SOLFEC-2.0 USER MANUAL

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Contents

Chapter 1

Installation

Clone Solfec-2.0 sources from GitHub:

```
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.xmf*); 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.xmf' 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, ...]* or *[[x0,y0], [x1,y1], ...]* or *[(x0,y0), (x1,y1), ...]* of points (where $ti < tj$, 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, ...*]
- **elements** - list of elements: [*e1, n1, n2, ..., ne1, me1, e2, n1, n2, ..., ne2, me2, ...*], where *e1* is the number of nodes of the first element, *n1, n2, ..., 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, ..., nf1, c1, f2, n1, n2, ..., nf2, c2, ...*], where *gcolor* is the global color for all not specified faces, *f1* is the number of nodes in the first specified face, *n1, n2, ..., 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 translate = (tx, ty, tz); 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 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); scale = $(px, py, px, factor)$, 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*

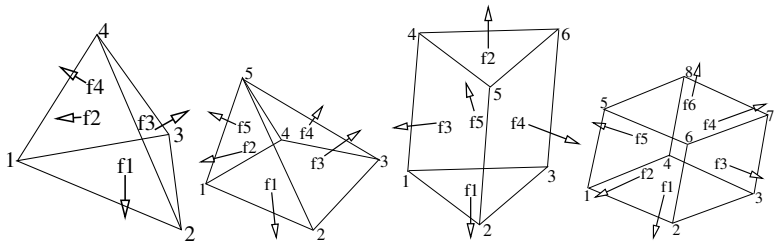

Figure 3.1: Mesh element types in Solfec-2.0.

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; 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 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 specifiedA*
- **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, ...]*; 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) = **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: $(\omega_x, \omega_y, \omega_z)$ = **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, ...*], 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 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. $dt_{\text{files}} = \text{dt\_fiels}\,(t)$ and $dt_{\text{history}} = \text{splnum}$, 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:

print_SPLINE(splnum)
print_MATERIAL(matnum)
print_MESH(bodnum)
print_ELLIP(bodnum)
print_RESTRAIN(resnum)
print_PRESCRIBE(prenum)
print_VELOCITIES()
print_FRICTIONS()
print_GRAVITY()
print_HISTORIES()
print_OUTPUTS()

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`