

# PARMEC USER MANUAL

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# Chapter 1

## Installation

Clone parmec sources from GitHub:

```
git clone https://github.com/tkoziara/parmec
```

Enter parmec directory:

```
cd parmec
```

Edit Config.mak file variables:

```
# C++ compiler (ISPC is assumed to be in the PATH; http://ispc.github.io)
CXX=g++

# Python paths
PYTHONINC=-I/usr/include/python2.7
PYTHONLIB=-L/usr/lib -lpython2.7

# HDF5 paths
HDF5INC=-I/usr/include
HDF5LIB=-L/usr/lib -lhdf5 -lhdf5_hl

# Debug version
DEBUG=no
```

Compile sources:

```
make
```

Parmec executable files are:

```
parmec4 (single precision)
parmec8 (double precision)
```

Parmec library files are:

```
libparmec4.a, parmec4.h (single precision library, header)
libparmec8.a, parmec8.h (double precision library, header)
```

To update parmec type:

```
make clean
git pull
make
```

## Chapter 2

# Running

PARMEC is a command line program. Typical usage:

1. Include `parmec` directory into your `PATH` variable.
2. Create a directory where your input file and output files will be stored (e.g. `mkdir test`).
3. Edit your Python input file in this directory (e.g. `test.py`); Chapter 4 documents all input commands.
4. Run PARMEC (e.g. `parmec4 path/to/test/test.py`, or `parmec8 path/to/test/test.py`).
5. Time histories can be generated during analysis using the `HISTORY` command; see Section 4.18.
6. Upon termination output file(s) is(are) created in the same directory (e.g. `path/to/test/test.dump`); see Section 4.19 and Chapter 5.
7. The output files can be viewed with OVITO, ParaView, or VisIt, as documented in Section 4.19 and Chapter 6.

## Chapter 3

# Implementation status

Individual features of parmec which are not implemented yet are marked as **(under development)**. Relatively complex features that have seen little testing are marked as **(experimental)**. Table 3.1 summarizes current status of automatic contact detection.

	SPHERE	MESH	OBSTACLE
SPHERE	OK	N/A	OK
MESH		N/A	N/A
OBSTACLE			N/A

Table 3.1: Current status of automatic contact detection.

# Chapter 4

## Input commands

PARMEC input language extends Python. Subroutines related to input processing are listed below. **In all cases below, when an object number is returned, indexing starts at 0 and increments on each call.**

### 4.1 ARGV

List command line arguments.

**list** = **ARGV** (**| nonparmec**)

- **list** - Python list (possibly empty) of command line arguments
- **nonparmec** - optional boolean flag enabling filtering out parmec arguments; default: True

### 4.2 RESET

Erase all data.

**RESET** ()

### 4.3 TSERIES

Create time series: a linear spline based on series of 2-points.

**tmsnum** = **TSERIES** (**points**)

- **tmsnum** - time series number
- **points** - a constant  $v0$ , or a list  $[t0, v0, t1, v1, \dots]$  or  $[[t0, v0], [t1, v1], \dots]$  or  $[(t0, v0), (t1, v1), \dots]$  of points (where  $t_i < t_j$ , when  $i < j$ ), or a path to a file storing pairs of times and values in format:

```
# comment 1 ...
# comment 2 ...
t0 v0
t1 v1
# comment 3 ...
```

```
t2 v2
...
```

## 4.4 MATERIAL

Create material.

**matnum** = MATERIAL (density, young, poisson)

- **matnum** - material number
- **density** - mass density
- **young** - Young modulus
- **poisson** - Poisson ratio

## 4.5 SPHERE

Create a spherical particle.

**parnum** = SPHERE (center, radius, material, color)

- **parnum** - particle number
- **center** - tuple  $(x, y, z)$  defining the center
- **radius** - radius
- **material** - material number
- **color** - positive integer surface color

## 4.6 MESH

Create a meshed particle.

**parnum** = MESH (nodes, elements, material, colors)

- **parnum** - particle number
- **nodes** - list of nodes:  $[x0, y0, z0, x1, y1, z1, \dots]$
- **elements** - list of elements:  $[e1, n1, n2, \dots, ne1, me1, e2, n1, n2, \dots, ne2, me2, \dots]$ , where  $e1$  is the number of nodes of the first element,  $n1, n2, \dots, ne1$  enumerate the element nodes, and  $me1$  is the material number. Similarly for the second and all remaining elements. Supported numbers of nodes per element are 4, 5, 6, and 8 for respectively *tetrahedron*, *pyramid*, *wedge*, and *hexahedron*, cf. Figure 4.1.
- **material** - material number
- **colors** - list of positive integer face colors:  $[gcolor, f1, n1, n2, \dots, nf1, c1, f2, n1, n2, \dots, nf2, c2, \dots]$ , where  $gcolor$  is the global color for all not specified faces,  $f1$  is the number of nodes in the first specified face,  $n1, n2, \dots, nf1$  enumerate the face nodes, and  $c1$  is the surface color of that face. Similarly for the second and all remaining faces. If only the global color is required, it can be passed as  $[gcolor]$  or as  $gcolor$  alone.

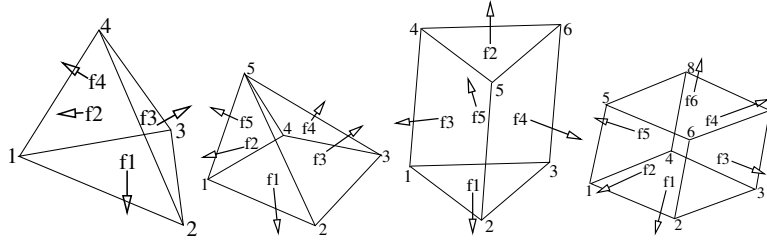


Figure 4.1: Mesh element types in Parmec.

## 4.7 ANALYTICAL

Create an analytical particle. Analytical particles have no shapes and are not involved in contact.

**parnum** = ANALYTICAL ( | inertia, mass, rotation, position, material, particle)

Note, that all parameters are optional.

- **parnum** - particle number
- **inertia** - inertia tensor passed as a list  $[Ixx, Iyy, Izz, Ixy, Ixz, Iyz]$ ; optional, if **particle** parameter is used; default  $[1, 1, 1, 0, 0, 0]$
- **mass** - scalar mass; optional, if **particle** parameter is used; default 1
- **rotation** - optional orientation matrix passed as a list  $[e1x, e1y, e1z, e2x, e2y, e2z, e3x, e3y, e3z]$ , where vectors  $e1, e2, e3$  are orthonormal; default  $[1, 0, 0, 0, 1, 0, 0, 0, 1]$
- **position** - optional position vector passed as a tuple  $(x, y, z)$ ; default  $(0, 0, 0)$
- **material** - material number; default 0
- **particle** - optional; if specified, an existing particle is converted into an analytical particle; its properties are inherited or overwritten, depending on whether any of the **inertia**, **mass**, **rotation**, **position** parameters are used; if initially specified, particle shape is inherited and its animated motion is included into the results

## 4.8 OBSTACLE

Create an obstacle.

**OBSTACLE** (triangles, color | point, linear, angular)

- **triangles** - list of triangle tuples  $[(t1x1, t1y1, t1z1, t1x2, t1y2, t1z2, t1x3, t1y3, t1z3), (t2x1, t2y1, t2z1, t2x2, t2y2, t2z2, t2x3, t2y3, t2z3), \dots]$  defining the obstacle
- **color** - positive integer surface color or a list  $[color1, color2, \dots]$  of colors for each individual triangle
- **point** - spatial reference point
- **linear** - linear velocity history callback:  $(v_x, v_y, v_z) = \mathbf{linear}(t)$
- **angular** - spatial angular velocity history callback:  $(\omega_x, \omega_y, \omega_z) = \mathbf{angular}(t)$



## 4.9 SPRING

Create a translational spring constraint. The applied force formula reads

$$\text{force}(t) = \text{direction}(t) \cdot [\text{spring}(\text{stroke}(t)) + \text{dashpot}(\text{velocity}(t)) \cdot |\text{sign}(\text{spring}(\text{stroke}(t)))|]$$

where

$$\text{direction}(t) = (\text{point2}(t) - \text{point1}(t)) / |\text{point2}(t) - \text{point1}(t)| \text{ or } \text{constant}(d_x, d_y, d_z) \text{ or } \text{tangent}$$

$$\text{stroke}(t) = \text{direction}(t) \cdot [\text{point2}(t) - \text{point1}(t)] - \text{direction}(0) \cdot [\text{point2}(0) - \text{point1}(0)]$$

$$\text{velocity}(t) = \text{direction}(t) \cdot \frac{d}{dt} [\text{point2}(t) - \text{point1}(t)]$$

$$\text{sign}(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$

The spring (stroke) and dashpot (velocity) relationships are defined by means of lookup tables; force (t) is applied at point2 (t), and  $-\text{force}(t)$  is applied at point1 (t); dashpot force is not applied when spring force is zero.

**sprnum = SPRING (part1, point1, part2, point2, spring | dashpot, direction, planar, unload, ylim)**

- **sprnum** - spring number
- **part1** - first particle number
- **point1** - tuple (x, y, z) defining a point moving with the first particle
- **part2** - second particle number;  $-1$  can be used to indicate a single-particle constraint
- **point2** - tuple (x, y, z) defining a second point, either moving with the second particle, or a spatial point
- **spring** - spring force lookup table [stroke<sub>1</sub>, force<sub>1</sub>, stroke<sub>2</sub>, force<sub>2</sub>, ..., stroke<sub>n</sub>, force<sub>n</sub>]; used for both loading and unloading when the **unload** table and the **yield** limits are not given
- **dashpot** - optional dashpot force lookup table [velocity<sub>1</sub>, force<sub>1</sub>, velocity<sub>2</sub>, force<sub>2</sub>, ..., velocity<sub>m</sub>, force<sub>m</sub>]; default:  $[-\infty, 0, +\infty, 0]$
- **direction** - optional constant direction (d<sub>x</sub>, d<sub>y</sub>, d<sub>z</sub>)
- **planar** - optional planar spring flag; when 'ON' spring direction

$$(\text{point2}(t) - \text{point1}(t)) / |\text{point2}(t) - \text{point1}(t)|$$

is projected onto a plane orthogonal to (d<sub>x</sub>, d<sub>y</sub>, d<sub>z</sub>); default: 'OFF'

- **unload** - spring unloading lookup table [stroke<sub>1</sub>, force<sub>1</sub>, stroke<sub>2</sub>, force<sub>2</sub>, ..., stroke<sub>n</sub>, force<sub>n</sub>]; must be monotonically increasing
- **ylim** - tuple (f<sub>yc</sub>, f<sub>yt</sub>) defining the compression, f<sub>yc</sub> < 0, and tension, f<sub>yt</sub> > 0, yield limits; the unloading curve begins to be used once either of these limits is crossed; default: (0, 0)

## 4.10 UNSPRING (under development)

**UNSPRING** (**tsprings**, **msprings**, **limits** | **entity**, **operator**, **abs**, **nsteps**, **nfreq**, **unload**)

Undoes user defined selection of springs (**msprings**) based on the value of spring entities experienced by a different user defined selection of springs (**tsprings**). Modifications to the spring curves occur during a simulation. Undone springs remain in the simulation but generate zero forces.

- **tsprings** - list of unique spring numbers whose spring entities are assessed against a criteria defined by **limits**; must be nonempty
- **msprings** - list of unique spring numbers which are to be modified if **tsprings** meet the **limits** criteria (springs defined in **tsprings** are not modified unless also specified in **msprings**); must be nonempty
- **limits** - tuple of (min, max) **tsprings** **operator** **entity** limit values which need to be exceeded for **msprings** to be modified; if either value is *None* then no failure limit is assumed e.g. (*None*, max) only has an upper failure limit; also min < max
- **entity** - scalar spring entity string: (spring stroke) 'STROKE', (spring total force) 'STF', (spring force without damping) 'SF', cf. 4.18 and 4.19; default: 'SF'
- **operator** - collective **tsprings** operator string: 'SUM', 'MIN', 'MAX'; default: 'SUM'
- **abs** - boolean, if *True* then spring forces are converted to absolute values before summation of the spring forces; default: *False*
- **nsteps** - int, number of time steps between calls of UNSPRING; default: 1
- **nfreq** - int, number of **nsteps** for which **tsprings** exceed **limits** before **msprings** are modified; default: 1
- **unload** - Python dictionary (i.e. **unload**[*key*] = *value*), where *key* (int) - unique spring number (must be present in **msprings**) and *value* (int) - time series number (TSERIES) defining the unload spring curve; an unloading curve must originate at zero and increase monotonically; once modification is activated, for each spring in **msprings**, the unloading curve is individually applied with a shift specific to the current displacement; both negative and positive displacement increments decrease total spring forces until zero; the spring force remains zero ever after; dashpot force is zero during unloading; default: instantaneous unloading to zero total force

By default, modification of **msprings** is based on the sum of the elastic spring force values across all spring numbers defined in **tsprings**. This is a sum of absolute values if **abs** = *True*. Forces in all **tsprings** must exceed the specific min/max values defined in **limits** for the spring curves to be modified (i.e. spring curve modification is an *and* operation, not *or*). For example:

```
tsprings = (1,2)
msprings = (3,4)
limits = (-1.0, 1.0)
UNSPRING(tsprings, msprings, limits)
```

results in the resultant elastic spring force (SF) being assessed against the (-1.0, 1.0) limits. For the spring curves of springs 3 and 4 to be modified, the sum of the forces of springs 1 and 2 must be outside of the (-1.0,1.0) limits for **nfreq** (=1) number of **nsteps** (=1).

## 4.11 GRANULAR

Define surface pairing for the granular contact interaction model.

**GRANULAR** (color1, color2, spring | damper, friction, rolling, drilling, kskn)

- **color1** - first color (positive, or color1 = 0 and color2 = 0 to redefine default parameters)
- **color2** - second color (positive, or color1 = 0 and color2 = 0 to redefine default parameters)
- **spring** - normal spring constant
- **damper** - optional normal damping ratio; default: 1.0
- **friction** - optional Coulomb's friction coefficient; default: 0.0; tuple  $(\mu_s, \mu_d)$  can be used to specify respectively static and dynamic friction coefficients; (experimental)
- **rolling** - optional rolling friction coefficient; default: 0.0; (under development)
- **drilling** - optional drilling friction coefficient; default: 0.0; (under development)
- **kskn** - optional ratio of normal to tangential spring and dashpot parameters; default: 0.5

## 4.12 RESTRAIN

Restrain particle motion.

**RESTRAIN** (parnum | linear, angular)

- **parnum** - particle number
- **linear** - list  $[x_1, y_1, z_1]$ ,  $[x_1, y_1, z_1, x_2, y_2, z_2]$ , or  $[x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3]$  defining directions of restrained linear motion; default:  $[0, 0, 0]$
- **angular** - list  $[x_1, y_1, z_1]$ ,  $[x_1, y_1, z_1, x_2, y_2, z_2]$ , or  $[x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3]$  defining directions of restrained spatial rotation; default:  $[0, 0, 0]$

## 4.13 PRESCRIBE

Prescribe particle motion. Prescribed motion overwrites this resulting from dynamics and restraints.

**PRESCRIBE** (parnum | linear, angular, kind)

- **parnum** - particle number
- **linear** - a tuple  $(i, j, k)$  of T SERIES numbers, or a callback:  $(v_x, v_y, v_z) = \mathbf{linear}(t)$ , defining linear velocity or acceleration history; default: *not prescribed*
- **angular** - a tuple  $(i, j, k)$  of T SERIES numbers, or a callback:  $(\omega_x, \omega_y, \omega_z) = \mathbf{angular}(t)$ , defining spatial angular velocity or acceleration history; default: *not prescribed*
- **kind** - string 'vv', 'va', 'av', or 'aa' indicating interpretation of respectively **linear** and **angular** time histories as either velocity or acceleration; default: 'vv'

## 4.14 VELOCITY

Set particle velocity.

### VELOCITY (parnum | linear, angular)

- **parnum** - particle number
- **linear** - linear velocity tuple  $(v_x, v_y, v_z)$ ; default:  $(0, 0, 0)$  at  $t = 0$
- **angular** - angular velocity tuple  $(\omega_x, \omega_y, \omega_z)$ ; default:  $(0, 0, 0)$  at  $t = 0$

## 4.15 GRAVITY

Set gravity.

### GRAVITY (gx, gy, gz)

- **gx** - constant  $x$  float number, or callback **gx**( $t$ ), or TSERIES number
- **gy** - constant  $y$  float number, or callback **gy**( $t$ ), or TSERIES number
- **gz** - constant  $z$  float number, or callback **gz**( $t$ ), or TSERIES number

## 4.16 DAMPING

Set global damping, applied as

$$\text{force} = -m \begin{bmatrix} -d_{vx}v_x \\ -d_{vy}v_y \\ -d_{vz}v_z \end{bmatrix}, \text{ torque} = -\mathbf{\Lambda}\mathbf{J}\mathbf{\Lambda}^T \begin{bmatrix} -d_{\omega x}\omega_x \\ -d_{\omega y}\omega_y \\ -d_{\omega z}\omega_z \end{bmatrix}$$

where  $m$  is scalar mass,  $v$  is linear velocity,  $\mathbf{\Lambda}$  is the rotation matrix,  $\mathbf{J}$  is the referential inertia matrix, and  $\omega$  is spatial angular velocity.

### DAMPING (linear, angular)

- **linear** - linear damping curve callback  $(d_{vx}, d_{vy}, d_{vz}) = \mathbf{linear}(t)$ , or a tuple  $(i, j, k)$  of TSERIES numbers
- **angular** - angular damping curve callback  $(d_{\omega x}, d_{\omega y}, d_{\omega z}) = \mathbf{angular}(t)$ , or a tuple  $(i, j, k)$  of TSERIES numbers

## 4.17 CRITICAL

Estimate critical time step.

### h = CRITICAL ()

- **h** - critical time step

## 4.18 HISTORY

Before running a simulation, request time history output.

**list = HISTORY (entity | source, point)**

- **list** - output time history list (empty upon initial request, populated during simulation)
- **entity** - entity name; global entities: (output time) 'TIME'; particle entities: (position) 'PX', 'PY', 'PZ', 'P|', (displacement) 'DX', 'DY', 'DZ', 'D|', (linear velocity) 'VX', 'VY', 'VZ', 'V|', (angular velocity) 'OX', 'OY', 'OZ', 'O|', (body force) 'FX', 'FY', 'FZ', 'F|', (body torque) 'TX', 'TY', 'TZ', 'T|'; spring entities: (spring stroke) 'STROKE', (spring total force) 'STF', (spring force without damping) 'SF';
- **source** - particle number  $i$ , or a list of particle numbers  $[i, j, \dots]$ , or a spatial sphere defined as tuple  $(x, y, z, r)$  (**under development**), or a spatial box defined as tuple  $(x_{\min}, y_{\min}, z_{\min}, x_{\max}, y_{\max}, z_{\max})$  (**under development**); in case of a list of particle numbers the output entity is averaged over the set of particles; in case of a spatial sphere or box the output entity is averaged over the set of particles passing through it (**under development**); default: 0 (useful when entity is 'TIME'); spring number or a list of numbers can be used as a source in case of spring entities
- **point** - optional referential point used in case of a single particle source; default: particle mass centre

**4.19 OUTPUT**

Before running a simulation, define scalar and/or vector entities included into the output file(s). PARMEC outputs:

- \*.dump files for spherical particles
- \*0.vtk.\* **and/or** (\*0.h5, \*0.xmf) files for obstacles and mesh based particles **not** specified as **a subset** in the OUTPUT command
- \*1.vtk.\*, \*2.vtk.\*, ... **and/or** (\*1.h5, \*1.xmf, \*2.h5, \*2.xmf, ...) files for mesh based particles specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls
- \*0rb.vtk.\* **and/or** (\*0rb.h5, \*0rb.xmf) for rigid body data of particles **not** specified as **a subset** in the OUTPUT command
- \*1rb.vtk.\*, \*2rb.vtk.\*, ... **and/or** (\*1rb.h5, \*1rb.xmf, \*2rb.h5, \*2rb.xmf, ...) files for rigid body data of particles specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls
- \*0cd.vtk.\* **and/or** (\*0cd.h5, \*0cd.xmf) for contact data including particles **not** specified as **a subset** in the OUTPUT command
- \*1cd.vtk.\*, \*2cd.vtk.\*, ... **and/or** (\*1cd.h5, \*1cd.xmf, \*2cd.h5, \*2cd.xmf, ...) files for contact data including particles specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls
- \*0sd.vtk.\* **and/or** (\*0sd.h5, \*0sd.xmf) for spring data including particles **not** specified as **a subset** in the OUTPUT command
- \*1sd.vtk.\*, \*2sd.vtk.\*, ... **and/or** (\*1sd.h5, \*1sd.xmf, \*2sd.h5, \*2sd.xmf, ...) files for spring data including particles specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls

**OUTPUT (entities | subset, mode, format)**

- **entities** - list of output entities; default: ['NUMBER', 'COLOR', 'DISPL', 'ORIENT', 'ORIENT1', 'ORIENT2', 'ORIENT3', 'LINVEL', 'ANGVEL', 'FORCE', 'TORQUE', 'F', 'FN', 'FT', 'SF', 'AREA', 'PAIR'] where:

- 'NUMBER' - scalar field of particle numbers (modes: 'SPH', 'MESH', 'RB'), or scalar field of spring numbers (modes: 'SD')
- 'COLOR' - scalar field of surface colors (modes: 'SPH', 'MESH'), or 2-component vector field of contact surface colors (modes: 'CD')
- 'DISPL' - 3-component vector field of displacements (modes: 'SPH', 'MESH', 'RB'), or scalar field of contact depths (modes: 'CD'), or scalar field of spring strokes (modes: 'SD')
- 'ORIENT' - 9-component tensor field representing rigid rotation matrix (modes: 'RB'), or 3-component vector field of spring orientations (modes: 'SD')
- 'ORIENT1', 'ORIENT2', 'ORIENT3' - three 3-component vector fields representing columns of rigid rotation matrix (orientation vectors) (modes: 'RB')
- 'LINVEL' - 3-component vector field of linear velocity (modes: 'SPH', 'MESH', 'RB')
- 'ANGVEL' - 3-component vector field of (spatially constant) angular velocity (modes: 'SPH', 'MESH', 'RB')
- 'FORCE' - 3-component vector field of (spatially constant) total body force (modes: 'SPH', 'MESH', 'RB')
- 'TORQUE' - 3-component vector field of (spatially constant) total body torque (modes: 'SPH', 'MESH', 'RB')
- 'F' - 3-component vector field of total contact forces (modes: 'CD'), or scalar field of total spring forces (modes: 'SD')
- 'FN' - 3-component vector field of normal contact forces (modes: 'CD')
- 'FT' - 3-component vector field of tangential contact forces (modes: 'CD')
- 'SF' - scalar field of spring force magnitude, without dashpot contribution (modes: 'CD', 'SD')
- 'AREA' - scalar field of contact area (modes: 'CD')
- 'PAIR' - 2-component vector field of particle pair numbers (modes: 'CD', 'SD')
- **subset** - optional particle number  $i$ , or a list of particle numbers  $[i, j, \dots]$ , to which this specification is narrowed down
- **mode** - optional output mode or list of output modes: 'SPH' for sphere output, 'MESH' for mesh output, 'RB' for rigid body output, 'CD' for contact data output, 'SD' for spring data output; default: ['SPH', 'MESH', 'RB', 'CD', 'SD']
- **format** - optional output format, e.g. 'VTK' or 'XDMF', or list ['VTK', 'XDMF'], where 'VTK' is the text based legacy VTK format, 'XDMF' is the HDF5/XML based XDMF format; default: 'XDMF'

## 4.20 DEM

Run DEM simulation.

**t = DEM (duration, step | interval, prefix, adaptive)**

- **t** - simulation runtime in seconds
- **duration** - simulation duration
- **step** - time step; initial if **adaptive** is used or constant otherwise

- **interval** - output interval (default: time step); tuple  $(dt_{\text{files}}, dt_{\text{history}})$  can be used to indicate different output frequencies of output files and time histories, respectively; callback functions or TSERIES numbers can also be used, e.g.  $dt_{\text{files}} = dt_{\text{files}}(t)$  and  $dt_{\text{history}} = \text{tmsnum}$ , prescribing variable interval frequencies, depending on current time;
- **prefix** - output file name prefix (default: input file name without the “.py” extension)
- **adaptive** - adaptive time step reduction factor; zero turns off adaptive time stepping, values  $> 0.0$  and  $\leq 1.0$  turn it on; default: 0.0 (experimental)

## Chapter 5

# Output files

(Under development)



## Chapter 6

# Output viewers

(Under development)