

SOLFEC-2.0 USER MANUAL

September 16, 2019

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Chapter 1

Installation

Clone Solfec-2.0 sources from [GitHub](https://github.com/parmes/solfec-2.0):

```
git clone https://github.com/parmes/solfec-2.0.git
```

Enter directory:

```
cd solfec-2.0
```

Edit Config.mak file variables:

```
# ISPC (http://ispc.github.io) and MPICXX compilers are assumed to be in the PATH

# Python {2 or 3} paths (Python is used to parse input files)
PYTHONINC=-I/usr/include/python2.7
PYTHONLIB=-L/usr/lib -lpython2.7

# HDF5 paths (HDF5 is used to write output files)
HDF5INC=-I/usr/include
HDF5LIB=-L/usr/lib -lhdf5 -lhdf5_hl

# Debug version
DEBUG=no
```

Compile sources:

```
make
```

Solfec-2.0 executables are:

```
solfec4 (single precision)
solfec8 (double precision)
```

To update the executables type:

```
make clean
git pull
make
```

Chapter 2

Running

Solfec-2.0 is a command line program utilizing MPI runtime environment and shared memory parallelism. For optimum performance, for an input model and a hardware platform at hand, you may want to test which degree of MPI parallelism per cluster node results in shortest runtimes. Typical usage:

1. Include solfec-2.0 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 3 documents all input commands.
4. Run Solfec-2.0 (e.g. `mpirun -np N solfec4 path/to/test/test.py`, or `mpirun -np N solfec8 path/to/test/test.py`, or use a batch script).
5. Time histories can be generated during analysis using the HISTORY command; see Section 3.12.
6. Upon termination output files are created in the same directory (e.g. `path/to/test/test.h5`, `path/to/test/test.xmlf`); see Section 3.13 and Chapter 4.

2.1 Version string

Running Solfec-2.0 without parameters, e.g.

```
./solfec4
```

results in the hint

```
VERSION: 2.4a49378 (2019-07-10)
SYNOPSIS: [mpirun -np N] solfec4 path/to/input/file.py
```

The version string has syntax “2.” (denoting Solfec-2.0’s primary version number) followed by a shorthand hexadecimal number (“4a49378” in this case) of a [GitHub commit](#) that most recently modified Solfec-2.0’s source code. This is followed by the date of that most recent modification of the source code.

Chapter 3

Input commands

Solfec-2.0 input language extends [Python](#) by subroutines listed below. In all cases, when an object number is returned, **indexing starts at 0** and increments on each call. Only **rank 0** MPI process reads the input file.

3.1 ARGV

List command line arguments.

list = **ARGV** (| **nonsolfec**)

- **list** - Python list (possibly empty) of command line arguments
- **nonsolfec** - optional boolean flag enabling filtering out Solfec-2.0 arguments; default: True

3.2 RESET

Erase all data.

RESET (| **outname**)

- **outname** - optional output file name (default: input file name without the “.py” extension); output name can include sub-directories, e.g. ‘an/alternative/path’ will result in output files ‘an/alternative/path.xmlf’ and ‘an/alternative/path.h5’ (relative to whence Solfec-2.0 was run) when XDMF output is used (see the OUTPUT command)

3.3 SPLINE

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

splnum = **SPLINE** (**points** | **cache**)

- **splnum** - spline number
- **points** - a list $[x0, y0, x1, y1, \dots]$ or $[[x0,y0], [x1,y1], \dots]$ or $[(x0,y0), (x1,y1), \dots]$ of points (where $t_i < t_j$, when $i < j$), or a path to a file storing pairs of (x, y) s in format:

```
# comment 1 ...
# comment 2 ...
x0 y0
x1 y1
# comment 3 ...
x2 y2
...
```

- **cache** - optional partial cache size; if **points** = file path and **cache** > 0 then only the cache size of points is stored in memory at any given time; this helps to save memory in case of a need for many large spline objects; default: 0 (entire spline is stored in memory)

3.4 MATERIAL

Create material.

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

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

3.5 MESH

Create a meshed body.

bodnum = MESH (nodes, elements, matnum, colors | transform)

- **bodnum** - body 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*, see Figure 3.1.
- **matnum** - 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.

- **transform** - optional transformation tuple, or a list of transformation tuples, e.g. [translate1, rotate1, translate2, scale2, rotate2, ...], where $\text{translate} = (tx, ty, tz)$; $\text{rotate} = (px, py, pz, ax, ay, az, angle)$, where px, py, pz define the point and ax, ay, az define the direction of the rotation axis while $angle$ defines the angle of rotation, or alternatively $\text{rotate} = (r_{11}, r_{21}, r_{31}, r_{12}, r_{22}, r_{32}, r_{13}, r_{23}, r_{33})$ is the rotation matrix (orthogonality is not checked, hence this matrix can be used for more general transformations); $\text{scale} = (px, py, pz, factor)$, where px, py, pz define the scaling centre point and $factor$ is the scaling factor; transformations are applied in the list order; default: *not specified*

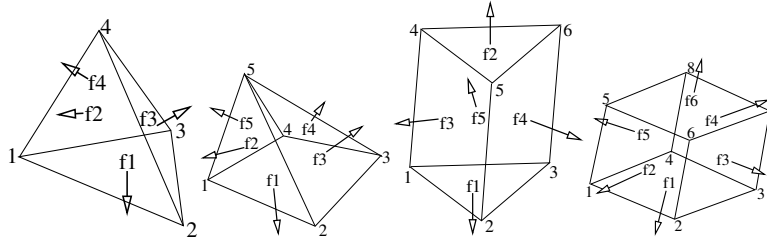


Figure 3.1: Mesh element types in Solfec-2.0.

3.6 ELLIP

Create a deformable ellipsoidal body.

bodnum = ELLIP (center, radius, matnum, color | rotate)

- **bodnum** - body number
- **center** - referential point (cx, cy, cz)
- **radius** - radius vector (rx, ry, rz)
- **matnum** - material number
- **color** - positive surface color
- **rotate** - optional transformation; $\text{rotate} = (px, py, pz, ax, ay, az, angle)$, where px, py, pz define the point and ax, ay, az define the direction of the rotation axis while $angle$ defines the angle of rotation, or alternatively $\text{rotate} = (r_{11}, r_{21}, r_{31}, r_{12}, r_{22}, r_{32}, r_{13}, r_{23}, r_{33})$ is the rotation matrix (orthogonality is not checked, hence this matrix can be used for more general transformations); default: *not specified*

3.7 RESTRAIN

Restrain body point or surface motion.

resnum = RESTRAIN (bodnum | point, color, direction)

- **resnum** - restraint number
- **bodnum** - body number
- **point** - optional referential point (px, py, pz) or list of points $[point1, point2, point3, ...]$; default: *not specified*

- **color** - optional surface color; default: *not specified*
- **direction** - optional direction (dx, dy, dz) ; default: *not specified*

3.8 PRESCRIBE

Prescribe body, point, or surface motion. Prescribed motion overwrites this resulting from dynamics and restraints.

prenum = PRESCRIBE (bodnum | point, color, linear, angular)

- **prenum** - prescribed motion number
- **bodnum** - body number
- **point** - optional referential point (px, py, pz) or list of points $[point1, point2, point3, \dots]$; default: *not specified*
- **color** - optional surface color; default: *not specified*
- **linear** - a tuple (i, j, k) of SPLINE numbers or floating point constant values, or a callback: $(v_x, v_y, v_z) = \text{linear}(t)$, defining linear velocity history; default: *not prescribed*
- **angular** - a tuple (i, j, k) of SPLINE numbers or floating point constant values, or a callback: $(\omega_x, \omega_y, \omega_z) = \text{angular}(t)$, defining spatial angular velocity history with respect to the entity (body or surface) mass center; default: *not prescribed*

3.9 VELOCITY

Set body velocity. The set of prescribed velocities is emptied upon each invocation of the RUN command. Multiple applications to one body are summed up.

VELOCITY (bodnum | linear, angular)

- **bodnum** - body number
- **linear** - linear velocity tuple (v_x, v_y, v_z) ; default: $(0, 0, 0)$ at $t = 0$
- **angular** - angular velocity tuple $(\omega_x, \omega_y, \omega_z)$, applied with respect to the referential mass center; default: $(0, 0, 0)$ at $t = 0$

3.10 FRICTION

Define surface pairing contact friction. Default values, for unspecified pairings, are: **static** = 0, **dynamic** = 0.

FRICTION (color1, color2 | static, dynamic)

- **color1** - first color (positive, or color1 = 0 and color2 = 0 to redefine default parameters for unspecified pairings)
- **color2** - second color (positive, or color1 = 0 and color2 = 0 to redefine default parameters for unspecified pairings)
- **static** - optional static Coulomb's friction coefficient; default: 0.0
- **dynamic** - optional dynamic Coulomb's friction coefficient; default: 0.0

3.11 GRAVITY

Set gravity.

GRAVITY (**gx**, **gy**, **gz**)

- **gx** - constant x float number, or callback $\mathbf{gx}(t)$, or SPLINE number
- **gy** - constant y float number, or callback $\mathbf{gy}(t)$, or SPLINE number
- **gz** - constant z float number, or callback $\mathbf{gz}(t)$, or SPLINE number

3.12 HISTORY

Before running a simulation, request time history output; or read history from an existing output file.

list = HISTORY (**entity** | **point**, **bodnum**, **filepath**)

- **list** - output time history list (empty upon initial request, populated during simulation)
- **entity** - entity name; global entities: (output time) 'TIME', (number of contacts) 'CONTACTS'; body entities: (position) 'PX', 'PY', 'PZ', '|P|', (displacement) 'DX', 'DY', 'DZ', '|D|', (linear velocity) 'VX', 'VY', 'VZ', '|V|', (Cauchy stress) 'SX', 'SY', 'SZ', 'SXY', 'SXZ', 'SYZ', '|S|' (von Mises norm);
- **point** - optional referential point (px, py, pz) or list of points [$point1$, $point2$, $point3$, ...] (in this case values are averaged over this set); default: *not specified*
- **bodnum** - body number; default: *not specified*
- **filepath** - optional file path to store the history in a text file; default: *not specified*

3.13 OUTPUT

Before running a simulation, define scalar and/or vector entities included into the output file(s). Solfec-2.0 outputs:

- *0.h5, *0.xmf files for bulk meshes of bodies **not** specified as **a subset** in the OUTPUT command
- *1.h5, *1.xmf, *2.h5, *2.xmf, ... files for bulk meshes of bodies specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls
- *0sf.h5, *0sf.xmf files for surface meshes of bodies **not** specified as **a subset** in the OUTPUT command
- *1sf.h5, *1sf.xmf, *2sf.h5, *2sf.xmf, ... files for surface meshes of bodies specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls
- *0cd.h5, *0cd.xmf files for contact data including bodies **not** specified as **a subset** in the OUTPUT command
- *1cd.h5, *1cd.xmf, *2cd.h5, *2cd.xmf, ... files for contact data including bodies specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls
- *0el.h5, *0el.xmf files for ellipsoidal particles including bodies **not** specified as **a subset** in the OUTPUT command
- *1el.h5, *1el.xmf, *2el.h5, *2el.xmf, ... files for ellipsoidal particles including bodies specified as subsets, where numbers 1, 2, ... match consecutive OUTPUT calls

OUTPUT (| entities, subset, modes)

- **entities** - list of output entities; default: ['NUMBER', 'COLOR', 'DISPL', 'LINVEL', 'STRESS', 'CF', 'CFN', 'CFT', 'AREA', 'BPAIR', 'CPAIR'] where:
 - 'NUMBER' - scalar field of body numbers (modes: 'MESH', 'SURF', 'EL')
 - 'COLOR' - scalar field of surface colors (modes: 'SURF', 'EL')
 - 'DISPL' - 3-component vector field of displacements (modes: 'MESH', 'SURF', 'EL')
 - 'LINVEL' - 3-component vector field of linear velocity (modes: 'MESH', 'SURF', 'EL')
 - 'STRESS' - 6-component tensor field representing Cauchy stress (modes: 'MESH', 'SURF', 'EL')
 - 'CF' - 3-component vector field of total contact forces (modes: 'CD')
 - 'CFN' - 3-component vector field of normal contact forces (modes: 'CD')
 - 'CFT' - 3-component vector field of tangential contact forces (modes: 'CD')
 - 'AREA' - scalar field of contact area (modes: 'CD')
 - 'BPAIR' - 2-component vector field of body pair numbers (modes: 'CD')
 - 'CPAIR' - 2-component vector field of color pair numbers (modes: 'CD')
- **subset** - optional body number i , or a list of body numbers $[i, j, \dots]$, to which this specification is narrowed down
- **modes** - optional output mode or list of output modes: 'MESH' for bulk mesh output, 'SURF' for surface mesh output, 'EL' for ellipsoid output, 'CD' for contact data output, ; default: ['MESH', 'EL', 'CD']

3.14 RUN

Run simulation.

t = RUN (duration, step | interval)

- **t** - simulation runtime in seconds
- **duration** - simulation duration; 0 can be used to output the initial model state
- **step** - simulation time step
- **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 SPLINE numbers can also be used, e.g. $dt_{\text{files}} = dt_fies(t)$ and $dt_{\text{history}} = splnum$, prescribing variable interval frequencies, depending on current time;

3.15 DELETE

Delete an object from simulation.

DELETE (objnum, objkind)

- **objnum** - object number
- **objkind** - object kind; one of: 'MESH', 'ELLIP', 'RESTRAIN', 'PRESCRIBE'

Chapter 4

Post-processing

The *.xmf HDF5/XML based [XDMF output format](#) can be viewed with [ParaView](#) and [VisIt](#). Sections below provide examples of using both softwares to visualize Solfec-2.0 results.

4.1 ParaView session viewing meshes

4.2 ParaView session viewing ellipsoidal particles

4.3 VisIt session viewing meshes

4.4 VisIt session viewing ellipsoidal particles

Chapter 5

Debug printing

For debugging purposes, the following Python commands are additionally defined:

<code>print _SPLINE(splnum)</code>
<code>print _MATERIAL(matnum)</code>
<code>print _MESH(bodnum)</code>
<code>print _ELLIP(bodnum)</code>
<code>print _RESTRAIN(resnum)</code>
<code>print _PRESCRIBE(prenum)</code>
<code>print _VELOCITIES()</code>
<code>print _FRICTIONS()</code>
<code>print _GRAVITY()</code>
<code>print _HISTORIES()</code>
<code>print _OUTPUTS()</code>

These commands print, to standard output, formatted definitions of the corresponding input data.

Chapter 6

Tests

Solfec-2.0 includes Python based self-consistency tests, located in `solfec-2.0/tests` directory. These can be invoked by typing:

```
make test
```

Tests can be extended by adding two files per test, as illustrated in Figures 6.1 and 6.1. The `output0` variable in Figure 6.2 contains the expected standard output of running:

```
../solfec4 material.py
```

from within the tests directory.

```
# Solfec-2.0 input command test: MATERIAL
matnum = MATERIAL (1E3, 1E9, 0.25, 0.0)
print_MATERIAL(matnum)
```

Figure 6.1: Test file 1: `solfec-2.0/tests/material.py`

```
# Solfec-2.0 unit test: MATERIAL input command
import unittest, os
output0 = \
'''MATERIAL_0_density = 1000
MATERIAL_0_young = 1e+09
MATERIAL_0_poisson = 0.25
MATERIAL_0_viscosity = 0
'''
class test(unittest.TestCase):
    def test(self):
        solfec = os.popen('../solfec4 material.py')
        output = solfec.read()
        solfec.close()
        self.assertEqual(output, output0)
```

Figure 6.2: Test file 2: `solfec-2.0/tests/test_material.py`