THE ARION UNSTRUCTURED GRIDS CFD SOLVER: THEORETICAL AND USER'S MANUAL

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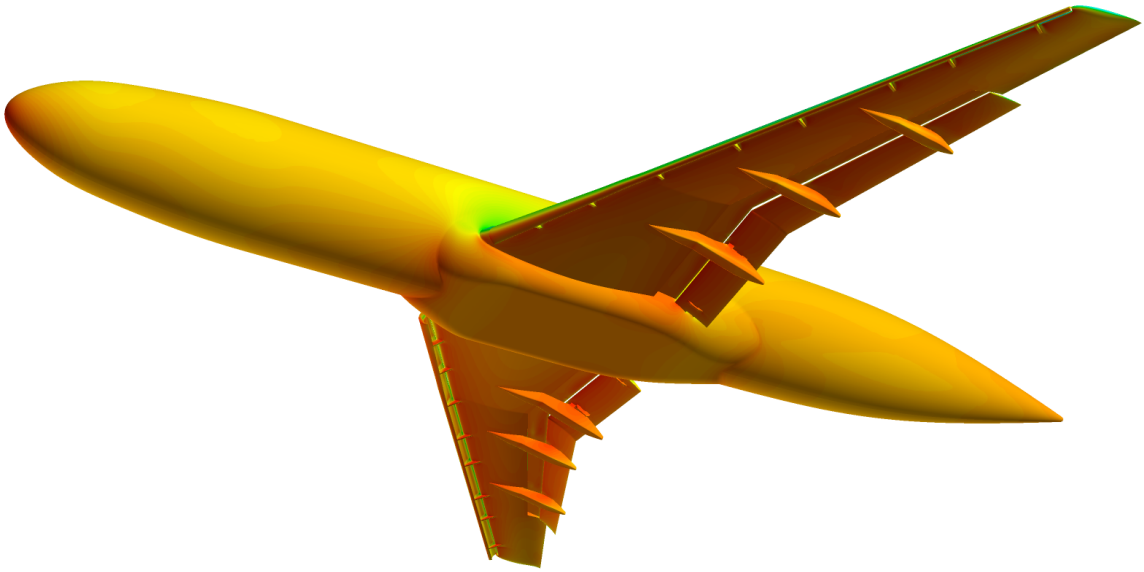

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Abstract

This manual describes the algorithms, methods, and input and output files of the **Arion** code. In addition, the manual serves as the user's manual of the code. The current version of the code has gone through a major revision. As of the current version, the code provides the capability to simulate inviscid, laminar, or turbulent steady flows of single-component or multi-component gas. Currently, the flow solver contains the HLLC approximate Riemann solver, the AUSM$^+$-up scheme, or the AUSM-DV schemes for the approximation of the convective fluxes. Turbulence may be modeled using either the k$-\omega$-TNT, the k$-\omega$-SST, or the Spalart-Allmaras turbulence models. The code provides the capability to simulate the flow of any perfect gas under a chemical equilibrium assumption. Near future versions of the code will support simulations under a chemical non-equilibrium assumption. The code is fully parallel using a distributed architecture. Domain decomposition is carried out using the Metis open source library. Convergence acceleration is obtained using a Krylov solver and a line search algorithm.

Chapter 1

Introduction

The **Arion** code is the Israeli CFD Center flow solver for unstructured grids. Along recent years, computational capabilities have been ported from the EZAir Suite of codes into the **Arion** code. This process shall continue in coming months and years at an accelerated pace. In addition, new capabilities are being introduced into the **Arion** code. The goal is to obtain a versatile flow solver that would possess the entire capabilities that the EZAir Suite of codes possesses. This manual describes the algorithms, methods, and input/output files of the **Arion** code. In addition, the manual serves as the user's manual of the code.

1.1 Current Release

The current version of the code has gone through a major revision. As of the current version, the code provides the capability to simulate inviscid, laminar, or turbulent steady flows of single-component or multi-component gas. Currently, the flow solver contains the HLLC approximate Riemann solver, the AUSM$^+$-up scheme, or the AUSM-DV schemes for the approximation of the convective fluxes. Turbulence may be modeled using either the k$-\omega$-TNT, the k$-\omega$-SST, or the Spalart-Allmaras turbulence models. The code provides the capability to simulate the flow of any perfect gas under a chemical equilibrium assumption. Near future versions of the code will support simulations under a chemical non-equilibrium assumption. The code is fully

parallel using a distributed architecture. Domain decomposition is carried out using the Metis open source library. Convergence acceleration is obtained using a Krylov solver and a line search algorithm.

1.2 Users's Manual Arrangement

The report is arranged in the following manner: Chapter 2 contains a description of the available physical models while Chapter 3 describes the turbulence models that are used in the code. Chapter 4 is dedicated to a detailed description of the computational methods. Chapter 5 briefly describes the boundary conditions while Chapter 6 describes the type and format of unstructured meshes that the code supports. Chapter 7 describes the parallelization of the code. Finally, Chapter 8 contains a detailed description of the input file syntax, and actually serves as the code's reference manual.

Chapter 2

Physical Models

2.1 Introduction

Computer simulations are generally based upon the numerical solution of the model equations in a discretized mode. The accuracy of the computations depends mainly on the physical modeling, the numerical algorithms, and the quality of the computational mesh. At its current developmental stage, the **Arion** code provides the capability to simulate single-component perfect gas flows, or multi-component perfect gas flows under chemical equilibrium. This chapter contains a description of the physical models that are available in the solver.

2.2 Single-Component Perfect Gas (SPG)

2.2.1 Governing Equations

The equations governing single-component, perfect gas fluid flow are derived from the laws of conservation of mass, momentum, and total energy. The set of five partial differential equations is known as the Navier-Stokes equations and can be represented in a conservation-law form that is convenient for numerical simulations, namely

$$\frac{\partial Q}{\partial t} + \frac{\partial \left(E_c - E_d\right)}{\partial x} + \frac{\partial \left(F_c - F_d\right)}{\partial y} + \frac{\partial \left(G_c - G_d\right)}{\partial z} = 0 \tag{2.1}$$

where Q is the vector of conserved mass, momentum, and energy

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{bmatrix} \tag{2.2}$$

where the density is denoted by ρ, the Cartesian velocity vector components are denoted by u,v and w, and E denotes the total (internal and kinetic) energy of the gas. The inviscid flux vectors, E_c, F_c, and G_c, are

$$E_c = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u\left(E + p\right) \end{bmatrix}, \quad F_c = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v\left(E + p\right) \end{bmatrix}, \quad G_c = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w\left(E + p\right) \end{bmatrix} \tag{2.3}$$

and the viscous flux vectors, E_d, F_d, and G_d, are

$$E_d = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yx} \\ \tau_{zx} \\ \beta_x \end{bmatrix}, \quad F_d = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{zy} \\ \beta_y \end{bmatrix}, \quad G_d = \begin{bmatrix} 0 \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{zz} \\ \beta_z \end{bmatrix} \tag{2.4}$$

where

$$\begin{aligned}
\tau_{xx} &= \lambda\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)+2\mu\frac{\partial u}{\partial x}\\
\tau_{yy} &= \lambda\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)+2\mu\frac{\partial v}{\partial y}\\
\tau_{zz} &= \lambda\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)+2\mu\frac{\partial w}{\partial z}\\
\tau_{xy} &= \tau_{yx} = \mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\\
\tau_{xz} &= \tau_{zx} = \mu\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)\\
\tau_{yz} &= \tau_{zy} = \mu\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)\\
\beta_x &= u\tau_{xx}+v\tau_{xy}+w\tau_{xz}+\kappa\frac{\partial T}{\partial x}\\
\beta_y &= u\tau_{yx}+v\tau_{yy}+w\tau_{yz}+\kappa\frac{\partial T}{\partial y}\\
\beta_z &= u\tau_{zx}+v\tau_{zy}+w\tau_{zz}+\kappa\frac{\partial T}{\partial z}
\end{aligned} \tag{2.5}$$

where T is the temperature. Stokes hypothesis, $\lambda = -\frac{2}{3}\mu$, is typically used to further simplify Equation (2.5).

Finally, in the perfect-gas model, the source-term vector, S, may only contain contributions from the turbulence model (see Chapter 3).

2.2.2 Integral Form For Moving Grids

For a three-dimensional flow through a finite volume Ω, enclosed by the boundary surface $\partial\Omega \equiv S$ that is moving with a grid velocity $\overline{V}_g$, the integral form of the conservation equations in an inertial frame of reference is given as:

$$\frac{\partial}{\partial t}\int_{\Omega} Q d\Omega + \oint_{S} d\overline{S}\cdot\overline{H} = 0 \tag{2.6}$$

where

$$\overline{H} = (E_c - E_d)\,\hat{i} + (F_c - F_d)\,\hat{j} + (G_c - G_d)\,\hat{k} \tag{2.7}$$

In Equation (2.6) the vector of dependent variables, Q, remains as in Equation (2.2).Similarly, the viscous flux vectors, E_d, F_d, and G_d, appearing in Equation (2.7), remain as in Equations (2.4) and (2.5) (see Section 2.2.1). In contrast, the inviscid flux vectors

take a form that reflects the motion of the grid as follows:

$$
\begin{aligned}
E_c &= \begin{bmatrix} \rho\left(u-u_g\right) \\ \rho u\left(u-u_g\right)+p \\ \rho v\left(u-u_g\right) \\ \rho w\left(u-u_g\right) \\ \left(E+p\right)\left(u-u_g\right)+u_g p \end{bmatrix} \\
F_c &= \begin{bmatrix} \rho\left(v-v_g\right) \\ \rho u\left(v-v_g\right) \\ \rho v\left(v-v_g\right)+p \\ \rho w\left(v-v_g\right) \\ \left(E+p\right)\left(v-v_g\right)+v_g p \end{bmatrix} \\
G_c &= \begin{bmatrix} \rho\left(w-w_g\right) \\ \rho u\left(w-w_g\right) \\ \rho v\left(w-w_g\right) \\ \rho w\left(w-w_g\right)+p \\ \left(E+p\right)\left(w-w_g\right)+w_g p \end{bmatrix}
\end{aligned}
\tag{2.8}
$$

where u_g, v_g, and w_g are the Cartesian components of the grid velocity vector $\overline{V}_g$. Note that currently the grid velocity vector is set to $\overline{V}_g \equiv 0$.

2.2.3 Equation of State

To close the system of fluid dynamics equations, it is necessary to establish relations between the thermodynamics variables, p, ρ, T, and the internal energy, e_I. Assuming a perfect gas, the pressure and temperature may be obtained from the following equation of state:

$$p = \rho R T \tag{2.9}$$

where R is the gas constant ($R = 287.0$ for air). By assuming further that the gas is a calorically perfect gas (and hence the specific heats C_p and C_v are constant), the

equation of state takes the form:

$$p = \rho\,(\gamma - 1)\,e_I \tag{2.10}$$

where e_I is the internal energy of the gas, and γ is the (constant) ratio of specific heats (c_p/c_v). In terms of the flow variables, the pressure and temperature are calculated using:

$$\begin{aligned} p &= (\gamma - 1)\left[E - \frac{1}{2}\rho\left(u^2 + v^2 + w^2\right)\right] \\ T &= \frac{\gamma - 1}{R}\left[e - \frac{1}{2}\left(u^2 + v^2 + w^2\right)\right] \end{aligned} \tag{2.11}$$

where $e = \frac{E}{\rho}$ is the specific total energy.

2.2.4 Transport Properties

In addition to the equation of state, it is also necessary to establish constitutive relations, namely, relations for the coefficient of viscosity, μ, and the coefficient of thermal conductivity, κ. In the single-component perfect gas (SPG) model, the Sutherland formulae are exclusively used to evaluate these coefficients. The **Arion** code provides two different ways to evaluate μ and κ.

The first (called "molecular.sutherland.air.1", see Table 8.14) is based on the following relations:

$$\begin{aligned} \mu &= C_{\mu_1}\frac{T^{\frac{3}{2}}}{T + C_{\mu_2}} \\ \kappa &= C_{\kappa_1}\frac{T^{\frac{3}{2}}}{T + C_{\kappa_2}} \end{aligned} \tag{2.12}$$

The default of the coefficients C_{μ_1}, C_{μ_2}, C_{κ_1}, and C_{κ_2} correspond to air and are given in Table 2.1. For the purpose of simulating a gas whose transport properties are different than air, the coefficients can be set by the user using the directives as described in Tables 8.17, 8.18, 8.19, 8.20.

Fluid type	C_{μ_1}	C_{μ_2}	C_{κ_1}	C_{κ_2}
Air	1.458×10^{-6}	110.4	2.495×10^{-3}	194

Table 2.1: Default coefficients for Sutherland formulae (type 1)

The second way to evaluate μ and κ (called "molecular.sutherland.air.2", see Table 8.14) is based on the following relations:

$$\begin{aligned} \mu &= \eta_0 \frac{T_0 + C_0}{T + C_0} \left(\frac{T}{T_0} \right)^{\frac{3}{2}} \\ \kappa &= \frac{c_p \mu}{Pr} \end{aligned} \tag{2.13}$$

where P_r is the Prandtl number. The default of the coefficients η_0, T_0, and C_0 correspond to air and are given in Table 2.2. The coefficients can be set by the user using the directives as described in Tables 8.21, 8.22, 8.23, and 8.24.

Fluid type	η_0	C_0	T_0	P_r
Air	1.827×10^{-5}	120	291.15	0.72

Table 2.2: Default coefficients for Sutherland formulae (type 2)

2.3 Multi-component Gas (MCG)

High-speed flows contain physical phenomena that generally may not be modeled by the perfect gas form of the Navier-Stokes equations presented in Section 2.2. Such phenomena include chemical and thermal non-equilibrium, vibrational and electronic excitation, and ionization. These phenomena require the use of a "real gas" model. This section presents the extended form of the Navier-Stokes equations governing the flow of a general gas in chemical and thermal non-equilibrium, and the thermodynamic and transport models that are used to describe the gas. Focus is given to the numerical algorithms that are used in the solution of the extended Navier-Stokes equations and

the finite-rate chemical kinetics and energy relaxation models that are employed to model non-equilibrium flow.

2.3.1 Basic Assumptions

The flow is modeled assuming that the continuum approximation is valid. Thermal equilibrium (*i.e.*, all energy modes are described by a single temperature) is assumed for general gases. For simulations involving air, the *two-temperature model* of Park [1] is employed to account for vibrational and electronic non-equilibrium. According to the two-temperature model, the translational and rotational energy modes are described by the translational temperature, T, while the vibrational and electronic energy modes of all species and the electron translational energy mode are described by a second temperature, denoted by T_v. The latter assumption considerably simplifies the system of equations by eliminating additional translational and vibrational energy equations for each polyatomic species and an energy equation for the free electrons. This model was shown to provide accurate results for aerodynamic coefficients and convective heat transfer rates in external flows of air at Mach numbers exceeding 20 [2]. It is therefore assumed adequate for the problems considered for simulation with the present code.

2.3.2 Governing Equations

Under the above assumptions, the extended three-dimensional Navier-Stokes equation set may be expressed in Cartesian coordinates as follows [3]:

$$\frac{\partial Q}{\partial t} + \frac{\partial \left(E_c - E_d\right)}{\partial x} + \frac{\partial \left(F_c - F_d\right)}{\partial y} + \frac{\partial \left(G_c - G_d\right)}{\partial z} = S \tag{2.14}$$

where Q is the vector of conserved variables,

$$Q = \begin{bmatrix} \rho u \\ \rho v \\ \rho w \\ E \\ \rho_1 \\ \vdots \\ \rho_N \\ E_v \end{bmatrix} \tag{2.15}$$

where u,v and w, denote the the Cartesian velocity vector components, E denotes the total (internal and kinetic) energy of the mixture, and E_v denotes the vibrational-electronic energy of the mixture. The mixture density, ρ, is given by a simple sum of the individual chemical species densities, ρ_s, namely,

$$\rho = \sum_{s=1}^{N} \rho_s = \sum_{s=1}^{N} \rho Y_s \tag{2.16}$$

where $Y_{s=1,\ldots,N}$ denote the individual chemical species mass fractions. Note that in the case of thermal equilibrium, the mixture vibrational-electronic energy is identically zero ($E_v = 0$) and the last equation in the set is omitted.

The convective (inviscid) flux vectors, E_c, F_c, and G_c, are

$$E_c = \begin{bmatrix} \rho u^2 + p \\ \rho uv \\ \rho uw \\ u\left(E+p\right) \\ \rho_1 u \\ \vdots \\ \rho_N u \\ uE_v \end{bmatrix}, \quad F_c = \begin{bmatrix} \rho uv \\ \rho v^2 + p \\ \rho vw \\ v\left(E+p\right) \\ \rho_1 v \\ \vdots \\ \rho_N v \\ vE_v \end{bmatrix}, \quad G_c = \begin{bmatrix} \rho uw \\ \rho vw \\ \rho w^2 + p \\ w\left(E+p\right) \\ \rho_1 w \\ \vdots \\ \rho_N w \\ wE_v \end{bmatrix} \tag{2.17}$$

and the diffusive (viscous) flux vectors, E_d, F_d, and G_d, are

$$E_d = \begin{bmatrix} \tau_{xx} \\ \tau_{yx} \\ \tau_{zx} \\ \beta_x \\ -J_{x,1} \\ \vdots \\ -J_{x,N} \\ \beta_{v,x} \end{bmatrix}, \quad F_d = \begin{bmatrix} \tau_{xy} \\ \tau_{yy} \\ \tau_{zy} \\ \beta_y \\ -J_{y,1} \\ \vdots \\ -J_{y,N} \\ \beta_{v,y} \end{bmatrix}, \quad G_d = \begin{bmatrix} \tau_{xz} \\ \tau_{yz} \\ \tau_{zz} \\ \beta_z \\ -J_{z,1} \\ \vdots \\ -J_{z,N} \\ \beta_{v,z} \end{bmatrix} \tag{2.18}$$

where

$$\begin{aligned}
\tau_{xx} &= \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) + 2\mu\frac{\partial u}{\partial x} \\
\tau_{yy} &= \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) + 2\mu\frac{\partial v}{\partial y} \\
\tau_{zz} &= \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) + 2\mu\frac{\partial w}{\partial z} \\
\tau_{xy} &= \tau_{yx} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \\
\tau_{xz} &= \tau_{zx} = \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\
\tau_{yz} &= \tau_{zy} = \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) \\
\beta_x &= u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - (q_x + q_{v,x}) - \sum_s (J_{x,s}h_s) \\
\beta_y &= u\tau_{yx} + v\tau_{yy} + w\tau_{yz} - (q_y + q_{v,y}) - \sum_s (J_{y,s}h_s) \\
\beta_z &= u\tau_{zx} + v\tau_{zy} + w\tau_{zz} - (q_z + q_{v,z}) - \sum_s (J_{z,s}h_s) \\
\beta_{v,x} &= -q_{v,x} - \sum_s (J_{x,s}e_{v,s}) \\
\beta_{v,y} &= -q_{v,y} - \sum_s (J_{y,s}e_{v,s}) \\
\beta_{v,z} &= -q_{v,z} - \sum_s (J_{z,s}e_{v,s})
\end{aligned} \tag{2.19}$$

the pressure is denoted by p, and h_s and $e_{v,s}$ are the specific enthalpy and vibrational energy of species s, respectively. The translational-rotational heat flux is given by $q = -\kappa\nabla T$ while $q_v = -\kappa_v\nabla T_v$ is the vibrational-electronic heat flux, where T, T_v are the translational and vibrational temperatures, respectively. The terms κ, κ_v are the

thermal conductivities associated with the various energy modes (*i.e.*, translational and vibrational-electronic).

The species mass diffusion fluxes, $J_{x,s}$, $J_{y,s}$, $J_{z,s}$ are modeled using Fick's law,

$$J_s = -\rho D_s \nabla Y_s \tag{2.20}$$

where D_s is the diffusion coefficient of species s with respect to the mixture (see Section 2.3.5). Stokes hypothesis, $\lambda = -\frac{2}{3}\mu$, is employed to further simplify Equation (2.19).

2.3.3 Integral Form For Moving Grids

For a three-dimensional flow through a finite volume Ω, enclosed by the boundary surface $\partial\Omega \equiv S$ that is moving with a grid velocity $\overline{V}_g$, the integral form of the conservation equations in an inertial frame of reference is given as:

$$\frac{\partial}{\partial t}\int_{\Omega} Q d\Omega + \oint_{S} d\overline{S} \cdot \overline{H} = 0 \tag{2.21}$$

where

$$\overline{H} = (E_c - E_d)\,\hat{i} + (F_c - F_d)\,\hat{j} + (G_c - G_d)\,\hat{k} \tag{2.22}$$

In Equation (2.21) the vector of dependent variables, Q, remains as in Equation (2.15). Similarly, the viscous flux vectors, E_d, F_d, and G_d, appearing in Equation (2.22), remain as in Equations (2.18) and (2.19) (see Section 2.3.2). In contrast, the inviscid

flux vectors take a form that reflects the motion of the grid as follows:

$$
\begin{aligned}
E_c &= \begin{bmatrix} \rho u\left(u-u_g\right)+p \\ \rho v\left(u-u_g\right) \\ \rho w\left(u-u_g\right) \\ \left(E+p\right)\left(u-u_g\right)+u_g p \\ \rho_1\left(u-u_g\right) \\ \vdots \\ \rho_N\left(u-u_g\right) \\ \left(u-u_g\right)E_v \end{bmatrix} \\
F_c &= \begin{bmatrix} \rho u\left(v-v_g\right) \\ \rho v\left(v-v_g\right)+p \\ \rho w\left(v-v_g\right) \\ \left(E+p\right)\left(v-v_g\right)+v_g p \\ \rho_1\left(v-v_g\right) \\ \vdots \\ \rho_N\left(v-v_g\right) \\ \left(v-v_g\right)E_v \end{bmatrix} \\
G_c &= \begin{bmatrix} \rho u\left(w-w_g\right) \\ \rho v\left(w-w_g\right) \\ \rho w\left(w-w_g\right)+p \\ \left(E+p\right)\left(w-w_g\right)+w_g p \\ \rho_1\left(w-w_g\right) \\ \vdots \\ \rho_N\left(w-w_g\right) \\ \left(w-w_g\right)E_v \end{bmatrix}
\end{aligned}
\tag{2.23}
$$

where u_g, v_g, and w_g are the Cartesian components of the grid velocity vector $\overline{V}_g$.

2.3.4 Thermodynamic Properties

The pressure, p, is obtained from Dalton's law of partial pressures for a mixture of thermally perfect gases,

$$p = \rho \sum_s R_s Y_s T + \rho R_e Y_e T_v \tag{2.24}$$

where $R_s = \frac{R_0}{W_s}$ is the specific gas constant of species s, with R_0 denoting the universal gas constant and W_s denoting the molecular weight of that species. The subscript e denotes the free electron species.

2.3.4.1 Thermal Equilibrium

If the gas is in thermal equilibrium (*i.e.*, $T = T_v$), then nine-term polynomials of temperature are used for calculating the specific enthalpy, h_s, and the heat capacity at constant pressure, $C_{p,s}$, of individual gaseous species [4]. The total energy is then given by:

$$E = \sum_s \rho Y_s h_s - p + \frac{1}{2}\rho\left(u^2 + v^2 + w^2\right) \tag{2.25}$$

2.3.5 Transport Properties

The transport properties of the mixture may be calculated with three different models. The first, most simple model, employs the Sutherland formulae (see Section 2.2.4) to evaluate the transport properties of standard air at low temperatures (up to 2,000 K). Therefore, it is recommended to use this model only for equilibrium air flows at relatively low speeds. A more elaborate model that accounts for the various components of the gas is based on Wilke's mixing rule [5] together with Blottner's [6] or Mcbride's [7] curve fits for approximating the viscosity, and Eucken's modified formula [8] for calculating the thermal conductivities of individual species. This model is suitable for air at temperatures of up to 10,000 K, and may not be used in simulation of ionized flows. For air at higher temperatures, arising typically in re-entry simulations, a second, more complex model is available owing to Gupta [9].

2.3.5.1 Wilke's Model

In this model, mixture transport properties are obtained using Wilke's mixing rule [5]:

$$\mu = \sum_s \frac{\mu_s X_s}{\phi_s} \quad , \quad \kappa = \sum_s \frac{\kappa_s X_s}{\phi_s} \tag{2.26}$$

where

$$\phi_s = \sum_r X_r \left[1 + \sqrt{\frac{\mu_s}{\mu_r}} \left(\frac{M_r}{M_s}\right)^{\frac{1}{4}}\right]^2 \left[\sqrt{8\left(1 + \frac{M_s}{M_r}\right)}\right]^{-1} , \tag{2.27}$$

the term X_s denotes the molar fraction of species s in the mixture, μ_s is the species coefficient of viscosity and κ_s is the species thermal conductivity for each energy mode (*i.e.*, translational and vibrational).

The species viscosities are calculated using Blottner's [6] curve-fits of temperature for components of air, or McBride [7] curve-fits for general gaseous species. The species thermal conductivities, κ_s^{tr} and κ_s^{vib}, are determined from a generalized Eucken's relation, according to Hirschfelder [8]:

$$\kappa_s^{tr} = \mu_s \left(\frac{5}{2} C_{v,s}^t + \frac{C_{v,s}^r}{Sc}\right) \tag{2.28}$$

$$\kappa_s^{vib} = \mu_s \left(C_{v,s}^{vib}\right) \tag{2.29}$$

The terms $C_{v,s}^t, C_{v,s}^r, C_{v,s}^{vib}$ denote the translational, rotational and vibrational specific heats at constant volume of species s, respectively, and Sc is a constant Schmidt number, assumed equal for all species.

Finally, the mass diffusion constant of species s with respect to the mixture, D_s, is replaced by a single binary coefficient, D, that is evaluated from a constant, user-supplied Schmidt number, as follows:

$$D = \frac{\mu}{\rho Sc} \tag{2.30}$$

2.3.6 Chemical Reaction Modeling

The local chemical composition of the mixture may be determined in three different methods, ordered here by increasing computational complexity:

1. *Frozen gas*: Under this assumption, the chemical composition remains fixed throughout the flow-field, and is set to the composition of the free-stream. This mode is suitable only for air at low temperatures (up to 2000 K), and for general gases that are known to be chemically non-reacting at the simulated conditions.

2. *Equilibrium gas*: Under this assumption, the local chemical composition is determined uniquely as a function of two thermodynamic variables (e.g., temperature and pressure) via minimization of Gibbs or Helmholtz free energy [10]. For enhanced efficiency, the equilibrium properties of the mixture are tabulated upon start-up, so that the cumbersome process of non-linear minimization is avoided throughout the normal operation of the program. The chemical equilibrium mode is applicable to flows at moderate speeds, where chemical reactions occur at a much faster rate than the traversal rate of the molecules through the domain of interest. The **Arion** code utilizes tabulation for the thermodynamic and molecular properties of the gas (see Section 8.8 for tabulation directives and options). Note, it is required to utilize the eos.table type for the equilibrium gas assumption (see Tables 8.8 and 8.9). In addition, it is required to addd the −−multi.component.gas directive and options (see Section 8.9).

3. *Non-Equilibrium flow*: Under this assumption, finite-rate chemical kinetics models (detailed ahead) are employed to calculate the local composition of the mixture from the solution of additional mass conservation equations for the individual components. This is the most accurate (and expensive) method for calculating the local composition of the gas. It should be used in high-speed flows of air, and in other cases where finite-rate chemistry effects are of interest (*e.g.*, combustion).

2.3.6.1 Equilibrium Gas Properties Tabulation

The tabulation of the equilibrium gas properties is conducted as described in Section 8.8, Tables 8.25-8.47. Note that viscosity, conductivity and heat capacity are also tabulated, based on the selected thermo/transport models.

2.3.6.2 Finite-rate Chemical Kinetics

A reaction mechanism composed of N_r reversible reactions may be generally described by the following chemical formulae:

$$\sum_{s=1}^{N} \nu'_{s,q} M_s \underset{c_{r,q}}{\overset{c_{f,q}}{\rightleftharpoons}} \sum_{s=1}^{N} \nu''_{s,q} M_s \quad \forall \quad q = 1 \ldots N_r \tag{2.31}$$

where $\nu'_{s,q}$ and $\nu''_{s,q}$ are the stoichiometric coefficients of species s (represented by the chemical symbol M_s), acting as a reactant or product in reaction q, respectively. The code currently assumes laminar chemistry, according to which the Arrhenius approach is used to describe the mean reaction rates (*i.e.*, based only on mean values of temperature and species mass fractions). The formula for the mean reaction rate for species s, S_s, appearing as a source-term in the respective species mass conservation equation, is then given by:

$$S_s = W_s \sum_{q=1}^{N_r} \left(\nu''_{s,q} - \nu'_{s,q}\right) \left[c_{f,q} \prod_{p=1}^{N} \left(\frac{\rho Y_p}{W_p}\right)^{\nu'_{p,q}} - c_{r,q} \prod_{p=1}^{N} \left(\frac{\rho Y_p}{W_p}\right)^{\nu''_{p,q}} \right] \tag{2.32}$$

where $c_{f,q}$ and $c_{r,q}$ are the forward and reverse rate coefficients of reaction q, respectively.

2.3.6.3 Reaction Rate Coefficients

The forward rate coefficients are expressed in Arrhenius form as:

$$c_q(T_c) = A_q T_c^{\gamma_q} e^{-(E_q/R_0 T_c)} \tag{2.33}$$

where γ_q and A_q are constants, E_q is the activation energy, and T_c is a controlling temperature to be defined later. Note that the default units of the Arrhenius coefficient and the activation energy are $[A] = (m^3/kmol)^{n-1}/sec$ and $[E] = (J/kmol/K)$, respectively. Other units may be specified via a "UNITS" directive at the beginning of the reaction rates file. The reverse rate coefficients may either be given explicitly in Arrhenius form, for instance, as in Dunn and Kang's 5-species, 11-reactions model [11], or they may be calculated via the equilibrium constant of the reaction, as follows:

$$c_{r,q}(T_{bc}) = \frac{c_{f,q}(T_{bc})}{K_{eq,q}(T_{bc})} \tag{2.34}$$

Where $K_{eq,q}$ denotes the equilibrium constant of reaction q, and T_{bc} is the reverse rate controlling temperature that is not necessarily equal to the forward controlling temperature, T_c. The equilibrium constant, K_{eq}, itself may be calculated in two methods: First, for air only, the constants may be approximated with Park's curve-fits [12] of the local number density. For a general gas, the equilibrium constant of reaction q may only be calculated from Gibbs' free energy,

$$K_{eq}(T) = \left(\frac{10^5}{R_0 T}\right)^{\nu_q} \exp\left[-\sum_s \left(\nu''_{s,q} - \nu'_{s,q}\right)\left(\frac{h_s}{R_s T} - \frac{s_s}{R_s}\right)\right] \tag{2.35}$$

where $\nu_q = \sum_s \left(\nu''_{s,q} - \nu'_{s,q}\right)$, and the dimensionless enthalpy and entropy are obtained from curve-fits, as described in section 2.3.4.

2.4 Gas Selection

2.4.1 Single Component Perfect Gas

As mentioned above, the **Arion** code provides the means to simulate the flow of any perfect gas. This is facilitated via a series of directives that allow to set the specific gas constant, (R, see Table 8.10), the the heat capacity ratio, (γ, see Table 8.11, and the Sutherland formulae coefficients as described in Section 2.2.4.

2.4.2 Multi Component Gas

In the case of a multi-component gas, the actual composition of the gas has to be defined using the appropriate directives. The reader is referred to Section 8.9 and the tables therein.

Chapter 3

Turbulence Models

The unsteady Navier-Stokes equations are generally considered to govern turbulent flows in the continuum flow regime. However, turbulent flow cannot be numerically simulated as easily as laminar flow. To resolve a turbulent flow by direct numerical simulation (DNS) requires that all relevant length scales be properly resolved. Such requirements place great demands on the computer resources, a fact that renders the possibility of conducting DNS analysis about complete aircraft configurations infeasible.

A practical approach to simulating turbulent flows is to solve the time-averaged Navier-Stokes equations. These equations are know as the "Reynolds averaged Navier-Stokes" (RANS) equations. The averaging of the equations of motion gives rise to new terms that are called the Reynolds stresses. To solve the averaged equations, the Reynolds stress tensor must be related to the flow variables through turbulence models. The models are used to "close" the system through an additional set of assumptions. The models are classified based on the number of additional partial differential equations that must be solved. The **Arion** code currently contains only one turbulence model, a two-equation model.

3.1 RANS Turbulence Model Equations

The **Arion** code treats the mean flow and turbulence models equations in a unified manner. To this end, the Navier-Stokes equation set is extended to include the turbulence model equations. Consequently, the discretization of the various fluxes can be conducted in the same manner.

The equations governing turbulent flows are obtained by Favre-averaging the Navier-Stokes equations and by modeling the Reynolds stress tensor. The unknown averaged Reynolds stress tensor is modeled either using the Boussinesq assumption via a linear eddy-viscosity model or by directly solving a transport equation for each of the Reynolds stress components via a second moment closure. The general form of the resulting Navier-Stokes equations and the turbulence model equations has the form (for simplicity of the representation, with no loss of generality, the formulation under the perfect gas physical model assumption is brought herein; it can be easily extended to any physical model):

$$\frac{\partial Q}{\partial t} + \frac{\partial \left(E_c - E_d\right)}{\partial x} + \frac{\partial \left(F_c - F_d\right)}{\partial y} + \frac{\partial \left(G_c - G_d\right)}{\partial z} = S \tag{3.1}$$

where S is the source term associated with the turbulence model only (once again, under the perfect gas physical model assumption). Hence, for turbulent flow simulations, Equation (3.1) replaces Equation (2.1).

In what follows, the symbol $(\bar{\ })$ indicates non-weighted averaging, the symbol $(\tilde{\ })$ signifies mass weighted Favre averaging, and the symbol $(\ '')$ denotes Favre fluctuations. Depending on whether the turbulence model has one, two, or m equations, the vector of dependent variables, Q, and the vector of source terms S now take the

form:

$$Q = \begin{bmatrix} \bar{\rho} \\ \bar{\rho}\tilde{u} \\ \bar{\rho}\tilde{v} \\ \bar{\rho}\tilde{w} \\ \tilde{E} \\ \bar{\rho}q_1 \\ \dots \\ \bar{\rho}q_m \end{bmatrix}, \qquad S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ s1 \\ \dots \\ s_m \end{bmatrix} \tag{3.2}$$

where q is the vector of turbulence model dependent variables and s, is the source terms vector. Note that the source terms differ from model to model. The vectors E_c, F_c, and G_c usually take the form:

$$E_c = \begin{bmatrix} \bar{\rho}\tilde{u} \\ \bar{\rho}\tilde{u}^2 + \bar{p} \\ \bar{\rho}\tilde{u}\tilde{v} \\ \bar{\rho}\tilde{u}\tilde{w} \\ \tilde{u}\left(\tilde{E} + \bar{p}\right) \\ \bar{\rho}\tilde{u}q_1 \\ \dots \\ \bar{\rho}\tilde{u}q_m \end{bmatrix}, \quad F_c = \begin{bmatrix} \bar{\rho}\tilde{v} \\ \bar{\rho}\tilde{u}\tilde{v} \\ \bar{\rho}\tilde{v}^2 + \bar{p} \\ \bar{\rho}\tilde{v}\tilde{w} \\ \tilde{v}\left(\tilde{E} + \bar{p}\right) \\ \bar{\rho}\tilde{v}q_1 \\ \dots \\ \bar{\rho}\tilde{v}q_m \end{bmatrix}, \quad G_c = \begin{bmatrix} \bar{\rho}\tilde{w} \\ \bar{\rho}\tilde{u}\tilde{w} \\ \bar{\rho}\tilde{v}\tilde{w} \\ \bar{\rho}\tilde{w}^2 + \bar{p} \\ \tilde{w}\left(\tilde{E} + \bar{p}\right) \\ \bar{\rho}\tilde{w}q_1 \\ \dots \\ \bar{\rho}\tilde{w}q_m \end{bmatrix} \tag{3.3}$$

Similarly, the vectors, E_d, F_d, and G_d, usually take the form:

$$E_d = \begin{bmatrix} 0 \\ \bar{\tau}_{xx} - \overline{\rho u'' u''} \\ \bar{\tau}_{yx} - \overline{\rho v'' u''} \\ \bar{\tau}_{zx} - \overline{\rho w'' u''} \\ \bar{\beta}_x \\ e_{d_1} \\ \dots \\ e_{d_m} \end{bmatrix}, \quad F_d = \begin{bmatrix} 0 \\ \bar{\tau}_{xy} - \overline{\rho u'' v''} \\ \bar{\tau}_{yy} - \overline{\rho v'' v''} \\ \bar{\tau}_{zy} - \overline{\rho w'' v''} \\ \bar{\beta}_y \\ f_{d_1} \\ \dots \\ f_{d_m} \end{bmatrix}, \quad G_d = \begin{bmatrix} 0 \\ \bar{\tau}_{xz} - \overline{\rho u'' w''} \\ \bar{\tau}_{yz} - \overline{\rho v'' w''} \\ \bar{\tau}_{zz} - \overline{\rho w'' w''} \\ \bar{\beta}_z \\ g_{d_1} \\ \dots \\ g_{d_m} \end{bmatrix} \tag{3.4}$$

where the vectors e_d, f_d, and g_d differ from model to model and

$$\begin{aligned}
\bar{\beta}_x &= \tilde{u}\left(\bar{\tau}_{xx} - \overline{\rho u'' u''}\right) + \tilde{v}\left(\bar{\tau}_{xy} - \overline{\rho u'' v''}\right) + \tilde{w}\left(\bar{\tau}_{xz} - \overline{\rho u'' w''}\right) + \left(\bar{\kappa} + \bar{\kappa}_t\right)\frac{\partial \tilde{T}}{\partial x} \\
\bar{\beta}_y &= \tilde{u}\left(\bar{\tau}_{yx} - \overline{\rho v'' u''}\right) + \tilde{v}\left(\bar{\tau}_{yy} - \overline{\rho v'' v''}\right) + \tilde{w}\left(\bar{\tau}_{yz} - \overline{\rho v'' w''}\right) + \left(\bar{\kappa} + \bar{\kappa}_t\right)\frac{\partial \tilde{T}}{\partial y} \\
\bar{\beta}_z &= \tilde{u}\left(\bar{\tau}_{zx} - \overline{\rho w'' u''}\right) + \tilde{v}\left(\bar{\tau}_{zy} - \overline{\rho w'' v''}\right) + \tilde{w}\left(\bar{\tau}_{zz} - \overline{\rho w'' w''}\right) + \left(\bar{\kappa} + \bar{\kappa}_t\right)\frac{\partial \tilde{T}}{\partial z}
\end{aligned} \tag{3.5}$$

The terms $\bar{\kappa}$ and $\bar{\kappa}_t$ are the averaged molecular and turbulent heat conductivities, respectively. The molecular heat conductivity is calculated using Sutherland's law (see Equation (2.12)) while the turbulent heat conductivity is calculated using

$$\bar{\kappa}_t = \frac{c_p \bar{\mu}_t}{Pr_t} \tag{3.6}$$

where $\bar{\mu}_t$ denotes the turbulent viscosity. The term c_p is the specific heat capacity at constant pressure, Pr is the Prandtl number set to $Pr = 0.72$, and Pr_t is the turbulent Prandtl number set to $Pr_t = 0.9$. The average turbulent viscosity, $\bar{\mu}_t$ differs from model to model.

3.2 The Spalart Allmaras Turbulence Model

The one-equation SA model was originally published in 1992 [13]. The original model, also known as the *standard* SA model (according to the TMR web site) heavily relies on calibration by references to a wide range of experimental data, including flows subjected to adverse pressure gradient. The rich body of empirical information that the model contains gives it advantages over other models when applied to 'complex' boundary layers approaching separation, and this has made the model popular for aeronautical practice. However, the *standard* SA model suffers from certain anomalies. To circumvent these anomalies, Edwards and Chandra [**?**] proposed a modification to the model, resulting in a far more robust model. Although the work by Edwards and Chandra concerns the incompressible form of the model, a compressible formulation of their model is adopted herein (denoted the *SA-Edwards* model). In addition, the EZAir code offers a second variant of the SA model, based on the work by Allmaras *et al* [14] with a slight modification as proposed in the work by Rumsey *et al* [**?**].

The second variant is denoted as the *SA-2020* model. Both models were desgined to overcome the above mentioned anomalies. The Spalart-Allmaras model that is implemented in **Arion** is the *SA-2020* variant of the model.

A unified formulation of the two aforementioned variants may be written as follows:

$$\frac{\partial \rho\tilde{\nu}}{\partial t} + \frac{\partial \rho\tilde{\nu}u_k}{\partial x_k} = \frac{\partial}{\partial x_k}\left[\frac{1}{\sigma}\left(\mu + \rho\tilde{\nu}\right)\frac{\partial \tilde{\nu}}{\partial x_k}\right] + P_{SA} - D_{SA} + SD_{SA} + C_{SA} \tag{3.7}$$

The model is comprised of a transport equation for the undamped eddy viscosity, $\tilde{\nu}$, where t denotes the time and x_j=[x,y,z] denote the Cartesian coordinates. The fluid density is denoted by ρ while the Cartesian velocity vector components are denoted by u_j=[u,v,w].

The production term, P_{SA}, and the destruction term, D_{SA}, are given as by:

$$P_{SA} = c_{b_1}\tilde{S}\rho\tilde{\nu} \tag{3.8}$$

and

$$D_{SA} = c_{w_1} f_w \rho \left(\frac{\tilde{\nu}}{d_w}\right)^2 \tag{3.9}$$

where d_w is the distance from the nearest wall. The near-wall damping function f_w is defined as:

$$f_w = g\left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6}\right)^{1/6} \tag{3.10}$$

where

$$g = r + c_{w2}\left(r^6 - r\right) \tag{3.11}$$

The laminar suppression term is given by

$$f_{t2} = c_{t3}\exp\left(-c_{t4}\chi^2\right) \tag{3.12}$$

The source diffusion term, SD_{SA} is given by:

$$SD_{SA} = \rho\frac{c_{b_2}}{\sigma}\frac{\partial \tilde{\nu}}{\partial x_k}\frac{\partial \tilde{\nu}}{\partial x_k} \tag{3.13}$$

The definition of the term C_{SA} is addressed later on.

The turbulent viscosity, μ_t, is defined as:

$$\mu_t = \rho\tilde{\nu} f_{v1} \tag{3.14}$$

where the the damping function, f_{v1}, is given by:

$$f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3} \tag{3.15}$$

where χ is defined by (ν being the kinematic viscosity):

$$\chi \equiv \frac{\tilde{\nu}}{\nu} \tag{3.16}$$

The model constants are given as follows:

$$\begin{gathered} c_{b1} = 0.1355, \quad c_{b2} = 0.622, \quad \kappa = 0.41, \quad \sigma = 2/3 \\ c_{w1} = \frac{c_{b1}}{\kappa^2} + \frac{1 + c_{b2}}{\sigma}, \quad c_{w2} = 0.3, \quad c_{w3} = 2, \quad c_{v1} = 7.1 \end{gathered} \tag{3.17}$$

3.2.1 SA-2020 Model

The *SA-2020* model is given in a fully consistent compressible formulation. The term $\tilde{S}$ is defined as

$$\tilde{S} = \begin{cases} \Omega_s + \bar{S} & \bar{S} \geq -c_{v_2}\Omega_s \\ \Omega_s + \dfrac{\Omega_s \left(c_{v_2}^2 \Omega_s + c_{v_3}\bar{S}\right)}{\left(c_{v_3} - 2c_{v_2}\right)\Omega_s - \bar{S}} & \text{Otherwise} \end{cases}$$

where

$$\Omega_s = \sqrt{0.5\left(2s_{ij}s_{ij} + 2\omega_{ij}\omega_{ij}\right)} \tag{3.18}$$

with c_{v_2}=0.7 and c_{v_3}=0.9. The term $\bar{S}$ is defined as:

$$\bar{S} = \frac{\tilde{\nu}}{\kappa^2 d_w^2} f_{v2} \tag{3.19}$$

where the function f_{v2} is defined as:

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}} \tag{3.20}$$

The parameter r is defined as:

$$r = \min\left(\frac{\tilde{\nu}}{\tilde{S}\kappa^2 d_w^2}, 10\right) \tag{3.21}$$

Finally, the term C_{SA} complements the fully consistent compressible formulation of the model, namely:

$$C_{SA} = -\frac{1}{\sigma}\left(\nu + \tilde{\nu}\right)\frac{\partial \rho}{\partial x_k}\frac{\partial \tilde{\nu}}{\partial x_k} \tag{3.22}$$

3.2.2 Boundary Conditions

To close the solution of the model, the boundary conditions are specified. The no-slip, wall boundary condition of $\tilde{\nu}$, denoted by $\tilde{\nu}_{wall}$, is specified by:

$$\tilde{\nu}_{wall} = 0 \tag{3.23}$$

The recommended far field inlet boundary condition of $\tilde{\nu}$, denoted by $\tilde{\nu}_\infty$, for external flows is given by: [15]:

$$\tilde{\nu}_\infty = 3\nu_\infty \; to \; 5\nu_\infty \tag{3.24}$$

This range of inflow values is appropriate for fully turbulent behavior, with $\tilde{\nu}_\infty = 3\nu_\infty$ being somewhat preferable at the lower Reynolds numbers regime. This is because it results in a free stream turbulent viscosity of $\mu_t/\mu \approx 0.2$, well below 1.0. Higher values may slightly help convergence at high Reynolds numbers by smoothing out the edges of turbulent regions, but not enough to motivate giving up the simple recommendation.

3.3 The k-ω-TNT Turbulence Model

The TNT turbulence model has two clear advantages over other two-equation turbulence models: it uses a topology-free approach, and it is insensitive to the specific turbulence dissipation rate free-stream boundary condition. The source term of the model is given by:

$$S = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ P_k - \beta_k \bar{\rho} k \omega \\ \alpha_\omega \frac{\omega}{k} P_k - \beta_\omega \bar{\rho} \omega^2 + \max(\mathcal{E}, 0) \end{Bmatrix} \tag{3.25}$$

The production term is denoted by P_k and it is based on the Boussinesq approximation while $\mathcal{E}$ is the cross diffusion term. The turbulent viscosity is defined as

$$\mu_t = \frac{\overline{\rho} k}{\omega} \tag{3.26}$$

The remaining model constants are $\sigma_k = 1.5$, $\sigma_\omega = 2.0$, $\sigma_d = 0.5$, $\beta_\omega = 0.075$, $\beta_k = 0.09$, $\alpha_\omega = \frac{\beta}{\beta^*} - \frac{\sigma_\omega \kappa^2}{\sqrt{\beta^*}}$, with $\kappa = 0.41$.
A description of the boundary conditions appears in Section 3.5.

3.4 The k-ω-SST Model

There are numerous suggestions in the literature for two-equation turbulence models, many being variations of a few baseline models. As most two equation models contain one equation for the turbulence kinetic energy, k, one important issue is the quantity chosen to represent the length scale. While ϵ is the most obvious and popular option, it is one that causes significant problems in practice, especially in near-wall flows approaching separation. In computational aerodynamics, the most popular alternative to ϵ itself is the turbulent specific dissipation rate, ω. The attraction of

ω-based models is rooted in the observation that it gives a superior representation of the near-wall behavior, especially in adverse pressure gradient regions. On the other hand, one serious flaw exhibited by ω based models is the extreme sensitivity to the value of ω at irrotational boundaries of shear flows and, by implication, also to the value in weak-shear regions within a complex shear flow. This, as well as other defects, have led Menter [16] to formulate a hybrid model which blends the k-ω model near-wall regions with the k-ϵ model in regions that are far from walls. In recent years, this model has become the most popular two-equation model in aeronautical CFD practice, especially in weakly separated flows. Again, over the years several variations and modifications to the original k-ω-SST model have appeared. The k-ω-SST-2003 (following the naming convention from the TMR website) has been chosen and implemented in the EZAir suite.

3.4.1 k-ω-SST-2003 Model

The transport form of the compressible k-ω-SST-2003 turbulence model contains two transport equations. A transport equation for the turbulence kinetic energy, k, and a second transport equation for the turbulent specific dissipation rate, ω. These transport equations take the following form:

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma_k \mu_t\right)\frac{\partial k}{\partial x_j}\right] + P_k - \beta^* \rho \omega k \tag{3.27}$$

$$\begin{aligned}\frac{\partial \rho \omega}{\partial t} + \frac{\partial \rho u_j \omega}{\partial x_j} &= \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma_\omega \mu_t\right)\frac{\partial \omega}{\partial x_j}\right] + \frac{\alpha_\omega}{\mu_t}\rho P_k - \beta \rho \omega^2 \\ &+ 2\left(1 - F_1\right)\frac{\rho \sigma_{\omega 2}}{\omega}\max\left(\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}, 0\right)\end{aligned} \tag{3.28}$$

where t denotes the time and x_j=[x,y,z] denote the Cartesian coordinates. The fluid density is denoted by ρ while the Cartesian velocity vector components are denoted

by u_j=[u,v,w]. The production term, denoted by P_k, is defined as

$$P_k = \mathfrak{R}_{ij} \frac{\partial u_i}{\partial x_j} \tag{3.29}$$

where $\mathfrak{R}_{ij} = \overline{\rho u_i'' u_j''}$ are the Reynolds stress tensor components.

The coefficient β^* is a constant equal to $\beta^* = 0.09$. The rest of the model coefficients, ϕ_c=($\sigma_k,\ \sigma_\omega,\ \alpha_\omega,\ \beta$) are blended according to

$$\phi_c = F_1 \phi_1 + (1 - F_1)\, \phi_2 \tag{3.30}$$

where the coefficients ϕ_1 and ϕ_2 are given in Table 3.1.

	σ_k	σ_ω	α_ω	β
ϕ_1	0.856	0.5	5/9	0.075
ϕ_2	1.0	0.856	0.44	0.0828

Table 3.1: SST coefficients

The F_1 function, proposed by Menter [16] himself, is given as:

$$F_1 = \tanh\left(\mathfrak{Z}_1{}^4\right) \tag{3.31}$$

with the argument $\mathfrak{Z}_1$ given by:

$$\mathfrak{Z}_1 = \min\left[\max\left(\frac{\sqrt{k}}{\beta^* \omega d_w}, \frac{500\mu}{\rho \omega d_w^2}\right), \frac{4\sigma_{\omega 2} \rho k}{\max\left(2\sigma_{\omega 2} \frac{\rho}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 10^{-10}\right) d_w^2}\right] \tag{3.32}$$

The turbulent viscosity is defined as

$$\mu_t = \frac{a_1 \rho k}{\max\left(a_1 \omega, S F_2\right)} \tag{3.33}$$

where S is:

$$S = \sqrt{2 S_{ij} S_{ij}} \tag{3.34}$$

with

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{3.35}$$

and the function F_2 is defined as follow:

$$F_2 = \tanh\left(\mathfrak{Z}_2{}^2\right) \tag{3.36}$$

with

$$\mathfrak{Z}_2 = \max\left(2\frac{\sqrt{k}}{\beta^*\omega d}, \frac{500\nu}{\omega d^2}\right) \tag{3.37}$$

In the k-ω-SST-2003 version, the production term, P_k is limited as follows

$$P_k = \min\left(P_k, 10\beta^*\rho\omega k\right) \tag{3.38}$$

A description of the boundary conditions appears in Section 3.5.

3.4.2 k-ω-SST-SAS Model

The k-ω-SST scale-adaptive-simulation (SAS) model is based on the formulation appearing in the work by Egorov and Menter [17]. The difference between the k-ω-SST model and the k-ω-SST-SAS model is the addition of the Q_{SAS} source term to the equation for ω, namely it is added to Equation 3.28, resulting in:

$$\begin{aligned}\frac{\partial\rho\omega}{\partial t} + \frac{\partial\rho u_j\omega}{\partial x_j} &= \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma_\omega\mu_t\right)\frac{\partial\omega}{\partial x_j}\right] + \frac{\alpha_\omega}{\mu_t}\rho P_k - \beta\rho\omega^2 \\ &+ 2\left(1 - F_1\right)\frac{\rho\sigma_{\omega 2}}{\omega}\max\left(\frac{\partial k}{\partial x_j}\frac{\partial\omega}{\partial x_j}, 0\right) + Q_{SAS}\end{aligned} \tag{3.39}$$

where Q_{SAS} is defined as:

$$Q_{SAS} = \max\left[\rho\xi\kappa S^2\left(\frac{L_l}{L_{vk}}\right)^2 - C\frac{2\rho k}{\sigma_\phi}\max\left(\frac{|\nabla\omega|^2}{\omega^2}, \frac{|\nabla k|^2}{k^2}\right), 0\right] \tag{3.40}$$

The modeled turbulence length scale, L_l, is given by

$$L_l = \sqrt{k} / \left(C_\mu^{1/4} \omega \right) \tag{3.41}$$

and the von Karman length scale, L_{vk}, is given by: ?

$$L_{vk} = \frac{\kappa S}{\left| \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} \right) \right|} \tag{3.42}$$

The model constants are $C = 2.0$, $\xi = 3.51$, $\kappa = 0.41$, $\sigma_\phi = 0.67$, and $C_\mu = 0.09$.

3.5 Boundary Conditions for the k-ω-TNT and k-ω-SST Turbulence Models

To close the solution of any of the k-ω models, the boundary conditions should be specified. The no-slip wall boundary conditions of k and ω, denoted by k_{wall} and ω_{wall}, respectively, are specified as follows:

$$k_{wall} = 0 \tag{3.43}$$

$$\omega_{wall} = 10 \frac{6\nu}{\beta_1 \left(\Delta d_1 \right)^2} \tag{3.44}$$

where Δd_1 denotes the distance between the center of the first cell neighboring the wall and the wall. The inflow boundary condition of k, denoted by k_∞ for external flows is

$$k_\infty = \frac{3}{2} \left(T_u \cdot U_\infty \right)^2 \tag{3.45}$$

where Tu represents the turbulence intensity and U_∞ is the magnitude of the inflow velocity. The inflow boundary condition of ω, denoted as ω_∞ is specified as follows:

$$\omega_\infty = \frac{\bar{\rho}_\infty k_\infty}{\left(\mu_t \right)_\infty} \tag{3.46}$$

with the recommended values of $(\mu_t)_\infty$ for external flows are as follows:

$$0.01 < \frac{(\mu_t)_\infty}{(\mu)_\infty} < 1.0 \tag{3.47}$$

3.6 Evaluation of the Reynolds Stress Tensor

The TNT model is a linear eddy viscosity model (LEVM), and therefore the Reynolds stress tensor that is added to the mean flow equations is defined based on the Boussinesq assumption, namely:

$$\Re_{ij} = \Re_{ij}^{LEVM} \tag{3.48}$$

where

$$\Re_{ij}^{LEVM} = 2\mu_t \left(S_{ij} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \right) - \frac{2}{3}\bar{\rho}k\delta_{ij} \tag{3.49}$$

and

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{3.50}$$

Note that the turbulence kinetic energy k is not available with the SA-Edwards model, therefore the term $\frac{2}{3}\bar{\rho}k\delta_{ij}$ is neglected when using the SA-Edwards model.

3.7 Turbulence-Mean-flow Coupling

In eddy-viscosity-based models, the coefficients of viscosity μ and thermal conductivity κ are replaced by the relations

$$\begin{aligned} \mu &= \bar{\mu}_l + \bar{\mu}_t \\ \kappa &= \bar{\kappa}_l + \frac{C_p\bar{\mu}_t}{Pr_t} \end{aligned} \tag{3.51}$$

to account for the effects of turbulence on the mean-flow. The turbulent Prandtl number is assumed constant ($Pr_t = 0.9$).

3.8 Hybrid RANS/LES Turbulence Models

Hybrid RANS/LES turbulence models provide the means to conduct complex, realistic flow simulations in an affordable manner. Among others, these types of flows include unsteady flows that exhibit massive flow separation. Such flows are know to be outside the validity bounds of RANS turbulence models. Arising from the need for an accurate description of complex, unsteady, separated flows while limited in computational resources has been the driving force behind the development of hybrid RANS/LES models. Hybrid models act in RANS mode near wall regions and switch to an LES mode further from walls, where accurate prediction of turbulent mixing is critical for the prediction of complex flow, *e.g.,* flows involving chemical reactions or combustion. Hybrid models relieve the need for a high grid resolution near the wall that is required by a pure LES model.

Currently, the Improved Delayed Detached Eddy Simulation (IDDES) family of hybrid RANS/LES models is available for use in the **Arion** flow solver. Two variant are supported, the first is based on the Spalart-Allmaras turbulence model, namely, SA-IDDES, and the second is based on the k-ω-SST turbulence model, namely, k-ω-SST-IDDES.

3.8.1 Subgrid Length Scale

The hybrid models that are implemented in the **Arion** flow solver require the calculation of a subgrid characteristic length that is usually associated with the local grid size and/or the local flow characteristics. The code provides 2 methods to set the subgrid characteristic length as described in the following sections. From here to forth, the LES subgrid length scale is denoted by Δ, evaluated using

$$\Delta = \min\left[\max\left(C_\omega d_w, C_\omega h_{\max}, h_{\min}\right), \Delta_{ls}\right] \tag{3.52}$$

The coefficient C_ω is set as $C_\omega = 0.15$, d_w is the distance between the cell center and the nearest wall, $h_{\max}$ is the largest distance to the nearest neighboring cell, $h_{\min}$ is the smallest distance to the nearest neighboring cell, and Δ_{ls} is another length

scale that can be either set to $h_{\max}$ or to the shear layer adapted length scale (Δ_{SLA}, described in the following section).

3.8.1.1 Shear Layer Adapted Length Scale

The Shear Layer Adapted (SLA) length scale is defined as:

$$\Delta_{\text{SLA}} = \tilde{\Delta}_{\omega} F_{\text{KH}}\left(\text{VTM}\right) \tag{3.53}$$

where VTM is the vortex tilting measure given by:

$$\text{VTM} = \frac{\left|(S\cdot\omega)\times\omega\right|}{\omega^2\sqrt{-Q_S}} \tag{3.54}$$

where S is the rate-of-strain tensor and Q_S denotes the second invariant of the tensor. The VTM can be viewed as a measure of how much the rate-of-strain tensor tilts the vorticity vector toward another direction. The function F_{KH} is aimed at unlocking the Kelvin-Helmholtz instability in the initial part of shear layers. The function satisfies $0 \leq F_{KH}\left(VTM\right) \leq 1$, $F_{KH}\left(0\right) = 0$, and $F_{KH}\left(1\right) = 1$.

3.8.2 The SA-IDDES Turbulence Model

The SA-IDDES formulation defers from the original SA turbulence model formulation by the destruction term (Equation 3.9) that now reads:

$$D_{SA} = c_{w_1} f_w \rho \left(\frac{\tilde{\nu}}{l_{IDDES}}\right)^2 \tag{3.55}$$

where l_{IDDES} is the IDDES length scale (see Section 3.8.4).

3.8.3 The k-ω-SST-IDDES Hybrid Turbulence Model

A unified formulation for the k-ω-SST-IDDES hybrid turbulence model source term is given by:

$$S = \begin{Bmatrix} P_k - \rho\dfrac{k^{1.5}}{l_k} \\ \dfrac{\alpha_\omega}{\mu_t}\rho P_k - \beta\rho\omega^2 + 2\left(1-F_1\right)\dfrac{\rho\sigma_{\omega 2}}{\omega}\max\left(\dfrac{\partial k}{\partial x_j}\dfrac{\partial \omega}{\partial x_j}, 0\right) \end{Bmatrix} \tag{3.56}$$

where l_{IDDES} is the IDDES length scale (see Section 3.8.4).

3.8.4 IDDES Formulation

The IDDES length scale, l_{IDDES} in Equations (3.55) and (3.56), is given by:

$$l_{IDDES} = \tilde{f}_d\left(1+f_e\right)l_{RANS} + \left(1-\tilde{f}_d\right)l_{LES} \tag{3.57}$$

The RANS model length scale is given by[1]:

$$\begin{cases} l_{RANS} = d_w & \text{SA model} \\ l_{RANS} = \dfrac{k^{1/2}}{\beta^*\omega} & \text{k-}\omega\text{-SST model} \end{cases} \tag{3.58}$$

while the LES length scale is given by:

$$l_{LES} = C_{DES}\Delta \tag{3.59}$$

with C_{DES} being:

$$C_{DES} = C_{DES1}F_1 + C_{DES2}\left(1-F_1\right) \tag{3.60}$$

where $C_{DES1} = 0.78$, $C_{DES2} = 0.61$, and the function F_1 is given in Equation (3.31). The function $\tilde{f}_d$ is a blending function given by:

$$\tilde{f}_d = \max\left[\left(1-f_{dt}\right), f_b\right] \tag{3.61}$$

[1]Note that when $\tilde{f}_d = 0$ the model reverts back to the original turbulence model

where

$$f_{dt} = 1 - \tanh\left[\left(C_{dt1}\mathbf{r}_{dt}\right)^{C_{dt2}}\right] \tag{3.62}$$

with $C_{dt1} = 20$ and $C_{dt2} = 3$ and

$$\mathbf{r}_{dt} = \frac{\nu_t}{\kappa^2 d_w^2 \sqrt{0.5\left(S^2 + \Omega^2\right)}} \tag{3.63}$$

where d_w is the distance to the nearest wall, S is the magnitude of the strain stress tensor, Ω is the magnitude of the vorticity vector, and $\kappa = 0.41$. The function f_b is given by:

$$f_b = \min\left[2\ exp\left(-9\alpha^2\right), 1.0\right] \tag{3.64}$$

where

$$\alpha = 0.25 - \frac{d}{\Delta_{ls}} \tag{3.65}$$

The function f_e is given by:

$$f_e = f_{e2} \max\left[\left(f_{e1} - 1\right), 0\right] \tag{3.66}$$

where

$$f_{e1} = \begin{cases} 2\ exp\left(-11.09\alpha^2\right) & \alpha \geq 0 \\ 2\ exp\left(-9.0\alpha^2\right) & \alpha < 0 \end{cases} \tag{3.67}$$

and

$$f_{e2} = 1 - \max\left(f_t, f_l\right) \tag{3.68}$$

The function f_t and f_l are given by:

$$f_t = \tanh\left[\left(C_t^2 \mathbf{r}_{dt}\right)^3\right] \tag{3.69}$$

and

$$f_l = \tanh\left[\left(C_l^2 \mathbf{r}_{dl}\right)^3\right] \tag{3.70}$$

where

$$\mathbf{r}_{dl} = \frac{\nu}{\kappa^2 d^2 \sqrt{0.5\left(S^2 + \Omega^2\right)}} \tag{3.71}$$

The coefficients C_l and C_t are set to $C_l = 5.0$ and $C_t = 1.87$

Chapter 4

Computational Methods

4.1 Spatial Discretization

A conservative cell-centered finite volume methodology is employed to discretize the governing equations. The computational domain is a unstructured hybrid grid that is discretized into N_{cv} non-overlapping control volumes. A control volume, C_v is defined by a grid volume element and $\partial\Gamma$ is the volume control surface, with $\mathbf{n} = [n_x, n_y, n_z]^T$ being the outward-pointing, unit normal vector to $\partial\Gamma$. Therefore, Equation (2.6) for a control volume C_v can be expressed as:

$$\frac{\partial}{\partial t}\int_{C_v} Q dV + \int_{\partial\Gamma} H dS = 0 \tag{4.1}$$

where H is the rotated flux, namely,

$$\begin{aligned} H &= H_c + H_d \\ H_c &= E_c n_x + F_c n_y + G_c n_z \\ H_d &= E_d n_x + F_d n_y + G_d n_z \end{aligned} \tag{4.2}$$

The term H_c is the convective part of the flux while H_d is the diffusive part of the flux. The semi-discrete form of Equation(4.1) for a non-deforming cell i is given by:

$$V_i \frac{dQ_i}{dt} = - \sum_{j \in N(i)} H_{ij} S_{ij} = R_i \tag{4.3}$$

where V_i denotes the cell volume, Q_i is the vector of cell-averaged conservative dependent variables, $N(i)$ denotes the set of cell i neighbors, H_{ij} is the rotated flux vector normal to the interface ij shared by cell i and cell j, and S_{ij} is the interface area. The number of cell neighbors, $N(i)$, depends on the type of the cell element. For example, a tetrahedron has 4 neighbors and therefore $N(i) = 4$ whereas for a hexahedron it is $N(i) = 6$. The term R_i signifies the residual of the equations. In what follows, the subscript "i" is dropped for compactness of the representation.

4.2 Flux Approximation Schemes

In flux difference splitting, the problem of computing the cell-face fluxes for a control volume is viewed as a series of one-dimensional Riemann problems along the direction normal to the control-volume faces. Because some of the details of the exact solution, obtained at considerable cost, are lost in the cell-averaged representation of the data, the solution of the full Riemann problem is usually replaced by methods referred to as approximate Riemann solvers. In what follows, the currently employed HLLC scheme is described in detail.

4.2.1 HLLC

The concept of average-state approximations was introduced by Harten, Lax and van-Leer [18] in 1983. The Harten, Lax and van-Leer (HLL) scheme is attractive because of its robustness, conceptual simplicity, and ease of coding, but it has the serious flaw of a diffusive contact surface. This is mainly because the HLL solver reduces the exact Riemann problem to two pressure waves and therefore neglects the contact surface. Toro *et al* [19] discussed this limitation, and proposed a modified

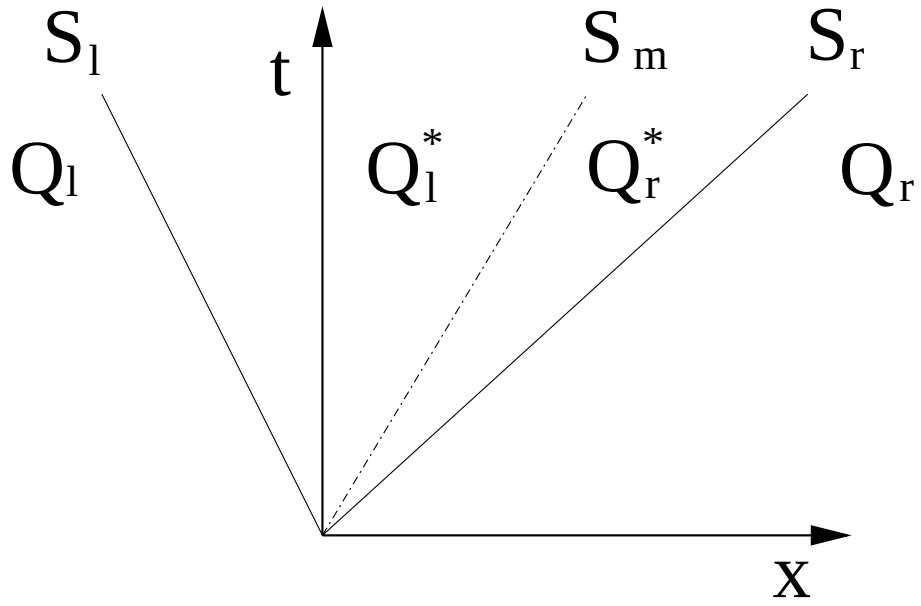

Figure 4.1: Wave structure of the HLLC approximate Riemann solver

three wave solver, named HLLC, where the contact discontinuity is explicitly present. The HLLC scheme is found to have the following properties:

1. Exact preservation of isolated contact discontinuities and shear waves.
2. Positivity preserving of a scalar quantity.
3. Enforcement of the entropy condition.

The resulting scheme greatly improves contact discontinuity resolution and has been successfully used to compute compressible viscous and turbulent flows [20].

The HLLC approximate Riemann solver that is implemented in the **Arion** code is as proposed by Batten *et al* [20]. The HLLC scheme assumes two intermediate states, $\mathbf{Q}_l^*$ and $\mathbf{Q}_r^*$ within the region bounded by the left moving wave, S_l, and the right moving wave, S_r (the subscripts "l" and "r" denote the left and right states of the approximate Riemann problem, respectively). The states $\mathbf{Q}_l^*$ and $\mathbf{Q}_r^*$ are split by the contact discontinuity, which moves with the velocity S_m (see Figure 4.1).

Two wave speed estimates can be used. In the first, the wave speeds S_l and S_r are computed according to Einfeldt *et al* [21] as follows:

$$S_l = \min[\lambda_{min}, \lambda_{min}^{Roe}] \tag{4.4}$$

$$S_r = \max[\lambda_{max}, \lambda_{max}^{Roe}] \tag{4.5}$$

where λ_{min} is the smallest eigenvalue and λ_{max} is the largest eigenvalue, evaluated at the interface. Similarly, λ_{min}^{Roe} and λ_{max}^{Roe} are the smallest and largest eigenvalues of Roe's average matrix [22], respectively. In the second, the wave speeds S_l and S_r are computed according to Davis [23] as follows:

$$S_l = \min[\lambda_{min}(L), \lambda_{min}(R)] \tag{4.6}$$

$$S_r = \max[\lambda_{max}(L), \lambda_{max}(R)] \tag{4.7}$$

The normal velocity to the interface, denoted by q, is defined as:

$$q = (u - u_g) n_x + (v - v_g) n_y + (w - w_g) n_z \tag{4.8}$$

The contact discontinuity speed S_m is evaluated according to Batten *et al* [20] by

$$S_m = \frac{\rho_r q_r (S_r - q_r) - \rho_l q_l (S_l - q_l) + p_l - p_r}{\rho_r (S_r - q_r) - \rho_l (S_l - q_l)} \tag{4.9}$$

This choice of S_m enforces the equality of the two star pressures, *i.e.*, $p^* = p_l^* = p_r^*$ which is obtained from

$$p^* = \rho_l (q_l - S_l)(q_l - S_m) + p_l = \rho_r (q_r - S_r)(q_r - S_m) + p_r \tag{4.10}$$

Introducing the intermediate left state vector

$$\mathbf{Q}_l^* = \begin{Bmatrix} \rho_l^* \\ (\rho u)_l^* \\ (\rho v)_l^* \\ (\rho w)_l^* \\ E_l^* \end{Bmatrix} = \Omega_l \begin{Bmatrix} \rho_l \left(S_l - q_l\right) \\ \left(S_l - q_l\right)(\rho u)_l + \left(p^* - p_l\right) n_x \\ \left(S_l - q_l\right)(\rho v)_l + \left(p^* - p_l\right) n_y \\ \left(S_l - q_l\right)(\rho w)_l + \left(p^* - p_l\right) n_z \\ \left(S_l - q_l\right) E_l - p_l q_l + p^* S_m \end{Bmatrix} \tag{4.11}$$

where $\Omega_l \equiv \left(S_l - S_m\right)^{-1}$. The left state flux vector becomes

$$\mathbf{H}_{c_l}^* \equiv \mathbf{H}_c\left(\mathbf{Q}_l^*\right) = \mathbf{Q}_l^* S_m + \begin{Bmatrix} 0 \\ p^* n_x \\ p^* n_y \\ p^* n_z \\ p^* S_m \end{Bmatrix} \tag{4.12}$$

and the corresponding intermediate right state vector and right flux vector are obtained from Equations (4.11), (4.12) by interchanging the subscripts $l \rightarrow r$. Finally, the numerical HLLC flux is defined as follow

$$\mathbf{H}_c\left(\mathbf{Q}_l, \mathbf{Q}_r\right) = \begin{Bmatrix} \mathbf{H}_c\left(\mathbf{Q}_l\right) & if\ S_l > 0 \\ \mathbf{H}_c\left(\mathbf{Q}_l^*\right) & if\ S_l \leq 0 < S_m \\ \mathbf{H}_c\left(\mathbf{Q}_r^*\right) & if\ S_m \leq 0 \leq S_r \\ \mathbf{H}_c\left(\mathbf{Q}_r\right) & if\ S_r < 0 \end{Bmatrix} \tag{4.13}$$

where $\mathbf{H}_c\left(\mathbf{Q}_l\right)$ and $\mathbf{H}_c\left(\mathbf{Q}_r\right)$ are the left and right analytic flux vectors, respectively.

4.2.2 AUSM

The advection upstream splitting method (AUSM) was first introduced in the year 1993 by Liou and Steffen [24]. The development of the AUSM was motivated by the desire to combine the efficiency of flux vector splitting methods (FVS) and the accuracy of flux differencing splitting methods (FDS). The key idea behind AUSM

schemes is the the fact that the inviscid flux vector consists of two physically distinct parts, namely the *convective* terms and the *pressure* terms. The convective terms can therefore be considered as passive scalar quantities convected by a suitably defined velocity. On the other hand, the pressure flux terms are governed by the acoustics wave speeds.

4.2.2.1 AUSM$^+$-up

Although AUSM schemes enjoy a demonstrated improvement in accuracy, efficiency, and robustness over existing schemes, they have been found to have deficiencies in some cases. In the year 1996, Liou improved the original AUSM, termed now the AUSM$^+$ [25]. Among the improvement features of the original AUSM scheme are the following properties: (1) exact resolution of a one-dimensional contact discontinuity and shock discontinuities, (2) positivity preserving of scalar quantities, (3) free of "carbuncle phenomenon".

In the year 2006, Liou introduced a sequel scheme to the AUSM$^+$ called the AUSM$^+$-up [26] extended for all speed flows. The AUSM$^+$-up is implemented in the **Arion** code and it is given as follows:

$$\mathbf{F}_c\left(\mathbf{Q}_l, \mathbf{Q}_r\right) = \mathbf{p}_{1/2} + \dot{m}_{1/2} \begin{Bmatrix} \boldsymbol{\psi}_l & \text{if } M_{1/2} > 0 \\ \boldsymbol{\psi}_r & \text{otherwise} \end{Bmatrix} \tag{4.14}$$

where

$$\boldsymbol{\psi}_{l/r} = \begin{Bmatrix} 1 \\ u_{l/r} \\ v_{l/r} \\ w_{l/r} \\ H_{l/r} \end{Bmatrix}, \tag{4.15}$$

the mass flux, $\dot{m}_{1/2}$ is defined as

$$\dot{m}_{1/2} = a_{1/2} M_{1/2} \begin{Bmatrix} \rho_l & \text{if } M_{1/2} > 0 \\ \rho_r & \text{otherwise} \end{Bmatrix}, \tag{4.16}$$

and the pressure flux, $\mathbf{p}_{1/2}$ is given as

$$\mathbf{p}_{1/2} = \begin{Bmatrix} 0 \\ p_{1/2}n_x \\ p_{1/2}n_y \\ p_{1/2}n_z \\ 0 \end{Bmatrix} \tag{4.17}$$

where

$$p_{1/2} = \mathcal{P}^{+}_{(5)}(M_l)p_l + \mathcal{P}^{-}_{(5)}(M_r)p_r - K_u\mathcal{P}^{+}_{(5)}(M_l)\mathcal{P}^{-}_{(5)}(M_r)(\rho_l + \rho_r)(f_a a_{1/2})(q_r - q_l) \tag{4.18}$$

is the interface pressure. The interface-normal velocity is denoted by q, H denotes the specific total enthalpy, and K_u is a constant that equals 0.75. The remaining functions are given below. The left/right Mach number at the interface, $M_{l/r}$, is defined as follows:

$$M_{l/r} = \frac{q_{l/r}}{a_{1/2}} \tag{4.19}$$

where $a_{1/2}$ is the speed of sound at the interface and it may be calculated by a simple average of a_l and a_r:

$$a_{1/2} = \frac{a_l + a_r}{2} \tag{4.20}$$

Next, the Mach number at the interface, $M_{1/2}$ is calculated as follows:

$$\begin{aligned}
\overline{M}^2 &= \frac{q_l^2 + q_r^2}{2a_{1/2}^2} \\
M_o^2 &= min\left(1, max\left(\overline{M}^2, M_\infty^2\right)\right) \\
f_a\left(M_o\right) &= M_o\left(2 - M_o\right) \\
\rho_{1/2} &= \frac{\rho_l + \rho_r}{2} \\
M_{1/2} &= \mathcal{M}^{+}_{(4)}\left(M_l\right) + \mathcal{M}^{-}_{(4)}\left(M_r\right) - \frac{K_p}{f_a} max\left(1 - \sigma\overline{M}^2, 0\right)\frac{p_r - p_l}{\rho_{1/2}a_{1/2}^2}
\end{aligned} \tag{4.21}$$

with the constants $K_p = 0.25$ and $\sigma = 1.0$. The split Mach numbers $\mathcal{M}_m^{+/-}$ are

polynomial functions of degree m (=1,2,4) of the Mach number, M, given as follows:

$$\begin{aligned}
\mathcal{M}_1^{\pm} &= \frac{1}{2}\left(M \pm |M|\right) \\
\mathcal{M}_2^{\pm} &= \pm\frac{1}{4}\left(M \pm 1\right)^2 \\
\mathcal{M}_{(4)}^{\pm}(M) &= \begin{cases} \mathcal{M}_{(1)}^{\pm} & if\ |M| > 0 \\ \mathcal{M}_{(2)}^{\pm}(1 \mp 16\beta\mathcal{M}_{(2)}^{\mp}) & otherwise \end{cases}
\end{aligned} \tag{4.22}$$

with the constant $\beta = 1/8$. Finally, the pressure polynomials are given as:

$$\mathcal{P}_{(5)}^{\pm}(M) = \begin{cases} \frac{1}{M}\mathcal{M}_{(1)}^{\pm} & if\ |M| \geq 1 \\ \mathcal{M}_{(2)}^{\pm}[(\pm 2 - M) \mp 16\alpha M\mathcal{M}_{(2)}^{\mp}) & otherwise \end{cases} \tag{4.23}$$

with the function $\alpha = \frac{3}{16}(-4 + 5f_a^2)$.

4.2.2.2 AUSM-DV

The AUSMDV [27] flux uses a blending function to combine the flux-difference (AUSMD) and flux-vector (AUSMV) versions of the basic AUSM flux to obtain a robust scheme that accurately resolves shock waves. The AUSMDV scheme has several properties that are favorable for hypersonic flows (*e.g.*, high-resolution of contact discontinuities, conservation of enthalpy for steady flows and applicability to chemically reacting flows). Therefore, this variant of the AUSM flux is recommended for simulations with the multi-component gas (MCG) physical model.

The AUSMDV flux is given as follows [27]. First, define the splittings of the interface-normal velocity, q, as follows:

$$q_l^{+} = \begin{cases} \alpha_l \frac{(q_l + a_m)^2}{4a_m} + (1 - \alpha_l)q_l^{pos} & \text{if } |q_l| \leq a_m, \\ q_l^{pos} & \text{otherwise} \end{cases} \tag{4.24}$$

$$q_r^{-} = \begin{cases} -\alpha_r \frac{(q_r - a_m)^2}{4a_m} + (1 - \alpha_r)q_r^{neg} & \text{if } |q_r| \leq a_m, \\ q_r^{pos} & \text{otherwise} \end{cases} \tag{4.25}$$

Where,

$$q_l^{pos} = \frac{1}{2}\left(q_l + |q_l|\right) \tag{4.26}$$

$$q_r^{neg} = \frac{1}{2}\left(q_r - |q_r|\right) \tag{4.27}$$

with q_l, q_r denoting the interface-normal velocities evaluated from the left and right states (cells), respectively. Furthermore, the interface speed of sound is given by

$$a_m = max(a_l, a_r); \tag{4.28}$$

and

$$\alpha_l = \frac{2(p_l/\rho_l)}{p_l/\rho_l + p_r/\rho_r} \tag{4.29}$$

$$\alpha_r = \frac{2(p_r/\rho_r)}{p_l/\rho_l + p_r/\rho_r} \tag{4.30}$$

are functions designed to avoid dissipation at contact discontinuities.

Then, the mass flux is simply defined as

$$\dot{m}_{1/2} = \rho_l q_l^+ + \rho_r q_r^- \tag{4.31}$$

Next, define the interface pressure as

$$p_{1/2} = p_l^+ + p_r^- \tag{4.32}$$

where the splittings of the pressure, p_l^+, p_r^- are given as follows:

$$p_l^+ = \begin{cases} p_l \frac{(q_l+a_m)^2}{4a_m^2}(2 - \frac{q_l}{a_m}) & \text{if } |q_l| \le a_m, \\ p_l \frac{q_l^{pos}}{q_l} & \text{otherwise} \end{cases} \tag{4.33}$$

$$p_r^- = \begin{cases} p_r \frac{(q_r-a_m)^2}{4a_m^2}(2 + \frac{q_r}{a_m}) & \text{if } |q_r| \le a_m, \\ p_r \frac{q_l^{neg}}{q_r} & \text{otherwise} \end{cases} \tag{4.34}$$

$$\tag{4.35}$$

Then, the momentum flux vector of AUSMDV is defined by blending of the AUSMD and AUSMV fluxes, as follows:

$$(\rho \mathbf{u} q)_{1/2} = \frac{1}{2}\left[(1+s)(\rho \mathbf{u} q)_{AUSMV} + (1-s)(\rho \mathbf{u} q)_{AUSMD}\right] + p_{1/2}\mathbf{n} \tag{4.36}$$

Where the momentum flux vectors of the AUSMV and AUSMD variants are given by:

$$(\rho \mathbf{u} q)_{AUSMV} = \rho_l q_l^+ \mathbf{u_l} + \rho_r q_r^- \mathbf{u_r} \tag{4.37}$$

$$(\rho \mathbf{u} q)_{AUSMD} = \frac{1}{2}\left[\dot{m}_{1/2}(\mathbf{u_l} + \mathbf{u_r}) - |\dot{m}_{1/2}|(\mathbf{u_r} - \mathbf{u_l})\right] \tag{4.38}$$

where $\mathbf{u}_{l/r} = (u, v, w)_{l/r}$ denote the velocity vectors evaluated from the left and right states (cells) of the interface, and $s = min\left[1, K\frac{|p_r - p_l|}{min(p_l, p_r)}\right]$ is the blending function. K is typically set equal to 10.

The total energy flux is defined by

$$(\rho H q)_{1/2} = \frac{1}{2}\left[\dot{m}_{1/2}(H_l + H_r) - |\dot{m}_{1/2}|(H_r - H_l)\right] \tag{4.39}$$

And the final expression for the interface-normal AUSMDV flux vector is:

$$\mathbf{F}_c(\mathbf{Q}_l, \mathbf{Q}_r) = \begin{Bmatrix} \dot{m}_{1/2} \\ (\rho u q)_{1/2} \\ (\rho v q)_{1/2} \\ (\rho w q)_{1/2} \\ (\rho H q)_{1/2} \end{Bmatrix} \tag{4.40}$$

4.2.3 Steger-Warming Flux Vector Splitting

The Steger-Warming scheme uses the homogeneous property of the inviscid flux vector, namely $E_c(\alpha Q) = \alpha E_c(Q)$, resulting in:

$$E_c(Q) = \frac{\partial E_c}{\partial Q} Q \equiv AQ \tag{4.41}$$

where A denotes the *Jacobian matrix* of the inviscid flux vector. The matrix A may be diagonalized, so that $A = L\Lambda R$, where L, R are the corresponding left- and right-eigenvectors of A, and Λ is a diagonal matrix composed of the eigenvalues of A. To produce an upwind-biased scheme, the inviscid flux is split into upstream (positive) and downstream (negative) contributions as follows:

$$E_{c,SW} = E_c^+ + E_c^- = A_l^+ Q_l + A_r^- Q_r \tag{4.42}$$

where l and r denote values from cells left and right of an interface, and $A_l^+ = (L\Lambda^+ R)_l$ and $A_r^- = (L\Lambda^- R)_r$. The positive and negative parts of the *n-th* eigenvalue of A are given by:

$$\lambda_n^{\pm} = \frac{1}{2}\left(\lambda_n \pm |\lambda_n|\right) \tag{4.43}$$

The discretization of the convective flux using the Steger-Warming scheme may yield non-physical solutions, specifically such that violate the second law of thermodynamics, *i.e.*, result in an impossible increase in entropy [28]. One way that such non-physical phenomena can be avoided is by redefining the eigenvalues in the following manner [29]:

$$\lambda_n^{\pm} = \frac{1}{2}\left(\lambda_n \pm \sqrt{(\lambda_n)^2 + (\epsilon a)^2}\right) \tag{4.44}$$

where ϵ is a constant typically set to 0.1-0.2, and a is the local speed of sound. The entropy correction is applied to all the eigenvalues, even though only the acoustic waves need to be corrected to prevent non-physical solutions. Applying the entropy correction to all the eigenvalues does not affect the accuracy of the solution and allows to use larger time steps in the pseudo-time integration of the equations [29].

The Steger-Warming Jacobian are highly recommended for use in supersonic flows, and in other, "numerically stiff" problems where the increased dissipation introduced by the Steger-Warming Jacobians may enhance overall robustness, without compromising accuracy.

4.2.4 Passive Scalar Approach

The **Arion** code implements the passive scalar approach [20] in spatial discretization of the various model equations (*e.g.*, turbulence, finite-rate chemistry, etc.). The passive scalar approach enables to treat the extended governing equation set (including the model equations) in a similar manner to that presented for the Navier-Stokes equations. For example, when using any of the $k-\omega$ models with the HLLC scheme, the left and right state vectors are extended as follows:

$$\mathbf{Q}_l^* = \begin{Bmatrix} \rho_l^* \\ (\rho u)_l^* \\ (\rho v)_l^* \\ (\rho w)_l^* \\ E_l^* \\ (\rho k)^* \\ (\rho \phi)^* \end{Bmatrix} = \Omega_l \begin{Bmatrix} \rho_l \left(S_l - q_l\right) \\ \left(S_l - q_l\right)(\rho u)_l + \left(p^* - p_l\right) n_x \\ \left(S_l - q_l\right)(\rho v)_l + \left(p^* - p_l\right) n_y \\ \left(S_l - q_l\right)(\rho w)_l + \left(p^* - p_l\right) n_z \\ \left(S_l - q_l\right) E_l - p_l q_l + p^* S_m \\ \rho k \\ \rho \phi \end{Bmatrix} \tag{4.45}$$

The HLLC inviscid flux is then easily evaluated using:

$$\mathbf{H}_{c_l}^* \equiv \mathbf{H}_c\left(\mathbf{Q}_l^*\right) = \mathbf{Q}_l^* S_m + \begin{Bmatrix} 0 \\ p^* n_x \\ p^* n_y \\ p^* n_z \\ p^* S_m \\ 0 \\ 0 \end{Bmatrix} \tag{4.46}$$

4.2.5 High Order Flux Approximations

For a first-order-accurate approximation, the left and right state vectors are simply calculated from cell-center values left and right of the interface, respectively. To obtain a higher order flux approximation, the left and right state vectors of the convective flux are evaluated using a linear reconstruction using Green's theorem or a Taylor

series expansion and least squares method. A cell-wise gradient of the primitive variables is constructed, followed by a second order Taylor series expansion, the left and right states are reconstructed. Let the vector $\boldsymbol{W} = (W_m; m = 1, ...7)$ denote the primitive variables vector (for a general $k - \omega$ turbulence model),

$$\boldsymbol{W} = [\bar{\rho}, \widetilde{u}, \widetilde{v}, \widetilde{w}, \bar{p}, k, \omega] \tag{4.47}$$

then the left and right primitive variables are reconstructed as follows:

$$(W_m)_L = (W_m)_i + (\psi_m)_i (\nabla W_m)_i \cdot \boldsymbol{d}_i^{ij} \tag{4.48a}$$

$$(W_m)_R = (W_m)_j + (\psi_m)_j (\nabla W_m)_j \cdot \boldsymbol{d}_j^{ij} \tag{4.48b}$$

where $\boldsymbol{d}_i^{ij}$ $\left(\boldsymbol{d}_j^{ij}\right)$ is the distance vector from the mid-point of face ij to the center of cell i (j), and ψ_m is the cell limiter that is used to suppress oscillations in the solution.

4.3 Diffusive Flux Vector Discretization

The diffusive flux vector normal to the interface, $\mathcal{H}_d$, is a function of the primitive variables vector, $\mathcal{W}$, evaluated at the mid-point of face ij, $\mathcal{W}_{ij}$, and of its derivatives. The vector $\mathcal{W}_{ij}$ is calculated by averaging of adjacent cell-center values (*i.e.*, $\mathcal{W}_i$ and $\mathcal{W}_j$).

4.4 Time Marching Schemes

The **Arion** code provides various possibilities for advancing Equation (4.3) in time. This section contains a brief description of the available schemes. The schemes may be classified as follows:

1. Explicit (single and multi stage) schemes
   (a) Explicit Euler
   (b) Third and fourth order Runge-Kutta schemes

2. Implicit schemes
   (a) Point Gauss-Seidel
3. Multi-stage implicit schemes
   (a) Third fourth and fifth order Runge-Kutta implicit schemes

4.4.1 Explicit schemes

4.4.1.1 Explicit Euler Scheme

Consider the semi-discrete equation[1]:

$$V\frac{dQ}{dt} = R \tag{4.49}$$

A simple, first-order Euler explicit time marching scheme is given by:

$$\Delta Q^n = \frac{\Delta t}{V} R^n \tag{4.50}$$

where ΔQ^n is the increment of the solution between time levels , namely,

$$\Delta Q^n = Q^{n+1} - Q^n \tag{4.51}$$

4.4.1.2 Runge-Kutta Schemes

Arion provides the choice of third or fourth order Runge-Kutta schemes. Consider the semi-discrete formulation as presented in Equation (4.49), the Runge-Kutta scheme formulation is as follows:

$$\begin{aligned} Q^{(0)} &= Q^n \\ Q^{(k)} &= Q^n + \alpha_k \frac{\Delta t}{V} R^{(k-1)}, \quad k = 1, \ldots, K \\ Q^{n+1} &= Q^{(K)} \end{aligned} \tag{4.52}$$

[1] Equation (4.3) without the index

where k is the Runge-Kutta sub-step number, $K = 3$ for third order and $K = 4$ for fourth order, and α_k are the appropriate weights.

4.4.1.3 Time-Accurate Third Order Runge-Kutta TVD

Arion provides the capability to use the third order, time-accurate, Runge-Kutta TVD scheme, defined as:

$$\begin{aligned} Q^{(1)} &= Q^n + \frac{\Delta t}{V} R^n, \\ Q^{(2)} &= \frac{3}{4} Q^n + \frac{1}{4} Q^{(1)} + \frac{1}{4} \frac{\Delta t}{V} R^{(1)}, \\ Q^{n+1} &= \frac{1}{3} Q^n + \frac{2}{3} Q^{(2)} + \frac{2}{3} \frac{\Delta t}{V} R^{(2)} \end{aligned} \tag{4.53}$$

4.4.2 Implicit Time Marching Formulation

The fine grid spacing required to resolve the normal viscous terms close to the body surface requires in turn very small time steps and therefore it rules out the use of explicit methods. In explicit time-marching schemes the maximum time step is proportional to the minimum grid spacing. As a result the time-step limit imposed by stability is very small. In contrast, even though the operation count per time step is high, it is more efficient to use implicit methods. The development of a non-iterative implicit algorithm for the solution of the Navier-Stokes equations requires a time linearization of the nonlinear vectors (R). The linearization procedure is simple since the equations are written in conservation-law form. Applying the first order Euler implicit method and utilizing the Delta form of the equations results in the following implicit scheme:

$$\left(\frac{V}{\Delta t} I - \frac{\partial R}{\partial Q} \right)^n \Delta Q^n = R^n \tag{4.54}$$

where R^n is the residual at time level n as define by Equation (4.3), I is the identity matrix, Δt is the time increment between levels n and $n + 1$, the term $\frac{\partial R}{\partial Q}$ is the Jacobian matrix. Note that the Jacobian matrix is first order and that it may be altered to improve stability.

Applying Equation (4.54) at every grid point results in a block-hepta-diagonal

matrix in three dimensions. The inversion of the matrix, or its approximation, may be conducted in various manners, resulting in a wide variety of implicit time marching schemes.

4.4.2.1 Point Gauss-Seidel

The exact, first order Jacobian matrix is retained only for the diagonal elements and the off diagonal Jacobian matrices are linearized based on the previous time step as follows:

$$\frac{\partial R}{\partial Q}\Delta Q \approx \left(\frac{\partial R}{\partial Q}\right)^{n} \Delta Q^{n} \tag{4.55}$$

Consequently, they can be moved to the right hand side.

4.4.2.2 Runge-Kutta Schemes

Runge-Kutta implicit schemes combine the explicit Runge-Kutta schemes as described in Section 4.4.1.2 with the PGS scheme that is described in Section 4.4.2.1 to form a robust implicit, multi-stage time marching scheme. note that this scheme requires the matrix inversions warranted by the PGS scheme at each stage and therefore requires more computer time per iteration.

4.5 Convergence Acceleration Methods

4.5.1 Krylov Methods

Krylov subspace methods were originally introduced as direct methods [30] for solving linear systems, but only gained popularity after being reintroduced as iterative methods [31]. Krylov methods are actually projection (Galerkin) methods for solving a linear set of equations $Ax = b$ using the Krylov subspace, K_j, spanned by:

$$K_j = span\left(r_0, Ar_0, A^2 r_0, ..., A^{j-1} r_0\right) \tag{4.56}$$

where $r_0 = b - Ax_0$. The main advantage of Krylov methods for large systems of equations, lies in the fact that they require only matrix-vector products to carry out

the iteration, and not the individual elements of A. This also makes them especially suitable for use with Newton's method.

The widely used Generalized Minimal RESidual (GMRES) Krylov method [32] employs Arnoldi basis vectors to form the trial subspace out of which the solution is constructed. One matrix-vector product is required per iteration to create each new trial vector, and the iterations are terminated based on an estimate of the residual that does not require explicit construction of intermediate residual vectors or solutions, which constitutes a major benefit of the algorithm. Several studies [33–35] have established the superiority of GMRES over other Krylov methods, especially in a Jacobian-Free Newton-Krylov framework. Consequently, GMRES is used to solve the large equation set arising in each Newton iteration, given by Equation 4.54.

4.5.1.1 Preconditioning

The intensive memory-pressure typically encountered in modern CFD codes has put an increased emphasis on quality preconditioning to complement Krylov methods. In fact, Krylov methods were shown to be efficient for large-scale problem only when coupled with effective preconditioning of the matrix A [33]. The **Arion** code employs the additive Schwartz method in which the action of the pre-conditioner is broken-down to smaller sub-pre-conditioners defined on individual geometric subdomains. The primary motivation for such an approach is its parallel scalability [36, 37]. Furthermore, domain-based parallelism is recognized as the form of data parallelism that most effectively exploits modern processors that possess a multi-level memory hierarchy [38].

Specifically, the **Arion** code makes use of the restricted additive Schwarz method (RASM), which eliminates interprocess communication during either the restriction or prolongation phase of the additive Schwarz technique [39], thus further increasing its suitability for massive-scale, distributed computations. The relatively small subsets of linear equations arising in the process of applying the preconditioner are solved with a local, block incomplete lower-upper (ILU) decomposition method.

4.5.1.2 Portable, Extensible Toolkit for Scientific Computation (PETSc)

PETSc, the Portable, Extensible Toolkit for Scientific Computation is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. PETSc is developed as open-source. Among the various solution methods that are available by the PETSc Toolkit, the **Arion** code utilizes certain Krylov solvers. The reader is referred to Section 8.13 for the PETSc directives that are supported by the **Arion** code.

4.5.2 Line Search

The **Arion** code uses the back-traced lines search algorithm as briefly described in this section. Let a general implicit iterative scheme be defined as:

$$\left(\frac{V}{\Delta t} - J^n\right)\Delta Q^n = R^n \tag{4.57}$$

where V is the cell volume, ΔQ^n is the vector of dependent variables correction term at iteration n, R is the residual vector, and J is the Jacobian matrix defined as:

$$J \triangleq \frac{\partial R}{\partial Q} \tag{4.58}$$

A relaxed updated solution may be given by

$$Q^{n+1} = Q^n + \alpha \Delta Q^n \tag{4.59}$$

where α is relaxation parameter. The relaxation parameter can manually prescribed or optimally calculated using a back-traced line search algorithm [40].

4.5.2.1 Back-Traced Line Search

Let the function $f(\alpha)$ be defined as

$$f(\alpha) = \frac{1}{2} R^T R \tag{4.60}$$

Consequently,

$$\begin{aligned} f(0) &= \frac{1}{2} R^{T^n} R^n \\ f(1) &= \frac{1}{2} R^{T^{n+1}} R^{n+1} \\ f'(0) &= R^{T^n} J^n \Delta Q^n \end{aligned} \tag{4.61}$$

Let the polynomial function satisfying the conditions in Equation 4.61 be defined as:

$$f(\alpha) = a\alpha^2 + b\alpha + c \tag{4.62}$$

The optimal relaxation parameter is such that minimizes the function f.

The algorithm that is implemented in the **Arion** code is as follows:

1. Solve the linear system:

$$J(Q^n)\,\Delta Q^n = -R(R^n)$$

2. Calculate the new residual:

$$R(Q^n + \Delta Q^n)$$

3. Check if the convergence is satisfactory:

$$f(Q^n + \Delta Q^n) < f(Q^n) + \beta\alpha \nabla f(Q^n)^T \Delta Q^n$$

4. If convergence is satisfactory, move on to the next Newton iteration. If not perform a line search:

$$\alpha | \min_{\alpha} f(Q^n + \alpha \Delta Q^n)$$

5. Repeat (go to 3) until the new residual is good enough or the maximum number of line search iterations is iteration reached or the minimum value of α is obtained.

The application of the lines search algorithm in the **Arion** code is in addition to

the Krylov methods (see Section 4.5.1). It is invoked through a directive (or a series thereof) to set the number of line search iterations, the convergence criterion constant, β, etc. The reader is referred to Section 8.12.2 for all of the relevant directives.

Chapter 5

Boundary Conditions

5.1 Introduction

The **Arion** code contains a wide variety of boundary conditions. Being an unstructured finite volume code, the notion of a ghost cell is utilized throughout. However, in certain cases the Jacobian and flux are explicitly dictated rather than calculated based on the ghost. In particular, the convection Jacobian and flux. In what follows, the subscript "g" signifies a ghost cell, the subscript "r" signifies a real cell where the flow is solved (a "real" cell), and the subscript "f" signifies the face (prescribed) value.

5.2 Wall Boundary Conditions

5.2.1 Impermeable Wall Conditions

Let $\hat{n}$ be the unit vector normal to the face of a boundary cell, with components (n_x, n_y, n_z). Then, the velocity in the ghost cell is taken as

$$\overline{V}_g = \overline{V}_r - 2\left(\overline{V}_r \cdot \hat{n} - \overline{V}_f \cdot \hat{n}\right)\hat{n} \tag{5.1}$$

The prescribed velocity vector $\overline{V}_f$ includes any motion of the boundary surface.

5.2.2 No-Slip Condition

The no-slip condition is much easier to implement:

$$\overline{V}_g = 2\overline{V}_f - \overline{V}_r \tag{5.2}$$

5.2.3 Adiabatic Wall

The temperature is set using:

$$T_g = T_r \tag{5.3}$$

while the pressure is set using

$$p_g = p_r \tag{5.4}$$

The density is evaluated using the equation of state.

5.2.4 Wall Function

The wall function follows the formulation of Nichols and Nelson [41] (see Table 5.2.1 for wall function activation).. The near-wall velocity profile is given by

$$\begin{aligned} y^+ = u^+ + y_0^+ \Bigg[\exp\left(\frac{\kappa}{\sqrt{\Gamma}}\left(\sin^{-1}\left(\frac{2\Gamma u^+ - \beta}{Q}\right) - \varphi\right)\right) \\ - 1 - \kappa u^+ - \frac{1}{2}(\kappa u^+)^2 - \frac{1}{6}(\kappa u^+)^3 \Bigg]. \end{aligned} \tag{5.5}$$

with

$$u^+ = \frac{u}{u_\tau}, \qquad y^+ = \frac{\rho_w u_\tau y}{\mu_w}, \qquad u_\tau = \sqrt{\frac{|\tau_w|}{\rho_w}}, \tag{5.6}$$

where u is the local tangential velocity magnitude, y is the wall-normal distance from the wall, and $\nu_w = \mu_w/\rho_w$ is the kinematic viscosity at the wall.

In addition,

$$\Gamma = \frac{r\,u_\tau^2}{2c_p T_w}, \qquad \beta = \frac{q_w \mu_w}{\rho_w T_w k_w u_\tau}, \qquad \varphi = \sin^{-1}\left(-\frac{\beta}{Q}\right), \tag{5.7}$$

$$Q = \sqrt{\beta^2 + 4\Gamma}, \qquad y_0^+ = e^{-\kappa B}. \tag{5.8}$$

The dimensionless parameter Γ models compressibility effects, whereas β models wall heat-transfer effects. The wall shear stress τ_w appears in the definitions of u^+, y^+, Γ, and β. The wall heat flux q_w appears only in the definition of β.

The temperature profile is given by

$$T = T_w \left(1 + \beta u^+ - \Gamma (u^+)^2\right). \tag{5.9}$$

For an adiabatic wall, the velocity and temperature equations are decoupled. The velocity equation is solved first for τ_w, and the temperature equation is then solved for T_w. For an isothermal wall, the equations are solved simultaneously for τ_w and q_w. Once the solution is obtained, the turbulent viscosity in the first off-wall cell is computed as

$$\mu_{t,w+1} = \mu_w \left.\frac{dy^+}{du^+}\right|_{w+1} - \mu_{w+1}. \tag{5.10}$$

Here, μ_w is the molecular viscosity at the wall, and the subscript $w+1$ denotes the value of a variable in the first cell adjacent to the wall. The turbulence variables at the first off-wall cell are then evaluated according to the selected model.

For k–ω models, the specific dissipation rate is computed as

$$\omega_{w+1} = \sqrt{\left(\frac{6\nu_w}{b_1\ d^2}\right)^2 + \left(\frac{u_\tau}{\sqrt{\beta^*}\,\kappa d}\right)^2}. \tag{5.11}$$

Where d is the distance from the wall. The turbulent kinetic energy depends on the k–ω variant. For the TNT model,

$$k_{w+1} = \frac{\mu_{t,w+1}\,\omega_{w+1}}{\rho_{w+1}}. \tag{5.12}$$

For the SST model the implicit relation is used,

$$k_{w+1} = \frac{\mu_{t,w+1}}{\rho_{w+1}} \max\left(\omega_{w+1}, \frac{\Omega_{w+1} F_2\left(k_{w+1}\right)}{a_1}\right). \tag{5.13}$$

For the Spalart–Allmaras model, the model variable is obtained from the implicit relation

$$\mu_{t,w+1} = \rho_{w+1}\,\hat{\nu}_{w+1}\,f_{v1}(\hat{\nu}_{w+1}). \tag{5.14}$$

Note that the wall-function procedure is applied only when $y^+ > 5$; otherwise, the wall shear stress and heat flux are computed in the same way as for a fully resolved wall.

5.3 Far Field Conditions

5.3.1 Turkel Type Conditions

The characteristic relations that are due-to Turkel are utilized. For supersonic inflow, the flow quantities at the inflow boundary are set based on the current values of the corresponding boundary:

5.3.1.1 Turkel Inlet

$$\rho_g = \rho_\infty \tag{5.15}$$

$$\overline{V}_g = \overline{V}_\infty \tag{5.16}$$

$$p_g = \frac{\rho_\infty}{\rho_r} p_r \tag{5.17}$$

5.3.1.2 Turkel Outlet

$$\rho_g = \rho_r + \frac{p_\infty - p}{a_\infty^2} \tag{5.18}$$

$$\overline{V}_g = \overline{V}_r \tag{5.19}$$

$$p_g = p_\infty \tag{5.20}$$

5.3.2 Riemann Type Conditions

Let q be the normal to the boundary face velocity. The Riemann invariants are calculated based on the following:

$$\begin{aligned} R^+ &= q_r - \frac{2}{\gamma - 1} a_\infty \\ R^- &= q_\infty - \frac{2}{\gamma - 1} a_r \end{aligned} \tag{5.21}$$

The ghost Riemann invariants are obtained using:

$$R_g = \frac{1}{2}\left(R^+ + R^-\right) \tag{5.22}$$

5.3.2.1 Riemann Inlet

$$\begin{aligned} \rho_g &= \frac{\rho_\infty}{a_\infty^{\frac{1}{\gamma-1}}} \left\{ \underbrace{\left[\frac{\gamma - 1}{4}\left(R^- - R^+\right) \right]^{\frac{1}{\gamma-1}}}_{a_g} \right\}^2 \\ p_g &= \sqrt{a_g}\rho_g\gamma \end{aligned} \tag{5.23}$$

5.3.2.2 Riemann Outlet

Let s be the entropy, the relations for ρ_g and p_g are given by:

$$\begin{aligned} s &= \frac{\rho^\gamma}{\gamma p} \\ \rho_g &= \left(a_g^2 s\right)^{\frac{1}{\gamma-1}} \\ p_g &= \sqrt{a_g}\rho_g\gamma \end{aligned} \tag{5.24}$$

5.3.3 Fixed (Supersonic Inlet)

$$\begin{aligned} \overline{V}_g &= \overline{V}_\infty \\ p_g &= p_\infty \\ T_g &= T_\infty \end{aligned} \tag{5.25}$$

5.3.4 Extrapolation (Supersonic Outlet)

$$\begin{aligned} \overline{V}_g &= \overline{V}_r \\ p_g &= p_r \\ T_g &= T_r \end{aligned} \tag{5.26}$$

5.3.5 Inlet

For supersonic inlet, a fixed boundary condition is applied (see Section 5.3.3). For subsonic inlet, the pressure is extrapolated from within the physical domain and the rest of the flow variables are fixed. This is automatically repeated every time step.

$$\begin{aligned} (\rho, u, v, w)_g &= (\rho, u, v, w)_\infty \\ p_g &= p_r \end{aligned} \tag{5.27}$$

5.3.6 Outlet

For supersonic outlet, an extrapolated boundary condition is applied (see Section 5.3.4). For subsonic outlet, a "Fixed," prescribed value is used for the pressure and the rest of the flow variables are extrapolated. This is automatically repeated every time step. Formally, this is a pressure outlet type boundary condition.

$$\begin{aligned} (\rho, u, v, w)_g &= (\rho, u, v, w)_r \\ p_g &= p_{bc} \end{aligned} \tag{5.28}$$

where p_{bc} is the prescribed pressure outlet. If no pressure outlet is prescribed then $p_{bc} \equiv p_\infty$.

5.3.6.1 Prescribed Mass Flow Rate

To obtain the prescribed mass flow rate at an outlet, the pressure is iteratively corrected in the following manner:

$$p_g = p_{bc} + \delta p \tag{5.29}$$

where p_{bc} is the prescribed pressure outlet (see Table 8.69). The pressure correction, δp, is calculated as follows:

$$\delta p_{new} = \omega \frac{|\dot{m}|^n \left(\dot{m}^n - \dot{m}_{bc}\right)}{\rho_{ave}^n A^2} + \delta p_{old} \tag{5.30}$$

where $\dot{m}^n$ is the computed mass flow rate at the current iteration, ρ_{ave}^n is the computed average density at the current iteration, A is the total area of the boundary, and δp_{new} and δp_{old} are the new and previous calculated pressure corrections, respectively. The parameter ω is a relaxation parameter (see Table 8.52). The mass flow rate is used in conjunction with the "outlet" boundary condition (see Table 8.51).

5.3.7 Inout

These boundary conditions are specific to low subsonic flows. With the exception of the pressure, these boundary conditions set "Fixed" conditions for inlet and "Extrapolation" conditions for outlet. Namely,

- **Inlet :**

$$\begin{aligned} (\rho, u, v, w)_g &= (\rho, u, v, w)_\infty \\ p_g &= p_r \end{aligned} \tag{5.31}$$

- **Outlet :**

$$\begin{aligned}(\rho, u, v, w)_g &= (\rho, u, v, w)_r \\ p_g &= p_\infty\end{aligned} \tag{5.32}$$

5.4 Stagnation Inlet

For subsonic flow, the stagnation inlet boundary condition is implemented as follows. The user prescribes the stagnation temperature and stagnation pressure (see Tables 8.68 and 8.69). Let the negative Riemann invariant be defined as:

$$R^- = q - \frac{2}{\gamma - 1} a \tag{5.33}$$

where $q = \overline{V} \cdot \hat{n}$ is the velocity normal to the face, a is the speed of sound, and γ is the ratio of specific heats.

Applying the Riemann invariance results in

$$R_g^- = q_g - \frac{2}{\gamma - 1} a_g = R_r^- \tag{5.34}$$

The subscript r pertains to the real flow cell, *i.e.*, extrapolated from the interior of the domain, while the subscript g pertains to the value at the ghost cell (boundary). By assuming a calorically perfect gas one can write on the boundary

$$c_p T_0 = c_p T_g + \frac{q_g^2}{2} \tag{5.35}$$

Consequently, the speed of sound at the ghost cell can be evaluated using

$$a_g = \sqrt{(\gamma - 1)\, c_p \left(T_0 - \frac{q_g^2}{2 c_p} \right)} \tag{5.36}$$

Substituting Equation 5.36 into Equation 5.34 results in a quadratic equation in q_g. The pressure, density, and temperature at the ghost cell are calculated using isentropic

relations.

5.5 Symmetry Boundary Conditions

Symmetric boundary conditions are treated exactly as an adiabatic impermeable wall.

Chapter 6

Computational Mesh

The **Arion** code is considered a hybrid code since it supports various cell element types. The code supports tetrahedra, hexahedra, prism, and pyramids. Mesh generation may be conducted by any unstructured grid generator, however, users must export the mesh using a Star-CD export or a CGNS export.

6.1 Star-CD Export

The Star-CD export results in three files. The first, a file containing the vertex information, having the extension ".vrt." The second, a file containing the cell elements, having the extension ".cel." And finally, a file containing the boundary elements (triangles or quads), having the extension ".bnd." The ".bnd" file contains the boundary elements as well as a name for each element. The naming is conducted by the user using the grid generation package (*e.g.,* Pointwise). The code supports two variations of the Star-CD format, the export by Pointwise and the export by CENTAUR (only 3-D export is supported).

6.2 CGNS Export

The CGNS export results in a single file. The file extension of the CGNS file is ".cgns."

6.3 Automated Mesh Adaptation

An automated mesh adaptation procedure is available in the **Arion** code. It requires the use of the Pointwise mesh generation package and can be facilitated through the EZOpt optimization software package. A feature based adaptation sensor that is proportional to an interpolation error is utilized. Using a series of options, a point cloud data file is generated and the mesh is re-generated using the previously generated computational mesh and the point cloud data. The method preserves the boundary layer mesh and it maintains smooth mesh size. The sensor function is given by:

$$S = K \left|\vec{h}\right|^p \left|\left[\hat{\vec{h}} \cdot \frac{\partial \hat{\Phi}}{\partial x_2} - \hat{\vec{h}} \cdot \frac{\partial \hat{\Phi}}{\partial x_1}\right]\right| \tag{6.1}$$

where $\hat{\vec{h}}$ is the distance vector between adjacent points and Φ is problem dependent. The parameters K and p may be prescribed by the user. Currently the **Arion** code supports sensor functions that depend on the Mach number, pressure, density, and velocity magnitude (Φ). The available adaptation options are described in Section 8.19.

Chapter 7

Parallelization

The **Arion** flow solver is designed to work in a distributed memory architecture using the MPI interface. The design of the code distinguishes between managing a simulation and solving the flow field. Within the distributed MPI universe, the first rank is responsible for managing the simulation and henceforth named 'manager rank'. The rest of the ranks are responsible for the flow solution and are named 'worker ranks'. The manager rank responsibility starts with the input analysis, and continuing with reading the initial geometric problem (the grid files), splitting the computational domain into parts and sending those parts to the worker ranks. Therefore, the worker ranks know only part of the computational domain, and pass boundary data among themselves. The manager rank is responsible for the the assembly of the 'restart' files, for timing all the worker threads, and for log output. Since there is a distinction between the manager rank and the worker ranks, one must have at least two ranks running, even if they reside on a single shared memory machine.

Chapter 8

Input File, Run Preparation, and Execution

8.1 Preface

The **Arion** code is driven through the command line with optionally additional input files having a certain syntax. An input file may be constructed using a simple text editor. The solver is invoked by typing the MPI command (depending on the MPI version of the actual machine): "mpirun [mpi options]... arion [−−f input_file] [command-line arguments]"

The input file is made of groups of directives, each group is marked by two consecutive − signs. Each group has a series of options, with each option marked with one − sign. Within the input file the sign ! means a remark until the end of the line. A brief help of all the options may be printed to the screen by using the −−h option. The latest additions to the code may be printed to the screen using the −−new option.

8.1.1 Scripting Language

The input file is a simple ASCII file with certain important rules. This chapter contains a detailed description of all the available command-line options. The syntax of each of the input options, or input file lines, follows the proceeding rules:

- The "# " symbol means that there is a comment until the next option. One may use as many comment lines as necessary.
- Each group of directives starts with two consecutive − signs, *i.e.*, −− followed by the group name and a series of options.
- Each option is marked with one − sign.
- An option may have no parameters, one parameter, or a few parameters.
- Parameters may be assigned values.

The proceeding description of the input options, or input file lines, makes use of the following symbols:

- The "$" symbol signifies a string input.
- The "#" symbol signifies a numerical input.
- The "|" symbol signifies a choice selection.
- The "..." symbol signifies an option that can be repeated.
- Input entries that are enclosed by curly brackets, { }, are required.
- Input entries that are enclosed by square brackets, [ ], are optional.

8.1.2 Basic Input File: Examples

8.1.2.1 Single Component Gas Example

Listing 8.1 contains a simple, single component gas, basic input file for a simple simulation of the ideal-gas flow about a two-dimensional airfoil.

```
--equation.of.state
   -name air
   -type eos.ideal.gas
   -ref.p 101325
   -ref.T 288

--bc
   -name RIE_FREE
   -type riemann

--bc
   -name IWALL
   -type impermeable.wall

--bc
   -name XZSYM
   -type 2d

--system
   -name ideal.gas.mf.inviscid
   -type ideal.gas.mf.inviscid
   -time.step 5 100 cfl.exponential 250
        -cell.gradient green.gauss.node
        -limiter mlp.2d
```

```
   -log convergence cfl residual log.residual

--solve
   -time.march           implicit.rk3.R.pgs
   -convection.flux      hllc.roe
   -convection.jacobian  hllc.roe
   -sweeps 4
   -spatial.order 2

   -iterations  2000
   -save      100
   -save.path ./save/

   -eos air
   -p     101325
   -T     288
   -Mach  0.8
   -alpha 1.25
   -beta  0
   -log convergence iter

--log
   -name convergence
   -prefix ./logs/convergence
   -per iter
   -screen

--plot
   -name naca0012
   -prefix ./plots/plot
   -interval 100
```

```
--uns
       -name naca0012-j129-uns-regular
       -prefix naca0012-j129-uns-regular/naca0012-j129-uns-regular
       -log convergence cl cd

--table
       -name P_table
       -prefix ./tables/table
       -interval 10
       -plane.bc 0 0 0 0 0.5 0 IWALL
```

Listing 8.1: Example of a simple **Arion** input file

8.1.2.2 Multi Component Gas Example

8.2 Grid Files

Currently, **Arion** supports the Star-CD and CGNS Version 3.4 exports only. A detailed description of the files is given in Chapter 6. Starting from Version 1.31, **Arion** uses the Metis open source library to convert the Star-CD or CGNS export to binary format. In addition, Metis assists in decomposing the computational domain into several partitions for the purpose of efficient parallel computations. The following section describes the use of the Metis library for conversion of the files to binary format. The conversion results in a new set of files with "+32" added to all file extensions, signifying that the integers are 32 bit wide.

The new set of files now contains 5 files. The vertex information has the extension".vrt+32." The cell elements file has the extension ".cel+32." The boundary elements file has the extension ".bnd+32." In addition, two new files are generated, one with the extension "nam+32" and the other with the extension "fac+32." As a result, the grid is read by the code in a fast manner.

8.3 Macros

8.3.1 Def

Def is a macros that starts with the directive −− def followed by a key and a value. The syntax is as described in Table 8.1.

Def		
Syntax	−−def $key $value	
Description	Sets a macro. Any '$key' or '${key}' in the options will be replaces by the $value .	
Parameters	$key	Key.
	$value	Value.
Examples	−−def mypath /Users/data/restart/	

Table 8.1: Def macro

8.4 Conversion

The conversion is conducted using the −−star2metis or −−cgns2metis directive as described in Table 8.2. Note that the Metis options that are described in Tables 8.2 and 8.3 are taken directly from the Metis runtime help. For further information the user is referred to the complete Metis User's Manual.

The conversion generates a new set of files, replacing the original files that were generated by the grid generation software package (*e.g.*, Pointwise). The actual files are not split but are reordered in a manner that prepares the files for a parallel read that is efficient in terms of domain decomposition.

Conversion		
Syntax	arion {−−star2metis | −−cgns2metis}$prefix #ranks $output [metis-options]...	
Description	Convert the Star-CD or CGNS files to the Arion binary format and use Metis to decompose the computational domain. See Table 8.3 for Metis options.	
Parameters	star2metis	Convert Star-CD files.
	star2cgns	Convert CGNS files.
	$prefix	Prefix of grid files.
	#ranks	Number of partitions.
	$output	Prefix of output files.
Examples	arion −−star2metis Star-CD-file-name 64 New-file-name	
	arion −−cgns2metis CGNS-file-name 64 New-file-name	

Table 8.2: Conversion

Metis Options

Metis Option	Description
-ptype {rb | kway}	Specifiy the scheme to be used for computing the k-way partitioning: rb - Recursive bisectioning, kway - Direct k-way partitioning [default].
-ctype {rm | shem}	Specify the scheme to be used to match the vertices of the graph; rm - Random matching, shem - Sorted heavy-edge matching [default].
-iptype {grow | random}	Specify the scheme to be used to compute the initial partitioning, (applies only when -ptype = rb); grow - Grow a bisection using a greedy scheme [default], random - Compute a bisection at random.
-objtype {cut | vol}	Specify the objective that the partitioning routines will optimize, (applies only when -ptype = kway); cut - Minimize the edgecut [default]; vol - Minimize the total communication volume.
-no2hop	Specify that the coarsening will not perform any 2-hop matchings when the standard matching fails to sufficiently contract the graph.
-contig	Specify that the partitioning routines should try to produce (applies only when -ptype = kway) partitions that are contiguous. Note that if the input graph is not connected this option is ignored.
-minconn	Specify that the partitioning routines should try to minimize the (applies only when -ptype = kway) maximum degree of the subdomain graph, i.e., the graph in which each partition is a node, and edges connect subdomains with a shared interface.

Table 8.3: Metis options

Metis Options (continued)

Metis Option	Description
-ufactor #x (where x is an integer)	Specify the maximum allowed load imbalance among the partitions. A value of x indicates that the allowed load imbalance is 1+x/1000. For -ptype=rb, the load imbalance is measured as the ratio of the 2*max(left,right)/(left+right), where left and right are the sizes of the respective partitions at each bisection. For -ptype=kway, the load imbalance is measured as the ratio of max_i(pwgts[i])/avgpwgt, where pwgts[i] is the weight of the ith partition and avgpwgt is the sum of the total vertex weights divided by the number of partitions requested. For -ptype=rb, the default value is 1 (i.e., load imbalance of 1.001) For -ptype=kway, the default value is 30 (i.e., load imbalance of 1.03).
-niter #i	Specify the number of iterations for the refinement algorithms at each stage of the uncoarsening process. Default is 10.
-ncuts #c	Specify the number of different partitionings that it will compute The final partitioning is the one that achieves the best edgecut or communication volume. Default is 1.
-seed #s	Select the seed of the random number generator.

Table 8.3: Metis options (continued)

8.4.1 Conversion Between Different Orderings

Arion provides the capabilities to start a simulation from a certain ordering and continue the simulation with a different ordering. This is conducted using the −−cnv2cnv directive as described in Table 8.4.

cnv2cnv		
Syntax	arion −−cnv2cnv $cnv1 $cnv2 $load-prefix $save-prefix {$system1-name}...	
Description	Converts **Arion** solution files between different orderings; creates new restart files.	
Parameters	$cnv1	Ordering type to convert from.
	$cnv2	Ordering type to convert to.
	$load-prefix	Prefix of input files.
	$save-prefix	Prefix of output files.
	$system1-name	Name of converted system.
Examples	arion −−cnv2cnv bin arion ./newsolution/oldfiles ./newsolution/newfiles ./restart/oldfiles	

Table 8.4: Conversion between different ordering (cnv2cnv) option

8.5 Parallel Options

The parallel input options section starts with the −−parallel directive, followed by a series of parallel options.

Cache		
Syntax	−cache #	
Description	Size of the cache memory (in bytes).	
Parameters	#	Cache size.
Examples	−cache 1000	

Table 8.5: Parallel cache option

Rank		
Syntax	[{{-rank #rank} | -all.ranks} | {-rank.span #rank_min #rank_-max} | {-rank.head #head} | {-rank.tail #tail}} {-threads | -parts | -load | -read.threads} #]...	
Description	Define how many OpenMP threads will be open on each rank.	
Parameters	#rank	Rank number.
	-threads	Number of threads for the current rank.
	-all.ranks	Means that all subsequent options hold for all the ranks.
	-rank.span	Means that all subsequent options hold for the span of ranks.
	-rank.head	Means that all subsequent options hold for the starting ranks.
	-rank.tail	Means that all subsequent options hold for the ending ranks.
	-threads	Set the number of solver threads on a specific (or all) rank.
	-read.threads	Use when memory is insufficient to read all the part in parallel (a significant amount of memory is needed to read a zone part, that is deallocated at the end of the read).
	-parts	Number of partitions.
	-load	Changes the load of a rank, by default all ranks have load 1.
	#	Load level for the current rank.
Examples	−rank 1 -threads 1	
	-rank 2 -threads 8	
	-all.ranks -threads 48	
	-rank 2 -load 4	

Table 8.6: Parallel rank option

8.6 Equation of State Options

The "Equation of State" input options section starts with the −−equation.of.state directive, followed by a series of equation.of.state input options. Each section is used to declare a specific fluid with its equation of state and constitutive laws (*e.g.* Sutherland's law). There could be more than one section, one per fluid type. It is first assigned a name to be used by the user. The current version of **Arion** provides the means to solve either a single component perfect gas fluid or a multi-component gas under the assumption of chemical equilibrium. Future versions will support multi-component gas under non-equilibrium conditions.

Name		
Syntax	−name $fluid	
Description	Name of flow medium.	
Parameters	$fluid	Flow medium.
Examples	−name air	

Table 8.7: equation.of.state name option

Type	
Syntax	−type $eos.type.fluid
Description	Choose the type of equation of state. Available types are listed in Table 8.9
Parameters	$eos.type.fluid Type of equation of state.
Examples	−type eos.ideal.gas

Table 8.8: equation.of.state type option

EOS Types	
EOS type	Description
eos.ideal.gas	Perfect gas (see Section 2.2.3 and Equation 2.10).
eos.table	Perfect gas under equilibrium assumption (required for multi-component.gas eqb system).
eos.mcg	Perfect gas under non-equilibrium or frozen chemistry assumption (required for multi-component.gas mcg or mcg.frozen system).

Table 8.9: EOS types

R		
Syntax	−R #	
Description	Set the specific gas constant (applicable to the eos.ideal.gas type only). Default is 287.22 (air).	
Parameters	#	Specific gas constant.
Examples	−R 287.22	

Table 8.10: equation.of.state R option

Gamma		
Syntax	−gamma #	
Description	Set the heat capacity ratio (γ, applicable to the eos.ideal.gas type only). Default is 1.4 (air).	
Parameters	#	Heat capacity ratio.
Examples	−gamma 1.4	

Table 8.11: equation.of.state gamma option

Ref		
Syntax	−ref.$ #	
Description	Set reference properties. These reference values are relevant in particular for the limiters.	
Parameters	-ref.p	Reference pressure. Default is 1.
	-ref.T	Reference temperature. Default is 1.
	-ref.length	Reference length. Default is 1.
	#	Reference value.
Examples	−ref.p 101325	
	-ref.length 0.5	

Table 8.12: equation.of.state ref option

8.7 Molecular Options

The "Molecular" input options section that is used to evaluate the viscosity and thermal conductivity coefficients, starts with the −−molecular directive, followed by a series of molecular input options. Each section is used to set the coefficients or to declare a specific type or constants for Sutherland's law. The coefficients can be evaluated in four different ways: The first, called molecular.const, sets the viscosity and thermal conductivity coefficients as constants, the second, called molecular.mcg, uses multi.component.gas molecular relations to calculate the transport properties. See the '−−multi.component.gas' directive for more information, specifically the '-trns' option (Section 8.9, Tables 8.40, 8.41, and 8.42). The third way, called molecular.sutherland.air.1, uses the direct coefficients for μ and κ (see Equation 2.12), namely, Mu = Cmu1 * $T^{(3/2)}$ / (Cmu2 + T) and Ka = Cka1 * $T^{(3/2)}$ / (Cka2 + T). The fourth way, called molecular.sutherland.air.2, uses Equation 2.13, namely, Mu = Eta0 * (T0 - C0) / (T - C0) * (T / T0)$^{(3/2)}$ and Ka = Cp * Mu / Prandtl.

In there is no molecular section in the input file, the molecular options depend on the type of the relevant flow system. For ideal gas, the default is as if molecular.sutherland.air.1 is selected. For multi component gas, the default is as if molecular.mcg is selected.

Name		
Syntax	−name $name	
Description	Set the name of the molecular thermodynamic relations.	
Parameters	$name	Name of molecular thermodynamic relations.
Examples	−name therm1	

Table 8.13: Molecular name option

Type		
Syntax	−type $type	
Description	Set the type of the molecular thermodynamic relations.	
Parameters	$type	Type of the molecular thermodynamic relations. Available types are:
	molecular.const	Constant viscosity and thermal conductivity coefficients, see Tables 8.15 and 8.16
	molecular.mcg	Use multi.component.gas molecular relations to calculate the transport properties (see '−−multi.component.gas' directive for more information, specifically at '-trns' option, Section 8.9, Tables 8.40, 8.41, and 8.42)
	molecular.sutherland.air.1	Use Equations 2.12 (see Section 2.2.4)
	molecular.sutherland.air.2	Use Equations 2.13 (see Section 2.2.4)
Examples	−type molecular.const	
	−type molecular.mcg	
	−type molecular.sutherland.air.1	
	−type molecular.sutherland.air.2	

Table 8.14: Molecular type option

Viscosity		
Syntax	−viscosity #mu	
Description	Set the viscosity coefficient.	
Parameters	#mu	Viscosity coefficient
Examples	−viscosity 1.78e-5	

Table 8.15: Molecular viscosity option

Conductivity		
Syntax	−conductivity #ka	
Description	Set the thermal conductivity coefficient.	
Parameters	#ka	Thermal conductivity coefficient
Examples	−conductivity 2.48e-2	

Table 8.16: Molecular conductivity option

Mu1		
Syntax	−Mu1 #Cmu1	
Description	Set the first coefficient for the Sutherland molecular viscosity formula; Default is 1.458e-06 (air, see Equation 2.12 and Table 2.1).	
Parameters	#Cmu1	First coefficient for the Sutherland formula
Examples	−Mu1 1.458e-06	

Table 8.17: Molecular Mu1 option

Mu2		
Syntax	−Mu2 #Cmu2	
Description	Set the second coefficient for the Sutherland molecular viscosity formula; Default is 110.3 (air, see Equation 2.12 and Table 2.1).	
Parameters	#Cmu2	Second coefficient for the Sutherland formula
Examples	−Mu2 110.3	

Table 8.18: Molecular Mu2 option

Ka1		
Syntax	−Ka1 #Cka1	
Description	Set the first coefficient for the Sutherland thermal conductivity formula; Default is 2.495e-03 (air, see Equation 2.12 and Table 2.1).	
Parameters	#Cka1	First coefficient for the Sutherland formula
Examples	−Ka1 2.495e-03	

Table 8.19: Molecular Ka1 option

Ka2		
Syntax	−Ka2 #Cka2	
Description	Set the second coefficient for the Sutherland thermal conductivity formula; Default is 194.0 (air, see Equation 2.12 and Table 2.1).	
Parameters	#Cka2	Second coefficient for the Sutherland formula
Examples	−Ka2 194.0	

Table 8.20: Molecular Ka2 option

Eta0		
Syntax	−Eta0 #Eta0	
Description	Set η_0 for the Sutherland molecular viscosity formula; Default is 1.827×10^{-5} (air, see Equation 2.13 and Table 2.2).	
Parameters	#Eta0	Coefficient for the Sutherland formula
Examples	−Eta0 1.827×10^{-5}	

Table 8.21: Molecular Eta0 option

C0		
Syntax	−C0 #C0	
Description	Set C_0 for the Sutherland molecular viscosity formula; Default is 120 (air, see Equation 2.13 and Table 2.2).	
Parameters	#C0	Coefficient for the Sutherland formula
Examples	−C0 120	

Table 8.22: Molecular C0 option

T0		
Syntax	−T0 #T0	
Description	Set T_0 for the Sutherland molecular viscosity formula; Default is 291.15 (air, see Equation 2.13 and Table 2.2).	
Parameters	#T0	Coefficient for the Sutherland formula
Examples	−T0 291.15	

Table 8.23: Molecular T0 option

Prandtl		
Syntax	−Prandtl #Prandtl	
Description	Set the Prandtl number; Default is 0.72 (air, see Equation 2.13 and Table 2.2).	
Parameters	#Prandtl	Prandtl number
Examples	−Prandtl 0.72	

Table 8.24: Molecular Prandtl option

8.8 Tabulate Options

The "Tabulate" input options section starts with the −−tabulate directive, followed by a series of tabulation input options. Tabulation is used in support of the chemical equilibrium model. Creating the eqb tables requires having a −−multi.component.gas section (see Section 8.9).

Name		
Syntax	−name $name	
Description	Set the name of the tabulation.	
Parameters	$name	Table name.
Examples	−name chem	

Table 8.25: Tabulate name option

Type		
Syntax	−type $type	
Description	Set tabulation type.	
Parameters	$type	Tabulation type, options are:
	create	Create new arion tables. Required: −distribution (see Table 8.27), −key (see Table 8.28), and −pT.chemistry as well (see Table 8.29).
	read	Read an existing arion tables. Required: −key as well (see Table 8.28).
	read.external	Read existing tabulation from non-arion engine. Required: −key as well (see Table 8.28).
Examples	−type create	

Table 8.26: Tabulate type option

Distribution		
Syntax	−distribution $distribution	
Description	Set the table distribution type.	
Parameters	$distribution	Distribution type, options are:
	linear	Linear table distribution.
	log	Logarithmic table distribution.
	tanh	Hyperbolic tangent table distribution (default).
Examples	−distribution tanh	

Table 8.27: Tabulate distribution option

Key	
Syntax	−key $key
Description	Set the table path for saving or loading.
Parameters	$key Table path.
Examples	−key /path/data/tables

Table 8.28: Tabulate key option

pT.chemistry	
Syntax	−pT.chemistry < -name p -n #n -min #min -max #max > < -name T -n #n -min #min -max #max >
Description	Create all tables using the given pressure and Temperature data.
Parameters	-name Paramemter name (p or T). -n #n Parameter resolution. -min #min Parameter minimum value. -max #max Parameter maximum value.
Examples	−pT.chemistry < -name p -n 400 -min 10000 -max 1e7 > < -name T -n 600 -min 250 -max 700 >

Table 8.29: Tabulate pT.chemistry option

8.9 Multi Component Gas Options

The "Multi Component Gas" input options section starts with the −−multi.component.gas directive, followed by a series of tabulation input options.

Name		
Syntax	−name $name	
Description	Set the name of the mcg (multi component gas) object.	
Parameters	$name	Multi component gas object name.
Examples	−name air	

Table 8.30: Multi component gas name option

Composition		
Syntax	−composition $composition composition.end	
Description	Set the composition mass fractions.	
Parameters	$compostion	The composition in mass fraction.
	composition.end	End of the composition.
Examples	−composition O2=0.23, NO=0, N=0, O=0, N2=0.77 composition.end	

Table 8.31: Multi component gas composition option

Composition molar		
Syntax	−composition molar $composition composition.end	
Description	Set the composition molar fractions.	
Parameters	$composition	The composition in mass fraction.
	composition.end	End of the composition.
Examples	−composition molar O2=0.21, NO=0, N=0, O=0, N2=0.79 composition.end	

Table 8.32: Multi component gas composition molar option

cy.eq	
Syntax	−cy.eq
Description	Equilibrate and override mcg composition based on inlet conditions (for applicable systems). If no composition is supplied in the −−bc section (see Section 8.10), the global composition is used for the equilibrium calculation. If a different composition is specified, only the species listed there will participate in the equilibrium mixing. Therefore, include all species that should be part of the equilibrium mixture, even if their concentration is set to zero.
Parameters	N/A
Examples	−cy.eq

Table 8.33: Multi component gas cy.eq option

cy.cutoff	
Syntax	−cy.cutoff
Description	Employ a cutoff to the mass fractions so that they are between 0 and 1.
Parameters	N/A
Examples	−cy.cutoff

Table 8.34: Multi component gas cy.cutoff option

Thrm.db		
Syntax	−thrm.db $thrm.db	
Description	Set the path to the thermal database.	
Parameters	$thrm.db	Path to the thermal database.
Examples	−thrm.db /path/data/thermo.inp	

Table 8.35: Multi component gas thrm.db option

Trns.db		
Syntax	−trns.db $trns.db	
Description	Set the path to the transport database.	
Parameters	$trns.db	Path to the transport database.
Examples	−trns.db /path/data/transport.dat	

Table 8.36: Multi component gas trns.db option

React.db	
Syntax	−react.db $react.db
Description	Set the path to the reactions database.
Parameters	$react.db Path to the reactions database.
Examples	−react.db /path/data/reactions.dat

Table 8.37: Multi component gas react.db option

Cantera.db	
Syntax	−cantera.db $cantera.db
Description	Set the path to the Cantera database file.
Parameters	$cantera.db Path to the Cantera database.
Examples	−cantera.db /path/data/cantera_file.yaml

Table 8.38: Multi component gas cantera.db option

Thrm		
Syntax	−thrm $thrm	
Description	Selects the method of calculating the thermodynamic properties.	
Parameters	$thrm	The method of calculating the thermodynamic properties. Possible options are:
	nasa	Use the NASA database to calculate thermodynamic properties (default).
	cantera	Use the cantera file to calculate thermodynamic properties.
Examples	−thrm cantera	
	−thrm nasa	

Table 8.39: Multi component gas thrm option

Trns		
Syntax	−trns $trns	
Description	Select the method of calculating the transport properties.	
Parameters	$trns	Transport properties, options are:
	wilke	Use Wilke's mixture rule to calculate the transport properties, and a constant Schmidt number for mass diffusivity (default). See Tables 8.41 and 8.42 for additional options.
	cantera	Use the Cantera mixture-averaged model to calculate the transport properties.
	cantera.multi	Use the Cantera multi-component model to calculate the transport properties.
Examples	−trns cantera	
	−trns cantera.multi	

Table 8.40: Multi component gas trns option

Viscosity		
Syntax	−viscosity $trns	
Description	Select the method for calculating the species viscosity (relevant only when wilke model is used, option are nasa or blottner).	
Parameters	$trns	Transport properties, options are:
	nasa	Use NASA 4 term curve fit (default).
	blottner	Use Blottner curve fit.
Examples	−viscosity nasa	
	−viscosity blottner	

Table 8.41: Multi component gas viscosity option

Conductivity		
Syntax	−conductivity $trns	
Description	Select the method for calculating the species thermal conductivity (relevant only when wilke model is used, option are nasa or eucken).	
Parameters	$trns	Transport properties, options are:
	nasa	Use NASA 4 term curve fit (default).
	eucken	Use Eucken formula (with Hirschfelder f_int fix).
Examples	−conductivity nasa	
	−conductivity eucken	

Table 8.42: Multi component gas conductivity option

Kinetics		
Syntax	−kinetics $kins	
Description	Select the method of calculating the reaction rates,.	
Parameters	$kins	Kinetics properties, options are:
	none	Disable chemical reactions.
	laminar	Use laminar model for chmeical reactions (default).
	cantera	Use Cantera to calculate the chemical reactions based on the reaction set in the Cantera file.
Examples	−kinetics none	
	−kinetics cantera	

Table 8.43: Multi component gas kinetics option

Eqconst		
Syntax	−eqconst $eqconst	
Description	Select the method of calculating the reverse reaction rates.	
Parameters	$eqconst	Method of calculating the reverse reaction rates, options are:
	arrhenius	Directly evaluate reverse reaction rates based on coefficients supplied with the -react.db option. If the reaction file contains the reverse rates, the code will automatically use them and override any other option.
	gibbs	calculate equilibrium constants for each reaction with Gibbs' free energy (default when no reverse rates are available).
Examples	−eqconst gibbs	

Table 8.44: Multi component gas eqconst option

Eq.engine		
Syntax	−eq.engine $eq.engine	
Description	Select the equilibrium solver.	
Parameters	$eq.engine	Equilibrium solver type, options are:
	internal	Use Arion internal solver (default).
	cantera	Use Cantera solver (usually much slower than the Arion internal solver).
Examples	−eq.engine internal	

Table 8.45: Multi component gas eq.engine option

Sc		
Syntax	−Sc #Sc	
Description	Set the Schmidt number.	
Parameters	#Sc	Schmidt number (default is 0.7).
Examples	−Sc 0.8	

Table 8.46: Multi component gas Sc option

Sc.trb		
Syntax	−Sc.trb #Sc	
Description	Set the turbulent Schmidt number.	
Parameters	#Sc	Turbulent Schmidt number (default is 1.0).
Examples	−Sc.trb 0.8	

Table 8.47: Multi component gas Sc.trb option

8.10 BC Options

Boundary conditions are set for each boundary cell, based on the name that has been assigned by the user (see Chapter 6). For each name, representing a group of boundary cells, the boundary conditions are set in two steps. First, assign the name, and second, assign the type. Each group starts with the −−bc directive, followed by the name and type as follows:.

Name		
Syntax	−name $name	
Description	Name of the boundary as set in Pointwise.	
Parameters	$name	Name of boundary.
Examples	−name WALL	

Table 8.48: BC name option

Type		
Syntax	−type $type	
Description	Type of boundary condition. See Chapter 5 and Table 8.50 for available types.	
Parameters	$type	Type of boundary condition.
Examples	−type noslip.wall	

Table 8.49: BC type option

Boundary Condition Types

BC type	Description (see Chapter 5 for details)
impermeable.wall	Impermeable wall.
noslip.wall	No slip wall.
nichols.wall.function	Nichols and Nelson wall function (see Section 5.2.1).
automatic.wall.function	same as nichols.wall.function.
riemann.inlet	Riemann type inlet boundary conditions.
riemann.outlet	Riemann type outlet boundary conditions.
riemann	Riemann type outer boundary conditions (automatic detection between riemann.inlet, riemann.outlet, fixed, and extrap).
turkel.inlet	Turkel type inlet boundary conditions (for subsonic flow only).
turkel.outlet	Turkel type outlet boundary conditions (for subsonic flow only).
turkel	Turkel type outer boundary conditions (automatic detection between turkel.inlet, turkel.outlet, fixed, and extap).
inlet	Inlet type outer boundary conditions.
outlet	Pressure outlet type outer boundary conditions.
inout	Inout outer boundary conditions (automatic detection between inlet and outlet).
extrap	Zero order extrapolation.
fixed	Fixed boundary conditions.
stagnation.inlet	Stagnation inlet.
symmetry	Symmetry type conditions.
2d	Two dimensional domain conditions.
axis	Axis for axisymmetric model.

Table 8.50: Boundary condition types

Mass.flow		
Syntax	−mass.flow #mdot	
Description	Targeted mass flow rate [kg/s]. Automatically adjusts the pressure boundary value in an attempt to yield the specified mass flow rate (see Section 5.3.6.1). Works only for the "outlet" type boundary condition. Can be used with −relax (see Table 8.52).	
Parameters	#mdot	Mass flow rate.
Examples	−mass.flow 10	

Table 8.51: BC mass.flow option

Relax		
Syntax	−relax #val	
Description	A relaxation parameter for the mass flow rate pressure adjustment (see Table 8.51). Use values smaller than 1 if the pressure changes too rapidly (see Section 5.3.6.1).	
Parameters	#val	Relaxation parameter.
Examples	−relax 0.5	

Table 8.52: BC relax option

Reference.pressure		
Syntax	−reference.pressure #ref	
Description	Set the mean-flow reference pressure (for force calculation), used to override free-stream reference pressure.	
Parameters	#ref	Reference pressure.
Examples	−reference.pressure 101325	

Table 8.53: BC reference.pressure option

Composition		
Syntax	−composition $composition composition.end	
Description	Override the composition mass fractions (for applicable systems, can specify only species fractions that are not zero).	
Parameters	$compostion	The composition in mass fraction.
	composition.end	End of the composition.
Examples	−composition O2=0.23, N2=0.77 composition.end	

Table 8.54: BC gas composition option

Composition Molar		
Syntax	−composition molar $composition composition.end	
Description	Override the composition molar fractions (for applicable systems, can specify only species fractions that are not zero).	
Parameters	$compostion	The composition in mass fraction.
	composition.end	End of the composition.
Examples	−composition molar O2=0.21, N2=0.79 composition.end	

Table 8.55: BC gas composition molar option

cy.eq	
Syntax	−cy.eq
Description	Equilibrate and override mcg composition based on inlet conditions (for applicable systems).
Parameters	N/A
Examples	−cy.eq

Table 8.56: BC gas cy.eq option

8.10.1 BC Log Options

Log	
Syntax	−log $log [log-options] ...
Description	Report in log file. See Table 8.58 for log options list.
Parameters	$log Log name.
Examples	−log coefficients cl cd

Table 8.57: Boundary conditions log option

BC Log Options	
Log type	Description
wet.surface	Wet surface area.
p.center.sum	Pressure center sum.
p.center.x	Center of pressure x coordinate.
p.center.y	Center of pressure x coordinate.
p.center.z	Center of pressure x coordinate.
p.center.xFy	Center of pressure x coordinate.
p.center.xFz	Center of pressure x coordinate.
p.center.yFx	Pressure center sum(y * dFx) / Fx coordinate.
p.center.yFz	Pressure center sum(y * dFz) / Fz coordinate.
p.center.zFx	Pressure center sum(z * dFx) / Fx coordinate.
p.center.zFy	Pressure center sum(z * dFy) / Fy coordinate .
fx	X coordinate direction force.

fy	Y coordinate direction force.
fz	Z coordinate direction force.
fx.pressure	Force in x direction due to pressure.
fy.pressure	Force in y direction due to pressure.
fz.pressure	Force in z direction due to pressure.
fx.friction	Force in x direction due to friction.
fy.friction	Force in y direction due to friction.
fz.friction	Force in z direction due to friction.
lift	Lift force.
drag	Drag force.
mx	Moment about X coordinate direction.
my	Moment about Y coordinate direction.
mz	Moment about Z coordinate direction.
cfx	X coordinate direction force coefficient.
cfy	Y coordinate direction force coefficient.
cfz	Z coordinate direction force coefficient.
cmx	Moment coefficient about X coordinate direction.
cmy	Moment coefficient about Y coordinate direction.
cmz	Moment coefficient about Z coordinate direction.
cl	Lift coefficient.
cd	Drag coefficient.
mass.flow	Mass flow rate.

Table 8.58: BC log options

8.10.2 Wall Distance Calculations

The following directives pertain to wall type boundary conditions. Normally, one would like to calculate wall distance based on whether a specific boundary has been assigned wall conditions. However, sometimes it is required to override this default. Note that the wall distance is used only for turbulence models that require wall distance. The following two directives are exactly for that. They should be used along with a wall boundary condition.

Wall.distance	
Syntax	−wall.distance
Description	Explicitly set wall distance search for a specific boundary. Default: for all walls.
Parameters	N/A
Examples	−wall.distance

Table 8.59: BC wall.distance option

No.wall.distance	
Syntax	−no.wall.distance
Description	Explicitly disable wall distance search for a specific boundary. Default: for all boundaries other than walls.
Parameters	N/A
Examples	−no.wall.distance

Table 8.60: BC no.wall.distance option

8.10.3 Free-Stream Conditions Override

Mach		
Syntax	−Mach #M	
Description	Override the free-stream Mach number.	
Parameters	#M	Free-stream Mach number.
Examples	−Mach 0.95	

Table 8.61: BC Mach option

Velocity.magnitude		
Syntax	−velocity.magnitude #V	
Description	Override the free-stream velocity [m/s].	
Parameters	#V	Free-stream velocity [m/s].
Examples	−velocity.magnitude 200	

Table 8.62: BC velocity.magnitude option

Alpha		
Syntax	−alpha #aoa	
Description	Override the free-stream angle of attack [degrees].	
Parameters	#aoa	Free-stream angle of attack [degrees].
Examples	−alpha 5	

Table 8.63: BC alpha option

Beta		
Syntax	−beta #beta	
Description	Override the free-stream side slip angle [degrees].	
Parameters	#beta	Free-stream side slip angle [degrees].
Examples	−beta 3	

Table 8.64: BC beta option

U		
Syntax	−u #u	
Description	Override the free-stream x coordinate direction velocity [m/s].	
Parameters	#u	Free-stream x coordinate direction velocity [m/s].
Examples	−u 150	

Table 8.65: BC u option

V		
Syntax	−v #v	
Description	Override the free-stream y coordinate direction velocity [m/s].	
Parameters	#v	Free-stream y coordinate direction velocity [m/s].
Examples	−v 20	

Table 8.66: BC v option

W		
Syntax	−w #w	
Description	Override the free-stream z coordinate direction velocity [m/s].	
Parameters	#w	Free-stream z coordinate direction velocity [m/s].
Examples	−w 10	

Table 8.67: BC w option

T		
Syntax	−T #T	
Description	Override the free-stream temperature [K]. In the case of the stagnation inlet (see Section 5.4) this directive pertains to the free-stream stagnation temperature.	
Parameters	#T	Free-stream temperature [K].
Examples	−T 300	

Table 8.68: BC T option

p		
Syntax	−p #p	
Description	Override the free-stream pressure [Pa]. In the case of the stagnation inlet (see Section 5.4) this directive pertains to the free-stream stagnation pressure.	
Parameters	#p	Free-stream pressure [Pa].
Examples	−p 105000	

Table 8.69: BC p option

Trb.intensity		
Syntax	−trb.intensity #ti	
Description	Override the free-stream turbulent intensity (in absolute fraction, not percentage).	
Parameters	#ti	Free-stream turbulent intensity (in absolute fraction, not percentage). Default is 0.001.
Examples	−trb.intensity 0.01	

Table 8.70: BC trb.intensity option

Trb.dnu		
Syntax	−trb.dnu #dnu	
Description	Override the free-stream turbulent Spalart-Allmaras model variable ($\tilde{\nu}$).	
Parameters	#dnu	Free-stream turbulent Spalart-Allmaras model variable.
Examples	−trb.dnu 0.1	

Table 8.71: BC trb.dnu option

8.11 System Options

A system refers to a "System of Equations," *e.g.,* Euler or Reynolds Averaged Navier-Stokes equations. Other examples may include, turbulence model equations or various physical model equations (not included in the current revision of the code). Each system starts with the directive −−system, followed by a series of options.

Certain systems require that an additional, complimentary system would be defined. For example, when simulating turbulent flows it is required to define a mean flow system that is consistent with the turbulence model selected and a second system to solve the actual turbulence model equations.

Type		
Syntax	−type $type	
Description	Type of equation set to be solved.	
Parameters	$type	Type of equation set. See Table 8.73 for equation system types.
Examples	−type ideal.gas.mf.inviscid −type ideal.gas.mf.tnt −type turbulent.kw.sst	

Table 8.72: System type option

System Types

System type	Description
ideal.gas.mf.inviscid	Solve the Euler equations assuming inviscid, perfect gas flow.
ideal.gas.mf.viscous	Solve the Navier-Stokes equations assuming laminar perfect gas flow.
ideal.gas.mf.tnt	Solve the Navier-Stokes equations assuming turbulent ideal gas flow (using the $k-\omega$-TNT turbulence model). This assumes an additional system for solving the $k-\omega$-TNT turbulence model equations.
ideal.gas.mf.sst	Solve the Navier-Stokes equations assuming turbulent ideal gas flow (using the $k-\omega$-SST turbulence model). This assumes an additional system for solving the $k-\omega$-SST turbulence model equations.
ideal.gas.mf.sa	Solve the Navier-Stokes equations assuming turbulent ideal gas flow (using the Spalart-Allmaras turbulence model) This assumes an additional system for solving the Spalart-Allmaras turbulence model equation.
turbulent.kw.tnt	Solve the $k-\omega$-TNT turbulence model equations.
turbulent.kw.sst	Solve the $k-\omega$-SST turbulence model equations.

turbulent.kw.sst.sas	Solve the $k-\omega$-SST-SAS turbulence model equations.
turbulent.kw.sst.iddes	Solve the $k-\omega$-SST-IDDES hybrid turbulence model equations (see Section 3.8).
turbulent.sa	Solve the Spalart-Allmaras turbulence model equation.
turbulent.sa.iddes	Solve the Spalart-Allmaras hybrid turbulence model equation (see Section 3.8).
eqb.inviscid	Solve the Euler equations assuming inviscid perfect gas flow under chemical equilibrium.
eqb.viscous	Solve the Navier-Stokes equations assuming laminar perfect gas flow under chemical equilibrium.
eqb.tnt	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under chemical equilibrium (requires subsequent mean-flow $k-\omega$-TNT model system).
eqb.sst	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under chemical equilibrium (requires subsequent mean-flow $k-\omega$-SST model system).
eqb.sa	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under chemical equilibrium (requires subsequent mean-flow Spalart-Allmaras model system).

mcg.inviscid	Solve the Euler equations assuming inviscid perfect gas flow under chemical non-equilibrium.
mcg.viscous	Solve the Navier-Stokes equations assuming laminar perfect gas flow under chemical non-equilibrium.
mcg.tnt	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under chemical non-equilibrium (requires subsequent mean-flow $k-\omega$-TNT model system).
mcg.sst	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under chemical non-equilibrium (requires subsequent mean-flow $k-\omega$-SST model system).
mcg.sa	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under chemical non-equilibrium (requires subsequent mean-flow Spalart-Allmaras model system).
mcg.frozen.inviscid	Solve the Euler equations assuming inviscid perfect gas flow under frozen chemistry.
mcg.frozen.viscous	Solve the Navier-Stokes equations assuming laminar perfect gas flow under frozen chemistry.
mcg.frozen.tnt	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under frozen chemistry (requires subsequent mean-flow $k-\omega$-TNT model system).

mcg.frozen.sst	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under frozen chemistry (requires subsequent mean-flow $k-\omega$-SST model system).
mcg.frozen.sa	Solve the Navier-Stokes equations assuming turbulent perfect gas flow under frozen chemistry (requires subsequent mean-flow Spalart-Allmaras model system).

Table 8.73: System types

Cell.gradient

Syntax	−cell.gradient $method	
Description	Method to calculate the cell center gradient that is required for high order approximations.	
Parameters	$method	Method for cell gradient calculation. See Table 8.75 for a list of available cell gradient methods.
Examples	−cell.gradient green.gauss.node	

Table 8.74: System cell.gradient option

Cell Gradient Types	
Cell Gradient type	Description
green.gauss.node	Calculate cell gradient based on the Green-Gauss Theorem using node reconstruction (default).
green.gauss.cell	Calculate cell gradient based on the Green-Gauss Theorem using cell center reconstruction.
least.square.1	Calculate cell gradient based on least square approximations using r (the distance) as the weight.
least.square.1.5	Calculate cell gradient based on least square approximations using $r^{1.5}$ as the weight.
least.square.2	Calculate cell gradient based on least square approximations using r^2 as the weight.

Table 8.75: Cell gradient types

Face.gradient		
Syntax	−face.gradient $method	
Description	Method to calculate the face gradient that is required for viscous fluxes calculations.	
Parameters	$method	Method for face gradient calculation. See Table 8.77 for a list of available face gradient methods.
Examples	−face.gradient diamond	

Table 8.76: System face.gradient option

Face Gradient Types	
Face Gradient type	Description
diamond	Calculate face gradient based on the Green-Gauss Theorem using a diamond-like shape (default).
thin.layer	Calculate face gradient based on the thin layer assumption.
hasselbacher	Calculate face gradient based on defect correction by Hasselbacher.

Table 8.77: Face gradient types

Limiter		
Syntax	−limiter $limiter	
Description	Type of limiter.	
Parameters	$limiter	Type of limiter. See Table 8.79 for limiter types.
Examples	−limiter venka.2d	

Table 8.78: Limiter option

Limiter Types	
Limiter type	Description
none	No limiter.
1st	First order.
venka.2d	Venkatakrishnan limiter (2D domain).
venka.3d	Venkatakrishnan limiter (3D domain).
mlp.2d	MLP-u2 limiter (2D domain).
mlp.3d	MLP-u2 limiter (3D domain).
minmod	Minmod limiter (2D, 3D).

Table 8.79: Limiter types

Venka.k		
Syntax	−venka.k #k	
Description	Change the Venkatakrishnan limiter coefficient. Default is 5.	
Parameters	#k	Venkatakrishnan limiter coefficient.
Examples	−venka.k 5	

Table 8.80: System venka.k option

Time.step		
Syntax	−time.step #initial #iterations {cfl.linear | cfl.exponential | cfl.tangential | dt.linear | dt.exponential | dt.tangential } #final	
Description	Set the CFL number or time step (first order single time stepping).	
Parameters	#initial	Initial CFL number or time step.
	#iterations	Number of iteration for which the CFL number or time step grows from #initial to #final.
	cfl.linear	Linear growth of the CFL number.
	cfl.exponentia	Exponential growth of the CFL number.
	cfl.tangential	Hyperbolic tangent growth of the CFL number.
	dt.linear	Linear growth of the time step.
	dt.exponentia	Exponential growth of the time step.
	dt.tangential	Hyperbolic tangent growth of the time step.
	#final	Final CFL number or time step.
Examples	−time.step 5 50 cfl.linear 10	

Table 8.81: System CFL option

Implicit.jacobi	
Syntax	−implicit.jacobi
Description	Use Jacobi instead of the default Gauss-Seidel.
Parameters	N/A
Examples	−implicit.jacobi

Table 8.82: System implicit.jacobi option

Convection.noslip.diagonal		
Syntax	−convection.noslip.diagonal {normal | analytic | implicit.on.noslip}	
Description	Select the way the diagonal convective jacobian is estimated on no-slip boundaries.	
Parameters	normal	The inviscid diagonal is evaluated directly based on the scheme.
	analytic	Use analytical Jacobian
	implicit.on.no	Implicit treatment of wall boundary conditions through the Jacobian.
Examples	−convection.noslip.diagonal analytic	

Table 8.83: System convection.noslip.diagonal option

Convection.impermeable.diagonal		
Syntax	−convection.impermeable.diagonal {normal | analytic | implicit.on.noslip}	
Description	Selects the way the diagonal convective jacobian is estimated on impermeable boundaries.	
Parameters	normal	The inviscid diagonal is evaluated directly based on the scheme.
	analytic	Use analytical Jacobian
	implicit.on.no	Implicit treatment of wall boundary conditions through the Jacobian.
Examples	−convection.impermeable.diagonal analytic	

Table 8.84: System convection.impermeable.diagonal option

Convection.symmetry.diagonal		
Syntax	−convection.symmetry.diagonal {normal | analytic | implicit.on.noslip}	
Description	Selects the way the diagonal convective jacobian is estimated on symmetry boundaries.	
Parameters	normal	The inviscid diagonal is evaluated directly based on the scheme.
	analytic	Use analytical Jacobian
	implicit.on.no	Implicit treatment of wall boundary conditions through the Jacobian.
Examples	−convection.symmetry.diagonal analytic	

Table 8.85: System convection.symmetry.diagonal option

Realizability.trb.w	
Syntax	−realizability.trb.w
Description	Adds realizability condition for omega (applies only to $k-\omega$-SST turbulence model).
Parameters	N/A
Examples	−realizability.trb.w

Table 8.86: System realizability.trb.w option

Realizability.trb.w.Smag	
Syntax	−realizability.trb.w.Smag
Description	Adds realizability condition for omega, based on the size of the strain-rate tensor (applies only to $k-\omega$-SST turbulence model).
Parameters	N/A
Examples	−realizability.trb.w.Smag

Table 8.87: System realizability.trb.w.Smag option

Source.mpk		
Syntax	−source.mpk #mpk	
Description	Limit turbulence model production (applies only to $k-\omega$ turbulence models).	
Parameters	#mpk	Upper limit for production term.
Examples	−source.mpk 5	

Table 8.88: System source.mpk option

Damp	
Syntax	−damp #damp-factor
Description	Set damping to the convection Jacobian. Values that are less than unity increase stability. Not recommended for turbulence model equations. The recommended damping factor is 0.5-1.0. Default is 1.
Parameters	#damp-factor Damping factor.
Examples	−damp 0.75

Table 8.89: System damp option

Relax	
Syntax	−relax #relax-factor
Description	Set relaxation to the solution increment. The recommended relaxation factor is 0.5-1.0. Default is 1.
Parameters	#relax-factor Relaxation factor.
Examples	−relax 0.75

Table 8.90: System relaxation option

iteration.convergence	
Syntax	−iteration.convergence #criterion
Description	Set the convergence criterion (log(Res/Res0)), default is ignored. For unsteady flows this would be the convergence of the whole simulation. For dual time this would be convergence of the iterations.
Parameters	#criterion Convergence criterion in terms of [log(Res/Res0)].
Examples	−iteration.convergence -5

Table 8.91: System iteration.convergence option

2d.tolerance	
Syntax	−2d.tolerance #tolerance
Description	Tolerance for two-dimensional detection.
Parameters	#tolerance Set the tolerance.
Examples	−2d.tolerance 1e-8

Table 8.92: System 2d.tolerance option

Geometric.tolerance	
Syntax	−geometric.tolerance #tolerance
Description	Geometric tolerance where needed.
Parameters	#tolerance Set the tolerance.
Examples	−geometric.tolerance 2e-7

Table 8.93: System geometric.tolerance option

Log	
Syntax	−log $log [log-options] ...
Description	Report in log file. See Table 8.95 for log options list.
Parameters	$log Log name.
Examples	−log coefficients cl cd

Table 8.94: System log option

Plot Functions	
Plot function	Description
cy	Species mass fraction (where applicable).
residual	Residual field.

relax	Relaxation field.
velocity	Velocity vector field (where applicable).
{u | v | w }	Velocity vector field components (scalars, where applicable).
dudx, dudy, dudz	Cell centered u-velocity derivatives.
dvdx, dvdy, dvdz	Cell centered v-velocity derivatives.
dwdx, dwdy, dwdz	Cell centered w-velocity derivatives.
r	Density field (where applicable).
p	Pressure field (where applicable).
Cp	Pressure coefficient (where applicable).
Cf	Skin-friction coefficient (where applicable).
Cf.signed	Signed skin-friction coefficient (where applicable).
T	Temperature field (where applicable).
{lim.r | lim.epsilon | lim.u | lim.v | lim.w}	Limiter fields (where applicable).
wall.distance	Wall distance field (where applicable).
mt	Turbulent viscosity field (where applicable).
qflux	Normal heat flux (where applicable).
total.enthalpy	Total enthalpy (where applicable).

total.temperature	Total temperature (where applicable).
total.pressure	Total pressure (where applicable).
enthalpy.conductance	Enthalpy conductance (where applicable).
mach	Mach number.
trb.k	Turbulent kinetic energy field (where applicable).
trb.w	Turbulent specific dissipation rate field (where applicable).
{trb.lim.k | trb.lim.w}	Turbulence model limiters (where applicable).
yplus	y^+ (where applicable).
rans.les	RANS / LES flag (where applicable).
hybrid.diss.factor	Central/upwind dissipation factor (where applicable).
resolved.reynolds.stress	Resolved stress (where applicable).
modeled.reynolds.stress	Modeled stress (where applicable).
integral.length	The turbulence integral length scale (where applicable).
cells.per.eddy	Cells per eddy (where applicable).
Tw	Magnitude of $\bar{\tau}_{wall}$ (where applicable).
Tw.vec	The vector $\bar{\tau}_{wall}$ (where applicable).
Tw{x | y | z }	X | Y | Z direction component of $\bar{\tau}_{wall}$.

cfl	CFL.
q.criterion	Q criterion.
lambda2	λ_2.
react.fraction	Cell reaction volume fraction (available for PaSR kinetics model).

Table 8.97: Plot functions

System Log Options

Log type	Description
cfl	System CFL.
dt	System Δt.
time	Time.
residual	System residual.
log.residual	System log of the residual.
minimal.timestep	Minimal time step (for non sp.petsc).
orig(minimal.timestep)	Minimal time step original cell index (for non sp.petsc).
cell(minimal.timestep)	Minimal time step zonal cell index (for non sp.petsc).
zone(minimal.timestep)	Minimal time step zone index (for non sp.petsc).
orig(res)	Original (ranked grid) cell index of the maximum residual.
primal(res)	Primal (input grid) cell index of the maximum residual.
cell(res)	Max residual zonal cell number.
zone(res)	Max residual zone number.
uns(res)	Max residual uns name.
max(mt)	Max of the turbulence viscosity (where applicable).
cell(mt)	Max turbulent viscosity cell number (where applicable).
zone(mt)	Max turbulent viscosity zone number (where applicable).
xyz(mt)	Adds maximal turbulent viscosity cell center coordinates.
petsc.iters	Petsc iteration number.
petsc.residual	Petsc residual.

Table 8.95: System log options

Plot	
Syntax	−plot $plot [plot-options] ...
Description	Functions to include in FV-UNS or CGNS file. See Table 8.97 for plot functions list.
Parameters	$plot Plot name.
Examples	−plot NACA0012 r p velocity residual

Table 8.96: System plot option

8.12 Solve Options

The Solve input options section starts with the −−solve directive, followed by a series of solve options.

Convection.flux		
Syntax	−convection.flux $method	
Description	Set the convection flux approximation method.	
Parameters	$method	Flux approximation method. See Table 8.99 for available convection flux types.
Examples	−convection.flux hllc.roe	

Table 8.98: Solve convection.flux option

Convection Flux Types	
Convection flux type	Description
hllc.roe	HLLC Roe.
hllc.davis	HLLC Davis.
ausm	AUSM.
ausm.up	AUSM^{+}-up.
ausm.dv	AUSM-DV.
slau2	SLAU2.
steger	Steger-Warming (for chemical equilibrium only).

Table 8.99: Convection flux types

Convection.jacobian	
Syntax	−convection.jacobian $jacobian
Description	Set the convection Jacobian. See Table 8.101 for available convection Jacobian types.
Parameters	$jacobian Jacobian.
Examples	−convection.jacobian hllc.roe

Table 8.100: Solve convection.jacobian option

Convection Jacobian Types	
Convection Jacobian type	Description
hllc.roe	HLLC Roe.
hllc.davis	HLLC Davis.
van.leer	van Leer.
steger	Steger-Warming Flux Vector Splitting.
rossow.low.mach	Low Mach number Rossow.
matrix.free	Matrix free.
steger	Steger-Warming.

Table 8.101: Convection Jacobian types

Spatial.order		
Syntax	−spatial.order #	
Description	Set the convection flux spatial order. Available options are either 1 for first order or 2 for second order.	
Parameters	#	Convection flux approximation order.
Examples	−spatial.order 2	

Table 8.102: Solve spatial.order option

Sweeps		
Syntax	−sweeps #	
Description	Set the number of sweeps within an iteration.	
Parameters	#	Number of sweeps. Can be any even number. Default is 6.
Examples	−sweeps 4	

Table 8.103: Solve sweeps option

Axisymmetric	
Syntax	−axisymmetric
Description	Set an axisymmetric simulation. The 2-D grid must be positioned in the $x-z$ plane and extruded by one node into the y-direction. Here, x represents the axis of rotation and z corresponds to the radius of rotation.
Parameters	N/A
Examples	−axisymmetric

Table 8.104: Solve axisymmetric option

Time March	
Syntax	−time.march $method
Description	Set the time marching method. See Table 8.106 for a list of available time marching methods.
Parameters	$method Time marching method.
Examples	−time.march implicit.pgs

Table 8.105: Solve time.march option

Time Marching Methods

Time marching method	Description
explicit.euler	Explicit Euler time marching scheme.
explicit.rk3	Third order Runge-Kutta explicit time marching scheme.
explicit.rk4	Fourth order Runge-Kutta explicit time marching scheme.
explicit.rk5	Fifth order Runge-Kutta explicit time marching scheme.
implicit.pgs	Implicit point Gauss-Seidel time marching scheme.
implicit.b2.pgs	Second order implicit B2 time marching scheme.
implicit.heun.R.pgs	Second order Runge-Kutta implicit point Gauss-Seidel time marching scheme.
implicit.rk3.R.pgs	Third order Runge-Kutta implicit point Gauss-Seidel time marching scheme.
implicit.rk4.R.pgs	Fourth order Runge-Kutta implicit point Gauss-Seidel time marching scheme.
implicit.rk5.R.pgs	Fifth order Runge-Kutta implicit point Gauss-Seidel time marching scheme.
implicit.rk3.R.petsc	Krylov-based Implicit (Runge-Kutta R, 3rd order).
implicit.rk4.R.petsc	Krylov-based Implicit (Runge-Kutta R, 4th order).
implicit.b2.petsc	Krylov-based Implicit (B2).

Table 8.106: Time marching methods

Time.accurate.explicit		
Syntax	−time.accurate.explicit #steps #time-step	
Description	Use 3rd order Runge-Kutta TVD (see Section 4.4.1.3) or Explicit Euler as a time-accurate method. Requires to set the time marching method (explicit.euler or explicit.rk3) as in Table 8.106.	
Parameters	#steps	Number of steps.
	#time-step	Time step.
Examples	−time.march explicit.rk3	
	−time.accurate.explicit 1000 0.0001	

Table 8.107: Solve time.accurate.explicit option

Iterations		
Syntax	−iterations #	
Description	Set the number of iterations. For unsteady flows this would be the number of iterations of the whole simulation. For dual time this would be the maximum iterations of the current time step.	
Parameters	#	Number of iterations.
Examples	−iterations 1000	

Table 8.108: Solve iterations option

Time.step.reduction	
Syntax	−time.step.reduction #attempts
Description	Set time the number of consecutive CFL reduction attempts when non-physical values are detected in the solution.
Parameters	#attempts Number of attempts.
Examples	−time.step.reduction 3

Table 8.109: Solve time.step.reduction option

Time.step.reduction.value	
Syntax	−time.step.reduction.value #value
Description	The minimal CFL/DT allowable for the reduction.
Parameters	#value Minimal allowable CFL/DT.
Examples	−time.step.reduction.value 0.1

Table 8.110: Solve time.step.reduction.value option

Dual.time		
Syntax	−dual.time #steps #time-step [1st.order | 2nd.order | auto.order]	
Description	Set dual time stepping simulation.	
Parameters	#steps	Number of physical time steps.
	#time-step	Physical time step (Δt).
	1st.order	First order temporal accuracy.
	2nd.order	Second order temporal accuracy.
	auto.order	Automatic temporal accuracy.
Examples	−dual.time 200 0.0001	

Table 8.111: Solve dual.time option

Global.minimal.timestep	
Syntax	−global.minimal.timestep
Description	Forces all the cells to use the global minimal time step that was calculated.
Parameters	N/A
Examples	−global.minimal.timestep

Table 8.112: Solve global.minimal.timestep option

Save		
Syntax	−save #	
Description	Set the intermittency of output of restart files.	
Parameters	#	Number of steps between output.
Examples	−save 10	

Table 8.113: Solve save option

Save.path		
Syntax	−save.path $path	
Description	Set the path for output of log and restart files.	
Parameters	$path	Path of log and restart files.
Examples	−save.path ./save/	

Table 8.114: Solve save.path option

Save.sequential	
Syntax	−save.sequential
Description	Adds iteration signature to the saves.
Parameters	N/A
Examples	−save.sequential

Table 8.115: Solve save.sequential option

Load.path		
Syntax	−load.path $path	
Description	Set the path for restart files.	
Parameters	$path	Path of restart files.
Examples	−load.path ./load/	

Table 8.116: Solve load.path option

Load.sequence		
Syntax	−load.sequence #iteration	
Description	Load a specific iteration.	
Parameters	#iteration	Iteration for load.
Examples	−load.sequence 1000	

Table 8.117: Solve load.sequence option

EOS		
Syntax	−eos $eos	
Description	Set the equation of state.	
Parameters	$eos	Equation of state. Currently, only perfect gases are supported.
Examples	−eos air	

Table 8.118: Solve eos option

Molecular	
Syntax	−molecular $molecular
Description	Set the name of the molecular viscosity and thermal conductivity.
Parameters	$molecular Molecular relations name.
Examples	−molecular air-suther

Table 8.119: Solve molecular option

P	
Syntax	−p #
Description	Set the free stream pressure.
Parameters	# Free stream pressure.
Examples	−p 101325

Table 8.120: Solve p option

T	
Syntax	−T #
Description	Set the free stream temperature.
Parameters	# Free stream temperature.
Examples	−p 288

Table 8.121: Solve T option

Mach		
Syntax	−Mach #	
Description	Set the free stream Mach number.	
Parameters	#	Free stream Mach number.
Examples	−Mach 0.8	

Table 8.122: Solve Mach option

Velocity.magnitude		
Syntax	−velocity.magnitude #	
Description	Set the free stream velocity magnitude.	
Parameters	#	Free stream velocity magnitude.
Examples	−velocity.magnitude 200	

Table 8.123: Solve velocity magnitude option

U		
Syntax	−u #	
Description	Set the free stream X coordinate direction velocity component.	
Parameters	#	Free stream X coordinate direction velocity component.
Examples	−u 200	

Table 8.124: Solve u option

V		
Syntax	−v #	
Description	Set the free stream Y coordinate direction velocity component.	
Parameters	#	Free stream Y coordinate direction velocity component.
Examples	−v 0	

Table 8.125: Solve v option

W		
Syntax	−w #	
Description	Set the free stream Z coordinate direction velocity component.	
Parameters	#	Free stream Z coordinate direction velocity component.
Examples	−w 20	

Table 8.126: Solve w option

Alpha		
Syntax	−alpha #	
Description	Set the free stream angle of attack.	
Parameters	#	Free stream angle of attack in degrees.
Examples	−alpha 10	

Table 8.127: Solve alpha option

Beta		
Syntax	−beta #	
Description	Set the free stream side slip angle.	
Parameters	#	Free stream side slip angle in degrees.
Examples	−beta 0	

Table 8.128: Solve beta option

Trb.intensity		
Syntax	−trb.intensity #	
Description	Set the free stream turbulence intensity.	
Parameters	#	Free stream turbulence intensity (in absolute fraction, not percentage).
Examples	−trb.intensity 0.01	

Table 8.129: Solve trb.intensity option

Trb.mt		
Syntax	−trb.mt #mt	
Description	Set the free stream turbulence viscosity.	
Parameters	#mt	Free stream turbulence viscosity (in absolute fraction from the molecular viscosity, not percentage).
Examples	−trb.mt 0.01	

Table 8.130: Solve trb.mt option

Reference.velocity	
Syntax	−reference.velocity #ref
Description	Set the reference velocity. Default is the mean flow free stream velocity.
Parameters	#ref Reference velocity.
Examples	−reference.velocity 300

Table 8.131: Solve reference.velocity option

Reference.mach	
Syntax	−reference.mach #ref
Description	Set the reference Mach number. Default is the mean flow free stream Mach number.
Parameters	#ref Reference Mach number.
Examples	−reference.mach 0.75

Table 8.132: Solve reference.mach option

Reference.pressure	
Syntax	−reference.pressure #ref
Description	Set the mean-Flow reference pressure, used to override free-stream pressure.
Parameters	#ref Reference pressure.
Examples	−reference.pressure 101325

Table 8.133: Solve reference.pressure option

Reference.velocity.trb		
Syntax	−reference.velocity.trb #ref	
Description	Set the reference velocity for the turbulence model (used to override the free-stream velocity).	
Parameters	#ref	Free-stream velocity [m/s].
Examples	−reference.velocity.trb 210	

Table 8.134: Solve reference.velocity.trb option

Reference.mach.trb		
Syntax	−reference.mach.trb #ref	
Description	Set the reference Mach number for the turbulence model (used to override the free-stream Mach number).	
Parameters	#ref	Free-stream Mach number.
Examples	−reference.mach.trb 0.7	

Table 8.135: Solve reference.mach.trb option

Reference.longitudinal		
Syntax	−reference.longitudinal #ref	
Description	Set the reference length for Reynolds number evaluation. Unused by the current version.	
Parameters	#ref	Reference length.
Examples	−reference.length 1.5	

Table 8.136: Solve reference.length option

Ref		
Syntax	−ref.$ # { # # }	
Description	Set the reference length, area, and reference point for force and moment coefficient calculations.	
Parameters	-reference.area	Reference area (scalar).
	-reference.len	Reference length (vector).
	-reference.point	Reference point (vector).
	#	Reference value.
Examples	−reference.len 0.325 0.1 0.325	
	−reference.point 1 0 0	

Table 8.137: Solve ref option

Plot	
Syntax	−plot [plot-options] ...
Description	Add to the fvuns or cgns file. See Table 8.139 for plot options list.
Parameters	N/A
Examples	−plot rank owner orig

Table 8.138: Solve plot option

Solve Plot Options	
Log type	Description
rank	Add the rank to the fvuns or cgns plot file.
part	Add the part to the fvuns or cgns plot file.
owner	Add ownership to the fvuns or cgns plot file.
orig	Add original node index to the fvuns or cgns plot file.

Table 8.139: Solve plot options

Log	
Syntax	−log $log [log-options] ...
Description	Report in log file. See Table 8.141 for log options list.
Parameters	$log Log name.
Examples	−log progress-logs iter step time

Table 8.140: Solve log option

Solve Log Options	
Log type	Description
iter	Iteration number.
step	Step number.
pos	Position # (iteration for steady state, step for dual time simulation).
time	Physical time for dual time simulation.
exec.time	Cumulative execution time.
iter.avg.time	iteration average time.
iteration.time	Iteration time.
step.time	Step time.
petsc.mem.usage	Petsc memory usage in mebibyte.
petsc.mem.malloc	Petsc memory malloc in mebibyte.

Table 8.141: Solve log options

Source.mom	
Syntax	−source.mom #fx #fy #fz
Description	Set a constant momentum source term of the form r × [fx, fy, fz] Where r is the local density.
Parameters	#fx #fy #fz External acceleration components.
Examples	−source.mom 1.0 1.0 1.0

Table 8.142: Solve source.mom option

Hyb.diss.min	
Syntax	−hyb.diss.min #value
Description	Set the minimum dissipation value for the hybrid upwind–central convection scheme used in LES/DES simulations (default value is 0.050000). Note that setting this value to 1 results in a purely upwind scheme.
Parameters	#value Minimum dissipation value.
Examples	−hyb.diss.min 0.5

Table 8.143: Solve hyb.diss.min option

Hyb.diss.type	
Syntax	−hyb.diss.type $type
Description	Sets the scheme for determining the dissipation factor in the hybrid upwind–central convection scheme. Note that multiple schemes may be active at the same time, and the final dissipation value is taken as the maximum over all active schemes. The options are listed in Table 8.145. Can use multiple types and the maximum between all prevails. Note that the IDDES $\tilde{f}_d$ is automatically activated when using the IDDES scheme.
Parameters	$type Dissipation factor type.
Examples	−hyb.diss.type ducros

Table 8.144: Solve hyb.diss.type option

Hybrid Dissipation Factor Types	
Dissipation Type	Description
iddes	IDDES.
ducros	Ducros shock sensor.
travin	Travin shock sensor.

Table 8.145: Hybrid Dissipation Factor Types

Grid.length.scale		
Syntax	−grid.length.scale $gridLengthScale	
Description	Set the grid length scale for IDDES simulation. The options are listed in Table 8.147.	
Parameters	$type	Dissipation factor type.
Examples	−grid.length.scale sla	

Table 8.146: Solve grid.length.scale option

Grid Length Scale Types	
Dissipation Type	Description
sla	Shear-Layer-Adapted grid length scale (see Section 3.8.1.1).
max.distance	Maximum distance between cell and it's neighbors.

Table 8.147: Grid Length Scale Types

Gravitation.acceleration		
Syntax	−gravitation.acceleration #gx #gy #gz	
Description	Set the gravitation acceleration [m/sec^2], used for weight calculation in the dof calculations (default is [0.00, 0.00, -9.81]).	
Parameters	#gx	Gravitation acceleration in the x-coordinate direction.
	#gy	Gravitation acceleration in the y-coordinate direction.
	#gz	Gravitation acceleration in the z-coordinate direction.
Examples	−gravitation.acceleration 0.0 0.0 -19.62	
	−gravitation.acceleration 0.0 -9.81 0.00	

Table 8.148: Solve gravitation.acceleration option

8.12.1 Wall Distance Evaluation

Wall distance evaluation is implemented by searching through a BVH (bounding volume hierarchy) tree. It is always exact in the sense that it calculates the distance from a given cell center to a wall boundary face surface. The tree can have various properties (number of children per trunk), the search can be conducted from the tree root or from the last leaf found. Furthermore, the boundary volume can be expressed in double or single precision (it does not affect the distance calculation which is always in double precision). The algorithm results can be verified against a different calculation using BVH or against brute force (when all options are searched). On top of the search, there is a load balancing algorithm which can still search from different ranks in case there is a significant load imbalance. In its current version, the wall distance evaluation is significantly faster than the previous versions.

Wall.distance		
Syntax	−wall.distance {exact | brute.force} [load.balance.rma | load.balance.async | no.load.balance] [BVH4 | BVH8] [from.root | from.leaf] [triangulated | not.triangulated] [double | float] [arion.exact.center | fast.exact.center | hiorder.exact]	
Description	Set the wall distance algorithm.	
Parameters	exact	Fast BVH (bounding volume hierarchy) tree search.
	brute.force	Sequential search on all options.
	load.balance.rma	Load balance between ranks (processes) using Remote Memory Access (default).
	load.balance.asyn	Load balance between ranks (processes) using asynchronous MPI messages.
	no.load.balance	No load balancing.
	BVH4/BVH8	BVH tree number of children per trunk (default BVH4).
	from.root/from.le	Search from tree root or from last searched leaf (default from.root).
	triangulated/not.t	Convert quad boundary faces to triangles (default: not.triangulated).
	double/float	Keep TREE boundary extents in double or single precision (default double).
	fast.exact.center/a	Algorithms for calculating the distance from a point to a polygon, maintained for backward compatibility (default fast.exact.center).
Examples	−wall.distance exact	

Table 8.149: Solve wall distance option

8.12.2 Line Search

Line.search iters	
Syntax	−line.search iters #iterations
Description	Set the number of line.search iterations default is 0 (no line search iterations).
Parameters	#iterations Number of line search iterations.
Examples	−line.search iters 1

Table 8.150: Solve line search iterations option

Line.search min.dq	
Syntax	−line.search min.dq #dq
Description	Set the minimal relaxation factor that the line search can use (optional, default is 0.1).
Parameters	#dq Minimal relaxation factor.
Examples	−line.search min.dq 1e-2

Table 8.151: Solve line search minimum dq option

Line.search poly.order		
Syntax	−line.search poly.order #order	
Description	Set the polynomial order of the back-traced line search curve-fitting, can be 2 or 3 (optional, default is 3).	
Parameters	#order	Order of back-traced line search curve-fitting polynomial.
Examples	−line.search poly.order 3	

Table 8.152: Solve line search polynomial order option

Line.search beta		
Syntax	−line.search beta #beta	
Description	Set the convergence check criterion constant in the line search algorithm (optional, default is 1.000000e-04).	
Parameters	#beta	Line search convergence criterion constant.
Examples	−line.search beta 1e-3	

Table 8.153: Solve line search beta option

Line.search flavor		
Syntax	−line.search flavor [meanflow | full | min]	
Description	Set the line search flavor, *i.e.*, how it is applied to the system of equations. Options are: meanflow, full, and min. (default is full).	
Parameters	meanflow	Apply line search to the mean flow system only.
	full	Apply line search to all systems.
	min	Apply line search to all systems and use the minimum dq value.
Examples	−line.search flavor min	

Table 8.154: Solve line search flavor option

8.13 PETSc Toolkit

The PETSc input option section starts with the −−petsc directive, followed by a series of petsc options. For advanced usage of the PETSc package the user is referred to the command line help or the online PETSc manual.

KSP_view	
Syntax	−ksp_view
Description	View internal Krylov solver iterations.
Parameters	N/A
Examples	−ksp_view

Table 8.155: Petsc ksp_view option

KSP_monitor_true_residual	
Syntax	−ksp_monitor_true_residual
Description	Monitor true (un-preconditioned) residuals.
Parameters	N/A
Examples	−ksp_monitor_true_residual

Table 8.156: Petsc ksp_monitor_true_residual option

KSP_norm_type		
Syntax	−ksp_norm_type [type]	
Description	Select type of norm used to determine convergence of Krylov solver.	
Types	none	Use no norm calculations.
	preconditioned	Use the preconditioned residual norm.
	unpreconditioned	Use the unpreconditioned residual norm.
	natural	Use the norm induced by the linear operator.
Examples	−ksp_norm_type none	

Table 8.157: Petsc ksp_norm_type option

KSP_max_it		
Syntax	−ksp_max_it #	
Description	Set maximum number of Krylov solver iterations.	
Parameters	#	Maximum number of Krylov iterations.
Examples	−ksp_max_it 20	

Table 8.158: Petsc ksp_max_it option

KSP_rtol		
Syntax	−ksp_rtol #	
Description	Set relative tolerance threshold for convergence (reduction in orders of magnitude).	
Parameters	#	Relative tolerance threshold for convergence.
Examples	−ksp_rtol 2e-2	

Table 8.159: Petsc ksp_rtol option

KSP_atol		
Syntax	−ksp_atol #	
Description	Set absolute tolerance threshold for convergence (absolute size of residual, use when residuals approach machine accuracy).	
Parameters	#	Aelative tolerance threshold for convergence.
Examples	−ksp_atol 1e-10	

Table 8.160: Petsc ksp_atol option

KSP_type	
Syntax	−ksp_type [type]
Description	Select Krylov solver (Linear Solvers and Krylov Methods (KSP)).
Types	Selected type list can be found in Table 8.162. For a complete list the user is referred to Petsc relevant user guide page.
Examples	−ksp_type fgmres

Table 8.161: Petsc ksp_type option

KSP Types	
Type	Description
gmres	Generalized Minimal Residual method.
fgmres	Flexible Generalized Minimal Residual method.

Table 8.162: Petsc KSP Types

KSP_gmres_restart	
Syntax	−ksp_gmres_restart #
Description	Set GMRES restart length (increase to improve convergence on account of memory and cpu time, default: 30).
Parameters	# GMRES restart length.
Examples	−ksp_gmres_restart 30

Table 8.163: Petsc ksp_gmres_restart option

PC_type	
Syntax	−pc_type [type]
Description	Set pre-conditioner (for additional information the reader is referred to Petsc relevant user guide page).
Types	Selected type list can be found in Table 8.166. For a complete list the user is referred to Petsc list of pre-conditioners.
Examples	−pc_type asm

Table 8.164: Petsc pc_type option

Sub_pc_type	
Syntax	−sub_pc_type [type]
Description	Select method used to invert the sub-domains created by the additive Schwartz pre-conditioner.
Types	Selected type list can be found in Table 8.166. For a complete list the user is referred to Petsc list of pre-conditioners.
Examples	−sub_pc_type ilu −sub_pc_type preonly

Table 8.165: Petsc sub_pc_type option

PC Types	
Type	Description
asm	Additive Schwarz.
ilu	Incomplete LU
preonly	Disable Krylov solver in computing inverse of asm sub-domains.

Table 8.166: Petsc PC Types

Sub_pc_factor_levels	
Syntax	−sub_pc_factor_levels #
Description	Set sub-domains pre-conditioner factor level.
Parameters	# Sub-domains pre-conditioner factor level.
Examples	−sub_pc_factor_levels 2

Table 8.167: Petsc sub_pc_factor_levels option

Sub_pc_factor_fill	
Syntax	−sub_pc_factor_fill #
Description	Indicate the amount of fill you expect in the factored matrix (for the sbu-domain).
Parameters	# Amount of fill you expect in the factored matrix.
Examples	−sub_pc_factor_fill 1

Table 8.168: Petsc sub_pc_factor_fill option

8.14 Domain Options

The Domain input options section starts with the −−domain directive, followed by a series of domain options. It is used to define a volumetric domain.

Name	
Syntax	−name $name
Description	Set the name of the domain.
Parameters	$name Domain name.
Examples	−name my_domain_name

Table 8.169: Domain name option

Init	
Syntax	−init $init_name
Description	Set the name of the init (see Section 8.15, Table 8.174).
Parameters	$init_name Init name (see Table 8.174).
Examples	−init my_init_name

Table 8.170: Domain init option

Type		
Syntax	−type $type $options	
Description	Set the type of the domain. Currently available types: 'box' and 'cylinder'. The options vary depending on the type. See Table 8.172 for specific options and examples for the 'box' shape and Table 8.173 for specific options and examples for the 'cylinder' shape.	
Parameters	$type	Domain type.
	$options	Options specific to the type. See Tables 8.172 and Table 8.173 for the available options.
Examples	−type box x.min 0 x.max 5 y.min -2 y.max 2 z.min -1 z.max 1	
	−type cylinder r.min 0.1 r.max 0.7 c1 0 0 0 c2 10 0 0	

Table 8.171: Domain type option

Box		
Syntax	−type box {[x.min #val] [x.max #val] [y.min #val] [y.max #val] [z.min #val] [z.max #val]}	
Description	Set a domain of type 'box'. The domain 'box' is a 3-D rectangular cuboid defined by min / max value on each axis. If one axis limits is not defined, then it is assumed to be $+\infty$ or $-\infty$ (depending on the context).	
Parameters	box	3D rectangular cuboid.
	x.min	Set x min.
	x.max	Set x max.
	y.min	Set y min.
	y.max	Set y max.
	z.min	Set z min.
	z.max	Set z max.
	#val	Value.
Examples	−type box x.min 0 x.max 5 y.min -2 y.max 2 z.min -1 z.max 1	
	−type box x.min 0 y.min -3 z.min -5	

Table 8.172: Domain box type option

Cylinder		
Syntax	−type cylinder [r.min #val] [r.max #val] [c1 #val.x #val.y #val.z] [c2 #val.x #val.y #val.z]	
Description	Set a domain of type 'cylinder'. The domain 'cylinder' is a 3D hollow cylinder defined by min radius / max radius (r.min and r.max, respectively) and 2 points of the center of the two bases (c1 and c2, respectively). If r.min is not defined it is assumed to be zero (and then the cylinder is filled rather than hollow). If one of the other limits is not defined, then it is assumed to be $+\infty$ or $-\infty$ (depending on the context).	
Parameters	cylinder	3D hollow cylinder.
	r.min	Set r min.
	r.max	Set r max.
	#val	Set the radius value.
	c1	Set beginning base of cylinder.
	c2	Set ending base of cylinder.
	#x.val	Set x value.
	#y.val	Set y value.
	#z.val	Set z value.
Examples	−type cylinder r.min 0.1 r.max 0.7 c1 0 0 0 c2 10 0 0	
	−type cylinder r.min 0.1 r.max 0.7 c1 0 0 0	

Table 8.173: Domain cylinder type option

8.15 Init Options

The Init input options section starts with the −−init directive, followed by a series of domain options. It is used to define a volumetric domain.

Name	
Syntax	−name $name
Description	Set the name of the init.
Parameters	$name Init name.
Examples	−init my_init_name

Table 8.174: Init name option

T	
Syntax	−T #T
Description	Override the free-stream temperature [K].
Parameters	#T Temperature.
Examples	−T 300

Table 8.175: Init T option

P	
Syntax	−p #p
Description	Override the free-stream pressure [pa].
Parameters	#p pressure.
Examples	−p 67000

Table 8.176: Init p option

U	
Syntax	−u #u
Description	Override the free-stream x direction velocity [m/s].
Parameters	#u velocity.
Examples	−u 150

Table 8.177: Init u option

V	
Syntax	−v #v
Description	Override the free-stream y direction velocity [m/s].
Parameters	#v velocity.
Examples	−v 0

Table 8.178: Init v option

W	
Syntax	−w #w
Description	Override the free-stream z direction velocity [m/s].
Parameters	#w velocity.
Examples	−w 10

Table 8.179: Init w option

Composition	
Syntax	−composition $composition composition.end
Description	Override the free-stream mcg composition (for applicable systems) mass fraction (can specify only species fractions that are not zero).
Parameters	$compostion The composition in mass fraction. composition.end End of the composition.
Examples	−composition O2=0.23, NO=0, N=0, O=0, N2=0.77 composition.end

Table 8.180: Init composition option

Composition Molar		
Syntax	−composition molar $composition composition.end	
Description	Override the free-stream mcg composition (for applicable systems) molar fraction (can specify only species fractions that are not zero).	
Parameters	$compostion	The composition in molar fraction.
	composition.end	End of the composition.
Examples	−composition molar O2=0.21, N2=0.79 composition.end	

Table 8.181: Init composition molar option

8.16 Var Options

The definition of a new function is conducted using the −−var directive, followed by a series of var options. The −−var directive is useful where there is a need for a varying scalar function (time or space dependent). The options are a constant function, a linear function, a trigonometric function, and a tabulated function. Table 8.182 describes the usage of the directive and its options. See Section 8.16.1 for examples and a detailed explanation of the usage.

var		
Syntax	−−var {[−name] $name} [id #id] {[const] #c | linear.{t|x|y|z} #a # b | {sin|cos|tanh}.{t|x|y|z} #a #b # c #d | table.{t|x|y|z} [#x #y]... table.end}	
Description	Add a function.	
Parameters	$name	var name.
	#id	Identification number (for internal use).
	const	Constant function.
	linear	Linear function.
	sin, cos, tanh	Trigonometric functions.
	#a, #b, #c, #d	Constants.
	t, x, y, z	Independent variables.
Examples	−−var −name new_const const 1	
	−−var −name linear_function linear.t 2 -1	
	−−var −name trigonometric_function tanh.t 3 5 7 9	
	−−var pressure table.z 0 101325 1000 89874.6 2000 79495.2 table.end	
	See Section 8.16.1 for more examples and a detailed explanation of the usage.	

Table 8.182: Var directive and its options

8.16.1 Var Examples

8.16.1.1 Constant Function

Directive	Function
−−var const_function const 5	const_function = 5

8.16.1.2 Linear Function

Directive	Function
−−var −name line linear.t 1 2	line.t = 1 + 2 * t

8.16.1.3 Trigonometric Function

Directive	Function
−−var −name trig sin.x 1 2 3 4	trig(x) = 1 + 2 * [sin(3x) + 4]

8.16.1.4 Tabulated Function

A tabulated function assumes linear variation between table entries. The directive: −−var −name my.table table.y 0 4 1 3 2 0 3 -6 table.end translates into the table [y, my.table(y)] whose entries are: (0, 4), (1, 3), (2, 0), (3 ,-6).

8.17 Vertex Option

The definition of a vertex is conducted using the −−vertex directive, followed by a series of vertex options. Table 8.183 describes the usage of the directive.

vertex	
Syntax	−−vertex {−name $name} {[−coordinates] #x #y #z] [−moves.with] [−coordinates.of]
Description	Add a 3D vertex. The coordinates can be either in observer frame or a certain UNS name. The vertex can move along with a UNS. Vertex that moves with a UNS can be defined directly from a UNS but they can not be referenced outside the UNS.
Parameters	$name Vertex name.
Examples	−−vertex −name nozzle −coordinates 0.4 0 0

Table 8.183: Vertex option

8.18 UNS Options

The UNS input options section starts with the −−uns directive, followed by a series of uns options.

Name	
Syntax	−name $name
Description	Name of flow case.
Parameters	$name Flow case name.
Examples	−name naca0012_laminar

Table 8.184: UNS name option

Prefix		
Syntax	{−prefix | −prefix.starcd | −prefix.cgns} $prefix	
Description	Set prefix of the flow case.	
Parameters	prefix	Used for manual conversion (conversion and decomposition has been conducted using star2metis or cgns2metis).
	prefix.starcd	Use original Star-CD export grid files (conversion and decomposition is conducted).
	prefix.cgns	Use original CGNS export grid files (conversion and decomposition is conducted).
	$prefix	Prefix of flow case.
Examples	−prefix ./naca0012/NACA0012-Str-Laminar-Rey500	

Table 8.185: UNS prefix option

Block		
Syntax	−block #block	
Description	Select block from within a multi-block Stat-CD file.	
Parameters	#block	Star-CD file block number.
Examples	−block 2	

Table 8.186: UNS block option

Base	
Syntax	−base #base
Description	Use only the specified base within the CGNS file. The user is referred to the CGNS format for further details.
Parameters	#base Base number.
Examples	−base 1

Table 8.187: UNS base option

Zone	
Syntax	−zone #zone
Description	Use only the specified zone within the CGNS file. The user is referred to the CGNS format for further details.
Parameters	#zone Zone number.
Examples	−zone 5

Table 8.188: UNS zone option

CRC	
Syntax	−crc $signature
Description	Use an explicit signature.
Parameters	#signature Signature.
Examples	−crc

Table 8.189: UNS crc option

Key	
Syntax	−key $prefix
Description	Save/load a key file. The file contains pre-calculated wall distance. If the file exists, the code reads it prior to execution. If the file does not exist, the code generates one.
Parameters	$prefix Prefix of the key file.
Examples	−key ./NACA0012-Str-Laminar-Rey500

Table 8.190: UNS key option

Geometric.tolerance	
Syntax	−geometric.tolerance #tolerance
Description	Geometric tolerance where needed (overrides global values).
Parameters	#tolerance Set the tolerance.
Examples	−geometric.tolerance 2e-7

Table 8.191: UNS geometric.tolerance option

Offset		
Syntax	−offset #x #y #z	
Description	Offset the grid.	
Parameters	#x	Offset in the x direction.
	#y	Offset in the y direction.
	#z	Offset in the z direction.
Examples	−offset 5 0 0	

Table 8.192: UNS offset option

Scale		
Syntax	−scale #x #y #z	
Description	Scale the grid.	
Parameters	#x	Scale in the x direction.
	#y	Scale in the y direction.
	#z	Scale in the z direction.
Examples	−scale 0.001 0.001 0.001	

Table 8.193: UNS scale option

Rotate [rad]	
Syntax	−rotate.{x|y|z}.rad #angle
Description	Rotate the grid around an axis at an angle [rad] (can concatenate rotations) .
Parameters	#angle Rotation angle [rad].
Examples	−rotate.x.rad 0.1 −rotate.y.rad 0.1

Table 8.194: UNS rotate option [rad]

Rotate [deg]	
Syntax	−rotate.{x|y|z}.deg #angle
Description	Rotate the grid around an axis at an angle [deg] (can concatenate rotations).
Parameters	#angle Rotation angle [deg].
Examples	−rotate.x.deg 10 −rotate.z.deg -10

Table 8.195: UNS rotate option [deg]

Vertex		
Syntax	{−<o>vertex | −vertex<o> | −vertex<o>:m | −<b>vertex | −vertex<b> | −vertex<b>:m} $name #x #y #z	
Description	Set named vertex in observer frame coordinates (<o>) or body frame coordinates (<b>) that moves along with the uns. The uns vertices are guaranteed to be 'known' iff they are defined prior to be referenced.	
Parameters	$name	Vertex name.
	#x, #y, #z	Vertex coordinates.
Examples	−<o>vertex v1 0 0 0	

Table 8.196: UNS vertex option

Log		
Syntax	−log $log [log-options] ...	
Description	Report in log file. See Tables 8.198 and 8.203 for log options list.	
Parameters	$log	Log name.
Examples	−log coefficients cl cd	

Table 8.197: UNS log option

UNS Log Options

Log type	Description
wet.surface	Wet surface area.
p.center.sum	Center of pressure.
p.center.x	Center of pressure x coordinate.
p.center.y	Center of pressure x coordinate.
p.center.z	Center of pressure x coordinate.
p.center.xFy	Center of pressure x coordinate.
p.center.xFz	Center of pressure x coordinate.
p.center.yFx	Pressure center sum(y * dFx) / Fx coordinate.
p.center.yFz	Pressure center sum(y * dFz) / Fz coordinate.
p.center.zFx	Pressure center sum(z * dFx) / Fx coordinate.
p.center.zFy	Pressure center sum(z * dFy) / Fy coordinate .
fx	X coordinate direction force.
fy	Y coordinate direction force.
fz	Z coordinate direction force.
fx.pressure	Force in x direction due to pressure.
fy.pressure	Force in y direction due to pressure.
fz.pressure	Force in z direction due to pressure.
fx.friction	Force in x direction due to friction.
fy.friction	Force in y direction due to friction.
fz.friction	Force in z direction due to friction.
lift	Lift force.
drag	Drag force.

mass.flow	Mass flow rate.
mx	Moment about X coordinate direction.
my	Moment about Y coordinate direction.
mz	Moment about Z coordinate direction.
cfx	X coordinate direction force coefficient.
cfy	Y coordinate direction force coefficient.
cfz	Z coordinate direction force coefficient.
mx.pressure	Adds moments around x axis (of this bc) induced by pressure.
my.pressure	Adds moments around y axis (of this bc) induced by pressure.
mz.pressure	Adds moments around z axis (of this bc) induced by pressure.
mx.friction	Adds moments around x axis (of this bc) induced by friction.
my.friction	Adds moments around y axis (of this bc) induced by friction.
mz.friction	Adds moments around z axis (of this bc) induced by friction.
cfx.pressure	Adds force coefficient in x direction (of this bc) induced by pressure.
cfy.pressure	Adds force coefficient in y direction (of this bc) induced by pressure.
cfz.pressure	Adds force coefficient in z direction (of this bc) induced by pressure.
cfx.friction	Adds force coefficient in x direction (of this bc) induced by friction.

cfy.friction	Adds force coefficient in y direction (of this bc) induced by friction.
cfz.friction	Adds force coefficient in z direction (of this bc) induced by friction.
cmx.pressure	Adds moments coefficient around x axis (of this bc) induced by pressure.
cmy.pressure	Adds moments coefficient around y axis (of this bc) induced by pressure.
cmz.pressure	Adds moments coefficient around z axis (of this bc) induced by pressure.
cmx.friction	Adds moments coefficient around x axis (of this bc) induced by friction.
cmy.friction	Adds moments coefficient around y axis (of this bc) induced by friction.
cmz.friction	Adds moments coefficient around z axis (of this bc) induced by friction.
cmx	Moment coefficient about X coordinate direction.
cmy	Moment coefficient about Y coordinate direction.
cmz	Moment coefficient about Z coordinate direction.
cl	Lift coefficient.
cd	Drag coefficient.

Table 8.198: UNS log options

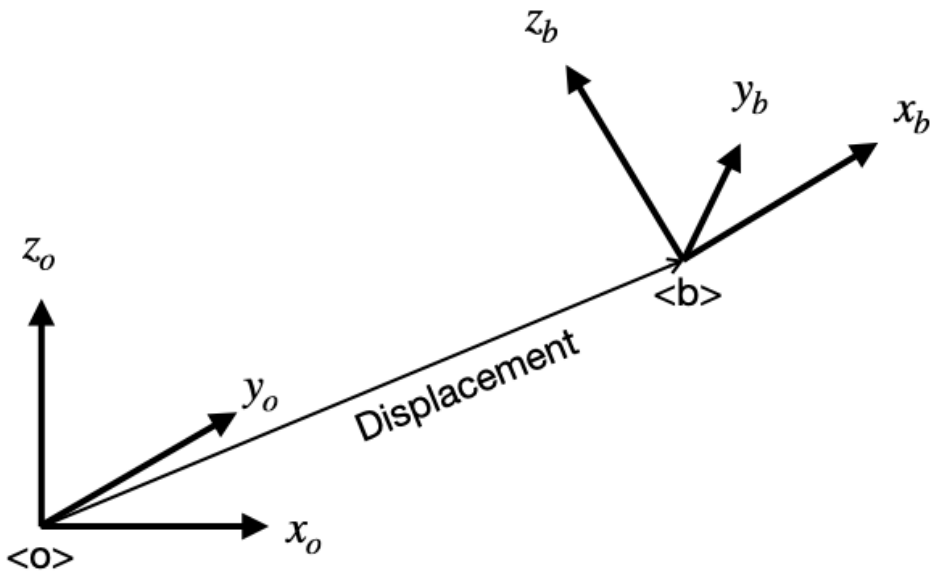

Figure 8.1: Observer and body reference frames

8.18.1 Motion Options

This section describes the directive to control motion. The current version of **Arion** supports the motion that is controlled by the equations of motion resulting from aerodynamics, inertial, and prescribed forces and moments acting on a certain body. A body is defined as the collection of surfaces in a certain UNS. The equations of motion can be overridden by the use of explicit values for acceleration, velocity, and position. The motion parameters are controlled using the −−var directive (it is strongly recommended to use the −−var directive, see Section 8.16). Using −−var enables first and second derivatives. Therefore, setting the position using vars automatically sets the velocity and acceleration. In what follows a certain terminology is adopted. For example the option "<o>initial.body.origin:m" is translated as follows: The '<o>' refers to observer reference frame ('<b>' refers to body reference frame, '<p>' refers to "parent" reference frame), 'initial.body.origin' is the actual option and ':m' refers to the dimensions (if SI system is used it can be omitted). Note that '<o/cg>' refers to the center of gravity in the observer reference frame. Figure 8.1 shows the observer and body reference frames.

Initial Position		
Syntax	−dof <o>initial.body.origin:m #x #y #z	
Description	Set the initial body frame origin in observer frame, it does NOT move the grid, just point to where the body axes origin are (start here).	
Parameters	#x #y #z	Origin of the body reference frame in observer frame.
Examples	−dof <o>initial.body.origin:m 5.5 0 0	

Table 8.199: UNS DOF initial position option

Initial Orientation		
Syntax	−dof {<o>initial.body.orientation:rad | <o>initial.body.orientation:deg} $\#\phi$ $\#\theta$ $\#\psi$	
Description	Set the initial body frame axes orientation in observer frame, it does NOT move the grid nor its orientation, it just sets the axes.	
Parameters	$\#\phi$ $\#\theta$ $\#\psi$	Origin of the body reference frame orientation in observer frame.
Examples	−dof <o>initial.body.orientation:deg 45 90 45	

Table 8.200: UNS DOF initial orientation option

From/Until		
Syntax	−dof [from #t] [until #t] {dof instruction}	
Description	Declare dof order, where from and until indicate the time span of the order effectiveness.	
Parameters	#t	Starting or ending time.
	instruction	Instruction, see Table 8.202 for a list of supported instructions.
Examples	−dof from 0.1 instruction (from Table 8.202)	
	−dof until 0.6 instruction (from Table 8.202)	
	−dof from 0.2 until 0.4 instruction (from Table 8.202)	

Table 8.201: UNS DOF from/until option

DOF-Instructions

Center of gravity	Description
<b>cg:m #x #y #z	Center of gravity in body reference frame where #x, #y, and #z are the coordinates thereof.
Mass and Inertia	**Description**
<o>mass:kg #m	Set the body mass where #m is the mass. Acts at the center of gravity.
{<b>inertia:kg*sq.m | <o/cg>inertia:kg*sq.m} #Ixx #Ixy #Ixy #Iyy #Iyz #Izz	Moment of inertia tensor where #Ixx, #Ixy, #Ixy, #Iyy, #Iyz, and #Izz are the inertia tensor components.
Displacement, Velocity, and Acceleration	**Description**
<p>displacement:m #dx #dy #dz	Override displacement where #dx #dy, and #dz are the displacement components.
<p>velocity:m/s #u #v #w	Override velocity where #u, #v, and #w are the velocity components.
<p>acceleration:m/sq.s #u.dot #v.dot #w.dot	Override the acceleration where #u.dot, #v.dot, and #w.dot are the acceleration vector components.

Angular orientation, velocity, and acceleration	Description
{<p>euler.angle:rad | <p>euler.angle:deg } $\#\phi$ $\#\theta$ $\#\psi$	Override the initial Euler angles where $\#\phi$, $\#\theta$, and $\#\psi$ are the angles.
{<b>angular.velocity:rad/sec | <b>angular.velocity:deg/sec } #p #q #r	Override angular velocity where #p, #q, and #r are the angular velocity components.
{<b>angular.acceleration:rad/sq.sec | <b>angular.acceleration:deg/sq.sec } #pdot #qdot #rdot	Override angular acceleration where #pdot, #qdot, and #rdot are the angular acceleration components.
Forces and Moments	**Description**
<b>explicit.force:N #fx #fy #fz {$vertex | {#x #y #z}}	Set an explicit force in body reference frame where #fx, #fy, and #fz are the force components and $vertex or #x, #y, and #z is the point of action
<b>explicit.pure.moment:Nm #Mx #My #Mz	Set an explicit moment where #Mx, #My, and #Mz are the component components.
aerodynamic.force	Add all of the aerodynamic forces of current uns.
aerodynamic.force.of $uns $bc	Add the aerodynamic forces of certain $bc of a certain $uns.

<o>weight	Add weight of current uns.
<o>weight.of $uns	Add weight of a certain $uns.

Table 8.202: DOF instrcutions

DOF Log Options

Log type	Description
<p>phi	ϕ-euler angle in parent frame.
<p>theta	θ-euler angle in parent frame.
<p>psi	ψ-euler angle in parent frame.
<b>p	p - angular velocity in body frame.
<b>q	q - angular velocity in body frame.
<b>r	r - angular velocity in body frame.
<b>p.dot	dp/dt - angular acceleration in body frame.
<b>q.dot	dq/dt - angular acceleration in body frame.
<b>r.dot	dr/dt - angular acceleration in body frame.
dof.all.angular	All angualr information.
<p>dx	x - translational offset in parent frame.

<p>dy	y - translational offset in parent frame.
<p>dz	z - translational offset in parent frame.
<p>u	u - translational velocity in observer frame.
<p>v	v - translational velocity in observer frame.
<p>w	w - translational velocity in observer frame.
<p>u.dot	du/dt - translational acceleration in observer frame.
<p>v.dot	dv/dt - translational acceleration in observer frame.
<p>w.dot	dw/dt - translational acceleration in observer frame.
dof.all.translational	All translational information.
<b>cg, <b>cg.x, <b>cg.y, <b>cg.z	Center of gravity in body frame.
<o>cg, <o>cg.x, <o>cg.y, <o>cg.z	Center of gravity in observer frame.
<o>mass	Mass.
<b>inertia, <b>ixx, <b>ixy, <b>ixz, <b>iyy, <b>iyz, <b>izz	Inertia tensor.
<b>all.inertia	All mass and inertia information.

<o>F, <p>F, <b>F	Force summation either in observer frame, parent frame, or body frame.
<b>M, <o>M	Moment summation either in body frame, or observer frame.
<o>all.force	All forces information.

Table 8.203: DOF log options

8.19 Point Cloud Data

The point cloud data input options section starts with the −−pcd directive, followed by a series of point cloud data options. This section describes the point cloud data options. A simple example of the point cloud section is brought in Listing 8.2. The reader is referred to Section 6.3 for a brief description of the adaptation method that is implemented in the **Arion** code.

```
--pcd
  -name mach-sensor
  -prefix mach-cycle-0
  -mach
  -power 1
  -k 1
  -percentage 2.5
  -decay 0.3
  -spacing 0.5
```

Listing 8.2: Example of a pcd section

Name		
Syntax	−name $name	
Description	Set the name of the point cloud data.	
Parameters	$name	Point cloud data name.
Examples	−name pcd1	

Table 8.204: PCD name option

Prefix	
Syntax	−prefix $prefix
Description	The point cloud data plot-file will be saved using the path prefix with '.fvuns' suffix.
Parameters	$prefix Point cloud data prefix.
Examples	−prefix ./pcfd/pcd

Table 8.205: PCD prefix option

Mach	
Syntax	−mach
Description	Set the grid adaptation criterion to Mach number.
Parameters	N/A
Examples	−mach

Table 8.206: PCD mach option

Pressure	
Syntax	−pressure
Description	Set the grid adaptation criterion to pressure.
Parameters	N/A
Examples	−pressure

Table 8.207: PCD pressure option

Density	
Syntax	−density
Description	Set the grid adaptation criterion to density.
Parameters	N/A
Examples	−density

Table 8.208: PCD density option

Velocity.magnitude	
Syntax	−velocity.magnitude
Description	Set the grid adaptation criterion to velocity magnitude.
Parameters	N/A
Examples	−velocity.magnitude

Table 8.209: PCD velocity.magnitude option

Power	
Syntax	−power #power
Description	Set the sensor power value (p). See Equation 6.1.
Parameters	#power Sensor power value.
Examples	−power 1

Table 8.210: PCD power option

K	
Syntax	−k #k
Description	Set the sensor constant (K). See Equation 6.1.
Parameters	#k Sensor constant.
Examples	−k 1

Table 8.211: PCD K option

Percentage	
Syntax	−percentage #percentage
Description	Set the refinement percentage (refine the top percentage% of the cells according to the value of sensor).
Parameters	#percentage Percentage of refined cells.
Examples	−percentage 2

Table 8.212: PCD percentage option

Spacing	
Syntax	−spacing #spacing
Description	Set the spacing.
Parameters	#decay Spacing (used by Pointwise to refine the mesh).
Examples	−spacing 0.5

Table 8.213: PCD spacing option

Decay	
Syntax	−decay #decay
Description	Set the decay.
Parameters	#decay Decay (used by Pointwise to refine the mesh).
Examples	−decay 0.3

Table 8.214: PCD decay option

8.20 Log Control Options

Log control options are used to set up the log outputs. For example, the options are used to set up the log file name. The log control options section starts with the −−log directive, followed by a series of options that are described in the following tables. It is important to note that the number of logs (and thus generated log files) is unlimited.

Name	
Syntax	−name $name
Description	Set the name of the log. This name is referred to by the specific −log options. It can be the predefined keywords: 'stdout', 'screen', or 'display': where it will be only shown on the screen. It can also be: 'stderr' where it will be only directed to the standard error stream.
Parameters	$name Log name.
Examples	−name convergence

Table 8.215: Log name option

Prefix	
Syntax	−prefix $prefix
Description	The log file path and name prefix. The '.log' suffix is added to obtain the actual log file name.
Parameters	$prefix Prefix.
Examples	−prefix ./logs/convergence

Table 8.216: Log prefix option

Per	
Syntax	−per $type
Description	Set when the log is printed based on the $type. The possibilities are: iter, produced every iteration (virtual time step); step, produced every step (physical time step); or pos, produced every 'pos' (depending on the simulation type).
Parameters	$type Type (iter, step, or pos).
Examples	−per pos

Table 8.217: Log per option

Stdout	
Syntax	−stdout
Description	Adds echo to the standard output as well as to the log file. One can also use the -screen or -display (the outcome is exactly the same).
Parameters	N/A
Examples	−screen

Table 8.218: Log stdout option

Stderr	
Syntax	−stderr
Description	Adds echo to the standard error as well as to the log file.
Parameters	N/A
Examples	−stderr

Table 8.219: Log stderr option

8.21 Plot Control Options

Plot control options are used to set up the plot outputs. The plot control options section starts with the −−plot directive, followed by a series of options that are described in the following tables.

Name	
Syntax	−name $name
Description	Set the name of the plot. This name is referred to by the specific −plot options.
Parameters	$name Plot name.
Examples	−name Alpha10

Table 8.220: Plot name option

Prefix	
Syntax	−prefix $prefix
Description	The plot file path and name prefix. The actual file number is composed from the prefix, and the $name as described in Table 8.184. The '.fvuns' or '.cgns' suffix is added to the plot file name. If the computational domain has been decomposed, the files are split as well and the number of the partition is added to the file name.
Parameters	$prefix Prefix.
Examples	−prefix ./plots/

Table 8.221: Plot prefix option

Interval	
Syntax	−interval #interval
Description	Set the interval (of iterations/steps) to create the plot files.
Parameters	#interval Plot interval.
Examples	−interval 100

Table 8.222: Plot interval option

Sequential/overwrite	
Syntax	−sequential / −overwrite
Description	Include position stamp in the plot files (or overwrite, without position stamp, default).
Parameters	N/A
Examples	−sequential

Table 8.223: Plot sequential/overwrite option

SIDS.Names	
Syntax	−sids.names
Description	Use SIDS-standard variable names for output variables (*e.g.*, 'Density', 'VelocityX' etc.).
Parameters	N/A
Examples	−sids.names

Table 8.224: Plot sids.names option

FVUNS/CGNS	
Syntax	−fvuns / −cgns
Description	Select the file format to use, default is: -cgns.
Parameters	N/A
Examples	−cgns −fvuns

Table 8.225: Plot fvuns/cgns option

BC		
Syntax	−bc {walls | all}	
Description	Include only boundaries in the cgns file (not applicable for fvuns files).	
Parameters	walls	Add only boundaries that are designated as walls to plot file.
	all	Add all boundaries to plot file.
Examples	−bc wall	
	−bc all	

Table 8.226: Plot bc option

8.22 Table Control Options

Table control options are used to set up the table outputs. The table control options section starts with the −−table directive, followed by a series of options that are described in the following tables.

Name	
Syntax	−name $name
Description	Set the name of the table. This name is referred to by the specific −table options.
Parameters	$name Table name.
Examples	−name Alpha10

Table 8.227: Table name option

Prefix	
Syntax	−prefix $prefix
Description	The table file path and name prefix. The '.tbl' suffix is added to obtain the actual table file name.
Parameters	$prefix Prefix.
Examples	−prefix ./tables/surface-pressure

Table 8.228: Table prefix option

Interval	
Syntax	−interval #interval
Description	Set the interval (of iterations/steps) to create the table files.
Parameters	#interval Table interval.
Examples	−interval 100

Table 8.229: Table interval option

Sequential/overwrite	
Syntax	−sequential / -overwrite
Description	Include position stamp in the table files (or overwrite, without position stamp, default).
Parameters	N/A
Examples	−sequential

Table 8.230: Table sequential/overwrite option

Horizontal/vertical	
Syntax	−horizontal / -vertical
Description	The table type (vertical is the default).
Parameters	N/A
Examples	−horizontal

Table 8.231: Table horizontal/vertical option

Point		
Syntax	−point #x #y #z	
Description	Create a table from a point where [x, y, z] is the point.	
Parameters	#x #y #z	Point.
Examples	−point 0 0 0	

Table 8.232: Table point option

Ray		
Syntax	−ray #x #y #z #vx #vy #vz	
Description	Create a table along a predefined ray.	
Parameters	#x #y #z	Ray origin.
	#vx #vy #vz	Ray direction.
Examples	−ray 0 0 0 1 1 1	

Table 8.233: Table ray option

Plane		
Syntax	−plane #x #y #z #nx #ny #nz	
Description	Create a table from a plane where [x, y, z] is a point on the plane and [nx, ny, nz] is the normal vector to the plane.	
Parameters	#x #y #z	Plane origin.
	#nx #ny #nz	Plane normal direction.
Examples	−plane 0 0 0 0 0 1	

Table 8.234: Table plane option

BC		
Syntax	−bc $bc	
Description	Create the table from a boundary condition.	
Parameters	$bc	Boundary condition name.
Examples	−bc STRUT	

Table 8.235: Table bc option

Plane.bc		
Syntax	−plane.bc #x #y #z #nx #ny #nz $bc-name	
Description	Create a table along an intersection between a plane and a boundary surface.	
Parameters	#x #y #z	Plane.bc origin.
	#nx #ny #nz	Plane.bc normal direction.
	$bc-name	The boundary surface name as assigned by the −−bc −name directive (see Section 8.10, Table 8.48).
Examples	−plane.bc 0 0 0 0 1 0 WALL	

Table 8.236: Table plane.bc option

8.23 Post Option

The post directive is utilized to read a solution and output all logs, plots, and tables without any flow calculations. The directive can be simply added to the input file. See Table 8.237 for the syntax.

Post	
Syntax	−−post
Description	Output all the logs, plots, and tables and quit.
Parameters	N/A.
Examples	−−post

Table 8.237: Post directive

8.24 Converge Options

The converge input options section starts with the −−converge directive, followed by a series of converge options. These options are used to determine simulation convergence other than residual convergence. For convergence **all** of the criteria of a certain section must be met. Different criteria convergence sections are evaluated independently. If one of the criteria convergence sections is met, the simulation is considered converged. For iteration based convergence only iteration duration is considered. Likewise, for time-accurate convergence, only time-span is considered. Once a convergence option has been named, it is used within the −−solve (see Section 8.12), −−uns (see Section 8.18) , or −−bc sections (see Section 8.10). See Table 8.239 for the syntax.

Name		
Syntax	−name $name	
Description	Set the convergence criterion name.	
Parameters	$name	Name of the convergence criterion.
Examples	−name coefficients	

Table 8.238: Converge name option

Converge		
Syntax	−converge $name $criterion {{amplitude.minmax #min #max} | {amplitude.range #range}} {{duration.i #iters} | {duration.t #time-span}}	
Description	Set a convergence criterion.	
Parameters	$name	Name of the convergence criterion.
	$criterion	Convergence criterion type (see Table 8.240 for criteria types).
	amplitude.minmax	Set minimum and maximum amplitude.
	#min	Minimum amplitude.
	#max	Maximum amplitude.
	amplitude.range	Set amplitude range of convergence criterion.
	#range	Amplitude range of convergence criterion.
	duration.i	Set the number of consecutive iterations that meet the criterion.
	#iters	Number of consecutive iterations to meet the criterion.
	duration.t	Set the time span that meets the criterion (for time-accurate simulations).
	#time-span	Time span to meet the criterion.
Examples	−converge coefficients cl amplitude.range 0.01 duration.i 1000	
	−converge coefficients cd amplitude.range 0.001 duration.i 1000	

Table 8.239: Converge converge option

Convergence Criteria Types

Convergence Criterion Type	Description (see Table 8.239)
f	Total force.
fx	Force in the x coordinate direction.
fy	Force in the y coordinate direction.
fz	Force in the z coordinate direction.
lift	Lift force.
drag	Drag force.
cf	Total force coefficient.
cfx	Force coefficient in the x coordinate direction.
cfy	Force coefficient in the y coordinate direction.
cfz	Force coefficient in the z coordinate direction.
cl	Lift coefficient.
cd	Drag coefficient.
m	Moment magnitude.
mx	Moment about the x coordinate direction.
my	Moment about the y coordinate direction.
mz	Moment about the z coordinate direction.
cm	Moment coefficient.
cmx	Moment coefficient about the x coordinate direction.
cmy	Moment coefficient about the y coordinate direction.
cmz	Moment coefficient about the z coordinate direction.

Table 8.240: Convergence criteria types

8.25 Run-time Options

Arion provides the capability to control the run while the application is running using the run-time options. This can be achieved by creating an ascii text file named 'arion.ins' containing one of the following run-time options:

Run-time Options

Option	Action
stop	Stop and save a restart.
kill	Immediately stop the run (even in dual-time mode) and save a restart.
plot	Dump the FVUNS or CGNS file as requested by the user at the next available opportunity.
table	Dump all tables requested by the user.
save	Save a restart.
time.step [$system] #cfl	Change to the specified constant CFL or virtual time step of all the systems or the specified $system.
dt #dt	Change to the specified physical time step (for dual time simulations).
iterations #iterations	Change the maximum number of iterations.
iteration.convergence #convergence	Change convergence criterion.
iteration.convergence $system #convergence	Change the convergence criterion of a systems.

Table 8.241: Run-time options

8.25.1 Run-time Options Examples

The examples in Table 8.242 provide the complete Unix/Linux command to create the 'arion.ins' file with the required content. Alternatively, the user may use an editor to create the file and enter the content. Note, once **Arion** identifies the existence of the file 'arion.ins' and reads its content, the file is erased.

Run-time Options Examples

Command	Result
echo stop > arion.ins	Stop and save a restart.
echo plot > arion.ins	Dump the FVUNS or CGNS file as requested by the user at the next available opportunity.
echo save > arion.ins	Save a restart.
echo time.step 50.0 > arion.ins	Change the CFL or time step to 50.0 (all systems).
echo time.step turbulent.kw.tnt 30.0 > arion.ins	Change the CFL or virtual time step for the k-ω-TNT turbulence model equations to 30.0.
echo dt 0.001	Change the physical time step to 0.001

Table 8.242: Run-time options examples

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