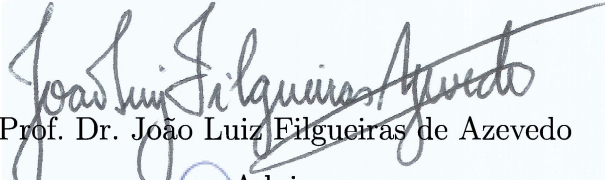


Thesis presented to Instituto Tecnológico de Aeronáutica, in partial fulfillment of the requirements for the degree of Doctor of Science in the Graduate Program of Ciências e Tecnologias Espaciais, Field of Sistemas Espaciais, Ensaios e Lançamentos.

Diego Ferolla de Abreu

**A STUDY OF TURBULENT SUPERSONIC JET FLOWS
AND THE INFLUENCE OF NOZZLE-EXIT BOUNDARY
CONDITIONS ON THE JET INITIAL DEVELOPMENT**

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2024

Cataloging-in Publication Data
Documentation and Information Division

Abreu, Diego Ferolla de

A Study of Turbulent Supersonic Jet flows and the Influence of Nozzle-Exit Boundary Conditions on the Jet Initial Development / Diego Ferolla de Abreu.

São José dos Campos, 2024.

177f.

Thesis of Doctor of Science – Course of Ciências e Tecnologias Espaciais. Area of Sistemas Espaciais, Ensaios e Lançamentos – Instituto Tecnológico de Aeronáutica, 2024. Advisor: Prof. Dr. João Luiz Filgueiras de Azevedo. Co-advisor: Dr. Carlos Junqueira Junior.

1. Turbulent flow. 2. Jet flow. 3. Computational fluid dynamics. 4. Reynolds number. 5. Numerical analysis. 6. Aerospace engineering. 7. Physics. I. Instituto Tecnológico de Aeronáutica. II. Title.

BIBLIOGRAPHIC REFERENCE

ABREU, Diego Ferolla de. **A Study of Turbulent Supersonic Jet flows and the Influence of Nozzle-Exit Boundary Conditions on the Jet Initial Development**. 2024. 177f. Thesis of Doctor of Science – Instituto Tecnológico de Aeronáutica, São José dos Campos.

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PUBLICATION TITLE: A Study of Turbulent Supersonic Jet flows and the Influence of Nozzle-Exit Boundary Conditions on the Jet Initial Development.

PUBLICATION KIND/YEAR: Thesis / 2024

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A STUDY OF TURBULENT SUPERSONIC JET FLOWS AND THE INFLUENCE OF NOZZLE-EXIT BOUNDARY CONDITIONS ON THE JET INITIAL DEVELOPMENT

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Dedicated to my grandparents, who are always so kind to me and encourage me to continue studying to go beyond, and to everyone else who supported me in this path.

Acknowledgments

I want to start by thanking my parents, Lilian and Gilberto, for all the support given to me since I was born. They always encouraged me to study and gave me the basis to reach so far. I also would like to thank my wife and life companion, Rafaela, who shared with me the most challenging times. For her patience and kindness. I also need to thank the newest member of my family, Kyubi. We did it! Thank you so much!

I thank my advisor, Prof. Dr. João Luiz F. Azevedo. It was in his first class when I was doing my specialization program at Embraer that I discovered that I wanted to work with computational fluid dynamics and that I wanted to do my Ph.D. work with him. I am grateful that he accepted me as his student, even with part-time dedication, due to my job at Embraer. Thank you, Azevedo!

I would also like to thank my co-advisor, Dr. Carlos Junqueira Junior. Since my first days at the Laboratory of Computational Aerodynamics, Junior supported me with the first simulations using the JAZzY code and teaching me the basics of Linux to the development of the FLEXI simulations and article writing.

The author acknowledges the computational resources from the Center for Mathematical Sciences Applied to Industry, CeMEAI, funded by Fundação de Amparo à Pesquisa do Estado de São Paulo, FAPESP, under the Research Grant No. 2013/07375-0. The author further acknowledges the National Laboratory for Scientific Computing (LNCC/MCTI, Brazil) for providing HPC resources of the SDumont supercomputer, under the Research Grant HFWBTF. This work was also granted access to the HPC resources of IDRIS under the allocation A0152A12067 made by GENCI.

I would like to thank my supervisor at Embraer, Prof. Dr. Luis Carlos de Castro Santos, who always encouraged me to do my Ph.D. work. He always stands by my side to continue developing this work.

I want to thank my colleagues from the Laboratory of Computational Aerodynamics for their support and partnership. I also want to thank my colleagues from Embraer, who supported me a lot and encouraged me to carry on with my studies. I finish the acknowledgment by thanking all my family and friends.

"Magic?"
"No. Something stronger. Engineering"
— ALITA, BATTLE ANGEL

Resumo

O avanço na capacidade computacional tem possibilitado a análise de escoamentos com alta complexidade geométrica e números de Reynolds elevados. Simulações de alta fidelidade, como a Simulação Numérica Direta (DNS) e a Simulação de Grandes Escalas (LES), têm se tornado opções atrativas para análises em mecânica dos fluidos. O presente estudo concentra-se na realização de LES de jatos supersônicos, que são a principal fonte de propulsão em veículos espaciais e aeronaves. Como resultado de sua operação, eles geram ruído e cargas dinâmicas. Para avaliar tais características do escoamento, é necessário obter flutuações de alta frequência, as quais podem ser obtidas por meio de simulações de alta fidelidade. Este trabalho realiza simulações de jatos supersônicos livres e seus objetivos incluem a investigação de configurações numéricas para a realização de simulações de alta fidelidade de jatos e a avaliação da influência de diferentes condições de contorno no desenvolvimento do jato. O trabalho apresenta uma análise da capacidade de dois métodos numéricos em resolver o jato supersônico. Para o mesmo número de graus de liberdade, os perfis de velocidade da simulação de alta ordem foram ligeiramente melhores do que das simulações de baixa ordem, levando a opção pelo método que permite discretização espacial de alta ordem. Um estudo é conduzido para identificar os requisitos de malha e ordem de precisão espacial para prever corretamente as propriedades turbulentas do escoamento. Os resultados mostram que a malha mais refinada, combinada com uma discretização espacial de terceira ordem de precisão, apresenta resultados em boa concordância com a referência experimental. O trabalho de pesquisa também endereça a investigação de opções de modelagem das características físicas da condição de entrada do jato. Uma revisão teórica das formulações de condição de entrada de jatos nos regimes subsônico e supersônico é apresentada, e três abordagens para a simulação de escoamentos de jatos supersônicos sem a inclusão do bocal no domínio computacional são propostas. A obtenção das características de entrada do jato requer simulações baseadas na formulação de Navier-Stokes com média de Reynolds (RANS). Os perfis de velocidade demonstram melhorias no desenvolvimento inicial do escoamento do jato com o aprimoramento das condições de entrada.

Abstract

Advancements in computational power have enabled the analysis of flows with large geometric complexity and high Reynolds numbers. High-fidelity simulations, such as Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES), have become attractive options for fluid mechanics analyses. The present study focuses on conducting LES of supersonic jets, which constitute the primary propulsion source for spacecraft and aircraft. As a consequence of their operation, they generate noise and dynamic loads. It is imperative to have the capability to calculate high-frequency fluctuations to assess such flow characteristics. The high-frequency fluctuations can be acquired through high-fidelity simulations. The present work performs simulations of free supersonic jet flows, aiming at investigating numerical configurations for conducting high-fidelity simulations of jets and at evaluating the influence of different boundary conditions on the jet development. The study analyzes the capability of two numerical methods in resolving the supersonic jet. For the same number of degrees of freedom, the velocity profiles from the high-order simulation were slightly superior than those from the low-order simulations, leading to the choice of the method allowing for high-order spatial discretization. A study is conducted to identify the mesh and spatial accuracy order requirements to correctly predict turbulent flow properties. The data demonstrate that the finer mesh, combined with third-order accurate spatial discretization, yield good agreement with the experimental data. The research also investigates modeling options for the physical characteristics of the jet inflow condition. A theoretical review of jet inlet formulations is presented for subsonic and supersonic regimes. Three approaches are proposed for simulating supersonic jet flows without including the nozzle in the computational domain. The calculation of jet inlet characteristics requires simulations based on the Reynolds-averaged Navier-Stokes (RANS) formulation. Velocity profiles show improvements in the initial development of jet flow with the enhancement of the inlet conditions.

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List of Symbols

Latin Symbols

c_p	specific heat at constant pressure
c_v	specific heat at constant volume
C_s	Smagorinsky constant
D	diameter
$\mathcal{D}$	derivative matrix
e	total energy per unit of mass
$\tilde{e}$	computable filtered total energy per unit of mass
$\check{e}$	filtered total energy per unit of mass according to Vreman's "System I"
f	frequency
$\mathbf{F}$	flux vector
$\mathcal{F}$	contravariant flux vector
$\hat{\mathcal{F}}^e$	inviscid part of the flux
$\mathcal{F}^*$	numerical interface flux
$\mathcal{F}$	contravariant flux vector
H	total specific enthalpy
J	Jacobian of the coordinate transformation
k	thermal conductivity coefficient
ℓ	Lagrange polynomial
$\mathbf{n}$	surface normal
p	pressure
$\bar{p}$	filtered pressure
Pr	Prandtl number
q	heat flux vector
$\check{q}$	computable filtered heat flux vector
$\mathbf{Q}$	vector of filtered conserved variables
r	radius
R	gas constant
s	Sutherland constant
S	strain rate

St	Strouhal number
t	time
t_s	time sample
T	temperature
$\tilde{T}$	computable filtered temperature
u	velocity fluctuation vector in polar coordinate system
u_i	velocity component in cartesian coordinate system
$\tilde{u}_i$	filtered velocity component in cartesian coordinate system
$\mathbf{u}$	velocity vector in cartesian coordinate system
$\mathbf{U}$	velocity in polar coordinate system
$\mathbf{x}$	position in cartesian coordinate system

Greek Symbols

γ	ratio of specific heats
δ	Kronecker delta
Δ	filter size
ϵ_{stab}	stabilization term
ζ	component of position in reference space
η	component of position in reference space
μ	dynamic viscosity coefficient
ξ	component of position in reference space
$\boldsymbol{\xi}$	position in reference space
ρ	density
$\bar{\rho}$	filtered density
σ	subgrid-scale stress tensor
τ	stress tensor
$\bar{\tau}$	filtered stress tensor
$\tilde{\tau}$	computable filtered stress tensor
ϕ	interpolating polynomial
ψ	test function
Ω	reference element

Subscripts

o	reference
SGS	subgrid-scale
h	discrete
j	jet
ff	farfield
x	longitudinal component
r	radial component
RMS	root mean square

θ	azimuthal component
ξ	computational domain
max	maximum
min	minimum

Superscripts

d	deviatoric
e	inviscid or Euler
m	modified
v	viscous
$\#$	split form

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1 Introduction

1.1 Scenario for Supersonic Jet Flow Applications

The complex interaction between the high-velocity and high-temperature supersonic jet flows with atmospheric air generates pressure fluctuations, which produce noise and cyclic loads when in contact with surfaces. Supersonic jet flows, which are originated from rocket engines, and commercial or military aircraft, generate a significant amount of noise and are a research subject for the aerospace community. The high-pressure fluctuations from rocket engines can damage launching structures or even be reflected back onto the vehicle. The noise emitted from aerospace engines close to the ground is one cause of Noise-Induced Hearing Loss (NIHL) in the exposed population.

In recent years, a new era of the aerospace market is beginning with the entrance of private companies, which is called “New Space” [1]. In the past, space exploration was restricted to government agencies and a few big companies, with financial assistance from governments. The early exploration of space required high investments, however, no direct profit was expected. With the entrance of private companies, a profitable and sustainable operation is required. In this sense, companies are putting much effort into producing reusable launchers, allowing cost savings and increasing launch frequencies. The viability of the reusable launchers is directly affected by the loads due to jet flow, and optimal design requires a correct prediction of these loads. The noise generated by the jets also became an important point of attention once spatial tourism became one funding opportunity for the business.

The evolution of the aerospace market relies on the additional payload capacity to be carried by the vehicles. There are studies to substitute current rocket launchers with hypersonic engines [1], for example, ramjets, to replace a large amount of oxygen carried in the launchers by the oxygen present in the atmosphere. When these new technologies are incorporated, another aspect of supersonic jets will require additional attention: the jet flowpath. When in close contact with surfaces, the development of the jet flowpath is modified from its free shear shape, resulting in different levels of pressure fluctuation and, consequently, noise and cyclic loads.

A significant investment of air forces in many countries is directed toward developing and operating supersonic aircraft. Within this application, the effect of noise due to supersonic jets on human health was investigated. The U.S. Department of Veteran Affairs observed increased expenses with hearing loss cases [2]. The Department of Navy measured the noise levels in diverse operations and observed that on carrier decks and inside aircraft cockpits, the noise levels were above safe levels for human health. For this reason, they have organized a Research and Development program to reduce supersonic jet noise. The International Civil Aviation Organization (ICAO), in its Environmental Report [3], presents numerous impacts of aircraft noise on the population living near airports. The socio-economic impact involves community noise annoyance, sleep disturbance, health impacts, and children's learning. The growth of the aviation market increases the challenges concerning socio-economic impacts due to the approximation of the population from the big cities to the aircraft operation near the current and newer airports [4].

The sustainable operation of supersonic military aircraft and aerospace launch vehicles requires sufficiently good predictions of pressure fluctuations to verify the design accomplishments of the requirements. There are many experiments performed to predict jet noise [5–8], both subsonic and supersonic, that can be used to develop semi-empirical correlations. The experiments can also be used together with numerical simulations, for example, the solution of the Navier-Stokes equations to potentially provide better predictions even for different conditions from the test.

1.2 Review of Turbulent Jet Flow Simulations

The numerical solution of Navier-Stokes equations for turbulent flows is performed mainly with three models: Direct Numerical Simulation (DNS), Large-Eddy Simulation (LES) and Reynolds-averaged Navier-Stokes (RANS). In the Direct Numerical Simulation, a numerical algorithm directly solves the Navier-Stokes equations. The turbulent eddies in the flow field are captured by sufficiently small mesh elements all over the domain. The smallest eddies are associated with high-frequency timescales, which impose restrictions on the timesteps of the simulation [9]. The computational costs of DNS are excessively high due to spatial and temporal requirements, which increase with the Reynolds number of the flow [10]. DNS is currently employed for the solution of general small Reynolds number flows and some high Reynolds number academic problems due to the high costs of the simulations.

Large-Eddy Simulation employs a spatial filter for the Navier-Stokes equations. The flow properties are filtered so that the large-scale flow is resolved and the small-scale flow is modeled. Adequate LES has nearly 80% of its energy scale simulated [9]. Within this approach, the turbulent scales associated with the fluid motion are simulated, which

is attractive due to its capability to simulate high-frequency fluctuations responsible for generating noise and cyclic loads. Due to the modeling of the smallest scales, which are associated with restrictive spatial and temporal requirements, the employment of the LES formulation is capable of simulating turbulent flows with considerably smaller computational costs than the DNS model. The differences in the computational costs are more relevant in free shear flows, where the eddies present in the domain are larger than those from wall-bounded flows.

The other approach for solving the Navier-Stokes equations is the Reynolds-averaged Navier-Stokes modeling. Due to the lower computational costs of this approach, it is the “workhorse” of industrial applications. The Reynolds averaging is applied to the Navier-Stokes equations to filter the high-frequency scales of motion associated with turbulence. Simultaneously, it permits the representation of small frequency scales associated with the mean flow field. Because the employment of this low-pass filter excludes all the turbulent scales from the equations, they need to be explicitly modeled. The closure of the RANS equations is performed with the turbulence models. The temporal filter of the RANS equations allows a significant reduction of the spatial and temporal requirements responsible for decreasing the costs of the simulations. Although the RANS equations present the lowest computational costs of the presented methodologies, they are not capable of reproducing some high-frequency fluctuations required for turbulent analyses involving cyclic load or noise generation.

The characteristics presented by the modeling options show that the LES model is a valuable alternative for studying turbulent flows. It has been a while since LES has been investigated to provide noise predictions of jet flows [11]. Even though this simulation strategy is more expensive than RANS simulations, with the growth of computational power, its application to some industrial problems has become feasible. This work is part of an effort in the research group to increase the application of high-fidelity simulations to industrial problems. In particular, in the specific case of the present effort, this is achieved by developing simulation capabilities to increase the accuracy of the prediction of unsteady problems based on the jet flow characteristics. The test case is the supersonic jet flow resulting, for instance, from the engine exhaust of supersonic aircraft or launch vehicles. The high-fidelity simulations, in the context of this work, are considered to be numerical simulations capable of effectively calculating the turbulent properties. The choice of numerical modeling to be investigated is the large-eddy simulation due to its capability to resolve high-energy turbulent scales, which is responsible for the definition of the main features of the flow field while still maintaining a reasonable computational cost.

There is a vast quantity of data in the literature on the simulation of jet flows [12–17]. In the present scenario, the majority of the work is concerned with the noise emitted by

subsonic jet flows at atmospheric air that represents the aircraft operation in takeoff. The concern about aircraft noise is associated with the demand to reduce noise levels near airports. Even though it is highly studied, there are plenty of topics to be investigated before high-fidelity simulations become feasible for industrial applications. One open topic for high-fidelity simulations is the imposition of boundary conditions for the inlet flow that efficiently reproduces the necessary jet characteristics entering the domain with an adequate computational cost. Bodony and Lele [11] performed an extensive review of LES and DNS of jet flows, which encompass the early developments of the jet flow simulations for aeroacoustic problems. Different options for imposing the inlet conditions were identified through the investigated simulations. The strategies for imposing the inlet condition were divided into two groups. The nozzle flow is resolved in the numerical simulations of the first group, while the free jet flow is exclusively simulated in the second group.

The numerical simulations performed with the nozzle geometry in the computational domain did not apply any additional model, such as forcing terms, to induce the flow transition according to Ref. [11]. The stagnation region close to the nozzle lip could produce enough disturbances to the flow leaving the nozzle and, consequently, anticipate the transition [18, 19]. In the numerical simulations in which only the free jet flow is simulated, some numerical models were employed to promote the transition from laminar to turbulent flows. The forcing terms [20, 21] are one example of the numerical models used to anticipate the flow transition. The forcing terms add velocity or pressure disturbances to the flow field in order to increase turbulence levels of the flow and promote the transition from laminar to turbulent flow. The correct imposition of the boundary layer thickness [22] improved the quality of the obtained simulations when compared to other inflow conditions. The absence of information from the nozzle-exit conditions from numerical experiments poses additional difficulties in validating the numerical algorithms.

The development of large-eddy simulations of jet flows has progressed significantly in the past few years. The influence of nozzle-exit boundary layer conditions on initially laminar jet flows was studied for a subsonic jet flow with a Mach number of 0.9 [12]. A constant area pipe represented the nozzle geometry, in which the imposed laminar flows were disturbed by a tripping-like forcing term inside the nozzle to produce highly disturbed flows [23]. The tripping parameters were adjusted to increase the disturbance levels from inlet conditions in the work presented in Ref. [22] compared to the flow from Ref. [12]. The jet inlet condition was improved by matching jet flow velocity parameters with the experimental data [24], including the momentum thickness and the shape factor of the boundary layer, the momentum-thickness-based Reynolds number, and the peak turbulence intensity. The computational mesh was generated with a high refinement level compared to other simulations [12, 22, 23] to adequately predict the jet flow. Subsonic

jet flows with the nozzle geometry in the computational domain were investigated with different mesh refinements in Ref. [14]. The numerical simulations were performed to evaluate the use of synthetic turbulence to enforce a boundary layer transition inside the nozzle and a wall model to represent the flow close to nozzle walls. Different tripping strategies are proposed in Refs. [25, 26]. A geometrical tripping is introduced in the nozzle surface to produce disturbances to the flow and promote the transition. A digital filter is employed to generate the turbulent inflow characteristic for a subsonic jet flow in Ref. [27].

The simulation of a supersonic jet flow with a Mach number of 1.4 was investigated in Ref. [28] and compared with an experimental reference [6]. The geometry of the nozzle was fully represented with its convergent-divergent geometry. The nozzle inlet condition was a laminar velocity profile with a hyperbolic tangent profile near the wall, providing an initial boundary layer thickness of $0.07D$, where D is the jet inlet diameter. Different from what was done in other studies [22–24], the inflow condition did not introduce any disturbance in the nozzle region. It was observed that the flow leaving the nozzle did not transition to a turbulent regime, resulting in the transition occurring outside the nozzle domain.

Three hot jet conditions were analyzed in Ref. [13]. The entire geometry of the nozzle was used in the simulations, and the inflow boundary condition of total pressure and temperature was imposed in the nozzle inlet. No artificial inflow turbulence or any other disturbance was imposed. The velocity profiles close to the jet inlet section present a similar behavior to those from Ref. [28], where the RMS values of the longitudinal velocity component fluctuations present a peak not observed in the experimental data. The first contact between the jet flow and the surrounding air produces peak RMS values of the velocity fluctuations when the jet flow is still in the laminar regime when leaving the nozzle.

A uniform inlet profile was imposed at the inlet section of the fully represented nozzle geometry in Refs. [29, 30]. The nozzle geometry was represented to generate a supersonic jet flow with a Mach number of 1.47 in Ref. [15]. The inflow condition prescribed the total pressure and total temperature in the nozzle inlet section without any disturbance to induce the transition to turbulence. Supersonic jet flows with three operating conditions for unheated and heated jet flows are investigated in Ref. [31]. The pressure and temperature conditions are imposed in the inlet section in order to match the Mach number of the operating condition in the jet outlet. No specific treatment was applied within the nozzle or boundary condition to resolve or model a turbulent boundary layer. Most of the numerical simulations for supersonic jet flow applications followed a different path to those from subsonic applications, where diverse features are employed to develop the flow inside the nozzle. In supersonic applications, the common approach is to represent

the nozzle geometry with the convergent-divergent section and impose the pressure and temperature to match the expected Mach number at the nozzle exit section.

Free jet flows, where the nozzle geometry is not included in the computational domain, have few applications in recent research efforts. In one research effort [17, 32], the simulations were performed with a uniform velocity profile to describe the nozzle outlet condition. The transition from laminar to turbulent occurs close to the jet inflow condition in the simulations, similar to the results observed for some simulations with the nozzle included in the computational domain [28]. In the simulations presented in Ref. [28], no forcing term is added to the calculations to increase the turbulence levels inside the nozzle.

1.3 Motivation

The research group in which this work was performed has experience developing large-eddy simulations of supersonic free jet flows [17, 32]. The previous experience showed the importance of the jet inlet condition in the development of the jet flow, which led to this effort to develop different inflow conditions that could improve the results from the numerical simulations. Recent jet simulations show no consensus on the best way to impose the jet inlet condition [13, 15, 17, 28, 31, 32]. Most of the presented strategies possess their benefits. However, they also present some drawbacks. It is essential to point out that the strategies presented are limited to jet flow applications, and the questions on inlet conditions are present in many high-fidelity simulations. An overview of turbulent inflow strategies for high-fidelity simulations is discussed for different applications in Ref. [33].

It is observed in the literature from jet flow simulations that the inclusion of the nozzle geometry in the computational domain is common practice from the most recent simulations [14, 15, 24, 28, 30, 34]. However, it is observed that the inclusion of the nozzle geometry to the computational domain without any additional forcing term to promote the transition inside the nozzle region may not be enough to provide adequate turbulent characteristics to the flow at the nozzle-exit section, which is observed in Refs. [13, 28, 31]. The mesh refinement inside the nozzle could not capture and reproduce the mechanisms associated with laminar-turbulent transition in Ref. [28]. For this reason, the flow leaving the nozzle presented a low level of turbulent intensity. A different result was obtained when the nozzle geometry was introduced to the computational domain with additional features to guarantee transition, as indicated in Refs. [14, 22–24, 26]. When a wall model or more refined meshes are used with a synthetic turbulence model or a tripping method, the nozzle-exit condition could provide a boundary layer similar to the experiment with higher levels of turbulence intensity.

In other words, the literature review indicates that additional features, beyond simply adding the nozzle geometry to the configuration under study, are necessary in order to produce an adequate condition for the nozzle-exit section. Additional numerical methods, such as forcing terms, wall modeling, and synthetic turbulence, are necessary to produce disturbances in the flow and promote the transition from laminar to turbulent inside the nozzle flow. The drawback of performing simulations with the nozzle geometry represented in the computational domain is the high computational costs associated with the fine near-wall mesh resolution. A general trend was observed that most simulations that could employ additional numerical features to develop the flow inside the nozzle domain evaluated subsonic flow regimes.

The literature review also indicates the need for more information from simulations that do not use the nozzle geometry in the computational domain. The best results obtained in the subsonic simulations employed the nozzle geometry in the computational domain. However, only some studies focused on the imposition of the nozzle-exit characteristics in simulations without the nozzle geometry. The numerical data from the simulations of supersonic jet flows with and without the nozzle geometry in the computational domain presented similar velocity profiles [17, 28, 32]. The few free jet flow studies and the small differences in the numerical results from the jet flow simulations with the nozzle geometry compared to the free jet flow simulations indicate a potential open subject of the jet flow simulations. The development of inflow conditions for free jet flows could improve the quality of the numerical simulation results while maintaining low computational costs.

1.4 Objectives

The objective of the present work is to investigate the simulation of the free, supersonic, perfect expanded, jet flows with a high-order numerical method and options for imposing the jet inflow condition. The work development includes evaluating the capabilities of a discontinuous Galerkin scheme implemented in the FLEXI numerical framework [35] to perform high-order simulations of the supersonic free jet flows. The evaluation compares velocity profiles obtained with the FLEXI numerical framework with the numerical data from the previously used JAZzY code [17, 32]. An accuracy evaluation study identifies the resolution requirements for the simulations with the discontinuous Galerkin scheme. The definition of the resolution requirements is a requisite for the investigation of jet inflow conditions due to its impact on the capability of the simulation to represent the features influenced by such condition.

Hence, in this context, the work has investigated three inflow conditions in order to address the effects on the quality of the numerical results from the simulations. The

investigated inflow conditions are expected to have a relatively small computational cost, when compared to equivalent simulations performed with the nozzle geometry introduced in the computational domain. The first inflow condition evaluated is the inviscid profile, which is the simplest one, and it is the same boundary condition employed in previous simulations [17, 32]. For this reason, the inviscid profile is considered the baseline against which the other calculations will be compared to. The second inflow condition has the mean flow properties obtained by a RANS simulation with a designed nozzle geometry. In the third inflow method, the mean flow properties from the nozzle RANS simulations are superimposed by a tripping method to generate an unsteady inflow condition.

1.5 Research Contributions

The present work investigates the simulation of supersonic jet flows using a high-order scheme and the influence of the inflow condition on the development of the free jet flow. The first contribution of the present research effort is the comparison of the jet flow simulation results obtained using two quite distinct numerical schemes, but maintaining the number of degrees of freedom as the reference parameter. One of the approaches is a 2nd-order, finite difference method, which represents the legacy form in which jet flows used to be addressed in our research group. The other methodology is a high-order, discontinuous Galerkin method, which is the primary simulation methodology of interest in the present work.

The second contribution of the present research is the investigation of the resolution requirements for the adequate simulation of free supersonic jet flows using the discontinuous Galerkin spectral element method [36, 37] implemented in the FLEXI numerical framework [35]. The numerical results from the simulations are compared with experimental data [6] to assess the capability of the two methods to represent flow physics. Finally, the third contribution of the research effort is the analysis of the influence of three inflow conditions on the initial development of the supersonic jet flows. Two inflow conditions were originally developed in the context of the present work, and they are compared to the specification of an inviscid jet profile, which has been used in previous investigations within the research group. The three numerical simulations are performed with the resolution requirements previously identified. The numerical results are again compared to available experimental reference data [6].

1.6 Overview of the Present Document

The present chapter introduces the reader to the motivation behind the development of this work, provides a brief review of the most recent developments about the topic, and then outlines the objective of the current work.

The second chapter of this work is focused on the physical formulation. The Navier-Stokes equations are presented to the reader, followed by the mathematical fundamentals of the spatial filtering process. The application of the filtering process to the Navier-Stokes equations is presented with the treatment of the additional terms and the subgrid-scale model used. The chapter concludes with a discussion of the physical characteristics of the inflow conditions.

The numerical methods are discussed in the third chapter. The FLEXI numerical framework is presented together with the formulation of the discontinuous Galerkin spectral element method. Discussions on the split formulation, Riemann solver, lifting scheme, shock capturing approach, and time marching method are presented. The chapter discusses the numerical formulation of the boundary conditions for the supersonic jet flow problem.

The fourth chapter presents details of the test case used in the work. The physical experiment is presented to the reader. The numerical model is discussed, with information on the geometry, mesh, and the numerical solver setup. The configuration of the nozzle simulations performed with the RANS formulation is also presented in this chapter.

The fifth chapter presents the results of the four studies conducted in this work. The first study compared the results from the FLEXI numerical framework with the previous numerical tool, JAZzY. Then, a resolution accuracy study is performed for the FLEXI numerical framework to identify the mesh and polynomial requirements for the correct large-eddy simulation of the supersonic free jet flow. The RANS simulations are performed to identify the mean properties of the flow at the nozzle-exit section to be imposed in the jet inlet section of the large-eddy simulations. Finally, the study is concluded by comparing the numerical results from the options of jet inflow condition analyzed.

In the sixth and final chapter, the work is concluded with the final remarks on the analysis of the numerical results and the presentation of opportunities for continuing the research on supersonic jet flows.

2 Physical Formulation

2.1 The Choice of the Physical Formulation

The Navier-Stokes equations represent every type of flow with all its characteristics. However, they cannot be exactly resolved. In the vast majority of the applications, the Navier-Stokes equations are resolved with the employment of different numerical methods. When employing a numerical method to solve a set of partial differential equations, such as the Navier-Stokes equations, the physical domain must be discretized into a finite number of elements. The time advance of the solution is also performed with a discrete time step.

When no modeling is employed and the spatial discretization and the time step are sufficiently small to capture all the smallest eddies of the turbulent flow, the simulation is called Direct Numerical Simulation (DNS). In this type of simulation, all turbulent structures from the frequency spectrum are represented, and no model is necessary. From Kolmogorov hypothesis [38], it is known that the ratio of the largest to smallest length scales varies with $\eta/L = Re^{-3/4}$ and $\tau/T = Re^{-1/2}$, where η and τ are the Kolmogorov microscales of length and time, L and T are the characteristic length and time of the largest eddies of the flow, and Re is the Reynolds number of the flow. From these relations, it is possible to see that the element size requirement in the numerical domain and time step restriction rapidly grows with the Reynolds number, which makes this simulation model computationally expensive for complex fluid flows at high Reynolds numbers.

A spatial filtering process can be applied to the Navier-Stokes equation in order to allow the resolution of the largest length scales of the flow, which are responsible for developing the mean flow field. The smallest length scales need to be modeled. This strategy is called Large-Eddy Simulation (LES), and it can provide three-dimensional unsteady data for turbulent flow with a significant reduction in computational costs compared to DNS. Due to the reduced computational costs of using the formulation compared to the DNS and its capacity to resolve most of the turbulent scales responsible for the development of the flow field, the Large-Eddy Simulation is selected for the performance of the simulations in the present work.

When the filtering process is employed in the Navier-Stokes equations, new terms

appear in the filtered equations, which brings a closure problem to the system of equations. There are different approaches to handle the closure problem for the filtered Navier-Stokes equations. In the present work, the “system I” of Vreman [39] defines the treatment for the energy conservation equation. The analysis of experimental references and the DNS simulation supports the choice of the new terms to be modeled. The closure problem is concluded by employing the Boussinesq hypotheses [40] to the remaining terms.

2.2 Navier-Stokes Equations

The Navier-Stokes equations are used in their conservative form. In the presence of discontinuities in the flow, the non-conservative form introduces errors when calculating the propagation velocity and intensity of the discontinuities [41] present in the flow field. The Navier-Stokes equations can be written as

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} &= 0, \\ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} &= 0, \\ \frac{\partial \rho e}{\partial t} + \frac{\partial (\rho e + p) u_j}{\partial x_j} - \frac{\partial \tau_{ij} u_i}{\partial x_j} + \frac{\partial q_j}{\partial x_j} &= 0, \end{aligned} \quad (2.1)$$

where variables t and $\mathbf{x} = (x_1, x_2, x_3)$ are the independent time and spatial coordinates of the three-dimensional domain, ρ is the density, $\mathbf{u} = (u_1, u_2, u_3)$ is the velocity vector, and p is the static pressure. The total energy per unit of volume is given by

$$\rho e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u_i u_i, \quad (2.2)$$

where e is the total energy per unit of mass and γ is the ratio of specific heats, obtained by $\gamma = c_p/c_v$, and its usual value is 1.4. The density, static pressure, and static temperature T of the fluid are correlated by the equation of state of ideal gases

$$p = \rho R T, \quad (2.3)$$

where R is the specific gas constant obtained by the relation $R = c_p - c_v$. For air, the specific gas constant has a value of 287.058 J/(kg·K). The properties c_p and c_v are the specific heats at constant pressure and volume, respectively.

The stress tensor, τ_{ij} , for a Newtonian fluid is given by

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij}. \quad (2.4)$$

The second viscosity coefficient, λ , receives its value from the Stokes hypothesis [42] of $\lambda = -2/3\mu$. The dynamic viscosity coefficient, μ , can be approximated using a kinetic theory in the way proposed by Sutherland [43],

$$\mu(T) \approx \mu_0 \left(\frac{T}{T_0} \right)^{3/2} \frac{T_0 + S}{T + S}, \quad (2.5)$$

where the reference values are $\mu_0 = 1.716 \times 10^{-5} \text{ N}\cdot\text{s}/\text{m}^2$, $T_0 = 273 \text{ K}$, and $S = 111 \text{ K}$, which is known as the Sutherland constant [42]. The viscosity coefficient approximation for air presents minor errors, below 2% [42], in the range of temperatures expected in the present work. The heat flux is given by

$$q_j = -\kappa \frac{\partial T}{\partial x_j}, \quad (2.6)$$

where κ is the thermal conductivity coefficient, given by $\kappa = \mu c_p / Pr$ and Pr is the Prandtl number. The computation of the specific heat ratio at constant pressure is performed by

$$c_p = \frac{\gamma R}{\gamma - 1}. \quad (2.7)$$

2.3 Filtering Process

2.3.1 Mathematical Formulation of the Filtering Process

The mathematical formulation of the filtering process is discussed in this section. The aspects discussed are restricted to the ideal case of homogeneous turbulence [40]. When employing a filtering process for homogeneous turbulence, it is required that the filter respect the physical properties of isotropy and homogeneity; in other words, the properties of the filter need to be independent of the position and the orientation of the reference frame in space. These properties result in the cut-off scale being constant and identical in all spatial directions. Additional information of the filtering process for inhomogeneous flows are presented in Ref. [44].

The separation of the scales is obtained using a low-pass filter. The low-pass filter is responsible for filtering the high-frequency eddies of the flow, which are associated with small length scales. The mathematical representation of a filtering in physical space is a convolution product. Employing the filtering process to a variable $a(x, t)$ leads to a resolved part $\bar{a}(x, t)$ that is mathematically defined by

$$\bar{a}(x, t) = \frac{1}{\Delta} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} G\left(\frac{x-v}{\Delta}, t-\iota\right) a(v, \iota) d\iota d^3v, \quad (2.8)$$

where the variable G represents the convolution kernel. The variables v and ι are dummy variables for the intermediate computation. The kernel G is characteristic of the filter type chosen and is associated with the cut-off scales in space and time. This relation can be symbolically represented by

$$\bar{a} = G \star a. \quad (2.9)$$

The non-resolved part of $a(x, t)$ is represented by $a'(x, t)$ that can be calculated by

$$a'(x, t) = a(x, t) - \bar{a}(x, t), \quad (2.10)$$

$$a'(x, t) = (1 - G) \star a. \quad (2.11)$$

2.3.2 Fundamental Properties of Filtering

There are three necessary properties to enable the usage of filters in the manipulation of the Navier-Stokes equations. They are consistency, linearity, and commutation with differentiation. The consistency property is associated with the filtering of a constant. This means that if a constant c is filtered, it should keep its value,

$$\bar{c} = c. \quad (2.12)$$

The consistency property is observed by the fact that the convolution product of a constant is unitary,

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} G(v, \iota) d\iota d^3v = 1. \quad (2.13)$$

The linearity means that the filter of a sum is equal to the sum of a mean. It is satisfied by the convolution form of the filtering,

$$\overline{a + b} = \bar{a} + \bar{b}. \quad (2.14)$$

The commutation with differentiation is also a property of the filtering process,

$$\frac{\partial \bar{a}}{\partial s} = \bar{\frac{\partial a}{\partial s}}, \quad s = x, t. \quad (2.15)$$

However, this property is only obtained with the restriction of the unbounded domain and with homogeneous convolution kernel [40].

It is important to discuss some properties that the filtering does not have. The filter presented in Eq. (2.8) is not from the class of Reynolds operator, since it does not satisfy the following property of this class of operator in general

$$\overline{ab} \neq \bar{a}\bar{b}. \quad (2.16)$$

The filter is not necessarily idempotent, also known as the projector property. Only some filters exhibit this property. This characteristic means that the additional application of the operator produces effects in the result, and the filtering of the fluctuation may not vanish from its large-scale component. These characteristics are represented by

$$\bar{\bar{a}} = G \star G \star a = G^2 a \neq \bar{a}, \quad (2.17)$$

$$\overline{a'} = G \star (1 - G) \star a \neq 0. \quad (2.18)$$

2.3.3 Classical Filters for Large-Eddy Simulation

Three convolution filters are largely employed for performing spatial scale separation [40]: the box filter, the Gaussian filter, and the sharp cutoff filter. The kernel in physical space for the box filter, which is also called the top hat filter, is calculated by

$$G(x - v) = \begin{cases} \frac{1}{\Delta} & |x - v| \leq \frac{\Delta}{2} \\ 0 & |x - v| > \frac{\Delta}{2} \end{cases}. \quad (2.19)$$

The Gaussian filter is calculated by

$$G(x - v) = \left(\frac{\varsigma}{\pi \Delta^2} \right)^{1/2} \exp \left(\frac{-\varsigma (x - v)^2}{\Delta^2} \right), \quad (2.20)$$

where the value of ς is usually 6 [40]. The last filter presented is the sharp cutoff filter, which is calculated by

$$G(x - v) = \frac{\sin(k_c(x - v))}{k_c(x - v)}, \quad (2.21)$$

and the constant k_c has the value $k_c = \pi/\Delta$. The kernel of the filters presented in this section is described in physical space, x . They can also be described in the spectral space, k . The representation of the filters in the spectral space is presented in Ref. [40].

The filters presented in Eqs. (2.19), (2.20), and (2.21) are symmetric fields and can only be applied to internal regions of the domain without discontinuities [45]. In the case of discontinuities, employing the symmetric filter results in a continuous filtered variable. It is also observed that the jump in the mean field contributes to the definition of the subgrid fluctuation. In the presence of shocks, this contribution dominates the subgrid fluctuation, affecting the subgrid model. The work in Ref. [46] presents options for non-centered filters to be employed where discontinuous flows are present. The application of filters in the boundaries requires additional treatments discussed in Refs. [47].

2.3.4 Favre Filtering

One alternative for compressible flows is to filter the system of equations weighted by density, which is employed to simplify the treatment of the new terms from the filtering process. The density-weighted filtering process is commonly referred to as the “Favre filtering” [40]. In the context of the Favre filtering, a filtered specific quantity could be written as

$$\tilde{a} = \frac{\overline{\rho a}}{\bar{\rho}}. \quad (2.22)$$

Nevertheless, it is important to point out that, differently from the non-resolved part, $a'(x, t)$, of a variable a , the employment of the Favre filtering produces the non-filtered property $a''(x, t)$, which has a different value from $a'(x, t)$. The density-weighted filtered variables, $\tilde{a}(x, t)$, are associated with the variable a by

$$a(x, t) = \tilde{a}(x, t) + a''(x, t). \quad (2.23)$$

The density-weighted filter operator is linear [40]. However, it does not commute with the derivative operator in space and time

$$\widetilde{\frac{\partial a}{\partial x}} \neq \frac{\partial \tilde{a}}{\partial x}, \quad (2.24)$$

$$\widetilde{\frac{\partial a}{\partial t}} \neq \frac{\partial \tilde{a}}{\partial t}. \quad (2.25)$$

2.4 Filtered Navier-Stokes Equations

2.4.1 Formulation of the Filtered Equations

In this section, the filtering process is employed for the Navier-Stokes equations in the conservative form to obtain the Filtered Navier-Stokes equations. The conservation of mass equation is the simplest one and, due to the use of the “Favre filtering”, the equation retrieves its original form with the filtered variables

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0. \quad (2.26)$$

The filtering process employed for the momentum equations produces additional terms. The result of the filtering process in the momentum equations is represented by

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} - \tilde{\tau}_{ij}) = 0, \quad (2.27)$$

where $\bar{\tau}_{ij}$ is the filtered stress tensor and $\check{\tau}_{ij}$ is the computable filtered stress tensor, which employs the density-weighted filtered variables

$$\check{\tau}_{ij} = \mu(\check{T}) \left[\left(\frac{\partial \check{u}_i}{\partial x_j} + \frac{\partial \check{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \check{u}_k}{\partial x_k} \delta_{ij} \right]. \quad (2.28)$$

The computable filtered stress tensor is added and subtracted to the momentum equations to represent the terms that involve variables that are computable in the resolution of the set of equations. The additional term present in the equation is the subgrid-scale stress tensor, σ_{ij} , given by

$$\sigma_{ij} = \bar{\rho} (\widetilde{u_i u_j} - \check{u}_i \check{u}_j), \quad (2.29)$$

where $\widetilde{\rho u_i u_j}$ is the filter of the triple product $\rho u_i u_j$ and $\check{\rho} \check{u}_i \check{u}_j$ is the computable filtered of the triple product that is added and subtracted to the momentum equations. In the present work, the modeling strategy proposed by Comte and Lesieur [40] is employed. It consists of the consideration of the deviatoric part of the subgrid-scale stress tensor, σ_{ij}^d while the terms from the main diagonal are considered together with the pressure. The last term in Eq. (2.27) is the difference between the filtered stress tensor, $\bar{\tau}_{ij}$, with the computable filtered stress tensor, $\check{\tau}_{ij}$. The computable filtered temperature, $\check{T}$, is explained together with the energy equation.

The last equation is the energy conservation. After the filtering process, many options exist to develop the energy conservation equation. The “system I” of Vreman [39] is the reference for this work. In the “system I” approach, there is an assumption that the computable filtered total energy per unit of volume, $\bar{\rho} \check{e}$, is calculated by

$$\bar{\rho} \check{e} = \frac{\bar{p}}{\gamma - 1} + \frac{1}{2} \bar{\rho} \widetilde{u_i u_i}, \quad (2.30)$$

instead of employing the filter of the triple product $\widetilde{\rho u_i u_i}$. If the filter of the triple product were employed, additional variables and models would be required to solve them. With this modeling choice, the filtered energy conservation equation [40] is given by

$$\begin{aligned} & \frac{\partial \bar{\rho} \check{e}}{\partial t} + \frac{\partial (\bar{\rho} \check{e} + \bar{p}) \check{u}_j}{\partial x_j} - \frac{\partial \check{\tau}_{ij} \check{u}_i}{\partial x_j} + \frac{\partial \check{q}_j}{\partial x_j} \\ & + B_1 + B_2 + B_3 - B_4 - B_5 - B_6 + B_7 = 0. \end{aligned} \quad (2.31)$$

The filtered heat flux vector with the filtered variables $\check{q}_j$ is calculated by

$$\check{q}_j = -\kappa \frac{\partial \check{T}}{\partial x_j}, \quad (2.32)$$

and the computable filtered temperature is obtained by the computable filtered total

energy per unit of volume and the equation of state, Eq. (2.3). It is given by

$$\tilde{T} = \frac{(\gamma - 1)}{R} \left[\tilde{e} - \frac{1}{2} \tilde{u}_i \tilde{u}_i \right], \quad (2.33)$$

and the B_i terms, with $i = 1, \dots, 7$, are the subgrid-scale terms [40]. They are calculated by

$$B_1 = \frac{1}{\gamma - 1} \frac{\partial}{\partial x_j} (\overline{\rho u_j} - \bar{\rho} \tilde{u}_j) = \frac{\partial c_v Q_j}{\partial x_j}, \quad (2.34)$$

$$B_2 = p \frac{\partial u_k}{\partial x_k} - \bar{p} \frac{\partial \tilde{u}_k}{\partial x_k} = \Pi_{\text{dil}}, \quad (2.35)$$

$$B_3 = \frac{\partial}{\partial x_j} (\sigma_{kj} \tilde{u}_k), \quad (2.36)$$

$$B_4 = \sigma_{kj} \frac{\partial}{\partial x_j} \tilde{u}_k, \quad (2.37)$$

$$B_5 = \overline{\tau_{kj} \frac{\partial}{\partial x_j} u_k} - \bar{\tau}_{kj} \frac{\partial}{\partial x_j} \tilde{u}_k = \epsilon_v, \quad (2.38)$$

$$B_6 = \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} \tilde{u}_i - \tilde{\tau}_{ij} \tilde{u}_i) = \frac{\partial \mathcal{D}}{\partial x_j}, \quad (2.39)$$

$$B_7 = \frac{\partial}{\partial x_j} (\bar{q}_j - \tilde{q}_j). \quad (2.40)$$

The filtered Navier-Stokes equations, Eqs. (2.26), (2.27) and (2.31), present all the subgrid-scale (SGS) terms and they differ significantly from the Navier-Stokes equations, except for the mass equation. An additional investigation of the SGS terms is necessary to simplify the equations and make them manageable. In Refs. [39, 48], 2-D shear layer flows with convective Mach numbers of 0.2 to 1.2 were investigated to assess the relevance of the subgrid-scale terms. The subgrid-scale terms were also calculated from the numerical results from a DNS of homogeneous isotropic turbulence at Mach number 0.52 [49].

In the DNS solution for the 2-D shear layer test cases [48], the amplitude of the terms associated with resolved and subgrid-scale fields were compared with the test data. The comparisons were based on the L_2 norm of the terms from the filtered equations. The authors classified the L_2 norm of the terms into four categories according to the influence of the term: large, medium, small, and negligible. At least one order of magnitude separates the norm in each classification. The final classification performed [48] is presented in Table 2.1, which is based on Ref. [40]. The recommendation was to model the terms with at least medium influence, resulting in the need to model the terms σ_{ij} , B_1 , B_2 , and B_3 . The conclusions obtained in Ref. [49] agree with those presented in Ref. [48]. One disagreement is observed between the two studies on the importance of the term B_2 . In terms of modeling, this disagreement has no practical effect. In the present work, the

subgrid-scale terms are treated in the same way performed in Ref. [48], in which the B_1 and B_2 terms are modeled together.

TABLE 2.1 – Classification of the subgrid-scale terms present in the filtered Navier-Stokes equations.

Influence of the term	System I
Large	convective $\overline{NS}$
Medium	diffusive $\overline{NS}$, σ_{ij} , B_1 , B_2 , B_3
Small	B_4 , B_5
Negligible	$\frac{\partial}{\partial x_j} (\overline{\tau_{ij}} - \tilde{\tau}_{ij})$, B_6 , B_7

After the removal of the terms with small or negligible influence from the equations, four terms remain to be modeled: σ_{ij} , B_1 , B_2 , and B_3 . Once σ_{ij} is modeled, the term B_3 is automatically modeled because it is the influence of the SGS Reynolds stress tensor in the energy equation. The terms B_1 and B_2 can be modeled together [48].

The developments of general tools behind the applications of LES were, in its majority, based on homogeneous turbulence [40]. Furthermore, the background on homogeneous turbulence was applied to quantify the interaction between the scales of turbulence. The investigation of the interaction between the scales of turbulence presented the behavior illustrated in Fig. 2.1, which is based on the work in Ref. [40]. The largest scales of turbulence can obtain kinetic energy from the mean flow. From a mechanism related to the instability of the largest eddies, the kinetic energy is transferred to smaller scales of turbulence. The region in which the transfer occurs is known as the inertial region. Then, the molecular viscosity dissipates the kinetic energy. It is also known that there is a transfer of energy from the smaller scales to larger ones. However, this transfer mechanism is weaker than the transfer from the largest eddies to the smaller ones.

One of the bases of the modeling of the SGS terms is that the filters are applied to the inertial region, and the smallest scales are isotropic. The isotropy of the smallest scales brings some universality to the models because they will present similar behavior independently from the largest scale flows. The consideration that the filter is applied to the inertial regions allows the smallest scales to dissipate the energy transferred through the filter.

Based on the explanation presented, the treatment of the SGS stress tensor is based on the Boussinesq hypothesis [40], which means that the dissipation from the smallest scales can be introduced as a Reynolds stress tensor that resembles the stress tensor with the subgrid-scale viscosity μ_{SGS} instead of the molecular viscosity. In practice, it is represented by an increment in the viscosity of the fluid. Some of the classical SGS models are concerned with the deviatoric part of the SGS stress tensor σ_{ij}^d [39] because the isotropic part is usually added to the pressure contribution. Therefore, the term σ_{ij}

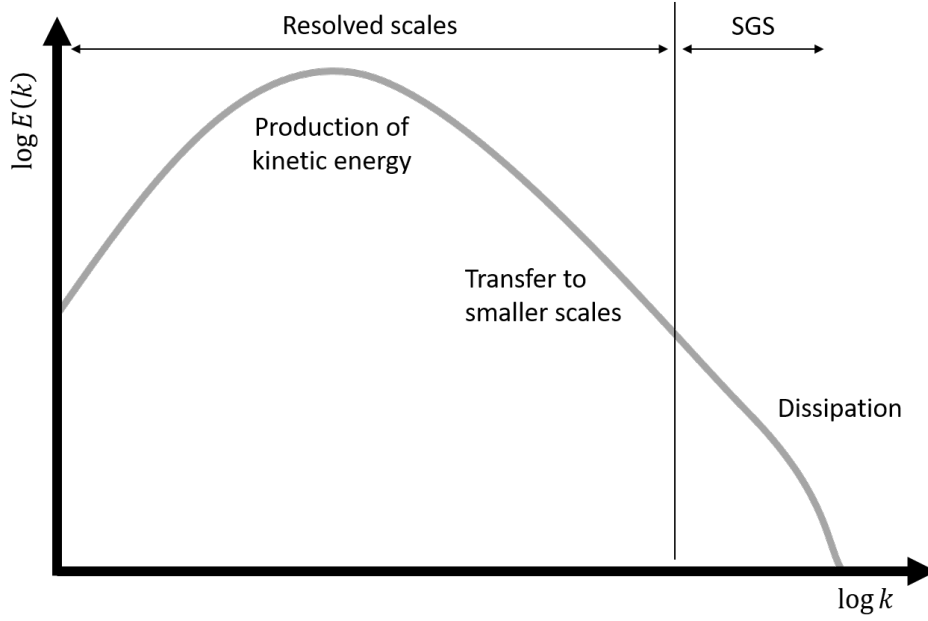


FIGURE 2.1 – Turbulent kinetic energy spectrum of a homogeneous turbulence problem.

in Eq. (2.27) is replaced by σ_{ij}^d . In this way, the contribution from the SGS stress tensor is given by

$$\sigma_{ij}^d = \sigma_{ij} - \frac{1}{3}\delta_{ij}\sigma_{kk} = -\bar{\rho}\nu_{sgs} \left[\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3}\delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right]. \quad (2.41)$$

The analysis of the isotropic part of the SGS stress tensor [50] showed that the $1/3\delta_{ij}\sigma_{kk}$ term should be neglected once its contribution is generally weak for the filtered pressure.

The contribution of the SGS heat flux needs also to be evaluated. The usual practice is to assume that the energy transfer from resolved scales to subgrid-scales is proportional to the gradient of resolved temperatures [40]. In this sense, the terms B_1 and B_2 from the energy equation are modeled by

$$B_1 + B_2 = \frac{\partial c_v Q_j}{\partial x_j} + \Pi_{dil} = -\frac{\partial}{\partial x_j} \left(\kappa_{sgs} \frac{\partial \tilde{T}}{\partial x_j} \right). \quad (2.42)$$

The variable κ_{sgs} is the SGS thermal conductivity coefficient, which can be associated with the SGS viscosity coefficient by

$$\kappa_{sgs} = \frac{\bar{\rho}\nu_{sgs}c_p}{Pr_{sgs}}, \quad (2.43)$$

where Pr_{sgs} is the SGS Prandtl number, which has a constant value of 0.9 [40].

The resultant set of filtered Navier-Stokes equations is given by

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0,$$

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tilde{\tau}_{ij}^m}{\partial x_j} &= 0, \\ \frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{e} + \bar{p}) \tilde{u}_j}{\partial x_j} - \frac{\partial \tilde{\tau}_{ij}^m \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{q}_j^m}{\partial x_j} &= 0, \end{aligned} \quad (2.44)$$

after the analysis of the subgrid-scale terms, the filtered Navier-Stokes formulation retrieves a form similar to the original Navier-Stokes equations, Eq. (2.1). The differences are in the modified filtered stress tensor $\tilde{\tau}_{ij}^m$, which is calculated by

$$\tilde{\tau}_{ij}^m = \left(\mu(\tilde{T}) + \bar{\rho} \nu_{sgs} \right) \left[\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right], \quad (2.45)$$

and the modified filtered heat flux vector $\tilde{q}_j^m$, which is calculated by

$$\tilde{q}_j^m = -(\kappa + \kappa_{sgs}) \frac{\partial \tilde{T}}{\partial x_j}. \quad (2.46)$$

2.4.2 Smagorinsky Model

The Smagorinsky model [51] is a simple closure used to calculate the anisotropic part of the SGS Reynolds stress tensor. The value for the SGS viscosity ν_{sgs} is calculated by

$$\nu_{sgs} = C_s^2 \Delta^2 |\check{S}|, \quad (2.47)$$

where $|\check{S}|$ is calculated by

$$|\check{S}| = (2\check{S}_{ij}\check{S}_{ij})^{1/2}, \quad (2.48)$$

and the computable strain rate, $\check{S}_{ij}$, is obtained by

$$\check{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \quad (2.49)$$

The value of C_s , which is the Smagorinsky constant, varies according to the type of the flow, but it usually presents values between 0.1 to 0.2. The value for the Smagorinsky constant can be estimated by considering the hypothesis of local equilibrium and the evaluation of the averaged SGS viscosity from eddy-damped quasi-normal Markovian theory (EDQNM), which gives a value of 0.148, used in the present work [44, 52]. The value for Δ , which is the filter size, is obtained from the cubic root of the volume. In the case of a regular hexahedral volume, the filter size can be calculated by

$$\Delta = (\Delta_x \Delta_y \Delta_z)^{1/3}. \quad (2.50)$$

In Ref. [17], three options of subgrid-scale models were employed to identify their

influence on supersonic jet flows. The classic Smagorinsky model [51], the Vreman model [53], and the dynamic Smagorinsky model [54] were evaluated. Few differences were observed between the velocity profiles of the simulations with different SGS models. Due to the reduced computational cost of the Smagorinsky model, especially compared to dynamic models, and few differences observed between the numerical results with different SGS models [17], the classic Smagorinsky model is employed in the present work.

2.5 Reynolds-Averaged Navier-Stokes Equations

2.5.1 Formulation of the Reynolds-Averaged Navier-Stokes Equations

The Reynolds-averaged Navier-Stokes (RANS) equations are another option for simplifying the Navier-Stokes equations, Eq. (2.1). The RANS formulation is obtained by the employment of the so-called Reynolds averaging process of the Navier-Stokes equations. The Reynolds average can be understood as a temporal low-pass filter that filters all the turbulent motion of the flow, dividing the equations into a mean resolved part and a non-resolved part. The concept for the employment of the Reynolds average is an attempt to approximate an ensemble average. In the ensemble average, an experiment is repeated multiple times, and the statistics of these multiple experiments are averaged to produce a single value. Because the ensemble average cannot be used in practical CFD simulations, a time averaging, or the Reynolds average, is employed. A time-filtered value, obtained by this process, of a variable, a , can be mathematically expressed as

$$\hat{a}(t) = \frac{1}{T_p} \int_t^{t+T_p} a(\tau) d\tau, \quad (2.51)$$

where the integration period, T_p , should be sufficiently large to allow high-frequency fluctuations to be averaged. The Reynolds-averaged Navier-Stokes equations are obtained with the expansion of all variables into the time-filtered variable variable, $\hat{a}(t)$, and the fluctuation part, $\tilde{a}(t)$, in the way presented in

$$a(t) = \hat{a}(t) + \tilde{a}(t). \quad (2.52)$$

Similarly to the strategy employed in LES formulation, a density-weighted time filtering is applied to the equations in order to simplify the treatment of the new terms. The density-weighted time filtering is referred to as the Favre average. An averaged specific quantity could be written as

$$\tilde{\tilde{a}} = \frac{\widehat{\rho a}}{\hat{\rho}}. \quad (2.53)$$

The expansion of all variables and the application of density-weighted time filtering al-

low the development of the equations, which results in three new terms: the Reynolds stress tensor, $\widehat{\rho\dot{u}_i\dot{u}_j}$, the Reynolds heat flux vector, $\widehat{\rho h\dot{u}_j}$, and the Reynolds dissipation terms, $\dot{u}_i(\tau_{ij} - \rho\dot{u}_i\dot{u}_j/2)$. It is important to point out that the change of variables to the density-weighted time-filtered quantities produces a different fluctuation part than the one obtained with the Reynolds-average process,

$$a(t) = \check{a}(t) + \acute{a}(t). \quad (2.54)$$

The new terms are treated with the Boussinesq hypothesis, leading to the Reynolds-averaged Navier-Stokes equations

$$\begin{aligned} \frac{\partial \hat{\rho}}{\partial t} + \frac{\partial \hat{\rho}\check{u}_j}{\partial x_j} &= 0, \\ \frac{\partial \hat{\rho}\check{u}_i}{\partial t} + \frac{\partial \hat{\rho}\check{u}_i\check{u}_j}{\partial x_j} + \frac{\partial \hat{p}}{\partial x_i} - \frac{\partial \hat{\tau}_{ij}^m}{\partial x_j} &= 0, \\ \frac{\partial \hat{\rho}\check{e}}{\partial t} + \frac{\partial (\hat{\rho}\check{e} + \hat{p})\check{u}_j}{\partial x_j} - \frac{\partial \hat{\tau}_{ij}^m\check{u}_i}{\partial x_j} + \frac{\partial \hat{q}_j^m}{\partial x_j} &= 0, \end{aligned} \quad (2.55)$$

where the modified viscous stress tensor is given by

$$\hat{\tau}_{ij}^m = \left(\mu(\check{T}) + \hat{\rho}\nu_t \right) \left[\left(\frac{\partial \check{u}_i}{\partial x_j} + \frac{\partial \check{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \check{u}_k}{\partial x_k} \delta_{ij} \right], \quad (2.56)$$

and the modified heat flux vector is calculated by

$$\hat{q}_j^m = -(\kappa + \kappa_t) \frac{\partial \check{T}}{\partial x_j}. \quad (2.57)$$

Two additional variables are present Eqs. (2.56) and (2.57), the turbulent viscosity coefficient, ν_t , and turbulent thermal conductivity coefficient, κ_t , which can be calculated by

$$\kappa_t = \frac{\hat{\rho}\nu_t c_p}{Pr_t}, \quad (2.58)$$

where Pr_t is the turbulent Prandtl number. The ν_t new variable needs to be modeled for the closure of the RANS equations.

2.5.2 Turbulence Model

The turbulence model in the RANS equations is highly important due to all information from turbulence originating from these models. In the LES formulation, the subgrid-scale models provide only the information from the dissipation region. In this sense, it is expected that the turbulence models are more sophisticated than the SGS models. In

practice, the turbulence models add transport equations to the RANS equations that calculate variables that provide the value of the turbulent viscosity. There is a vast number of options for turbulence models [55]. They vary concerning the variables calculated in the transport equations and the number of transport equations resolved. In this work, the turbulent variables are calculated by the Spalart-Allmaras (SA) [56] turbulence model. The SA turbulence model can produce good estimates of wall-bounded flows, which is the case for the nozzle flow that is solved with the RANS equations, with a reduced cost compared to other turbulence models because it only solves one transport equation. The SA turbulence model used in the CFD commercial software CFD++ [57] is presented in Ref. [56]. The calculation of the turbulent viscosity is performed by

$$\nu_t = \tilde{\nu} f_{v1}, \quad (2.59)$$

and requires the calculation of the empirical function f_{v1} ,

$$f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad (2.60)$$

and the calculation of the $\tilde{\nu}$. The $\tilde{\nu}$ is the working variable of the turbulence model and is obtained by the transport equation

$$\begin{aligned} \frac{\partial \tilde{\nu}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\nu}}{\partial x_j} = c_{b1} [1 - f_{t2}] \check{S} \tilde{\nu} + \frac{1}{c_\sigma} [\nabla \cdot ((\nu + \tilde{\nu}) \nabla \tilde{\nu}) + c_{b2} (\nabla \tilde{\nu})^2] \\ - \left[c_{w1} f_w - \frac{c_{b1}}{\kappa_k^2} f_{t2} \right] \left[\frac{\tilde{\nu}}{d_w} \right]^2 + f_{t1} \Delta U^2. \end{aligned} \quad (2.61)$$

The calculation of the empirical function f_{v1} requires the intermediate variable χ ,

$$\chi \equiv \frac{\tilde{\nu}}{\nu}, \quad (2.62)$$

and the empirical constant c_{v1} .

The modified vorticity rate $\check{S}$ is calculated by

$$\check{S} \equiv S_\omega + \frac{\tilde{\nu}}{\kappa_k^2 d_w^2} f_{v2}, \quad (2.63)$$

and requires the calculation of the empirical function f_{v2} , which is calculated by

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}. \quad (2.64)$$

The variable S_ω is the magnitude of the vorticity, and d_w is the distance of the element to the nearest wall. The empirical function f_w and the intermediate variables g_i and r_i

are calculated by

$$f_w = g_i \left[\frac{1 + c_{w3}^6}{g_i^6 + c_{w3}^6} \right]^{1/6}, \quad (2.65)$$

$$g_i = r_i + c_{w2} (r_i^6 - r_i), \quad (2.66)$$

$$r_i \equiv \frac{\tilde{\nu}}{\check{S} \kappa_k^2 d_w^2}. \quad (2.67)$$

The last two empirical functions t_{t2} and f_{t1} are calculated by

$$f_{t2} = c_{t3} \exp(-c_{t4} \chi^2), \quad (2.68)$$

$$f_{t1} \equiv 0. \quad (2.69)$$

The constants that completes the set of equation are $c_{b1} = 0.1355$, $c_\sigma = 2/3$, $c_{b2} = 0.622$, $\kappa_k = 0.41$, $c_{w1} = c_{b1}/\kappa_k^2 + (1 + c_{b2})/c_\sigma$, $c_{w2} = 0.3$, $c_{w3} = 2$, $c_{v1} = 7.1$, $c_{t3} = 1.1$, $c_{t4} = 2$, $c_{r1} = 1.0$, $c_{r2} = 12.0$, and $c_{r3} = 1.0$.

2.6 Boundary Treatments for High-Fidelity Simulations

2.6.1 Inflow Conditions for Scale Resolving Simulations

The high-fidelity simulations can resolve small structures present in the turbulent flows that influence the development of the flow field. However, besides the high computational costs, the high-fidelity simulations present additional difficulties in developing the calculations compared to other simulation models. One difficulty when employing such methods is ensuring that the simulations can realistically represent the flow characteristics of the problem of interest. There are many problems in which it is not feasible to reproduce the complete physical model responsible for generating the flow to be analyzed. For example, in the analysis of the jet flows, there is a whole path for the fluid prior to the nozzle. In the physical experiments of jet flows, the test bench usually presents an installation composed of a reservoir where the fluid, in high pressure, is stored. The installation also has a series of pipes that lead the high-pressure fluid to the nozzle geometry, going through the valves that control the flow rate. The nozzle increases the flow velocity to produce the jet flow downstream of the nozzle exit section.

The alternative to the simulation of the complete test bench is to impose an inflow condition that represents the physical flow produced in the installation. The main difficulty in using that approach is representing all the flow features produced in the boundary condition in the installation. Examples of main features from mean flow are the boundary layer thickness, shape factor, and local total pressure. The mean flow features are relatively easy

to reproduce since they are statistical properties. However, when performing high-fidelity simulations, the flow is time-dependent and able to resolve, at some level, high-frequency fluctuations. In the case of turbulent flows, the distribution of mean turbulent intensity and mean turbulent kinetic energy, in a similar way done for RANS simulations, is no longer enough to reproduce the flow characteristics. The boundary condition should reproduce turbulent information [33], for example, single-point autocorrelations, two-point spatial correlations, and spectral distribution of turbulent kinetic energy, among others. Besides the need for the boundary conditions to produce high-order statistics, they should be capable of avoiding the generation of spurious features, *e.g.*, noise in the flow field.

A review of inflow methodologies for high-fidelity simulations is presented in Ref. [33]. Diverse options to generate an inflow condition adequate for high-fidelity simulations are discussed. The inflow conditions are grouped into different categories according to some major characteristics of the method. The turbulence library-based methods are characterized by requiring an “*a priori*” set of data to be introduced in the inflow section of the simulation to be performed. One alternative simulation can be used to generate the inflow data for the main simulation. In such applications, the precursor simulation is performed before the principal simulation to generate the flow in the inflow condition with adequate turbulent characteristics. An example of the precursor simulation is presented in Fig. 2.2, where it is possible to observe that data from one section of the flow in the precursor simulation is stored to be employed in the principal simulation. The present strategy was employed in the work presented in Refs. [58, 59]. Another option of a database for the inflow condition is to use experimental data or a previously performed simulation with a higher level of fidelity than the principal simulation. For example, stored DNS data can be employed for a LES calculation. The library-based approach can provide good quality results since it represents realistic turbulent data [60]. However, since the turbulence-based library is generated for a specific flow at a high cost, it lacks practical application, which results in few applications of the methods. One other drawback of the method is the stored data. Since the precursor simulations or experiments are performed at different moments than the primary simulation, data exchange is performed through data files that need to be stored somewhere. The amount of stored data is significant for scale-resolving simulations with large running times. The process of opening and closing files is also a restriction for obtaining high simulation performance.

Concurrent simulations are alternatives to generate the data for the principal simulation. The methods that employ such an approach are called recycling-rescaling-based methods. They employ a concurrent spatially evolving simulation that creates its inflow condition by rescaling and reintroducing the velocity field from a downstream station at the inflow section. The present approach only requires storing a small amount of data since the two simulations are performed simultaneously. It is even possible to perform

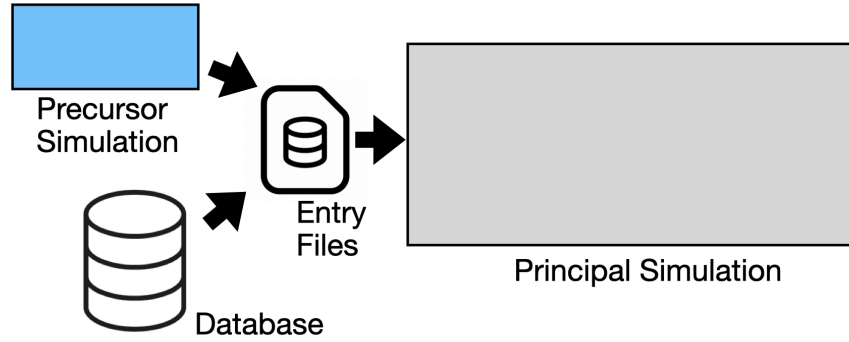


FIGURE 2.2 – Example of the library-based methods employed for generating inflow conditions.

the two simulations together as a unique simulation. In the strategy, a small portion of the domain is simulated in the precursor simulation. The outlet flow is recycled to the inflow section of the domain, producing a continuous flow. For most applications, it is necessary to introduce forcing terms in the domain to guarantee that the flows do not present different characteristics due to energy loss through the continuous flow process. In Fig. 2.3, an example of concurrent simulations is presented. The recycling strategy of the concurrent simulation and the transposition of the outflow data can be observed in the principal simulations. Examples of good results obtained with this approach are presented in the work in Refs. [61–63]. In such an approach, the amount of stored data is reduced since the simulations are performed at the same time. The library-based and recycling-rescaling-based methods share a similar characteristic, the high cost of the auxiliary simulation due to the mesh requirements of the wall-bounded flows. The auxiliary simulations can be even more expensive than the principal simulations.

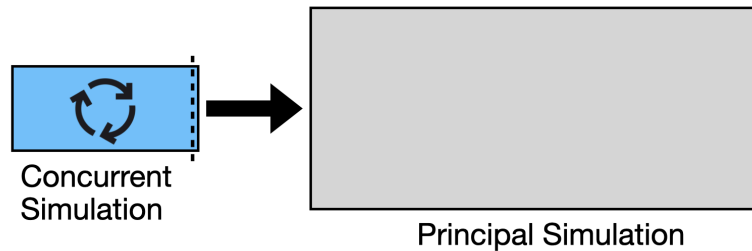


FIGURE 2.3 – Example of the concurrent simulation employed for generating inflow conditions.

The turbulent flows are obtained after a transition process from the laminar regime. The free stream flow when reaching an airfoil is laminar close to the leading edge, and after some disturbances, it transitions from laminar to turbulent. An alternative to obtain a fully turbulent flow is to induce the transition of the flow from laminar to turbulent, introducing disturbances to the flow. An example of tripping is presented in Fig. 2.4. One characteristic of the tripping method is that, unlike the library-based or the recycling-

rescaling-based methods, when a tripping method is employed, it requires a development length to reach the turbulent characteristics expected for the flow. The tripping methods rely on the employment of a numerical tripping [23, 64, 65] or geometrical tripping [26, 66]. A numerical algorithm is required to introduce the disturbances to the flow field in numerical tripping. Since it does not modify the mesh geometry, it is simpler and cheaper than the geometrical tripping. The geometrical tripping geometrically modifies the physical domain to add the tripping devices, for example, a step, gap, and cylinders. The tripping methods are capable of obtaining good results after the development region. However, they require adjustments to the intensity of the numerical perturbations or the tripping devices to reach satisfactory results.

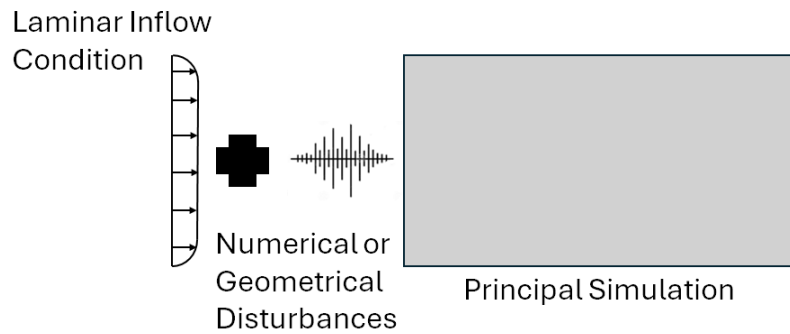


FIGURE 2.4 – Example of the transition induced method employed for generating inflow conditions.

The capability to inject realistic turbulent fluctuations without relying on a turbulence library or an auxiliary simulation is desirable for most applications. As a result, creating a turbulent inflow has drawn much interest, particularly in recent years. The synthetic turbulence methods employ different formulations to recreate turbulent structures. An artificial turbulence inflow should be able to introduce turbulent structures that are appropriate for the particular issue being researched. Matching inflow properties entails meeting the phase information, Reynolds stress tensor, turbulent kinetic energy spectrum, and intended mean velocity profile. The synthetic turbulence method is represented in Fig. 2.5. One characteristic of the synthetic turbulence methods is that none of the methods already employed could generate realistic turbulence. For this reason, the methods require a development region to progress the turbulence characteristics of the flow from those imposed in the inlet section to realistic turbulence. The development length required by the different synthetic turbulent methods is one measure of the quality of the methods. Small distances reflect that the turbulence generated by the method was closer than expected. Several methods were investigated to generate synthetic turbulence for diverse problems. The deterministic inner and outer layer method [67, 68], the Fourier modes-based methods [69–72], the proper orthogonal decomposition methods [73, 74] and the vortex and synthetic eddy methods [75–78] are examples of synthetic turbulence inflow

methods investigated.

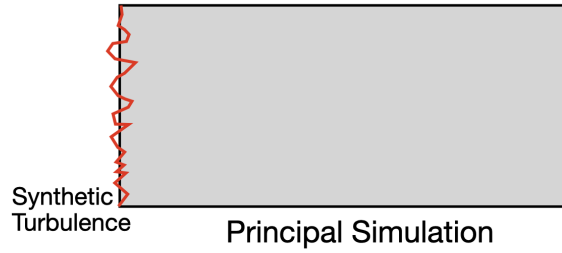


FIGURE 2.5 – Example of the synthetic turbulence method employed for generating inflow conditions.

The methods discussed in this section can be employed for different problems. They present different computational costs and capabilities to represent the turbulent characteristics of the inflow condition, making the choice of the right method for each problem difficult. The next section investigates the methods applied to recent jet flow applications.

2.6.2 Review of Inflow Treatments for Jet Flows

The employment of large-eddy simulations for the simulation of jet flows started some decades ago. The work developed by Bodony and Lele in Ref. [11] presents an extensive review of the LES and DNS of jet flows. The authors observed that the jet flow simulations presented multiple options regarding the imposed inflow condition. Bodony and Lele [11] observed two major approaches to developing the jet flow inflow conditions in the review. The first approach relied on the representation of the nozzle geometry in the computational domain to permit the flow development from the nozzle inlet condition to the jet inlet section, where the jet flow begins. The second group reproduced only the free jet flow in the simulations. In the second group, Bodony and Lele [11] observed that the simulations set up the necessity of introducing forcing terms to destabilize the flow and yield transition from a laminar to a turbulent state. One type of force term employed in subsonic flows is the vortex ring forcing [20], which introduces solenoidal disturbances given by

$$\begin{aligned}
 u_x &= u_x + \sum_{n=0}^9 \alpha \epsilon_n \cos(n\theta + \phi_n) \left[2 \frac{r_0}{r} \frac{r - r_0}{\Delta_0} \exp \left(-\ln(2) \left(\frac{\Delta(x, r)}{\Delta_0} \right)^2 \right) \right] U_j, \\
 u_r &= u_r + \sum_{n=0}^9 \alpha \epsilon_n \cos(n\theta + \phi_n) \left[-2 \frac{r_0}{r} \frac{x - x_0}{\Delta_0} \exp \left(-\ln(2) \left(\frac{\Delta(x, r)}{\Delta_0} \right)^2 \right) \right] U_j, \quad (2.70)
 \end{aligned}$$

in the incoming shear layer. The radius r is given by $r = \sqrt{y^2 + z^2}$, $\Delta(x, r)^2 = (x - x_0)^2 + (r - r_0)^2$, and $x_0 = 0.8r_0$. ϵ_n and ϕ_n are uniform random variables in time, between -1 and 1 , and between 0 and 2π . In the inflow boundary condition, a hyperbolic-tangent

velocity profile,

$$u(r) = \frac{U_j}{2} + \frac{U_j}{2} \tanh \left(\frac{r_0 - r}{2\delta_\theta} \right), \quad (2.71)$$

is imposed to represent the laminar flow leaving the nozzle. The results obtained with the inflow method were validated with experimental data concerning the flow field characteristics, velocity spectra, and acoustics levels. The boundary condition did not provide an adverse impact on the results of the simulations.

The jet flow numerical simulations presented in Ref. [79] analyzed two subsonic jet velocities. The jet flows reproduced the operating conditions of 0.4 and 0.9 Mach numbers. The hyperbolic tangent velocity profile [80]

$$u(r) = \frac{1}{2}U_j \left\{ 1 - \tanh \left[\frac{r_0}{4\delta_2} \left(\frac{r}{r_0} - \frac{r_0}{r} \right) \right] \right\}, \quad (2.72)$$

is applied in the jet inlet condition of the jet flow simulations. The variable δ_2 is the momentum thickness of the boundary layer in the inlet section of the jet flow. The authors of the work investigated two strategies for imposing the forcing term. For the 0.9 Mach number simulation, a random value from the δ_2 , specified as a function of the time and azimuthal angle, was imposed. The mean value of δ_2 is specified to $0.08r_0$. The same velocity profile at the inlet is employed for the 0.4 Mach number simulation with a value of $\delta_2 = 0.1r_0$. The forcing term is obtained by identifying disturbances using inviscid linear stability theory. Three modes were chosen to reproduce the fluctuations: the most unstable mode f_0 , one of its subharmonics $f_0/2$, and a helical mode, which possesses an azimuthal wave number $\beta = 1.0$ in the unstable frequency f_0 . The inlet disturbance vector a' is given by

$$a' = \Re[A_0\hat{a}_0 \exp(-i\omega_0 t) + A_1\hat{a}_1 \exp(i(-\omega_0 t/2 + 2.7)) + A_h\hat{a}_h \exp(i(-\omega_0 t + \beta\phi))], \quad (2.73)$$

where $\hat{a}$ is the eigenfunction vector from the linear stability theory. They are normalized for the maximum magnitude of the longitudinal velocity eigenfunction equals 1. The constants are $\omega_0 = 2\pi f_0$, $A_0 = 0.0025$, $A_1 = 0.0025$ and $A_h = 0.0005$. The velocity profiles from the simulation performed with a jet inlet Mach number of 0.9 were validated with DNS data. The Mach number 0.4 simulations also employed two subgrid-scale models, which provided slightly different turbulence and sound level distributions. The two inflow strategies could generate simulations that agree with the numerical references.

The velocity, total temperature, and static pressure profiles were imposed in the inflow boundary condition of the simulations presented in Ref. [21]. The Crocco-Busemann relation obtains the values for the density variable. The inlet profile used is the same from previous work [79], Eq. (2.72), with $\delta_2 = 0.09r_0$ and the same turbulence seeding method

based on linear stability theory, Eq. (2.73), is employed. Some differences were observed in the velocity profiles and the sound pressure levels compared to the experimental references [81]. The lack of initial shear layer turbulence in the numerical simulations may be associated with the differences between the experimental data and the numerical simulations [21]. The large-eddy simulations of a supersonic jet flow were performed without introducing the nozzle geometry in Refs. [17, 32]. The imposition of the inflow condition was performed by representing the velocity profile with a “top hat” profile, which applies all the properties fixed to the specific values of the jet inlet. The imposition of the boundary conditions was performed using the 1-D characteristic relations for the 3-D Euler equations. The inlet condition does not consider any disturbance-forcing method. The proposed inflow condition induced the flow transition in the region close to the jet inflow station in the numerical simulations. The numerical simulations presented an underresolved behavior with a significantly shorter potential core length than the experimental reference. Large RMS values of the longitudinal velocity component fluctuations are observed in the lipline of the jet flow field close to the inlet section, which is not present in the experimental reference.

It is observed that after the review presented in Ref. [11], the strategy of modeling the nozzle geometry in the computational domain became the predominant option to develop the turbulent characteristics of the flow prior to the jet inlet section. In the early stages of developing LES of jet flows, some work has been able to extract valuable results from available computational resources. In the numerical simulations analyzed in Refs. [18, 82], the subsonic and supersonic jet flow were investigated with the external nozzle walls represented in the computational domain. This strategy added to the flow of the external wall and, consequently, the nozzle lip. The longitudinal velocity profile is imposed with temperature in the inflow boundary condition, and the tangential velocity is set to zero. Pressure is obtained by

$$\frac{\partial p}{\partial t} + (u - c) \frac{\partial p}{\partial x} = 0, \quad (2.74)$$

in subsonic flows and by direct imposition for supersonic flows. The velocity profile is defined to have a boundary layer thickness of $0.035D_j$ and a momentum thickness of $0.004D_j$. The simulations investigated different operating conditions, defined by inflow velocities and temperature, which produced different levels of agreement with experimental data. The numerical simulations reduced the numerical errors with grid refinement and produced a good agreement with the experimental reference after some adjustments were made to the numerical schemes. Some spurious peaks are presented in the jet flow field and the authors have evidence that physical inflow forcing devices can handle the peak values.

Subsonic jet flows were investigated in Ref. [19, 83] with the internal walls of the nozzle

represented in the computational domain. Different approaches for imposing the inflow condition are investigated. One approach was to impose the total pressure and enthalpy in the inlet section of the nozzle. Two other approaches are investigated. The addition of a synthesized inlet turbulence and the specification of a total pressure profile to produce a velocity profile. The synthesized inlet turbulence is obtained by the imposition of velocity fluctuation obtained by random Fourier nodes and specified turbulent kinetic energy and turbulent dissipation rate. The velocity components v_i are generated by the sum of 30 Fourier modes,

$$v_i(x) = 2 \sum_{n=1}^{30} \hat{u}_n \cos(k_n x + \varphi_n) \sigma_n. \quad (2.75)$$

The variables $\hat{u}_n$, φ_n , and σ_n are the amplitude, phase and direction of the n Fourier mode. The amplitude of each mode,

$$\hat{u}_n = \sqrt{E(k_n) \Delta k_n}, \quad (2.76)$$

is calculated from a model turbulence energy spectrum function $E(k_n)$ obtained by isotropic turbulence. The model turbulence energy spectrum function is obtained by the imposed turbulent kinetic energy and dissipation rate, and the Δk_n represents an interval of the spectrum around k_n . The velocity fluctuation at time step m , u_i^m , is obtained from the velocity components v_i by

$$u_i^m = a u_i^{m-1} + b (v_i^m + v_i^{m-1}), \quad (2.77)$$

where a and b define a low-pass filter for the synthesized velocity components, $a = \exp^{\Delta t/\tau}$ and $b = \sqrt{1.0 - a}/2$, τ is a defined time scale for the frozen turbulence. No information on the total pressure profile is provided. It was observed that the three inflow methodologies did not significantly change the acoustic predictions from the numerical simulations performed.

Subsonic jet flows were analyzed with the nozzle represented by a constant radius pipe in Refs. [12, 22–24, 84]. The simulations were conducted for initially laminar flows with the imposition of a laminar boundary layer profile in the nozzle inflow condition. The work presented in Ref. [12] investigated a Mach number 0.9 jet flow using different boundary layer thicknesses in the nozzle inlet. The laminar Blasius profile is imposed by a polynomial approximation,

$$u_x(r) = U_j \frac{r_0 - r}{\delta} \left[2 - 2 \left(\frac{r_0 - r}{\delta} \right)^2 + \left(\frac{r_0 - r}{\delta} \right)^3 \right], \quad \text{if } r \geq r_0 - \delta, \\ u_x(r) = U_j, \quad \text{if } r < r_0 - \delta. \quad (2.78)$$

The radial and tangential velocities are imposed to zero, the pressure is defined, and the temperature is obtained by a Crocco-Busemann relation. The boundary layer thickness employed has values of $\delta = 0.025r_0$, $0.05r_0$, $0.1r_0$ and $0.2r_0$. Two levels of pressure random noise were added to the nozzle interior domain, from $-0.4r_0 \leq x \leq -0.2r_0$. The jet inlet plane is positioned at $x = 0.0$. The random pressure was added only to the boundary layer thickness $\delta = 0.05r_0$ with amplitudes of 250 and 2000 Pa. The inlet pressure of the flow is $1 \times 10^5 Pa$. It was observed that the boundary layer thickness affected the potential core length of the jet flows and the levels of turbulent intensities in the centerline of the jet flow. The development of the shear layer was affected by the introduction of the noise in the nozzle interior.

The inflow condition presented in Ref. [12] was improved in Ref. [23], where a tripped exit boundary layer was reproduced by using two tripping methods inside the nozzle domain. The Blasius velocity profile, Eq. (2.78), was employed with a boundary layer thickness of $0.15r_0$. The tripping methods in Ref. [23] are referred to as noise-tripping and ring-tripping methods. The noise-tripping introduces velocity fluctuations that are fully random in time and space. The tripping influences the flow in $-1.1r_0 < x < -0.9r_0$ and inside the boundary layer of the Blasius profile, $r_0 - \delta < r < r_0$. The jet inlet is positioned at $x = 0.0$. The three velocity components, in cylindrical coordinates, are disturbed according to

$$\begin{Bmatrix} u_x \\ u_r \\ u_\theta \end{Bmatrix} = \begin{Bmatrix} u_x \\ u_r \\ u_\theta \end{Bmatrix} + \alpha U_j \begin{Bmatrix} 3\epsilon_x(x, r, \theta, t) \\ \epsilon_r(x, r, \theta, t) \\ 2\epsilon_\theta(x, r, \theta, t) \end{Bmatrix}. \quad (2.79)$$

The variables ϵ_x , ϵ_r , and ϵ_θ are random numbers between -1 and 1 . The constant *alpha* is an adjustment constant for the jet velocity U_j . The value $\alpha = 0.00625$ is used to adjust the peak of axial velocity fluctuation. The ring tripping is implemented divergence-free to minimize spurious acoustic waves. It is based on vortical disturbances uncorrelated in the azimuthal direction. An annular velocity is calculated by

$$\begin{Bmatrix} u_x^{ring} \\ u_r^{ring} \end{Bmatrix} = \frac{2r_{ring}}{rb} \exp\left(-\ln(2)\frac{a^2}{b^2}\right) \begin{Bmatrix} x_{ring} - x \\ r - r_{ring} \end{Bmatrix}, \quad (2.80)$$

and then the values are inserted in

$$\begin{Bmatrix} u_x \\ u_r \end{Bmatrix} = \begin{Bmatrix} u_x \\ u_r \end{Bmatrix} + \epsilon_\alpha(\theta, t) \alpha U_j \begin{Bmatrix} u_x^{ring} \\ u_r^{ring} \end{Bmatrix}, \quad (2.81)$$

to generate the tripping in the boundary layer. The variable a is calculated by $a^2 = (x - x_{ring})^2 + (r - r_{ring})^2$, and the value of b may vary according to the simulation. The vortex ring core is located at $x_{ring} = -0.95r_0$ and at $r_{ring} = r_0\delta/2 + \epsilon_r(\theta, t)\delta/6$. The

variables ϵ_r and ϵ_α are random numbers from -1 to 1 . The value of *alpha* may change between the simulations. There were no significant differences in the numerical simulation results due to the choice of the tripping method.

In the analysis of highly disturbed subsonic jets presented in Ref. [22], the velocity profile presented in Eq. (2.78) is used with the ring tripping method presented in Eq. (2.81). A strong influence of the jet inlet boundary layer in the mixing layer properties of the jet flow was observed. In Ref. [24], the laminar velocity profile, Eq. (2.78), and the turbulent velocity profile,

$$u_x(r) = U_j \left\{ \sin \left[\frac{\pi}{2} \left(\frac{r_0 - r}{\delta_{T2}} \right)^{\beta 2} \right] \right\}^{\gamma 2}, \quad \text{if } r \geq r_0 - \delta_{T2},$$

$$u_x(r) = U_j, \quad \text{if } r < r_0 - \delta_{T2}, \quad (2.82)$$

were used with the ring-tripping method, Eq. (2.81), to produce “experiment-like” boundary layer in the nozzle-exit section. The turbulent profile presented in Eq. (2.82) used the constants $\beta 2 = 0.423$, $\gamma 2 = 0.82$, and $\delta_{T2} = 0.1328r_0$. In addition to the inflow methods, the computational mesh was significantly refined compared to other meshes employed in the numerical simulations of jet flows. The numerical mesh employed in the work reached 3.1×10^9 points to discretize the computational domain. With the combination of the inflow method with the computational mesh and the high-order scheme, they could produce an excellent agreement with one of the experimental references.

The jet flow simulation presented in Refs. [15, 29–31] imposed the inflow condition at the nozzle inlet section by a total pressure and temperature characteristic condition. Because of the nozzle geometry in the computational domain, the flow entering the nozzle is subsonic. Based on the 1-D characteristic relations for the 3-D Euler equations, the adequate imposition for subsonic flows is the total pressure and temperature. No inflow profile is imposed in the inlet of the numerical simulations. In the jet flow numerical simulations presented in Refs. [28, 34], a similar approach of imposing a total pressure and temperature in the nozzle inlet is employed. However, they also imposed a velocity profile to match the boundary layer in the nozzle outlet.

The ensemble of synthetic turbulence with wall modeling inside the nozzle was employed in the numerical simulation in Ref. [14] to produce nozzle outlet conditions that better match the flow in the experimental reference. The digital filtering technique proposed in Ref. [85] was adapted to employ an unstructured grid to develop synthetic turbulence to generate realistic turbulence by the nozzle-exit section. The model requires estimates of the amplitude of the fluctuations, length, and time scales. After the flow leaves the tripping region, it enters a region where the wall modeling is employed. The modeling strategy is based on traditional approaches, discussed in Refs. [86, 87]. The

method is based on a wall-stress modeling approach where the numerical methods solve a RANS model near the wall and a LES model in the rest of the domain. In addition to the two methods, the effect of near-wall mesh refinement is investigated. It is concluded in Ref. [14] that the best agreement with the experimental reference was achieved using the three numerical features.

In Refs. [25, 26], the geometrical tripping is used to develop the flow inside the nozzle. The effect of including gaps in the nozzle interior was investigated to produce the tripping necessary to transition the flow. In Ref. [25], no wall modeling strategy is employed with the step approach. Therefore, an increase in the local mesh refinement is necessary to obtain the levels of turbulence increment due to the steps introduced in the domain. Ref. [26] introduces the steps with two wall modeling strategies. One of them is to solve the near-wall region with RANS and the outer free flow with LES, similar to the performed in Ref. [14]. In the second one, the wall-modeled LES is effectively introduced, which requires additional mesh refinement in the near wall region. Both methodologies produce adequate results, with some advantages in the first strategy for thermal and vibrational analyses, while the second methodology is more suitable for acoustics analyses.

The majority of the strategies presented that use any forcing term to improve the unsteady data for the simulations rely on tripping methodologies to induce the transition or increase the turbulence intensity of the flow. Only two strategies presented in Refs. [14, 18, 82] tried to generate some synthetic turbulence to provide an inflow condition closer to the desired condition. In previous experience of the research group [17, 32], an inviscid profile was imposed in the inflow condition of the supersonic jet flow. It is observed that a steady radial velocity profile is commonly employed for inflow conditions. In addition, tripping methods are the most used in practice to increase the turbulent levels of the flow. The present work evaluates two new inflow conditions with the inviscid profile: a steady viscous profile and an unsteady viscous profile, generated with a tripping method.

3 Numerical Methods

The solution of the filtered Navier-Stokes equations is obtained using a numerical approach. The research group has experience developing LES of supersonic jet flows. A solver based on the finite difference method on structured meshes, named JAZzY solver [17, 32], was developed to perform the jet flow simulations. The research group also employed a high-order solver on unstructured meshes, the FLEXI numerical framework [88, 89], based on the discontinuous Galerkin scheme to perform LES of wall-bounded flows. The high-order solver is also an option for performing LES of the supersonic jet flows. As part of the research effort here described, the results from the numerical simulations performed with the two methods are compared to support the selection of the solver to be employed in the continuation of the present work. The fundamentals that characterize the two numerical methods are introduced in this section. The complete description of the JAZzY solver is presented in Refs. [17, 90]. The main characteristics of the FLEXI numerical framework are discussed in the present chapter. The discussion of the boundary conditions used in the numerical simulations performed in the present research is presented at the end of the chapter.

3.1 Fundamental Aspects of the Numerical Schemes

The research group has two numerical solvers capable of performing LES of supersonic jet flows. The two solvers are based on distinct numerical methods. The JAZzY solver [17, 90] uses a finite difference scheme to discretize the filtered Navier-Stokes equations. The FLEXI numerical framework [35] uses the discontinuous Galerkin scheme. The fundamental aspects of the two numerical methods are discussed to support the selection of the numerical solver to be employed for the jet flow simulations in the present research work. The numerical methods were developed to solve partial differential equations. One example of one-dimensional conservation law is given by

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \quad x \in \Omega, \quad (3.1)$$

where the domain Ω is subject to a set of boundary conditions at the boundaries $\partial\Omega$, the variable $u(x, t)$ is the solution, and $f(u)$ is the flux.

The first scheme discussed is the finite difference method (FD) employed in the JAZzY solver. The domain is divided into multiple grid elements, x^k , where $k = 1, \dots, K$, and the spatial derivative can be approximated by multiple options. The solution in the grid points is represented by $u_h(x^k, t)$. The conservation law can be described by

$$\frac{\partial u_h(x^k, t)}{\partial t} + \frac{f_h(x^{k+1}, t) - f_h(x^{k-1}, t)}{\Delta x} = 0, \quad (3.2)$$

where $\Delta x = x^{k+1} - x^{k-1}$ is the grid size. In the present example, the derivative of the flux is approximated by a second-order difference approximation. The numerical accuracy of the difference approximation can be defined by an analysis of a Taylor series expansion [91]. The choice of the difference approximation scheme can modify the order of accuracy and introduce some level of numerical dissipation to the scheme. One difficulty of this scheme is its dependency on a certain well-defined structure of the computational mesh. Generating structured meshes in complex geometries is a challenging task, and depending on the complexity of the geometry to be analyzed, the process can be unfeasible.

The discontinuous Galerkin finite element method (DG-FEM) is the discretization scheme employed in the FLEXI numerical framework. The DG-FEM method can be described by first introducing some fundamentals of the classic finite element methods (FEM) and, then, discussing the differences that lead to the DG-FEM schemes. In the finite element methods, the element D^k can be defined between the interval $[x^k, x^{k+1}]$. Inside the element, the solution can be expressed by

$$u_h(x, t) = \sum_{n=1}^{N_p} u_n \psi_n(x), \quad (3.3)$$

where $\psi_n(x)$ is a locally defined basis function. If the basis function is defined to be linear

$$u_h(x, t) = \sum_{i=0}^1 u(x^{k+i}) \ell_i^k(x), \quad (3.4)$$

where the Lagrange polynomial ℓ is defined by

$$\ell_i^k(x) = \frac{x - x^{k+1-i}}{x^{k+i} - x^{k+1-i}}. \quad (3.5)$$

In such an example, each element shares at least one node with others. In practice, only the boundary nodes share one node, while all interior elements share the two nodes with

other elements. If the solution of a numerical method could solve the residue

$$\mathcal{R}_h(x, t) = \frac{\partial u_h}{\partial t} + \frac{\partial f_h}{\partial x}, \quad (3.6)$$

the solution of the equation is found. An alternative is to define a space of test functions, V_h , and to ensure that the residual is orthogonal to all test functions $\phi_h(x)$ in this space, which can be expressed by

$$\int_{\Omega} \mathcal{R}_h(x, t) \phi_h(x) dx = 0. \quad (3.7)$$

A global representation of the numerical solution can be obtained by employing the linear shape function $N_i(x_j) = \delta_{ij}$ in a way that

$$u_h(x) = \sum_{k=1}^K u^k N^k(x), \quad (3.8)$$

and the linear shape function can also be employed in the test functions

$$\phi_h(x) = \sum_{k=1}^K \phi^k(x^k) N^k. \quad (3.9)$$

The Galerkin schemes are a class of finite element methods where the spaces spanned by the basis and test functions are the same.

When Eqs. (3.8) and (3.9) are inserted back at Eq. (3.7), they result in

$$\int_{\Omega} [\phi^p N^p(x)] \frac{\partial}{\partial t} [u^k(t) N^k(x)] dx + \int_{\Omega} [\phi^p N^p(x)] \frac{\partial}{\partial x} [f_h^k N^k(x)] dx = 0, \quad (3.10)$$

which, after some manipulation, can be written by

$$\mathcal{M} \frac{\partial}{\partial t} [u^k(t)] + \mathcal{S} f_h^k = 0, \quad (3.11)$$

where $\mathcal{M}$ and $\mathcal{S}$ are the mass and stiffness matrix given by

$$\mathcal{M}_{pk} = \int_{\Omega} N^p(x) N^k(x) dx, \quad (3.12)$$

$$\mathcal{S}_{pk} = \int_{\Omega} N^p(x) \frac{\partial}{\partial x} [N^k(x)] dx. \quad (3.13)$$

In addition to the mass and stiffness matrices, the solution vector and the flux vector complete the system. The mass and stiffness matrices can be resolved to provide the values of the solution in the domain, which represents the global behavior of the finite element method.

In the discontinuous Galerkin scheme, each mesh element has a dedicated set of interior

and interface nodes. The space of basis functions is defined as the space of piecewise polynomial functions, which can be described by

$$\int_{D^k} \mathcal{R}_h(x, t) \ell_i^k(x) dx = 0, \quad (3.14)$$

for the test functions $\ell_i^k(x)$. This approach led to a local scheme, so only information from the elements is required. The employment of numerical fluxes performs the continuity of the information to connect the elements at the interfaces. It is done by employing Gauss's theorem to the flux term in the residual, obtaining

$$\int_{D^k} \frac{\partial u_h^k}{\partial t} \ell_j^k dx - \int_{D^k} f_h^k \frac{\partial \ell_j^k}{\partial t} dx + [f_h^k \ell_j^k]_{x^k}^{x^{k+1}} = 0. \quad (3.15)$$

In Eq. (3.15), the last term corresponds to the flux, and the Lagrange polynomials are evaluated at the boundaries of the element. Each element sharing a node has its value. A numerical flux f^* can unify the flux values between the two elements. Determining the numerical flux can also introduce information on the flow type. If the same development of Eq. (3.11) is employed to Eq. (3.15), the local elementwise scheme is obtained

$$\mathcal{M}^k \frac{\partial}{\partial t} [u^k(t)] + \mathcal{S}^k f_h^k + f^*(x^{k+1}) \ell^k(x^{k+1}) + f^*(x^k) \ell^k(x^k) = 0, \quad (3.16)$$

where the mass and stiffness matrices are given by

$$\mathcal{M}_{ij}^k = \int_{D^k} \ell_i^k(x) \ell_j^k(x) dx, \quad (3.17)$$

$$\mathcal{S}_{ij}^k = \int_{D^k} \ell_i^k(x) \frac{\partial}{\partial x} \ell_j^k(x) dx. \quad (3.18)$$

The comparison of the two numerical schemes indicates the advantages and disadvantages of each method. The finite difference scheme is simpler than the discontinuous Galerkin finite element method. Due to the simplicity of the FD scheme, the numerical solver is fast due to the minimum calculations performed. The scheme has a low memory consumption, and due to the centered scheme, it has no intrinsic artificial dissipation. The choice of the artificial dissipation method performs the numerical stabilization of the method. The advantages of the DG-FEM are the capability to simulate general geometries with an unstructured topology and the intrinsic high-order capability of the method.

The choice of the numerical solver used in the present research is based on multiple aspects. One advantage of the FLEXI numerical framework is the capability to perform high-order simulations without the need to implement new features. The geometrical flexibility would allow using the numerical framework to solve other problems of interest to the research group [88, 89, 92]. The comparison of the jet flow numerical results

from the two solvers, presented in Sec. 5.1.1, indicate slight improvements when the FLEXI numerical framework is used with a third-order accurate spatial discretization when simulations with the same degrees-of-freedom are analyzed. For the three reasons presented, the FLEXI numerical framework was chosen as the numerical solver for the research effort.

3.2 FLEXI Numerical Framework

3.2.1 Discontinuous Galerkin Spectral Element Method

In this section, the DG-FEM numerical formulation employed in the FLEXI numerical framework [35] is presented. Different DG-FEM implementation options are employed in the multiple numerical frameworks used in the literature. The set of choices from the characteristics of the DG-FEM scheme used in the FLEXI numerical framework is called the discontinuous Galerkin spectral element method (DGSEM) [36, 37]. The implementation of the DGSEM in the FLEXI numerical framework uses exclusively hexahedral elements to discretize the domain. The hexahedral elements from the physical domain are mapped to a reference unit cube. The solutions and fluxes are represented by a nodal basis with the choice of tensor-product of one-dimensional Lagrange basis functions applied to the reference unit cube element. The choice of the tensor-product of one-dimensional Lagrange basis functions is more efficient regarding the number of operations and memory consumption than other options [37]. The volume and surface integrals are substituted by a Gauss-Legendre quadrature. The solution and fluxes are approximated by interpolation at the nodes of the Gauss-Legendre or Gauss-Lobatto-Legendre quadrature points. The computational efficiency is increased with the collocation of the integration and interpolation nodes.

The use of hexahedral elements limits the flexibility of the mesh generation process, even with an unstructured mesh architecture. The choice of hexahedral elements reduces the cost per degree of freedom compared to other DG-FEM choices using tetrahedral elements [93]. The dispersion and dissipation properties of the DGSEM scheme used in the FLEXI numerical framework are presented in Ref. [94]. The fundamentals of the DGSEM scheme are developed in search of the semi-discrete approach of both the weak and strong forms of the method. The two forms are presented because the weak form is more commonly used than the strong form [35]. The strong form is employed in the present work due to the employment of the split DG formulation, described in Sec. 3.2.2, which requires some characteristics that can only be obtained with the strong formulation.

3.2.1.1 Discontinuous Galerkin Formulation

The discontinuous Galerkin spectral element method implemented in the FLEXI numerical framework requires the physical domain Ω to be discretized into multiple non-overlapping hexahedral elements Ω_h . The numerical algorithm is capable of solving curved surfaces. The numerical computations are performed on a reference cube $E = [-1, 1]^3$. It is necessary to define a transfinite map $\vec{x} = \mathcal{X}(\vec{\xi}, t)$. The transfinite map is calculated at the beginning of the numerical computation. The transfinite map presents different formulations as a function of the shape of the hexahedral element in the physical domain. The coordinates in physical space $\vec{x}$ and in the computational domain $\vec{\xi}$ are given by

$$\vec{x} = (x_1, x_2, x_3)^T, \quad (3.19)$$

$$\vec{\xi} = (\xi^1, \xi^2, \xi^3)^T. \quad (3.20)$$

The Jacobian, $\mathcal{J}$, of the mapping between the physical and the computational domain, is the determinant of the Jacobian matrix, $\nabla_{\xi}\mathcal{X}$. The ∇_{ξ} operator represents the nabla operator evaluated in the computational domain. The contravariant basis vector $\mathcal{J}\vec{a}^i$ is also defined and calculated so that the divergence-free is ensured [95]. The contravariant basis vector is calculated by

$$\mathcal{J}\vec{a}_n^i = -\hat{x}_i \cdot \nabla_{\xi} \times (x_l \nabla_{\xi} x_m), \quad i = 1, 2, 3, \quad n = 1, 2, 3, \quad (n, m, l) = \text{cyclic}, \quad (3.21)$$

where $\hat{x}_i$ is the unit vector in the i th Cartesian direction. Besides mapping the physical domain to the computational domain, it is necessary to map the governing equations to the computational domain.

The filtered Navier-Stokes equations, Eq. (2.44) are represented in vector form

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot \vec{F}(\vec{u}, \nabla \vec{u}) = 0, \quad (3.22)$$

where $\vec{u} = [\bar{\rho}, \bar{\rho}\tilde{u}_1, \bar{\rho}\tilde{u}_2, \bar{\rho}\tilde{u}_3, \bar{\rho}\tilde{e}]^T$ is the vector of filtered conserved variables and $\vec{F}$ is the flux vector. The flux vector can be divided into the advective, or Euler, and the viscous fluxes, $\vec{F}^e$ and $\vec{F}^v$, respectively. The flux vector division is obtained by $\vec{F} = \vec{F}^e - \vec{F}^v$. The fluxes with the filtered variables may be written as

$$\vec{F}_i^e = \begin{bmatrix} \bar{\rho}\tilde{u}_i \\ \bar{\rho}\tilde{u}_1\tilde{u}_i + \delta_{1i}\bar{p} \\ \bar{\rho}\tilde{u}_2\tilde{u}_i + \delta_{2i}\bar{p} \\ \bar{\rho}\tilde{u}_3\tilde{u}_i + \delta_{3i}\bar{p} \\ (\bar{\rho}\tilde{e} + \bar{p})\tilde{u}_i \end{bmatrix} \quad \vec{F}_i^v = \begin{bmatrix} 0 \\ \tilde{\tau}_{1i}^m \\ \tilde{\tau}_{2i}^m \\ \tilde{\tau}_{3i}^m \\ \tilde{\tau}_{ij}^m\tilde{u}_i - \tilde{q}_i^m \end{bmatrix}, \quad \text{for } i = 1, 2, 3. \quad (3.23)$$

In the continuity of the formulation, the flux vectors are written as one to keep a compact notation. The flux term, or the divergence terms, can be mapped from physical space to reference space by

$$\nabla \cdot \vec{F} = \frac{1}{\mathcal{J}} \sum_{i=1}^3 \frac{\partial}{\partial \xi^i} \mathcal{J} \vec{a}^i \cdot \vec{F}, \quad (3.24)$$

which brings the contravariant fluxes $\vec{\mathcal{F}}$

$$\vec{\mathcal{F}}^i = \mathcal{J} \vec{a}^i \cdot \vec{F}. \quad (3.25)$$

The governing equations, Eq. (3.22), can be mapped on the reference space using the equations

$$\mathcal{J}(\vec{\xi}) \frac{\partial}{\partial t} \vec{u}(\vec{\xi}, t) + \nabla_{\xi} \cdot \vec{\mathcal{F}}(\vec{u}(\vec{\xi}, t), \nabla \vec{u}(\vec{\xi}, t)) = 0. \quad (3.26)$$

The discontinuous Galerkin formulation is obtained by the multiplication of Eq. (3.26) by the test function $\phi = \phi(\vec{\xi})$, integration over the reference element E , and application of Green's identity to separate interior and boundary contributions, which results in

$$\frac{\partial}{\partial t} \int_E \mathcal{J} \vec{u} \phi d\vec{\xi} + \int_{\partial E} \left(\vec{\mathcal{F}} \cdot \vec{N} \right)^* \phi dS - \int_E \vec{\mathcal{F}} \cdot (\nabla_{\xi} \phi) d\vec{\xi} = 0, \quad (3.27)$$

or with a second application of Green's identity to the interior flux terms that results in

$$\frac{\partial}{\partial t} \int_E \mathcal{J} \vec{u} \phi d\vec{\xi} + \int_{\partial E} \left(\left(\vec{\mathcal{F}} \cdot \vec{N} \right)^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi dS + \int_E \nabla_{\xi} \vec{\mathcal{F}} \cdot \phi d\vec{\xi} = 0. \quad (3.28)$$

In Eq. (3.27), the discontinuous Galerkin scheme is presented in the weak form, and in Eq. (3.28) the strong form is presented. In the discontinuous Galerkin equations, $\vec{N}$ is the unit normal vector of the faces of the elements in the reference space. The $(\cdot)^*$ superscript indicates the need to handle the properties in the interface of the elements since each element may have a different value. In the implementation used in this work, the approximate Riemann solver of Roe [96] treats the properties in the interfaces. Initially, the semi-discrete approach in weak form is discussed. Then, the approach for the strong form is also discussed. Analytically and discretely, the weak and the strong formulations are identical for the DGSEM if the Legendre-Gauss-Lobatto quadrature is used. If the Gauss-Legendre quadrature is employed, special attention should be given to the internal fluxes [36]. The strong form is the starting point for the implementation of the Split DG formulation discussed in the Sec. 3.2.2.

3.2.1.2 Approximation of the Solution and Fluxes

In each element, the solution is approximated by a polynomial tensor-product basis. The polynomial degree has an order N in each space direction. The solution is given by

$$\vec{u} \approx \sum_{m,n,o=0}^N \hat{u}_{mno} \psi_{mno}(\vec{\xi}), \quad (3.29)$$

where $\hat{u}$ are the nodal degrees of freedom and ψ_{mno} is the basis function defined by a composition of the one-dimensional Lagrange polynomials ℓ

$$\psi_{mno}(\vec{\xi}) = \ell_m(\xi^1) \ell_n(\xi^2) \ell_o(\xi^3), \quad (3.30)$$

$$\ell_j(\xi) = \prod_{\substack{i=0 \\ i \neq j}}^N \frac{(\xi - \xi_i)}{(\xi_j - \xi_i)}, \quad j = 0, \dots, N, \quad (3.31)$$

with the property

$$\ell_j(\xi_i) = \delta_{ij}, \quad j = 0, \dots, N, \quad (3.32)$$

that is defined by a nodal set $\{\xi_i\}_{i=0}^N$ defined in the interval $\xi \in [-1, 1]$.

The same approach is performed for the contravariant fluxes. They are approximated by interpolation at the nodal points

$$\vec{\mathcal{F}}(\vec{u}(\vec{\xi}, t))^l = \sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^l \psi_{mno}(\vec{\xi}), \quad l = 1, 2, 3, \quad (3.33)$$

the polynomial coefficients are calculated as the transformed physical fluxes

$$\hat{\mathcal{F}}_{mno}^l = \sum_{d=1}^3 \mathcal{J} a_d^l(\xi^1, \xi^2, \xi^3) F_d(\vec{u}(\xi^1, \xi^2, \xi^3)). \quad (3.34)$$

The interpolation is formally equal to a discrete projection, which means it is exact only up to a maximum polynomial degree of the integration. The maximum polynomial degree of the integration depends on the distribution of points used. For example, $(N+1)$ Gauss points could integrate polynomials of degree $N_{int} = (2N+1)$ exactly. The problem of interest from this work has non-linear fluxes. It may have non-linear metric terms, which leads to truncation error polynomials representation of the functions and aliasing errors of the high-order terms.

3.2.1.3 Semi-Discrete Approach in Weak Form

Once the approximation for the solution and the fluxes are defined, it is possible to return to Eq. (3.27) and discuss how each term is developed. The first term is the time derivative integral, which is responsible for evolving the solution in time. The second term, the surface integral, deals with a balance of the fluxes through the surfaces of the element. The third, and last term, deals with calculations within the element.

The time derivative integral has the solution vector approximated by the numerical solution, Eq. (3.29), and the choice for the test function is $\phi = \psi_{ijk}$. Then, the integral is separated into three directions and approximated by a Gauss-Legendre quadrature.

$$\begin{aligned}
\frac{\partial}{\partial t} \int_E \mathcal{J} \vec{u} \phi d\vec{\xi} &= \frac{\partial}{\partial t} \int_E \mathcal{J} \left(\sum_{m,n,o=0}^N \hat{u}_{mno} \psi_{mno} \right) \psi_{ijk} d\vec{\xi} \\
&= \frac{\partial}{\partial t} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 J \left(\sum_{m,n,o=0}^N \hat{u}_{mno} \psi_{mno} \right) \psi_{ijk} d\xi^1 d\xi^2 d\xi^3 \\
&= \frac{\partial}{\partial t} \sum_{\lambda,\mu,\nu=0}^N \mathcal{J} \left(\sum_{m,n,o=0}^N \hat{u}_{mno} \psi_{mno} \right) \psi_{ijk} \omega_\lambda \omega_\mu \omega_\nu \\
&= \frac{\partial}{\partial t} \sum_{\lambda,\mu,\nu=0}^N \mathcal{J} \left(\sum_{m,n,o=0}^N \hat{u}_{mno} \underbrace{\ell_m(\xi_\lambda^1)}_{=\delta_{m\lambda}} \underbrace{\ell_n(\xi_\mu^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_\nu^3)}_{=\delta_{o\nu}} \right) \psi_{ijk} \omega_\lambda \omega_\mu \omega_\nu \\
&= \frac{\partial}{\partial t} \sum_{\lambda,\mu,\nu=0}^N \mathcal{J} \hat{u}_{\lambda\mu\nu} \underbrace{\ell_i(\xi_\lambda^1)}_{=\delta_{i\lambda}} \underbrace{\ell_j(\xi_\mu^2)}_{=\delta_{j\mu}} \underbrace{\ell_k(\xi_\nu^3)}_{=\delta_{k\nu}} \omega_\lambda \omega_\mu \omega_\nu, \tag{3.35}
\end{aligned}$$

the time integral can be reduced even more due to the collocation of the integration and interpolation nodes and the property from the Lagrange polynomial, Eq. (3.32),

$$\frac{\partial}{\partial t} \int_E \mathcal{J} \vec{u} \phi d\vec{\xi} = \mathcal{J}(\vec{\xi}_{ijk}) \omega_i \omega_j \omega_k \frac{\partial \hat{u}_{ijk}}{\partial t}. \tag{3.36}$$

One aspect to mention about this equation is that the Gauss-Legendre quadrature can integrate exactly the time derivative integral if the Jacobian is linear in $\vec{\xi}$, which is the case for linear and bilinear hexahedra [97]. For other types of hexahedral elements, an additional integration error is introduced. This error is usually called mass lumping [37]. In the case of the Gauss-Lobatto points, the solution is mass-lumped due to the reduced integration order, $(2N - 1)$, compared to the Gauss points.

The volume integral term, the third term in Eq. (3.27), is manipulated in a similar way to the performed for the time derivative term, Eq. (3.36). The development of the equation refers to the general contravariant flux $\vec{\mathcal{F}}$, but it can be readily extended to the split in the advective and viscous fluxes. The volume integral term can be separated into

the three contravariant flux directions to handle each direction independently

$$\int_E \vec{\mathcal{F}} \cdot (\nabla_{\xi} \phi) d\vec{\xi} = \sum_{d=1}^3 \int_E \vec{\mathcal{F}}^d \frac{\partial \phi}{\partial \xi^d} d\vec{\xi}, \quad (3.37)$$

and only one of the directions is investigated due to the similarities between the developments. The manipulation of Eq. (3.37) starts with the insertion of the approximation to the flux, Eq. (3.33), and the choice for the test function is $\phi = \psi_{ijk}$. Then, substituting the volume integral with the integral in each direction and approximating the three integrals by the Gauss-Legendre quadrature and manipulating the terms from the ψ_{lmn} and ψ_{ijk} , in a similar way performed in the manipulation of Eq. (3.36),

$$\begin{aligned} \int_E \vec{\mathcal{F}}^1 \frac{\partial \phi}{\partial \xi^1} d\vec{\xi} &= \int_E \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \psi_{mno} \right) \frac{\partial \psi_{ijk}}{\partial \xi^1} d\vec{\xi} \\ &= \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \psi_{mno} \right) \frac{\partial \psi_{ijk}}{\partial \xi^1} d\xi^1 d\xi^2 d\xi^3 \\ &= \sum_{\lambda,\mu,\nu=0}^N \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \underbrace{\ell_m(\xi_{\lambda}^1)}_{=\delta_{m\lambda}} \underbrace{\ell_n(\xi_{\mu}^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_{\nu}^3)}_{=\delta_{o\nu}} \right) \frac{\partial \psi_{ijk}}{\partial \xi^1} \omega_{\lambda} \omega_{\mu} \omega_{\nu} \\ &= \sum_{\lambda,\mu,\nu=0}^N \hat{\mathcal{F}}_{\lambda\mu\nu}^1 \frac{d\ell_i(\xi)}{d\xi} \bigg|_{\xi=\xi^1} \underbrace{\ell_j(\xi_{\mu}^2)}_{=\delta_{j\mu}} \underbrace{\ell_k(\xi_{\nu}^3)}_{=\delta_{k\nu}} \omega_{\lambda} \omega_{\mu} \omega_{\nu} \\ &= \omega_j \omega_k \sum_{\lambda=0}^N \hat{\mathcal{F}}_{\lambda jk}^1 \frac{d\ell_i(\xi)}{d\xi} \bigg|_{\xi=\xi^1} \omega_{\lambda}. \end{aligned} \quad (3.38)$$

Gathering the information from the three coordinates and defining the differentiation matrix

$$D_{ij} = \frac{d\ell_j}{d\xi} \bigg|_{\xi=\xi^i}, \quad i, j = 0, \dots, N, \quad (3.39)$$

which allows to substitute

$$\sum_{\lambda=0}^N \frac{d\ell_j}{d\xi} \bigg|_{\xi=\xi^i} \omega_{\lambda} = \sum_{\lambda=0}^N D_{\lambda i} \omega_{\lambda}, \quad (3.40)$$

it is possible to reach the final volume integral term

$$\begin{aligned}
\int_E \vec{\mathcal{F}} \cdot (\nabla_\xi \phi) d\vec{\xi} &= \omega_j \omega_k \sum_{\lambda=0}^N \hat{\mathcal{F}}_{\lambda j k}^1 D_{\lambda i} \omega_\lambda \\
&+ \omega_i \omega_k \sum_{\mu=0}^N \hat{\mathcal{F}}_{i \mu k}^2 D_{\mu j} \omega_\mu \\
&+ \omega_i \omega_j \sum_{\nu=0}^N \hat{\mathcal{F}}_{i j \nu}^3 D_{\nu i} \omega_\nu.
\end{aligned} \tag{3.41}$$

The sum of one-dimensional integrals calculates the term for the surface integral. The manipulation of the boundary term in Eq. (3.27) starts by splitting the area integral into the two coordinates

$$\begin{aligned}
\int_{\partial E} (\vec{\mathcal{F}} \cdot \vec{N})^* \phi dS &= \left[\int_{-1}^1 \int_{-1}^1 (\vec{\mathcal{F}} \cdot \vec{N})^* \phi d\xi^2 d\xi^3 \right]_{\xi^1=-1}^1 \\
&+ \left[\int_{-1}^1 \int_{-1}^1 (\vec{\mathcal{F}} \cdot \vec{N})^* \phi d\xi^1 d\xi^3 \right]_{\xi^2=-1}^1 \\
&+ \left[\int_{-1}^1 \int_{-1}^1 (\vec{\mathcal{F}} \cdot \vec{N})^* \phi d\xi^1 d\xi^2 \right]_{\xi^3=-1}^1.
\end{aligned} \tag{3.42}$$

The first term on the right side is the only term evaluated due to the similarities between the manipulation of the three directions. Investigating the contravariant flux term, which is computed with Riemann solvers, in the boundaries of the element $\xi^1 = \pm 1$ with normal vector $\vec{N}^\pm = (\pm 1, 0, 0)^T$, the numerical flux reduces to

$$\begin{aligned}
(\vec{\mathcal{F}} \cdot \vec{N}^\pm) &= \pm \vec{\mathcal{F}}^1 = \sum_{n=1}^3 \mathcal{J} a_n^1(\pm 1, \xi^2, \xi^3) F_n(\pm 1, \xi^2, \xi^3) \\
&= (\vec{F} \cdot \vec{n}^\pm) \hat{s}^\pm,
\end{aligned} \tag{3.43}$$

in which $\vec{n}^\pm$ is the normal vector in the physical domain, given by $n^\pm = \frac{\pm \mathcal{J} a_n^1}{\hat{s}^\pm}$, and the surface element in the physical space is calculated by $\hat{s}^\pm = \sqrt{\sum_{n=1}^3 (\mathcal{J} a_n^1(\pm 1, \xi^2, \xi^3))^2}$. The contravariant flux can be replaced by the surface element and the numerical flux function f^*

$$(\vec{\mathcal{F}} \cdot \vec{N}^\pm) = (\vec{F} \cdot \vec{n}^\pm) \hat{s}^\pm = f^*(u^L, u^R, \vec{n}^\pm) \hat{s}^\pm. \tag{3.44}$$

The numerical flux is approximated in the face of the element by extrapolating the interior nodes when using the Gauss-Legendre quadrature or by the nodes positioned in the face

when employing the Gauss-Lobatto-Legendre quadrature.

$$f^*(\pm 1, \xi^2, \xi^3) \hat{s}^\pm = \sum_{j,k=0}^N [f^* \hat{s}]_{j,k}^{\pm \xi^1} \ell_j(\xi^2) \ell_k(\xi^3) \quad (3.45)$$

where $+\xi^1$ is associated with the positive face in the ξ -direction and $-\xi^1$ is associated with the negative face in the ξ direction. The test function $\phi = \psi_{ijk}$ is employed, and the integrals are approximated by the Gauss quadrature, leading to

$$\begin{aligned} \left[\int_{-1}^1 \int_{-1}^1 (\vec{\mathcal{F}} \cdot \vec{N})^* \phi d\xi^2 d\xi^3 \right]_{\xi^1=-1}^1 &= \left[\int_{-1}^1 \int_{-1}^1 f^*(u^L, u^R, \vec{n}) \hat{s} \phi d\xi^2 d\xi^3 \right]_{\xi^1=-1}^1 \\ &= \sum_{\mu, \nu=0}^N \left(\sum_{n,o=0}^N [f^* \hat{s}]_{n,o}^{+\xi^1} \underbrace{\ell_n(\xi_\mu^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_\nu^3)}_{=\delta_{o\nu}} \right) \ell_i(1) \underbrace{\ell_j(\xi_\mu^2)}_{=\delta_{j\mu}} \underbrace{\ell_k(\xi_\nu^3)}_{=\delta_{k\nu}} \omega_\mu \omega_\nu \\ &\quad - \sum_{\mu, \nu=0}^N \left(\sum_{n,o=0}^N [f^* \hat{s}]_{n,o}^{-\xi^1} \underbrace{\ell_n(\xi_\mu^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_\nu^3)}_{=\delta_{o\nu}} \right) \ell_i(-1) \underbrace{\ell_j(\xi_\mu^2)}_{=\delta_{j\mu}} \underbrace{\ell_k(\xi_\nu^3)}_{=\delta_{k\nu}} \omega_\mu \omega_\nu \\ &= \left([f^* \hat{s}]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s}]_{j,k}^{-\xi^1} \ell_i(-1) \right) \omega_j \omega_k \quad (3.46) \end{aligned}$$

and putting together all the three directions

$$\begin{aligned} \int_{\partial E} (\vec{\mathcal{F}} \cdot \vec{N})^* \phi dS &= \left([f^* \hat{s}]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s}]_{j,k}^{-\xi^1} \ell_i(-1) \right) \omega_j \omega_k \\ &\quad + \left([f^* \hat{s}]_{i,k}^{+\xi^2} \ell_j(1) - [f^* \hat{s}]_{i,k}^{-\xi^2} \ell_j(-1) \right) \omega_i \omega_k \\ &\quad + \left([f^* \hat{s}]_{i,j}^{+\xi^3} \ell_k(1) - [f^* \hat{s}]_{i,j}^{-\xi^3} \ell_k(-1) \right) \omega_i \omega_j. \quad (3.47) \end{aligned}$$

The semi-discrete formulation of the scheme is obtained by gathering the Eqs. (3.36), (3.41) and (3.47)

$$\begin{aligned} \mathcal{J}(\vec{\xi}_{ijk}) \omega_i \omega_j \omega_k \frac{\partial \hat{u}_{ijk}}{\partial t} &+ \left([f^* \hat{s}]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s}]_{j,k}^{-\xi^1} \ell_i(-1) \right) \omega_j \omega_k \\ &+ \left([f^* \hat{s}]_{i,k}^{+\xi^2} \ell_j(1) - [f^* \hat{s}]_{i,k}^{-\xi^2} \ell_j(-1) \right) \omega_i \omega_k + \left([f^* \hat{s}]_{i,j}^{+\xi^3} \ell_k(1) - [f^* \hat{s}]_{i,j}^{-\xi^3} \ell_k(-1) \right) \omega_i \omega_j \\ &- \omega_j \omega_k \sum_{\lambda=0}^N \hat{\mathcal{F}}_{\lambda jk}^1 D_{\lambda i} \omega_\lambda - \omega_i \omega_k \sum_{\mu=0}^N \hat{\mathcal{F}}_{i \mu k}^2 D_{\mu j} \omega_\mu - \omega_i \omega_j \sum_{\nu=0}^N \hat{\mathcal{F}}_{i j \nu}^3 D_{\nu k} \omega_\nu = 0, \quad (3.48) \end{aligned}$$

which, after some manipulation, the following form is reached

$$\begin{aligned} \mathcal{J}(\vec{\xi}_{ijk}) \frac{\partial \hat{u}_{ijk}}{\partial t} &+ \left([f^* \hat{s}]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s}]_{j,k}^{-\xi^1} \ell_i(-1) \right) \frac{1}{\omega_i} \\ &+ \left([f^* \hat{s}]_{i,k}^{+\xi^2} \ell_j(1) - [f^* \hat{s}]_{i,k}^{-\xi^2} \ell_j(-1) \right) \frac{1}{\omega_j} + \left([f^* \hat{s}]_{i,j}^{+\xi^3} \ell_k(1) - [f^* \hat{s}]_{i,j}^{-\xi^3} \ell_k(-1) \right) \frac{1}{\omega_k} \\ &- \sum_{\lambda=0}^N \hat{\mathcal{F}}_{\lambda j k}^1 D_{\lambda i} \frac{\omega_{\lambda}}{\omega_i} - \sum_{\mu=0}^N \hat{\mathcal{F}}_{i \mu k}^2 D_{\mu j} \frac{\omega_{\mu}}{\omega_j} - \sum_{\nu=0}^N \hat{\mathcal{F}}_{i j \nu}^3 D_{\nu i} \frac{\omega_{\nu}}{\omega_k} = 0. \end{aligned} \quad (3.49)$$

The semi-discrete form of the discontinuous Galerkin in weak form can be further simplified by the introduction of one-dimensional precomputed operators

$$\hat{\ell}_i = \frac{\ell_i}{\omega_i}, \quad \hat{D}_{ij} = \frac{-\omega_i}{\omega_j} D_{ij}, \quad i, j = 0, \dots, N, \quad (3.50)$$

which results in

$$\begin{aligned} \frac{\partial \hat{u}_{ijk}}{\partial t} &= -\frac{1}{\mathcal{J}} \left[\sum_{\lambda=0}^N \hat{\mathcal{F}}_{\lambda j k}^1 \hat{D}_{\lambda i} + \left([f^* \hat{s}]_{j,k}^{+\xi^1} \hat{\ell}_i(1) - [f^* \hat{s}]_{j,k}^{-\xi^1} \hat{\ell}_i(-1) \right) \right. \\ &+ \sum_{\mu=0}^N \hat{\mathcal{F}}_{i \mu k}^2 \hat{D}_{\mu j} + \left([f^* \hat{s}]_{i,k}^{+\xi^2} \hat{\ell}_j(1) - [f^* \hat{s}]_{i,k}^{-\xi^2} \hat{\ell}_j(-1) \right) \\ &\left. + \sum_{\nu=0}^N \hat{\mathcal{F}}_{i j \nu}^3 \hat{D}_{\nu i} + \left([f^* \hat{s}]_{i,j}^{+\xi^3} \hat{\ell}_k(1) - [f^* \hat{s}]_{i,j}^{-\xi^3} \hat{\ell}_k(-1) \right) \right]. \end{aligned} \quad (3.51)$$

Equation (3.51) concludes the development of the semi-discrete approach of the discontinuous Galerkin formulation in the strong form. This form is largely employed. However, due to additional properties that are obtained from the strong form with the Legendre-Gauss-Lobatto quadrature, which is discussed in Sec. 3.2.2, the choice in the present work is to work with the strong form, that is described in the following section.

3.2.1.4 Semi-Discrete Approach in Strong Form

In the development of the semi-discrete approach for the strong form of the DGSEM, Eq. (3.28), the time derivative integral is the same as those developed for the weak form, Eq. (3.36). The volume and surface derivatives differ between the two forms. Therefore, they are discussed in this section. Following the same sequence from the weak form, the volume integral is the first term discussed. In the strong form, the volume integral term is the same as the original conservation equation. It is manipulated in a similar way performed for the weak form. The volume integral term can be separated into the three

contravariant flux directions to handle each direction independently

$$\int_E \nabla_\xi \vec{\mathcal{F}} \cdot \phi d\vec{\xi} = \sum_{d=1}^3 \int_E \frac{\partial \vec{\mathcal{F}}^d}{\partial \xi^d} \phi d\vec{\xi}, \quad (3.52)$$

and only one of the directions is investigated due to the similarities between the manipulation. The ξ^1 -component of the volume integral requires the choice for the test function to be $\phi = \psi_{ijk}$, the substitution of the volume integral with the integral in each direction, and the approximation of the three integrals by the Gauss-Legendre quadrature

$$\begin{aligned} \int_E \frac{\partial \vec{\mathcal{F}}^1}{\partial \xi^1} \phi d\vec{\xi} &= \int_E \frac{\partial}{\partial \xi^1} \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \psi_{mno} \right) \psi_{ijk} d\vec{\xi} \\ &= \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \frac{\partial}{\partial \xi^1} \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \psi_{mno} \right) \psi_{ijk} d\xi^1 d\xi^2 d\xi^3 \\ &= \sum_{\lambda,\mu,\nu=0}^N \frac{\partial}{\partial \xi^1} \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \ell_m(\xi_\lambda^1) \ell_n(\xi_\mu^2) \ell_o(\xi_\nu^3) \right) \psi_{ijk} \omega_\lambda \omega_\mu \omega_\nu \\ &= \sum_{\lambda,\mu,\nu=0}^N \left(\sum_{m,n,o=0}^N \hat{\mathcal{F}}_{mno}^1 \frac{\partial \ell_m(\xi_\lambda)}{\partial \xi} \bigg|_{\xi=\xi^1} \underbrace{\ell_n(\xi_\mu^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_\nu^3)}_{=\delta_{o\nu}} \right) \psi_{ijk} \omega_\lambda \omega_\mu \omega_\nu \\ &= \sum_{\lambda,\mu,\nu=0}^N \sum_{m=0}^N \hat{\mathcal{F}}_{m\mu\nu}^1 \frac{\partial \ell_m(\xi_\lambda)}{\partial \xi} \bigg|_{\xi=\xi^1} \underbrace{\ell_i(\xi_\lambda^1)}_{=\delta_{i\lambda}} \underbrace{\ell_j(\xi_\mu^2)}_{=\delta_{j\mu}} \underbrace{\ell_k(\xi_\nu^3)}_{=\delta_{k\nu}} \omega_\lambda \omega_\mu \omega_\nu \\ &= \omega_i \omega_j \omega_k \sum_{m=0}^N \hat{\mathcal{F}}_{mjk}^1 \frac{d\ell_m(\xi)}{d\xi} \bigg|_{\xi=\xi^1}. \end{aligned} \quad (3.53)$$

The obtained equation can be further simplified by employing the same differentiation matrix, Eq. (3.39), from the weak form. Gathering the volume integrals from the three coordinates

$$\begin{aligned} \int_E \nabla_\xi \vec{\mathcal{F}} \cdot \phi d\vec{\xi} &= \omega_i \omega_j \omega_k \sum_{m=0}^N \hat{\mathcal{F}}_{mjk}^1 D_{mi} \\ &= \omega_i \omega_j \omega_k \sum_{n=0}^N \hat{\mathcal{F}}_{ink}^1 D_{nj} \\ &= \omega_i \omega_j \omega_k \sum_{o=0}^N \hat{\mathcal{F}}_{ijo}^1 D_{ok}. \end{aligned} \quad (3.54)$$

In the surface integral of the strong form, a new term arises, that is, the interior contribution $\vec{\mathcal{F}}^{int}$. Once more, the sum of one-dimensional integrals calculates the term for the surface integral. The manipulation of the boundary term begins with the split of

the area integral into the two coordinates

$$\begin{aligned}
\int_{\partial E} \left((\vec{\mathcal{F}} \cdot \vec{N})^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi dS &= \left[\int_{-1}^1 \int_{-1}^1 \left((\vec{\mathcal{F}} \cdot \vec{N})^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi d\xi^2 d\xi^3 \right]_{\xi^1=-1}^1 \\
&+ \left[\int_{-1}^1 \int_{-1}^1 \left((\vec{\mathcal{F}} \cdot \vec{N})^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi d\xi^1 d\xi^3 \right]_{\xi^2=-1}^1 \\
&+ \left[\int_{-1}^1 \int_{-1}^1 \left((\vec{\mathcal{F}} \cdot \vec{N})^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi d\xi^1 d\xi^2 \right]_{\xi^3=-1}^1.
\end{aligned} \tag{3.55}$$

The first term on the right side is the only term evaluated due to the similarities between the manipulation of the three directions. In the same way, performed for the weak form, the contravariant is substituted by the surface element and the numerical flux function, which is approximated in the face element by extrapolating the interior nodes from the Gauss-Legendre quadrature. The test function $\phi = \psi_{ijk}$ is used, and the integrals are approximated by the Gauss quadrature, leading to

$$\begin{aligned}
&\left[\int_{-1}^1 \int_{-1}^1 \left((\vec{\mathcal{F}} \cdot \vec{N})^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi d\xi^2 d\xi^3 \right]_{\xi^1=-1}^1 \\
&= \left[\int_{-1}^1 \int_{-1}^1 \left(f^*(u^L, u^R, \vec{n}) \hat{s} - \hat{\mathcal{F}}^1 \right) \phi d\xi^2 d\xi^3 \right]_{\xi^1=-1}^1 \\
&= \sum_{\mu, \nu=0}^N \left(\left(\sum_{n,o=0}^N [f^* \hat{s}]_{n,o}^{+\xi^1} \underbrace{\ell_n(\xi_\mu^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_\nu^3)}_{=\delta_{o\nu}} \right) - \hat{\mathcal{F}}^1 \Big|_{+\xi^1} \right) \underbrace{\ell_i(1)}_{=\delta_{j\mu}} \underbrace{\ell_j(\xi_\mu^2)}_{=\delta_{k\nu}} \underbrace{\ell_k(\xi_\nu^3)}_{=\delta_{k\nu}} \omega_\mu \omega_\nu \\
&- \sum_{\mu, \nu=0}^N \left(\left(\sum_{n,o=0}^N [f^* \hat{s}]_{n,o}^{-\xi^1} \underbrace{\ell_n(\xi_\mu^2)}_{=\delta_{n\mu}} \underbrace{\ell_o(\xi_\nu^3)}_{=\delta_{o\nu}} \right) - \hat{\mathcal{F}}^1 \Big|_{-\xi^1} \right) \underbrace{\ell_i(-1)}_{=\delta_{j\mu}} \underbrace{\ell_j(\xi_\mu^2)}_{=\delta_{k\nu}} \underbrace{\ell_k(\xi_\nu^3)}_{=\delta_{k\nu}} \omega_\mu \omega_\nu \\
&= \left([f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{-\xi^1} \ell_i(-1) \right) \omega_j \omega_k \tag{3.56}
\end{aligned}$$

and putting together all the three directions

$$\begin{aligned}
\int_{\partial E} \left((\vec{\mathcal{F}} \cdot \vec{N})^* - \vec{\mathcal{F}}^{int} \cdot \vec{N} \right) \phi dS &= \left([f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{-\xi^1} \ell_i(-1) \right) \omega_j \omega_k \\
&+ \left([f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{+\xi^2} \ell_j(1) - [f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{-\xi^2} \ell_j(-1) \right) \omega_i \omega_k \\
&+ \left([f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{+\xi^3} \ell_k(1) - [f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{-\xi^3} \ell_k(-1) \right) \omega_i \omega_j.
\end{aligned} \tag{3.57}$$

The semi-discrete formulation of the scheme in strong form is obtained by gathering

the Eqs. (3.36), (3.54) and (3.57)

$$\begin{aligned}
& \mathcal{J}(\vec{\xi}_{ijk}) \omega_i \omega_j \omega_k \frac{\partial \hat{u}_{ijk}}{\partial t} + \left([f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{-\xi^1} \ell_i(-1) \right) \omega_j \omega_k \\
& + \left([f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{+\xi^2} \ell_j(1) - [f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{-\xi^2} \ell_j(-1) \right) \omega_i \omega_k \\
& + \left([f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{+\xi^3} \ell_k(1) - [f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{-\xi^3} \ell_k(-1) \right) \omega_i \omega_j \\
& + \omega_i \omega_j \omega_k \sum_{m=0}^N \hat{\mathcal{F}}_{mjk}^1 D_{mi} + \omega_i \omega_j \omega_k \sum_{n=0}^N \hat{\mathcal{F}}_{ink}^2 D_{nj} + \omega_i \omega_j \omega_k \sum_{o=0}^N \hat{\mathcal{F}}_{ijo}^3 D_{ok} = 0, \quad (3.58)
\end{aligned}$$

which, after some manipulation, the following form is reached

$$\begin{aligned}
& \mathcal{J}(\vec{\xi}_{ijk}) \frac{\partial \hat{u}_{ijk}}{\partial t} + \left([f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{+\xi^1} \ell_i(1) - [f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{-\xi^1} \ell_i(-1) \right) \frac{1}{\omega_i} \\
& + \left([f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{+\xi^2} \ell_j(1) - [f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{-\xi^2} \ell_j(-1) \right) \frac{1}{\omega_j} \\
& + \left([f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{+\xi^3} \ell_k(1) - [f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{-\xi^3} \ell_k(-1) \right) \frac{1}{\omega_k} \\
& + \sum_{m=0}^N \hat{\mathcal{F}}_{mjk}^1 D_{mi} + \sum_{n=0}^N \hat{\mathcal{F}}_{ink}^2 D_{nj} + \sum_{o=0}^N \hat{\mathcal{F}}_{ijo}^3 D_{oi} = 0. \quad (3.59)
\end{aligned}$$

With the strong form of the discontinuous Galerkin equations, only the one-dimensional precomputed operator $\hat{\ell}_j$ in Eq. (3.50) need to be employed to obtain the final form of the semi- discrete approach in strong form

$$\begin{aligned}
\frac{\partial \hat{u}_{ijk}}{\partial t} = & -\frac{1}{\mathcal{J}} \left[\sum_{m=0}^N \hat{\mathcal{F}}_{mjk}^1 D_{mi} + \left([f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{+\xi^1} \hat{\ell}_i(1) - [f^* \hat{s} - \hat{\mathcal{F}}^1]_{j,k}^{-\xi^1} \hat{\ell}_i(-1) \right) \right. \\
& + \sum_{n=0}^N \hat{\mathcal{F}}_{ink}^2 D_{nj} + \left([f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{+\xi^2} \hat{\ell}_j(1) - [f^* \hat{s} - \hat{\mathcal{F}}^2]_{i,k}^{-\xi^2} \hat{\ell}_j(-1) \right) \\
& \left. + \sum_{o=0}^N \hat{\mathcal{F}}_{ijo}^3 D_{ok} + \left([f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{+\xi^3} \hat{\ell}_k(1) - [f^* \hat{s} - \hat{\mathcal{F}}^3]_{i,j}^{-\xi^3} \hat{\ell}_k(-1) \right) \right]. \quad (3.60)
\end{aligned}$$

Equation (3.60) concludes the introduction of the discontinuous Galerkin spectral element method. From this point, it is necessary to describe how the semi-discrete formulation is modified to incorporate the split DG, which is one alternative to enhance the robustness of the numerical method. The split DG formulation is one method employed only for the Euler portion of the flux of the Navier-Stokes equations. The split DG formulation requires some properties that are only obtained with the strong form of the discontinuous Galerkin method. For this reason, the strong form is used in the numerical framework. It is necessary to introduce how the viscous fluxes are handled since there is no direct calculation of the second-order derivatives. The discontinuities in the boundaries

are treated with the employment of a Riemann solver and it concludes the presentation of the discontinuous Galerkin scheme used within the FLEXI numerical framework.

3.2.2 Split DG Formulation

The split DG formulation is one option to enhance the stability of the simulations. The formulation used in this work is based on the work presented in Ref. [98], in which the authors proposed an alternative approach to calculate the advective flux. The split form of the advective flux for the DG-FEM is an additional form to enhance the robustness of the scheme to other classic stability enhancement methodologies, such as the filtering process and over-integration. In the split DG formulation proposed in Ref. [98], the advective flux of the Navier-Stokes equations is calculated with alternative formulations of the non-linear terms. The Euler flux presented in Eq. (3.23) is presented in the divergence form, which is the commonly employed form. Nevertheless, the Euler flux can be reinterpreted in different ways in an equivalent split form.

Different split form approximations of derivatives of products can be obtained for a particular splitting. For example, when the derivative of a product of two variables is split, it can be approximated by

$$\frac{\partial ab}{\partial x} = \alpha \frac{\partial ab}{\partial x} + (1 - \alpha) \left(\frac{\partial a}{\partial x} b + a \frac{\partial b}{\partial x} \right), \quad (3.61)$$

which is called quadratic splitting due to the multiplication of two variables. A similar splitting form can be obtained for the product of three variables, which is called the cubic splitting

$$\begin{aligned} \frac{\partial abc}{\partial x} = & \alpha \frac{\partial abc}{\partial x} + \beta \left[a \frac{\partial bc}{\partial x} + \frac{\partial a}{\partial x} bc \right] + \kappa \left[b \frac{\partial ac}{\partial x} + \frac{\partial b}{\partial x} ac \right] \\ & + \delta \left[c \frac{\partial ab}{\partial x} + \frac{\partial c}{\partial x} ab \right] + \varepsilon \left[bc \frac{\partial a}{\partial x} + ac \frac{\partial b}{\partial x} + ab \frac{\partial c}{\partial x} \right]. \end{aligned} \quad (3.62)$$

With the two split forms for the product of two and three variables, it is possible to compose equivalent forms of the non-linear operators from the Euler fluxes, which can enhance the stability of the spatial discretization. In Ref. [98], the split forms developed in Refs. [99], [100], [101] and [102] are discussed. Only the split form presented by Pirozzoli [102] is discussed in the present work. It is the reference for the development of the split form used in the simulations performed.

Pirozzoli [102] developed a split form that followed the proposals in Ref. [101] with the enthalpy form of the energy equation. The total specific enthalpy is defined as $H = e + p/\rho$.

The cubic splitting is employed to the inviscid fluxes to obtain the following split form

$$\vec{F}_1^{e,PI} = \begin{bmatrix} \frac{1}{2}((\bar{\rho}\tilde{u}_1)_x + \bar{\rho}(\tilde{u}_1)_x + \tilde{u}_1(\bar{\rho})_x) \\ \frac{1}{4}[(\bar{\rho}\tilde{u}_1^2)_x + \bar{\rho}(\tilde{u}_1^2)_x + 2\tilde{u}_1(\bar{\rho}\tilde{u}_1)_x + \tilde{u}_1^2(\bar{\rho})_x + 2\bar{\rho}\tilde{u}_1(\tilde{u}_1)_x] + \bar{p}_x \\ \frac{1}{4}[(\bar{\rho}\tilde{u}_1\tilde{u}_2)_x + \bar{\rho}(\tilde{u}_1\tilde{u}_2)_x + \tilde{u}_1(\bar{\rho}\tilde{u}_2)_x + \tilde{u}_2(\bar{\rho}\tilde{u}_1)_x + \tilde{u}_1\tilde{u}_2(\bar{\rho})_x \\ + \bar{\rho}\tilde{u}_1(\tilde{u}_2)_x + \bar{\rho}\tilde{u}_2(\tilde{u}_1)_x] \\ \frac{1}{4}[(\bar{\rho}\tilde{u}_1\tilde{u}_3)_x + \bar{\rho}(\tilde{u}_1\tilde{u}_3)_x + \tilde{u}_1(\bar{\rho}\tilde{u}_3)_x + \tilde{u}_3(\bar{\rho}\tilde{u}_1)_x + \tilde{u}_1\tilde{u}_3(\bar{\rho})_x \\ + \bar{\rho}\tilde{u}_1(\tilde{u}_3)_x + \bar{\rho}\tilde{u}_3(\tilde{u}_1)_x] \\ \frac{1}{4}[(\bar{\rho}\tilde{u}_1\bar{H})_x + \bar{\rho}(\tilde{u}_1\bar{H})_x + \tilde{u}_1(\bar{\rho}\bar{H})_x + \bar{H}(\bar{\rho}\tilde{u}_1)_x + \tilde{u}_1\bar{H}(\bar{\rho})_x \\ + \bar{\rho}\tilde{u}_1(\bar{H})_x + \bar{\rho}\bar{H}(\tilde{u}_1)_x] \end{bmatrix}. \quad (3.63)$$

The same approach is applied to the other two directions to complete the inviscid flux function in split form. The concepts presented in the development of the split form of Pirozzoli [102] are adapted to the DGSEM in Ref. [98]. It is important to emphasize that adapting the split form from Ref. [102] to the DGSEM requires using the strong formulation of the discontinuous Galerkin method on Legendre-Gauss-Lobatto nodes. It was shown in Ref. [103] that the DGSEM with these characteristics possesses the summation-by-parts (SBP) property. The DGSEM with the Legendre-Gauss-Lobatto nodes satisfies the diagonal summation-by-parts property [98], which is essential to obtain a conservative approximation for the split forms.

The split DG formulation is exclusively employed for the advective fluxes from the Navier-Stokes equations, presented in Eq. (3.60). The Euler fluxes for the ξ^1 -component direction are

$$\hat{\mathcal{F}}_{\xi^1}^e = \sum_{m=0}^N D_{mi} \hat{\mathcal{F}}_{mjk}^{e,1} + \left([f^{e,*} \hat{s} - \hat{\mathcal{F}}^{e,1}]_{j,k}^{+\xi^1} \hat{\ell}_i(1) + [f^{e,*} \hat{s} - \hat{\mathcal{F}}^{e,1}]_{j,k}^{-\xi^1} \hat{\ell}_i(-1) \right). \quad (3.64)$$

From this point, the implementation of the split form to the DGSEM is presented. The volume and surface integrals are modified to include the split form. In Refs. [104] and [105], the authors presented that the differencing operator with the diagonal SBP property could be written as an equivalent finite volume differencing formulation

$$\sum_{m=0}^N \hat{\mathcal{F}}_{mjk}^d D_{mi} = \frac{\bar{\mathcal{F}}_{(i+1)jk}^d - \bar{\mathcal{F}}_{ijk}^d}{\omega_i}, i, j, k = 0, \dots, N, d = 1, 2, 3, \quad (3.65)$$

employing consistent auxiliary fluxes $\{\bar{\mathcal{F}}_{(ii)jk}^1\}_{ii,j,k=0}^{(N+1),N,N}$, with similar definition for the other two components. The result is important because it immediately conserves diagonal norm SBP discretizations [98]. The flux differencing formulation provides the desired conservation property and allows discretizations that conserve entropy. In Refs. [104] and [105], a diagonal norm SBP operator, Eq. (3.65), is employed with a two-point en-

tropy conserving flux function, $\mathcal{F}_{EC}^\# = \mathcal{F}_{EC}^\#(u_{ijk}, u_{mjk})$, to obtain a high-order accurate discretization

$$\frac{\bar{\mathcal{F}}_{(i+1)jk}^d - \bar{\mathcal{F}}_{ijk}^d}{\omega_i} \approx 2 \sum_{m=0}^N D_{mi} \mathcal{F}_{EC}^{\#,d}(u_{ijk}, u_{mjk}). \quad (3.66)$$

In addition to treating the volume fluxes, the numerical surface flux is also treated with the split form of the flux function. It is done by substituting the numerical surface flux function with the numerical volume flux function $F^\#$ and adding a stabilization term $Stab(u_-, u_+)$ in a way that introduces dissipation at the interface, which depends on the difference between the two states, leading to

$$f^*(u_-, u_+) = f^\#(u_-, u_+) - Stab(u_-, u_+), \quad (3.67)$$

where the values from the stabilization term are based on the local Lax-Friedrichs numerical flux function

$$Stab(u_-, u_+) = \frac{1}{2} \lambda_{max}[u_-, u_+], \quad (3.68)$$

where λ_{max} is the maximum wave speed at the interface. The manipulations lead the Euler flux to be rewritten as

$$\begin{aligned} \hat{\mathcal{F}}_{\xi^1}^e &= 2 \sum_{m=0}^N D_{mi} \hat{\mathcal{F}}^{\#,e,1}(u_{ijk}, u_{mjk}) \\ &\quad + \left([f^{\#,e,*} \hat{s} - Stab(u_-, u_+) - \hat{\mathcal{F}}^{e,1}]_{j,k}^{+\xi^1} \hat{\ell}_i(1) \right. \\ &\quad \left. + [f^{\#,e,*} \hat{s} - Stab(u_-, u_+) - \hat{\mathcal{F}}^{e,1}]_{j,k}^{-\xi^1} \hat{\ell}_i(-1) \right). \end{aligned} \quad (3.69)$$

The arithmetic mean is employed to a generic nodal quantity a_i , $i = 0, \dots, N$, which can be written by

$$\{\{a\}\}_{im} = \frac{1}{2}(a_i + a_m). \quad (3.70)$$

The translation of the quadratic and cubic split forms into the equivalent numerical volume flux generates a high-order accurate and consistent DGSEM discretization of the split DG formulation. The averages are taken in each spatial direction to simplify the notation of the volume fluxes.

$$\hat{\mathcal{F}}_1^\#(U_{ijk}, U_{m,j,k}) = \{\{\bar{\rho}\}\} = \frac{1}{2}(\bar{\rho}_{ijk} + \bar{\rho}_{mjk}), \quad (3.71)$$

$$\hat{\mathcal{F}}_2^\#(U_{ijk}, U_{i,m,k}) = \{\{\bar{\rho}\}\} = \frac{1}{2}(\bar{\rho}_{ijk} + \bar{\rho}_{imk}), \quad (3.72)$$

$$\hat{\mathcal{F}}_3^\#(U_{ijk}, U_{i,j,m}) = \{\{\bar{\rho}\}\} = \frac{1}{2}(\bar{\rho}_{ijk} + \bar{\rho}_{ijm}) \quad (3.73)$$

The split form of the advective flux from Pirozzoli [102] modified for the use on the

DGSEM scheme is described by

$$\hat{\mathcal{F}}_i^\# = \begin{bmatrix} \{\{\bar{\rho}\}\}\{\{\tilde{u}_i\}\} \\ \{\{\bar{\rho}\}\}\{\{\tilde{u}_i\}\}\{\{\tilde{u}_1\}\} + \delta_{1i}\{\{\bar{p}\}\} \\ \{\{\bar{\rho}\}\}\{\{\tilde{u}_i\}\}\{\{\tilde{u}_2\}\} + \delta_{2i}\{\{\bar{p}\}\} \\ \{\{\bar{\rho}\}\}\{\{\tilde{u}_i\}\}\{\{\tilde{u}_3\}\} + \delta_{3i}\{\{\bar{p}\}\} \\ \{\{\bar{\rho}\}\}\{\{\tilde{u}_i\}\}\{\{\bar{h}\}\} \end{bmatrix}, \text{ for } i = 1, 2, 3. \quad (3.74)$$

Recent LES of turbulent channel flow using the split DG formulation [88] indicated significant improvement in the stability of the simulations.

3.2.3 Lifting Scheme

The viscous fluxes from the Navier-Stokes equations include second-order derivatives, which means that the viscous fluxes depend on the gradients of the solution. In Ref. [106], it was observed that the discontinuous approximation of purely elliptic problems is unstable if the local polynomial derivatives inside the elements are employed. The lifting of the gradients is one option to stabilize the numerical scheme. The BR1 [106] and BR2 [107] schemes are two well-known lifting schemes for fluid dynamics applications. In general, the lifting schemes add to the system of equations up to three additional equations for the gradient of the solution in each space direction

$$\begin{aligned} Q^d &= \frac{\partial u}{\partial x_d}, \\ Q^d - \frac{\partial}{\partial x_d} u &= 0, \quad d = 1, 2, 3. \end{aligned} \quad (3.75)$$

The additional equations are treated in the same way as the filtered Navier-Stokes equations. They are transformed into the reference space using the mapping function

$$\begin{aligned} Q^d - \frac{1}{\mathcal{J}} \sum_{i=1}^3 \frac{\partial}{\partial \xi^i} ((\mathcal{J}a)_d^i u) &= 0, \\ Q^d - \frac{1}{\mathcal{J}} \nabla_\xi \cdot \mathcal{U}^d &= 0, \end{aligned} \quad (3.76)$$

where $\mathcal{U}^d = ((\mathcal{J}a)_d^1, (\mathcal{J}a)_d^2, (\mathcal{J}a)_d^3)^T u$. The equations are discretized in the same way employed in the conservation equation. The weak form of the scheme is given by

$$\int_E \mathcal{J} Q^d \phi d\vec{\xi} + \int_E \mathcal{U}^d \cdot (\nabla_\xi \phi) d\vec{\xi} - \int_{\partial E} u^* n_d \hat{s} \phi dS = 0, \quad (3.77)$$

where $(\mathcal{U}^d \cdot \vec{N})^* = u^* n_d \hat{s}$. The strong form of the additional equations is given by

$$\int_E \mathcal{J} Q^d \phi d\vec{\xi} + \int_E (\nabla_{\xi} \cdot \mathcal{U}^d) \phi d\vec{\xi} - \int_{\partial E} (u^* - u^{int}) n_d \hat{s} \phi dS = 0, \quad (3.78)$$

where the residual of the gradient equation is recovered in the volume integral. The surface integral is called, in some references, the lifting term. It is associated with the jump of the flux in the interfaces, and it is null when a continuous solution is obtained at the element interface.

The flux of the gradient equation is simply the solution u , with the numerical flux u^* . For the BR1 and BR2 schemes, they are computed by

$$u^* = \frac{1}{2} (u^L + u^R),$$

$$\mathcal{F}^{*,v} (u^L, u^R, \nabla_x u^L, \nabla_x u^R) = \frac{1}{2} (\mathcal{F}^v (u^L, \nabla_x u^L) + \mathcal{F}^v (u^R, \nabla_x u^R)). \quad (3.79)$$

The BR1 scheme directly employs the arithmetic mean of the solution and the numerical flux with a weak form of the gradient equations. The use of the BR1 scheme is unstable for some classes of problems [97]. The BR2 scheme was developed to be applied to a larger variety of problems. It employs local lifting operators to handle the instabilities of the BR1 scheme. The BR2 scheme is employed with the strong form of the gradient equations, adding a penalty parameter η_{BR2} to the lifting term. It is shown that the stability of the scheme is obtained for η_{BR2} larger than the number of element faces. The volume flux is lifted with all element sides for consistency. The semi-discrete approach for the gradient equations of the additional equations in strong form is given by

$$Q_{ijk}^d = \frac{1}{\mathcal{J}} \left[\left(\sum_{m=0}^N D_{mi} \mathcal{U}_{mjk}^{d,1} + \sum_{n=0}^N D_{nj} \mathcal{U}_{ink}^{d,1} + \sum_{o=0}^N D_{ok} \mathcal{U}_{ijo}^{d,1} \right) \right. \\ \left. + [H^*]_{jk}^{+\xi^1} \hat{\ell}_i(1) + [H^*]_{jk}^{-\xi^1} \hat{\ell}_i(-1) \right. \\ \left. + [H^*]_{ik}^{+\xi^2} \hat{\ell}_j(1) + [H^*]_{ik}^{-\xi^2} \hat{\ell}_j(-1) \right. \\ \left. + [H^*]_{ij}^{+\xi^3} \hat{\ell}_k(1) + [H^*]_{ij}^{-\xi^3} \hat{\ell}_k(-1), \right. \quad (3.80)$$

where

$$[H^*]_{jk}^{+\xi^1} = [(u^* - u^{int}) n_d \hat{s}]_{jl}^{+\xi^1}. \quad (3.81)$$

It is necessary to interpolate the volume contribution to each surface separately for the

BR2 scheme, taking into account only the local surface flux

$$[Q^d]_{jk}^{+\xi^1} = \sum_{i=1}^N \frac{1}{\mathcal{J}} \left[\left(\sum_{m=0}^N D_{mi} \mathcal{U}_{mjk}^{d,1} + \sum_{n=0}^N D_{nj} \mathcal{U}_{ink}^{d,1} + \sum_{o=0}^N D_{ok} \mathcal{U}_{ijo}^{d,1} \right) + \eta_{BR2} [H^*]_{jk}^{+\xi^1} \hat{\ell}_i(1) \right] \ell_i(+1) \quad (3.82)$$

with the stabilization parameter multiplying the surface flux. To keep things simple, we only display the derivations for the element face in the $+\xi^1$ direction; the other faces are handled similarly. The computational cost of the BR2 scheme is higher than that of the BR1 scheme. However, its improved stability is required for the development of the simulations. In the FLEXI numerical framework [35], a modified version of the BR2 scheme is implemented [97] in order to improve the computational efficiency of the method.

3.2.4 Riemann Solver

One well-known Riemann solver is the one proposed by Roe [96]. In his scheme, Roe proposes to approximate the solution of the Riemann problem by an exact solution to an approximated problem. The Riemann problem is characterized by a discontinuity in the flow, which can be described by

$$u(x) = \begin{cases} u^L & \text{if } x < 0 \\ u^R & \text{if } x > 0. \end{cases} \quad (3.83)$$

In the present discussion, the Roe approximate Riemann solver is applied to a hyperbolic system of conservation laws

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0, \quad (3.84)$$

where $\mathbf{u}(x, t)$ is the vector of conserved variables and $\mathbf{f}(\mathbf{u})$ is the flux vector. In the proposed approximate Riemann solver, the original Riemann problem is substituted by an approximated problem

$$\frac{\partial \mathbf{u}}{\partial t} + \tilde{A}(\mathbf{u}^L, \mathbf{u}^R) \frac{\partial \mathbf{u}}{\partial x} = 0, \quad (3.85)$$

in conjunction with the initial conditions. The $\tilde{A}(\mathbf{u}^L, \mathbf{u}^R)$ matrix is the Roe constant matrix, which is required to satisfy four properties:

- The matrix is a linear mapping from the vector space of $\mathbf{u}$ to the vector space of $\mathbf{f}$
- As $\mathbf{u}^L \rightarrow \mathbf{u}^R \rightarrow \mathbf{u}$, $\tilde{A}(\mathbf{u}^L, \mathbf{u}^R) \rightarrow A(\mathbf{u})$, where $A = \partial \mathbf{f} / \partial \mathbf{u}$
- For any value of $\mathbf{u}^L$ and $\mathbf{u}^R$, $\tilde{A}(\mathbf{u}^L, \mathbf{u}^R) \times (\mathbf{u}^L - \mathbf{u}^R) = \mathbf{f}^L - \mathbf{f}^R$

- The eigenvectors of $\tilde{A}$ are linearly independent.

The numerical flux of the Roe scheme is given by

$$F^{Roe}(\mathbf{u}^L, \mathbf{u}^R) = \frac{1}{2}[\mathbf{f}(\mathbf{u}^L) + \mathbf{f}(\mathbf{u}^R)] - \frac{1}{2} \sum_{k=1}^p |\tilde{a}_k| \tilde{\mathcal{A}}_k \hat{r}_k, \quad (3.86)$$

where $\tilde{a}_k = \tilde{a}_k(\mathbf{u}^L, \mathbf{u}^R)$ and $\hat{r}_k = \hat{r}_k(\mathbf{u}^L, \mathbf{u}^R)$ are the eigenvalues and the eigenvectors of the Roe constant matrix $\tilde{A} = \tilde{A}(\mathbf{u}^L, \mathbf{u}^R)$ and the coefficients $\tilde{\mathcal{A}}_k$ are the components of the jump $\mathbf{u}^R - \mathbf{u}^L$ on these eigenvectors, namely,

$$\mathbf{u}^R - \mathbf{u}^L = \sum_{k=1}^p \tilde{\mathcal{A}}_k \hat{r}_k. \quad (3.87)$$

The equation can be further developed by defining

$$|\tilde{A}| = \hat{R} |\hat{\lambda}| \hat{R}^{-1}, \quad (3.88)$$

with $|\hat{\lambda}| = \text{diag}(|\tilde{a}_1|, \dots, |\tilde{a}_p|)$ and $\hat{R}$ is the matrix of the right eigenvectors $\hat{r}_k$, then

$$|\tilde{A}(\mathbf{u}^L, \mathbf{u}^R)|(\mathbf{u}^R - \mathbf{u}^L) = \sum_{k=1}^p |\tilde{a}_k| \tilde{\mathcal{A}}_k \hat{r}_k. \quad (3.89)$$

The numerical flux, with the present notation, can be written by

$$F^{Roe}(\mathbf{u}^L, \mathbf{u}^R) = \frac{1}{2}[\mathbf{f}(\mathbf{u}^L) + \mathbf{f}(\mathbf{u}^R)] - \frac{1}{2} |\tilde{A}(\mathbf{u}^L, \mathbf{u}^R)|(\mathbf{u}^R - \mathbf{u}^L). \quad (3.90)$$

The Roe approximate Riemann solver, when in the vicinity of the stagnation or sonic speed regions, can generate zero artificial dissipation. The sonic speed region, where shock waves are present, is the region where artificial dissipation is most necessary to stabilize the simulation. This characteristic was already identified by Roe [96], and some options were developed to overcome such conditions. The options to handle such conditions are called entropy corrections or entropy fixes. An entropy fix to the Roe scheme was proposed in Ref. [108]. The numerical flux with the entropy fix is formulated by

$$F^{HH2}(\mathbf{u}^L, \mathbf{u}^R) = \frac{1}{2}[\mathbf{f}(\mathbf{u}^L) + \mathbf{f}(\mathbf{u}^R)] - \frac{1}{2} \sum_{k=1}^p q^{HH2}(\tilde{a}_k) \tilde{\mathcal{A}}_k \hat{r}_k, \quad (3.91)$$

where

$$q^{HH2}(\tilde{a}_k) = \begin{cases} \frac{1}{2} \left(\frac{\tilde{a}_k^2}{\delta_k} + \delta_k \right) & \text{if } |\tilde{a}_k| < \delta_k \\ |\tilde{a}_k| & \text{if } |\tilde{a}_k| \geq \delta_k, \end{cases} \quad (3.92)$$

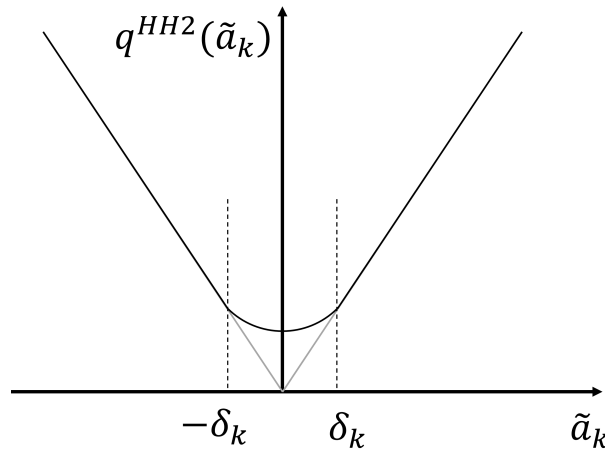


FIGURE 3.1 – Entropy fix proposed to the Roe scheme.

with

$$\delta_k = \max\{0, \tilde{a}_k - a_k(\mathbf{u}^L), a_k(\mathbf{u}^R) - \tilde{a}_k\}. \quad (3.93)$$

This modification ensures sufficient artificial dissipation even in sonic speed regions. The entropy fix formulation requires guaranteeing that the coefficient of the artificial dissipation term, which is based on the Roe characteristic speed for that particular characteristic variable, $\tilde{a}_k$, which is one eigenvalue of the Roe matrix, $\tilde{A}$, is never zero. Important improvements were obtained with the modified Roe scheme. This scheme is called the Roe scheme with an entropy fix in the FLEXI numerical framework [35]. The Roe approximate Riemann solver with entropy fix was chosen to be employed in the present work due to improved robustness when compared to the original Roe approximate Riemann solver.

3.2.5 Shock Capturing Method

The problem of interest in this work is a supersonic perfectly expanded jet flow. The perfectly expanded condition assures that the shock waves present in the simulations are weak. However, even weak shock waves can destabilize the numerical scheme. The shock waves produce numerical errors in the solution that can destabilize the numerical algorithm, which could lead to large errors and, eventually, to a divergence of the method.

It is necessary to have alternatives to deal with the shock waves that may arise inside the cell elements. Different strategies are available in the literature. Usually, the local order of accuracy is reduced from the spatial discretization to avoid the instabilities associated with the shock waves and the high-order schemes [109]. Another option is the addition of artificial dissipation [110]. An artificial viscosity method, which increases the artificial viscosity locally when a shock wave is identified, is proposed in Ref. [111]. The strategy used in the present work is the one described in Ref. [112]. In this strategy, once a shock wave indicator reaches a defined threshold inside an element, the formulation of

the element is changed to a finite volume scheme with multiple sub-cells, each possessing one of the nodes of the DG formulation. The approach was called the Finite Volume (FV) sub-cell shock-capturing method.

The formulation of the finite volume method for the conservation law in the reference space is developed. For each discontinuous Galerkin element E , $(N + 1)^3$ sub-cells, κ_{ijk} , where N is the polynomial degree, are calculated in the same control volume

$$\int_{\kappa_{ijk}} \mathcal{J} \frac{\partial \vec{u}}{\partial t} d\vec{\xi} + \int_{\kappa_{ijk}} \nabla_{\xi} \cdot \mathcal{F}(\vec{u}) d\vec{\xi} = 0, \quad \forall \kappa_{ijk} \in E, \quad (3.94)$$

which can be further developed by applying the divergence theorem to the last term in the left-hand side of the equation

$$\int_{\kappa_{ijk}} \mathcal{J} \frac{\partial \vec{u}}{\partial t} d\vec{\xi} + \int_{\partial \kappa_{ijk}} \mathcal{F}(\vec{u}) \cdot n dS_{\xi} = 0. \quad (3.95)$$

The solution inside the element with the DG formulations is obtained by substituting the solution with the nodal representation and by the change of the integral to the Gauss-Legendre quadrature

$$\begin{aligned} \int_E \vec{u} d\vec{\xi} &= \int_E \sum_{i,j,k=0}^N \hat{u}_{ijk} \psi_{ijk} d\vec{\xi} = \sum_{\lambda,\mu,\nu=0}^N \sum_{i,j,k=0}^N \hat{u}_{ijk} \underbrace{\ell_i(\xi_{\lambda}^1)}_{=\delta_{i\lambda}} \underbrace{\ell_j(\xi_{\mu}^2)}_{=\delta_{j\mu}} \underbrace{\ell_k(\xi_{\nu}^3)}_{=\delta_{k\nu}} \omega_{\lambda} \omega_{\mu} \omega_{\nu} \\ &= \sum_{i,j,k=0}^N \hat{u}_{ijk} \omega_i \omega_j \omega_k, \end{aligned} \quad (3.96)$$

where ω are the Gauss-Legendre quadrature weights. When the FV sub-cells are employed, the solution is given by

$$\int_E \vec{u} d\vec{\xi} = \sum_{i,j,k=0}^N \int_{\kappa_{ijk}} \hat{u}_{ijk} d\vec{\xi} = \sum_{i,j,k=0}^N \hat{u}_{ijk} \omega_i \omega_j \omega_k. \quad (3.97)$$

One advantage of the present formulation is that even using high-order polynomials, when changing to finite volume sub-cells, the number of degrees of freedom of the simulation is kept constant, and the process is local for each cell. Once the shock wave indicator reaches the threshold, only the identified cells are modified to a finite volume formulation, and the communication with neighbor discontinuous Galerkin cells is kept the same.

The shocks are identified using an indicator method, which measures gradients of some properties in the flow field, *e.g.*, pressure or density, to identify when a discontinuity is present in the flow field. The Finite Volume sub-cell shock-capturing method implemented in the FLEXI numerical framework presents multiple indicators available: the Persson

indicator [111], the JST indicator [113] and the Ducros indicator [114]. In the present work, the indicator based on the switching function of Jameson-Schmidt-Turkel [113] is chosen as the principal indicator for the method. It was adapted to be applied to the discontinuous Galerkin scheme by

$$\mathcal{I}_{\text{JST}}(i, j, k) = \frac{p_{\min,ijk} - 2p_{ijk} + p_{\max,ijk}}{p_{\min,ijk} + 2p_{ijk} + p_{\max,ijk}}, \quad (3.98)$$

where $p_{\min,ijk} = \min(p_{i \pm \delta_{id}, j \pm \delta_{jd}, k \pm \delta_{kd}}, d = 1, 2, 3)$ is the minimal pressure in the adjacent node values of the node ξ_{ijk} and $p_{\max,ijk}$ is the maximal value. The presented indicator gives a value for each FV sub-cell or degree of freedom in the DG scheme. In order to be used with the DG scheme, one value for the whole element must be added. The average is obtained by a weighted average of the nodal values

$$\mathcal{I}_{\text{JST}} = \frac{1}{V_E} \sum_{i,j,k=0}^N \mathcal{I}_{\text{JST}}(i, j, k) V_{i,j,k}, \quad (3.99)$$

where $V_E = \sum_{i,j,k=0}^N V_{i,j,k}$. V_E is the volume of the discontinuous Galerkin element and $V_{i,j,k}$ are the volume of the finite volume sub-cells. One strategy adopted to avoid a constant switching between the DG and the FV formulation is the definition of an upper and a lower threshold to trigger the switch of the formulations. Once the indicator crosses the upper threshold, the formulation changes to the FV formulation. After the formulation is changed to FV, it is only switched back to DG after the indicator gets lower than the lower threshold. The idea behind the thresholds is illustrated in Fig. 3.2.

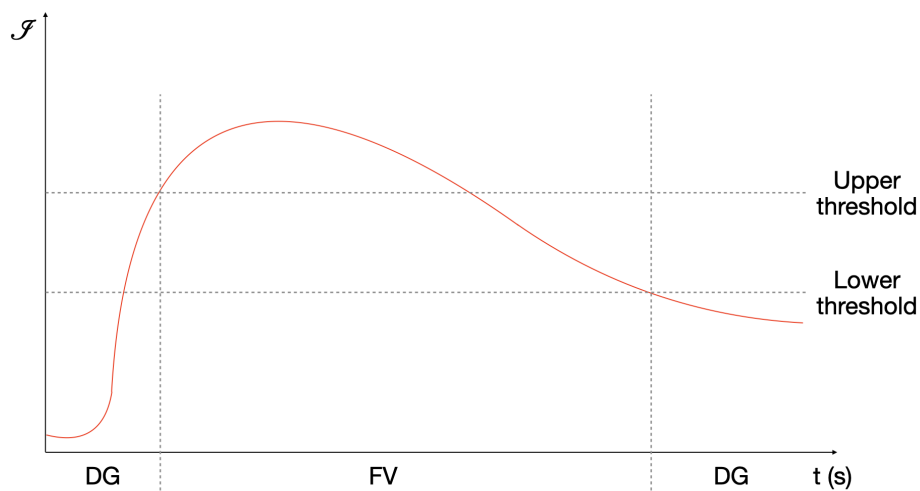


FIGURE 3.2 – Solution to minimize the switching between the FV and DG formulation by employing two thresholds.

In the present work, one additional indicator is verified before the FV sub-cells are

switched back to the DG formulation. The Persson indicator [111] is employed as a second check. The fundamental assumption from the Persson indicator is that the coefficients or modes of a smooth solution decay very quickly. As oscillations occur when a discontinuity is approximated using polynomials, it is suggested in Ref. [111] to use the amount of power of the highest mode as a smoothness indicator. The indicator contrasts the total solution up to this mode with the portion of the solution solely represented in the highest polynomial mode. The solution is expressed in a modal hierarchical basis of polynomials up to degree p by

$$u_m = \sum_{i=1}^{N(p)} u_i \Psi_i. \quad (3.100)$$

In addition to the solution approximation, a truncated expansion of the same solution, containing only the terms up to order $p - 1$, is given by

$$u_{m,t} = \sum_{i=1}^{N(p-1)} u_i \Psi_i. \quad (3.101)$$

The definition of the indicator for each element is

$$S = \frac{(u_m - u_{m,t}, u_m - u_{m,t})_{L_2}}{(u_m, u_m)_{L_2}}. \quad (3.102)$$

In the equation, $(\cdot)_{L_2}$ is the L_2 inner product. The truncation to the modes between a and b is defined by

$$[u_{m,t}]_a^b = \sum_{i=N(a-1)+1}^{N(b)} u_i \Psi_i, \quad (3.103)$$

and the indicator is

$$S = \frac{([u_{m,t}]_p^p, [u_{m,t}]_p^p)_{L_2}}{([u_{m,t}]_1^p, [u_{m,t}]_1^p)_{L_2}}. \quad (3.104)$$

Finally, this indicator is generalized by

$$\mathcal{I}^{\text{Persson}} = \max \left\{ \frac{([u_{m,t}]_i^i, [u_{m,t}]_i^i)_{L_2}}{([u_{m,t}]_1^i, [u_{m,t}]_1^i)_{L_2}}, i = p - k, \dots, p \right\}. \quad (3.105)$$

The reconstruction of the finite volume properties is done with second-order accuracy. However, this method also requires additional treatment in the presence of discontinuities, which is done by employing slope limiters. The two slope limiters investigated in Ref. [109] are the minmod [115] and the Sweby [116] limiters. These two slope limiters are available in the FLEXI numerical framework. The minmod limiter [115] is employed for FV reconstruction in the present work.

3.2.6 Time Marching Method

The development of a time-dependent solution requires a numerical algorithm to advance the solution in time. Multiple methods exist for the solution of the systems of partial differential equations. The common use is to separate the process with independent space and time discretizations, which is called the method of lines [117]. In the present work, the differential equations are advanced in time with Runge-Kutta methods (RK).

3.2.6.1 Runge-Kutta Methods

The Runge-Kutta methods are an important family of time-integration methods. They can reach high-order accuracy and large stability levels for explicit schemes. The Runge-Kutta methods perform multiple intermediate stages to advance one time step. The Runge-Kutta methods perform the numerical solution of the initial value problem

$$\frac{du}{dt} = f(u, t), \quad \text{with initial condition } u(t_0) = u_0 \quad (3.106)$$

and the general form of the K-stage Runge-Kutta method [117] is

$$\begin{aligned} u^1 &= u^n \\ u^2 &= u^n + \Delta t \alpha_2 f^1 \\ &\vdots \\ u^K &= u^n + \Delta t \alpha_K f^{(K-1)} \\ u^{(n+1)} &= u^n + \Delta t \sum_{k=1}^K \beta_k f^k, \end{aligned} \quad (3.107)$$

where α_k , β_1 , and β_k , with $k = 2, \dots, K$, are the intermediate and final weights of the methods, and

$$\sum_{k=1}^K \beta_k = 1. \quad (3.108)$$

The notation $f^k = f(u^k)$ is employed in the equations. The general form of the method indicates that many possibilities are available. One example of a fourth-order accurate Runge-Kutta method is obtained with the use of the intermediate and final weights [117]

$$\begin{aligned} \alpha_2 &= 1/2 & \alpha_3 &= 1/2 & \alpha_4 &= 1 \\ \beta_1 &= 1/6 & \beta_2 &= \beta_3 = 1/3 & \beta_4 &= 1/6. \end{aligned} \quad (3.109)$$

3.2.6.2 Low-Storage Runge-Kutta Methods

It may be observed from the classical Runge-Kutta methods, as indicated in Eq. (3.107), that one disadvantage of the method is that it requires a large memory to store the residuals calculated in the intermediate steps to later employ in the approximation on the last step of the method. One alternative class of Runge-Kutta methods is capable of reducing the memory requirements by storing fewer intermediate solutions than the classical Runge-Kutta methods. This class of Runge-Kutta methods is called the Low-Storage Runge-Kutta methods (LSRK). One example of a LSRK method is the Runge-Kutta scheme with five stages and fourth-order accuracy from Carpenter and Kennedy [118]. The Carpenter and Kennedy Runge-Kutta method belongs to a subclass of the LSRK methods known as the 2N-storage schemes because it needs to store only twice the number of variables required to solve the problem.

The 2N-storage schemes are formulated by

$$\begin{aligned} \left(\frac{\partial \hat{u}}{\partial t}\right)_i^{temp} &= \frac{\partial}{\partial t} \hat{u}_{ijk}(t + dt RKc_i) + \left(\frac{\partial \hat{u}}{\partial t}\right)_{i-1}^{temp} RKA_i \\ u_i &= u_{i-1} + \left(\frac{\partial \hat{u}}{\partial t}\right)_i^{temp} RKb_i, \end{aligned} \quad (3.110)$$

where RKA , RKb and RKc are the coefficients of the method and $\left(\frac{\partial \hat{u}}{\partial t}\right)_i^{temp}$ are the intermediate residuals that are additionally stored. The present work performs the simulations with second-order and third-order accurate spatial discretizations. A cost-effective Runge-Kutta scheme that presents a similar temporal order of accuracy is the 3-3LSRK scheme [103], which performs three intermediate stages and has a third order of accuracy. The values of the coefficients for the Runge-Kutta method used in the present work are presented in Tab. 3.1.

TABLE 3.1 – Runge-Kutta coefficients for the scheme employed in the present work.

Stage i	RKA_i	RKb_i	RKc_i
1	0	$\frac{1}{3}$	0
2	$\frac{5}{9}$	$\frac{15}{16}$	$\frac{1}{3}$
3	$\frac{153}{128}$	$\frac{8}{15}$	$\frac{3}{4}$

3.3 Boundary Conditions

3.3.1 Weakly Imposed Boundary Conditions

In the current work, the boundary conditions are weakly imposed, which means that, instead of imposing the properties in the face of the boundary elements, which is the strong imposition of the boundary condition, the external contribution of the boundary condition is imposed by the numerical flux through the boundary faces of the domain. Strongly imposed conditions tend to over-constrain the inner solution, which usually results in oscillations [119]. The solutions of weakly enforced boundary conditions are consistent with the order of accuracy of the interior solution but feel the influence of the boundary through the numerical fluxes. This leads to better solutions away from the boundaries [119–121].

The weakly imposed Dirichlet condition is the only type of boundary condition used for all boundaries of the computational domain in the present work. In this type of boundary condition, the state of the external contribution of the numerical flux is fixed to a defined state, for example, the free stream. This state is used to calculate the advective fluxes of the external face, while the viscous fluxes are calculated using gradients from interior nodes. The Roe Riemann solver, presented in Sec. 3.2.4, is, then, applied to obtain the numerical flux through the boundaries. According to Ref. [122], the behavior of the weakly imposed Dirichlet-type condition is similar to one-dimensional non-reflecting characteristic boundary conditions. While the reference state of the far field condition is the same among the numerical simulations, the reference state from the jet inflow section presents three different options. The next section discusses the implementation of the three inflow conditions, and, in the sequence, the far field condition is discussed.

3.3.2 Jet Inflow Condition

The influence of the inflow condition on the development of the supersonic jet flow is assessed by investigating three inflow conditions. The boundary condition employed in the jet inflow section is the weakly enforced solution of a Riemann problem with a Dirichlet condition. In the three inflow conditions, the reference state differs from each other. In the first condition, an inviscid profile is imposed. The second condition imposes the viscous steady state profile obtained from an “*a priori*” RANS simulation of a supersonic nozzle. In the third condition, the steady viscous profile from the RANS simulation is used together with a tripping method, which introduces a disturbance to the velocity properties inside the boundary layer.

3.3.2.1 Inviscid Profile

The inviscid inflow condition imposes constant properties in the jet inlet section. Due to the shape of the velocity vector in the inlet section of the domain, composed of the jet inlet and the far field inlet, this inflow condition is commonly referred to as the “top-hat” profile. The inviscid inflow profile was previously employed in the reference work performed with the second-order solver [17, 32], and it is the simplest inflow profile to be imposed. The reference state can be provided in either dimensional or non-dimensional values in the FLEXI numerical framework. The characteristics of the flow field are provided in primitive variables that are converted to the conserved variables before the calculation of the external contribution of the numerical flux in the elements bounded by the boundary conditions. The primitive variables provided are the density, the three components of the velocity vector, and the static pressure.

3.3.2.2 Viscous Steady State Profile from the RANS Simulation

The present section discusses the algorithm employed to transfer the data from the RANS simulation to the LES inflow condition. Firstly, it is necessary to discuss about the data output from the RANS simulation. The RANS simulation from the supersonic nozzle flow was post-processed, and the radial profiles from the density, axial velocity component, radial velocity component, and pressure were obtained. The numerical values are gathered in the vertices of the grid cells, which means that data is available from the wall to the center of the nozzle. The radial profiles from the RANS simulation as a function of the radial position are provided in a matrix in the FLEXI numerical framework code. The radial position is the distance from the wall. In the wall surface, it has a null value, and in the jet centerline, it is equal to $d_{wall}/D_j = 0.5$.

The properties are gathered from the RANS simulation in the face nodes from the elements bounded by the jet inlet condition. The face node position is a function of the numerical meshes and the polynomial order of accuracy. In that sense, it is unlikely that the same positions where the data was gathered from the RANS simulations correspond to the same location of the face nodes from the LES calculations. An interpolation process is performed to exchange data from the RANS simulation to the LES face nodes. The interpolation process employed is the piecewise cubic Hermite interpolation [123]. The piecewise cubic Hermite interpolation allows the interpolation of the function and its derivative.

In the general cubic Hermite interpolation, given a set of points, it is possible to interpolate the function by solving the following equation

$$q(z) = a + b(z - x_L) + c(z - x_L)^2 + d(z - x_L)^2(z - x_R), \quad (3.111)$$

where a , b , c , and d are the coefficients that define the shape of the function between the interval $[x_L, x_R]$. The derivative is interpolated by

$$q(z)' = b + 2c(z - x_L) + d(2(z - x_L)(x - x_R) + (z - x_L)^2), \quad (3.112)$$

the two equations can be interpreted as

$$\begin{aligned} q(x_L) &= y_L & q(x_R) &= y_R \\ q(x_L)' &= s_L & q'(x_R) &= s_R, \end{aligned}$$

where y_L and y_R are the values of the function at x_L and x_R , and s_L and s_R are the derivatives of the function at the same positions. It is necessary to determine the values of the coefficients a , b , c , and d to close the two interpolation equations. They are defined by

$$a = y_L \quad (3.113)$$

$$b = s_L \quad (3.114)$$

$$c = \frac{y_L' - s_L}{x_R - x_L} \quad (3.115)$$

$$d = \frac{s_R + s_L - 2y_L'}{(x_R - x_L)^2} \quad (3.116)$$

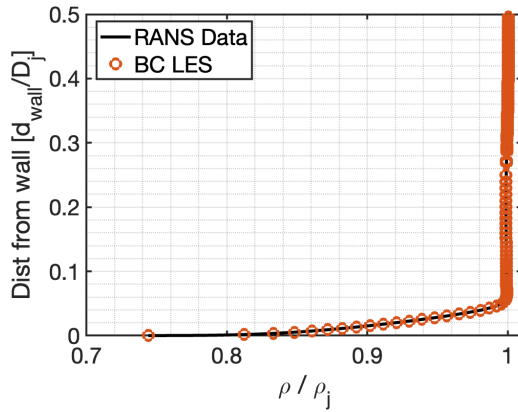
$$y_L' = \frac{y_R - y_L}{x_R - x_L}. \quad (3.117)$$

The closure of the equations depends on the definition of the slope of the function. The present work employed Lagrange polynomials. The derivative of a function can be approximated by

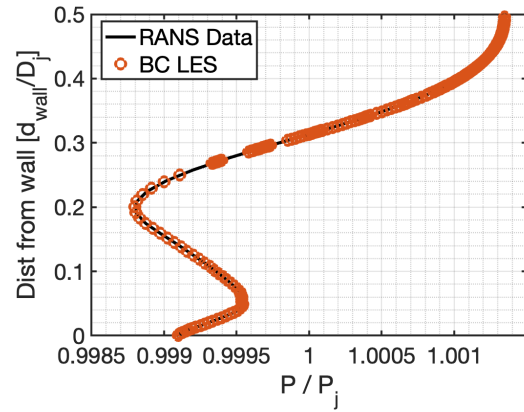
$$s(x) = \frac{2x - x_b - x_c}{(x_a - x_b)(x_a - x_c)}y_a + \frac{2x - x_a - x_c}{(x_b - x_a)(x_b - x_c)}y_b + \frac{2x - x_a - x_b}{(x_c - x_a)(x_c - x_b)}y_c, \quad (3.118)$$

where y_a , y_b and y_c are the values of a function at x_a , x_b and x_c , respectively. By putting together the equations, it is possible to identify the interpolation of the RANS data to the face nodes from the LES calculations. Examples of the interpolation results from the RANS profile are presented in Fig. 3.3.

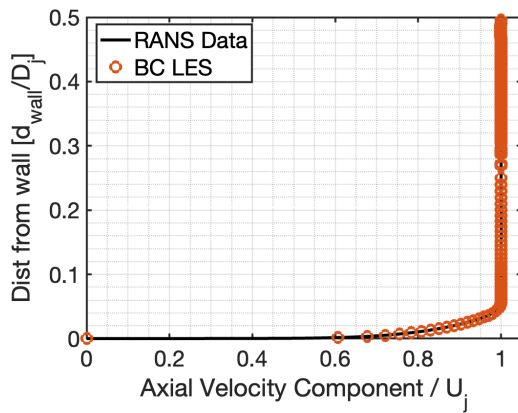
Once the data is interpolated from the RANS data, it is necessary to convert the velocity values from the polar coordinate system to the Cartesian coordinate system employed to compute the numerical flux function. The transformation from the polar coordinate system to the Cartesian coordinate system is performed by first identifying the quadrant of the face node. Then, the local angle θ is defined. Once it is defined, it is possible to transform the radial velocity component into the u_2 and u_3 velocity components. After these steps are completed, the primitive variables are converted to conserved variables,



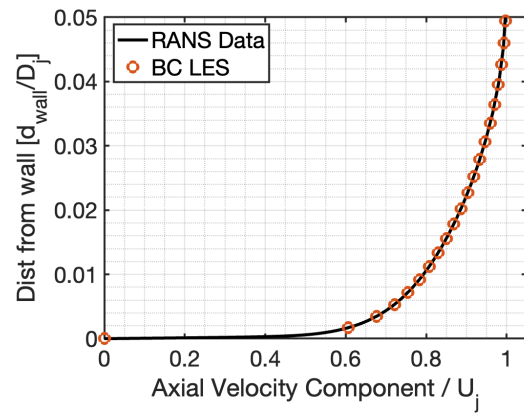
(a) Density variable.



(b) Pressure Variable.



(c) Longitudinal velocity component.



(d) Detail of the longitudinal velocity component.

FIGURE 3.3 – Examples of the interpolation process applied to the RANS data to obtain the values of the face nodes from the LES boundary condition.

which are provided for the numerical flux function calculations.

3.3.2.3 Unsteady Viscous Profile

The third and last inflow condition evaluated is the unsteady viscous profile. In this inflow condition, the same viscous profile obtained from the RANS simulation is superimposed by the tripping method presented in Ref. [23]. The tripping method employed is referred to in its original work as “noise tripping” since it employs a random variable independent of time and position, which does not ensure the development of divergence-free velocity distribution. The authors suggest another tripping method, referred to as “vortex-ring tripping”, that is expected to be divergence-free. Due to small differences obtained from the two methods, it was opted to implement the “noise tripping” in the present work due to its simplicity.

The tripping method in Ref. [23] is calculated by

$$\begin{Bmatrix} u_x \\ u_r \\ u_\theta \end{Bmatrix} = \begin{Bmatrix} u_{x,RANS} \\ u_{r,RANS} \\ 0.0 \end{Bmatrix} + \alpha U_j \begin{Bmatrix} 3\epsilon_x(x, r, \theta, t) \\ \epsilon_r(x, r, \theta, t) \\ 2\epsilon_\theta(x, r, \theta, t) \end{Bmatrix}, \quad \text{for } d_w < \delta_{BL}, \quad (3.119)$$

where u_x , u_r , and u_θ are the axial, radial, and tangential velocity components in a cylindrical coordinate system. The variables $u_{x,RANS}$ and $u_{r,RANS}$ are the axial and radial velocity components from the RANS simulation of the supersonic nozzle flow. The variable U_j is the jet inlet velocity, α is a constant that adjusts the intensity of the tripping method. The variables ϵ_x , ϵ_r , and ϵ_θ are three random variables independent in space and time. They have values that are between $[-1, 1]$. The variables d_{wall} is the distance from the wall, and δ_{BL} is the boundary layer thickness. The constant α value is the same employed in Ref. [23] and has a value of 0.00625.

The three inflow conditions from the jet inlet boundary condition are described. A comparison between the three profiles investigated in the present work is presented in Sec. 5.3 in Fig. 5.23.

3.3.3 Far Field Condition

The far field condition employs the same weakly imposed Dirichlet-type boundary condition used in the jet inflow condition with a different reference state. In the far field boundary condition, the density and pressure are defined to match the ambient conditions of the physical experiments. Even though the surrounding air is a quiescent flow, it is a common practice for jet flow simulations [28, 31] to impose a small Mach number to avoid strong reflections due to null velocity at the boundaries. The far field Mach number is approximately 0.01 in the present work. The axial velocity component has a value of $M = 0.01$ and the velocity components in the other two directions are set to zero.

The weakly imposed boundary conditions cannot avoid the reflection of all disturbances. A sponge zone is employed to prevent any disturbance from reaching the boundaries of the domain. The sponge zone investigates the differences between the properties from the flow field to a defined reference state, which is usually the same as the boundaries of the free stream, and it affects the flow field to reach the defined state. In this work, the sponge zone is implemented as a source term [122]. The sponge zone employs a ramping function, σ_{sp}

$$\sigma_{sp}(x^*) = 6x^{*5} - 15x^{*4} + 10x^{*3}, \quad (3.120)$$

$$x^* = \frac{x - x_0}{\Delta x_{sp}}, \quad (3.121)$$

to progressively increase the strength of the source term. x_0 is the beginning of the ramp

and Δx_{sp} is the width of the ramp. The source term added to the equations has the form of

$$-d_{sp}\sigma_{sp}(u_{ref} - \vec{u}), \quad (3.122)$$

where d_{sp} is a free damping parameter, which varies from 0 to 1, and u_{ref} is the defined state from the sponge region. Pruett et al. [124] proposed a modification to the base flow state to consider the moving average base flow. In this case,

$$\frac{\partial u_{ref}}{\partial t} = \frac{\vec{u}(t_n) - u_{ref}(t_{n-1})}{\Delta}, \quad (3.123)$$

where Δ is the filter width. The equation for $\frac{\partial V}{\partial t}$ is integrated using the same Runge-Kutta scheme described in the previous section.

4 Simulation of a Supersonic Jet Flow

4.1 Characteristics of Jet Flows

Jet flows are largely present in industrial applications. For example, the supersonic jet flows provide thrust for launch vehicles to leave the atmosphere and supersonic aircraft to fly at high speed. There are two possible geometries for nozzles to generate the jet flow. The convergent nozzle can be used for both subsonic and supersonic regimes. However, inside the nozzle, the flows cannot reach supersonic velocities. The maximum velocity is obtained in the throat with a Mach number of 1. If the static pressure in the throat is still higher than the ambient pressure, the jet flow will continue to expand and increase its velocity after leaving the nozzle. The convergent-divergent geometry is used to obtain supersonic flows inside the nozzle. Once after passing the nozzle throat, the flow can expand and increase its velocity.

The supersonic jet flows, leaving a convergent-divergent nozzle, have three operating conditions: underexpanded, perfectly expanded, and overexpanded [42]. The difference between the operating conditions is regarding the exit pressure. For the underexpanded condition, the pressure at the nozzle exit section is higher than the ambient pressure, and the jet flow will continue to expand by the effect of expansion waves and gain velocity after leaving the nozzle. The perfectly expanded condition is the design point for nozzles. In this condition, the nozzle can provide the flow in the exit section with the atmospheric pressure, which means that the jet is uniformly supersonic, with weak shock or expansion waves observed. For the overexpanded condition, the nozzle will allow the flow to reach lower pressures than the ambient pressure. When the flow leaves the nozzle, it will present a set of shock waves to decrease the velocity and equal the ambient pressure.

The overexpanded and underexpanded operating conditions are complex flows once the shock and expansion waves are strong. The simulation of these two conditions would require deeper investigations of shock-capturing methods and Riemann solvers, which are not the focus of this work. For this reason, the choice of the perfectly expanded is the right one. The attention concerning the simulations can be headed to the imposition of jet inlet conditions. In the experimental work presented in Ref. [6], diverse operating

conditions for supersonic round jet flows were investigated. From the operating conditions tested, a supersonic perfectly expanded condition with Mach number 1.4 is selected as the experimental reference for the simulations performed in the present work. The nozzle exit diameter employed in the tests has 0.0508 m, which gives a Reynolds number based on the exit diameter of 1.58×10^6 .

4.2 Design of the Computational Model

4.2.1 Definition of the Computational Geometry

The geometry employed to develop the numerical meshes has a divergent shape. The free jet flow is simulated without the presence of internal or external nozzle surfaces. Two geometries were used in the simulations. They represent the same divergent shape with small differences in the external dimensions. The first is based on previously used geometry [17], and the second is a simplification to reduce the number of internal volumes in the mesh. The discontinuous Galerkin spectral element method (DGSEM) performance optimization is obtained through a set of characteristics, one of which is the domain discretization exclusively in hexahedral elements. The mesh generation strategy may require an integrated generation of geometry and mesh. The open-source geometry and mesh generator used in this work is the Gmsh [125]. The strategy to generate the mesh is based on the multiblock process. The generation of hexahedral elements requires that the domain be divided into six-sided volume blocks. Consequently, the blocks that define the edges of the mesh are pre-defined in the geometry.

The two geometries are called G1 and G2 in this work. The visualization of a cut plane for the two geometries is presented in Fig. 4.1. The cut plane indicate the 2-D block structure employed in the generation of the two numerical meshes. The sketch identifying the points that differentiate the two geometries is presented in Fig. 4.2. The inlet section is positioned at the point P_{il} with $x/D_j = 0.0$, and the centerline extends up to section $x/D_j = 40.0$, P_{ir} . In the external face of the domain, the leftmost corner, P_{el} , is located at $x/D_j = -0.95$ and $r/D_j = 5.65$ for the G1 geometry, and at $x/D_j = -0.95$ and $r/D_j = 8.0$ for the G2 geometry. The rightmost corner, P_{er} , is located at $x/D_j = 36.6$ and $r/D_j = 12.5$ for the G1 geometry and at $x/D_j = 40.0$ and $r/D_j = 12.5$ for the G2 geometry. The three dimensional view is presented in Fig. 4.3. In the geometry definition process, a rectangular core is defined, and then the upcoming volumes connect to the faces and edges of the core. In the process, there is no issue if the surfaces of the volumes are straight or curved. The multiblock generation process can handle curved surfaces as well as straight surfaces. In Fig. 4.4, the structure of the computational domain in the core is presented with a zoom in the inlet section where the inlet condition is highlighted in red.

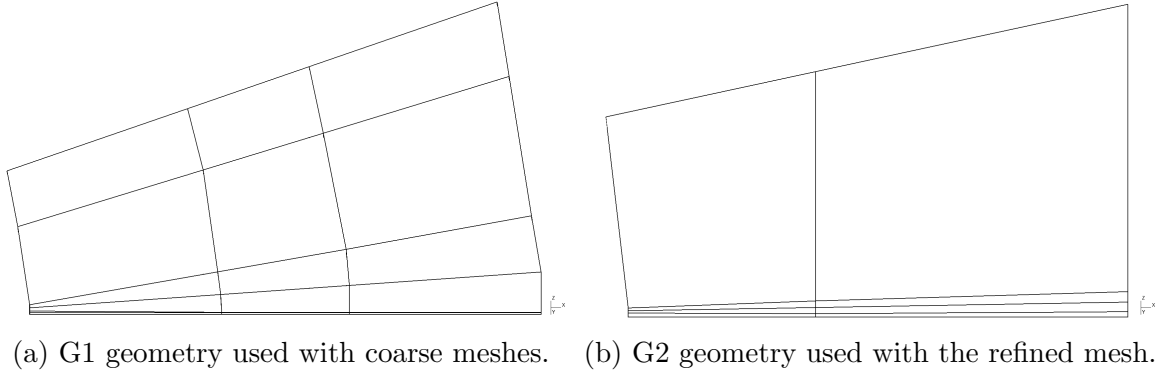
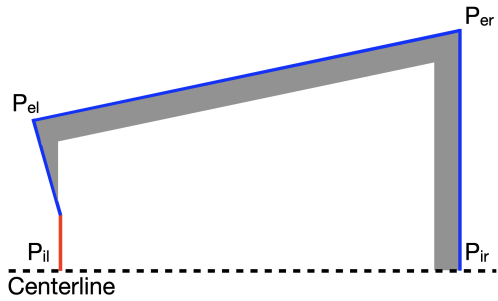


FIGURE 4.1 – 45-degree cut plane of the two geometries employed to generate the numerical meshes.



(a) 2-D Sketch.

Geometry	P_{il}		P_{ir}	
	x/D_j	r/D_j	x/D_j	r/D_j
G1	0.0	0.0	40.0	0.0
G2	0.0	0.0	40.0	0.0
Geometry	P_{el}		P_{er}	
	x/D_j	r/D_j	x/D_j	r/D_j
G1	-0.95	5.65	36.6	12.5
G2	-0.95	8.0	40.0	12.5

(b) Dimensions of the two geometries.

FIGURE 4.2 – 2-D sketch of the computational geometries employed in the present work. The points that define the physical domain are identified, and the dimensions are presented in the table. The two face groups and the sponge zone are identified with different colors.

4.2.2 Generation of the Numerical Mesh

Three meshes are generated for the LES simulations performed in this work of the free jet flows. In the same way that G1 geometry is based on previously generated geometry [17], the M1 and M2 meshes, which are generated over G1 geometry, are also based on previously generated meshes. The first two meshes were generated to provide the same degrees of freedom of the reference mesh with the DGSEM using linear (degree 1) and quadratic (degree 2) polynomials for the spatial representation of the numerical solution. The reference mesh, developed in the work presented in Ref. [17], was designed with 50×10^6 points to be employed with a finite difference solver, which presents one degree of freedom for each mesh point. Within the DGSEM scheme, the number of degrees of freedom for each element depends on the polynomial degree used to approximate the solution and the fluxes. The numerical simulation presents 8 degrees of freedom per element with a linear polynomial, and 27 degrees of freedom per element with a quadratic polynomial. The number of degrees of freedom for each element is associated with the internal nodes in each direction. The specification of a linear polynomial demands

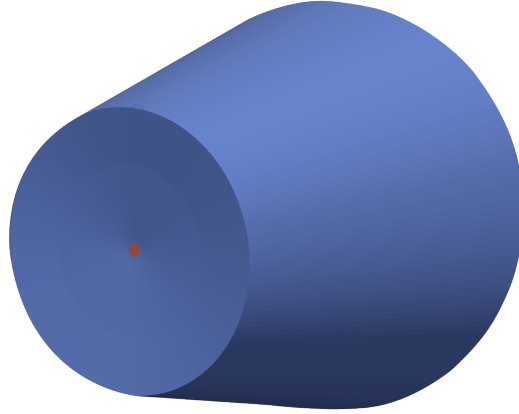
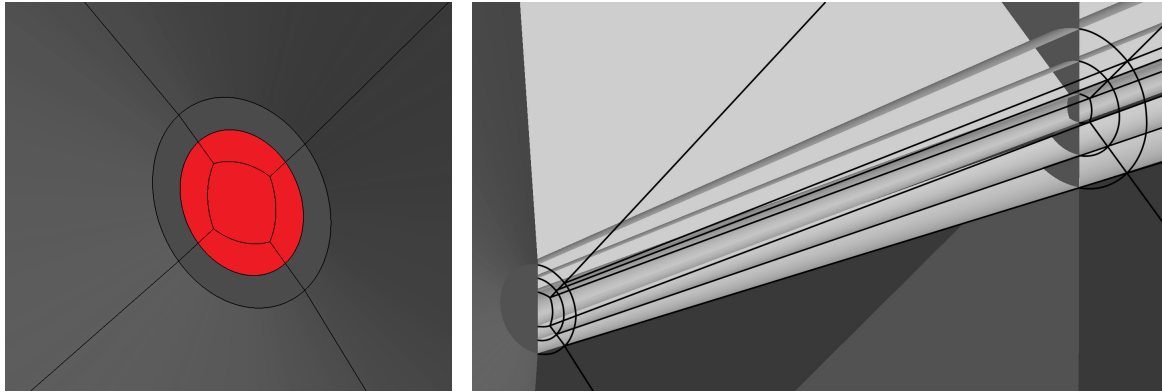


FIGURE 4.3 – 3-D view of the computational geometry. In red is the surfaces of the jet inflow and in blue the surfaces of the far field.



(a) Highlight of the inlet section.

(b) Multiblock structure of the domain.

FIGURE 4.4 – Structure of the six-sided volumes within the domain with a highlight in the inlet section in red from the G2 geometry.

two nodes in each direction, and the quadratic polynomial demands three nodes in each direction, which total the values specified for three-dimensional simulations. Specifying the same number of degrees of freedom for the three simulations requires that the M1 and M2 meshes have fewer elements than the reference mesh. The number of elements for the M1 mesh, which will be used with a linear polynomial, is 6.2×10^6 elements, and the M2 mesh, which will be used with a quadratic polynomial, is 1.8×10^6 elements. The cut plane of the M1 and M2 geometries are presented in Fig. 4.5a and 4.5b. The three meshes are generated with the Gmsh mesh generator [125].

The generation of the M1 and M2 mesh tried to reproduce the points distribution of the reference mesh [17], which was limited to an axisymmetric structured topology. The topology restricts the distribution of points, forcing a high number of points close to the jet centerline. The multi-block strategy still has some limitations regarding excessive elements in regions in which the flow simulated is smooth. However, it provides more significant opportunities to include elements where they are necessary.

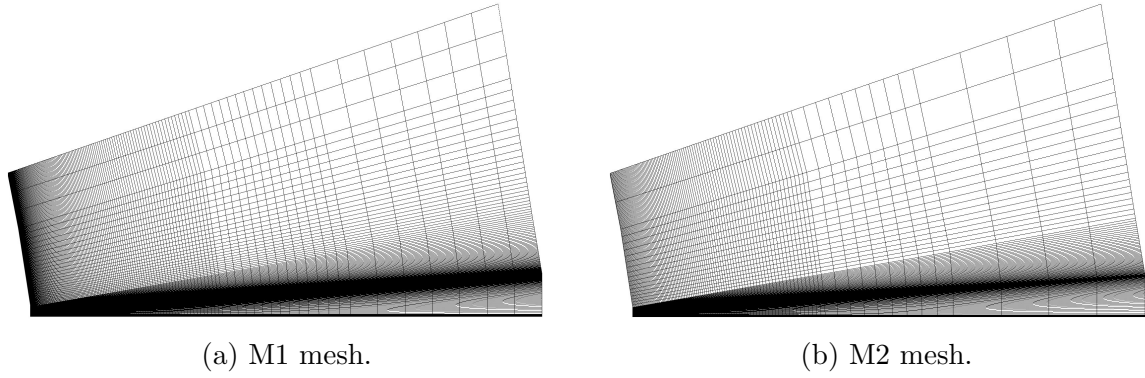


FIGURE 4.5 – Cut planes of the two meshes generated over G1 geometry.

The M3 mesh was generated together with G2 geometry after the analysis of the numerical results from the simulations using the M1 and M2 meshes. The block structure employed in the development of the M3 numerical mesh is presented in Fig. 4.6. The grid design attempts to capture with high precision the region of $0.0 \leq x/D_j \leq 15.0$ at the centerline of the jet, identified by the region *a* in Fig. 4.6. Then, a large stretching of the distribution of the elements, region *b*, is specified to reduce the total amount of elements and to coarser the mesh close to the boundaries to dissipate oscillations reaching the boundary domain that could destabilize the simulation. The mean longitudinal velocity component contours obtained from the simulations of the M1 and M2 meshes indicate that a surface with one degree of opening angle would better represent the middle surface of the jet mixing layer. Two regions are defined from this surface, *d*, and *e*, to ensure a refinement level around the jet mixing layer. They have a geometrical stretching in the inlet section $x/D_j = 0$ to enable local refinement in the shear layer region with large refinement in the nozzle lip and a uniform distribution in $x/D_j = 15$, where larger structures dominate the flow. The internal section of the mixing layer connects to one hexahedral block, region *c*. That core block has dimensions defined to keep the largest element in the mixing layer the same size. The external section, region *f*, is employed above the regions representing the mixing layer, and they connect to the external domain. The region presents a large stretching of the distributions of the element, similar to what is performed for region *b*. A cut plane of the M3 mesh is presented in Fig. 4.7.

The grid refinement in the radial direction of the mixing layer, regions *d* and *e*, of M3 mesh is defined based on the literature [12, 13, 17, 24, 31]. The grid spacing in the radial and axial directions along the mixing layer is $\Delta r_0/D_j = 0.001$ and $\Delta x_0/D_j = 0.005$, respectively. Each region of the mixing layer contains 50 elements. The centerline presents 651 elements set in geometrical stretching distribution between $x/D_j = 0.0$ and $x/D_j = 15.0$, region *a*. The azimuthal direction accommodates 180 elements evenly distributed, the M1 mesh also accommodates 180 elements, and the M2 mesh accommodates 90 elements equally distributed. In each part represented by the region *c*, one-quarter of

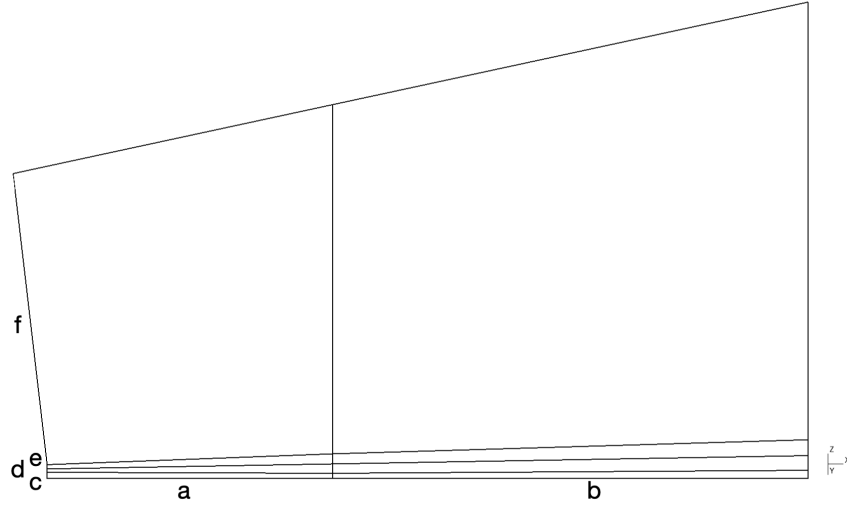


FIGURE 4.6 – Cut plane of the M3 mesh with the block structure employed in the development of the numerical mesh.

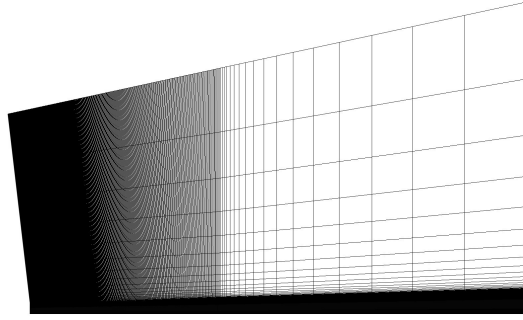
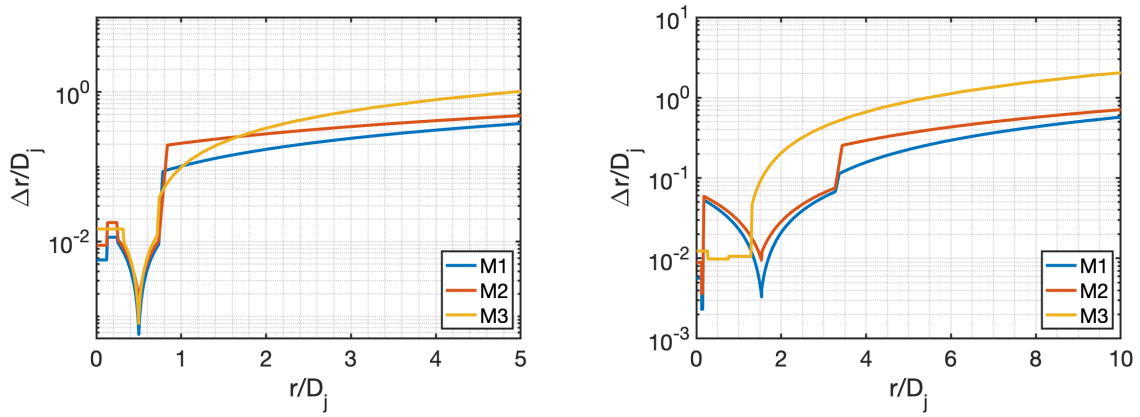


FIGURE 4.7 – Cut plane of the M3 mesh generated over G2 geometry.

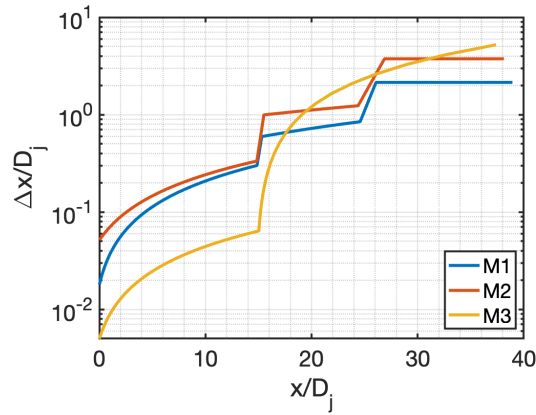
the elements from the azimuthal direction are inserted, which means 45 elements in each part. In region b , 21 elements are distributed with a stretching ratio of 1.26, and in region f , 21 elements are distributed with a stretching ratio of 1.35. Figures 4.8a and 4.8b present the radial mesh refinement in two longitudinal positions, $x/D_j = 0$ and $x/D_j = 15$, for the three numerical meshes used in this work. Figure 4.8c illustrates the axial mesh refinement along the jet centerline. Table 4.1 summarizes the three meshes generated for the LES study of supersonic jet flows. The three numerical meshes used in the present work are linear meshes. Linear meshes are generated with a polynomial degree of one connecting adjacent nodes.

TABLE 4.1 – Summary of meshes generated for LES of supersonic jet flow.

Mesher	Geometry	# Elements (10^6)
M1	G1	1.8
M2	G1	6.2
M3	G2	15.4



(a) Radial mesh refinement at $x/D_j = 0.0$. (b) Radial mesh refinement at $x/D_j = 15.0$.



(c) Axial mesh refinement at $r/D_j = 0.0$.

FIGURE 4.8 – Radial and longitudinal (axial) mesh refinement from the three meshes employed in the present work.

4.2.3 Boundary Conditions

The numerical formulations of the boundary conditions were previously explained in Sec. 3.3. This section discusses the details of the regions where the boundary conditions are imposed and the reference states. The two boundary surfaces present in the computational domain are jet inflow and far-field. The surfaces are represented by the red and blue lines, respectively, in Fig. 4.2. The boundary condition imposed for both surfaces is the weakly enforced solution to a Riemann problem with a Dirichlet condition. The Riemann solver used to impose the boundary condition is the same one employed to calculate the numerical flux between element interfaces. The difference between the two boundary conditions is the reference state.

For the jet inflow condition, three reference states are applied. The inviscid profile is the baseline. It has a uniform distribution of the properties. The reference primitive variables for the boundary condition are given in Table 4.2. The other two reference states use the radial profile from the nozzle simulation with the RANS formulations. The profile

provided is a mean flow profile for all primitive variables. The numerical procedure to take the values from the RANS simulation to the LES boundary condition is presented in Sec. 3.3, and the profiles of the mean properties are presented in Sec. 5.2. The third reference state applied the formulation of the noise tripping [23], Eq. 2.79, to introduce disturbances to the mean velocity values from the RANS simulation.

Based on Refs. [28, 31], a small longitudinal velocity component with $M = 0.01$ is imposed for the far-field boundary condition. The sponge layer model [122], presented in Sec. 3.3 is imposed around the far-field boundaries, represented by the gray region in Fig. 4.2, to damp oscillations that could reach the boundary condition and be reflected to the jet flow. The description of the non-dimensional variables imposed in the far-field boundary conditions is presented in Table 4.2.

TABLE 4.2 – Reference state from the two uniform boundary conditions used in the simulations.

Properties Boundary condition	Pressure [p/p_∞]	Temperature [T/T_∞]	Mach Number [-]
Free stream	1.0	1.0	0.01
Jet inlet	1.0	1.0	1.4

4.3 Numerical Simulation Settings

In the development of this work, six large-eddy simulations of the same operating condition are performed. The operating condition is the supersonic perfectly expanded jet flow with Mach number 1.4 and the Reynolds number based on the jet inlet diameter 1.58×10^6 . Table 4.3 summarizes the free jet simulations performed in the present work. Three numerical analyses are performed.

The S1 simulation is run with a linear polynomial, which yields second-order accurate spatial discretization and M1 mesh using the inviscid profile. The total number of degrees of freedom from the simulation is approximately 50×10^6 . The S2 simulation is run with a quadratic polynomial, which yields third-order accurate spatial discretization and M2 mesh using the inviscid profile. The total number of degrees of freedom from the simulation is approximately 50×10^6 . The S3 and S4 simulations are run with linear and quadratic polynomials, with the M3 mesh and an inviscid profile. The total degrees of freedom are approximately 120×10^6 and 410×10^6 . The S5 and S6 simulations uses a similar setup to the S4 simulation with differences in the inflow strategy. The S5 simulation use the steady viscous profile from the nozzle simulation and the S6 simulation use the unsteady viscous profile.

All simulations are performed with the same time marching method, a third-order

TABLE 4.3 – Summary of simulations settings.

Simulation	Mesh	Order of Accuracy	Inflow Methodology	Total # of dof (10^6)
S1	M1	2 nd order	Inviscid Profile	≈ 50
S2	M2	3 rd order	Inviscid Profile	≈ 50
S3	M3	2 nd order	Inviscid Profile	≈ 120
S4	M3	3 rd order	Inviscid Profile	≈ 410
S5	M3	3 rd order	Steady Viscous Profile	≈ 410
S6	M3	3 rd order	Unsteady Viscous Profile	≈ 410

accurate standard Runge-Kutta scheme with three stages, described in Sec. 3.2.6. The time step used in the simulation has a fixed value based on a fraction of the limit of stability for the Courant–Friedrichs–Lewy (CFL) number for the Runge-Kutta method. The CFL number stability limit varies with the polynomial degree used to discretize the solution. The increase in the polynomial degree decreases the maximum CFL for the simulation. The maximum CFL value for the second-order accurate simulations is 1.2285 and for third-order accurate simulations 1.0485. It was observed that the attempt to use the maximum CFL produced instabilities that did not allow the simulation to progress. The second-order accurate simulations could get closer to the maximum CFL value observed with simulation S1. For the S3 simulation, there was excessive caution in the definition of the time step, which led to a small CFL value. For other third-order accurate simulations, the fraction of the maximum CFL number is always below 0.5. The imposition of the steady viscous profile in the S5 simulation and the unsteady viscous profile in the S6 simulation reduced the maximum CFL when compared to the S4 simulation, and they also required a reduction of the fraction of the maximum CFL number to obtain stable simulations. The fraction of the CFL and the non-dimensional time step that produced stable simulations are presented in Table 4.4.

The simulation procedure involves two steps. The reference time for the development of the simulations is the non-dimensional flow-through time (FTT). The FTT is the time required for one particle with the jet velocity to move through one jet diameter. The first step is the initialization of the jet flow. This step is responsible for advancing the simulation from its initial condition to statistically steady conditions. The initial step requires approximately 240 FTT to reach the statistically steady condition when the initial condition is a steady flow and approximately 100 FTT when the initial condition is an already developed jet flow simulation. The initialization of a previously developed simulation was applied to S4 to S6 simulations. In the sequence, the simulations run an additional time to collect data for the statistical analysis of the flow field. For the flow-field analysis, a time sample of approximately 114 FTT is ideal for accurate results. The six numerical simulations could be performed for the 114 FTT. The information is summarized in Table 4.4.

TABLE 4.4 – Summary of temporal settings and acquisition data sampling.

Simulation	Fraction of maximum CFL	Non-dimensional time step ($\times 10^5$)	Interval data acquisition (FTT)
S1	0.71	37.87	≈ 114
S2	0.46	29.59	≈ 114
S3	0.39	29.59	≈ 114
S4	0.49	23.67	≈ 114
S5	0.26	7.40	≈ 114
S6	0.27	7.40	≈ 114

The configuration of the sub-cell shock-capturing method explained in Sec. 3.2.5 significantly influenced the stability of the simulations. The second-order accurate simulations allowed high values of the threshold of the shock indicator. The resultant amount of finite volume cells in the domain was small. The change in the spatial discretization accuracy, from second-order to third-order accuracy, substantially modified the simulations' stability, which required the reduction of the thresholds from the shock indicator. The consequence of reducing the thresholds is the increment of the cells being resolved with finite volume formulation. The sub-cell shock capturing has two thresholds: the upper threshold indicates when the formulation changes from DG to FV, and the lower threshold indicates when the formulation returns from FV to DG. The thresholds used in the simulations and an average fraction of cells being resolved with finite volume formulations are presented in Table 4.5.

TABLE 4.5 – Summary of the shock indicator parameters.

Simulation	Upper Threshold	Lower Threshold	Fraction of FV cells(%)
S1	0.02500	0.01000	0.3
S2	0.01400	0.00500	18.4
S3	0.02500	0.01000	0.2
S4	0.00050	0.00015	65.7
S5	0.00025	0.00010	71.5
S6	0.00025	0.00010	71.2

The numerical simulations were performed in different high-performance computing (HPC) centers. Computational resources from the Euler [126], SDumont [127], and Jean-Zay [128] clusters were employed in the numerical simulations. The initial tests, S1 and S2 simulations, were mainly run in the Euler cluster. The most demanding simulations, S3, S4, S5, and S6 simulations, were run in the Jean-Zay cluster due to the larger capacity available. In the Jean-Zay cluster, a total of 12M CPU.h was used for tests and the run of the simulations.

4.4 Post-Processing of the Numerical Data

Mean of flow properties and root mean square (RMS) fluctuations are calculated along the centerline, lipline, and four streamwise positions. The centerline is defined as the line in the center of the geometry $r/D_j = 0.0$, whereas the lipline is a surface parallel to the centerline and located at the nozzle diameter, $r/D_j = 0.5$. The data extracted from the lipline are an azimuthal mean from 120 equally spaced positions. The calculation of the mean properties is performed with the azimuthal average by

$$(\bar{\cdot})_i = \frac{1}{120nt} \sum_{m=1}^{120} \sum_{n=1}^{nt} (\cdot)_i^{mn}, \quad (4.1)$$

where i indicate the variable position and nt the time sample. The fluctuation in each point uses the azimuthal average of that position, *i.e.*, central moments

$$(\cdot)_i'^{mn} = (\cdot)_i^{mn} - (\bar{\cdot})_i. \quad (4.2)$$

The four surfaces in the streamwise positions are at $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$. The surface properties are also an azimuthal average using 120 equally spaced positions. Figure 4.9 illustrates a snapshot of the jet flow with the lines and surfaces of data analyses. Instantaneous longitudinal velocity component contours help identify the data analysis position in the jet flow.

Spectral analysis is also conducted. The Power Spectral Density (PSD) of the longitudinal and radial velocity fluctuations is performed in the centerline and lipline in the four streamwise planes. The data acquisition frequency of the simulations is 200 kHz. Due to the employment in the PSD analysis of the non-dimensional velocity fluctuation, the frequency need also to used in non-dimensional form. The non-dimensional frequency is obtained with the same length reference, which is the jet inlet diameter (D_j) and the jet inlet velocity (U_j). The non-dimensional frequency value of the data acquisition is 21.124. In the lipline, the PSD results are an average of the 120 points evenly spaced. No window function is used in the velocity fluctuation signal. PSD is calculated by the employment of the fast Fourier transform (FFT), Eq. (4.3). The PSD results are presented as a function of the non-dimensional frequency, the Strouhal number (St), Eq. (4.4). In the equations, $f(t)$ is the dimensional frequency, $f(t^*)$ is the non-dimensional frequency, nt is the time sample, $\text{fft}(u/U_j)$ is the fast Fourier transform of non-dimensional velocity fluctuation u/U_j , D_j is the jet inlet diameter, and U_j is the jet inlet velocity.

$$PSD = 2 \frac{1}{f(t^*) nt} \text{abs}[\text{fft}(u/U_j)]^2 \quad (4.3)$$

$$St(f) = \frac{f(t^*)D_j}{U_j} \quad (4.4)$$

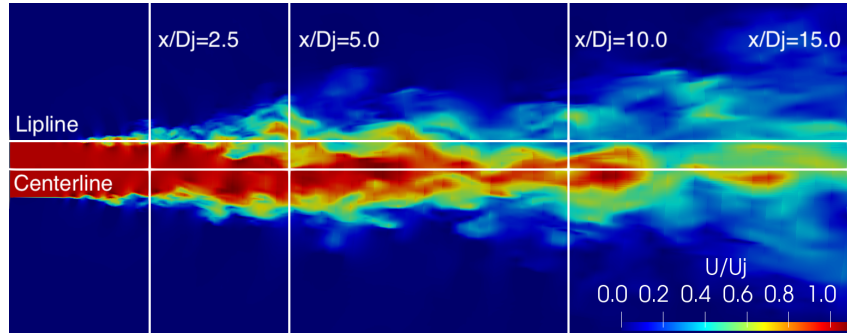


FIGURE 4.9 – Snapshot of the instantaneous longitudinal velocity component with the reference of the positions of the centerline, lipline and the four streamwise positions of data analyses at $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$

4.5 Nozzle Design for the Generation of the Inflow Condition

The nozzle design is performed to generate an inflow condition for the jet flow. There is a necessity to design the numerical nozzle because it does not present the same shape from experiments [6]. The nozzle shape is based on a diffuser with a small opening angle to produce a small velocity increment along the nozzle. This strategy is based on the use of straight pipes for subsonic cases. The nozzle design is performed with Reynolds-averaged Navier-Stokes (RANS) formulation. The RANS formulation is solved by a finite volume formulation implemented in the commercial software CFD++ [57]. The RANS equations are solved with a second-order accurate discretization, using an HLLE Riemman solver [129] and minmod limiter [130]. The equation of state is solved for a perfect gas. The relaxation procedure uses an implicit backward Euler, modified for implementation within a Message Passing Interface (MPI) framework, called in the solver as point implicit. The turbulence closure is performed with the Spalart-Allmaras [56] model.

The simulations are performed exclusively with the nozzle geometry in the 3-D computational domain. The nozzle design aims to define a nozzle geometry capable of providing a highly uniform flow in the nozzle exit section with the properties specified in the experiments [6]. Due to the growth of the boundary layer, an iterative process is necessary to match the nozzle inflow condition, opening angle, outflow condition, and outflow uniformity. The parameters that are being adjusted are presented in Fig. 4.10, in which the black line represents the symmetry axis, the red line represents the nozzle inlet section, the blue line represents the nozzle walls, and the green line represents the nozzle exit section.

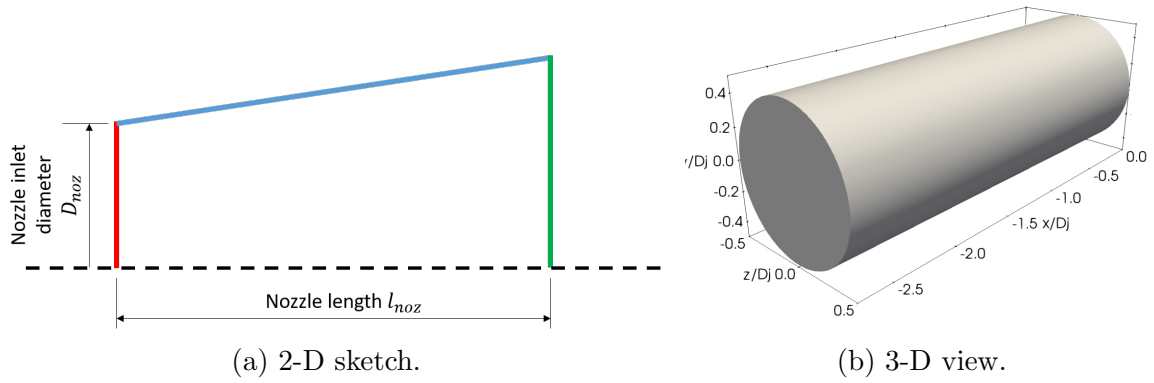


FIGURE 4.10 – 2-D schematic representation and 3-D view of the nozzle geometry used for the generation of a mean flow profile for the jet inflow condition.

The meshes generated for the RANS simulations are based on the same multi-block strategy used for the jet meshes. The mesh is specified to present a Y^+ close to unit [131] with geometrical growth until a maximum estimate for the boundary layer height. A region with constant-size cells is in the interior of the nozzle. The estimate for $Y^+ = 1$ is obtained for a first cell with a height equal to $3 \times 10^{-5} D_j$. The discretization in the nozzle azimuth direction presents a cell every 2° . The nozzle axis has approximately 50 elements per nozzle exit diameter. The mesh sizes varied according to the nozzle length. They have the total number of cells varying from 0.5×10^6 to 1.6×10^6 . The cut plane of the mesh used in the nozzle simulations is presented in Fig. 4.11.

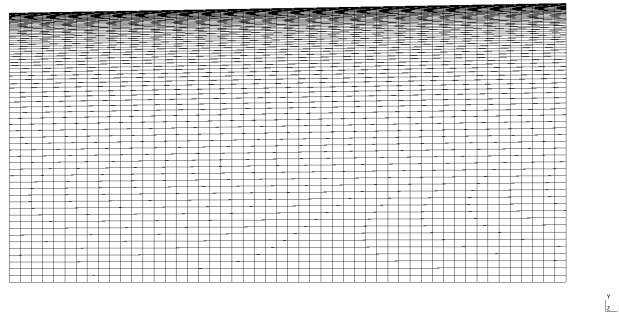


FIGURE 4.11 – Cut plane of the mesh of the nozzle for the definition of the inflow condition for the jet simulation.

The boundary conditions used are Supersonic inlet, red line in Fig. 4.10, with all primitive variables prescribed, supersonic outlet, the green line in Fig. 4.10, in which no condition is prescribed, and all the information comes from the domain cells. The boundary condition for the wall is a no-slip condition. Due to the high refinement in the near-wall region, no wall model is required. The simulation is performed for 2000 iterations with a Courant-Friedrichs-Lewy number (CFL) ramping from 1 in the first iteration to 100 in the 100th iteration.

5 Results and Discussion

In the present section, the three numerical analyses performed in the work are presented. In the first analysis, an accuracy assessment is performed to identify which numerical method is more suitable for the calculations. The numerical data from the simulations performed with the JAZzY solver [17, 32, 90] are compared to two simulations performed with the FLEXI numerical framework [35]. The three simulations have the same degrees of freedom and similar mesh topologies. The second part of this analysis presents an assessment of the “*hp*” refinement, which is performed with the FLEXI numerical framework to identify the mesh and polynomial refinements for the development of the jet flow simulations. In this part of the analysis, the two simulations evaluated previously are compared to two additional simulations. The second analysis performed involves the RANS simulations of the nozzle flow. The RANS simulations are employed to design a nozzle geometry capable of providing outlet conditions that match those obtained in the reference physical experiments of Bridges and Wernet [6]. A total of 15 nozzle designs are investigated, and the nozzle outflow condition is obtained. The last analysis performed in the present work compares three different inflow conditions that influence on the development of the supersonic jet flow. The inviscid inflow condition, applied to the simulations performed in the previous analyses, is compared to the viscous profile obtained from the RANS simulations of the nozzle flow and to an unsteady viscous profile, which is obtained by the superimposition of a tripping method to the viscous profile.

5.1 Accuracy Assessment of the Jet Flow Simulations

Two analyses are performed to build the foundations for investigating the influence of the inflow conditions on the development of the jet flow. In the first analysis, the reference numerical data, which was obtained from a second-order accurate solver from the research laboratory named JAZzY [17, 32, 90], is compared with the numerical data from the FLEXI numerical framework to understand the characteristics that the two methods present for the solution of supersonic jet flows. In order to perform a fair comparison between the two methods, the M1 and M2 meshes are employed. These two meshes were generated with a topology based on the finest mesh used in the simulations with the

JAZzY solver. The simulations that employ the M1 and M2 meshes are the S1 and S2. A summary of the settings of the two simulations is presented in Tab. 4.3. The S1, S2, and numerical reference were performed with the same degrees of freedom, approximately 50×10^6 . The numerical data are compared to the experimental data from Bridges and Wernet [6].

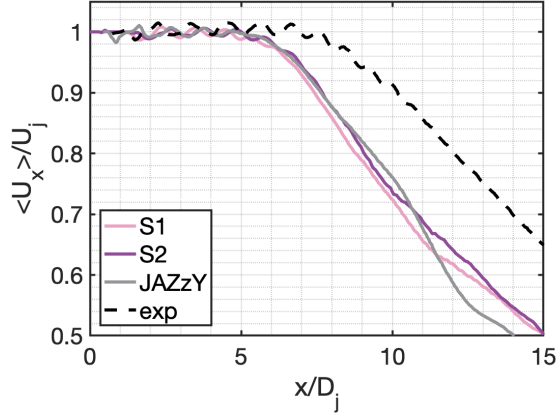
In the second analysis, an accuracy assessment is performed with the FLEXI numerical framework to identify the “*hp*” refinement required by the discontinuous Galerkin spectral element method to produce correct large-eddy simulations of the supersonic jet flows. The numerical data from the S1 and S2 simulations are compared with the numerical data of the S3 and S4 simulations. The S3 and S4 simulations employ a more refined mesh, M3 mesh, which was generated with a different mesh topology. The second mesh topology, explained in detail in Sec. 4.2.2, presents a higher level of local mesh refinement when compared to the M1 and M2 meshes. The degrees of freedom from the four simulations vary between 50×10^6 and 410×10^6 . The study focuses on the establishment of the mesh and solver settings for the inflow condition investigation.

5.1.1 Comparison of the Results from Different Numerical Methods

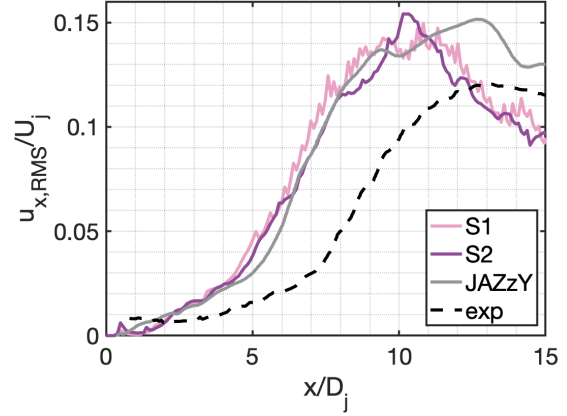
The comparison between the two numerical methods is performed via the investigation of the velocity profiles at different regions of the jet flow field. The three simulations were performed with the same degrees of freedom. The simulations performed with the FLEXI framework [35], which are refereed as S1 and S2, employed the M1 and M2 meshes and second and third-order accurate spatial discretizations. The numerical simulation performed with the JAZzY solver [17, 32, 90] employed a 50×10^6 point mesh with a second-order accurate spatial discretization. The velocity distributions are investigated in the regions presented in Fig. 4.9.

The longitudinal velocity component distributions at the jet centerline and jet lipline are presented in Fig. 5.1. the three numerical simulations present similar mean longitudinal velocity component distribution at the jet centerline, Fig. 5.1a. The simulations present slight differences near the inlet section. The S1 and S2 simulations present nearly constant velocity values up to $x/D_j = 1.5$, while the simulation fromn the JAZzY solver presents a first local minimum before $x/D_j = 1.0$. The S1 simulation presents an early change in the velocity slope, with slight differences from the other two simulations. The velocity distribution from the S2 simulation and those obtained with JAZzY solver are close up to $x/D_j = 11.0$, where a second change in the velocity slope occurs for the simulation obtained with JAZzY. The mean velocity distributions from the three numerical simulations present different velocity values in the potential core region and a shorter potential core when compared to the experimental reference, which may indicate a dissi-

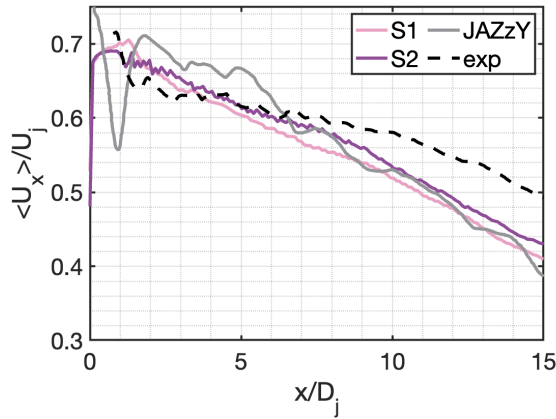
pative behavior from the numerical simulations. The jet potential core is the region of the jet with a longitudinal velocity higher than $0.95U_j$, where U_j is the jet inlet velocity. The length of the potential core is the distance in the centerline of the jet from the inlet section to the position where the velocity reaches the boundary of the potential core, $U = 0.95U_j$.



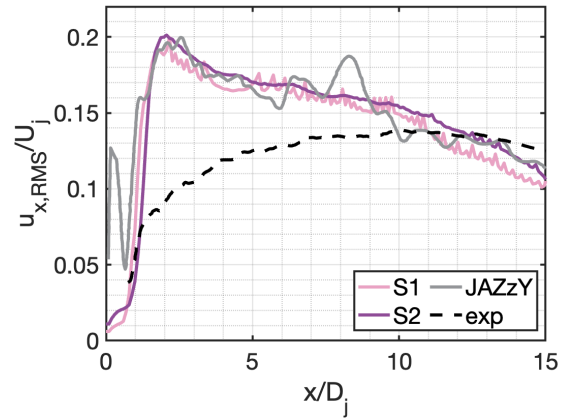
(a) Averaged U_x profile along the centerline.



(b) RMS values of u_x along the centerline.



(c) Averaged U_x profile along the lipline.



(d) RMS values of u_x along the lipline.

FIGURE 5.1 – Velocity distributions at the jet centerline from the numerical simulations that compare the numerical methods. The mean longitudinal velocity component distributions are on the left, and the distributions of the RMS values of longitudinal velocity component fluctuation are on the right. The velocity distributions at the jet centerline ($r/D_j = 0$) are on the top, while the velocity distributions at the jet lipline ($r/D_j = 0.5$) are on the bottom.

The root mean square (RMS) values of the longitudinal velocity fluctuation distribution at the jet centerline are presented in Fig. 5.1b. Similar to what was observed from Fig. 5.1a, the three numerical simulations present a similar velocity profiles of velocity fluctuation up to $x/D_j = 11.0$. In the early development of the jet flow, at $x/D_j < 2.0$, the RMS values of velocity fluctuation from the simulation obtained by the JAZzY solver indicate an early increase compared to the other two simulations. However, for $x/D_j > 2.0$, the other two calculations, using the FLEXI numerical framework, present a local increase

of velocity and, hence, their slope is higher than the one obtained from the simulation using the JAZzY solver. Moreover, in a small distance, $2.0 < x/D_j < 4.0$, the RMS values of the velocity fluctuation from the S1 and S2 simulations get higher than those from the simulations performed with the JAZzY solver. The peak of RMS values from the S2 and S1 simulations are observed at $x/D_j \approx 10.0$ and $x/D_j \approx 11.0$, respectively. In contrast, the peak RMS value from the simulation from the JAZzY solver is reached at $x/D_j \approx 13.0$. Large velocity values from the simulation performed with the JAZzY are observed after the peak RMS values. Moreover, the velocity values for the simulation obtained with JAZzY are larger than those obtained in the S1 and S2 simulations. In the simulation from JAZzY, the slope of the RMS values from the velocity fluctuation after the peak does not present similar levels to the S1 and S2 simulations. The RMS values from the longitudinal velocity fluctuation of the three numerical simulations are larger than those presented by the experimental reference in almost all the longitudinal lengths investigated, $0.0 \leq x/D_j \leq 15.0$. The change in the distribution of RMS values slope occurs at a longitudinal position closer to the inlet section, $x/D_j \approx 2.0$, and the peak RMS values, $u_{x,RMS}/D_j \approx 0.15$, are larger than those obtained in the physical experiments, $u_{x,RMS}/D_j \approx 0.12$.

The mean longitudinal velocity component distributions at the jet lipline, Fig. 5.1c, present larger differences between the numerical simulations distributions than those observed at the jet centerline, Fig. 5.1a. The velocity distributions from the S1 and S2 simulations present a nearly constant slope after the development region ($x/D_j < 1.0$). The mean velocity distribution from the numerical reference presents larger slope changes than the simulations performed with the FLEXI numerical framework. In one region, the velocity levels are below those from the S1 and S2 simulations, $x/D_j \approx 1.0$. In one other region, $1.5 < x/D_j < 6.5$, the velocity values exceed those of the S1 and S2 simulations. After $x/D_j \approx 7.0$, the velocity values from the three numerical simulations are close. The mean velocity values from the S1 and S2 simulations agree with the experimental reference of $x/D_j = 7.0$. After that region, the velocity values from the three numerical simulations are underestimated when compared to the experimental reference.

The RMS values of the longitudinal velocity fluctuation component distributions at the lipline, Fig. 5.1d, from the three numerical simulations present a different behavior at the nozzle vicinity. While the S1 and S2 simulations present one constant velocity slope towards the peak RMS values, the RMS values from the simulation performed with the JAZzY solver oscillates in the region $0 < x/D_j < 2.0$. After the peak RMS value at $x/D_j = 2.0$, similar RMS values of the longitudinal fluctuation are obtained from the three numerical simulations. Also, the velocity slope of the three simulations is nearly equal. All numerical studies overestimate the velocity profile of RMS values along the lipline.

In addition to the velocity distribution at the jet centerline and lipline, the radial profiles of the longitudinal velocity component and some components of the Reynolds stress tensor are presented in four longitudinal positions $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$, indicated in Fig. 4.9. The radial distributions of the mean longitudinal velocity component, mean of the longitudinal component of the Reynolds stress tensor, mean of the radial component of the Reynolds stress tensor, and mean of the Reynolds shear stress tensor component are presented in Fig. 5.2. The evolution of the mean longitudinal velocity component profile on the streamwise direction is presented in Figs. 5.2a to 5.2d. In the first station, at $x/D_j = 2.5$, the velocity distribution from the three numerical simulations differs. The velocity distribution from the simulation performed with JAZzY presents a larger velocity spreading that can be observed by the higher slope in the profile compared to the other velocity profiles. The velocity distribution from the S1 simulation has a higher slope than the S2 simulation, which has a velocity distribution that agrees with the experimental reference. At the second, $x/D_j = 5.0$, third, $x/D_j = 10.0$, and fourth stations, $x/D_j = 15.0$, the velocity distributions from the three numerical simulations are similar. The comparison with the experimental reference indicates a larger velocity spreading in the three stations, with a large difference at the jet centerline, where a large velocity difference is observed after the third station.

The radial distribution of the Reynolds stress tensor component associated with the longitudinal velocity fluctuation is presented in Figs. 5.2e to 5.2h. In the first station, the peak values from the three numerical simulations are located at similar radial positions, with the largest value from the numerical reference, and the second largest value from the S2 simulations. The peak values from the three numerical simulations are up to two times the experimental reference values. A larger region of high Reynolds stress tensor component values is observed from the numerical simulations when compared to a similar region from the experimental reference. The profiles from the next station present a distinction between the numerical solutions. The Reynolds stress tensor component from the S1 and S2 simulations are closer to the experimental data. In contrast, the profile from the simulations performed with the JAZzY solver continue to present large values, that are close to twice the value from the experimental reference. In the next section, $x/D_j = 10.0$, the numerical profiles at the lipline match with the experimental data. However, at the jet centerline, the Reynolds stress tensor component profiles present larger values than experimental data. In the last section, the radial profiles from the numerical simulations have an almost constant distribution, while the experimental data has a larger value than the three numerical simulations close to $r/D_j = 0.6$.

The radial profiles of the Reynolds stress tensor component associated with the radial velocity fluctuation are presented in the four longitudinal sections in Figs. 5.2i to 5.2l. In the first two sections, the profiles present similar behavior. The values from the

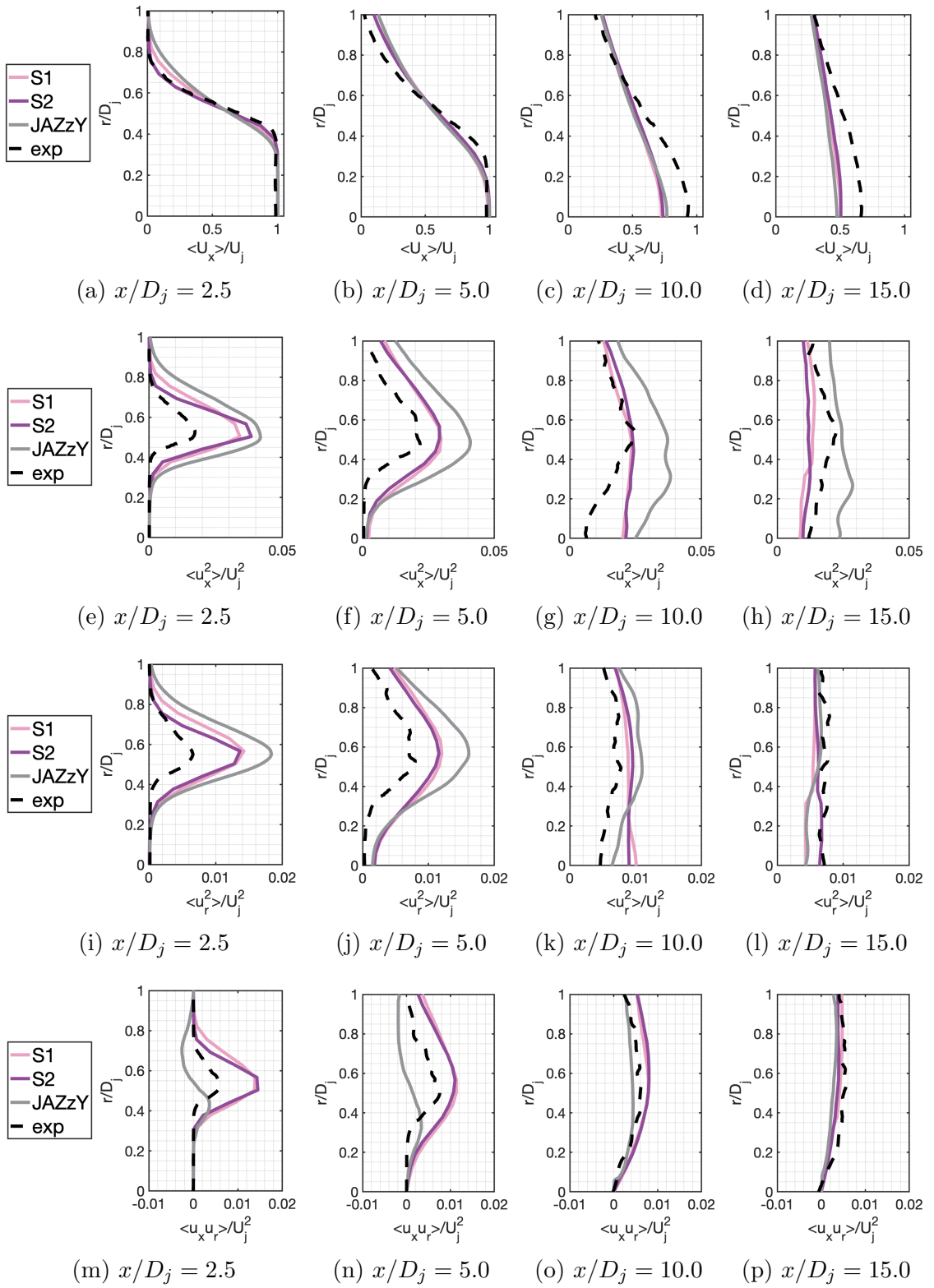


FIGURE 5.2 – Radial velocity and Reynolds stress tensor component profiles from the numerical simulations that compare the numerical methods. From top to bottom, the mean longitudinal velocity component, the mean of the Reynolds stress tensor components associated with the longitudinal and radial velocities, and the mean of the Reynolds shear stress tensor component are presented. From left to right, the data from $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$ are presented.

numerical reference are higher than those of the others. The S1 and S2 numerical simulations generated similar data that overpredict the experimental reference profile. In the third section, $x/D_j = 10.0$, the Reynolds stress tensor component values from the three numerical simulations get closer between themselves. However, the numerical reference present smaller values when compared to the other two simulations close to the centerline. Nonetheless, the profiles from the numerical reference present larger values than the obtained from the simulation with the FLEXI numerical framework above the lipline. The values of the radial profile of the Reynolds stress tensor component are above the experimental reference, with smaller differences than what was identified in previous sections. In the fourth section, Reynolds stress tensor profiles present similar values between the numerical simulations and the experimental reference in all radial locations.

The Reynolds shear stress tensor component is analyzed in Figs. 5.2m to 5.2p. In the first section, the values from the simulation performed with the JAZzY solver present different trends from those from FLEXI simulations and the experimental reference. The profile of the Reynolds shear stress tensor component from the simulation performed with JAZzY presents a small positive value before the lipline. Then, it presents a negative value, which are not observed from the other numerical profiles. The Reynolds shear stress tensor component profiles from the S1 and S2 simulations are more consistent with the experimental data, and they only present a positive peak. The peak value is significantly larger than the one presented in the experimental data. In the second section, the profiles from the numerical simulations are closer to the experimental reference than those from the first section. The profiles obtained from the calculations performed with JAZzY sustained the inversion of the sign, while the profiles obtained from the FLEXI simulations are always positive. In the third and fourth sections, the Reynolds shear stress tensor component profiles from the three numerical simulations agree with the experimental reference.

Except for the initial development of the mixing layer, the mean longitudinal velocity component profiles present the same trend when using the same amount of degrees of freedom. Few differences are observed in the RMS values of the longitudinal velocity fluctuation distribution at the centerline for $x/D_j > 11.0$ and at the lipline for $x/D_j < 2.0$. The radial profiles of the mean longitudinal velocity component show similar behavior. The differences are observed in the Reynolds stress tensor components, especially close to the jet inlet section. In summary, the presented data show that the FLEXI numerical framework could predict the jet flow field with small improvements compared to the simulation performed with the JAZzY solver. The FLEXI numerical framework also presents the intrinsic high-order algorithm associated with the polynomial degree that represents the numerical solution inside the elements. Due to the benefits obtained with the FLEXI numerical framework, it is employed in the following analyses of the present work.

5.1.2 Assessment of the “*hp*” Refinement for Jet Flow Simulations

The mesh and polynomial “*hp*” refinements required for developing supersonic jet flows are investigated. The requirements change according to the numerical methods. Therefore, the present study is focused on the DGSEM implemented in the FLEXI numerical framework. The accuracy assessment compares the two simulations investigated in the previous analysis, S1, and S2, with the S3 and S4 simulations. The S1 simulation is performed with M1 mesh and a linear polynomial degree, yielding a second-order accurate spatial discretization. The S2 simulation is performed with M2 mesh and a quadratic polynomial degree that yields a third-order accurate spatial discretization. The M1 and M2 meshes share the same topology. They possess different refinement levels. The two simulations have approximately 50×10^6 degrees of freedom. The S3 and S4 simulations are performed with M3 mesh. In the S3 simulation, the M3 mesh is simulated with a linear polynomial degree, and in the S4 simulation, the M-4 mesh is simulated with a quadratic polynomial degree. The two simulations have approximately 120×10^6 and 410×10^6 degrees of freedom.

Due to axisymmetry of the jet flow the results are presented in the polar coordinate system $\mathbf{U} = (U_x, U_r, U_\theta)$. A qualitative analysis is performed with contours of instantaneous and statistical properties. A quantitative analysis is performed with the longitudinal and radial distributions at the centerline, lipline, and the four streamwise planes. In the quantitative analysis, the results of the four simulations are compared with experimental data. A signal analysis is performed with the power spectral density of the velocity fluctuation in the lipline.

5.1.2.1 Instantaneous Flow Field

The instantaneous contours of velocity and pressure from the jet flow field are investigated to visualize the flow features presented by the numerical simulations. The instantaneous longitudinal velocity component contours presented in Fig. 5.3 show that in the mixing layer from the S3, Fig. 5.3c, and S4, Fig. 5.3d, calculations present smaller eddies than those in the mixing layer from the of the S1, Fig. 5.3a, and S2, Fig. 5.3b, simulations. The velocity contours along the lipline of the jet flow indicate that the first turbulent structures occur closer to the jet inlet section for the S3 and S4 simulations than in the S1 and S2 calculations. In the S1 and S2 calculations, the interaction of the shock waves is weak, producing few changes to the velocity distribution in the interior of the jet flow. The higher resolution from S3 and S4 simulations than the S1 and S2 calculations reproduce more intense shock interactions, which affects the flow in the interior of the jet flow. The many velocity changes in the interior of the jet flow identify the shock interactions.

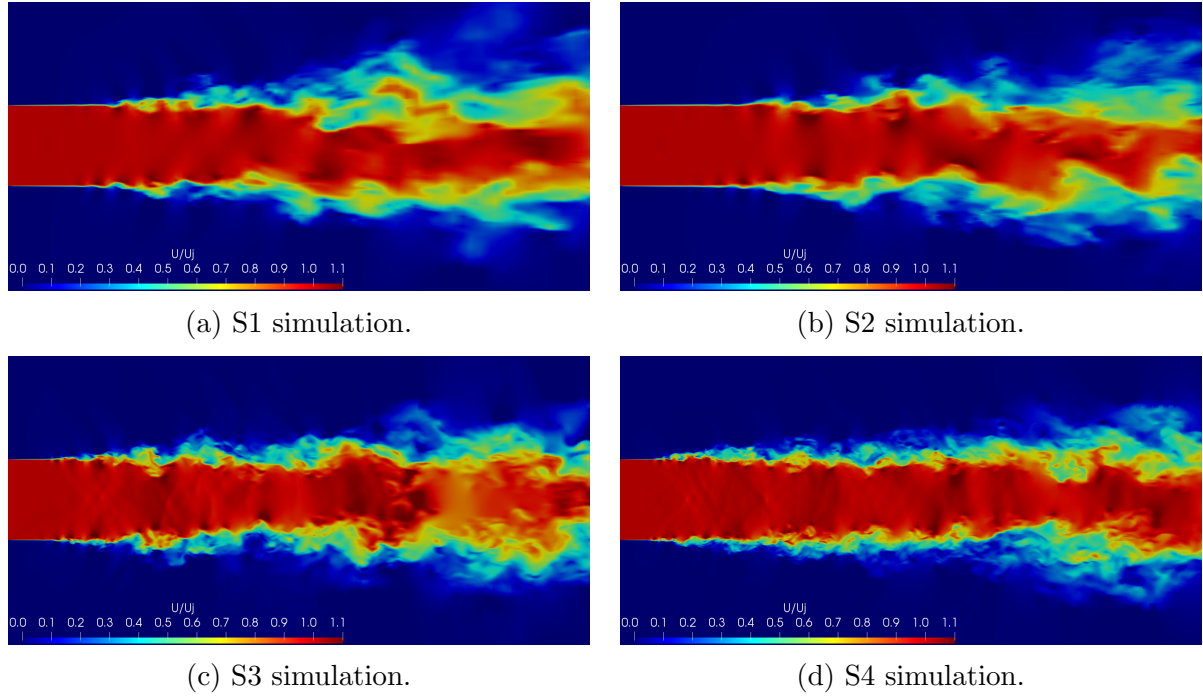


FIGURE 5.3 – Instantaneous longitudinal velocity component contours on a plane through the centerline of the jet. Contours presented from S1 to S4 simulations (a-d).

The vorticity contours, presented in Fig. 5.4 highlight the turbulent structures generated by the interaction between the high-speed flow with the surrounding air and the interaction between the shock waves and the mixing layer. The pressure contours highlight the interaction between the shock waves in the interior of the jet flow and the pressure wave propagation external to the jet flow. The vorticity calculated by the S1 simulation, Fig. 5.4a, indicates weak vortices close to the jet inlet section that almost dissipate when it advances in the domain. The increase in the order of accuracy from S1 to S2 simulation, Fig. 5.4b, can produce better-defined vortices and sustain the presence of the turbulent eddies with the advance in the domain. In the S1 and S2 simulations, the pressure contours indicate the presence of large-scale pressure waves associated with the vortical structures reproduced in the mixing layer. The simulations that used the M3 mesh, the S3 and S4 simulations, could represent additional features in the pressure and vorticity contours when compared to the snapshots from S1 and S2. The vorticity contours from the S3 simulation, Fig. 5.4c, show that the simulation can reproduce small-scale vortices close to the jet inlet section that develop into larger eddies in the mixing layer of the flow. More shock waves are present, which produce a series of pressure changes in the interior of the jet flow. The S4 simulation, Fig. 5.4d, presents the best-defined eddies in the mixing layer and shock waves in the interior of the jet flow from the four simulations analyzed. The comparison among the pressure contours and vorticity magnitude contours from the four simulations indicates an eventual reduction of numerical dissipation, with the capability of the high-resolved simulations to maintain the flow features correctly represented

for longer distances and to include the representation of smaller features present in the flowfield.

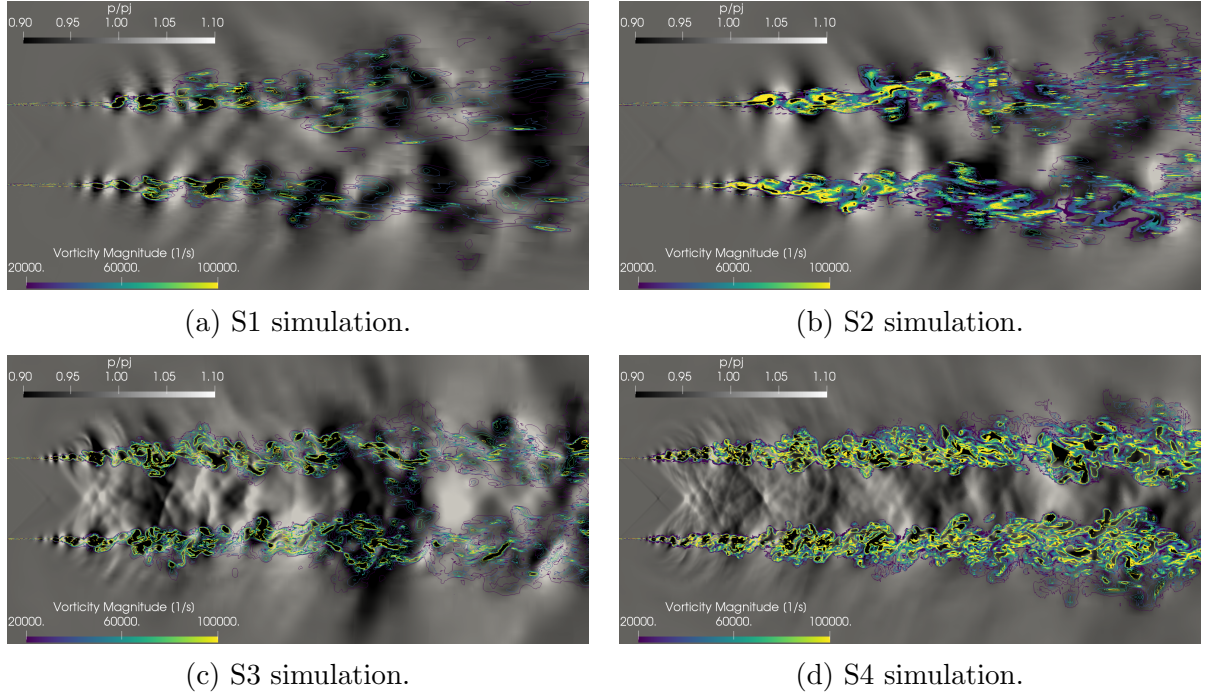


FIGURE 5.4 – Snapshots of pressure with superimposed contours of vorticity magnitude on a plane through the centerline of the jet flow. Contours presented from S1 to S4 simulations (a-d).

It was present in Table. 4.5 that the third-order accurate simulations required additional elements to be solved with a finite volume algorithm through the shock-capturing method to produce stable solutions. Figure 5.5 presents the region where the finite volume elements are employed. The region in the flow where the discontinuous Galerkin formulation is employed is presented in gray, while the red cells indicate the elements resolved with a finite volume formulation. The second-order accurate simulations S1 and S3, Figs. 5.5a and 5.5c, present almost no elements resolved with finite volume formulation. The third-order accurate simulations S2 and S4, Figs. 5.5b and 5.5d, require a significant quantity of elements in the mixing layer to be resolved with a finite volume formulation. Even though the focus is to solve the shock waves with a finite volume formulation, due to weak shock waves in the perfectly expanded operating condition, few elements are resolved with finite volume formulation in the shock waves. Other work from literature [15] presents a similar behavior with the shock indicator, where it triggers in the mixing layer.

5.1.2.2 Mean Flow Field

The contours of the mean longitudinal velocity component, presented in Fig. 5.6, provide some qualitative information on the distinct calculations of the potential core from

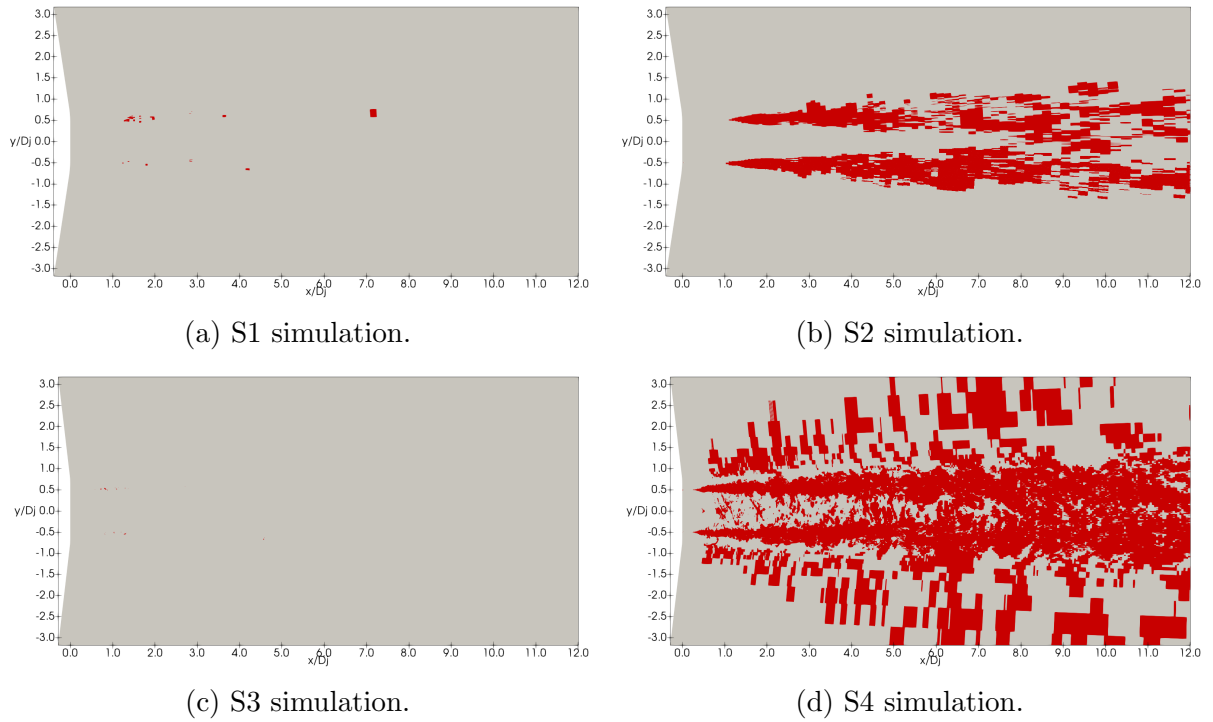


FIGURE 5.5 – Instantaneous identification of DG and FV elements at a cut plane in the center of the jet. Gray contour represents DG elements and red contour represents FV elements. Contours presented from S1 to S4 simulations (a-d).

each simulation. Comparing the velocity contours in Fig. 5.6a and Fig. 5.6b, from S1 and S2 simulations, one can observe that the S2 simulation presents a slightly longer core. Both simulations present a subtle velocity change associated with the shock waves. The velocity contours from the simulations performed with the more refined mesh, Figs. 5.6c and 5.6d, present longer jet cores, larger shock waves, and the mixing layer development commences closer to the jet inlet condition than the contours from the S1 and S2 simulations. The comparison of the velocity contours from simulations S3 and S4 shows a longer potential core with a narrow mixing layer when increasing the resolution from the S3 to S4 simulations.

A deeper investigation of the mixing layer can be performed by visualizing the contours of the root mean square (RMS) values of the longitudinal velocity fluctuation, presented in Fig. 5.7. Due to the interaction between the jet flow and the surrounding air, the turbulence levels in the mixing layer are higher than in other parts of the flow, and the longitudinal velocity fluctuation presents information on the turbulence levels. In the contours presented in Figs. 5.7a and 5.7b, from the S1 and S2 simulations, the values of the peak of RMS of the longitudinal velocity component and the spreading of velocity fluctuation in the longitudinal and transversal directions are similar. The velocity contours from the S3 and S4 simulations, Figs. 5.7c and 5.7d, show some differences in the mixing layer development. The commencement of the development of the shear layer and the

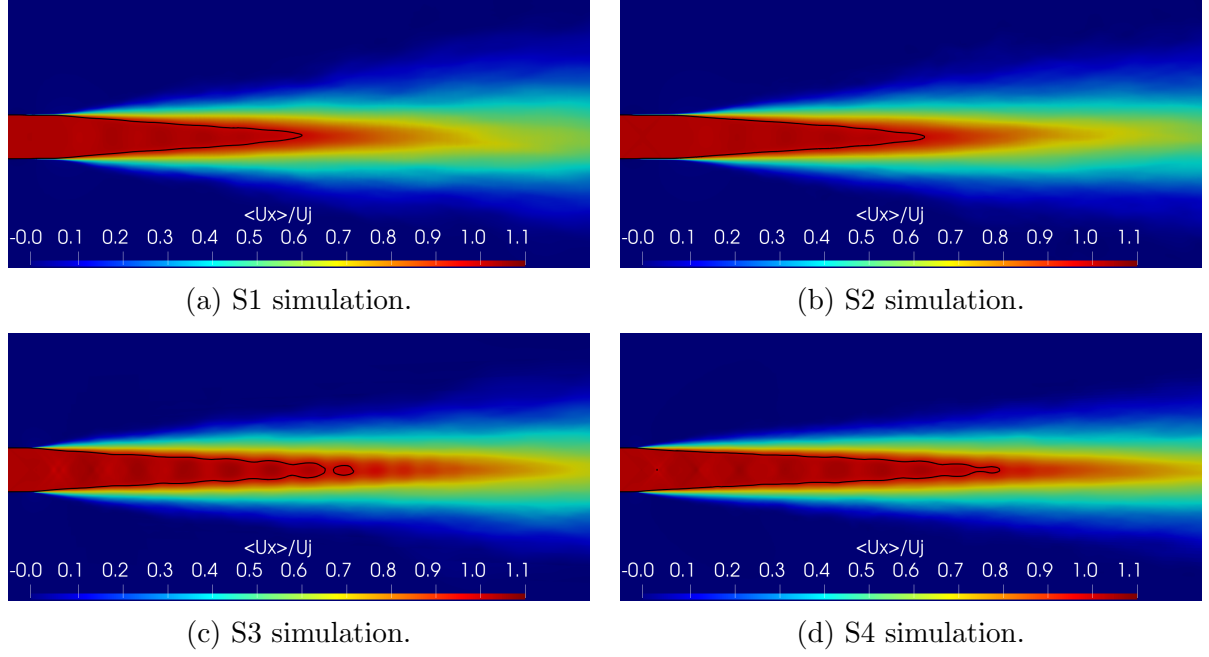


FIGURE 5.6 – Contours of mean non-dimensional longitudinal velocity component for the simulations performed. The black contour indicate the boundaries of the jet potential core, $U = 0.95U_j$. Contours presented from S1 to S4 simulations (a-d).

peak values occurs close to the inlet section. The contours present minor transversal spreading of velocity fluctuation, which can be observed by the long region unaffected by the mixing layer in the centerline and the narrow region with high fluctuation.

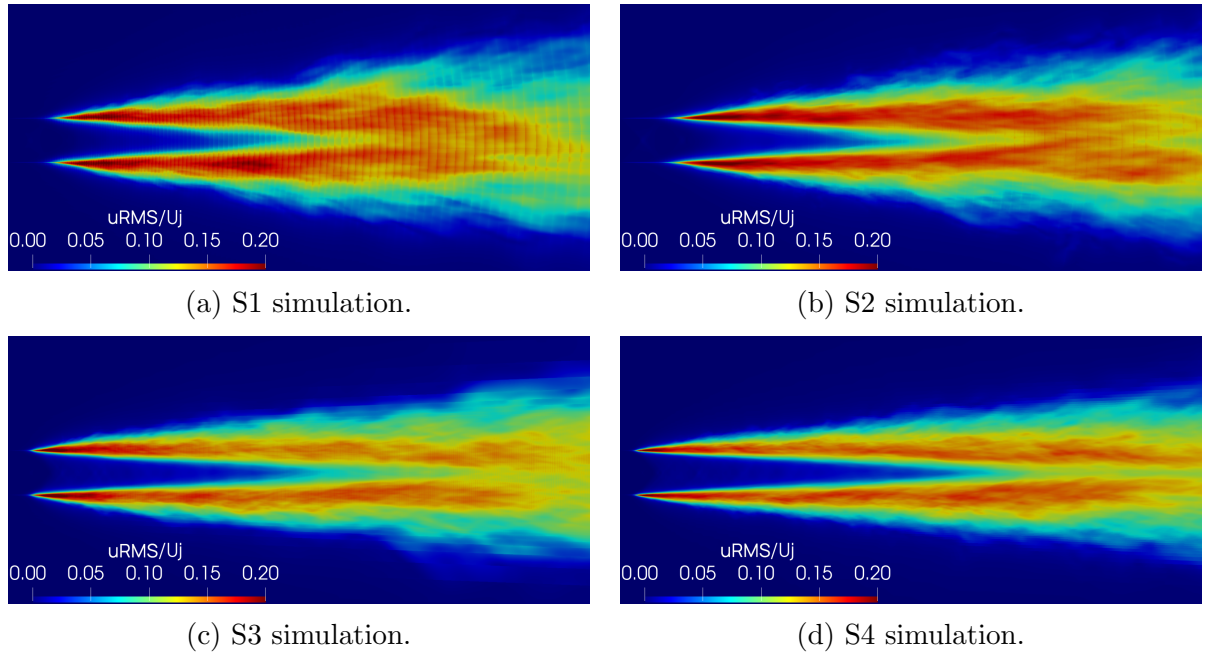


FIGURE 5.7 – Contours of root mean square values of non-dimensional longitudinal velocity component fluctuations. Contours presented from S1 to S4 simulations (a-d).

The contours of mean pressure highlight the differences in the simulations concerning

the shock waves present in the jet core, Fig. 5.8. The contours from the S1 simulation, Fig. 5.8a, indicate a non-uniform pressure distribution, which is associated with the lack of *hp*-resolution of the simulation and the interpolation from the simulation data nodes to probes set employed for the statistical analyses. The pressure contours from the S2 simulation, Fig. 5.8b, present a smoother transition when compared to the contours from the S1 simulation, and additional shock waves are present. Significant differences appear when comparing the pressure contours from the S3 and S4 simulations, Figs. 5.8c and 5.8d, with the contours from the S1 and S2 simulations. A high number of shock structures are present in the flow with high resolution. The first shock wave is closer to the inlet section in the S3 simulation than in the S2 simulation contours. The first shock waves from the S3 and S4 simulations present a smaller thickness when compared to the pressure contours from the S1 and S2 simulations. The better-defined shock waves are associated with a better resolution from the S3 and S4 simulations when compared to the S1 and S2 simulations. The pressure contours from the S4 simulation indicate thin shock waves compared to the S3 simulation. However, the shock waves from the S3 simulation present larger pressure differences between the repetitions than those of the S4 simulation, which may be associated with an unsteady position of the shock waves.

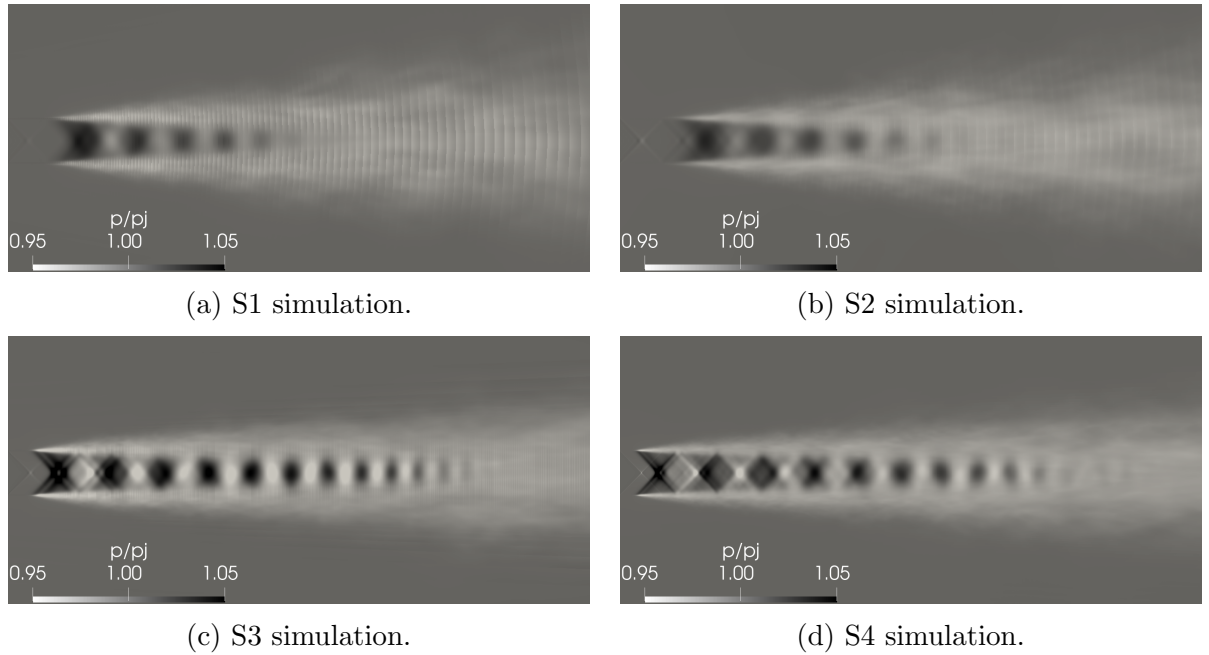


FIGURE 5.8 – Mean non-dimensional pressure contours from the simulations performed. Contours presented from S1 to S4 simulations (a-d).

5.1.2.3 Longitudinal Distributions of the Longitudinal Velocity Component

The flow visualization assists the understanding of the significant characteristics of the flow. However, retaining detailed flow field information is only possible with a quantitative

analysis. Figure 4.9 presents the regions where the jet flow information is compared to experimental data. In Fig. 5.9, the longitudinal distributions of the longitudinal velocity component and the Reynolds stress tensor components at the centerline are presented, and in Fig. 5.10, the longitudinal distributions at the lipline are presented. The longitudinal distributions from the four numerical simulations are compared with experimental data [6].

Figures 5.9a and 5.9b present the mean longitudinal velocity component distribution and the RMS values of the longitudinal velocity fluctuation distribution at the centerline of the jet flow. The velocity values are only affected by the shock waves close to the jet inlet section, inside the potential core of the jet flow. Close to the potential core length, the velocity distribution presents a negative slope associated with the mixing layer of the jet flow spreading the velocity from the jet core. The S1 and S2 simulations present a shorter potential core length when compared to the S3 and S4 simulations. The short potential core length, which occurs right after the velocity slope change, is close to $x/D_j = 7.0$. The change in the slope from the experimental data is only observed downstream of the jet flow. The velocity distribution from the S2 simulation indicates a slightly longer potential core when compared with the S1 simulation. The velocity distribution from the S3 and S4 simulations is closer to the experimental reference when compared to the S1 and S2 simulations. The potential core length is close to $x/D_j = 8.0$, and there is a visible influence of the set of shock waves through the jagged distribution in the potential core. In the S1 and S2 simulations, a series of shock waves with small peak-to-peak velocity amplitude can be observed up to the section $x/D_j \approx 6$, while in the S3 simulation, the set of shock waves extends up to $x/D_j \approx 10$. The S4 simulation presents a better agreement with experimental data when compared to the other simulations. The potential core from the S4 simulation is longer than the potential core from the S3 simulation. The peak-to-peak velocity amplitude in the potential core from the S4 simulation is smaller than those obtained in the S3 simulation. The potential core length is used as a parameter to assess the error of the numerical simulations. The error assessment of numerical data with experimental data is presented in Tab. 5.1.

TABLE 5.1 – Summary of potential core length for all simulations.

Simulation	Potential core length (x/D_j)	Error to experimental data (%)
S1	6.6	25.0
S2	6.9	21.6
S3	7.7	12.5
S4	8.5	3.4

The RMS values of the longitudinal velocity fluctuation distribution at the jet centerline, Fig. 5.9b, indicate improvements from the velocity values of the numerical simulations

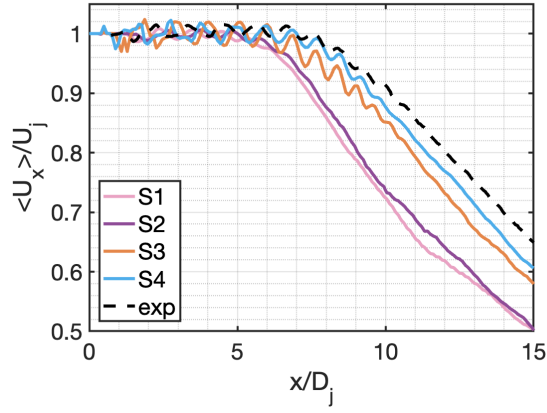
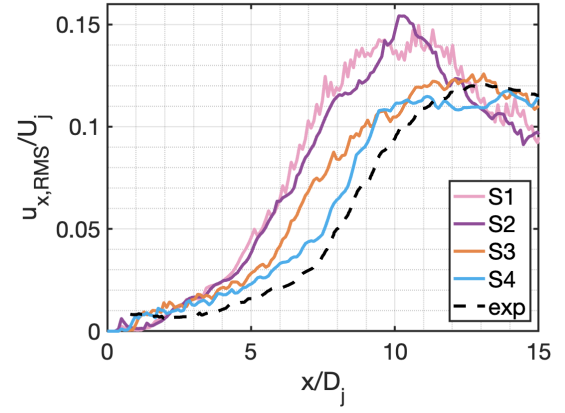
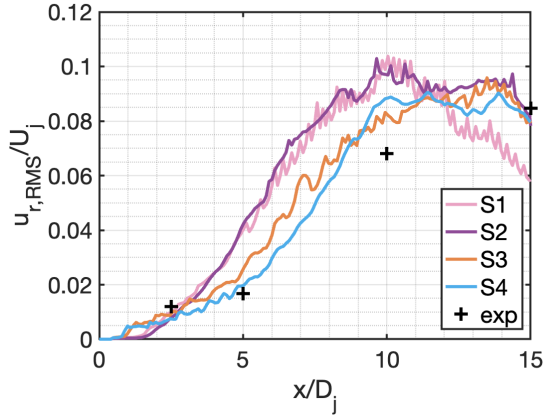
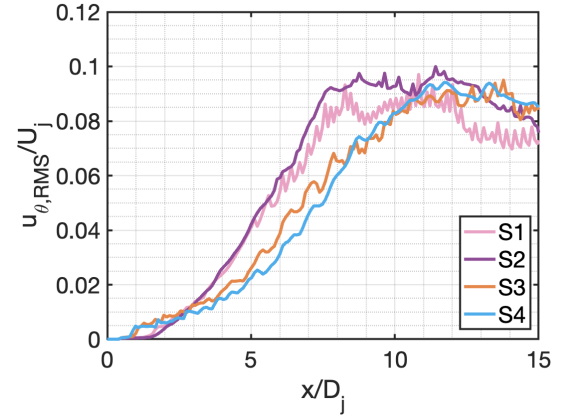
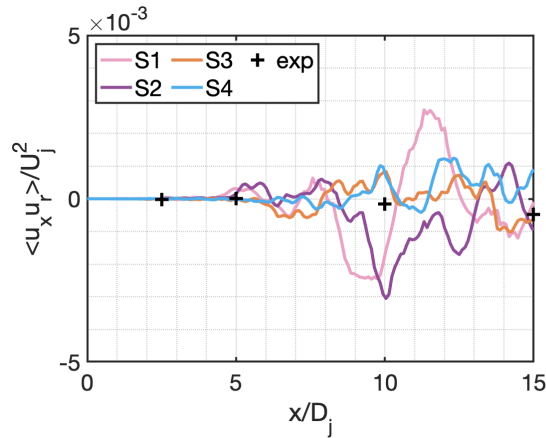
(a) Averaged U_x profile along jet centerline.(b) RMS values of u_x along jet centerline.(c) RMS values of u_r along jet centerline.(d) RMS values of u_θ along jet centerline.(e) Averaged $u_x u_r$ profile along jet centerline.

FIGURE 5.9 – Longitudinal distributions of the mean longitudinal velocity component distribution (a), RMS values of longitudinal velocity fluctuation (b), RMS values of radial velocity fluctuation (c), RMS values of the tangential velocity fluctuation (d), and mean Reynolds shear-stress component (e) at the jet centerline, $r/D_j = 0.0$.

with increased resolution compared to the experimental reference. The longitudinal velocity fluctuation distributions from the S1 and S2 simulations present an increase in the velocity slope occurring closer to the jet inlet section than the S3 and S4 simulations and the experimental data. The velocity fluctuation distribution from the S1 simulation presents oscillation in the velocity distribution associated with employing a relatively coarse mesh and linear polynomial degree with the probe processing employed to interpolate data in the flow field. The results with large mesh refinement or third-order accurate scheme do not present a similar oscillation. The velocity fluctuation of the S3 simulation presents a reduced maximum RMS value when compared to the maximum values from the S1 and S2 simulations. The reduced peak values from the velocity fluctuation distribution and the change in the velocity slope occurring far from the inlet section led the velocity fluctuation distribution to approach the experimental reference. In the longitudinal velocity fluctuation, the S4 simulation provided results that match the experimental reference better than the other numerical simulations.

The RMS values of the radial velocity fluctuation distribution, Fig. 5.9c, present similar characteristics observed by the RMS values of the longitudinal velocity fluctuation. The increase in the velocity fluctuation from the S3 and S4 simulations occurs farther from the inlet section, and they present smaller peak values. The difference between the peak values from the S3 and S4 simulations compared to those from the S1 and S2 simulations is proportionally smaller than those obtained from the RMS values of the longitudinal velocity fluctuation. The radial velocity distributions present one difference from the S1 and S2 simulations. The velocity slope after the peak value is smaller than that from the S2 simulation. The other three simulations have similar velocity levels at this region. The RMS values of the tangential velocity fluctuation distribution, Fig. 5.9d, present a similar behavior to the RMS values of the radial velocity distribution with similar peak values from the four simulations and similar velocity slopes after the peak values. The mean Reynolds shear-stress component, Fig. 5.9e, experimental reference indicates that negligible stress is obtained at the centerline, which is the case for all simulations for $x/D_j < 5.0$. However, for $x/D_j > 5.0$, an oscillation is observed from all numerical data. The oscillation amplitude is higher for the S1 and S2 simulations when compared to the S3 and S4 simulations.

Figures 5.10a and 5.10b present the distribution of the mean longitudinal velocity component and the RMS values of the longitudinal velocity fluctuation at the lipline of the jet flow. The mean longitudinal velocity component distribution at the lipline, Fig. 5.10a, indicate that in the region $0 < x/D_j < 5.0$ the four simulations and the experimental data present similar values. The velocity distributions from the S1 and S2 simulations present a change in the velocity slope, which resulted in small mean velocity velocities. The change in the velocity slope occurs after the position $x/D_j \approx 5.0$ for the

S1 simulation and for $x/D_j \approx 7.0$ for the S2 simulations. The mean velocity distributions from the S3 and S4 simulations indicate similar velocity values along the longitudinal region evaluated.

The distributions presented for the RMS values of the longitudinal velocity fluctuation at the lipline, Fig. 5.10b, have different behavior than the previous analyses from Figs. 5.9a, 5.9b, and 5.10a. The four simulations present an abrupt change in the slope of the velocity fluctuation distribution in the region $0.0 < x/D_j < 2.0$. After the abrupt increase in the velocity fluctuation levels, the distributions reach maximum velocity fluctuation values significantly larger than those from the experimental reference. After reaching the maximum value, an inversion in the velocity distribution slope is observed. The velocity slope inversion led to the S1, S2, and S3 simulations to present velocity fluctuation levels above the experimental reference for $x/D_j > 12.0$. The S3 and S4 simulations present a similar velocity fluctuation behavior in the lipline. In these two simulations, the abrupt change in the velocity slope occurs in a station even closer to the jet inlet section, $x/D_j \approx 0.5$, when compared to the change in the slope from the S1 and S2 simulations, $x/D_j \approx 1.0$, and reaches its peak close to $x/D_j = 1.0$. The velocity fluctuation distribution from the S4 simulation never reaches velocity values below those of experimental data. The velocity fluctuation distribution shows that the growth in the velocity fluctuation occurs closer to the jet inlet section with increased resolution, except for the S1 and S2 simulations. Even though the S1 simulation is simulated with a second-order accurate spatial discretization, it has a more refined mesh than the S2 simulation, which may be responsible for allowing the simulation to capture smaller eddies than those of the S2 simulation. Once the same mesh is employed with different spatial discretization accuracy, the third-order accurate method could better reproduce the turbulent eddies than the second-order accurate, allowing the simulation to anticipate the transition mechanism. The results from the velocity fluctuation in the lipline indicate important differences to the experimental data, which are associated with the inviscid profile imposed in the jet inlet section and not related to a lack of accuracy of the numerical method.

The RMS values of the radial velocity fluctuation distributions are compared with the experimental data at the lipline in Fig. 5.10c. The velocity fluctuation distribution presents a similar shape observed in the longitudinal velocity fluctuation distribution, Fig. 5.10b, with a sudden increase of the velocity fluctuation close to the inlet section. The difference between the radial and the longitudinal velocity distribution is that in the radial velocity distribution, there is a larger difference in the peak values between the S3 and S4 simulations and the S1 and S2 simulations. The S1 and S2 simulations produce peak velocity fluctuations above the experimental reference, but the S3 and S4 simulations produce nearly twice the peak value from experimental data. The same behavior is observed in the RMS values of the tangential velocity fluctuation distribution, Fig. 5.10d.

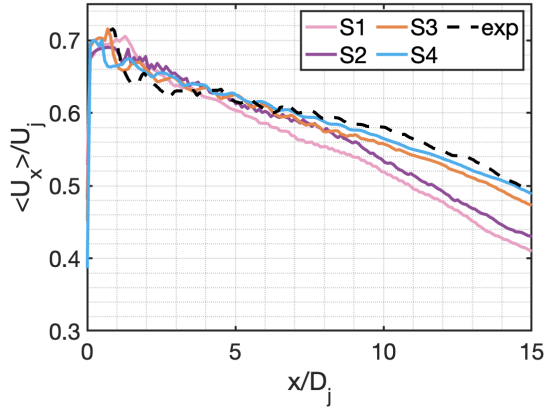
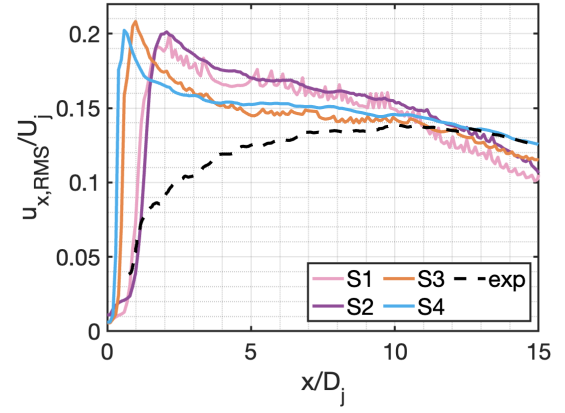
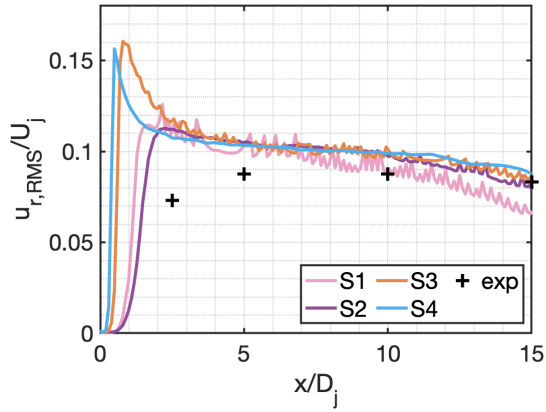
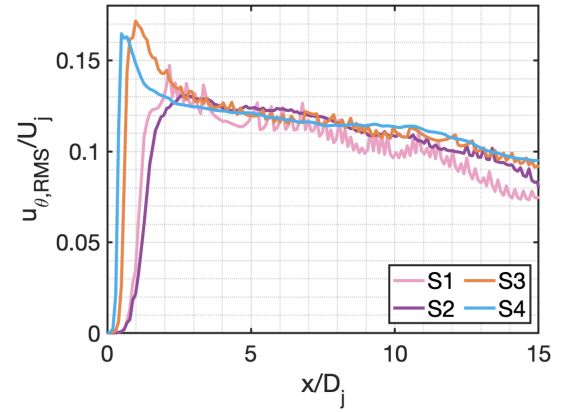
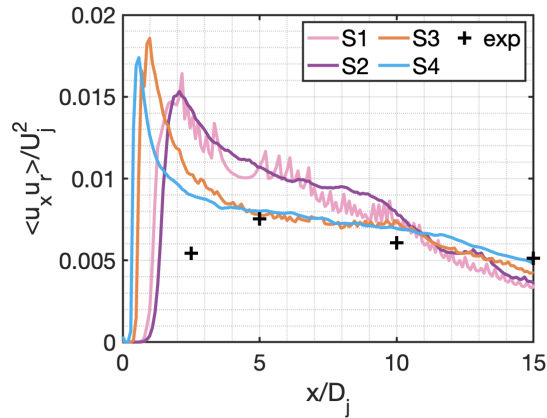
(a) Averaged U_x profile along jet lipline.(b) RMS values of u_x along jet lipline.(c) RMS values of u_r along jet lipline.(d) RMS values of u_θ along jet lipline.(e) Averaged $u_x u_r$ profile along jet lipline.

FIGURE 5.10 – Longitudinal distributions of the mean longitudinal velocity component distribution (a), RMS values of longitudinal velocity fluctuation (b), RMS values of radial velocity fluctuation (c), RMS values of the tangential velocity fluctuation (d), and mean Reynolds shear-stress component (e) at the jet lipline, $r/D_j = 0.5$.

The Reynolds shear-stress component from the four simulations is compared with the experimental data in Fig. 5.10e. The peak values from the numerical simulations are higher than twice the values from the experimental reference in the region of the jet inlet. At the same time, they could get closer to experimental data at $x/D_j > 5.0$.

5.1.2.4 Radial Profiles of the Longitudinal Velocity Component and Reynolds Stress Tensor

Figure 5.11 presents a set of radial profiles from the four simulations compared with experimental data. The radial profiles were obtained in four longitudinal positions: $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$. The variables investigated are the mean longitudinal velocity component and three components from the Reynolds stress tensor: the mean squared longitudinal velocity fluctuation component, the mean squared radial velocity fluctuation component, and the mean shear-stress tensor component. The mean longitudinal velocity component distributions, Figs. 5.11a to 5.11d, present information on the development of the mean flow field of the jet flow. In Fig. 5.11a, which is the closest station to the jet inlet section, the profiles from the four simulations present a similar shape when compared with the experimental data, with a larger slope in the region $0.4 < r/D_j < 0.8$, which indicate a larger velocity spreading of the jet. The mean longitudinal velocity component profiles from the S2 simulation could provide a better agreement with experimental reference at this position. The behavior agrees with the postponed change of the velocity fluctuation slope presented in Fig. 5.10b. The analysis of the profiles of the mean longitudinal velocity component at station $x/D_j = 5.0$, Fig. 5.11b, indicates a larger jet spreading from the simulations compared to the experimental data, characterized by the larger slope profile in $0.3 < r/D_j < 1.0$ from the numerical simulations compared to the experimental data. The four simulations present profiles with a similar shape between themselves. At station $x/D_j = 10.0$, Fig. 5.11c, the differences in the mean velocity profiles are apparent. The S1 and S2 simulations present a larger velocity reduction at the jet centerline than the S3 and S4 simulations. The region of small velocity values extends up to $r/D_j = 0.8$, where the S1 and S2 velocity distributions reach the values of the other simulations. The mean velocity profiles from S3 and S4 simulations present a larger velocity reduction in the centerline than the experimental data. In the last section, $x/D_j = 15.0$, presented in Fig. 5.11d, the velocity profiles present a similar behavior to those observed in Fig. 5.11c, where the largest velocity reduction in the centerline is observed from the S1 and S2 simulations, then the S3 and S4 present similar velocity levels and, above them, the experimental data. Extending above $r/D_j = 1.0$, all the simulations and the experimental reference present similar velocity levels.

The radial progression of the mean squared longitudinal velocity fluctuation, Figs. 5.11e to 5.11h, indicate a clear division in the velocity distribution from the S1 and S2

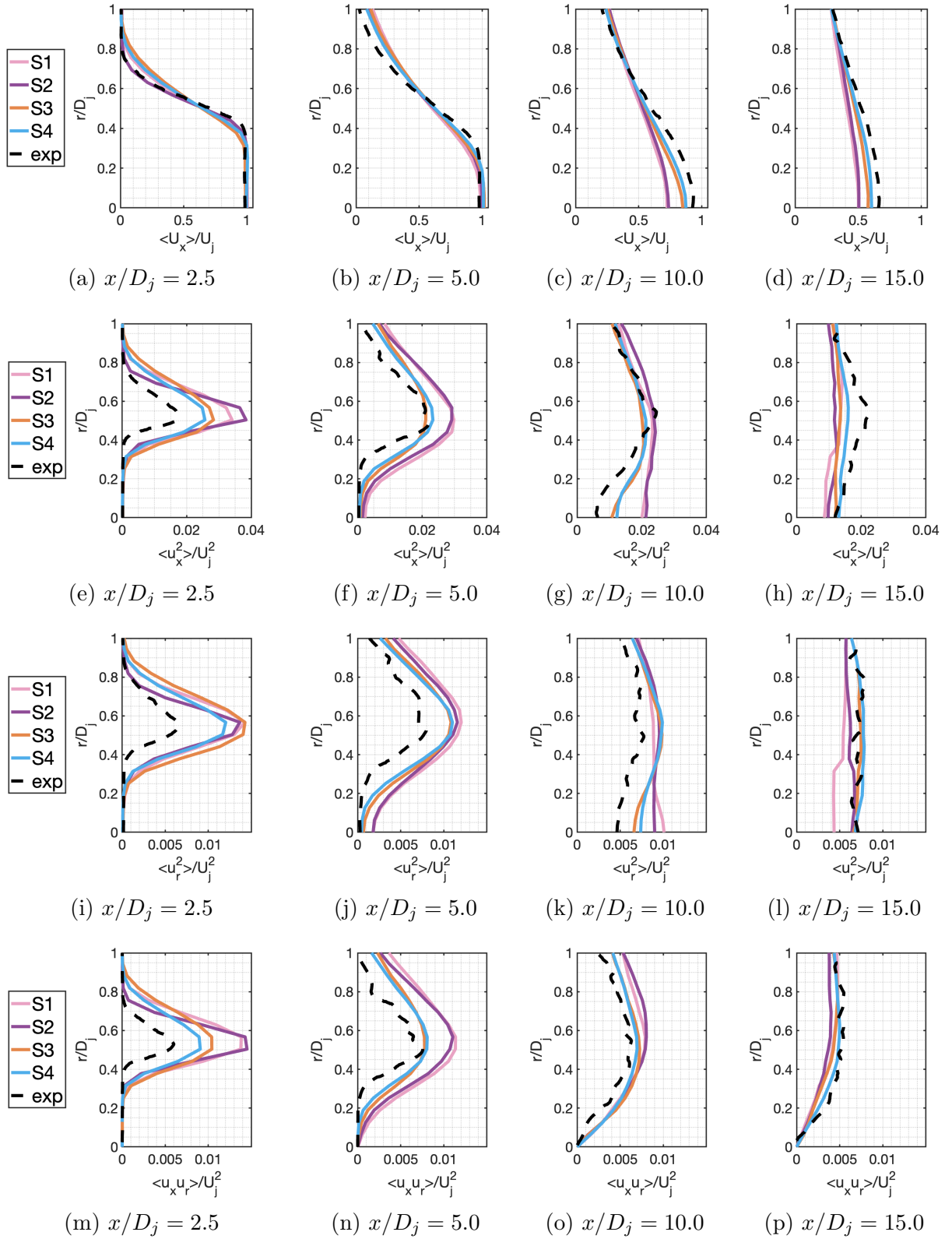


FIGURE 5.11 – Radial distributions of the mean longitudinal velocity component, mean of longitudinal velocity fluctuation squared, mean of radial velocity fluctuation squared and mean shear-stress tensor component (from top to bottom) presented in four streamwise positions $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$ (from left to right).

simulations and the S3 and S4 simulations. In the first section, Fig. 5.11e, close to the jet lipline, the velocity fluctuation profiles from the S3 and S4 simulations have a small peak compared to those from the S1 and S2 simulations. The four simulations generally present a larger fluctuation value than the experimental data. The velocity fluctuation in the second station, Fig. 5.11f, shows that the peak values from the S3 and S4 simulations are similar to the peak values of the experimental data. The S3 and S4 simulations have a wider high-velocity fluctuation region than the experimental reference. The velocity fluctuation distribution from the S1 and S2 simulations present larger peak values and spreading than the other two numerical simulations and the experimental reference. In the section $x/D_j = 10.0$, the peak of velocity fluctuation and the velocity distribution above the mixing layer have similar levels between all the numerical simulations and the experimental data. Close to the centerline, the values of velocity fluctuation differ between the S1 and S2 simulations with the S3 and S4 simulations and the experimental data. In the last section, Fig. 5.11h, the levels of velocity fluctuation between all the numerical simulations are very similar, with small differences to the experimental data only in the jet lipline.

The distributions of the Reynolds stress tensor component associated with the radial velocity component are presented in Figs. 5.11i, 5.11j, 5.11k, and 5.11l. The profiles are similar to those presented by the longitudinal velocity component. In Fig. 5.11i, the peak values are obtained close to the jet lipline, $r/D_j = 0.5$, with nearly twice the values reported by the experimental data. The peak values of all simulations are close in this station. In the second station analyzed, Fig. 5.11j, the velocity fluctuation values from the numerical simulations continue to be close between themselves, and they got closer to the experimental reference. The velocity distribution in the section $x/D_j = 10.0$, Fig 5.11h, presents some differences in the profiles of the simulations. The S1 and S2 simulations present larger values in the centerline than the S3 and S4 simulations. The S3 and S4 simulations present larger radial velocity fluctuation values than the experimental reference. The profiles of radial velocity fluctuation of the simulations match the numerical simulations close to $r/D_j = 0.2$ with larger values compared to the experimental reference up to $r/D_j = 1.0$. In the last section, Fig. 5.11l, the radial velocity distribution of all the simulations agrees with the experimental reference.

The last component of the Reynolds stress tensor evaluated in this radial basis is the shear-stress component, Figs. 5.11m, 5.11n, 5.11o, and 5.11p. The radial distributions from section $x/D_j = 2.5$, Fig. 5.11m, distinguish the simulation data into two groups. The peak values from the S1 and S2 simulations are nearly three times larger than those of the experimental reference, while the peak values from the S3 and S4 simulations are nearly twice those from the experimental reference. The shear-stress tensor profile from the numerical simulations indicates a larger spreading when compared to the experimental

reference, which presents small values close to the lipline. The radial distribution in the section $x/D_j = 5.0$, Fig. 5.11n show a better agreement with experimental data from the peak values of the S3 and S4 simulations with a reduction in the differences between the S1 and S2 simulations. Even with an agreement in the peak values, a larger spreading is observed directed to the jet centerline and the external flow. The shear-stress distributions from the sections $x/D_j = 10.0$ and $x/D_j = 15.0$, Figs. 5.11o and 5.11p, indicate an agreement of the numerical data with experimental data concerning the peak values and the profiles.

The general behavior of the Reynolds stress tensor components indicates more considerable differences in the initial development of the jet flows, $x/D_j < 5.0$, with larger peak values and increased mixing layer. The overprediction of the Reynolds stress tensor component may be associated to the choice of the inflow condition for the jet flow. In the section $x/D_j = 10.0$, there are similarities in the shape of the radial profiles far from the jet centerline, where the numerical simulations present more significant velocity fluctuation levels than the experimental data. In the last section analyzed, $x/D_j = 15.0$, all the components of the Reynolds stress tensor agree with experimental data. The mean longitudinal Reynolds stress tensor component profile behaviors are similar to the experimental data in the first section, $x/D_j = 2.5$. In the second section, at $x/D_j = 5.0$, the derivative of the mean longitudinal velocity with the radial position is larger than the experimental data, which is associated with a larger jet spreading, resulting in a smaller core of the jet and larger velocity values far from the jet lipline. In stations, $x/D_j = 10.0$ and $x/D_j = 15.0$ similar mean velocity values are observed between the numerical simulations and the experimental data for radial positions larger than $r/D_j = 5$. In contrast, in the centerline of the jet, smaller mean velocity values are obtained.

5.1.2.5 Power Spectral Density Analyses

The analysis performed with the mean velocities and the components of the Reynolds stress tensor provides insight into the characteristics of the flow field. The study of turbulence shows that more information is needed to characterize a turbulent flow. In turbulent motion, many eddies are present in the fluid and are responsible for the velocity fluctuations observed in previous results. These eddies exist in different sizes and possess different velocities. The quantity of these eddies and the sizes and velocities are proportional to the Reynolds number of the flow. There are different ways to evaluate the sizes and velocities, or frequency, of the turbulent eddies. The power spectral density (PSD) is one tool that investigates the frequencies of the turbulent eddies and indicates the power associated with each frequency. Another way to perform such studies is through the turbulent kinetic energy spectrum, where a spatial analysis is performed, and the energy contained in specific length scales is determined. The present work performs the PSD of

the longitudinal and radial velocity fluctuations at the centerline and lipline at the four longitudinal positions. Experimental data are available for the lipline PSD values in three of the four stations. The experimental reference is only available for a short interval of frequencies, which is positioned in the smallest frequency range, which does not contribute significantly to the analysis of the identification of the influence of the spatial filter in the numerical data.

Figure 5.12 presents the PSD of the longitudinal velocity component fluctuation at the centerline of the jet flow in the four longitudinal locations of interest. The analysis of the PSD data in the centerline shows a noisy signal. The PSD data can be investigated by comparison with the distribution of the longitudinal velocity fluctuation at the jet centerline, Fig. 5.9b. In the first station, Fig. 5.12a, small power of the velocity signal is observed in all the frequencies, which agrees with the small level of RMS values of the longitudinal velocity fluctuation at $x/D_j = 2.5$. In $x/D_j = 5.0$, Fig. 5.12b, an increase in the power level in the high frequencies is observed, which agrees with the increment presented in the centerline distribution. It is possible to observe that the power levels of S1 and S2 simulations are slightly above S3 and S4, and this last one has the smaller power level in this position for most of the frequencies. This sequence is also observed at the centerline distribution. In $x/D_j = 10.0$, Fig. 5.12c, the power levels increased significantly from all the simulations in the smallest frequencies, which is also observed in the results from $x/D_j = 15.0$, Fig. 5.12a. The high power levels present in these last two stations are represented by the centerline distribution, where the RMS values of the longitudinal velocity component fluctuation presented a large increment in the fluctuation levels.

The PSD data from the longitudinal velocity fluctuation at the jet lipline are presented in Fig. 5.13. Due to the employment of the azimuthal average, the time sample is substantially increased, and the PSD value distributions present a smaller noise level. The experimental reference is available for three positions. The PSD data in $x/D_j = 2.5$, Fig. 5.13a present two interesting observations. The power distribution from S1 and S2 simulations present a peak level close to $St = 0.5$. In the literature [28], it is discussed that when some frequencies in the middle of the range present a peak of power, these frequencies are associated with the transition phenomena. This is interesting because at the lipline distribution of RMS values of longitudinal velocity fluctuation, in $x/D_j = 2.5$ for the S1 and S2 simulations, the two simulations present the largest values of velocity fluctuation, which may be correlated to the transition phenomena. The power levels from the S3 and S4 simulations do not present this peak because they have already passed from the peak RMS values from the velocity fluctuation distribution. The second interesting point is that a clear distinction between the capability of the S1 and S2 simulations to capture high-frequency fluctuations is smaller than the capacity from the S3 and S4 simulations. In $x/D_j = 5.0$, the first comparison with experimental data is available, Fig.

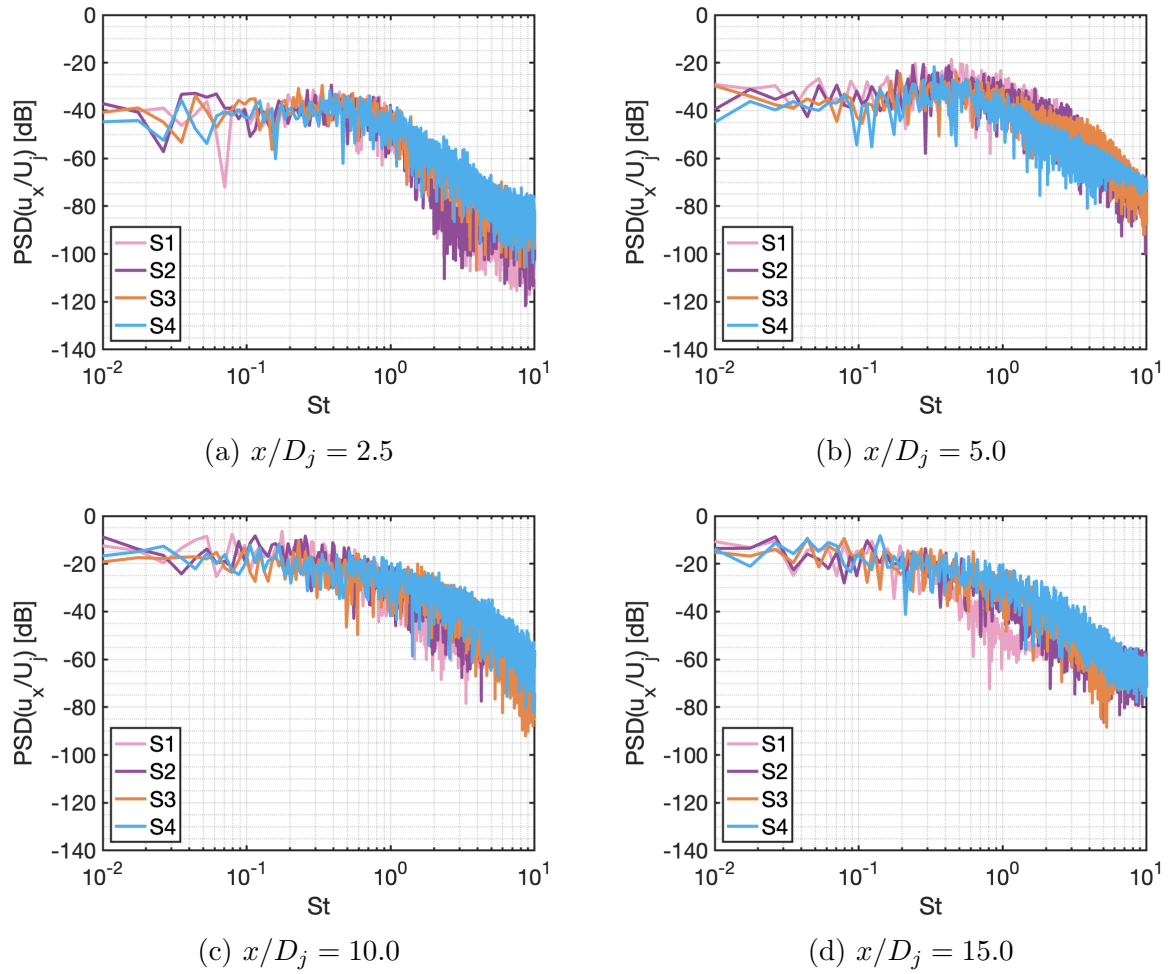


FIGURE 5.12 – Power spectral densities of the longitudinal velocity component fluctuation at four streamwise planes: $x/D_j = 2.5$ (a), $x/D_j = 5.0$ (b), $x/D_j = 10.0$ (c), and $x/D_j = 15.0$ (d). PSDs obtained in the centerline of the jet flow.

5.13b. In the range of the experimental data, all simulations present similar levels of velocity fluctuation, which are in good agreement with experimental data. Once more, it is possible to observe the higher capacity of the S3 and S4 simulations to capture high-frequency data when compared to the data from the S1 and S2 simulations. The results in $x/D_j = 10.0$ and $x/D_j = 15.0$, Figs. 5.13c and 5.13d, present similar information. The numerical simulations agree with experimental data for the smallest frequencies, and the S3 and S4 simulations are able to capture the high frequencies better. One difference that appears is due to the coarsening of the mesh close to $x/D_j = 15.0$, where the S3 and S4 simulations fail to simulate the highest frequencies of eddies present in the flow.

The PSD data from the radial velocity component fluctuation, Figs. 5.14 and 5.15, present some differences when compared to the results from the longitudinal velocity component fluctuations, Figs. 5.12 and 5.13. In the first two positions at the centerline of the jet flow, Figs. 5.14a and 5.14b, low power levels are observed for all frequencies. However, the power levels in the medium frequencies, $St \approx 0.5$, are highlighted. It is also

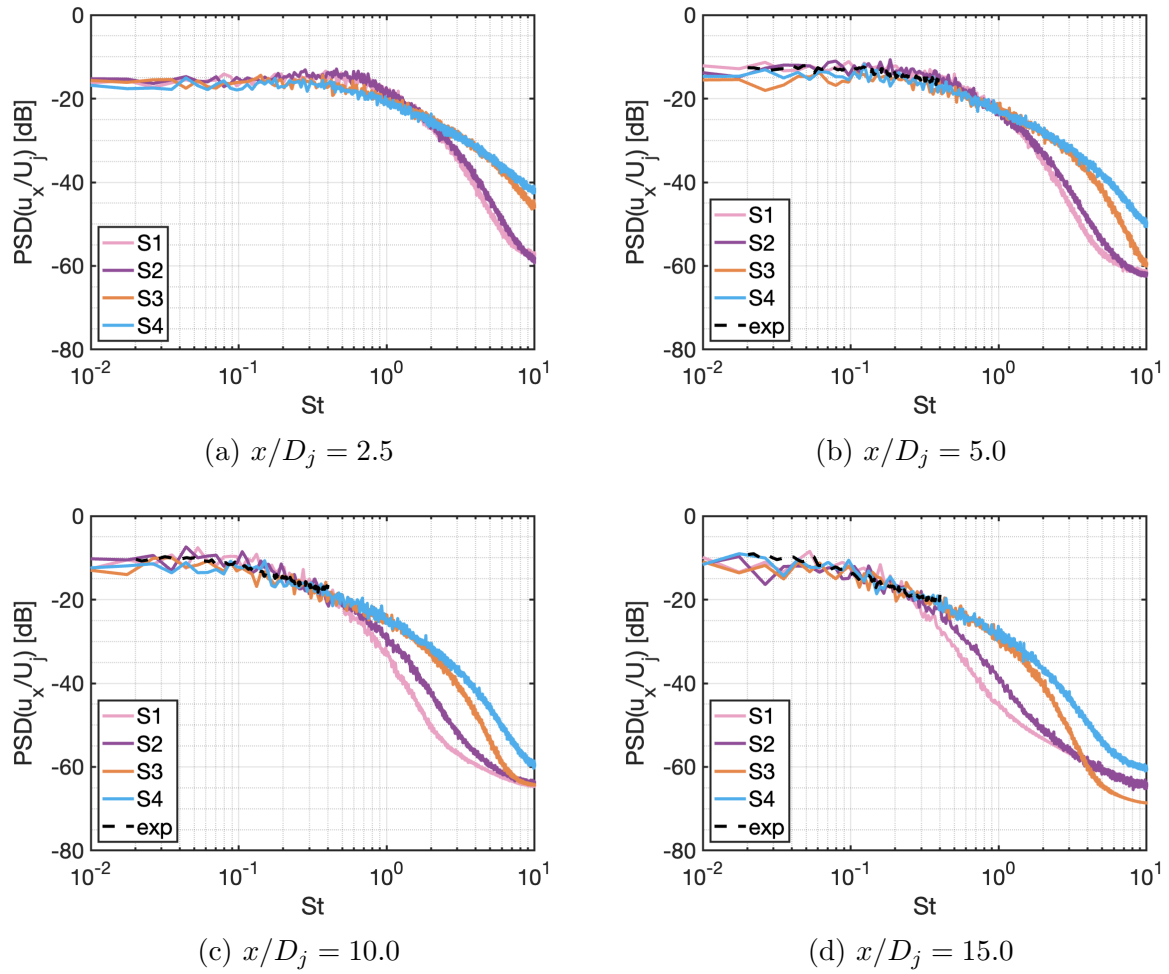


FIGURE 5.13 – Power spectral densities of the longitudinal velocity component fluctuation at four streamwise planes: $x/D_j = 2.5$ (a), $x/D_j = 5.0$ (b), $x/D_j = 10.0$ (c), and $x/D_j = 15.0$ (d). PSDs obtained in the lipline of the jet flow.

possible to observe the overall power growth from Fig. 5.14a to Fig. 5.14b. The power levels from the third station, Fig. 5.14c, indicate similar results for the smallest frequencies and a division in the values for the highest frequencies, with the S3 and S4 simulations being able to present the largest levels. In the last station, Fig. 5.14d, the difficulty of the S1 simulation to reproduce the highest frequencies of eddies is evident. The differences between the S2, S3, and S4 simulations are similar to the third station.

The PSD data from the radial velocity component fluctuation at the lipline, Fig. 5.15, present once more comparison with experimental data. In the first station, Fig. 5.15a, the peak of power level close to $St = 0.5$ is present once more for the S1 and S2 simulations, and the difference in the power levels of the highest frequency is also present. In the second station, Fig. 5.15b, the comparison of the numerical power levels with experimental data indicates that there is a slight difference between the S1 and S2 simulations with S3 and S4 simulations. The PSD values indicate a better agreement between the PSD of the S3 and S4 simulations and the experimental reference. In the third station, Fig.

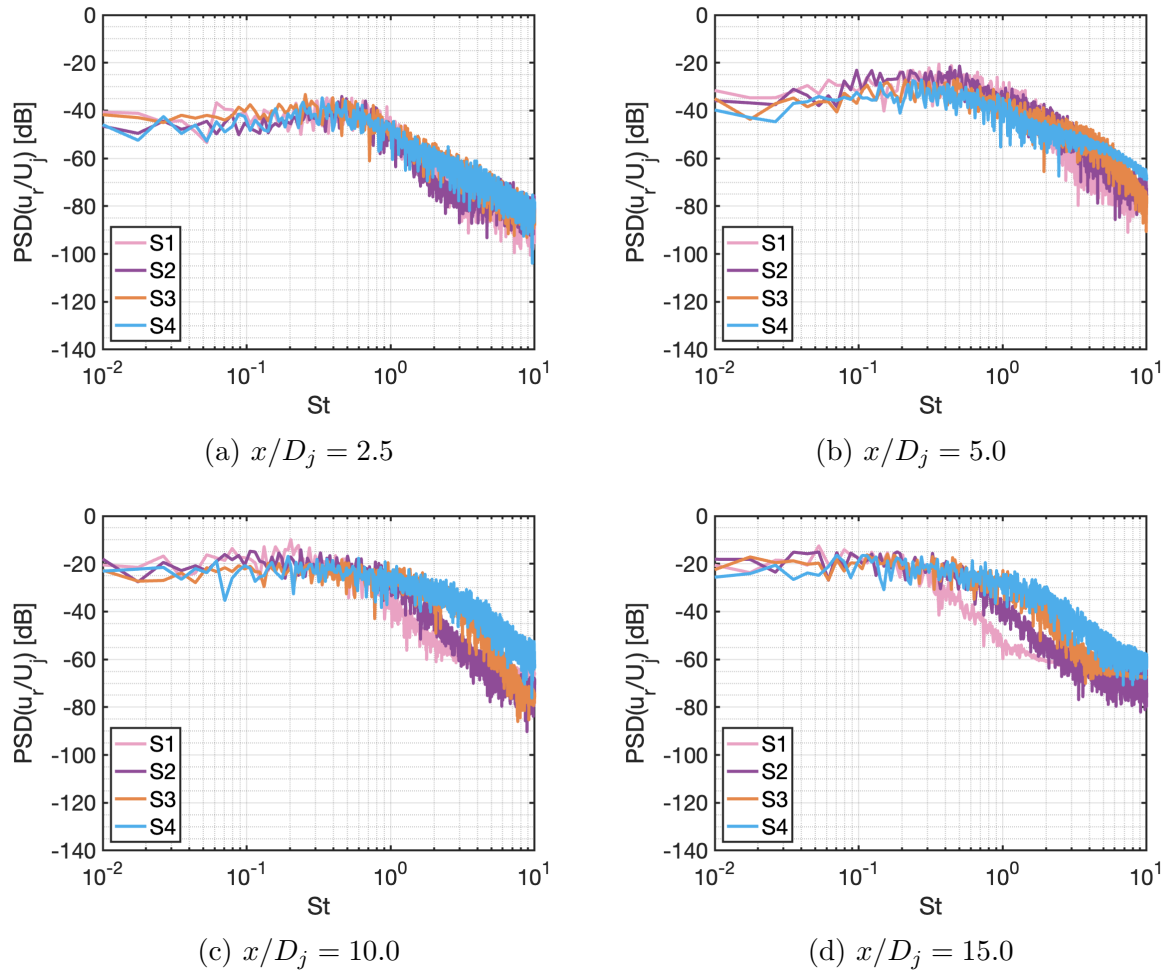


FIGURE 5.14 – Power spectral densities of the radial velocity component fluctuation at four streamwise planes: $x/D_j = 2.5$ (a), $x/D_j = 5.0$ (b), $x/D_j = 10.0$ (c), and $x/D_j = 15.0$ (d). PSDs obtained in the centerline of the jet flow.

5.15c, all the simulations are closer and agree with experimental data for the smallest frequencies. However, for the largest frequencies, there is a significant difference between the simulations. In the last station, Fig. 5.15d, The S1 and S2 simulations fail to capture the highest eddies present in the range of the experimental data. The PSD data from the S3 and S4 simulations show a good agreement with experimental data and a sustain of the power levels with higher frequencies.

The analysis of the “ hp ” requirements for the supersonic jet flow simulation is conducted with four numerical simulations that employ three numerical meshes and two spatial discretization orders of accuracy. The results indicate that the S1 and S2 simulations are under-resolved in a large-eddy simulation perspective. Due to the large mesh size, the simulations cannot capture the smallest eddies that affect the flow field. For this reason, they present a set of differences with experimental data: shorter jet potential core length, the postponed development of the mixing layer, larger radial velocity spreading, and difficulty in capturing the highest frequencies eddies. The employment of the

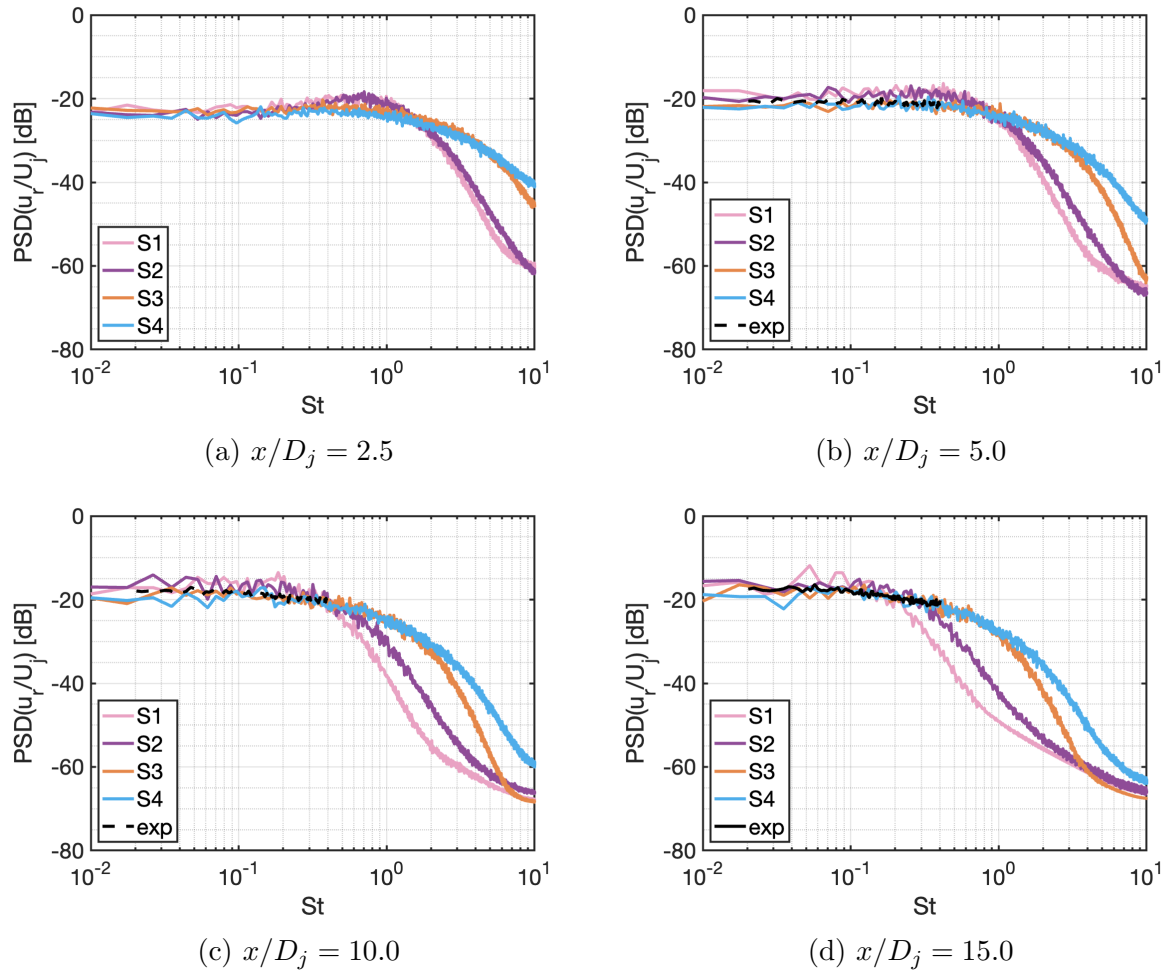


FIGURE 5.15 – Power spectral densities of the radial velocity component fluctuation at four streamwise planes: $x/D_j = 2.5$ (a), $x/D_j = 5.0$ (b), $x/D_j = 10.0$ (c), and $x/D_j = 15.0$ (d). PSDs obtained in the lipline of the jet flow.

M3 mesh in the S3 and S4 simulations produced significant improvements to the jet flow simulations, which were visible in all the properties investigated. The increment in the spatial order of accuracy from second-order to third-order produced additional improvements that led to the error of the potential core of the jet reaching a value of 3.4%. The benefits are also visible in other properties investigated. It is possible to continue refining the computational mesh or increasing the spatial order of accuracy to improve the results even more. However, in the context of scale resolving flows, the LES “ hp ” convergence leads to a DNS. The focus of an LES simulation is to effectively simulate around 80% of the energy spectrum [9], which, according to the numerical data presented, is close to the obtained with the largest resolution simulation performed. Due to the overall best agreement with the experimental data obtained and the highest capacity to reproduce small eddies present in the flow field, essential for capturing the flow field characteristics in a large-eddy simulation perspective, the S4 simulation is selected as the base for the inflow condition studies.

5.2 Nozzle Design using a RANS Formulation

The nozzle design is the process responsible for determining the nozzle geometry. According to the experimental reference [6], the nozzle geometry employed in the tests presents a convergent-divergent shape, and the nozzle was designed through the method of characteristics. The method of characteristics applies the isentropic relations of the shock waves to determine the nozzle geometry that optimizes the flow. The optimization technique based on the method of characteristics presents limited flexibility in the design of the nozzle geometry. For a specified Mach number and nozzle exit diameter, the nozzle length is an output of the method, as well as the shape of the nozzle walls. Even though the nozzle from the experiments was designed with the same methods of characteristics, the characteristics of the flow leaving the nozzle were not specified. Due to the installation upstream of the nozzle geometry, the flow leaving the nozzle can significantly vary.

The objective of this part of the work is to investigate the influence of the inflow condition on the development of the supersonic jet flows. The fulfillment of the objective is reached by the investigation of three inflow profiles to represent the nozzle-exit condition. The inviscid profile employed in previous analyses is compared to a viscous profile. The viscous profile is obtained by using a largely employed methodology from subsonic jet flow simulations, where a constant diameter pipe is employed as the nozzle geometry [14, 24]. The methodology modified for supersonic nozzle flows represents the nozzle geometry by a divergent shape with a small opening angle. The experimental work of Bridges and Wernet [6] presents no information regarding the boundary layer thickness. In the present work, a value of $0.05D_j$ could influence the jet flow field, and it is the target for the development of the jet flow.

The nozzle design is an iterative process employed to determine the nozzle dimensions and the inflow condition in the nozzle inlet section. The process begins with determining an initial nozzle geometry and the nozzle inflow condition. The nozzle inflow condition is an inviscid profile with specified velocities, pressure, and temperature. All the properties are specified since it is a supersonic inflow boundary. Two initial geometries are evaluated with nozzle length $l_{noz} = 1.0D_j$ and $1.5D_j$. The two nozzles have the inlet diameter $D_{noz} = 0.9651D_j$. The jet inlet condition is calculated using the isentropic relations. The simulation for the nozzle with a short length is called *cfg1*, and the simulation with the long nozzle is called *cfg2*. The term *cfg* is an abbreviation of configuration. Fig. 5.16a presents the Mach number distribution at the nozzle centerline. The Mach number distributions show that, due to the presence of shock waves in the interior of the nozzle represented by the velocity decay after local peak values close to $x/D_j = -0.6$ and $x/D_j = -1.1$, for *cfg1* and *cfg2*, respectively, the isentropic relations are not adequate for the predictions of the inlet condition of the jet flow. The nozzle exit flow could not reach

the ambient pressure in the outlet condition, and therefore, the velocity value obtained is smaller than the one obtained in the experiments, $M = 1.4$. The increase in the nozzle exit velocity is obtained by increasing the inlet velocity. The constraint adopted to increase the Mach number at the nozzle inlet section is to keep the same total pressure of the exit section. The simulation for the short nozzle with the second inflow predicted is called *cfg3* and the long nozzle *cfg4*. The Mach number distributions for the four nozzle geometries are presented in Fig. 5.16a. The nozzle velocity in the exit section increased, getting close to the specified condition. The higher velocity at the nozzle-exit section shows that the total pressure is a better reference for the predictions of the inlet condition.

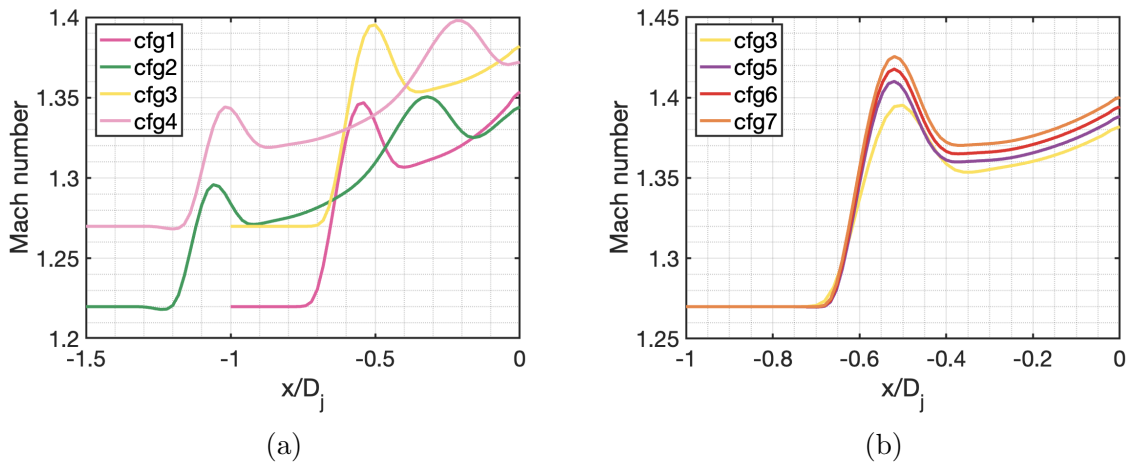


FIGURE 5.16 – Mach number profiles along the centerline of the nozzle for the preliminary nozzle geometries analyzed. (a) Comparison of two nozzle lengths and inlet conditions. (b) Comparison of four nozzle inlet diameters.

The second investigation performed in the nozzle design assesses the influence of the nozzle inlet diameter. Because the outlet diameter is fixed to the jet inlet, the change in the inlet diameter modifies the nozzle opening angle for a fixed nozzle length. The test was performed using the *cfg3* as a reference, and the nozzle inlet diameter is reduced to $D_{noz} = 0.9633D_j$, $0.9616D_j$ and $0.9599D_j$. The simulations are named *cfg5*, *cfg6*, and *cfg7*. Figure 5.16b presents the Mach number distributions at the nozzle centerline. The Mach number distribution at the centerline of the nozzle shows that the increase in the nozzle angle increases the exit velocity. However, as a side effect of this change, strong shock waves appear in the nozzle, which would produce larger values of pressure distortion when compared to the pressure values from the short nozzles in the exit section. The pressure distortion is associated with the amplitude of the pressure distribution at the nozzle exit section. A flow with high distortion would produce a large amplitude in the pressure distribution. The flow with little distortion present and almost constant pressure distribution. The amplitude of the Mach number change in the shock position can be employed to identify the shock wave intensity. Since one requisite defined for the nozzle design is to produce minimum levels of velocity increment, the analysis of the nozzle

opening angle indicates that keeping the nozzle opening angle small is one alternative to comply with the requirements.

The influence of employing a nozzle geometry with curved walls is evaluated. Two curved wall nozzle geometries are designed with nozzle length $l_{noz} = 1.0D_j$ and $1.5D_j$, nozzle inlet diameter $D_{noz} = 0.9651D_j$, and the radius of the circular segments are $r_{wall} \approx 28.65$ and $r_{wall} \approx 59.06$. Due to the choice of inlet conditions, the curved wall geometry simulations are compared with *cfg3* and *cfg4*. The curved walls simulations are called *cfg8* with $l_{noz} = 1.0D_j$ and *cfg9* for the $l_{noz} = 1.5D_j$. The Mach number distributions along the jet centerline are presented in Fig. 5.17a and the boundary layer profiles at the nozzle exit section are presented in Fig. 5.17b. The Mach number distribution along the nozzle centerline shows that the velocity distribution presents small velocity amplitudes for the short nozzles. It can also be observed that only one shock wave appears at the beginning of the nozzle. After the position of the shock wave, a monotonic velocity increment is observed. The straight nozzle does not present the same behavior. The first shock wave appears in a position farther from the nozzle inlet section when compared to the position of the shock wave from the curved wall nozzle. The straight walls also present a second shock wave close to the nozzle exit section. The Mach number distribution from the long nozzles indicates the opposite behavior. The curved wall nozzle presented a strong shock wave close to the inlet section, which is identified by the large velocity amplitude close to $x/D_j = -1.2$, and the velocity increment also had a large slope. The straight long nozzle presented two weak shock waves. In general, the straight wall nozzles presented velocity distributions with smaller velocity amplitudes, which are associated with a more uniform flow distribution when compared to the curved walls that presented large velocity amplitudes. The boundary layer profiles, presented in Fig. 5.17b, show that the shorter nozzle produced boundary layers with approximately $0.02D_j$ thickness, and the simulations with a longer nozzle produced boundary layers with approximately $0.025D_j$ thickness. The two boundary layers obtained do not present the expected thickness of $0.05D_j$.

The curved wall study indicates that the boundary layer thickness at the outlet section of the nozzle was not large enough to comply with the requisites. For this reason, it is necessary to increase the nozzle length. The nozzle design evaluates geometries with a nozzle length $l_{noz} = 3.0D_j$. Once a new length is selected, it is necessary to analyze the nozzle angle again. The baseline nozzle inlet diameter considered is $D_{noz} = 0.9633D_j$. The simulation from the baseline nozzle is named *cfg10*. From the baseline, four other nozzle inlet diameters are created. Two had smaller inlet diameters, and two had larger inlet diameters. The four simulations, with nozzle inlet diameter $D_{noz} = 0.9686D_j$, $0.9738D_j$, $0.9581D_j$ and $0.9529D_j$ are named *cfg11*, *cfg12*, *cfg13*, and *cfg14*. The Mach number distributions at the nozzle centerline are presented in Fig. 5.18a, and the boundary layer

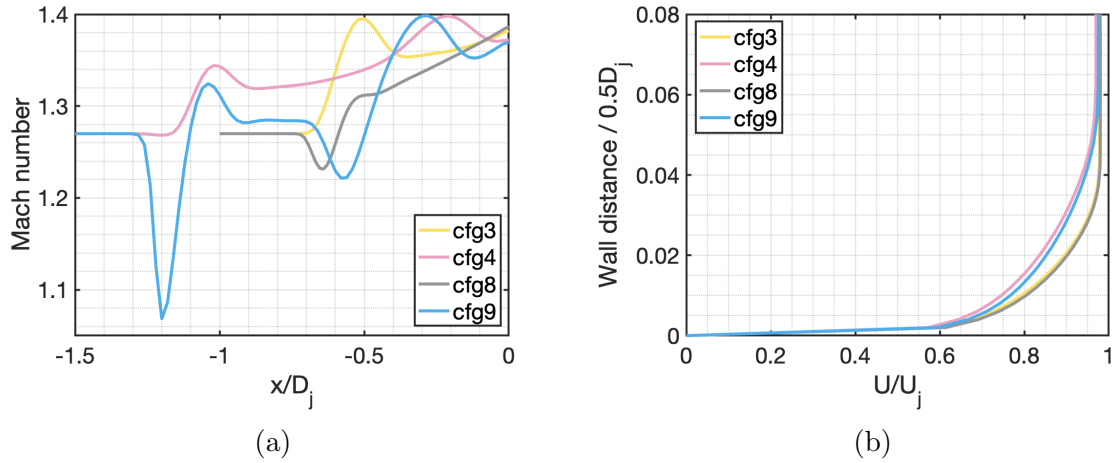


FIGURE 5.17 – Comparison of the simulations with straight walls and curved walls. (a) Mach number distribution along nozzle centerline. (b) Comparison of boundary layer profile in the nozzle exit section.

profiles at the nozzle outlet section are presented in Fig. 5.18b. The inlet velocity is calculated using the isentropic relations to ensure that all nozzles present some equity for comparison. Using the isentropic relations allowed the nozzles to provide a similar velocity at the outlet section. The velocity distribution agrees well with previous data on different nozzle angles, in which larger angles are responsible for larger velocity increments in the nozzle. Because it is desired to have the minimum impact on nozzle expansion, the Mach number distribution from *cfg12* indicates that this geometry should be used. However, it was observed that the first shock wave from *cfg11* was smaller than those of *cfg12* and that the velocity difference was small, so it was decided to conclude the nozzle design by selecting the nozzle geometry employed in *cfg11* that has the nozzle length $l_{noz} = 3.0D_j$ and nozzle inlet diameter $D_{noz} = 0.9686D_j$. The analysis of the nozzle boundary layer profile at the nozzle-exit section, Fig. 5.18b, shows that the boundary layer thickness increased, reaching values close to $0.05D_j$ and complying with the requisites.

The Mach number distribution presented in Fig. 5.18a shows that the nozzle exit Mach number did not reach the required value of 1.4, which indicates the necessity to adjust the inlet boundary condition. The adjustment is performed by changing the nozzle inlet velocity, keeping the same total pressure of the nozzle outlet section. After some iterations, it was observed that by adjusting the nozzle length from $l_{noz} = 3.0D_j$ to $2.75D_j$, the static pressure distribution at the outlet section could reach a more uniform distribution than considering the total nozzle length of $l_{noz} = 3.0D_j$. For this reason, the nozzle length was changed to $l_{noz} = 2.75D_j$. After completing the adjustment process, the final velocity profiles are presented in Figs. 5.19a and 5.19b. The final nozzle design is called *cfg15*. In Fig. 5.19a, the Mach number distribution at the centerline is presented, and in Fig. 5.19b, the boundary layer profile is presented. It is possible to observe from the development

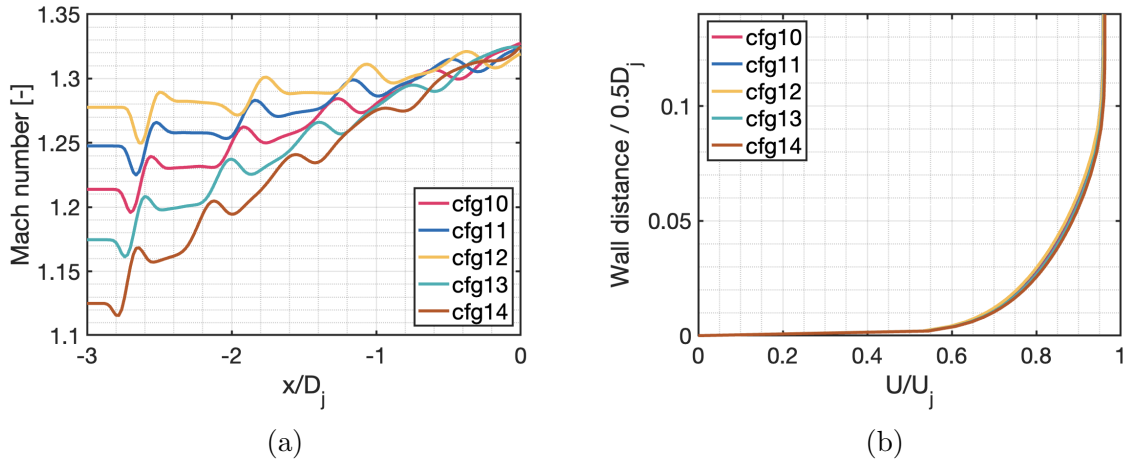


FIGURE 5.18 – Comparison of the simulations with longer nozzle length and five inlet diameters. (a) Mach number distribution along nozzle centerline. (b) Comparison of boundary layer profile in the nozzle exit section.

of the velocity in the center of the nozzle that the target is reached, which means the velocity at the centerline is the same as in the experimental tests. The analysis of the boundary layer profile indicates a few impacts of the reduction of the nozzle length to the boundary layer thickness. The radial Mach number and pressure distributions at the nozzle exit section are also presented in Figs. 5.20a and 5.20b.

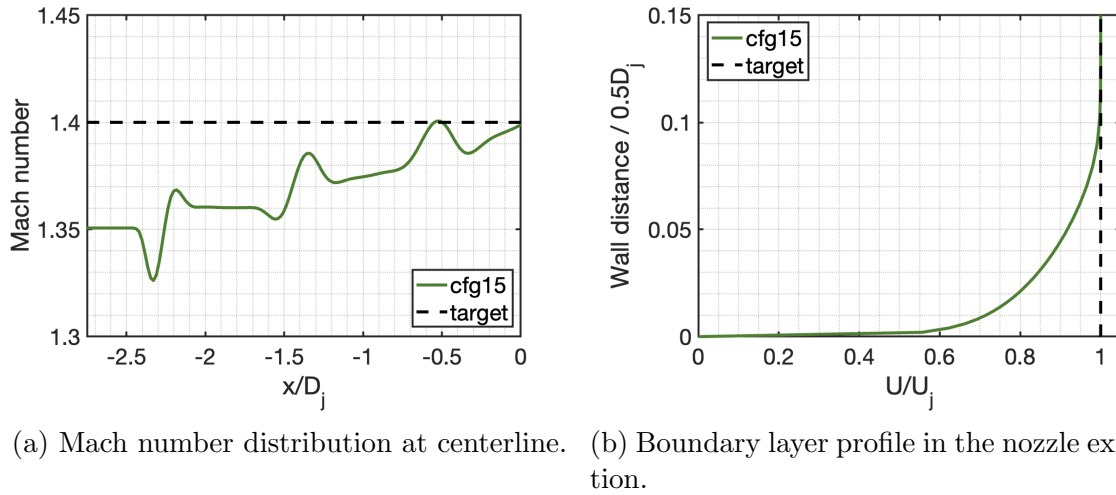


FIGURE 5.19 – Data from the final nozzle design, *cfg15*, with adjusted inlet condition.

The level of velocity and pressure uniformity are investigated in the two figures. The velocity contours, represented by the Mach number, and the pressure contours are presented in Figs. 5.21 and 5.22. The Mach number contours, Fig. 5.21, show the series of shocks and the uniform velocity growth. A few distortions can be observed in the velocity contours. The pressure contours, Fig. 5.22, show similar behavior to the velocity contours, with a progressive reduction in the static pressure and a uniform distribution in the outlet

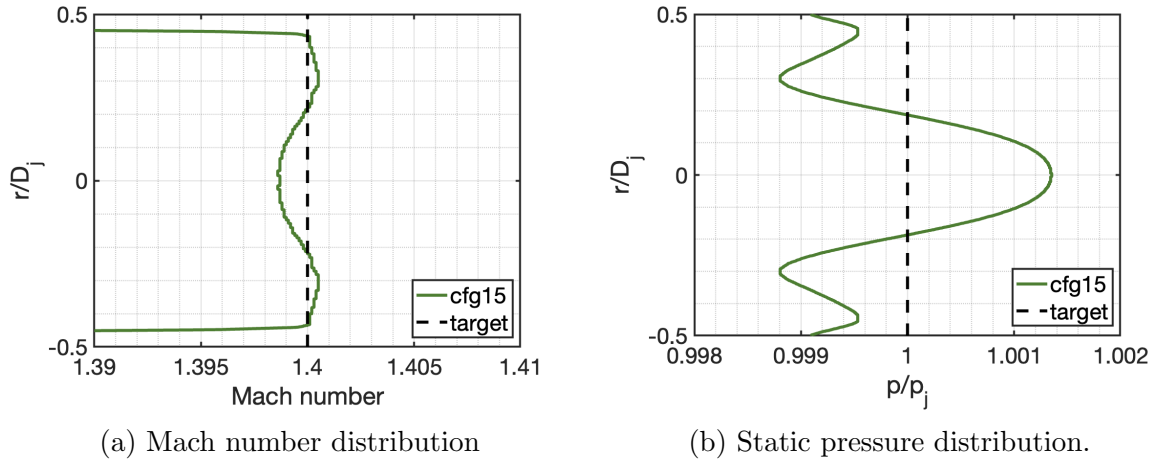


FIGURE 5.20 – Data from the final nozzle design, *cfg15*, with adjusted inlet condition, at the outlet section.

section. The nozzle design is concluded. The outlet radial profiles from the five primitive variables, density, three velocity components, and pressure, are organized into tables to be applied to the inlet condition for the LES of the jet flow. The radial distribution of the primitive variables is presented in Table. 5.2.

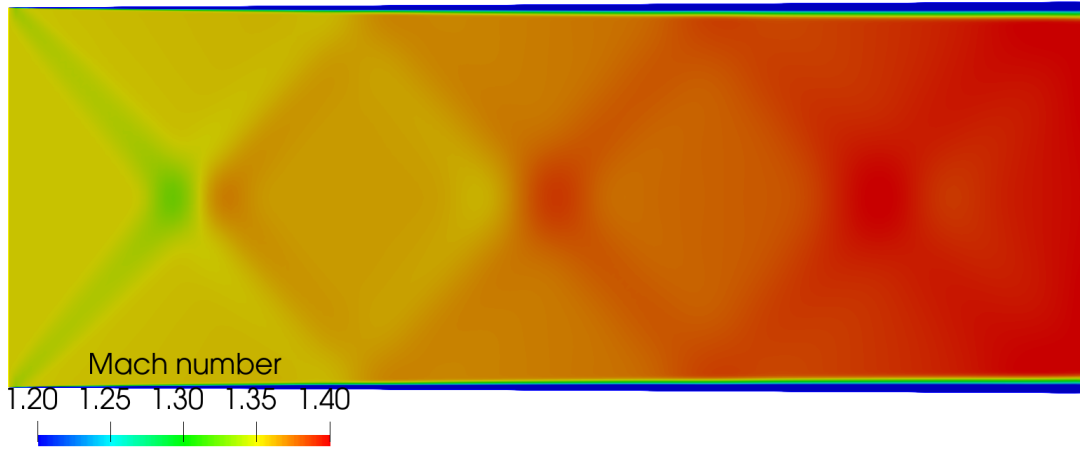


FIGURE 5.21 – Mach number contours for the final nozzle design, *cfg15*.

TABLE 5.2 – Mean profiles obtained from the nozzle RANS simulations for defining the inflow conditions for the free jet flow calculations.

r/D_j	ρ/ρ_j	p/p_j	U/U_j	V/U_j
0.000000	0.743957	0.999097	0.000000	0.000000
0.000030	0.744316	0.999097	0.048308	0.000253
0.000065	0.745532	0.999097	0.101493	0.000532
0.000102	0.747925	0.999097	0.161258	0.000846

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TABLE 5.2 – Mean profiles obtained from the nozzle RANS simulations for defining the inflow conditions for the free jet flow calculations (cont.).

r/D_j	ρ/ρ_j	p/p_j	U/U_j	V/U_j
0.000148	0.751824	0.999097	0.226523	0.001188
0.000197	0.757307	0.999097	0.293251	0.001537
0.000254	0.763859	0.999097	0.354457	0.001857
0.000317	0.770489	0.999097	0.404356	0.002118
0.000390	0.776440	0.999097	0.442302	0.002316
0.000472	0.781560	0.999097	0.471268	0.002467
0.000567	0.786031	0.999097	0.494470	0.002587
0.000673	0.790077	0.999097	0.514140	0.002689
0.000795	0.793875	0.999097	0.531634	0.002779
0.000933	0.797540	0.999097	0.547756	0.002861
0.001089	0.801150	0.999098	0.562987	0.002938
0.001266	0.804756	0.999098	0.577629	0.003011
0.001467	0.808394	0.999099	0.591868	0.003081
0.001695	0.812091	0.999100	0.605834	0.003148
0.001953	0.815867	0.999101	0.619619	0.003213
0.002248	0.819740	0.999103	0.633295	0.003276
0.002583	0.823729	0.999105	0.646918	0.003337
0.002961	0.827850	0.999108	0.660540	0.003395
0.003392	0.832122	0.999111	0.674204	0.003451
0.003880	0.836563	0.999115	0.687954	0.003505
0.004435	0.841197	0.999120	0.701830	0.003555
0.005063	0.846044	0.999126	0.715874	0.003603
0.005778	0.851135	0.999133	0.730127	0.003647
0.006589	0.856499	0.999142	0.744631	0.003688
0.007510	0.862164	0.999153	0.759426	0.003724
0.008555	0.868169	0.999165	0.774556	0.003755
0.009742	0.874557	0.999176	0.790060	0.003780
0.011091	0.881380	0.999189	0.805980	0.003800
0.012620	0.888688	0.999208	0.822346	0.003812
0.014356	0.896550	0.999234	0.839194	0.003815
0.016327	0.905008	0.999263	0.856536	0.003807
0.018563	0.914123	0.999287	0.874358	0.003785
0.021104	0.923952	0.999315	0.892613	0.003747
0.023986	0.934540	0.999351	0.911186	0.003689
0.027260	0.945843	0.999389	0.929850	0.003611

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TABLE 5.2 – Mean profiles obtained from the nozzle RANS simulations for defining the inflow conditions for the free jet flow calculations (cont.).

r/D_j	ρ/ρ_j	p/p_j	U/U_j	V/U_j
0.030976	0.957734	0.999430	0.948205	0.003510
0.035195	0.969889	0.999472	0.965567	0.003391
0.039982	0.981542	0.999512	0.980793	0.003269
0.045419	0.991184	0.999538	0.992112	0.003177
0.051589	0.996925	0.999536	0.998058	0.003161
0.058594	0.998910	0.999535	0.999823	0.003226
0.066547	0.999225	0.999526	1.000046	0.003341
0.075575	0.999199	0.999491	1.000048	0.003474
0.085823	0.999148	0.999437	1.000062	0.003614
0.097457	0.999106	0.999373	1.000081	0.003750
0.110663	0.999054	0.999296	1.000119	0.003862
0.125656	0.998986	0.999198	1.000158	0.003930
0.141878	0.998893	0.999092	1.000189	0.003946
0.158211	0.998816	0.998980	1.000214	0.003905
0.174650	0.998739	0.998873	1.000249	0.003806
0.191185	0.998688	0.998807	1.000285	0.003659
0.207817	0.998705	0.998808	1.000295	0.003472
0.224537	0.998714	0.998883	1.000208	0.003254
0.241344	0.998782	0.999019	1.000123	0.003012
0.258228	0.998969	0.999205	1.000119	0.002756
0.275187	0.999148	0.999428	1.000073	0.002498
0.292215	0.999302	0.999676	0.999948	0.002244
0.309307	0.999514	0.999937	0.999879	0.002000
0.326457	0.999702	1.000195	0.999794	0.001768
0.343660	0.999872	1.000439	0.999653	0.001549
0.360912	1.000026	1.000659	0.999626	0.001344
0.378206	1.000153	1.000848	0.999553	0.001152
0.395537	1.000256	1.001003	0.999430	0.000971
0.412901	1.000341	1.001124	0.999428	0.000799
0.430292	1.000392	1.001215	0.999383	0.000632
0.447703	1.000434	1.001279	0.999353	0.000471
0.465131	1.000460	1.001319	0.999331	0.000312
0.482570	1.000469	1.001342	0.999318	0.000155
0.500000	1.000511	1.001349	0.999372	0.000000

FIGURE 5.22 – Pressure contours for the final nozzle design, *cfg15*.

5.3 Influence of the Inflow Condition on the Development of Jet Flows

5.3.1 Inflow Condition Options for the Jet Flow Simulations

The influence of the inflow condition on the development of the Mach number 1.4 perfectly expanded supersonic jet flow is assessed with the numerical setup from the S4 simulation. The numerical setup uses the M3 mesh with a quadratic polynomial degree. The S4 simulation is the numerical reference for the inflow condition analysis since it employs the most straightforward inflow condition with constant properties independent of the radial and azimuthal position, which is called the “inviscid profile” in the work. The first alternative to the inviscid profile is the imposition of a mean radial profile obtained from the RANS simulation of the divergent section of a supersonic nozzle flow, designed to provide low-pressure distortion and a thick boundary layer, which is called steady viscous profile in the continuity of the work. The radial data of the mean radial profile is given in Tab. 5.2. The choice of the steady viscous profile is based on a cost-saving simulation due to the high computational costs of an LES nozzle flow simulation. In most applications of the nozzle geometries in the LES simulations of supersonic jet flows [13, 28, 31], the nozzle flow could not develop to the expected flow condition at the nozzle outlet section due to the coarse mesh employment. The under-resolved simulations do not produce turbulent flow at the nozzle outlet section. The development of the RANS simulation of the nozzle flow ensures that the mean flow leaving the nozzle has a turbulent profile, which is the focus of the second alternative. The third inflow option is the superimposition of a tripping method to the mean RANS profile, which is referred to by unsteady viscous profile. In the classical approach [14, 23], the tripping is imposed into a region inside the

nozzle geometry, and there is a development length for the flow to evolve to the expected condition. In the approach used in this work, the tripping method is imposed in the jet inflow boundary condition. The comparison of the inflow characteristics of the three options employed in this work is presented in Fig. 5.23. In the case of the unsteady viscous profile, presented in blue in Fig. 5.23, are snapshots that exemplify what can be obtained in the simulations. The gray lines indicate the range in which the velocity values can vary through the employment of the tripping method. In Fig. 5.23, the Figs. 5.23c and 5.23e present the longitudinal and radial velocity profiles for the complete length from the wall to the center of the inlet section and Figs. 5.23d and 5.23f present a detailed chart from the boundary layer.

5.3.2 Instantaneous Flow Field

The instantaneous longitudinal velocity component contours from the S4, S5, and S6 simulations are presented in Fig. 5.24. The velocity contours from the S4 simulation are the same as presented in Fig. 5.3d. It is presented once more to make it easier the comparison of the three numerical contours. Few differences can be observed between the velocity contours. The velocity gradient from the boundary layer imposed by the inflow condition is observed from the S5 and S6 velocity contours, where none is observed in the S4 contours. The first eddies in the mixing layer appear close to the jet inlet section in Figs. 5.24b and 5.24c. The quality of the visualization of the eddies from the S5 and S6 simulations is at the same level as those from the S4 simulation.

The instantaneous pressure field contours with the vorticity magnitude contours are presented in Fig. 5.25. The contours from the S5, Fig. 5.25b, and S6 simulations, 5.25c, are compared with the contours from the S4 simulation, Fig. 5.4d, which is reintroduced in Fig. 5.25. The pressure contours highlight the difference between the shock waves of the simulations. In the S4 simulation, a strong shock appears in the early development of the jet flow. The shock wave is identified by a thin white contour region at the centerline in Fig. 5.25a. The pressure flow field from the S5 and the S6 simulations do not present the shock wave in the same position as the S4 simulation. The shock waves are weaker in the contours from the S5 and S6 simulations compared to the contours of the S4 simulation. In the S5 and S6 simulation contours, the shock waves are represented by a light gray contour instead of the white contour from the S4 simulation. The vorticity magnitude contours present a thicker region close to the jet inlet section from the S5 and S6 simulations than the S4 simulation. The thick vorticity region is associated with the thick boundary layer entering the flow. It can also be observed the presence of small structures of the flow close to the jet inlet section in Figs. 5.25b and 5.25c than in Fig. 5.25a.

Due to the steady and unsteady viscous profiles employed in the S5 and S6 numerical

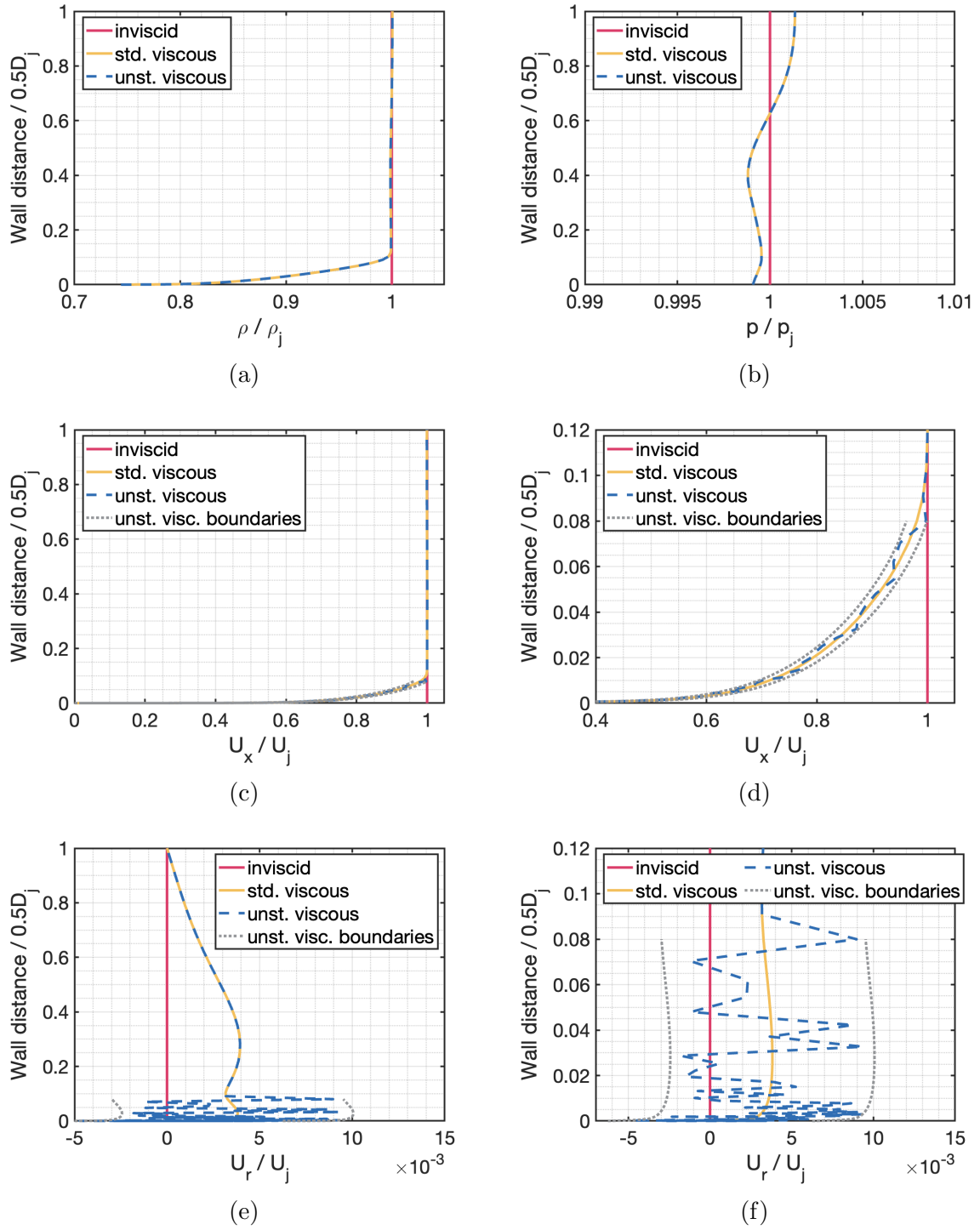
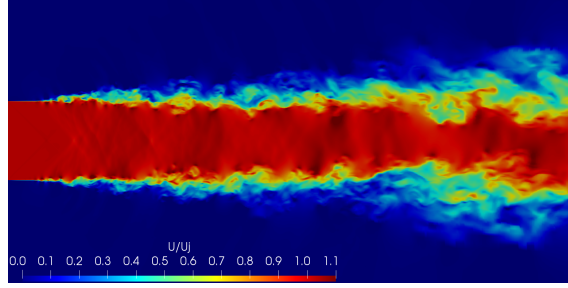
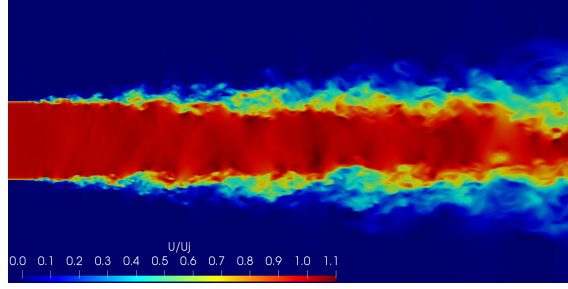


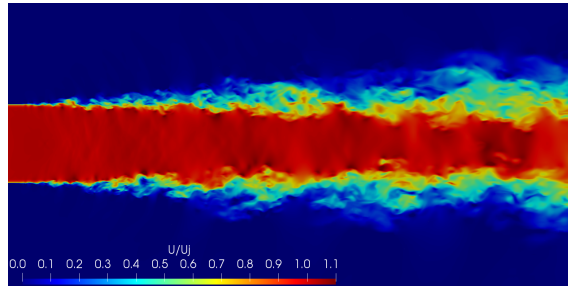
FIGURE 5.23 – Inlet flow profiles from the three boundary conditions investigated in the work. The density (a) and pressure (b) radial profiles are presented on top. The complete radial profile of the axial velocity component (c) and a detail of the boundary layer (d) are presented in the middle. The complete radial profile of the radial velocity component (e) and a detail of the boundary layer (f) are presented on bottom.



(a) S4 simulation.



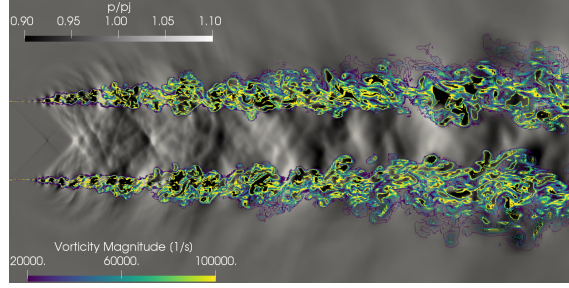
(b) S5 simulation.



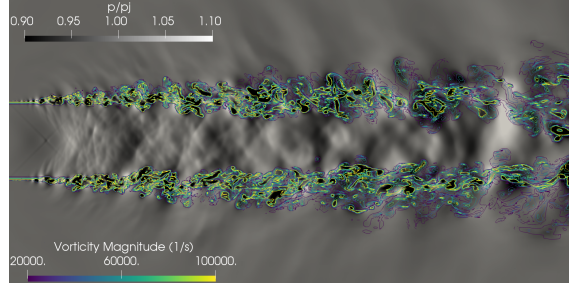
(c) S6 simulation.

FIGURE 5.24 – Instantaneous longitudinal velocity component contours on a plane through the centerline of the jet.

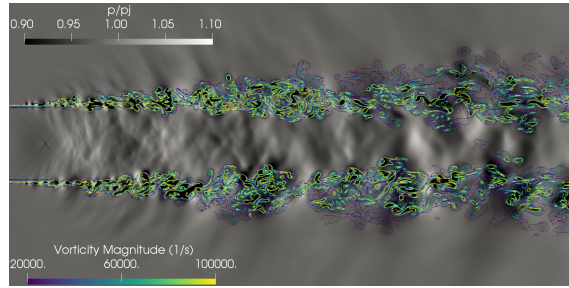
simulations, the numerical method presented instabilities that affected the highly-resolved simulations. The thresholds of the shock indicator were adjusted from the values employed in the S4 simulation. It was necessary to reduce the thresholds, Tab. 4.5, which resulted in a large amount of elements solved with the FV approach. An instantaneous snapshot presenting the distribution of the DG and FV cells is presented in Fig. 5.26 for the S5 and S6 simulations with the snapshots from the S4 simulation, previously presented in Fig. 5.5d. In the same way, presented in the previous visualization, the gray-contoured elements are solved with the DG approach, and the red-contoured elements are solved with the FV approach. Even though many cells are solved with the FV approach, no significant difference is observed among the three numerical calculations.



(a) S4 simulation.



(b) S5 simulation.

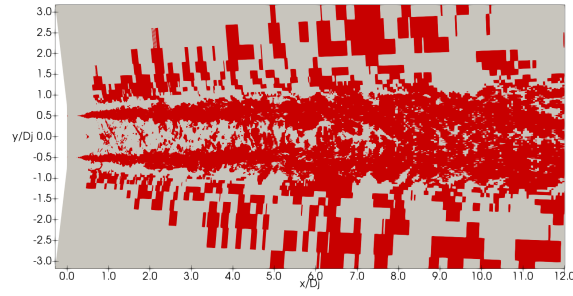


(c) S6 simulation.

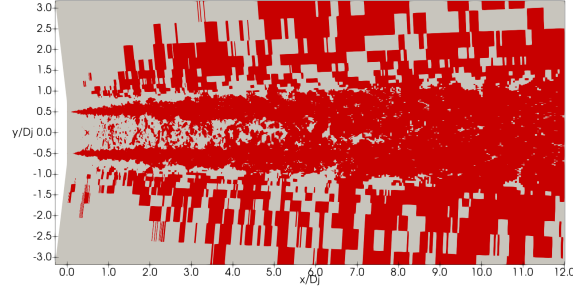
FIGURE 5.25 – Instantaneous pressure contours with contours of vorticity magnitude on a plane through the centerline of the jet.

5.3.3 Mean Flow Field

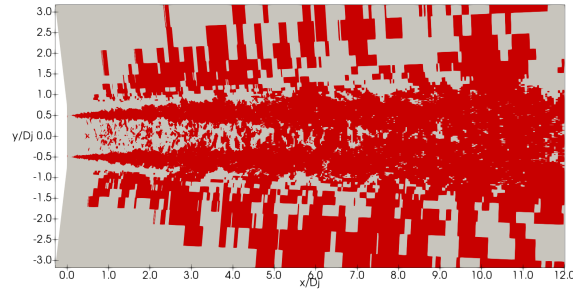
The comparison of the mean longitudinal velocity component contours from the S5 and S6 simulations with the S4 simulation, Fig. 5.27, present the same differences between the simulations observed from the instantaneous longitudinal velocity component contours comparisons, Figs. 5.24. The velocity contours from the S4 simulation are the same from Fig. 5.6d. The local velocity effect associated with the boundary layer from the S5 and S6 simulations inflow condition is present, and the mixing layer occurs closer to the jet inlet section. Figure 5.28 presents the RMS values of the longitudinal velocity fluctuation contours from the S5 and S6 simulations. The velocity fluctuation comparison with those from the S4 simulation, Fig. 5.28b, highlights the early mixing layer from the simulations with the mean RANS profile, the S5 and S6 simulations. They also present smaller values in the region of high-velocity fluctuation, which indicates a reduction in the peak velocity fluctuations produced by the simulation with the inviscid profile. The velocity contours



(a) S4 simulation.



(b) S5 simulation.

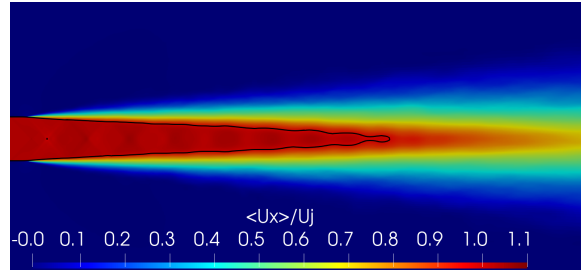


(c) S6 simulation.

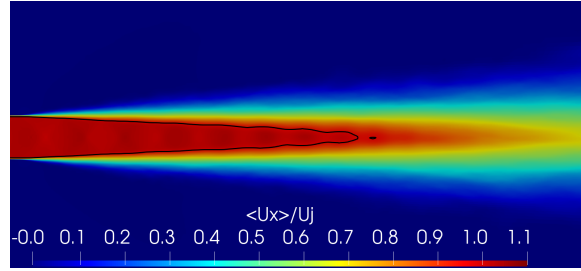
FIGURE 5.26 – Instantaneous identification of DG and FV elements on a plane through the centerline of the jet. Gray contour represents DG elements and red contour represents FV elements.

from the S5 and S6 simulations present negligible differences.

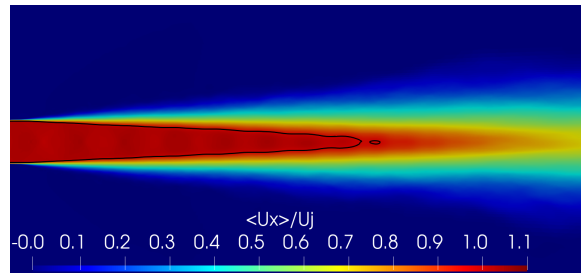
The mean pressure contours from the S5 and S6 simulations, Fig. 5.29 highlights the differences between the simulations with the viscous profile and the simulation with the inviscid profile observed in the instantaneous pressure flow field, Figs. 5.25. The first shock wave does not present the same intensity as those from the S4 simulation, which is indicated by lighter dark contours in the S5 and S6 pressure contours. Another aspect observed is that the region with darker pressure contours is thicker in the S5 and S6 simulations, indicating that the shock wave has a large displacement compared to the shock wave from the S4 simulation. Besides these differences in the first shock waves, no significant difference is observed in other regions of the flow field.



(a) S4 simulation.



(b) S5 simulation.

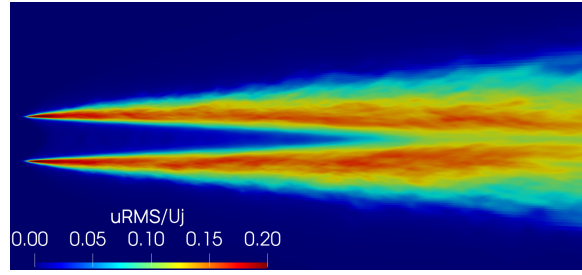


(c) S6 simulation.

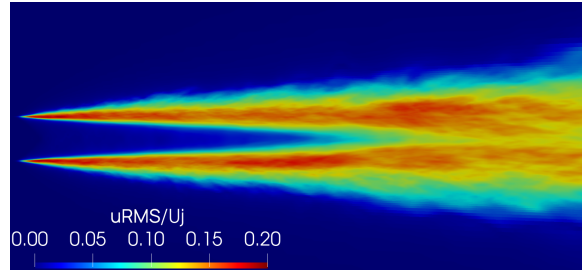
FIGURE 5.27 – Mean longitudinal velocity component contours on a plane through the centerline of the jet. The black contour indicate the boundaries of the jet potential core, $U = 0.95U_j$.

5.3.4 Longitudinal Distributions of the Longitudinal Velocity Component

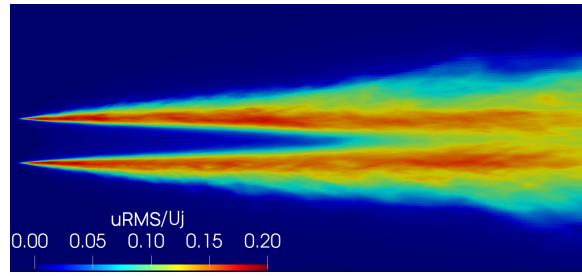
The mean longitudinal velocity component distributions and RMS values of the longitudinal velocity component fluctuation, radial velocity component fluctuation, and tangential velocity component fluctuation distributions, and the mean Reynolds shear stress tensor component distribution at the centerline of the jet flow are presented in Fig. 5.30. The mean longitudinal velocity component distributions at the jet centerline, Fig. 5.30a, indicate a similar behavior using the three inflow conditions up to $x/D_j = 7.0$. One slight difference observed in that region is the smaller velocity amplitudes associated with the shock waves from the S5 and S6 simulations compared to the S4 simulation. For distances larger than $x/D_j > 7.0$, lower velocity levels are observed from the simulations that employ the viscous inflow profile. A slightly longer potential core is observed from the S4 simulation, which employs the inviscid profile compared to the other two simulations.



(a) S4 simulation.



(b) S5 simulation.



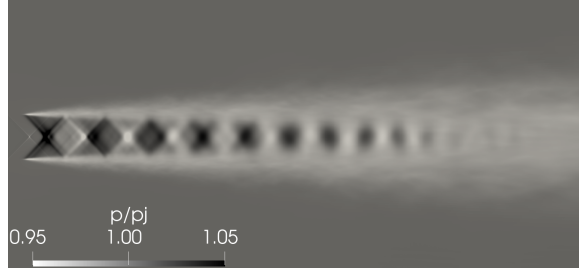
(c) S6 simulation.

FIGURE 5.28 – RMS values of the longitudinal velocity fluctuation contours on a plane through the centerline of the jet.

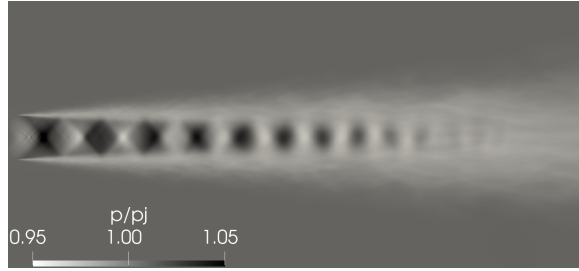
When comparing the S5 and S6 simulations, it is observed that the superimposition of the tripping method to the viscous profile could produce a longer potential core. However, not long enough to produce the same length as those from the S4 simulation.

The RMS values of the longitudinal velocity component fluctuation distributions at the jet centerline are presented in Fig. 5.30b. The velocity fluctuation distribution follows a similar behavior observed from the mean velocity distribution. The velocity fluctuation distribution is nearly identical up to $x/D_j = 7.0$. After that section, the RMS values of the axial velocity distributions from the S5 and S6 simulations separate from the S4 simulation, presenting larger values. In the region of the peak of the axial velocity fluctuation distribution, $11.0 < x/D_j < 13.0$, it is observed that the S5 simulation presents the largest values of velocity fluctuation, and the S4 simulation presents the lowest values.

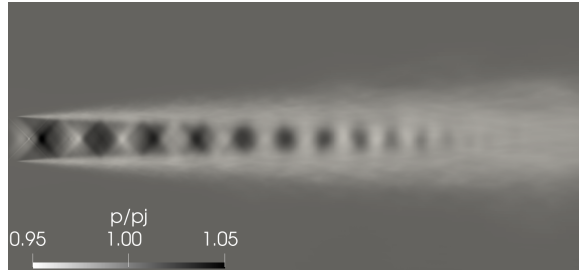
The RMS values of the radial velocity component fluctuation distributions, Fig. 5.30c, present similarities when comparing the simulations with the three inflow options than the distribution of the RMS values of the longitudinal velocity fluctuation. The differences



(a) S4 simulation.



(b) S5 simulation.



(c) S6 simulation.

FIGURE 5.29 – Mean pressure contours on a plane through the centerline of the jet.

among the RMS values in relation to the peak values of the three simulations are smaller than those of the longitudinal velocity fluctuation in all the investigated lengths of the jet flow field. When comparing to the experimental data, it is seen that the difference in $x/D_j = 10.0$ is significantly larger than the difference observed from the longitudinal velocity fluctuation distributions. The RMS values of the tangential velocity component fluctuation distributions, Fig. 5.30d, present a similar behavior to the distributions for the radial velocity fluctuation with even smaller differences between the three numerical simulations. It is impossible to distinguish the peak values from the three numerical simulations. The three simulations generated similar profiles of the mean Reynolds shear stress component distributions, Fig. 5.30e. The largest oscillation amplitudes are observed from the S5 simulations, while the S4 and S6 present similar values.

The velocity distributions at the jet lipline present important differences with the imposition of the inflow conditions studied. The mean longitudinal velocity component distributions and RMS values of the longitudinal velocity component fluctuation, radial velocity component fluctuation, and tangential velocity component fluctuation distribu-

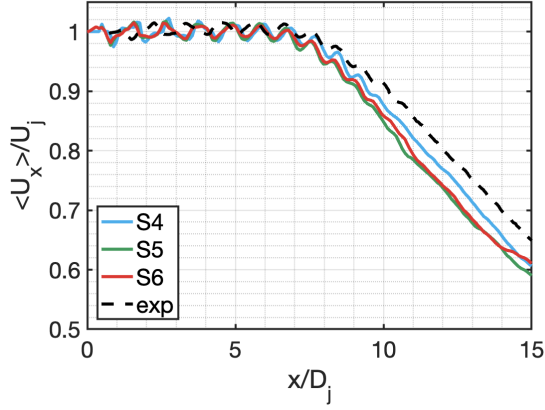
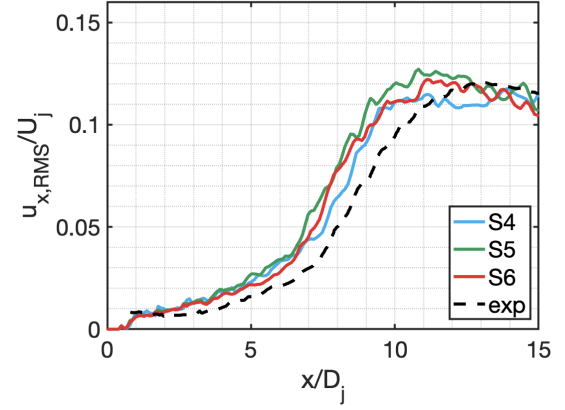
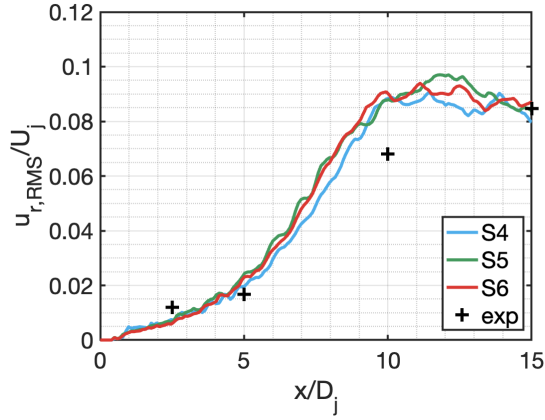
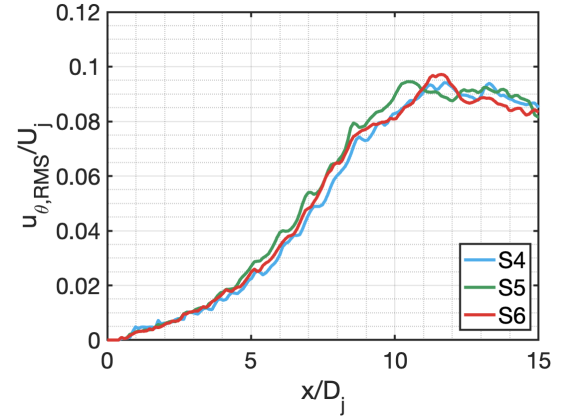
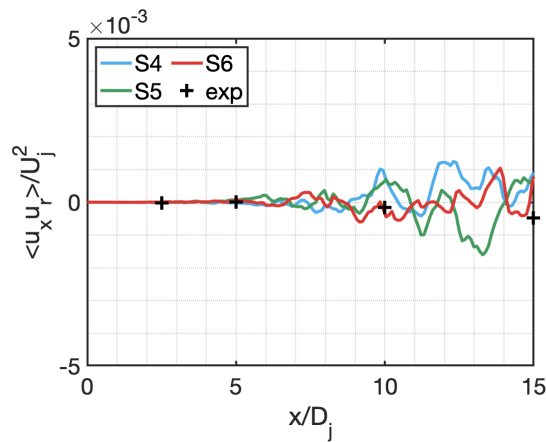
(a) Averaged U_x profile along jet centerline.(b) RMS values of u_x along jet centerline.(c) RMS values of u_r along jet centerline.(d) RMS values of u_θ along jet centerline.(e) Averaged $u_x u_r$ profile along jet centerline.

FIGURE 5.30 – Velocity and Reynolds stress tensor component distributions at the centerline of the jet flow for the inflow condition studies.

tions, and the mean Reynolds shear stress tensor component distribution at the lipline of the jet flow are presented in Fig. 5.31. The inflow conditions have an important role on the profiles along the lipline, which can be observed from the mean axial velocity component distributions, Fig. 5.31a. The mean axial velocity distribution from the S4 simulation presents large velocity values close to the jet inflow section, $x/D_j = 0.0$, due to the lack of a boundary layer inflow profile. When the boundary layer is imposed in the viscous profiles, S5 and S6 simulations, low-velocity levels are observed close to the inflow section. The different velocity levels are observed up to axial station $x/D_j = 7.0$. Compared to the experimental data, the lower velocity levels from the S5 and S6 numerical simulations may indicate that the thickness of the boundary layer obtained from the designed nozzle is larger than the thickness obtained in the physical experiments. For $x/D_j > 7.0$, the velocity values from the S6 simulation are close to the mean values from the S4 simulation, and the values from the S5 simulations are slightly below those from the other two simulations.

The RMS values of the longitudinal velocity component fluctuation distributions at the lipline, Fig. 5.31b, present one small improvement towards the experimental reference with the viscous inflow profiles. The imposition of the viscous inflow profile could slightly reduce the peak RMS value of the velocity fluctuation distribution. The velocity fluctuation distribution from the S5 simulation could provide a smaller peak than the S4 velocity distributions. The S6 simulation provided slightly smaller peak values than the S5 simulation. After the peak value, the velocity fluctuation distributions presented similar values. The axial velocity fluctuation distribution detail near the inlet section is presented in Fig. 5.32. When investigated in detail, it is possible to observe that when the viscous velocity profile is imposed, the axial velocity fluctuation increases closer to the inlet section than with the inviscid profile, S4 simulation. Insignificant differences are observed from the S5 and S6 simulations.

The RMS values of the longitudinal, radial, and tangential velocity fluctuation distributions, Figs. 5.31b, 5.31c, and 5.31d, present the same behavior among the three simulations with different intensities in each variable investigated. The high-velocity fluctuation peak presented by the S4 simulation is reduced by including the viscous profile from the S5 and S6 simulations. The difference in the distribution of the RMS values of the longitudinal velocity fluctuation from the simulations is small. However, the difference is significant for the RMS values of the radial velocity fluctuation, which presents a reduction of the peak in 30%. The RMS values of the radial velocity fluctuation distribution have a shape with an almost constant behavior after the inlet section. The introduction of the tripping method was able to reduce the peak values in the RMS values of the three velocity component fluctuations. The mean Reynolds shear-stress tensor component distribution, Fig. 5.31e, presents a similar shape to those from the radial velocity component

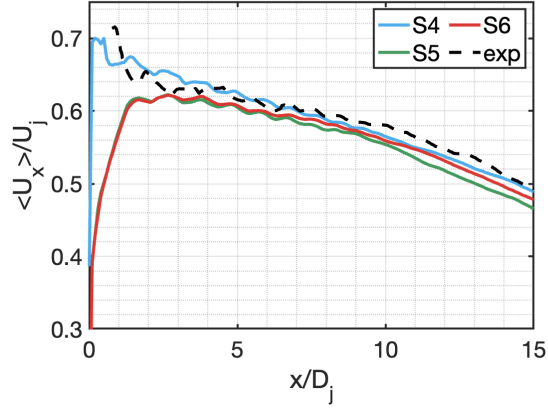
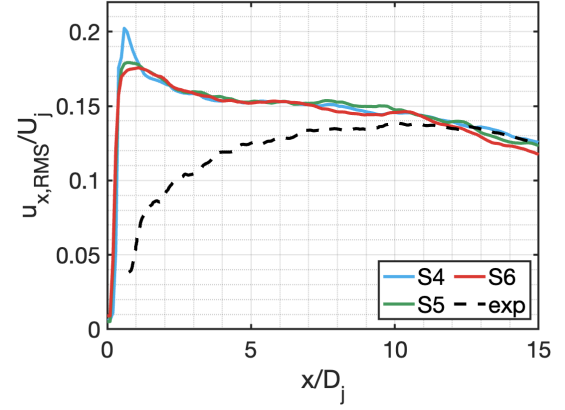
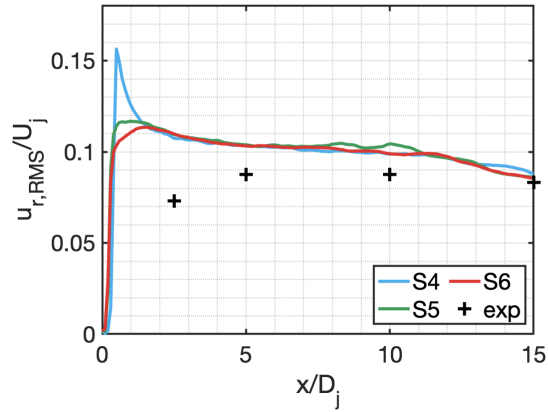
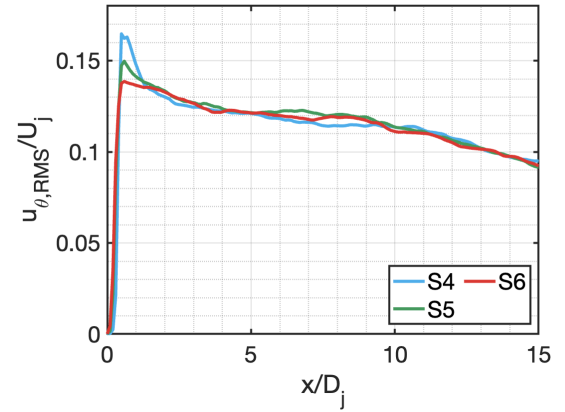
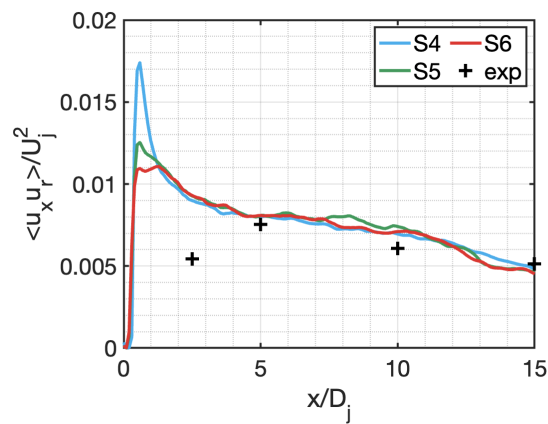
(a) Averaged U_x profile along jet lipline.(b) RMS values of u_x along jet lipline.(c) RMS values of u_r along jet lipline.(d) RMS values of u_θ along jet lipline.(e) Averaged $u_x u_r$ profile along jet lipline.

FIGURE 5.31 – Velocity and Reynolds stress tensor component distributions at the lipline of the jet flow for the inflow condition studies.

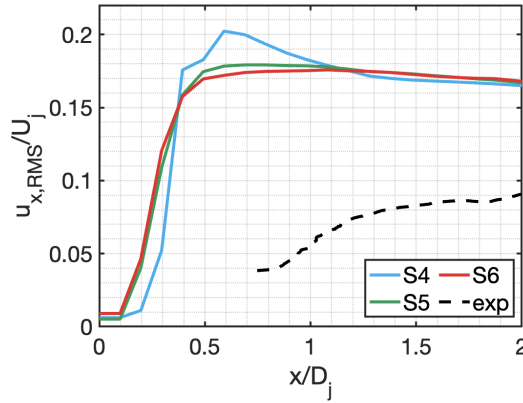


FIGURE 5.32 – Detail of the region close to the jet inflow boundary condition from the distribution of the RMS values of axial velocity component fluctuation at the jet lipline, Fig. 5.31b.

fluctuation distribution, Fig. 5.31c, with a large reduction when compared to the simulation with the inviscid profiles with the viscous profile. In the region of $x/D_j < 5.0$, the values from the three numerical simulations are above those from the experiments. For $x/D_j > 5.0$, the numerical simulations agree with the experimental data.

5.3.5 Radial Profiles of the Longitudinal Velocity Component and Reynolds Stress Tensor

The radial profiles of the mean longitudinal velocity component, Reynolds stress tensor component associated with the longitudinal velocity, Reynolds stress tensor component associated with the radial velocity, and Reynolds shear stress tensor component are presented in Fig. 5.33 in four longitudinal positions, $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$. The development of the mean flow investigated by the mean longitudinal velocity component profiles is presented in Figs. 5.33a to 5.33d. Due to the velocity range in the radial profiles of the mean longitudinal velocity component, it is hard to observe any important difference between the three numerical simulations. One consistent characteristic between the radial profiles from the four positions is that the velocity levels from the S5 and S6 simulations are lower than those from the S4 simulation. The differences are more pronounced in the mixing layer region in the first axial position, Fig. 5.33a, between $0.4 < r/D_j < 0.8$. The numerical profiles consistently present a larger spreading than the experimental data that can be observed by the larger velocity slope, when compared to the experimental data, in the mixing region in the first two axial positions. The last two positions also show a reduced velocity close to the jet centerline.

The Reynolds stress tensor component associated with the longitudinal velocity component, $\langle u_x^2 \rangle$, radial profiles are investigated in Figs. 5.33e to 5.33h. In the first two

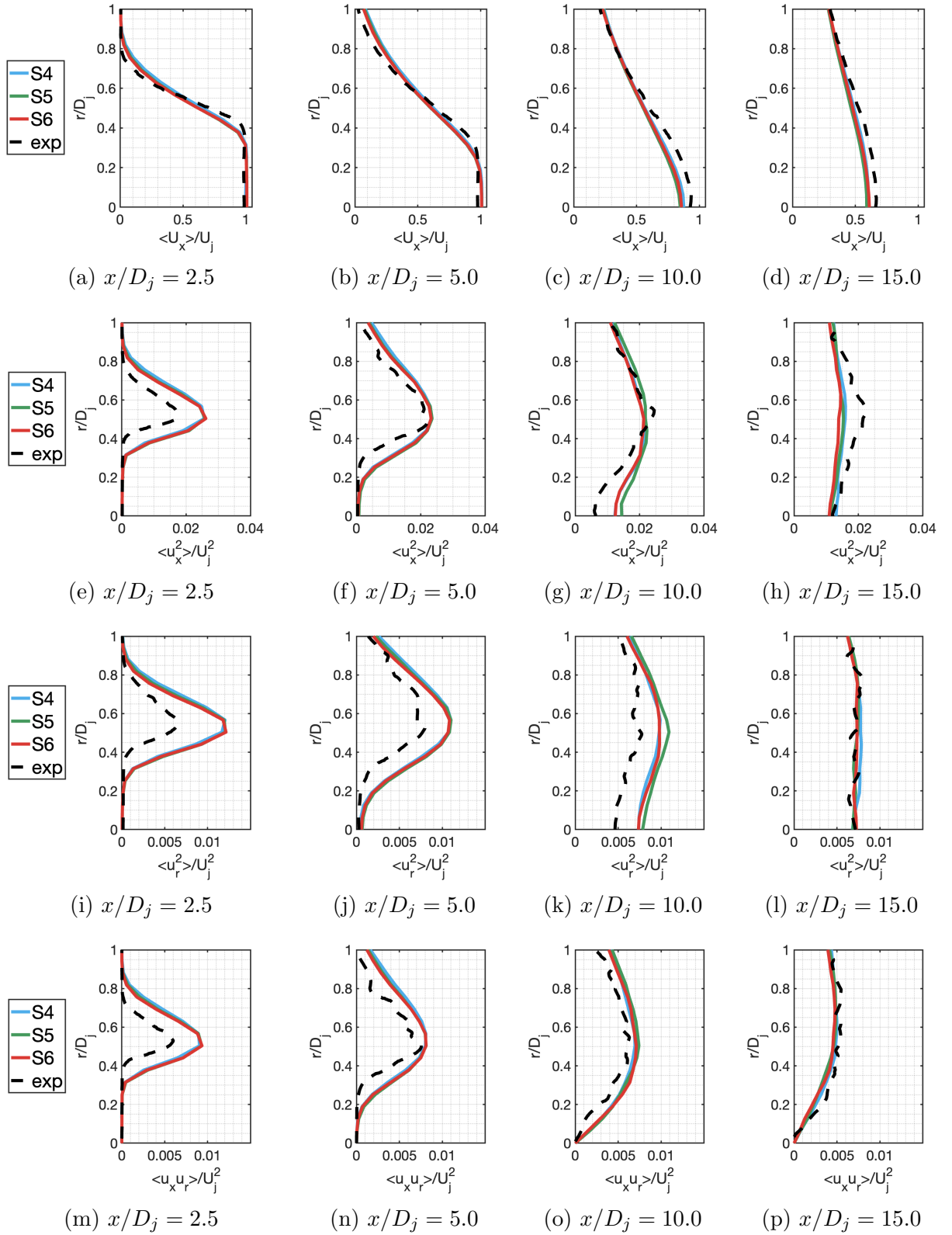


FIGURE 5.33 – Radial distributions of the mean longitudinal velocity component, mean of longitudinal velocity fluctuation squared, mean of radial velocity fluctuation squared and mean shear-stress tensor component (from top to bottom) presented in four streamwise positions $x/D_j = 2.5$, $x/D_j = 5.0$, $x/D_j = 10.0$, and $x/D_j = 15.0$ (from left to right).

longitudinal positions, Figs. 5.33e and 5.33f, it is possible to observe that the shape of the radial profiles is displaced in the radial direction. The profile from the S4 simulation presents the mixing layer occurring at a higher radial position than the mixing layer from the S5 and S6 simulations. The difference in the mixing layer position is due to the absence of a boundary layer in the inviscid inflow profile. The comparison of the simulation profiles with the experimental data indicates larger levels of Reynolds stress tensor along the radial interval investigated predicted by the numerical simulations. The third axial position, Fig. 5.33g, presents one characteristic that the radial profiles from the S4 and S6 simulations match, while the radial profile from the S5 simulation presents larger Reynolds stress component values along the different radial positions than the S4 and S5 simulations. The numerical profiles present larger values close to the jet lipline than the experimental data. The experimental data present a peak region close to $r/D_j = 0.55$ that does not occur in the numerical profiles. In higher radial positions, the numerical and experimental profiles are similar. In the last position evaluated, Fig. 5.33h, the three simulations produced similar radial profiles for the Reynolds stress tensor longitudinal component. The numerical axial component of the Reynolds stress tensor is consistently below the experimental levels.

The Reynolds stress tensor component associated with the radial velocity component, $\langle u_r^2 \rangle$, radial profiles are investigated in Figs. 5.33i to 5.33l. The behavior of the radial component of the Reynolds stress tensor is similar to that observed from the axial component. In the first two sections, Figs. 5.33i and 5.33j, the radial profile from the S4 simulation is displaced in the radial direction to the profiles from the S5 and S6 simulations. The numerical profiles present larger values than the experimental data for all radial positions. In the third position, Fig. 5.33k, it is possible to observe that the profile from the S6 simulation is closer to the profile from the S4 simulation than that of the S5 simulation. The numerical profiles continue to present larger values than the experimental data. In the last section, Fig. 5.33l, the numerical and experimental profiles present nearly the same values for the radial component of the Reynolds stress tensor.

The Reynolds shear-stress tensor component, $\langle u_x u_r \rangle$, radial profiles are investigated in Figs. 5.33m to 5.33p. It is possible to observe, once more, the displacement in the radial direction between the radial profile from the S4 simulations and the S5 and S6 simulations in the first two positions, Figs. 5.33m and 5.33n. The numerical profiles also present larger values than the experimental data. In the third longitudinal position, Fig. 5.33o, the three numerical profiles are similar, and they present slightly larger values than those of the experimental reference with a similar shape. In the last longitudinal position, Fig. 5.33p, the three numerical and experimental profiles are similar in the shear-stress tensor component values and distribution shape.

5.3.6 Power Spectral Density Analyses

The PSD of the longitudinal velocity fluctuation from the three simulations with different jet inlet boundary conditions are presented at the centerline, Fig. 5.34, and at the lipline, Fig. 5.35, of the jet flow in the same four longitudinal positions where the radial profiles were investigated. In the same way, presented in the accuracy assessment study, there is no experimental data for the jet centerline. The PSD values at the jet centerline present similarities between the three flows. The PSD values of the three numerical simulations indicate the minor influence of the inflow condition in the spectral distribution of the velocity fluctuation in the four sections investigated. In the first longitudinal station, Fig. 5.34a, it is possible to observe a difference in the PSD values from the S5 simulation in the higher frequencies, where it is possible to observe large values in that region when compared to the other two simulations. In the next station, Fig. 5.34b, it is possible to observe an inversion of the trend, with the values from the S5 simulation being above those from the other two simulations in the higher frequencies. In the last two stations investigated, no difference can be visualized from the PSD values of the three numerical simulations.

The analysis of the PSD values of the longitudinal velocity component fluctuation at the jet lipline, Fig. 5.35, indicates even fewer differences among the three numerical simulations when compared to the centerline PSD values. It is important to point out that with the three boundary conditions investigated, no difference is observed in the range of frequencies where experimental data is available, which means that the PSD values from the three numerical simulations agree with the experimental reference. The only difference among the PSD values of the longitudinal velocity fluctuation component from the three numerical simulations appears at the highest frequencies in the last station, $X/D_j = 15.0$, where the imposition of the inviscid profile could produce slightly higher PSD values than the simulations with the viscous inflow profiles.

The PSD values of the radial velocity component fluctuation from the three simulations with different inflow conditions are presented at the centerline, Fig. 5.36, and at the lipline, Fig. 5.37, of the jet flow field in the four longitudinal locations investigated in the multiple analyses. The PSD values obtained at the jet centerline show negligible influence of the inflow boundary condition at the four positions investigated. At the centerline of the jet flow, there is no experimental data to be compared with the numerical values.

The PSD values at the lipline, Fig. 5.37, show once more no influence of the inlet condition on the spectral distribution of the velocity fluctuation of the radial velocity component. The three simulations reproduced the same velocity fluctuations associated with the frequency distribution. When compared with the experimental data available, no difference is observed in the range of the frequency with data available. The PSD

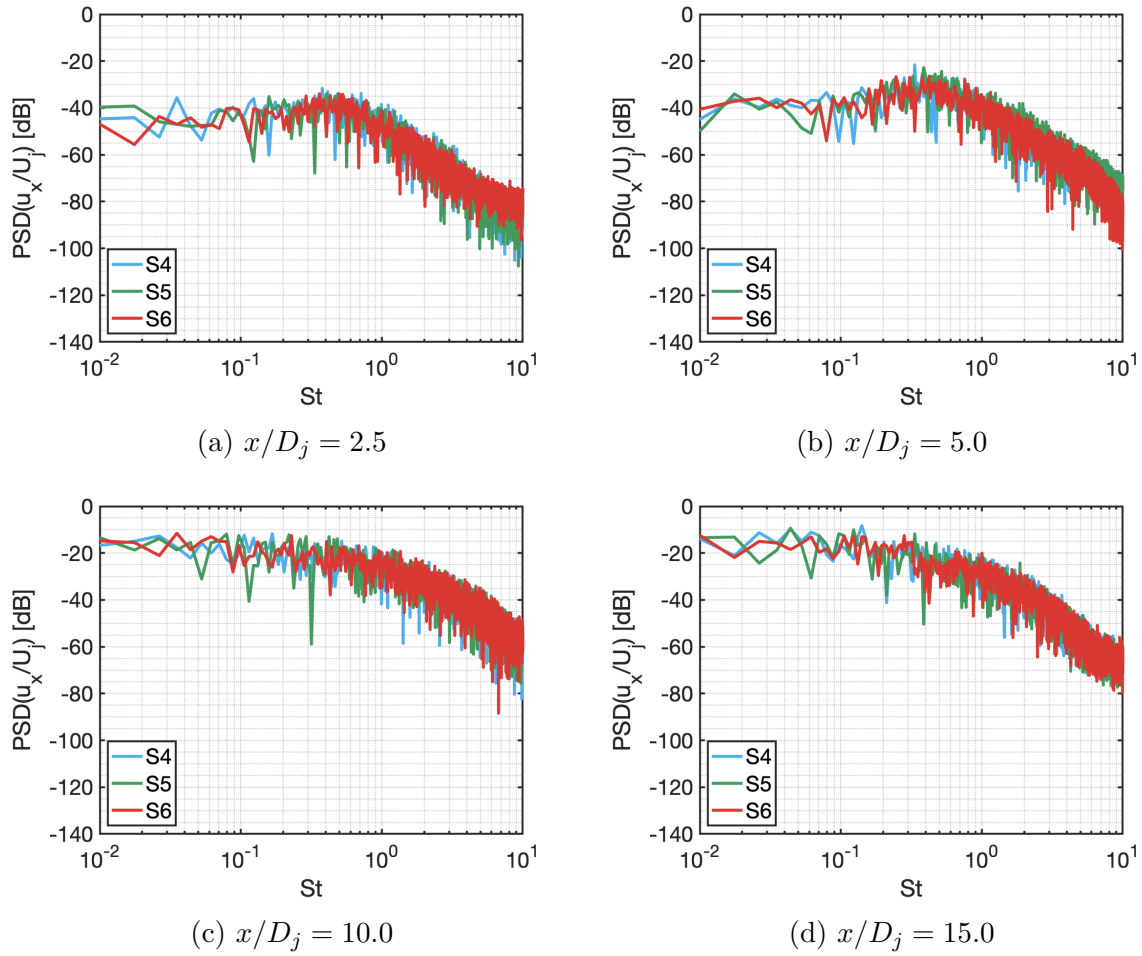


FIGURE 5.34 – Power spectral densities of the longitudinal velocity component fluctuation at four streamwise planes. PSDs obtained in the centerline of the jet flow.

values from the three numerical simulations agree with the experimental reference.

5.3.7 Discussion of the Numerical Results

The influence of three options for the imposition of the jet inflow condition was evaluated in the present work. The inviscid profile was the first one, and it is a straightforward implementation because it considers a uniform flow in the inlet section. The imposed properties have constant values in the radial and azimuthal directions. The second option imposed the mean properties obtained from a RANS simulation of the nozzle flow. In the RANS simulation, the divergent shape of a supersonic nozzle was modeled to adjust the thickness of the boundary layer in the exit station and the level of uniformity of the pressure profile. The strategy of modeling only the divergent section of the nozzle was based on the imposition of a constant section pipe employed in the LES of subsonic jet flows. The density, pressure, longitudinal velocity, and radial velocity components were tabulated and input in the inflow condition of the LES simulations. The last option was

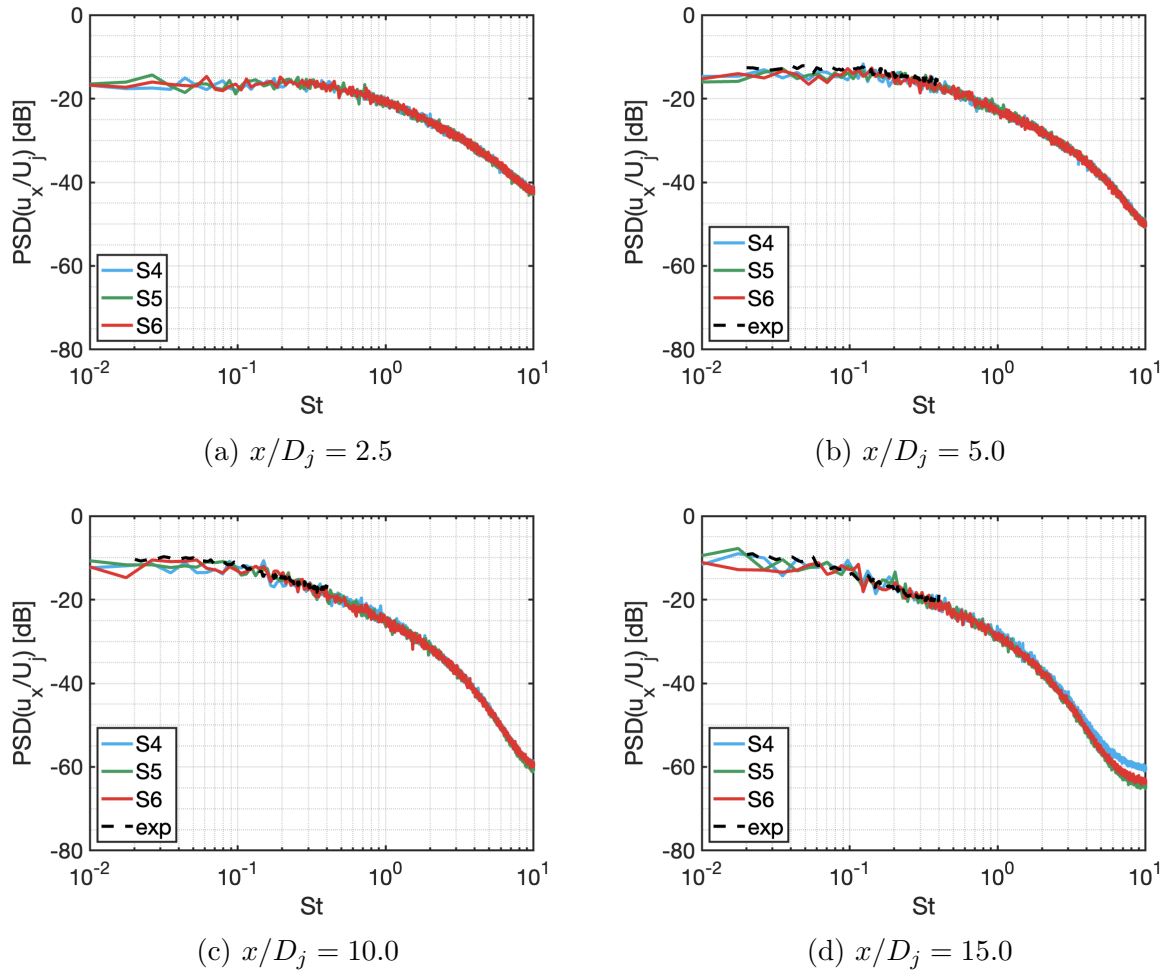


FIGURE 5.35 – Power spectral densities of the longitudinal velocity component fluctuation at four streamwise planes. PSDs obtained in the lipline of the jet flow.

to apply the mean profile from the RANS simulation and superimpose a tripping method to introduce a disturbance in the inlet condition to promote an early increase in the turbulence properties in the mixing layer and avoid the high peak values observed when the inviscid profile is imposed.

The “*hp*” requirement study showed that, generally, the agreement between the numerical data from the S4 simulation and experimental data was good, with important differences only associated with the flow at the jet lipline close to the inlet section. The numerical values from the S4, S5, and S6 simulations, which were performed with the same numerical mesh, polynomial degree, and the three inflow conditions, indicate that, in general, the inflow condition has a negligible impact on the flow field of the jet. What was observed is an influence only in the lipline close to the jet inlet section. The imposition of the mean RANS profile was able to significantly modify the mean flow in the jet lipline and reduce the peak of the velocity fluctuations obtained by the interaction between the high-velocity flow and the surrounding air. The imposition of the tripping

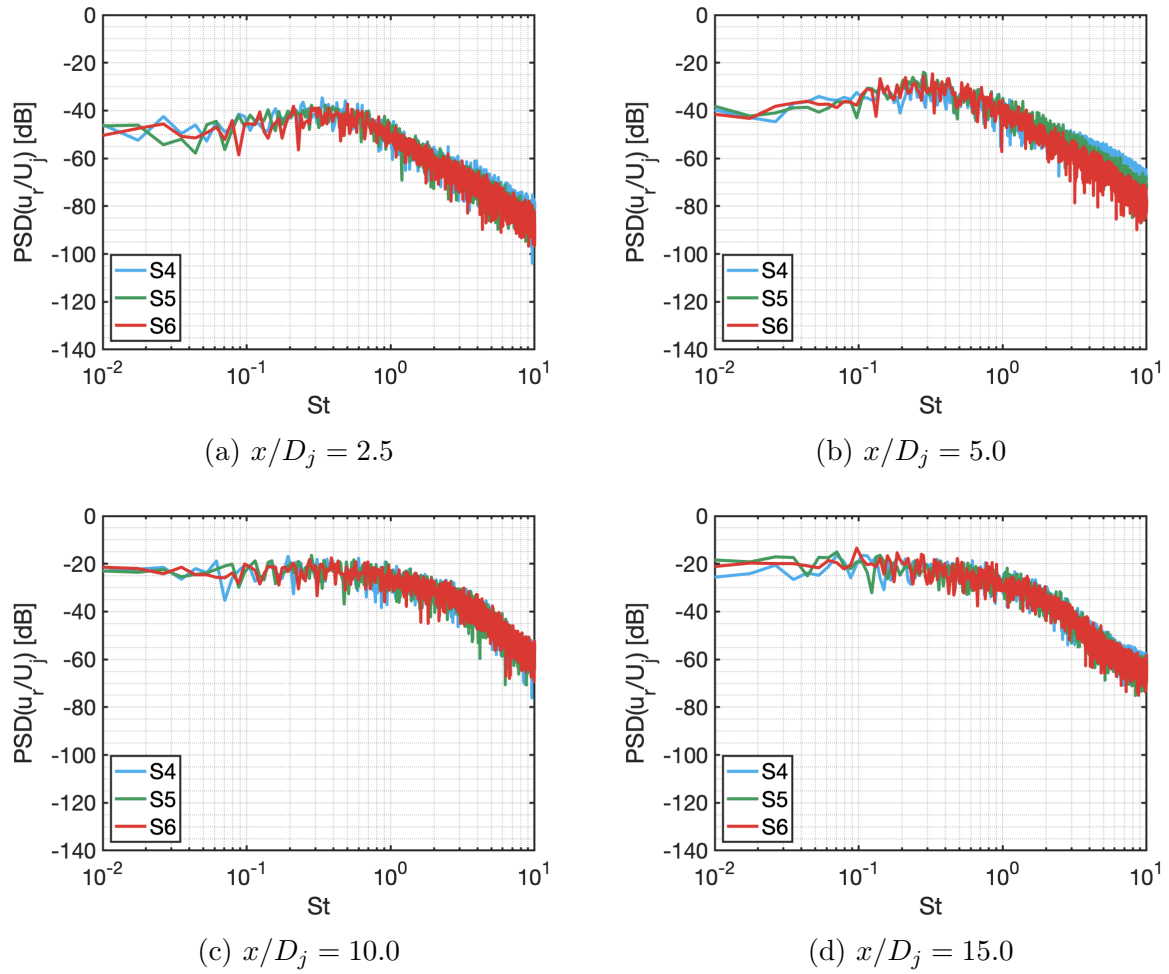


FIGURE 5.36 – Power spectral densities of the radial velocity component fluctuation at four streamwise planes. PSDs obtained in the centerline of the jet flow.

procedure produced a slight reduction in the peak of velocity fluctuation at the lipline when compared to the imposition of the viscous profile only. The tripping procedure was used with the same parameters from the reference work [23] where it was based, and it may be weak for the supersonic jet flow application. The present study reached its objective to assess the influence of the inflow condition on the simulation of jet flows. It showed that, for the evaluated options, the numerical simulations could produce a flow field close to the experimental data without introducing the nozzle domain into the computations. The costs of the simulations increased due to the necessity of reducing the time steps to maintain the stability of the simulations. However, this cost increase is small compared to the insertion of the nozzle geometry in the physical domain.

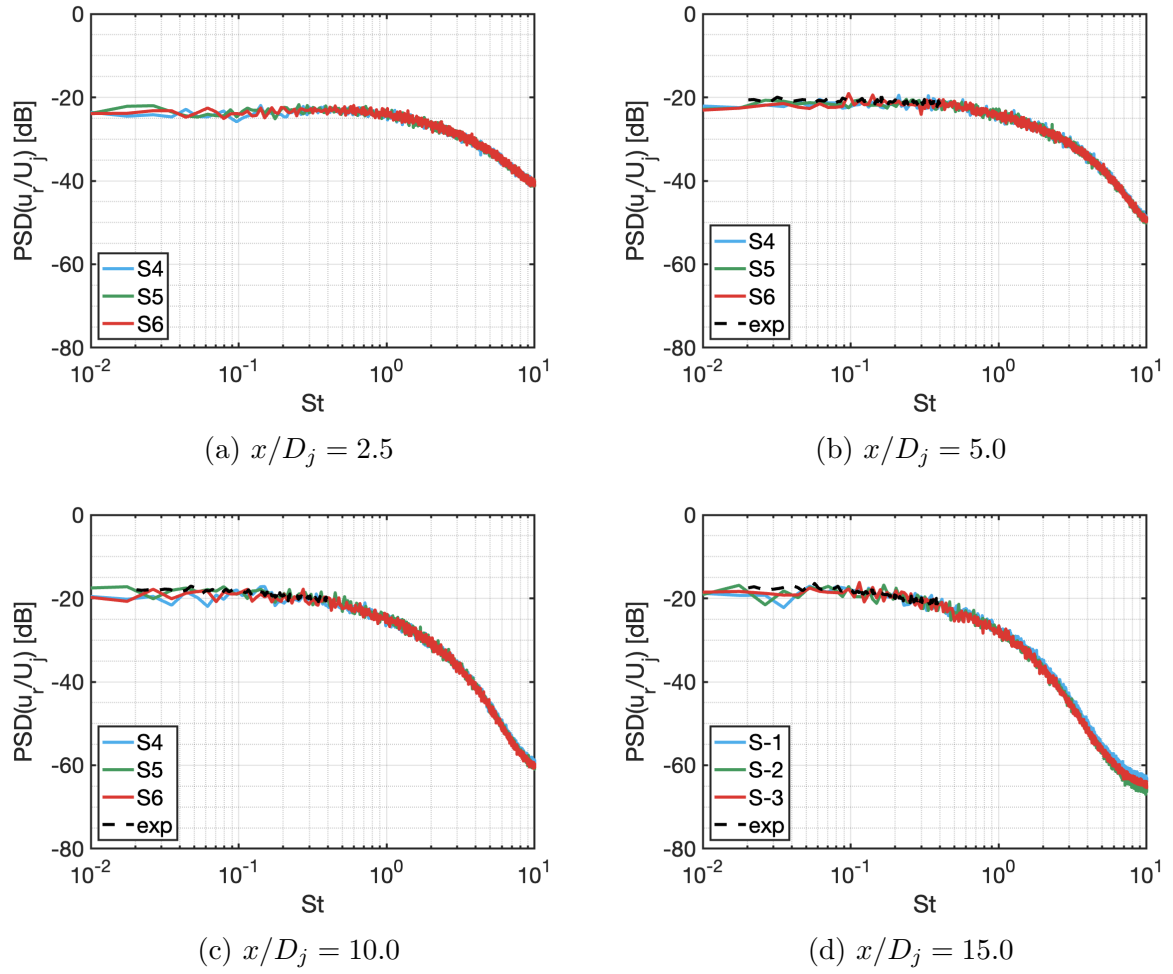


FIGURE 5.37 – Power spectral densities of the radial velocity component fluctuation at four streamwise planes. PSDs obtained in the lipline of the jet flow.

6 Conclusions

6.1 Concluding Remarks

In the present work, studies are conducted to assess the resolution requirements and the influence of the inflow condition on the initial development of a perfectly expanded supersonic jet flow with a Mach number 1.4 and a Reynolds number based on the jet inlet diameter of 1.58×10^6 . The first study compared the results of the jet flow simulations using two different numerical methods available to the author for performing high-fidelity simulations. In the sequence, an accuracy assessment study was performed with the DGSEM scheme, available in the FLEXI numerical framework, to identify the polynomial and mesh refinement (“*hp*”) requirements for the large-eddy simulations of the supersonic perfectly expanded jet flow. The third study evaluated the effects of different inlet boundary conditions on the supersonic jet flow of interest.

The first study compares data from the supersonic jet flow simulations of interested using two different numerical schemes: a centered second-order finite difference scheme for structured meshes [17, 90] and a discontinuous Galerking spectral element method scheme for unstructured meshes [35–37]. The JAZzY finite difference solver was developed in the research group in which this work was performed, and the FLEXI numerical framework is an open-source academic code which implements the discontinuous Galerkin scheme. The discontinuous Galerkin scheme was chosen due to its innate capacity to apply high-order spatial discretization through the change of the polynomial degree that represents the numerical solution of the element. The two methods were compared using a fixed number of degrees of freedom. The reference simulation used a mesh with 50×10^6 points. Hence, two other simulations were performed with the FLEXI numerical framework using 50×10^6 DOFs. In 3-D, when the solution is approximated by linear polynomial degrees, there are 8 degrees of freedom per element. The solution approximated by a quadratic polynomial has 27 DOFs per element. This aspect has to be considered when generating a DGSEM mesh. Therefore, in the current work, the meshes generated for the FLEXI numerical framework are coarser than the mesh used in the JAZzY code. It was also necessary to perform a small adjustment in the central part of the mesh to accomplish the requirement

of exclusively hexahedral elements. The final meshes for the DGSEM simulations have 6.2×10^6 for the second-order accurate simulation, and 1.8×10^6 elements for the third-order accurate simulation.

The comparison of the numerical results indicates similar characteristics presented by the three numerical simulations. The simulations produced a potential jet core that was significantly shorter than the physical test results. The distribution of velocity fluctuation in the lipline and centerline shows different peak levels and positions compared to experimental data. The velocity profiles from the simulation performed with the JAZzY solver were generally better than those obtained with the second-order accurate FLEXI simulation and slightly worse than those obtained from the third-order accurate FLEXI simulation. The flexibility of the DGSEM scheme to handle high-order discretizations allowed better results for the same number of degrees of freedom when compared to second-order accurate simulations. Therefore, the discontinuous Galerkin was chosen for the work development.

An “*hp*” refinement study was conducted to identify the necessary requirements for a large-eddy simulation of the supersonic jet flow using the discontinuous Galerkin scheme. Three numerical meshes and two polynomial degrees were used in four simulations. Two meshes are the same employed in the previous study of the numerical method comparison. The third mesh is improved based on the preliminary calculations from the simulations with 50×10^6 DOFs. The improvement is performed using a new topology that increases the refinement in specific regions of interest, such as the shear layer. The third mesh is also more refined than the first two meshes. It has a total of 15.4×10^6 elements. The three numerical meshes employed are linear meshes. Two simulations are performed with the third mesh. They have used linear and quadratic polynomial degrees to obtain second- and third-order accurate spatial discretizations. The numerical simulations performed with the third mesh have 120×10^6 DOFs when simulated with second-order accurate spatial discretization, and 410×10^6 DOFs when simulated with the third-order accurate spatial discretization.

The simulations run with 50×10^6 DOFs present similar behavior and are underresolved compared to the experimental data. One can observe a short potential core and a mismatch of the velocity profiles along the lipline. The “*hp*” discretization can be related to the LES filter cutoff, which means that coarse “*hp*” refinement is equivalent to modeling or neglecting a larger portion of the energy spectrum of turbulence. Hence, the calculations could not develop the eddies that caused the flow to transition in the mixing layer, which modified the turbulence transition. The consequence is a short potential core, which is the length in the centerline from the inlet section to the position where the jet reaches 95% of its initial velocity. The numerical data also present a more significant mean velocity reduction along the lipline. The power spectral densities of the longitudinal

velocity component fluctuations indicate a power reduction occurring at smaller frequencies than those of the other simulations. Such behavior is also associated with the lack of resolution from the numerical simulations, since large mesh elements cannot simulate small eddies that are associated with high frequency behavior.

The mesh refinement produced significant improvements even when simulated with second-order accurate spatial discretizations. The potential jet core is improved, matching the references. The rate of velocity reduction in the centerline and the lipline of the jet flow have similar values to those from the experimental reference. The transition of the mixing layer was anticipated, occurring closer to the inlet section and resulting in turbulent levels closer to experimental data after the peak values. The power spectral density showed that the numerical simulation could match the experimental data in the three positions where experimental data was available. In the higher frequencies, the simulation could sustain high PSD levels. The change to a quadratic polynomial degree, which yields a third-order accurate spatial discretization, increased the quality of the simulations, except for the velocity distribution at the lipline close to the jet inlet section, which got farther from the experimental results when compared with the velocity profiles from the other numerical simulations. The highly-resolved simulation required an adjustment to the shock indicator, which increased the number of elements being resolved with the shock-capturing method. However, it did not affect the practical result since the numerical results got close to the experimental data. The overall agreement with the experimental data, in terms of mean flow and turbulent quantities, indicates that the simulation with the third numerical mesh, with 15.4×10^6 elements and a quadratic polynomial degree resulting in 410×10^6 degrees of freedom is the best configuration for the LES of supersonic jet flows and, consequently, for the development of the study of the influence of the inflow condition.

The third study developed in this work is the nozzle design, which employed the RANS formulation in the calculations. The target of the design process was to obtain a nozzle with only a divergent shape that could provide a thick boundary layer and low-pressure distortion at the nozzle exit section. The goal is to obtain the outlet profiles from the nozzle simulations to impose in the inlet condition of the jet flow LES. The two constraints of the design were the nozzle exit diameter and the properties that should be delivered in the nozzle exit section. The design parameters evaluated were the nozzle length, inlet diameter, the opening angle, and the inflow condition. The design of nozzles with curved walls was also evaluated. The final nozzle design could deliver a thick boundary layer and the target values in the outlet section with minimum pressure distortion. The radial profiles of density, pressure, longitudinal, and radial velocity components were identified for the inflow condition of the large-eddy simulation of the jet flow.

The evaluation of inlet BCs on the LES of the perfectly expanded jet flow, which is the

main study of this work, was conducted with the analysis of three numerical simulations that used the same mesh and spatial order of accuracy with different jet inlet boundary conditions. The first condition applied, the inviscid profile, where the properties are uniform in the boundary condition, is the most straightforward condition employed in the resolution study. The second condition imposes the steady viscous velocity profile obtained at the outlet section from the RANS simulation of the nozzle flow. The reduction of interpolation errors was obtained using a piecewise cubic interpolation between the profile and the large-eddy simulation mesh. The third condition used the mean profile from the RANS simulations with the superimposition of a tripping method [23] in the boundary layer of the profile.

The imposition of the mean flow profile obtained from the RANS simulation in the inlet condition significantly changed the mean velocity and root mean square of the velocity fluctuation distributions at the lipline, with insignificant changes in the velocity profiles in other regions of the flow field. The mean longitudinal velocity component distribution presented a significant change due to the boundary layer from the mean profile. It presented a reduction in the initial region of the jet flow, close to the jet inlet section, reaching values smaller than those from the physical experiments, indicating that the boundary layer thickness imposed was larger than those from the experiments. The improvement obtained was in the root mean square of the longitudinal velocity fluctuation distribution, where the peak values were reduced, and the transition was anticipated. The imposition of the mean profile from the RANS simulation compared to the inviscid profile resulted in a slight reduction of the jet potential core.

The imposition of the viscous profile superimposed by the tripping algorithm produced few modifications to the result with only the mean profile. It could slightly diminish the peak value of the root mean square of the longitudinal velocity fluctuation, and it could recover some of the drawbacks observed. For example, the potential core grows with the tripping. The cost of the simulations with the newer boundary conditions has increased due to the necessity of reducing the time step to maintain the same stability levels. The numerical results indicate that the inflow condition significantly affects the jet flow development investigated in the present work. Compared to the inviscid inflow profile, the imposition of the viscous profile could improve the jet flow field towards the experimental reference. The tripping method attempts to overcome the lack of unsteady physics from the RANS computation. However, due to a lack of a specific adjustment on the tripping parameters for the jet flow of interest, the transition of the flow field could not be promoted in a manner closer to the observed in the experiments.

The influence of the inflow condition on the development of large-eddy simulations of supersonic jet flows was assessed, and improvements were obtained without the inclusion of the nozzle geometry in the computational domain. The strategy of imposing a mean

profile from the RANS simulation of the nozzle flow could affect the mean velocity and root mean square velocity distributions at the lipline of the jet flow. These improvements were obtained with insignificant changes in the velocity data in other regions of the flow field. The imposition of the tripping method did not produce significant improvements when compared to the mean profile from the RANS simulation. However, it could slightly improve the numerical results obtained with the viscous profile in some specific areas, for example, the potential core length, which makes the option of tripped mean profile the best approach among the options investigated in the current study.

6.2 Future Research

The development of the present work has shown opportunities to keep evolving the large-eddy simulations of supersonic jet flows using the discontinuous Galerkin schemes. Some of the opportunities do not require large developments to the numerical framework, which was employed in the simulations in the present work. Others require additional development within the framework. One of the possibilities for the continuation of the present work would be the development of tools to perform the acoustic analysis of the simulated jet flows. In the acoustic analysis, the pressure data is gathered to be used together with a Ffowcs-Williams and Hawkings [132] acoustic analogy formulation to identify the sound pressure levels predicted by the jet flows by the numerical simulations. The unsteady data for the Ffowcs-Williams and Hawkings tool was gathered, and it is stored within the database from the jet flow simulations. The development of acoustic tools could expand the range of analysis to be performed with the present numerical framework.

During the execution of the present research effort, three opportunities were identified to improve the quality of the numerical results and the computational costs of the simulations. The first opportunity is associated with the tripping method imposed on the inflow condition. In the present work, the parameters of the tripping method were the same as the reference methodology [23], which were adjusted to induce the transition in a region inside the nozzle of a subsonic jet flow. It is observed from the numerical results that the imposition of the viscous profile with the tripping method did not produce significant differences from the imposition of only the viscous profile. Understanding the capability of the tripping method to improve the jet flow field demands an adjustment of the tripping method parameters to the application of the free supersonic jet flows.

One essential opportunity for reducing the computational costs of the simulations is to take advantage of the capability of the discontinuous Galerkin scheme to work with unstructured meshes. Due to the need to work with hexahedral elements in discretizing the computational domain, the mesh generation process with Gmsh [125] required a multi-

block strategy. In the multiblock strategy, the blocks are connected. The distribution of elements is kept constant between the blocks, which means that the generation of a high mesh refinement with the interior of the jet flow region results in the propagation to regions of the far field where they are not necessary, which ends up increasing the number of elements present in the computational domain and consequently a high computational cost. The discontinuous Galerkin implementation used in the FLEXI numerical framework [35] permits the simulation of meshes with hanging nodes or non-conforming meshes. With this capability, it is possible to significantly reduce the number of elements in the numerical meshes without affecting the quality of the jet flow solution. The open-source Gmsh mesh generator does not work with non-conforming meshes with hexahedral elements. In the development of the work, the Numeca Hexpress [133] commercial mesh generator was identified as an option for generating non-conforming meshes. It should be interesting to evaluate the capacity of the FLEXI framework to resolve the meshes generated with the Numeca Hexpress mesh generator.

The third and last direct option for the continuity of the work is using a new option for the shock-capturing method. In the present work, the option employed was the sub-cell finite volume shock-capturing method [112], which was explained in detail in Sec. 3.2.5. In a few words, it uses a shock indicator to identify if shock waves are present in the vicinity of the cells. This indicator has an upper and lower threshold. When the indicator levels surpass the upper thresholds, the cell changes from the discontinuous Galerkin formulation to a finite volume formulation with a second-order reconstruction and limiters to handle the shock waves. When the indicator reduces below the lower threshold, the elements return to be evaluated by the discontinuous Galerkin formulation. The process should work well in a static shock wave because the same elements would be treated with each formulation.

In time-dependent calculations, which is the case for large-eddy simulations, there is a constant change in the formulation employed in the cells. This change can destabilize the numerical simulations, and the alternative to overcome this characteristic is to increase the upper threshold and decrease the lower threshold, leading to many elements resolved with a finite volume formulation. During the development of the work, another shock-capturing approach was developed, and it became available in the FLEXI framework after the simulations of the present work were performed. The new approach [134] follows a similar strategy of employing finite volume formulation to handle shock waves in the elements. However, instead of switching between the two formulations, the new approach employs a blending function to smoothly change between the two numerical schemes. This shock-capturing method may enable the reduction of the thresholds of the shock indicator and consequently increase the number of cells resolved with the discontinuous Galerkin formulation, increasing the overall accuracy of the simulation. The second approach was

not investigated during the development of the present work due to a lack of computational resources and time to conclude the work. When the second shock-capturing approach became available from the FLEXI developers [134], the computational resources, that the author could use, were only sufficient to conclude the simulations with the first approach. The tests and rerun of the simulations with the new approach would demand an amount of computational resources and time that the author would not have.

A second reason for the large amount of finite-volume cells in the domain may be the use of linear meshes. When the linear meshes are employed with second-order accurate spatial discretizations, the simulations are stable with a small number of cells being calculated with FV formulation. When the linear meshes are simulated with a third-order accurate spatial discretization, it is observed that a large number of cells need to be simulated with FV formulation to keep the simulations stable. During the development of the work, it was decided to generate linear meshes due to the absence of walls in the computational domain, and consequently, it should have no drawback in simplifying the mesh generation. It should also be interesting to reevaluate this option with the simulation of high-order meshes together with high-order property-reconstructing polynomials.

The present work focused on developing large-eddy simulations of the perfectly expanded supersonic jet flows. This condition was chosen due to the weak shock waves in the interior of the jet flow. The perfectly expanded supersonic condition is a design point, meaning that one operating condition presents such behavior for a nozzle geometry. The nozzles usually operate in subexpanded or overexpanded conditions, where the exit pressure does not match the ambient pressure. In these operating conditions, stronger shock waves are formed in the jet flows. The knowledge developed in the present work concerning the simulation of supersonic jet flows can be the starting point for the simulations with other operating conditions. In Ref. [6], the experimental data for other operating conditions are also available.

There are other interesting options for developing the inflow condition for the jet flow simulations that could provide additional improvements to the initial development of the jet flows. The synthetic turbulence model is an option that should be studied. The synthetic turbulence models introduce unsteady information to the inflow condition that respects some turbulent properties from a reference model, such as the turbulent kinetic energy spectrum. There are many options to generate synthetic turbulence [33]. For example, in Sec. 2.6.1, the synthetic turbulence model [19, 83] employs Fourier modes to reproduce a turbulent kinetic energy spectrum from isotropic turbulence. In the present work, three boundary conditions were evaluated, and improvements were discussed. The chosen options are simpler and cheaper than the more sophisticated options. Due to the focus on performing the best simulation with reduced computational cost, the first alternatives investigated are the simplest. With the knowledge that these alternatives

are not sufficient to represent the physics of the nozzle-exit condition, more sophisticated methods should certainly be investigated.

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FOLHA DE REGISTRO DO DOCUMENTO			
1. CLASSIFICAÇÃO/TIPO TD	2. DATA 27 de agosto de 2024	3. DOCUMENTO Nº DCTA/ITA/TD-041/2024	4. Nº DE PÁGINAS 177
5. TÍTULO E SUBTÍTULO: A study of turbulent supersonic jet flows and the influence of nozzle-exit boundary conditions on the jet initial development			
6. AUTOR(ES): Diego Ferolla de Abreu			
7. INSTITUIÇÃO(ÕES)/ÓRGÃO(S) INTERNO(S)/DIVISÃO(ÕES): Instituto Tecnológico de Aeronáutica – ITA			
8. PALAVRAS-CHAVE SUGERIDAS PELO AUTOR: Large-Eddy Simulation; Jet Flows; Inflow Conditions; Computational Fluid Dynamics			
9. PALAVRAS-CHAVE RESULTANTES DE INDEXAÇÃO: Escoamento turbulento; Escoamento de jato; Dinâmica dos fluidos computacional; Números de Reynolds; Análise numérica; Engenharia aeroespacial; Física			
10. APRESENTAÇÃO: (X) Nacional () Internacional ITA, São José dos Campos. Curso de Doutorado. Programa de Pós-Graduação em Ciências e Tecnologias Espaciais. Área de Sistemas Espaciais, Ensaios e Lançamentos. Orientador: Prof. Dr. João Luiz Filgueiras de Azevedo; coorientador: Dr. Carlos Junqueira Junior. Defesa em 19/06/2024. Publicada em 2024.			
11. RESUMO: Advancements in computational power have enabled the analysis of flows with large geometric complexity and high Reynolds numbers. High-fidelity simulations, such as Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES), have become attractive options for fluid mechanics analyses. The present study focuses on conducting LES of supersonic jets, which constitute the primary propulsion source for spacecraft and aircraft. As a consequence of their operation, they generate noise and dynamic loads. It is imperative to have the capability to calculate high-frequency fluctuations to assess such flow characteristics. The high-frequency fluctuations can be acquired through high-fidelity simulations. The present work performs simulations of free supersonic jet flows, aiming at investigating numerical configurations for conducting high-fidelity simulations of jets and at evaluating the influence of different boundary conditions on the jet development. The study analyzes the capability of two numerical methods in resolving the supersonic jet. For the same number of degrees of freedom, the velocity profiles from the high-order simulation were slightly superior than those from the low-order simulations, leading to the choice of the method allowing for high-order spatial discretization. A study is conducted to identify the mesh and spatial accuracy order requirements to correctly predict turbulent flow properties. The data demonstrate that the finer mesh, combined with third-order accurate spatial discretization, yield good agreement with the experimental data. The research also investigates modeling options for the physical characteristics of the jet inflow condition. A theoretical review of jet inlet formulations is presented for subsonic and supersonic regimes. Three approaches are proposed for simulating supersonic jet flows without including the nozzle in the computational domain. The calculation of jet inlet characteristics requires simulations based on the Reynolds-averaged Navier-Stokes (RANS) formulation. Velocity profiles show improvements in the initial development of jet flow with the enhancement of the inlet conditions.			
12. GRAU DE SIGILO: (X) OSTENSIVO () RESERVADO () SECRETO			