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An assessment of OpenFOAM solver on RANS simulations of round supersonic free jets

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Abstract

Numerical performance of *rhoCentralFoam*, a compressible solver in *OpenFOAM*, was studied by modeling round supersonic free jets with varying nozzle exit conditions through Reynolds-Averaged Navier-Stokes approach. To understand the behavior and accuracy of the solver, simulations were conducted at four different nozzle pressure ratios (i.e. NPR=2.8, 3.4, 4 and 5), corresponding to over-, perfectly-, moderately under- and highly under-expanded exit conditions, respectively. The simulated results were subsequently validated against qualitative and quantitative experimental results and good overall agreements can be observed, in terms of the shock structures along the jet core as well as the mixing characteristics through velocity decay and shear layer growth. In particular, the predicted lengths of the first shock cell were within 4% of those measured from experiments. However, the jet shear layers determined from k- ω SST model showed wider spread and hence over-estimating the jet mixing behavior. Nevertheless, the discrepancies were still deemed to be within acceptable range (<10%). In addition, results obtained from comparisons with commercial CFD solver also demonstrate certain advantages in numerical accuracy for *rhoCentralFoam* solver, under the present simulation conditions.

Keywords: Supersonic; jets; compressible flow; RANS simulations; *rhoCentralFoam*; OpenFOAM;

Nomenclatures

List of symbols

a	Speed of the fastest traveling waves (m/s)
c	Speed of sound (m/s), $c = \sqrt{\gamma p / \rho}$
c_p	Specific heat capacity at constant pressure (J/(kg·K))
c_v	Specific heat capacity at constant volume (J/(kg·K))
D	Internal diameter of the CD nozzle outlet (m)
E	Specific total energy (J/kg)
e	Specific internal energy (J/kg)
$\mathbf{d}_{ON}$	Vector from the owner cell centre to neighbour cell centre (m)
k	Turbulent kinetic energy in k- ω SST RANS model (m ² /s ²)
Ma	Mach number
Ma_d	Design Mach number at perfect expansion
Ma_j	Jet Mach number
$\mathbf{n}_f$	Unit normal vector of a face
P_t	Total pressure at CD nozzle inlet (Pa)
P_{amb}	Atmospheric pressure (Pa)
p	Fluid pressure (Pa)
Pr_t	Turbulent Prandtl number
R	Ideal gas constant for air (J/(kg·K))
$r_{f,i}$	Relative smoothness of a solution at face f of the i^{th} control volume
S_f	Surface area of a particular cell (m ²)
T	Fluid temperature (K)
$\mathbf{u}$	Flow Velocity (m/s)
$\mathbf{U}$	Time-averaged flow velocity (m/s)
$\mathbf{W}$	Set of flow variables in hyperbolic conservation laws, $\mathbf{W} = \{W_1, W_2 \dots W_n\}$
x	Streamwise direction in Cartesian coordinates
y	Spanwise direction (perpendicular to x) in Cartesian coordinates
z	Spanwise direction (lateral) in Cartesian coordinates

Greek Letters

Ω	An arbitrary face of a cell in consideration
α_{eff}	Effective heat conduction term in rhoCentralFoam
γ	Heat capacity ratio, $\gamma = 1.4$
κ	Molecular thermal conductivity (W/(m·K))
κ_{eff}	Effective thermal conductivity (W/(m·K))
κ_t	Turbulent thermal conductivity (W/(m·K))

μ	Fluid dynamic viscosity (kg/(m·s))
μ_{eff}	Effective viscosity (sum of the dynamic and eddy viscosities, kg/(m·s))
μ_t	Eddy viscosity evaluated with <i>k-ω SST model</i> (kg/(m·s))
σ	Viscous stress tensor
ω	Specific rate of turbulence dissipation in <i>k-ω shear stress transport model</i>
ρ	Fluid density (kg/m ³)
Δt	Time step of an iteration (s)
<hr/>	
Subscript	
f	Flow variables/quantities associated with the face f
i	Variables/quantities at i^{th} -control volume
O	Variables associated with owner cells in <i>rhoCentralFoam</i>
N	Variables associated with neighbour cells in <i>rhoCentralFoam</i>
<hr/>	
Superscript	
$+$	Flow variables/quantities evaluated at the ‘positive’ side of a face
$-$	Flow variables/quantities evaluated at the ‘negative’ side of a face
0	Flow variables/quantities at time zero (beginning of an iteration)
$*$	Intermediate flow variables/quantities from the predictor/corrector step
KNP	Kurganov-Noelle-Petrova (KNP) central-upwind flux scheme
T	Transpose of a matrix
<hr/>	
Others	
$F()$	Flux function of a given set of conserved variables
$F_{inv}()$	Inviscid component of the flux function
$F_v()$	Viscous component of the flux function
$\Phi()$	Function for computation of numerical fluxes at a face
$\Psi()$	Limiter function in total variation diminishing reconstruction
$\Psi_{van\ Leer}()$	The van Leer Limiter function
$\overline{}$	Cell average value of a variable

1 Introduction

Computational Fluid Dynamics (CFD) has grown to become an important toolset in modeling and analyzing a diverse range of flow problems, occurring both in nature and in engineering applications [41,48,53,60]. Significant progresses have been made in key aspects of CFD over the years, such as more realistic and accurate mathematical formulation of numerical models, improvement upon computational efficiency, its ability for large-scale parallelization as well as its accessibility and availability to the users. The open source CFD toolbox, *OpenFOAM*, is certainly a representative of the latter initiative. First released in 2004 (i.e. *OpenFOAM v1.0*), *OpenFOAM* has gained popularity lately among the scientific and engineering communities, as it constantly expands and improves upon the available solvers and pre- and post-processing utilities with collective efforts from the community [12,28,29]. For instance, *OpenFOAM* now has more than 80 solvers, each designed to simulate a specific category of flow phenomena from incompressible and compressible flows to fluid-structure interaction and chemically-reacting flows [12].

Being open source, *OpenFOAM* offers some distinct advantages over commercial CFD packages. Firstly, the solver codes are well-structured, and yet flexible which allow user modifications and/or additions with a top-down approach (despite a relatively steep learning curve at the initial stage). For instance, Vuorinen et al. [57] discussed in detail on the implementation of an explicit 4th-order Runge-Kutta time-marching method without significant changes to the original solver. Secondly, the entire *OpenFOAM* toolbox is published under general public license, and thus can be used freely for non-commercial purposes. Consequently, a number of notable computational fluid dynamics studies have been published recently based on *OpenFOAM* toolbox, such as Doolan [8], Lysenko et al. [16], Flores et al. [24], Robertson et al. [50], Vuorinen et al. [55-57], Lee et al. [61], among many others. While a significant number of these studies focused on incompressible flow phenomena and fluid-structure interactions,

utilizing OpenFOAM-based compressible solvers for high speed compressible flows has gained remarkable traction over the past few years as well. Some of these works would include studies conducted by Shen et al., [15], Arisman et al. [11] as well as Hinman and Johansen [60–62].

On the other hand, there has been an increased interest in the study of high-speed compressible flows recently, due to several recent initiatives to improve aviation efficiency and to control and mitigate aviation noises in the industry [23,45]. Strategies to achieve better propulsion efficiency and noise control demand a comprehensive understanding on the flow dynamics and structures of transonic and supersonic jet flows, which still pose major challenges today despite active research in the area. Furthermore, development of an innovative solution to noise reduction in supersonic jets would likely paint an encouraging outlook towards supersonic commercial jetliners in the future [36]. Therefore, it is expected that significant computational efforts will continue to be directed to the investigation and understanding of supersonic jet flows.

More than often, researchers develop in-house codes to examine supersonic jet flows and the associated acoustics [1,32,33,46,51], as both the presence of strong gradients in the flow properties (i.e. shocks and contact discontinuities) and high sensitivity of acoustic signatures to pressure and temperature fluctuations require careful numerical treatments [13], which can be a daunting undertaking if the solver were to be designed from scratch. The *OpenFOAM* toolbox however, provides a useful alternative, whereby researchers can either rely on the existing compressible solvers or modify segments of the code for better performance on their targeted flow problems.

Vuorinen et al. [57] implemented selective-scale discretization and 4th-order Runge-Kutta as spatial and temporal discretization methods together with enhanced Cook-Cabot shock capturing model, so as to

investigate the transient Mach disk development as well as the mixing characteristics along the jet shear layers of highly under-expanded supersonic jets. The Implicit Large-Eddy Simulation (ILES) code developed based on the *OpenFOAM* solver was able to predict satisfactorily the variations of shock cell structures (such as the Mach disk length) at different Nozzle Pressure Ratios (NPRs), as well as capturing the helical mode of the shear layer growth of the under-expanded jet flows.

More recently, Lee et al. [61] proposed a low-dissipative reconstruction scheme for the density-based compressible solver '*rhoCentralFoam*', in order to resolve fine turbulent structures at smooth flow regions. Using the modified Ducros shock sensor as a switch, the hybrid scheme combined the central-upwind Kurganov-Tadmor flux scheme with 4th-order central scheme to reduce numerical dissipation in the solver. They demonstrated noticeable improvements in capturing coherent structures in the flow by using the 'hybrid' solver, through the classical Shu-Osher and forward-facing step problems.

The above studies have clearly indicated that the compressible flow solvers, modified on top of the *OpenFOAM* solver code and structure, are capable of numerically modeling supersonic flows with sufficient degree of accuracy and robustness. Nonetheless, equally crucial is the validation of *OpenFOAM* solvers without any modifications, as suggested by Roberson et al. [50] who performed elaborate validations on *OpenFOAM*'s default incompressible solvers, turbulence modeling approaches and pressure-velocity coupling methods in the study. Inspired by their validation work on incompressible solvers and the fact that similar work on compressible solvers in *OpenFOAM* being relatively limited, the present study aims to carry out a detailed validation of the *rhoCentralFoam* solver, one of the latest additions to *OpenFOAM* compressible solver family, on Reynolds Averaged Navier-Stokes (RANS) simulations of both perfectly and imperfectly expanded supersonic jets. The present paper will first provide some accounts on the theoretical foundation and implementations specific to the

rhoCentralFoam solver in *OpenFOAM*. Subsequently, the simulated results will be qualitatively and quantitatively validated against experimental measurements, followed by a scalability study on its parallel computing performance and lastly a brief comparison between results obtained from commercial CFD solver under similar conditions. As such, the assessment would provide researchers with useful reference on the performance of *rhoCentralFoam* and thus an enhanced knowledge and insight when they either make direct use of or modify the high-speed compressible solvers in *OpenFOAM* for their intended studies.

2 Numerical methods in OpenFOAM

2.1 Mesh topology

A convergent-divergent nozzle (CD nozzle) is used to produce the desired supersonic jet flows for the present numerical study. The geometry of CD nozzle is taken from an ongoing experimental study on supersonic jet flows [27,49], so that the simulation results can be compared and validated against the available qualitative and quantitative measurements. Based on the nozzle expansion, the designed exit Mach number is approximately $Ma_d = 1.45$. Readers are advised to refer to the study by Wu and New [34] for a detailed description of the CD nozzle.

A preliminary comparison carried out by the authors between axisymmetric (2D) and fully 3D simulations on the similar supersonic jet flows suggested that axisymmetric results tend to predict longer lengths for both the shock cells and the jet potential core than those from 3D simulations [8]. Hence, in order to minimize such effects and have a more realistic assessment on the *OpenFOAM* solver, the present numerical simulations were carried out in a fully 3D domain. As shown in Fig. 1, the computational domain extends from the nozzle inlet to 40D downstream of the nozzle outlet in the streamwise direction and on the other hand, 10D from the nozzle centerline in the cross-stream

Figure 1 Simulation domain along both the streamwise and cross-stream directions for the present study

direction (D is the internal diameter of the nozzle outlet, where $D = 12.7mm$). Note that the origin $(0,0,0)$ is defined at the center of the nozzle outlet, as indicated in Fig. 1.

The present approach in mesh construction followed closely to the strategy employed by Shen and Tam [30,31] in their study of jet screech tones. Broadly speaking, the topology was split into two distinct regions, namely the coarse outer layer and the dense core layer, as can be seen from both Figs. 1 and 2(b). To better capture the jet mixing characteristics along the jet shear layers, an additional level of mesh refinement was applied within the dense core, which corresponded approximately to the linear growth behavior of supersonic jet shear layers [6]. Furthermore, the grid spacing was increased by a factor of 1.5 at every $10D$ interval along the streamwise direction, starting from $\Delta x = D/48$ at the nozzle outlet until $\Delta x = D/16$ at the far-field (see Fig. 1). A summary of the near-field grid sizes between the present mesh and those from similar past studies in Table 1 demonstrates comparable mesh densities along circumferential and streamwise directions respectively, and thus the constructed mesh is deemed sufficient for the intended numerical simulations on supersonic jets. Last but not least, a growth factor of no more than 1.15 was imposed upon the entire mesh domain to avoid abrupt changes in grid size between adjacent cells which may introduce unwanted numerical instabilities.

Studies	$\Delta r_{min...} \Delta r_{max}$	$\Delta x_{min...} \Delta x_{max}$	Cell Type	Re_D
Present study	$D/72...D/54$	$D/48...D/36$	Hexahedral	$\sim 10^6$
Vuorinen et al.[56]	$D/70...D/50$	$D/35...D/25$	Hexahedral	$\sim 10^5$
Munday et al.[17]	$D/50...D/35$	$D/50...D/35$	Hexahedral	$\sim 10^6$
Rana et al.[62]	$D/33$	$D/33$	Hexahedral	$\sim 2.4 \times 10^4$
Dauplain et al.[1]	$D/35...D/30$	$D/35...D/30$	Tetrahedral	$\sim 10^6$

Table 1 Comparison on the mesh density between the present and previous studies in region close to the nozzle outlet

2.2 Initial and boundary conditions

With a constant stagnation temperature, the supersonic jet flows can be perfectly-, over- or under-expanded at the nozzle exit depending on the exact NPR used. The expression for NPR and its relation to jet Mach number (Ma_j) are illustrated in Eq. 2-1 below:

$$NPR = \frac{P_t}{P_{atm}} = \left(1 + \frac{(\gamma - 1)}{2} Ma_j^2\right)^{\frac{\gamma}{\gamma - 1}} \quad (2-1)$$

where P_t and P_{atm} are the inlet total pressure and atmospheric pressure, respectively and $\gamma = 1.4$. Despite the fact that CD nozzles are designed to operate at perfectly-expanded conditions for optimal efficiency, the jet flow often experiences over- or under-expansion as it is susceptible to imperfections in manufacturing, physical fluctuations in the atmosphere and also large-scale disturbances in the flow. Consequently, it is necessary to investigate all three different jet flow conditions for a complete assessment of the solver performance with the presence (or the absence) of various shock systems. Since the CD nozzle in the present design underwent perfect-expansion at $NPR=3.4$, numerical simulations were performed with four different NPRs (i.e. $NPR = 2.8, 3.4, 4.0$ and 5.0), which corresponded to over-, perfectly-, moderately under- and highly under-expanded jet flows respectively.

Figure 2 Three-dimensional mesh topology for the present supersonic jet with (a) boundary conditions and (b) zoomed-in view on dense core and coarse outer layer

For these pressure-driven supersonic jet flows, total pressure and temperature are specified at the nozzle inlet and non-reflective conditions are applied to all far-field boundaries [i.e. left, circumference and right boundaries, as shown in Fig. 2(a).] It is worthwhile to highlight that non-reflecting boundary condition is crucial in preventing artificial pressure ‘build-ups’ adjacent to the boundaries, which could otherwise lead to unphysical phenomenon and numerical instability. Remarkably, there are a number of prescribed boundary conditions available for compressible high-speed flows in *OpenFOAM* and Table 2 lists the boundary conditions utilized for the present simulations in *OpenFOAM* terms.

	Pressure (P)	Velocity (U)	Temperature (T)
Nozzle Inlet	<i>'totalPressure'</i>	<i>'zeroGradient'</i>	<i>'totalTemperature'</i>
Far-field	<i>'waveTransmissive'</i>	<i>'waveTransmissive'</i>	<i>'zeroGradient'</i>

Table 2 Pressure, velocity and temperature boundary conditions for the numerical simulations of supersonic jet flows

2.3 The *RhoCentralFoam* solver

The presence of shocks and other flow discontinuities (e.g. slip lines) can be detrimental to the numerical stability and accuracy of compressible solvers, if the numerical flux schemes are not properly designed and implemented. *RhoCentralFoam*, on the other hand, is an explicit density-based solver implementing a central upwind flux scheme proposed by Kurganov and Tadmor [4] and Kurganov et al. [5], and is among one of the latest additions to *OpenFOAM*'s solver library to enhance its capability in modeling compressible flows with discontinuities. In a recent numerical study by Gutiérrez-Marcantonia et al. [35], *rhoCentralFoam* has demonstrated promising ability in capturing normal and oblique shocks in supersonic flows up to Mach number of 5. In this section, the theoretical background and implementation will be briefly outlined.

A general form of hyperbolic conservation laws can be written as:

$$\frac{\partial \mathbf{W}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{W}) = 0 \quad (2-2)$$

whereby $\mathbf{W} = \{W_1, K, W_n\}$ is the set of conserved variables and $\mathbf{F}(\mathbf{W})$ is the flux function.

Integrating Eq. 2-2 over the i^{th} control volume Ω_i with volume $|\Omega_i|$ yields

$$\frac{d\overline{\mathbf{W}}_i}{dt} = -\frac{1}{|\Omega_i|} \iiint_{\Omega_i} \nabla \cdot \mathbf{F}(\mathbf{W}) dV \quad (2-3)$$

where $\overline{\mathbf{W}}_i$ represents the cell average of $\mathbf{W}$ over Ω_i :

$$\overline{\mathbf{W}}_i \equiv \frac{1}{|\Omega_i|} \iiint_{\Omega_i} \mathbf{W} dV \quad (2-4)$$

In finite volume method, volume integral on the right-hand side of Eq. 2-3 can be transformed using Gauss Theorem into a surface integral over $\partial\Omega_i$, the surface of Ω_i . If Ω_i is a polyhedron with m faces, the surface integral can be approximated by performing a summation over the faces using the face centre values $\mathbf{W}_f$.

$$\iiint_{\Omega_i} F(\mathbf{W}) dV = \iint_{\partial\Omega_i} F(\mathbf{W}) \cdot d\mathbf{S} \approx \sum_f F(\mathbf{W}_f) \cdot \mathbf{S}_f \quad (2-5)$$

Note that $\mathbf{S}_f$ refers to the face area normal vector of face f of Ω_i .

2.2.1 URANS equations

The unsteady Reynolds-averaged Navier Stokes (URANS) equations can be cast in the general form of Eq. 2-2. It consists of mass, momentum and energy conservation equations. The flux function $F(\mathbf{W})$ is split into the inviscid component F_{inv} and the viscous component F_v which have to be handled differently.

$$\mathbf{W} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{bmatrix}, \quad F(\mathbf{W}) = \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \\ \rho E \mathbf{u} + p \mathbf{u} \end{bmatrix} - \begin{bmatrix} \mathbf{0} \\ \boldsymbol{\sigma} \\ \boldsymbol{\sigma} \cdot \mathbf{u} + \kappa_{eff} \nabla T \end{bmatrix} \quad (2-6)$$

As usual, ρ , $\mathbf{u}$, p and T refer to the density, velocity, pressure and temperature, respectively. The specific total energy E is the sum of the specific internal energy e and the specific kinetic energy $(\mathbf{u} \cdot \mathbf{u})/2$. Based on ideal gas law, $p = (\gamma - 1)\rho e$ whereby γ is the ratio of specific heat capacities taken to be 1.4.

The viscous-turbulent stress tensor $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} = \mu_{eff} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2I}{3} \nabla \cdot \mathbf{u} \right) \quad (2-7)$$

where μ_{eff} is the sum of the dynamic and turbulent/eddy viscosities, i.e. $\mu_{eff} = \mu + \mu_t$. The dynamic viscosity μ is computed as a function of temperature using the Sutherland transport model [58] while the turbulent viscosity μ_t is calculated using the two-equation $k - \omega$ shear stress transport (SST) turbulence model [25]. The $k - \omega$ SST model has been shown to produce reliable results for various transonic and supersonic flow phenomena in the numerical studies [6,19,20,40].

Similarly, the effective thermal conductivity κ_{eff} appearing in the energy equation is defined as $\kappa_{eff} = \kappa + \kappa_t$. The molecular thermal conductivity κ is obtained from the modified Eucken correlation and the turbulent thermal diffusivity $\kappa_t = c_p \mu_t / Pr_t$ where c_p is the specific heat capacity at constant pressure and Pr_t is the turbulent Prandtl number taken to be the default value of 1.0. In *rhoCentralFoam*, the heat conduction term $\kappa_{eff} \nabla T$ is expressed in a slightly different form as $\alpha_{eff} \nabla e$ whereby $\alpha_{eff} \equiv \kappa_{eff} / c_v$ (not to be mistaken for effective thermal diffusivity $\kappa_{eff} / \rho c_p$).

2.2.2 Computation of numerical fluxes

From Eq. 2-5, it is apparent that the fluxes have to be computed at each cell interface. The viscous flux F_v terms can be approximated using linear interpolation. The treatment of the inviscid flux terms is more involved. Due to the possible presence of discontinuities such as shocks and slip lines within the flow, the physical flux F_{inv} in Eq. 2-5 needs to be replaced by a numerical flux $\Phi(W_f^+, W_f^-)$. W_f^+ and W_f^- refer to the positive-sided and negative-sided interpolations of W at face f , respectively. The convention for positive (+) and negative (-) sides is determined by the direction of the face normal vector. In *OpenFOAM*, each face is assigned a unique face normal vector which points out from the owner cell (denoted as '+' side) and into the neighbour cell (denoted as '-' side) as illustrated in Fig. 3.

Figure 3 Definition of the '+' and '-' sides of an arbitrary cell in *OpenFOAM*

Therefore, $\mathbf{W}_f^+$ is the owner-biased interpolation while $\mathbf{W}_f^-$ is the neighbour-biased interpolation. It must be noted that this is opposite to the traditional convention whereby the cell into which the normal vector points to is taken to be the '+' side.

In *rhoCentralFoam* solver, the Kurganov-Noelle-Petrova (KNP) central upwind scheme [5] shown below is used as the numerical flux scheme.

$$\Phi^{KNP}(\mathbf{W}^+, \mathbf{W}^-) = \frac{a^+ F(\mathbf{W}^+) - a^- F(\mathbf{W}^-)}{a^+ - a^-} + \left(\frac{a^+ a^-}{a^+ - a^-} \right) [\mathbf{W}^- - \mathbf{W}^+] \quad (2-8)$$

Note that the sign convention in Eq. 2-8 differs from the original form [5] because of the aforementioned difference in the definition of '+' and '-' sides. Here, a^+ and a^- refer to the fastest wave-speeds along the face normal direction. As a result, a^+ should be interpreted as the fastest wave-speed in the direction of the face normal vector (towards the '-' side) and a^- as the fastest wave-speed in the direction opposite to the face normal vector (towards the '+' side). The wave-speeds are computed as follows.

$$a^+ = \max \{ \mathbf{u}^+ \cdot \mathbf{n}_f + c^+, \mathbf{u}^- \cdot \mathbf{n}_f + c^-, 0 \} = \max \{ u_n^+ + c^+, u_n^- + c^-, 0 \} \geq 0 \quad (2-9a)$$

$$a^- = \max \{ \mathbf{u}^+ \cdot \mathbf{n}_f - c^+, \mathbf{u}^- \cdot \mathbf{n}_f - c^-, 0 \} = \max \{ u_n^+ - c^+, u_n^- - c^-, 0 \} \leq 0 \quad (2-9b)$$

where c is the local speed of sound (i.e. $c = \sqrt{\gamma p / \rho}$) and $\mathbf{n}_f$ denotes the unit normal vector of the face.

2.2.3 Spatial interpolation and Total Variation Diminishing (TVD)

The owner- and neighbour-biased interpolation of variables is carried out using total variation diminishing (TVD) schemes [2]. For simplicity, the TVD interpolations at face f are given below for a scalar variable W .

$$W_f^+ = \overline{W}_O + (1 - w_f) \psi(r_{f,O}) (\overline{W}_N - \overline{W}_O) \quad (2-10a)$$

$$W_f^- = \overline{W}_N + w_f \psi(r_{f,N}) (\overline{W}_O - \overline{W}_N) \quad (2-10b)$$

$\overline{W}_O$ and $\overline{W}_N$ refer to cell averages of the owner and neighbour cells, respectively, and $W_f = w_f \overline{W}_O + (1 - w_f) \overline{W}_N$ refers to the linear interpolation of $\overline{W}_O$ and $\overline{W}_N$ at the face f using the central difference weights w_f and $(1 - w_f)$. The factor $r_{f,i}$ is a measure of the relative smoothness of the solution. $r_{f,i}$ is computed in *OpenFOAM* using following expression which is applicable to both structured and unstructured meshes [37]. $(\nabla W)_i$ refers to the gradient computed at cell i and $\mathbf{d}_{ON} \equiv \mathbf{x}_N - \mathbf{x}_O$ is the vector from the owner cell center to the neighbour cell center.

$$r_{f,i} = \frac{2(\nabla W)_i \cdot \mathbf{d}_{ON}}{\overline{W}_N - \overline{W}_O} - 1 \quad \text{where } i = O, N \quad (2-11a)$$

Since accurate capturing of shocks and discontinuities depend directly upon the interpolation, the van Leer limiter function was chosen for the study, as suggested by Greenshields et al. [11]:

$$\psi_{\text{van Leer}}(r) = \frac{|r| + r}{1 + r} \quad (2-11b)$$

2.2.4 Solution procedures

The URANS equations are solved sequentially. Variables with a superscript '0' refer to values from the current time step. Flux terms calculated using the KNP numerical flux scheme (Eq. 2-8) are indicated

with a superscript 'KNP'.

The mass conservation equation is solved first for density using explicit time discretization as shown below followed by its implementation in *OpenFOAM*.

$$\frac{\overline{\rho_i} - \overline{\rho_i^0}}{\Delta t} + \frac{1}{|\Omega_i|} \sum_f \Phi_{\rho}^{KNP} = 0 \quad (2-12a)$$

$$fvm::ddt(\rho) + fvc::div(phi) \quad (2-12b)$$

The momentum is solved next using an explicit predictor step for $\rho \mathbf{u}$ and an implicit corrector step for $\mathbf{u}$. Summing together the predictor and corrector steps yields the complete governing equation. In the following expressions, variables with a superscript '*' refer to predicted intermediate values. The predictor and corrector steps for momentum equation as well as their corresponding *OpenFOAM* implementations are given below.

i. Predictor step (explicit)

$$\frac{(\rho \mathbf{u})_i^* - (\rho \mathbf{u})_i^0}{\Delta t} + \frac{1}{|\Omega_i|} \sum_f \Phi_{\rho \mathbf{u}}^{KNP} = 0 \quad (2-13a)$$

$$fvm::ddt(\rho U) + fvc::div(phi U p) \quad (2-13b)$$

ii. Corrector step (implicit)

$$\frac{\overline{\rho_i \mathbf{u}_i} - \overline{\rho_i \mathbf{u}_i^*}}{\Delta t} - \frac{\overline{\rho_i^* \mathbf{u}_i} - \overline{\rho_i^0 \mathbf{u}_i^0}}{\Delta t} = \frac{1}{|\Omega_i|} \sum_f (\mu_{eff} \nabla \mathbf{u})_f \cdot \mathbf{S}_f + \frac{1}{|\Omega_i|} \sum_f \left[\mu_{eff} \left((\nabla \mathbf{u}^0)^T - \frac{2I}{3} \nabla \cdot \mathbf{u}^0 \right) \right]_f \cdot \mathbf{S}_f \quad (2-14a)$$

τ_{MC}

$$fvm::ddt(\rho, U) - fvc::ddt(\rho, U) = fvm::laplacian(\mu_{eff}, U) + fvc::div(\tau_{MC}) \quad (2-14b)$$

It is worth highlighting that the intermediate value for velocity $\overline{u_i^*}$ is computed as $\overline{u_i^*} = \overline{(\rho u)_i^*} / \overline{\rho_i}$.

Similarly, the energy equation is solved using an explicit predictor step for ρE and an implicit corrector step for e . These steps and their corresponding *OpenFOAM* implementations are given below.

i. Predictor step (explicit)

$$\frac{\overline{(\rho E)_i^*} - \overline{(\rho E)_i^0}}{\Delta t} + \frac{1}{|\Omega_i|} \sum_f \Phi_{\rho E}^{KNP} = \frac{1}{|\Omega_i|} \sum_f \left[\left(\mu_{eff} \left(\nabla u \right) + \tau_{MC} \right) \cdot u^0 \right]_f \cdot S_f \quad (2-15a)$$

$$fvm::ddt(\rho E) + fvc::div(phiEp) == fvc::div(sigmaDotU) \quad (2-15b)$$

ii. Corrector step (implicit)

$$\frac{\overline{\rho_i e_i} - \overline{\rho_i e_i^*}}{\Delta t} - \frac{\overline{\rho_i e_i^*} - \overline{\rho_i^0 e_i^0}}{\Delta t} = \frac{1}{|\Omega_i|} \sum_f (\alpha_{eff} \nabla e)_f \cdot S_f \quad (2-16a)$$

$$\begin{aligned} fvm::ddt(\rho, e) - fvc::ddt(\rho, e) == \\ fvm::laplacian(turbulence->alphaEff(), e) \end{aligned} \quad (2-16b)$$

Evaluation of the term $\sigma \cdot u$ in Eq. 2-15a requires the approximation of u^0 at the face f . This is achieved by using the weighting factors from the KNP flux scheme (Eq. 2-8) as shown below.

$$u_f^0 = \left(\frac{a^+}{a^+ - a^-} \right) u^{0+} + \left(\frac{-a^-}{a^+ - a^-} \right) u^{0-} \quad (2-17)$$

Lastly, the intermediate value of the specific internal energy $\overline{e_i^*}$ is computed as

$$\overline{e_i^*} = \overline{(\rho E)_i^*} / \overline{\rho_i} - (\overline{u_i} \cdot \overline{u_i}) / 2.$$

3 Results and Discussion

3.1 Mesh independence study

To investigate the effects of mesh density on the simulation performance of *rhoCentralFoam*, as well as to ensure that the final results are independent of the mesh size, a mesh independence study was first carried out with a single NPR of 4. Since the jet flow is moderately under-expanded with the formation of shock structures at this particular NPR (recall that the CD nozzle in the present design undergoes perfect expansion at NPR=3.4), it is regarded as a meaningful representative of the supersonic jet flows with discontinuities for the mesh independence study.

Beginning with a relatively coarse mesh setup of approximately 20million cells, two levels of global refinement were applied with an increment factor of approximately 1.2 between successive meshes. For consistency in modeling the boundary layer development along the nozzle wall, the first cell distance to the nozzle wall was maintained constant throughout the CD nozzle such that the wall y -plus was estimated to be approximately $y^+ \approx 3$ at the nozzle exit. Moreover, more than 20 cells were allocated in the viscous sub-layer regardless of the mesh refinement level. Furthermore, the present simulations were marched explicitly in time (*since rhoCentralFoam is an explicit solver*) and the physical time step (Δt) was limited such that the maximum Courant number did not exceed 0.5. This is to prevent any numerical instabilities being produced across the flow discontinuities, which could deteriorate the solution accuracy. Finally, solution convergence was achieved after three ‘flow-through’ periods (i.e. time estimated for the jet core to convect from exit to end of simulation domain) and the changes in maximum centerline velocity were determined to be within 0.5% between two consecutive iterations [34]. Interestingly, such small time steps, as mandated by the supersonic flow velocity and the much refined mesh size along the jet core, also help alleviate possible instabilities associated with numerical stiffness in regions of low flow speed (i.e. Mach < 0.3) [15]. On the other hand, if only steady-state (or

fully developed) solutions are of interest, an implicit solver, either steady-state or transient, becomes computationally more efficient since a much larger time step can often be used to achieve converged solutions. However, preconditioning of the solution matrices is essential when simulating ‘all-speed’ flows with such implicit solver, due to the possible presence of numerical stiffness at low speed regions. For instances, it is noteworthy that Shen et al. [14, 15] have successfully incorporated preconditioning schemes into a modified a *DensityBasedTurbo* solver in *OpenFOAM*, such that the modified solver is capable of simulating ‘all-speed’ flow problems with desired accuracy and efficiency.

Figure 4 shows comparisons of both the jet exit velocity profiles and jet centerline velocity developments in terms of Mach number for all three meshes. Good agreements can be observed between the three meshes (i.e. coarse, 1st refinement and 2nd refinement) and furthermore, the predicted averaged exit velocity at $Ma \approx 1.46$ corresponds reasonably well with the design Mach number of 1.45. The satisfactory convergence on the mesh independence test corroborates the findings by Dauplain et al. [1], in which they have conducted a similar test on an impinging supersonic jet and concluded that stable shock structures can be captured with a mesh size of approximately $D/30$.

Though a closer examination of the comparison reveals some small and yet noticeable differences in the centerline velocity development towards the end of the potential core between the meshes [see Fig. 4(b)], the magnitude differences remain relatively insignificant and the discrepancy quickly subsided over a short downstream distance (about $2D$ from the end of potential core). Therefore, mesh density equivalent to the first refinement (approximately 24million cells) was subsequently adopted for simulating the supersonic jet flows at other NPRs.

Figure 4 Mesh independence study of the under-expanded supersonic jet flows at $NPR=4$

3.2 Overall shock structures and first shock cell length

When the actual NPR deviates from the designed value, a system of shocks emanating from the nozzle lip would be produced within the jet potential core. Figure 5 shows the isometric view of the Mach number contour for $NPR=2.8, 3.4, 4$ and 5 . Note that the contours are clipped along the nozzle centre plane to reveal the near-field shock structures more clearly. Since the formation and development of the shock structures of an imperfectly-expanded supersonic jet have been discussed extensively in the past literatures [3,21,38,39], only the most pertinent features will be highlighted here.

At $NPR=2.8$, the jet flow at the CD nozzle exit expands below the atmospheric pressure (i.e. over-expanded) and thus, immediately undergoes compression through the steep oblique shocks originating from the nozzle lip with a Mach disk forming symmetric about the jet centerline. This is followed by a series of periodic expansion and compression events until the pressure of the jet core reaches equilibrium with the atmosphere, as can be observed in Fig. 5(a). When the NPR increases to 3.4 in Fig. 5(b), the perfectly-expanded jet flow is essentially free of discernible shock structures within the jet

Figure 5 Near-field shock structures of the supersonic jet flows at NPR=2.8, 3.4, 4 and 5

potential core. Further increasing the NPR values will again result in the formation of periodic shock cells similar to those observed at over-expanded condition, as can be seen from Figs. 5(c) and (d). However, being under-expanded at the nozzle exit for both NPR=4 and 5, the jet flows first expand through Prandtl-Meyer expansion waves before turning towards the oblique shocks and Mach disk, giving rise to the differences in the shape and length of the shock cells between over- and under-expanded conditions [39]. Furthermore, it is also interesting to note that the boundary of the shock cell of the largest NPR exhibits a ‘barrel’-like shape, which is a distinct flow feature for highly under-expanded supersonic jet. In their comprehensive survey and review of under-expanded supersonic jet flows, Franquet et al. [21] determined that moderately under-expanded free jet flows were achieved typically with $2 \lesssim NPR \lesssim 4$, while highly under-expanded ones ranged from $4 - 5 \lesssim NPR \lesssim 7$. Clearly, observations on the shock structures from the present RANS simulations are consistent with the results

from past studies, which provides confidence for subsequent quantitative comparisons with the experimental measurements.

As shown in Fig. 6, the distances from the nozzle exit to the first Mach disk were estimated from both the RANS simulation results and experimental Schlieren images captured using in-house facilities for the imperfectly-expanded condition. Note that the distance is non-dimensionalized with the nozzle exit internal diameter. It should also be highlighted that when a Mach disk is not present for a moderately under-expanded jet flow (i.e. $NPR=4$), the intercepting point of the two oblique shocks is used for the distance measurement instead, where they can be clearly identified from both numerical and experimental results. Generally speaking, the simulation results agree quite well with the experimental Schlieren images, though simulations slightly over-predict the first shock cell length regardless of the exit conditions. The consistent over-estimation of the shock cell length in numerical simulations could be attributed to the use of Reynolds-averaged two-equation $k-\omega$ SST model, which is known to under-predict shear flows with strong velocity and pressure gradients, leading to a possibly longer jet potential core [9,19,51]. Nonetheless, the predicted lengths are deemed to be satisfactory since the differences in the magnitude remain to be no more than 4% from the experimental measurements.

Moreover, the accuracy of the simulation results in capturing near-field shock structures can also be validated with a comparison of the jet centerline velocity with quantitative digital particle image velocimetry (DPIV) measurements conducted for the over-expanded condition [27]. As seen from Fig. 7, both jet flows undergo a series of expansion and compression immediately after the nozzle exit with comparable periodicity and length in the developmental cycle. It should be highlighted that only the gross trends in the centerline velocity development are compared and discussed here to complement

Figure 6 Comparison of the distance from CD nozzle exit to the Mach disk for over- and under-expanded jet flows between (a) experimental Schlieren measurement (these Schlieren images were captured using in-house facilities) and (b) RANS simulations in *rhoCentralFoam*

the validation from Schlieren images because DPIV measurements of supersonic flows are highly sensitive towards seeding conditions and flow discontinuities, which made measurements inherently challenging [26]. Nonetheless, the comparison here sufficiently demonstrates the ability of the present simulations to capture both the shock occurrences and the drastic velocity variations across them.

Figure 7 Comparison of the jet centerline velocity developments between numerical simulation and DPIV measurement (Lim et al., [27]) within the first two shock cell for over-expanded condition (NPR=2.8).

3.3 Streamwise velocity decay

Besides the near-field shock structures of the supersonic jet flows which *rhoCentralFoam* has captured relatively accurately, another important aspect in assessing numerical accuracy of a free jet flow pertains to the streamwise velocity decay, which is a useful indicator on the jet mixing characteristics. Figure 8 compares the velocity profiles extracted at five locations of $x/D=1, 2, 4, 7$ and 10 downstream of the nozzle exit from simulation results with those derived experimentally from Pitot tube measurements [59] at over-expanded (NPR=2.8) and moderately under-expanded (NPR=4) conditions, respectively. Note that the profiles are differentiated by shifting each of the downstream locations to the right with a magnitude of 2 and two NPRs are selected for comparisons here to highlight the contrasting jet exit conditions.

Firstly, it can be observed from Fig. 8 that the velocity profiles transit gradually from a sharp ‘top-hat’ like shape into a ‘parabola’ like shape with increasing jet widths for both of the NPRs –a direct consequence to the continuous entrainment and mixing of the jet flows with ambient fluid as they convect downstream. This is typical of a free jet being exhausted into a quiescent medium [22,33,47,54].

Figure 8 Comparison of the velocity profiles extracted at locations of $x/D=1, 2, 4, 7$ and 10 downstream of the nozzle exit from both numerical simulations and experimental Pitot tube measurements (Wei et al., [59]) for (a) over-expanded $NPR=2.8$ and (b) under-expanded $NPR=4$

Secondly, the velocity profiles from the simulation results generally agree very well with the experiments up to $x/D=10$ distance downstream for both NPRs. However, a closer examination reveals that while the two profiles remain close to each other throughout the locations for the over-expanded condition, discrepancies grow larger with increasing downstream distance for the under-expanded test case. This could be due to the relatively larger errors arising from the flow passing through stronger periodic shocks in the under-expanded case, which subsequently accumulate over the distance. Thirdly, observing the jet velocity further away from the symmetry (i.e. $y=0$) beyond $x/D=4$ downstream, results from the numerical simulations decrease more slowly (eventually to nearly zero in regions where mixing does not take place) than those from the Pitot tube measurements regardless of the NPRs used, which indicate a greater jet spread predicted by *rhoCentralFoam*.

To confirm that *rhoCentralFoam* predicts a greater extent of the jet spread into the ambient fluid, Mach contour lines are further extracted from the simulation results and plotted together with Pitot tube measurements [59], as shown in Fig. 9. Clearly when the velocity along the shear layer drops to a merely fraction of the centerline velocity (i.e. approximately below $Mach = 0.3$ in the figure), the

Figure 9 Comparison of the near-field Mach contour lines along the jet centre plane derived from both numerical simulations and experimental Pitot tube measurements (Wei et al., [59]) for (a) over-expanded NPR=2.8 and (b) over-expanded NPR=4

simulation results deviate progressively from the experiments with a wider jet spread away from the jet symmetry. Moreover, the discrepancies are found to be greater for the under-expanded jet flow, which corroborates the observations made from streamwise velocity decay in Fig. 8.

3.4 Shear layer development

Mixing behavior and characteristics along the shear layer of a free jet can also be accurately represented and examined through flow quantities such as the turbulent kinetic energy or the Reynolds shear stress. Fortunately, by using $k-\omega$ SST RANS model, turbulent kinetic energy (k) is evaluated during the solution process and explicitly available as an output variable. It is however significantly more difficult to obtain highly accurate turbulent kinetic energy experimentally due to inherent experimental limitations. Still, some useful quantitative information of the jet shear layer can be explored based through time-averaged Schlieren images and subsequently used for validating the numerical results. Take for instance, the approximate angle at which the jet shear layers grow outwards after being exhausted into the ambient.

Figure 10 shows the turbulent kinetic energy contour maps for all four NPRs from the RANS results. Both the magnitude of turbulent kinetic energy along the shear layer and the length of the jet potential core, as indicated by the merging point of the two shear layers, increase with increasing NPR value. This is within expectation since the jet flow velocity is directly proportional to its nozzle pressure ratio. More importantly, the jet shear layers appear to grow in a relatively linear manner over $x/D=12$ downstream distance regardless of the jet exit conditions, which is in accordance with both the experimental observations by Papamoschou and Roshko [18] and the time-dependent RANS simulations by Rona and Zhang [5]. The latter argued that a uniform growth rate (i.e. linear growth) of the jet shear layers would be expected when jet flapping and high-frequency asymmetric screech mode were removed, or in this case, averaged.

Following from the good overall agreements, the shear layer growth angles are estimated from the turbulent kinetic energy results with an outlining criterion at 10% of the maximum turbulent kinetic energy level. The angles are subsequently compared with those determined from time-averaged Schlieren images through similar image processing techniques. Table 3 summarizes the differences between simulation and experimental results captured using in-house facilities. Coupled with $k-\omega$ SST turbulence model, *rhoCentralFoam* consistently over-predicts the angle of shear layer growth, though still within an acceptable range of no greater than 8%. The reason for such over-predicted characteristics are two-fold - Firstly, the Reynolds-averaged turbulent model hardly captures any coherent structures developed along the shear layers. Instead the turbulent mixing effect is averaged and numerically diffused across several cells. Secondly, additional numerical diffusion is introduced with TVD schemes, which are essential in ensuring numerical stability across flow discontinuities. Therefore, to achieve better accuracy in modeling the jet shear layer development requires high-order numerical

Figure 10 Growth of the jet shear layers at exit conditions of (a) over-expanded NPR=2.8, (b) perfectly-expanded NPR=3.4, (c) moderately under-expanded NPR=4 and (d) highly under-expanded NPR=5. The angles are estimated based on turbulent kinetic energy k .

Nozzle Pressure Ratio	Estimated shear layer growth angle (degree)	
	<i>rhoCentralFoam</i> simulation	Experimental Schlieren
NPR2.8	5.9	5.7
NPR3.4	5.8	5.6
NPR4.0	5.4	5.2
NPR5.0	5.4	5.0

Table 3 Growth angle of the jet shear layer determined from both numerical simulation and experimental Schlieren images captured using in-house facilities.

schemes with significantly less numerical diffusion, especially so when compressibility effects become significant at high NPR values, which possibly explains the larger discrepancies observed between simulation and experimental results at NPR=5 [7,44]. Nevertheless, the present simulations based on $k-\omega$ SST model are deemed sufficient for a quick exploration on the shear layer development and mixing characteristics at the near-field region of a supersonic jet flow with shocks.

3.5 Scalability on High Performance Computing cluster

Similar to the parallel scalability study conducted by Robertson et al. [50] on incompressible solvers in *OpenFOAM*, a scalability study was performed using clusters from National Supercomputing Centre of Singapore (NSCC). The simulation domain was decomposed into corresponding number of sub-domains with the default '*hierarchical*' method in *OpenFOAM* and the actual simulation was run for a physical time of '2e-05' seconds from the fully developed solution and subsequently the consumed CPU core time was logged in the system and scaled according to the number of CPU cores. Figure 11 shows the speed increase in multiples of 24 (i.e. each computing node in the cluster has 24 cores) against the number of cores employed in parallel computation. *RhoCentralFoam* solver in *OpenFOAM* exhibits promising scalability over a range of core numbers with 24million cells. As can be seen from the figure, the speed-up grows almost linearly with number of cores paralleled from 96 to 288 cores: below 96 cores, it becomes computationally saturated with each core having more than 250K cells and beyond 288 cores on the other hand, time is spent unnecessarily on inter-core communication. Hence, the present scalability test suggests that the range of cell counts to be allocated to each core lies within ' $117K < \text{No. of cells per core} < 250K$ '. Interestingly, this is remarkably close to the range of ' $110K < \text{No. of cells per core} < 230K$ ' determined by Robertson et al. [50]. So, the determined range is likely a plausible choice for parallelizing default 2nd-order solvers and even a reasonable starting point for customized high-order solves in *OpenFOAM*.

Figure 11 Scalability of *rhoCentralFoam* solver with the present structured mesh (approximately 24million cells) on NSCC cluster

3.6 Comparison of *rhoCentralFoam* solver with commercial CFD solver

Last but not least, a brief comparison between a well-established commercial CFD solver (ANSYS Fluent™ v18.2) and *rhoCentralFoam* solver is carried out to complete the assessment on the numerical accuracy and stability of *rhoCentralFoam*. Several steps were taken to ensure an appropriate and consistent comparison between the two solvers. First of all, simulation domain and its associated mesh topology identical to the one used in *rhoCentralFoam* was created and loaded into the commercial CFD solver. Secondly, total pressure and pressure far-field were imposed as the inlet and outlet boundary conditions, respectively. Thirdly, a monotonicity-preserving ASUM-based flux scheme [42,43] was activated to capture discontinuities in the flow with 2nd-order accuracy. Lastly, a courant number limit of 0.5 was used to achieve desirable solution convergence at every time step, similar to the adjustable time step control in *rhoCentralFoam*.

As seen from Fig. 12, good overall agreement can be observed between the two solvers for both over- and under-expanded jet flows, in terms of the near-field shock structures, the extent and width of the jet mixing as well as the approximate length of the jet potential core. Nevertheless, there exist a number

Figure 12 Comparison of the Mach number contour along the jet centerline plane extracted from (a) commercial solver ANSYS FluentTM and (b) *rhoCentralFoam* solver for over- and under-expanded jet exit conditions

of distinct differences between the results as well. Take for instance, the predicted jet velocity is relatively higher in the commercial solver at NPR=2.8. Recall that the velocity profiles extracted from *rhoCentralFoam* at various downstream locations match quite well with the experimental measurements [see Fig. 8(a)], thus the predicted jet velocity from the commercial solver may differ more significantly from the experimental measurements in over-expanded conditions. In addition, a slight asymmetry in the jet spread can be discerned for the commercial solver result at NPR=5. Such asymmetry could be due to a small but lopsided pressure 'build-up' close to the far-field boundary, which in return feeds inadvertently to the flow asymmetry.

Figure 13 Comparison of the CPU core time consumption between *rhoCentralFoam* and ANSYS Fluent™ running in parallel with similar numerical set-ups.

Last but not least, Figure 13 shows the comparison on the CPU core time used between *rhoCentralFoam* and ANSYS Fluent™ solvers for simulating the jet flows in parallel with 48, 72 and 96 cores, respectively. A total number of 2000 iterations were run from the fully-developed solution in both solvers, using explicit time marching with a constant time step of ' $1e-09$ ' second and the recorded core consumptions were scaled with the simulation that expended the longest core time (i.e. *rhoCentralFoam* with 48 cores). It can be observed that ANSYS Fluent™ solver performs noticeably faster with 48 cores than *rhoCentralFoam*, and remains to be more efficient when the number of cores increases to 72, though the differences narrow between the two. This can be possibly attributed to both the optimized parallelization architecture in ANSYS Fluent™ and the poor performance of *rhoCentralFoam* solver when the individual core becomes computationally saturated. Further increasing the number of cores to 96 will see significant improvement in parallel performance of both solvers, but more importantly, *rhoCentralFoam* becomes equally efficient as its ANSYS Fluent™ counterpart. In fact, a closer examination reveals that *rhoCentralFoam* solver performs fractionally faster at 96 cores in the present test. Recall from the scalability study earlier that *rhoCentralFoam* exhibits optimal parallel performance

approximately from 96 cores to 288cores (see Fig. 11). Hence, the comparison corroborates further with the findings in the scalability study where a range of ' $117K < \text{No. of cells per core} < 250K$ ' is recommended for *rhoCentralFoam* solver, based on the present simulations of supersonic jet flows.

4 Conclusions

In the present study, RANS simulations on round supersonic free jets are performed based on *rhoCentralFoam* solver in *OpenFOAM*. To assess the numerical stability and accuracy of the density-based *rhoCentralFoam* solver towards different exit conditions, four NPRs of 2.8, 3.4, 4 and 5 are specified at the nozzle inlet, corresponding to over-, perfectly-, moderately under- and highly under-expanded conditions, respectively.

The development of the shock structures at imperfectly expanded conditions is in good agreement qualitatively with the studies in the past literature, in which the jets experience periodic compression and expansion to form a series of shock cells. More importantly, though numerical simulations consistently over-estimate the lengths of the first shock cell as compared to experimental Schlieren images, the discrepancies remain within 4%. This observation is further confirmed by overlapping the simulated jet centerline velocity results with DPIV measurements. Hence, *rhoCentralFoam* is capable of accurately predicting the overall shock structures of the supersonic jet flows for all the NPRs tested.

Subsequently, velocity profiles along downstream locations of $x/D=1, 2, 4, 7$ and 10 are extracted and compared with the experimental Pitot tube measurements. Quantitatively, the streamwise velocity decay is found to agree quite well at both the over- and moderately under-expanded conditions. However, the differences increase with increasing NPR value, possibly due to greater numerical errors in resolving stronger shocks (and hence greater flow discontinuities) in the jet flow. Moreover, the

predicted growth angles of the jet shear layers are greater than those derived from experimental Schlieren images. Particularly, the discrepancy becomes noticeable at approximately 10% as the jet flow becomes highly under-expanded. This could be attributed to strong compressibility effects along jet shear layers which the low order flux scheme coupled with RANS turbulence model do not capture well.

As part of the overall assessment, a scalability study was conducted and the results suggest that *rhoCentralFoam* solver exhibit excellent scalability when each core is allocated with ' $117K < \text{No. of Cores} < 250K$ '. Interestingly, the finding coincides very well with the study conducted by Robertson et al. [49] on incompressible solvers in *OpenFOAM*. Last but not least, a brief comparison between the results from *rhoCentralFoam* and the commercial CFD solver, ANSYS FluentTM, reveals that *rhoCentralFoam* performs equally well or even better in modeling supersonic jet flows with comparable parallel performance at recommended core loads.

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