HORSES3D

A **H**igh-**Or**der (DG) **S**pectral **E**lement **S**olver **User Manual**

Numath group

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Compiling the code

- Clone the git repository or copy the source code into a desired folder.
- Go to the folder Solver.
- Run configure script.

```
$ ./configure
```

• Install using the Makefile:

```
$ make all <<Options>>
```

with the desired options (bold are default):

- MODE=DEBUG/RELEASE
- COMPILER=ifort/gfortran
- COMM=PARALLEL/SEQUENTIAL
- ENABLE_THREADS=NO/**YES**
- WITH_MKL=y/n

For example:

```
$ make all COMPILER=ifort COMM=PARALLEL
```

- The ENABLE-THREADS=YES flag enables shared memory simulations using OpenMP.
- \bullet The COM=PARALLEL flag enables distributed memory simulations using MPI.
- To compile the code linking it with METIS (that is an option for creating the mesh partitions of MPI runs), it is needed that before compilation and running, an environment variable called METIS_HOME is found. This variable must contain the path to the HDF5 installation folder (it must have been compiled with the same compiler as HORSES3D).
- To compile the code linking it with HDF5 (necessary for reading HOPR meshes), it is needed that before compilation and running, an environment variable called HDF5_ROOT is found. This variable must contain the path to the METIS installation folder (it must have been compiled with the same compiler as HORSES3D). In addition, the lib folder must be added to the environment variable LD_LIBRARY_PATH.
- If you use environment modules, it is advised to use the HORSES3D module file:

```
$ export MODULEPATH=$HORSES_DIR/utils/modulefile:$MODULEPATH
```

where \$HORSES_DIR is the installation directory.

• It is advised to run the *make clean* or *make allclean* command if some options of the compilation rutine needs to be changed and it has been compiled before.

Input and Output Files

DONT USE TABS!

2.1 Input Files

- Control file (*.control)
- Mesh file (*.mesh / *.h5 / *.msh)
- Polynomial order file (*.omesh)
- Problem File (ProblemFile.f90)

Notes on the GMSH format (*.msh) and general workflow using GMSH.

- Curved geometry supported up to polynomial order 5.
- Curved geometry should be generated using following options: tools -i, options -i, mesh -i, general -i, element order.
- HORSES3D can read mesh format 4.1 and 2.2 (legacy format).
- The solution to most of the problems mesh reading is to load it in GMSH and export to format 2.2 to have a clean ASCII file.

2.2 Output Files

- Solution file (*.hsol)
- Horses mesh file (*.hmesh)
- Boundary information (*.bmesh)
- Partition file (*.pmesh)
- Polynomial order file (*.omesh)
- Monitor files (*.volume / *.surface / *.residuals)

Running a Simulation

3.1 Control File (*.control) - Overview

The control file is the main file for running a simulation. A list of all the mandatory keywords for running a simulation and some basic optional keywords is presented in Table 3.1. The specific keywords are listed in the other chapters.

Table 3.1: General keywords for running a case.

Keyword	Description	Default value
solution file name	CHARACTER: Path and name of the output file. The name of	Mandatory
	this file is used for naming other output files.	keyword
simulation type	CHARACTER: Specifies if HORSES3D must perform a 'steady-	'steady-state'
	state' or a 'time-accurate' simulation.	
time integration	CHARACTER: Can be 'implicit', 'explicit', or 'FAS'. The latter	'explicit'
	uses the Full Algebraic Storage (FAS) multigrid scheme, which	
	can have implicit or explicit smoothers.	
polynomial order	INTEGER: Polynomial order to be assigned uniformly to all the	_*
	elements of the mesh. If the keyword polynomial order file is	
	specified, the value of this keyword is overridden.	
polynomial order i	INTEGER: Polynomial order in the i, j, or k component for all	_*
polynomial order j	the elements in the domain. If used, the three directions must be	
polynomial order k	declared explicitly, unless you are using a polynomial order file.	
	If the keyword <i>polynomial order file</i> is specified, the value of this	
	keyword is overridden.	
polynomial order file	CHARACTER: Path to a file containing the polynomial order of	_*
	each element in the domain.	
restart	LOGICAL: If .TRUE., initial conditions of simulation will be read	Mandatory
	from restart file specified using the keyword restart file name.	keyword
cfl	REAL: A constant related with the convective Courant-	_**
	Friedrichs-Lewy (CFL) condition that the program will use to	
	compute the time step size.	
defl	REAL: A constant related with the diffusive Courant-Friedrichs-	_**
	Lewy (DCFL) condition that the program will use to compute the	
	time step size.	
dt	REAL: Constant time step size.	_**
final time	REAL: This keyword is mandatory for time-accurate solvers	_
mesh file name	CHARACTER: Name of the mesh file. The currently supported	Mandatory
	formats are .mesh (SpecMesh file format) and .h5 (HOPR hdf5	keyword
	file format).	
mesh inner curves	LOGICAL: Specifies if the mesh reader must suppose that the	.TRUE.
	inner surfaces (faces connecting the elements of the mesh) are	
	curved. This input variable only affects the hdf5 mesh reader.	
number of time steps	INTEGER: Maximum number of time steps that the program will	Mandatory
	compute.	keyword

Table 3.1: General keywords for running a case - continued.

Keyword	Description	Default value
output interval	INTEGER: In steady-state, this keyword indicates the interval of	Mandatory
	time steps to display the residuals on screen. In time-accurate	keyword
	simulations, this keyword indicates how often a 3D output file	
	must be stored.	
convergence tolerance	REAL: Residual convergence tolerance for steady-state cases	Mandatory
		keyword
partitioning	CHARACTER: Specifies the method for partitioning the mesh in	'metis'
	MPI simulations. Options are: 'metis' (the code must have been	
	linked to METIS at compilation time, see Chapter 1), or 'SFC' (to	
	use a space-filling curve method, no special compilation is needed	
	for this option).	
manufactured solution	CHARACTER: Must have the value '2D' or '3D'. When this key-	_
	word is used, the program will add source terms for the conser-	
	vative variables taken into account an exact analytic solution for	
	each primitive variable j (ρ, u, v, w, p) of the form:	
	$j = j_C(1) + j_C(2)\sin(\pi j_C(5)x) + j_C(3)\sin(\pi j_C(6)y) +$	
	$j_C(4)\sin(\pi j_C(7)z)$	
	Where $j_C(i)$ are constants defined in the file ManufacturedSolu-	
	tions.f90. Proper initial and boundary conditions must be im-	
	posed (see the test case). The mesh must be a unit cube.	

^{*} One of these keywords must be specified

3.2 Boundary conditions

The boundary conditions are specified as blocks in the control file. The block start with a the keywords '#define' and ends with '#end'. Inside the block the options are specified as a pair of keywords and values, just as the normal body of the rest of the file.

Each boundary condition can be individually defined or if multiple boundaries are set with the same definition, it could be done on the same block (with the name separated by a double under score '-' sign). The name of each boundary must match with the one specified at the mesh file.

The block in general can be seen below. Table 3.2 show the values for the type keyword, and the possible value for the parameters depends on the boundary condition.

Table 3.2: Keywords for Boundary Conditions.

Keyword	Description	Default value
type	CHARACTER: Type of boundary condition to be applied. Op-	N/A
	tions are: Inflow, Outflow, NoSlipWall, FreeSlipWall, Periodic,	
	User-defined.	

By default, NoSlipWall is adiabatic. Isothermal wall can be activated with the following block:

It is also possible to set a moving wall with the keyword wall velocity = value.

^{**} For Euler simulations, the user must specify either the CFL number or the time-step size. For Navier-Stokes simulations, the user must specify the CFL and DCFL numbers or the time-step size.

For periodic boundary conditions, the second boundary that must be used as a complement must be specified by the keyword 'coupled boundary'. These two boundaries must have the same node position in all directions but one. For mesh files generated by commercial software where this strict rule is not imposed a comparison based on the minimum edge size of the face element can be used by a boolean parameter in the normal body of the control file (not in the block body), with the keyword 'periodic relative tolerance'.

Spatial Discretization

HORSES3D uses a high-order discontinuous Galerkin Spectral Element (DGSEM) method. As part of the numerical method, several options of volume and surface discretization options can be selected. Some options are only available in certain solvers.

Table 4.1: Keywords for spatial discretization.

the solution. Options are:	'Gauss'
f inviscid fluxes. Options are:	'Standard'
function to use in numerical otions are:	_
compressible Navier–Stokes)	
compressible Navier–Stokes)	
fluxes. Options are:	'BR2'
1	ncompressible Navier–Stokes) ncompressible Navier–Stokes) fluxes. Options are:

Table 4.1: Keywords for spatial discretization - continued.

Keyword	Description	Default value
riemann solver	CHARACTER: Riemann solver for inviscid fluxes. Options are: • Central	Mandatory keyword
	 Roe (Only for compressible Navier–Stokes) Standard Roe (Only for compressible Navier–Stokes) 	
	• Roe-Pike (Only for compressible Navier–Stokes)	
	• Low dissipation Roe (Only for compressible Navier–Stokes)	
	• Lax-Friedrichs (Only for compressible and Incompressible Navier–Stokes)	
	• ES Lax-Friedrichs (Only for compressible Navier–Stokes, not including RANS)	
	• u-diss (Only for compressible Navier–Stokes, not including RANS)	
	• Rusanov (Only for compressible Navier–Stokes)	
	• Matrix dissipation (Only for compressible Navier–Stokes)	
	• Viscous NS (Only for compressible Navier–Stokes, not including RANS)	
	• Exact (Only for Incompressible Navier-Stokes, and Multiphase)	

Restarting a Case

Table 5.1: Keywords for restarting a case.

T7 1	Table 5.1. Neywords for restarting a case.	D C 1: 1
Keyword	Description	Default value
restart	LOGICAL: If .TRUE., initial conditions of simulation will be read	Mandatory
	from restart file specified using the keyword restart file name.	keyword
restart file name	CHARACTER: Name of the restart file to be written and, if key-	Mandatory
	word $restart = .TRUE.$, also name of the restart file to be read	keyword
	for starting the simulation.	
restart polorder	INTEGER: Uniform polynomial order of the solution to restart	same as case's
	from. This keyword is only needed when the restart solution is of	
	a different order than the current case.	
restart nodetype	CHARACTER: node type of the solution to restart from (Gauss	same as case's
	or Gauss-Lobatto). This keyword is only needed when the restart	
	node type is different than the current case.	
restart polorder file	CHARACTER: File containing the polynomial orders of the solu-	same as case's
	tion to restart from. This keyword is only needed when the restart	
	solution is of a different order than the current case.	
get discretization error of	CHARACTER: Path to solution file. This can be used to estimate	_
	the discretization error of a solution when restarting from a higher-	
	order solution.	

Physics related keyword

6.1 Compressible flow

Table 6.1: Keywords for compressible flow (Euler / Navier-Stokes).

Keyword	Description	Default value
Mach number	REAL:	Mandatory
		keyword
Reynolds number	REAL:	Mandatory
		keyword
Prandtl number	REAL:	0.72
Turbulent Prandtl number	REAL:	Equal to
		Prandtl
AOA theta	REAL: Angle of attack (degrees), based on the spherical coordi-	0.0
	nates polar angle (θ) definition	
AOA phi	REAL: Angle of attack (degrees), based on the spherical coordi-	0.0
	nates azimuthal angle (φ) definition	
LES model	CHARACTER(*): Options are:	None
	• Vreman	
	• Wale	
	Smagorinsky	
	• None	
Wall model	CHARACTER:	linear

6.1.1 Shock-capturing

The shock-capturing module helps stabilize cases with discontinuous solutions, and may also improve the results of under-resolved turbulent cases. It is built on top of a *Sensors* module that detects problematic flow regions, classifying them according to the value of the sensor, s, mapped into the interval $a \in [0, 1]$,

$$a = \begin{cases} 0, & \text{if } s \le s_0 - \Delta s/2, \\ \frac{1}{2} \left[1 + \sin\left(\frac{s - s_0}{\Delta s}\right) \right], & \text{if } s_0 - \Delta s/2 < s < s_0 + \Delta s/2, \\ 1, & \text{elsewhere.} \end{cases}$$

The values of $s_0 = (s_1 + s_2)/2$ and $\Delta s = s_2 - s_1$ depend on the sensor thresholds s_1 and s_2 .

At the moment, flow regions where $a \leq 0$ are considered smooth and no stabilization algorithm can be imposed there. In the central region of the sensor, with 0 < a < 1, the methods shown in the next table can be used and even scaled with the sensor value, so that their intensity increases in elements with more instabilities. Finally, the higher part of the sensor range can implement a different method from the table; however, the intensity is set to the maximum this time.

All the methods implemented introduce artificial dissipation into the equations, which can be filtered with an SVV kernel to reduce the negative impact on the accuracy of the solution. Its intensity is controlled with the parameters μ (similar to the viscosity of the Navier-Stokes equations) and α (scaling of the density-regularization term of the Guermond-Popov flux), which can be set as constants or coupled to the value of the sensor or to a Smagorinsky formulation.

Table 6.2: Keywords for shock-capturing algorithms in the Navier-Stokes equations.

Keyword	Description	Default value
Enable shock-capturing	LOGICAL: Switch on/off the shock-capturing stabilization	.FALSE.
Shock sensor	CHARACTER: Type of sensor to be used to detect discontinuous regions Options are:	Integral
	• Zeros: always return 0	
	• Ones: always return 1	
	• Integral: integral of the sensor variable inside each element	
	• Integral with sqrt: square root of the Integral sensor	
	• Modal: based on the relative weight of the higher order modes	
	• Truncation error: estimate the truncation error of the approximation	
	• Aliasing error: estimate the aliasing error of the approximation	
	• GMM: clustering sensor based on the divergence of the velocity and the gradient of the pressure	
Shock first method	CHARACTER: Method to be used in the middle region of the sensor $(a \in [0,1])$. Options are:	None
	• None: Do not apply any smoothing	
	• Non-filtered: Apply the selected viscous flux without SVV filtering	
	• SVV: Apply an entropy-stable, SVV-filtered viscous flux	
Shock second method	CHARACTER: Method to be used in the top-most region of the sensor $(a = 1)$. Options are:	None
	• None: Do not apply any smoothing	
	• Non-filtered: Apply the selected viscous flux without SVV filtering	
	• SVV: Apply an entropy-stable, SVV-filtered viscous flux	
Shock viscous flux 1	CHARACTER: Viscous flux to be applied in the elements where $a \in [0, 1]$. Options are:	_
	• Physical	
	• Guermond-Popov (only with entropy variables gradients)	

Table 6.2: Keywords for shock-capturing algorithms in the Navier-Stokes equations – continuation.

Keyword	Description	Default value
Shock viscous flux 2	CHARACTER: Viscous flux to be applied in the elements where $a=1$. Options are:	_
	Physical	
	• Guermond-Popov (only with entropy variables gradients)	
Shock update strategy	CHARACTER: Method to compute the variable parameter of the specified shock-captruing approach in the middle region of the sensor. Options are:	Constant
	• Constant	
	• Sensor	
	ullet Smagorinsky: only for non-filtered and SVV	
Shock mu 1	$REAL/CHARACTER(*)$: Viscosity parameter μ_1 , or C_s in the case of LES coupling	0.0
Shock alpha 1	<i>REAL</i> : Viscosity parameter α_1	0.0
Shock mu 2	<i>REAL</i> : Viscosity parameter μ_2	μ_1
Shock alpha 2	<i>REAL</i> : Viscosity parameter α_2	α_1
Shock alpha/mu	REAL: Ratio between α and μ . It can be specified instead of α itself to make it dependent on the corresponding values of μ , and it is compulsory when using LES coupling	_
SVV filter cutoff	REAL/CHARACTER(*): Cutoff of the filter kernel, P. If "automatic", its value is adjusted automatically	"automatic"
SVV filter shape	CHARACTER(*): Options are:	Power
	• Power	
	• Sharp	
	• Exponential	
SVV filter type	CHARACTER(*): Options are:	High-pass
	• Low-pass	
	• High-pass	

Table 6.2: Keywords for shock-capturing algorithms in the Navier-Stokes equations – continuation.

Keyword	Description	Default value
Sensor variable	CHARACTER(*): Variable used by the sensor to detect shocks. Options are:	rhop
	• rho	
	• rhou	
	• rhov	
	• rhow	
	• u	
	• v	
	• w	
	• p	
	• rhop	
	• grad rho	
	• div v	
Sensor lower limit	REAL: Lower threshold of the central sensor region, s_1	Mandatory keyword (ex- cept GMM)
Sensor higher limit	$REAL$: Upper threshold of the central sensor region, s_2	Mandatory keyword (ex- cept GMM)
Sensor TE min N	INTEGER: Minimum polynomial order of the coarse mesh used for the truncation error estimation	1
Sensor TE delta N	Polynomial order difference between the solution mesh and its coarser representation	1
Sensor TE derivative	CHARACTER*: Whether the face terms must be considered in the estimation of the truncation error or not. Options are:	Isolated
	Non-isolated	
	• Isolated	
Sensor number of clusters	INTEGER: Maximum number of clusters to use with the GMM sensor	2
Sensor min. steps	INTEGER: Minimum number of time steps that an element will remain detected. The last positive value will be used if the sensor "undetects" an element too early	1

Spectral Vanishing Viscosity

The introduction of an SVV-filtered artificial flux helps dissipate high-frequency oscillations. The baseline viscous flux can be chosen as the Navier-Stokes viscous flux or the flux developed by Guermond and Popov. In any case, this flux is expressed in a modal base where it is filtered by any of the following three filter kernels:

- power: $\hat{F}_i^{\text{1D}} = (i/N)^P$,
- exponential: $\hat{F}_i^{\text{1D}} = 0$ if $i \leq P$, $\hat{F}_i^{\text{1D}} = \exp\left(-\frac{(i-N)^2}{(i-P)^2}\right)$ elsewhere.

The extension to three dimensions allows the introduction of two types of kernels based on the one-dimensional ones:

• high-pass: $\hat{F}_{ijk}^{H} = \hat{F}_{i}^{1D} \hat{F}_{i}^{1D} \hat{F}_{k}^{1D}$,

$$\bullet \text{ low-pass: } \hat{F}_{ijk}^{\mathrm{L}} = 1 - \left(1 - \hat{F}_i^{\mathrm{1D}}\right) \left(1 - \hat{F}_j^{\mathrm{1D}}\right) \left(1 - \hat{F}_k^{\mathrm{1D}}\right),$$

being the low-pass one more dissipative and, thus, more suited to supersonic cases. The high-pass filter, on the other hand, works better as part of the SVV-LES framework for turbulent cases.

The cutoff parameter P can be set as "automatic", which uses a sensor to differentiate troubled elements from smooth regions. The stabilisation strategy then depends on the region:

• smooth regions: P = 4, $\mu = \mu_2$, $\alpha = \alpha_2$,

• shocks: P = 4, $\mu = \mu_1$, $\alpha = \alpha_1$.

In addition to this, the viscosity μ_1 can be set to "Smagorinsky" to use the implemented SVV-LES approach. In this case, the $\mu = \mu_{\rm LES}$ viscosity is computed following a Smagorinsky formulation with $C_s = \mu_2$ and the viscosity parameters do not depend on the region anymore,

$$\mu = C_s^2 \Delta^2 |S|^2, \quad \alpha = \alpha_1.$$

6.1.2 Acoustic

The Ffowcs Williams and Hawkings (FWH) acoustic analogy is implemented as a complement to the compressible NS solver. It can run both during the execution of the NS (in-time) or as at a post-process step. The version implemented includes both the solid and permeable surface variations, but both of them for a static body subjected to a constant external flow, i.e. a wind tunnel case scenario. The specifications for the FWH are divided in two parts: the general definitions (including the surfaces) and the observers definitions. The former is detailed in Table 6.3, while the latter are defined in a block section, similar to the monitors (see Chapter 12):

```
#define acoustic observer 1
   name = SomeName
   position = [0.d0, 0.d0, 0.d0]
#end
```

To run the in-time computation, the observers must be defined in the control file. Beware that adding an additional observer will require to run the simulation again. To use the post-process computation, the solution on the surface must be saved at a regular time. Beware that it will need more storage. To run the post-process calculation the horses.tools binary is used, with a control file similar to the one use for the NS simulation (without monitors), and adding the keywords "tool type" and "acoustic files pattern", as explained in Table 6.3.

Table 6.3: Keywords for acoustic analogy

Keyword	Description	Default value
acoustic analogy	CHARACTER(*): This is the main keyword for activating the	_
	acoustic analogy. The only options is: "FWH".	
acoustic analogy permeable	LOGICAL: Defines if uses a permeable or solid approach.	.FALSE.
acoustic solid surface	CHARACTER(*): Array containing the name of each bound-	_
	ary to be used as a surface for integration. In the form:	
	'[bc1,bc2,bc3]'. Mandatory for using the solid surface variant.	
acoustic surface file	CHARACTER(*): Path to a fictitious surface that will be used	_
	for integration. It must be tailor-made for the mesh. Mandatory	
	for using the permeable surface variant.	
observers flush interval	INTEGER: Iteration interval to flush the observers information	100
	to the files.	
acoustic solution save	LOGICAL: Defines whether it saves the NS solution on the sur-	.FALSE.
	face. Mandatory for post-process computation.	
acoustic save timestep	REAL: Controls the time or iteration at which the FWH will be	_
	calculated (and saved if specified). If the key is missing it will be	
	done at each timestep.	
acoustic files pattern	CHARACTER(*): Pattern to the path of all the saved solutions	_
	on the surface (To be used in horses.tools for the post-process	
	calculation).	
tool type	CHARACTER(*): Necessary for post-process calculation. De-	_
	fines the type of post-process of horses.tools. For the FWH anal-	
	ogy the value must be "fwh post"	

6.2 Incompressible Navier-Stokes

Among the various incompressible Navier-Stokes models, HORSES3D uses an artificial compressibility formulation, which converts the elliptic problem into a hyperbolic system of equations, at the expense of a non divergence–free velocity field. However, it allows one to avoid constructing an approximation that satisfies the inf–sup condition. This methodology is well suited for use as a fluid flow engine for interface–tracking multiphase flow models, as it allows the density to vary spatially.

The artificial compressibility system of equations is

$$\rho_t + \vec{\nabla} \cdot (\rho \vec{u}) = 0, \tag{6.1}$$

$$(\rho \vec{u})_t + \vec{\nabla} \cdot (\rho \vec{u} \vec{u}) = -\vec{\nabla} p + \vec{\nabla} \cdot \left(\frac{1}{\text{Re}} \left(\vec{\nabla} \vec{u} + \vec{\nabla} \vec{u}^T \right) \right) + \frac{1}{\text{Fr}^2} \rho \vec{e}_g, \tag{6.2}$$

$$p_t + \rho_0 c_0^2 \vec{\nabla} \cdot \vec{u} = 0, \tag{6.3}$$

The factor ρ_0 is computed as $max(\rho_1/\rho_1, \rho_2/\rho_1)$.

This solver is run with the binary horses3d.ins.

Table 6.4: Keywords for incompressible Navier-Stokes solver

Keyword	Description	Default value
reference velocity (m/s)	REAL: Reference value for velocity	_
number of fluids $(1/2)$	INTEGER: Number of fluids present in the simulation	1
maximum density (kg/m ³)	REAL: Maximum value used in the limiter of the density	Huge(1.0)
minimum density (kg/m ³)	REAL: Minimum value used in the limiter of the density	-Huge(1.0)
artificial compressibility factor	<i>REAL</i> : Artificial compressibility factor c_0^2 .	_
gravity acceleration (m/s ²)	REAL: Value of gravity acceleration	_
gravity direction	REAL: Array containing direction of gravity. Eg. $[0.0, -1.0, 0.0]$.	_

The incompressible Navier Stokes solver has two modes: with 1 fluid and with 2 fluids. The required keywords are listed below.

Table 6.5: Keywords for incompressible Navier-Stokes solver. Mode with 1 fluid

Keyword	Description	Default value
density (kg/m ³)	REAL: Density of the fluid	_
viscosity (pa.s)	REAL: Viscosity of the fluid	_

Table 6.6: Keywords for incompressible Navier-Stokes solver. Mode with 2 fluids

Keyword	Description	Default value
fluid 1 density (kg/m ³)	REAL: Density of the fluid 1	_
fluid 1 viscosity (pa.s)	REAL: Viscosity of the fluid 1	_
fluid 2 density (kg/m ³)	REAL: Density of the fluid 2	_
fluid 2 viscosity (pa.s)	REAL: Viscosity of the fluid 2	_

6.3 Multiphase

The multiphase flow solver implemented in HORSES3D is constructed by a combination of the diffuse interface model of Cahn–Hilliard with the incompressible Navier–Stokes equations with variable density and artificial compressibility. This model is entropy stable and guarantees phase conservation with an accurate representation of surface tension effects. The modified entropy-stable version approximates:

$$c_t + \vec{\nabla} \cdot (c\vec{u}) = M_0 \vec{\nabla}^2 \mu, \tag{6.4}$$

$$\sqrt{\rho} \left(\sqrt{\rho} \vec{u} \right)_t + \vec{\nabla} \cdot \left(\frac{1}{2} \rho \vec{u} \vec{u} \right) + \frac{1}{2} \rho \vec{u} \cdot \vec{\nabla} \vec{u} + c \vec{\nabla} \mu = -\vec{\nabla} p + \vec{\nabla} \cdot \left(\eta \left(\vec{\nabla} \vec{u} + \vec{\nabla} \vec{u}^T \right) \right) + \rho \vec{g}, \tag{6.5}$$

$$p_t + \rho_0 c_0^2 \vec{\nabla} \cdot \vec{u} = 0, \tag{6.6}$$

where c is the phase field parameter, M_0 is the mobility, μ is the chemical potential, η is the viscosity and c_0 is the artificial speed of sound. The factor ρ_0 is computed as $max(\rho_1/\rho_1, \rho_2/\rho_1)$. Mobility M_0 is computed from the control file parameters chemical characteristic time t_{CH} , interface width ϵ and interface tension σ with the formula $M_0 = L_{ref}^2 \epsilon/(t_{CH}\sigma)$.

The term $M_0 \vec{\nabla}^2 \mu$ can be implicity integrated to reduce the stiffnes of the problem with the keyword time integration = IMEX. This is only recomended if the value of M_0 is very high so that the time step of the explicit scheme is very small.

This solver is run with the binary horses3d.mu.

Table 6.7: Keywords for multiphase Navier-Stokes solver

Keyword	Description	Default value
fluid 1 density (kg/m ³)	REAL: Density of the fluid 1	_
fluid 1 viscosity (pa.s)	REAL: Viscosity of the fluid 1	_
fluid 2 density (kg/m ³)	REAL: Density of the fluid 2	_
fluid 2 viscosity (pa.s)	REAL: Viscosity of the fluid 2	_
reference velocity (m/s)	REAL: Reference value for velocity	_
maximum density (kg/m ³)	REAL: Maximum value used in the limiter of the density	Huge(1.0)
minimum density (kg/m ³)	REAL: Minimum value used in the limiter of the density	-Huge(1.0)
artificial compressibility factor	<i>REAL</i> : Artificial compressibility factor c_0^2 .	_
gravity acceleration (m/s ²)	REAL: Value of gravity acceleration	_
gravity direction	<i>REAL</i> : Array containing direction of gravity. Eg. $[0.0, -1.0, 0.0]$.	_
velocity direction	REAL: Array containing direction of velocity used for the outflow	_
	BC. Eg. [1.0, 0.0, 0.0].	
chemical characteristic time (s)	$REAL: t_{CH}$ controls the speed of the phase separation	_
interface width (m)	$REAL: \epsilon$ controls the interface width between the phases	_
interface tension (N/m)	<i>REAL</i> : σ controls the interface tension between the phases	_

6.4 Particles

WARNING: Lagrangian particles do not support MPI.

HORSES3D includes a two-way coupled Lagrangian solver. Particles are tracked along their trajectories, according to the simplified particle equation of motion, where only contributions from Stokes drag and gravity are retained,

$$\frac{dy_i}{dt} = u_i, \quad \frac{du_i}{dt} = \frac{v_i - u_i}{\tau_p} + g_i, \tag{6.7}$$

where u_i and y_i are the *ith* components of velocity and position of the particle, respectively. Furthermore, v_i accounts for the continuous velocity of the fluid at the position of the particle. We consider spherical Stokesian particles, so their mass and aerodynamic response time are $m_p = \rho_p \pi D_p^3/6$ and $\tau_p = \rho_p D_p^2/18\mu$, respectively, ρ_p being the particle density and D_p the particle diameter.

Each particle is considered to be subject to a radiative heat flux I_o . The carrier phase is transparent to radiation, whereas the incident radiative flux on each particle is completely absorbed. Because we focus on relatively small volume fractions, the fluid-particle medium is considered to be optically thin. Under these hypotheses, the direction of the radiation is inconsequential, and each particle receives the same radiative heat flux, and its temperature T_p is governed by

$$\frac{d}{dt}(m_p c_{V,p} T_p) = \frac{\pi D_p^2}{4} I_o - \pi D_p^2 h(T_p - T), \tag{6.8}$$

where $c_{V,p}$ is the specific heat of the particle, which is assumed to be constant with respect to temperature. T_p is the particle temperature and h is the convective heat transfer coefficient, which for a Stokesian particle can be calculated from the Nusselt number $Nu = hD_p/k = 2$.

In practical simulations, integrating the trajectory of every particle is too expensive. Therefore, particles are agglomerated into parcels, each of them accounting for many particles with the same physical properties, position, velocity, and temperature. The evolution of the parcels is tracked with the same set of equations presented for the particles.

The two-way coupling means that fluid flow is modified because of the presence of particles. Therefore, the Navier-Stokes equations are enriched with the following source terms:

$$S = \beta \begin{bmatrix} 0 \\ \sum_{n=1}^{N_p} \frac{m_p}{\tau_p} (u_{1,n} - v_1) \delta(\mathbf{x} - \mathbf{y}_n) \\ \sum_{n=1}^{N_p} \frac{m_p}{\tau_p} (u_{2,n} - v_2) \delta(\mathbf{x} - \mathbf{y}_n) \\ \sum_{n=1}^{N_p} \frac{m_p}{\tau_p} (u_{3,n} - v_3) \delta(\mathbf{x} - \mathbf{y}_n) \\ \sum_{n=1}^{N_p} \pi D_p^2 h(T_{p,n} - T) \delta(\mathbf{x} - \mathbf{y}_n) \end{bmatrix},$$
(6.9)

where δ is the Dirac delta function, N_p is the number of parcels, β is the number of particles per parcel and $u_{i,n}$, $\mathbf{y}_{i,n}$, $T_{p,n}$ are the velocity, spatial coordinates, and temperature of the parcel nth. The dimensionless form of the Navier Stokes equations can be seen in the appendix at the end of this document.

Particles are solved in a box domain inside the flow domain. The box is defined with the keywords "minimum box" and "maximum box". The boundary conditions for the particles are defined with the keyword "bc box". Possible options are inflow/outflow, periodic and wall (with perfect rebound).

Table 6.8: Keywords for particles Navier-Stokes solver		
Keyword	Description	Default value
lagrangian particles	LOGICAL: If .true. activates particles	.false.
stokes number	REAL: Stokes number which for Stokesian particles is $St =$	_
	$\frac{\rho_p D_p^2 u_o}{18 L_o \mu_o}$	
Gamma	<i>REAL</i> : Ratio between specific heat of particles and fluid Γ	_
	$c_{v,p}/c_v$	
phi_m	<i>REAL</i> : Ratio between total mass of particles and fluid $\phi_m = \frac{m_p N_p}{\rho_o L_o^3}$	_
Radiation source	<i>REAL</i> : Non dimensional radiation source intensity $I_o^* = \frac{I_o D_p}{4k_o T_o}$	_
Froude number	<i>REAL</i> : Froude number $Fr = \frac{u_o}{\sqrt{g_o L_o}}$	_
high order particles source term	LOGICAL: source term with high order dirac delta or averaged	.false.
	in the whole element	
number of particles	INTEGER: Total number of parcels in the simulation	_
particles per parcel	<i>REAL</i> : β particles per parcel	_

Table 6.9: Keywords for particles Navier-Stokes solver - continued

Keyword	Keywords for particles Navier-Stokes solver - continued Description	Default value
Gravity direction	INTEGER: Array with direction of gravity. Only required if Fr	_
v	number is specified.[0,0,-1]	
particles file	CHARACTER(*): Path to file with initial position of the par-	_
•	ticles. If not provided, initialization without particles inside the	
	domain. Not compatible with injecting particles in the domain	
	(see keyword below).	
vel and temp from file	LOGICAL: If .true. Initial velocity and temperature of particles	_
-	read from file. If .false., initial velocity and temperature of parti-	
	cles are the same as flow at the position of the particle.	
injection	LOGICAL: If .true. injection of particles through a face of the	_
	box.	
particles injection	INTEGER: Array with a vector indicating the direction of the	_
	injection. Eg., $[0,1,0]$	
particles per step	INTEGER: Number of particles injected per time step.	_
particles iter period	INTEGER: Iteration period for particles injection. Set to 1 to	_
	inject particles every time step.	
particles injection velocity	REAL: Array with particles injection non dimensional velocity.	_
	Eg., [0.d0, 1.d0, 0.d0]	
particles injection temperature	REAL: Particles injection non-dimensional temperature	_
minimum box	REAL: Array with minimum x,y,z coordinates of box with parti-	_
	cles. Eg., $[0.d0,0.d0,0.d0]$	
maximum box	REAL: Array with maximum x,y,z coordinates of box with parti-	_
	cles. Eg., [4.d-2,1.6d-1,4.d-2]	
bc box	INTEGER: Array with boundary conditions for particles box in	_
	the form [yz,xz,xy]. 0 is inflow/outflow, 1 is wall, 2 is periodic.	
	Eg., [2,0,2]. In this example planes yz and xy are periodic, while	
	plane xz is inflow/outflow for particles.	

6.5 Complementary Modes

6.5.1 Wall Function

The wall function overwrites the viscous flux on the specified boundaries based on an specific law using a Newman condition. It must be used as a complement of no slip boundary condition. Table 6.10 shows the parameters that can be set in the control file. The frictional velocity is calculated using the instantaneous values of the first node (either Gauss or Gauss-Lobatto) of the element neighbour of the face element (at the opposite side of the boundary face). Currently is only supported for the compressible Navier-Stokes solver.

The standard wall function uses the Reichardt law, solving the algebraic non-linear equation using the newton method to obtain the frictional velocity. The ABL function uses the logarithmic atmospheric boundary layer law, using the aerodynamic roughness; the frictional velocity is without using any numerical method.

Table 6.10: Keywords for Wall Function

Keyword	Description	Default value
Wall Function	CHARACTER(*): This is the main keyword for activating the	_
	wall function. Identifies the wall law to be used. Options are:	
	 Standard: uses the Reichardt law. ABL: uses the atmospheric boundary layer law. 	
Wall Function Boundaries	CHARACTER(*): Array containing the name of each boundary	_
	to be used. In the form: '[bc1,bc2,bc3]'. Mandatory for using the	
	wall function.	
Wall Function kappa	REAL: von Karman constant	0.38
Wall Function C	REAL: Log law 'C' constant	4.1
Wall Function Seed	REAL: Initial value for the newton method	1.0
Wall Function Damp	REAL: Initial value damp for the newton method	1.0
Wall Function Tolerance	REAL: Tolerance for the newton method	10^{-10}
Wall Function max iter	INTEGER: Maximum number of iterations for the newton	100
	method	
Wall Roughness	REAL: Aerodynamic roughness for the ABL wall function.	_
	Mandatory value for the ABL law.	
Wall Plane Displacement	REAL: Plane displacement due to roughness for the ABL wall	0.0
	function	

6.5.2 Tripping

A numerical source term is added to the momentum equations to replicate the effect of a tripping mechanism used commonly in explerimental tests. The forcing is described via the product of two independent functions: one that depends streamwise and vertical directions (space only) and the other one describing the spanwise direction and time (space and time). It can be used for the compressible NS, both LES and RANS. The keywords for the trip options are listed in table 6.11.

Table 6.11: Keywords for Tripping model

Keyword	Description	Default value
use trip	LOGICAL: This is the main keyword for activating the trip	.FALSE.
trip time scale	REAL: Time interval between the change of the time dependent	Mandatory
	part of the trip.	
trip number of modes	INTEGER: Number of Fourier modes in the spanwise direction of	Mandatory
	the trip.	
trip z points	INTEGER: Number of points to create the Fourier Transforma-	Mandatory
	tion of the spanwise direction, it must be greater than the number	
	of modes and should be ideally equal to the number of discretiza-	
	tion points of the mesh in the same direction.	
trip attenuation	$REAL\ ARRAY(2)$: Length scale of the gaussian attenuation of	Mandatory
	the trip, the first position is the streamwise direction and the	
	second is the wall-normal direction.	
trip zone	CHARACTER(*) ARRAY(:): Boundary condition name that	Mandatory
	constrains at least one surface where the trip center is located.	
	It can be ither one or two boundary conditions, the latter used to	
	generate a trip in two different positions (i.e. pressure and suction	
	sides of an airfoil).	
trip center	REAL: Position of the origin of the trip in the streamwise direc-	Mandatory
	tion.	
trip center 2	REAL: Position of the origin of the second trip, if used, in the	_
	streamwise direction.	
trip amplitude	REAL: Maximum time varying amplitude of the trip.	1.0
trip amplitude steady	REAL: Maximum steady amplitude of the trip.	0.0
random seed 1	INTEGER: Number used to initialize the random number gen-	930187532
	erator of the trip. It can vary in different simulations but must	
	remain constant for a restart.	
random seed 2	INTEGER: Number used to initialize the random number gen-	597734650
	erator of the trip. It can vary in different simulations but must	
	remain constant for a restart.	

Implicit Solvers with Newton linearisation

7.1 General Keywords

The keywords for the implicit solvers are listed in table 7.1

Table 7.1: Keywords for implicit solvers.

Keyword	Description	Default value
time integration	CHARACTER: This is the main keyword for activating the implicit solvers. The value of it should be set to 'implicit' for the BDF solvers and to 'rosenbrock' for Rosenbrock schemes.	'explicit'
linear solver	 CHARACTER: Specifies the linear solver that has to be used. Options are: 'petsc': PETSc library Krylov-Subspace methods. Available in serial, but use with care (PETSc is not thread-safe, so OpenMP is not recommended). Only available in parallel (MPI) for preallocated Jacobians (see next section). 'pardiso': Intel MKL PARDISO. Only available in serial or with OpenMP. 'matrix-free gmres': A matrix-free version of the GM-RES algorithm. Can be used without preconditioner or with a recursive GMRES preconditioner using 'preconditioner=GMRES'. Available in serial and parallel (OpenMP+MPI) 'smooth': Traditional iterative methods. One can select either 'smoother=WeightedJacobi' or 'smoother=BlockJacobi'. 'matrix-free smooth': A matrix-free version of the previous solver. Only available with 'smoother=BlockJacobi'. 	'petsc'

7.2 Keywords for the BDF Methods

The BDF methods implemented in HORSES3D use a Newton's method

Table 7.2: Keywords for the BDF solvers.

Keyword	Description	Default value
bdf order	INTEGER: If present, the solver uses a BDF solver of the specified order. BDF1 - BDF5 are available, and BDF2 -	1
	BDF5 require constant time steps.	D17.00
jacobian by convergence	LOGICAL: When .TRUE., the Jacobian is only computed	.FALSE.
	when the convergence falls beneath a threshold (hard-coded). This improves performance.	
compute jacobian every	INTEGER: Forces the Jacobian to be computed in an in-	Inf
	terval of iterations that is specified.	
print newton info	LOGICAL: If .TRUE., the information of the Newton iterations will be displayed.	'.FALSE.'
implicit adaptive dt	LOGICAL: Specifies if the time-step should be computed according to the convergence behavior of the Newton iterative method and the linear solver.	.FALSE.
newton tolerance	REAL: Specifies the tolerance for the Newton's method.	10^{-6} for time-accurate simulations, or $MaxResidual \times a$ for steady-state simulations, where a is the keyword $newton$
		factor
newton max iter	INTEGER: Maximum number of Newton iterations for BDF solver.	30
linsolver max iter	INTEGER: Maximum number of iterations to be taken by the linear solver. This keyword only affects iterative linear solvers.	500
newton factor	$REAL$: In simulations that are not time-accurate, the tolerance of the Newton's method is a function of the residual: $MaxResidual \times a$, where a is the specified value.	10^{-3}
linsolver tol factor	<i>REAL</i> : The linear solver tolerance is a function of the absolute error of the Newton's method: $tol = e _{\infty} * a^i$, where e is the absolute error of the Newton's method, i is the Newton iteration number, and a is the specified value.	0.5
newton first norm	REAL: Specifies an assumed infinity norm of the absolute error of the Newton's method at the iteration 0 of the time step 1. This can change the behavior of the first Newton iterative method because of the dependency of the linear system tolerance on the absolute error of the Newton's method (see keyword linsolver tol factor).	0.2

$7.3 \quad \text{Keywords for the Rosenbrock-Type Implicit Runge-Kutta Methods} \\$

Table 7.3: Keywords for the Rosenbrock schemes.

Keyword	Description	Default value
rosenbrock scheme	CHARACTER: Rosenbrock scheme to be used. Currently, only	_
	the $RO6-6$ is implemented.	

7.4 Jacobian Specifications

The Jacobian must be defined using a block of the form:

#define Jacobian type = 2

```
\begin{array}{ll} \text{print info} = .\text{TRUE.} \\ \text{preallocate} = .\text{TRUE.} \\ \text{\#end} \end{array}
```

Table 7.4: Keywords for Jacobian definition block.

Keyword	Description	Default value
type	INTEGER: Specifies the type of Jacobian matrix to be computed.	Mandatory
	Options are:	Keyword
	1. Numerical Jacobian: Uses a coloring algorithm and a finite difference method to compute the DG Jacobian matrix (only available with shared memory parallelization).	
	2. Analytical Jacobian: Available with shared (OpenMP) or distributed (MPI) memory parallelization for advective and/or diffusive nonlinear conservation laws, BUT only for the standard DGSEM (no split-form).	
print info	LOGICAL: Specifies the verbosity of the Jacobian subroutines	.TRUE.
preallocate	LOGICAL: Specifies if the Jacobian must be allocated in prepro-	.FALSE.
	cessing (.TRUE only available for advective/diffusive nonlinear	
	conservation laws) or every time it is computed (.FALSE.)	

Explicit Solvers

Explicit time integration schemes available in HORSES3D. The main keywords to use it are shown in Table 8.1.

Table 8.1: Keywords for the multigrid solver.

Keyword	Description	Default value
time integration	CHARACTER: This is the main keyword to activate the multi-	'explicit'
	grid solvers. The value of it should be set to 'FAS' for the Full	
	Approximation Scheme (FAS) nonlinear multigrid solvers and to	
	'AnisFAS' for anisotropic FAS schemes.	
simulation type	CHARACTER: Specifies if HORSES3D must perform a 'steady-	'steady-state'
	state' or a 'time-accurate'. If 'time-accurate' the solver switches	
	to BDF integration and uses FAS as a pseudo problem solver.	
	Compatible only with 'FAS'.	
explicit method	CHARACTER: Select desired Runge-Kutta solver. Options are:	RK3
	'Euler', 'RK3', 'RK5', 'RKOpt', 'SSPRK33' and 'SSPRK43'.	
rk order	INTEGER: Order of Runge-Kutta method optimized for steady-	2
	state solver ('RKOpt'). Possible orders are from 2 to 7.	
limit timestep	LOGICAL: Activate the possitivity limiter of Zhang and Shu (only	.false.
	for SSPRK methods).	
limiter minimum	REAL: Minimum value of density and pressure allowed by the	1e-13
	limiter.	

Nonlinear p-Multigrid solver (FAS)

The code has an implementation of the Full Approximation Scheme (FAS) nonlinear p-multigrid method. The main keywords to use it are shown in Table 9.1.

Table 9.1: Keywords for the multigrid solver.

Keyword	Description	Default value
time integration	CHARACTER: This is the main keyword to activate the multi-	'explicit'
	grid solvers. The value of it should be set to 'FAS' for the Full	
	Approximation Scheme (FAS) nonlinear multigrid solvers and to	
	'AnisFAS' for anisotropic FAS schemes.	
simulation type	CHARACTER: Specifies if HORSES3D must perform a 'steady-	'steady-state'
	state' or a 'time-accurate'. If 'time-accurate' the solver switches	
	to BDF integration (the exact method can be set using 'bdf or-	
	der' option) and uses FAS as a local steady-state problem solver.	
	Compatible only with 'FAS'.	
multigrid levels	INTEGER: Number of multigrid levels for the computations.	Mandatory
		keyword
delta n	INTEGER: Interval of reduction of polynomial order for creating coarser multigrid levels.	1
multigrid output	LOGICAL: If .TRUE., the residuals at the different multigrid lev-	.FALSE.
	els will be displayed.	
mg sweeps	INTEGER: Number of smoothing sweeps to be taken.	1*
mg sweeps pre	INTEGER: Number of pre-smoothing sweeps to be taken.	1*
mg sweeps post	INTEGER: Number of post-smoothing sweeps to be taken.	1*
mg sweeps coarsest	INTEGER: Number of pre- and post-smoothing sweeps to be	Average
	taken on the coarsest multigrid level.	between pre-
		sweeps and
		post-sweeps
mg sweeps exact	INTEGER(:): Alternative to 'mg sweeps'. Defines exact number	1*
	of pre- and post- smoothing sweeps to be taken on each level.	
	Index of the array indicates the MG level for the sweeps to be	
	performed, e.g. [1,4] performs 1 pre-sweep and 1 post-sweep on	
	level 1 and 4 pre-post-sweeps on level 2.	
mg sweeps pre exact	INTEGER(:): Alternative to 'mg sweeps pre'. Defines exact num-	1*
	ber of pre-smoothing sweeps to be taken on each level. Index of	
	the array indicates the MG level for the sweeps to be performed,	
	e.g. [1,4] performs 1 pre-sweep on level 1 and 4 pre-sweeps on	
	level 2.	
mg sweeps post exact	INTEGER(:): Alternative to 'mg sweeps post'. Defines exact	1*
	number of post-smoothing sweeps to be taken on each level. Index	
	of the array indicates the MG level for the sweeps to be performed,	
	e.g. [1,4] performs 1 post-sweep on level 1 and 4 post-sweeps on level 2.	

Table 9.1: Keywords for the multigrid solver - continued.

Keyword	Description	Default value
mg smoother	CHARACTER: The smoothing technique to be used. The key-	RK3
	words and possible explicit smoothers are the same as the 'ex-	
	plicit method' in 8.1. For the semi-implicit residual relaxation use 'BIRK5'.	
fasfmg residual	REAL: When this keyword is used, the code uses a full multigrid	
lasinig residuar	(FMG) method to obtain an initial condition for the simulation.	
	The initial condition has the specified residual.	
fasfmg save solutions	LOGICAL: Save the solutions that are obtained at the different	.FALSE.
	FMG levels. Only usable when fasfmg residual is used.	
postsmooth option	CHARACTER: When this keyword is used, the code performs	_
	extra post-smoothing sweeps, so that the final residual after com-	
	pleting the post-smoothing is lower than the residual achieved by	
	the pre-smoothing. The options are:	
	• f-cycle: Do the extra post-smoothing with an FMG cycle.	
	• <i>smooth</i> : Do normal smoothing.	
smooth fine	REAL: Extra pre-smoothing is performed on a multigrid level of	_
	order P , until a residual is obtained $\ \tilde{\mathbf{g}}^P\ _{\infty} < \eta \ \tilde{\mathbf{g}}^{\tilde{N}}\ _{\infty}$, where	
	N is the polynomial order of the next (coarsest) grid, and η is the	
	specified value.	
max mg sweeps	INTEGER: Maximum number of smoothing sweeps to be per-	10000
	formed. This only makes sense if one uses the keywords postsmooth option and/or smooth fine.	
mg initialization	LOGICAL: Sets the initial explicit residual smoothing with RK3	.FALSE.
ing initialization	and local time stepping.	·IIILSE.
initial residual	REAL: Threshold for the $\ \tilde{\mathbf{g}}^P\ _{\infty}$ after which solver switches from	1.0
	the 'mg initialization' settings to user specified.	
initial cfl	REAL: CFL and DCFL number for initial residual smoothing.	0.1

^{*} The user must specify mg sweeps pre and mg sweeps post, or mg sweeps.

p-Adaptation Methods

The p-adaptation methods are used when the p-adaptation region is specified in the control file:

```
#define p-adaptation
   Truncation error type = isolated
   truncation error
                         = 1.d-2
   Nmax
                         = [10, 10, 10]
                         = [2, 2, 2]
   Conforming boundaries = [InnerCylinder, sphere]
   order across faces = N*2/3
                         = .FALSE.
   increasing
   write error files
                        = .FALSE.
                         = .FALSE.
   adjust nz
   mode
                        = time
   interval
                         = 1.d0
   restart files
                        = .TRUE.
                         = 1
   max N decrease
   padapted mg sweeps pre
   padapted mg sweeps post
   padapted mg sweeps coarsest = 20
#end
```

Table 10.1: Keywords for the p-adaptation algorithms.

Keyword	Description	Default value
truncation error type	CHARACTER: Can be either "isolated" or "non-isolated".	isolated
truncation error	REAL: Target truncation error for the p-adaptation algorithm.	Mandatory
		keyword
coarse truncation error	REAL: Truncation error used for coarsening.	same as trun-
		cation error
Nmax	INTEGER(3): Maximum polynomial order in each direction for	Mandatory
	the p-adaptation algorithm.	keyword
Nmin	INTEGER(3): Minimum polynomial order in each direction for	[1,1,1]
	the p-adaptation algorithm.	
conforming boundaries	CHARACTER(*): Specifies the boundaries of the geometry that	_
	must be forced to be conforming after the p-adaptation process.	
order across faces	CHARACTER: Mathematical expression to specify the maximum	N-1
	polynomial order jump across faces. Currently, only $N*2/3$ and	
	N-1 are supported.	
increasing	LOGICAL: If .TRUE. the multi-stage FMG adaptation algorithm	.FALSE.
	is used.	

Table 10.1: Keywords for the p-adaptation algorithms - continued.

Keyword	Description	Default value
write error files	LOGICAL: If .TRUE., the program writes a file per element con-	.FALSE.
	taining the directional tau-estimations. The files are stored in	
	the folder ./TauEstimation/. When the simulation has several	
	adaptation stages, the new information is just appended.	
adjust nz	LOGICAL: If .TRUE., the order across faces is adjusted in the	.FALSE.
	directions xi, eta, and zeta of the face (being zeta the normal	
	direction). If .FALSE., the order is only adjusted in the xi and	
	eta directions. The adjustment currently consists (hard-cod ed)	
	in allowing jumps in the polynomial order of at most 1.	
mode	CHARACTER: p-Adaptation mode. Can be static, time or iter-	static
	ation. Static p-adaptation is performed once at the beginning of	
	a simulation for steady or unsteady simulations. Unsteady adap-	
	tation can be by time or by iteration.	
interval	INTEGER/REAL: In dynamic p-adaptation cases, this keyword	$huge \ number$
	specifies the iteration (integer) or time (real) interval for p-	
	adaptation.	
restart files	LOGICAL: If .TRUE., the program writes restart files before and	.FALSE.
	after the p-adaptation.	
max N decrease	INTEGER: Maximum decrease in the polynomial order in every	$N-N_{min}$
	p-adaptation procedure.	
post smoothing residual	<i>REAL</i> : Specifies the maximum allowable deviation of $\partial_t q$ after the	_
	p-adaptation procedure.	
post smoothing method	CHARACTER: Either RK3 or FAS.	RK3, if the
		last keyword
		is activated
estimation files	CHARACTER: Name of the folder that contains the error esti-	_
	mations obtained with the multi tau-estimation (section 10.1).	
estimation files number	INTEGER(2): First and last estimation stages to be used for	Mandatory if
	p-adaptation.	last keyword
		is used.
padapted $\ll keyword \gg$	MULTIPLE: Specifies control file keywords that should be re-	_
	placed after the adaptation procedure. Currently, only 'mg sweeps	
	', 'mg sweeps pre', 'mg sweeps post', and 'mg sweeps coarsest' are	
	supported.	

10.1 Multiple truncation error estimations

A static p-adaptation procedure can be driven by a set of error estimations, which have to be performed beforehand in a simulation with the following block:

```
#define multi tau-estimation
truncation error type = isolated
interval = 10
folder = MultiTau
#end
```

Immersed boundary method

The immersed boundary is activated during the simulation if the following lines are specified in the control file:

```
#define IBM
   name
                                    = myIBM
   active
                                    = . true.
                                    = 1.0 d-6
   penalization
   semi implicit
                                    = . false.
   number of objects
   number of interpolation points = 15
   band region
                                    = . true.
   band region coefficient
                                    = 1.3
                                    = . true.
   compute distance
   clip axis
                                    = 1
   aab
                                    = . false.
   describe
   plot obb
                                    = . false.
   plot kdtree
                                    = . false.
   plot mask
                                    = . true.
   plot band points
                                    = . false.
#end
```

A folder called 'IBM' must be created.

Table 11.1: Keywords for the immersed boundary method.

Keyword	Description	Default value
name	CHARACTER: name assigned to immersed boundary method job	
active	LOGICAL: When .TRUE. the immersed boundary method is ac-	.FALSE.
	tive.	
penalization	<i>REAL</i> : Specifies the value of the penalization term, <i>i.e.</i> η .	Δt
semi implicit	LOGICAL: The source term is treated in a semi-implicit manner.	.FALSE.
number of objects	INTEGER: Specifies the maximum number of objects inside a leaf	5
	of the KD-tree.	
number of interpolation	INTEGER: Number of points used for the interpolation of the	15
points	variables' values on the surface. It's needed for the computation	
	of the forces.	
band region	LOGICAL: If it's true, the band region is computed, otherwise it	.FALSE.
	is not.	
band region coefficient	INTEGER: A region n-times the oriented bounding box is created	1.5
	(where n is the band region coefficient): all the points inside this	
	region belong to the band region. The band region's points are	
	used for the interpolation. It must be greater then 1 and 'band	
	region' must be .true	

Table 11.1: Keywords for the immersed boundary method - continued.

Keyword	Description	Default value
compute distance	LOGICAL: If it's true, the distance between the points in the	.FALSE.
	band region and the stl file is computed, otherwise it is not. If	
	the distance is not required, turn it off since it is an expansive	
	operation.	
clip axis	INTEGER: It's the axis along which the stl is cut. It is only	0
	needed if the forces are computed so that the integration of the	
	variables is performed only on the portion of the stl surface lying	
	inside the mesh. 1 corresponds to x-axis, 2 with y-axis and 3 with	
	z-axis	
aab	LOGICAL: The Axis Aligned Box is computed instead of the Ori-	.FALSE.
	ented Bounding box. It is recommended when 'clip axis' $\neq 0$.	
describe	LOGICAL: The immersed boundary parameters are printed on	.FALSE.
	the screen.	
plot obb	LOGICAL: The oriented-bounding box is plotted.	.FALSE.
plot kdtree	LOGICAL: The kd-tree is plotted.	.FALSE.
plot mask	LOGICAL: The degrees of freedom belonging to the mask are	.FALSE.
	plotted.	
plot band points	LOGICAL: The band region's points are plotted.	.FALSE.

11.0.1 STL file

Immersed boundary requires, along with the mesh, a STL file. It must be put in the MESH folder with the mesh. The STL file name must be in lowercase character. In some programs, like AutoCAD, a STL file has always positive coordinates: the mesh should be built according to this consideration.

In the case of 2D simulations, the STL can be automatically cut by horses3D through the addition of the line *clip axis* (described in the previous section) so that only the STL portions inside the mesh are considered.

 Keyword
 Description
 Default value

 number of stl =
 INTEGER: Number of stl files.
 1

 stl file name =
 CHARACTER: The name of the STL file, without extension; it has to be inside the folder "MESH" .
 Mandatory keyword

 stl file nameN =
 CHARACTER: The name of the Nth-STL file (where N starts from 2), without extension; for the first STL just use "stl file name". It has to be inside the folder "MESH" .
 none

Table 11.2: Keywords for stl files.

11.0.2 Computing forces

In order to compute the forces on a body, the monitor should be defined as usual but the "Marker=" has to be equal to the name of the stl file on which the user wants to compute the forces. Given a STL file called "stlname", the monitor should be:

```
#define surface monitor 1
marker = stlname
.
.
.
.
#end
```

The result of this operation is a .tec file inside the RESULTS folder. This file contains a scalar or a vector data projected on the body surface.

11.0.3 Moving bodies

If one or more of the stl files move, then the following lines must be added:

Table 11.3: Keywords for a moving stl.

Keyword	Description	Default value
stl name	CHARACTER: name of the moving stl; it has to be equal to the	mandatory
	name of one of the stl files.	keyword
type	CHARACTER: Type of motion, it can be ROTATION or LIN-	Mandatory
	EAR.	keyword
angular velocity	REAL: Specifies the angular velocity. It must be in [Rad]/[s]	Mandatory
		keyword
		for rotation
		type
velocity	REAL: Specifies the translation velocity. It must be in [m]/[s]	Mandatory
		keyword for
		linear type
motion axis	REAL: Specifies the axis along which the rotation/translation oc-	Mandatory
	curs.	keyword

Monitors

The monitors are specified individually as blocks in the control file. The only general keyword that can be specified is explained in Table 12.1.

Table 12.1: Keywords for monitors.

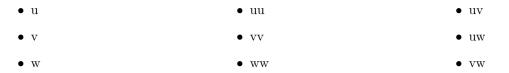
Keyword	Description	Default value
monitors flush interval	INTEGER: Iteration interval to flush the monitor information to	100
	the monitor files.	

12.1 Residual Monitors

12.2 Statistics Monitor

#define statistics
initial time = 1.d0
initial iteration = 10
sampling interval = 10
dump interval = 20
@start
#end

By default, the statistic monitor will average following variables:



A keyword preceded by @ is used in real-time to signalize the solver what it must do with the statistics computation:

• @start	• @stop	• @dump
• @pause	• @reset	

After reading the keyword, the solver performs the desired action and marks it with a star, e.g. @start*. **ATTENTION:** Real-time keywords may not work in parallel MPI computations. I depends on how the system is configured.

12.3 Probes

```
#define probe 1
  name = SomeName
  variable = SomeVariable
  position = [0.d0, 0.d0, 0.d0]
#end
```

Table 12.2: Keywords for probes.

Keyword	Description	Default value
name	CHARACTER: Name of the monitor.	Mandatory
		Keyword
variable	CHARACTER: Variable to be monitored. Implemented options	Mandatory
	are:	Keyword
	• pressure	
	• velocity • w	
	• u • mach	
position	REAL(3): Coordinates of the point to be monitored.	Mandatory
		Keyword

12.4 Surface Monitors

Table 12.3: Keywords for probes.

Keyword	Descrip	otion	Default value
name	CHARACTER: Name of the monitor.		Mandatory
			Keyword
marker	CHARACTER: Name of the boundary where a variable will be monitored.		Mandatory
			Keyword
variable	CHARACTER: Variable to be monitored. Implemented options are:		Mandatory
			Keyword
	• mass-flow	• force	
	• flow	• lift	
	• pressure-force	• drag	
	• viscous-force	• pressure-average	
reference surface	REAL: Reference surface [area] for the monitor. Needed for "lift" and "drag" computations.		_
direction	REAL(3): Direction in which the	_	
direction	Needed for "pressure-force", "visc		
	specified for "lift" (default [0.d0,1]		
	[1.d0,0.d0,0.d0])		

12.5 Volume Monitors

Volume monitors compute the average of a quantity in the whole domain. They can be scalars(s) or vectors(v).

```
#define volume monitor 1
   name = SomeName
   variable = SomeVariable
#end
```

Table 12.4: Keywords for volume monitors.

Keyword	Description		Default value
name	CHARACTER: Name of the monitor.		Mandatory
			Keyword
variable	CHARACTER: Variable to be monitored. The variable can be scalar (s) or vectorial (v). Implemented options are:		Mandatory
			Keyword
	 (s) kinetic energy (s) kinetic energy rate (s) enstrophy (s) entropy (s) entropy rate 	(s) mean velocity(v) velocity(v) momentum(v) source	

Advanced User Setup

Advanced users can have additional control over a simulation without having to modify the source code and recompile the code. To do that, the user can provide a set of routines that are called in different stages of the simulation via the Problem file (*ProblemFile.f90*). A description of the routines of the Problem File can be found in section 13.1.

13.1 Routines of the Problem File: ProblemFile.f90

- UserDefinedStartup: Called before any other routines
- UserDefinedFinalSetup: Called after the mesh is read in to allow mesh related initializations or memory allocations.
- UserDefinedInitialCondition: called to set the initial condition for the flow. By default it sets an uniform initial condition, but the user can change it.
- UserDefinedState1, UserDefinedNeumann: Used to define an user-defined boundary condition.
- UserDefinedPeriodicOperation: Called before every time-step to allow periodic operations to be performed.
- UserDefinedSourceTermNS: Called to apply source terms to the equation.
- UserDefinedFinalize: Called after the solution computed to allow, for example error tests to be performed.
- UserDefinedTermination: Called at the end of the main driver after everything else is done.

13.2 Compiling the Problem File

The Problem File file must be compiled using a specific Makefile that links it with the libraries of the code. If you are using the horses/dev environment module, you can get templates of the Problemfile.f90 and Makefile with the following commands:

\$ horses-get-problemfile

Otherwise, search the test cases for examples.

To run a simulation using user-defined operations, create a folder called SETUP on the path were the simulation is going to be run. Then, store the modified *ProblemFile.f90* and the *Makefile* in SETUP, and compile using:

```
$ make <<Options>>
```

where again the options are (bold are default):

- MODE=DEBUG/RELEASE
- COMPILER=ifort/gfortran
- COMM=PARALLEL/SEQUENTIAL
- ENABLE_THREADS=NO/YES

Postprocessing

For postprocessing the Simulation Results

14.1 Visualization with Tecplot Format: horses2plt

HORSES3D provides a script for converting the native binary solution files (*.hsol) into tecplot ASCII format (*.tec), which can be visualized in Pareview or Tecplot. It can also export the solution to the more recent VTKHDF format; however, note that this feature does **not** export boundary information or mesh files. Usage:

\$ horses2plt SolutionFile.hsol MeshFile.hmesh <<Options>>

The options comprise following flags:

Table 14.1: Flags for horses2plt.

Flag	Description	Default value
output-order=	INTEGER: Output order nodes. The solution is interpolated into	Not Present
	the desired number of points.	
output-basis=	CHARACTER: Either Homogeneous (for equispaced nodes, or	Gauss*
	Gauss.	
output-mode=	CHARACTER: Either multizone or FE. The option multizone	multizone
	generates a Tecplot zone for each element. The option FE gener-	
	ates only one Tecplot zone for the fluid and one for each boundary	
	(ifboundary-file is defined). Each subcell is mapped as a linear	
	finite element. This format is faster to read by Paraview and	
	Tecplot.	
output-variables=	CHARACTER: Output variables separated by commas.A com-	Q
	plete description can be found in Section 14.1.1.	
dimensionless	Specifies that the output quantities must be dimensionless	Not Present
partition-file=	CHARACTER: Specifies the path to the partition file (*.pmesh)	Not Present
	to export the MPI ranks of the simulation.	
boundary-file=	CHARACTER: Specifies the path to the boundary mesh file	Not Present
	(*.bmesh) to export the surfaces as additional zones of the Tecplot	
	file.	
output-type=	CHARACTER: Specifies the type of output file: tecplot or vtkhdf.	tecplot

^{*} Homogeneous when --output-order is specified

Additionally, depending on the type of solution file, the user can specify additional options.

14.1.1 Solution Files (*.hsol)

For standard solution files, the user can specify which variables they want to be exported to the Tecplot file with the flag --output-variables=. The options are:

• Q (default)	• <i>V</i>	\bullet Nav	• <i>u_x</i>	• <i>c</i> _ <i>y</i>
• <i>rho</i>	• <i>Ht</i>	• <i>N</i>	• <i>v_x</i>	• <i>c_z</i>
• <i>u</i>	ullet $rhou$	• <i>Ax_Xi</i>	• w_x	
• <i>v</i>	• <i>rhov</i>	\bullet Ax_Eta	• <i>u</i> _ <i>y</i>	ullet $omega$
• w	\bullet $rhow$	\bullet Ax_Zeta	• <i>v_y</i>	 omega_x
• p	\bullet $rhoe$	\bullet Three Axes	• w ₋ y	$ullet$ $omega_y$
• T	• <i>c</i>	• Axes	• <i>u_z</i>	$ullet$ $omega_z$
• Mach	$\bullet Nxi$	$\bullet mpi_rank$	• <i>v_z</i>	V
• <i>s</i>	• Neta	• <i>eID</i>	• w_z	$ullet$ $omega_abs$
$\bullet Vabs$	• Nzeta	$\bullet \ gradV$	• c_x	ullet $Qcrit$

14.1.2 Statistics Files (*.stats.hsol)

Statistics files generate following variables by default (being Sij the components of the Reynolds Stress tensor):

• Umean	• Sxx	• Sxy
• Vmean	• Syy	• Sxz
• Wmean	• Szz	• Syz

14.2 Extract geometry

Under construction.

14.3 Merge statistics tool

Tool to merge several statistics files. The usage is the following:

 $\label{thm:condition} \$\ \, \text{horses.mergeStats}\ \ *.\ \, \text{hsol}\ \, --\text{initial-iteration=INTEGER}\ \, --\text{file-name=CHARACTER}\ \, \\ \text{Some remarks:}$

- Only usable with statistics files that are obtained with the "reset interval" keyword and/or with individual consecutive simulations.
- Only constant time-stepping is supported.
- Dynamic p-adaptation is currently not supported.

Appendices

Non-dimensional Navier Stokes equations

To illustrate the roles of various terms in the governing equations, we present here the non-dimensionalized governing compressible Navier Stokes equations with particles. We define the non-dimensional variables as

$$x_i^* = x_i/L_o, \quad y_i^* = y_i/L_o, \quad t^* = tu_o/L_o, \quad \rho^* = \rho/\rho_o, \quad u_i^* = u_i/u_o$$
 (14.1)

$$v_i^* = v_i/u_o, \quad p^* = p/\rho_o u_o^2, \quad e^* = e/u_o^2 \quad T^* = T/T_o, \quad T_p^* = T_p/T_o,$$
 (14.2)

$$\mu^* = \mu/\mu_o, \quad \kappa^* = \kappa/\kappa_o \quad g_i^* = g_i/g_o \tag{14.3}$$

where the subscript o denotes a reference value. Under these scalings, the Navier Stokes equations become

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial \rho^* u_j^*}{\partial x_j^*} = 0, \tag{14.4}$$

$$\frac{\partial \rho^* u_i^*}{\partial t^*} + \frac{\partial \rho^* u_i^* u_j^*}{\partial x_j^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{Re} \frac{\partial \tau_{ij}^*}{\partial x_j^*} + \frac{1}{Fr^2} g_i^* - \beta \frac{\mu^* \phi_m}{N_p St} \sum_{n=1}^{N_p} (u_i^* - v_{i,n}^*) \delta(\mathbf{x}^* - \mathbf{y}_n^*), \tag{14.5}$$

$$\frac{\partial \rho^* e^*}{\partial t^*} + \frac{\partial u_j^* (\rho^* e^* + p^*)}{\partial x_j^*} = \frac{1}{Re} \left[\frac{\partial \tau_{ij}^* u_j^*}{\partial x_i^*} + \frac{1}{(\gamma - 1) Pr M_o^2} \frac{\partial}{\partial x_j^*} \left(k^* \frac{\partial T^*}{\partial x_j^*} \right) \right] + \\
+ \beta \frac{\phi_m}{3N_p} \frac{Nu}{(\gamma - 1) Pr M_o^2 St} \sum_{n=1}^{N_p} (T_{p,n}^* - T^*) \delta(\mathbf{x}^* - \mathbf{y}_n^*). \tag{14.6}$$

Where $Re = \frac{\rho_o L_o u_o}{\mu_o}$ is the Reynolds number, $Fr = \frac{u_o}{\sqrt{g_o L_o}}$ is the Froude number, $\phi_m = \frac{m_p N_p}{\rho_o L_o^3}$, $St = \frac{\tau_p}{\tau_f}$ is the Stokes number which for Stokesian particles is $St = \frac{\rho_p D_p^2 u_o}{18 L_o \mu_o}$, the Prandtl number (which is assumed constant and equal to 0.72) $Pr = \frac{\mu_o c_p}{k_o}$, the Nusselt number $Nu = \frac{hD_p}{k_o} = 2$ (for Stokesian particles) and the Mach number $M_o = \frac{u_o}{\sqrt{\gamma R T_o}}$.

Non-dimensional particle equations

The non dimensional set of equations for the particles reads:

$$\frac{dy_i^*}{dt^*} = v_i^*, \quad \frac{dv_i^*}{dt^*} = \frac{\mu^*}{St} \left(u_i^* - v_i^* \right) + \frac{1}{Fr^2} g_i^*. \tag{14.7}$$

$$\frac{dT_p^*}{dt^*} = \frac{\gamma}{3\Gamma St Pr} \left(I_o^* - Nu(T_p^* - T^*) \right), \tag{14.8}$$

where $I_o^* = \frac{I_o D_p}{4k_o T_o}$ and $\Gamma = c_{v,p}/c_v$ is the ratio of the particle specific heat capacity to the fluid isochoric specific heat capacity.