HORSES3D

A \mathbf{H} igh- \mathbf{Or} der (DG) \mathbf{S} pectral \mathbf{E} lement \mathbf{S} olver \mathbf{User} \mathbf{Manual}

Andrés Rueda Many others (future?)

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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**
- $\ \mathrm{PLATFORM} \!\!=\!\! \mathrm{MACOSX}/\mathbf{LINUX}$
- ENABLE_THREADS=NO/**YES**

For example:

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

• If you use environment modules, it is advised to use the HORSES3D module file:

 $\label{lem:modulefile:MODULEPATH=SHORSES_DIR/utils/modulefile:$MODULEPATH$ where $HORSES_DIR$ is the installation directory.$

Input and Output Files

2.1 Input Files

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

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 NSLITE3D 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 polynomial order file 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.	
dcfl	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
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.	
Number of boundaries	INTEGER: Specifies the number of boundaries of the geometry.	Mandatory
	This keyword must be followed by an equal number of lines in the	keyword
	control file that define the boundary conditions as follows:	
	$boundary Name 1\ boundary Value 1\ boundary Type 1$	
	$boundary Name 2\ boundary Value 2\ boundary Type 2$	

^{*} One of these keywords must be specified

3.2 Boundary conditions

Under construction.

^{**} 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.

Restarting a Case

Table 4.1: Keywords for restarting a case.

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 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

5.1 Compressible flow

Table 5.1: 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	
LES model	CHARACTER(*): Options are:	None	
	SmagorinskyNone		
Wall model	CHARACTER(*):	linear	

5.2 Incompressible Navier-Stokes

5.3 Cahn-Hilliard

Implicit Solvers

6.1 General Keywords

The keywords for the implicit solvers are listed in table 6.1

Table 6.1: 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'
jacobian by convergence	LOGICAL: When .TRUE., the Jacobian is only computed when the convergence falls beneath some threshold (see keyfords: blah and blah blah). This improves performance but can introduce big numerical errors for time-accurate simulations.	.FALSE.
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. 	'petsc'
	 '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 	
	 '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'. 	
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.

Table 6.1: Keywords for implicit solvers - continued.

Keyword	Description	Default value
newton tolerance	REAL: Specifies the tolerance for the Newton method.	10^{-6} or
		for time-
		accurate sim-
		ulations and
		$MaxResidual \times$
		10^{-3} for
		steady-state
		simulations
max newton iter	INTEGER: Maximum number of Newton iterations for BDF	30
	solver.	
compute jacobian every	INTEGER: Forces the Jacobian to be computed in an interval of	Inf
	iterations that is specified.	
bdf order	INTEGER: If present, the solver uses a BDF solver of the specified	1
	order. BDF1 - BDF5 are available, and BDF2 - BDF5 require	
	constant time steps.	

6.2 Jacobian Specifications

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

```
#define Jacobian
  type = 2
  print info = .TRUE.
  preallocate = .TRUE.
#end
```

Table 6.2: Keywords for Jacobian definition block.

Keyword	Description	Default value
type	INTEGER: Specifies the type of Jacobian matrix to be computed. Options are:	Mandatory Keyword
	1. Numerical Jacobian: Uses coloring algorithm for computing Jacobian (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.	
print info	LOGICAL: Specifies the verbosity of the Jacobian subroutines	.TRUE.
preallocate	LOGICAL: Specifies if the Jacobian must be allocated in preprocessing (.TRUE only available for advective/diffusive nonlinear conservation laws) or every time it is computed (.FALSE.)	.FALSE.

. TRUE.=Preallocate / .FALSE.=Perform allocation every time the Jacobian is constructed

Multigrid

Table 7.1: Keywords for the multigrid solver.

Keyword	word Description	
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 levels will be displayed.	.FALSE.

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.
   adjust nz
                        = .FALSE.
   mode
                        = time
                        = 1.d0
   interval
   restart files
                        = .TRUE.
                        = 1
   max N decrease
   padapted mg sweeps pre
   padapted mg sweeps post
   padapted mg sweeps coarsest = 20
#end
```

Table 8.1: 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.	
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.	

Table 8.1: Keywords for the p-adaptation algorithms - continued.

Keyword	Description	Default value
adjust nz	LOGICAL: If .TRUE., the order accross 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-	
C1	adaptation.	DALCE
restart files	LOGICAL: If .TRUE., the program writes restart files before and	.FALSE.
	after the p-adaptation.	$N - N_{min}$
max N decrease	INTEGER: Maximum decrease in the polynomial order in every p-adaptation procedure.	$N-N_{min}$
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
T		last keyword
		is activated
estimation files	CHARACTER: Name of the folder that contains the error esti-	_
	mations obtained with the multi tau-estimation (section 8.1).	
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.	

8.1 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
```

Monitors

9.1 Statistics Monitor

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

By default, the statistic monitor will average following variables:

•	u	•	uu	•	uv
•	V	•	VV	•	uw
•	W	•	ww	•	vw

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

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

9.2 Probes

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

Table 9.1: Keywords for probes.

Keyword	Description	Default value
name	CHARACTER: Name of the monitor.	Mandatory
		Keyword

Table 9.1: Keywords for the p-adaptation algorithms - continued.

Keyword	Description			Default value
variable	CHARACTER:	Variable to be monitored.	Implemented options	Mandatory
	are:			Keyword
	• pressure	• V	• k	
	• velocity	• w		
	• u	• mach		
position	$\mid REAL(3)$: Coor	dinates of the point to be r	nonitored.	Mandatory
				Keyword

9.3 Surface Monitors

Table 9.2: Keywords for probes.

Keyword	D	Description		
name	CHARACTER: Name of th	CHARACTER: Name of the monitor.		
			Keyword	
marker	CHARACTER: Name of the	ne boundary where a variable will be	Mandatory	
	monitored.		Keyword	
variable	CHARACTER: Variable to	CHARACTER: Variable to be monitored. Implemented options		
	are:		Keyword	
	• mass-flow	• force		
	• flow	• lift		
	• pressure-force	ullet drag		
	• viscous-force	• pressure-average		
reference surface	REAL: Reference surface [a and "drag" computations.	REAL: Reference surface [area] for the monitor. Needed for "lift" and "drag" computations.		
direction	REAL(3): Direction in whi	REAL(3): Direction in which the force is going to be measured.		
	Needed for "pressure-force"	Needed for "pressure-force", "viscous-force" and "force". Can be		
	specified for "lift" (default	$[0.\mathrm{d}0,\!1.\mathrm{d}0,\!0.\mathrm{d}0])$ and "drag" (default		
	[1.d0,0.d0,0.d0])			

9.4 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 9.3: Keywords for volume monitors.

Keyword	Descr	ription	Default value
name	CHARACTER: Name of the monitor.		Mandatory
			Keyword
variable	CHARACTER: Variable to be monitored. The variable can be		Mandatory
	scalar (s) or vectorial (v). Implemented options are:		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 10.1.

10.1 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 the end of the main driver after everything else is done.

10.2 Compiling the Problem File

The Problem Fie 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-makefile
- \$ 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

- $\bullet \ \mathrm{PLATFORM} \!\!=\!\! \mathrm{MACOSX}/\mathbf{LINUX}$
- $\bullet \ \, \text{ENABLE_THREADS=NO/YES} \\$

Postprocessing

For postprocessing the Simulation Results

11.1 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. Usage:

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

The options comprise following flags:

Table 11.1: 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-mesh is defined). Each subcell is mapped as a lin-	
	ear 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 11.1.1.	
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-mesh=	CHARACTER: Specifies the path to the boundary mesh file	Not Present
	(*.bmesh) to export the surfaces as additional zones of the Tecplot	
	file.	

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

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

11.1.1 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>	• T	$\bullet Vabs$	• rhou
• <i>rho</i>	• <i>w</i>	\bullet $Mach$	• <i>V</i>	\bullet $rhov$
• <i>u</i>	• <i>p</i>	• <i>S</i>	• <i>Ht</i>	\bullet rhow

• *Ax_Xi* \bullet rhoe• *u_x* • *v_z* \bullet $omega_y$ \bullet Ax_Eta • c • *v_x* • w_z \bullet Ax_Zeta \bullet Nxi• w_x • *c_x* \bullet $omega_z$ \bullet Neta \bullet ThreeAxes • c_y u_y • Nzeta \bullet Axes $\bullet \ omega_abs$ v_y • *c_z* $\bullet \ mpi_rank$ \bullet Nav• w_y \bullet omega• N \bullet gradV• *omega_x* • *u_z* ullet Qcrit

11.1.2 Statistics Files (*.stats.hsol)

Statistics files generate following variables by default:

Umean
Sxx
Vmean
Syy
Sxz
Wmean
Szz
Syz

11.2 Extract geometry

Under construction.

11.3 Merge statistics tool