Solfec User Manual

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Chapter 1

Introduction

Solfec is a computational code aimed at simulation of multi-body systems with constraints. It implements an instance of the Contact Dynamics (CD) method by Moreau [13] and Jean [7], hence the constraints are handled implicitly. One of the main goals of the software is to provide a user friendly platform for testing formulations and solution methods for the (dynamic) frictional contact problem. It is also meant to serve as a development platform for other aspects of time-stepping methods (e.g. contact detection, time integration). The code implements several kinematic models (rigid, pseudo-rigid, finite element), few contact detection algorithms, several time integrators and a couple of constraint solvers (e.g. penalty, Gauss-Seidel). A distributed memory and a serial versions of the code are available. Solfec is an open-source software and can be downloaded from http://code.google.com/p/solfec.

Basics

It will be useful to introduce some basic notions here. Let us have a look at a figure below



There are four bodies in the figure. Placement of each point of every body is determined by a configuration \mathbf{q}_i . Velocity of each point of every body is determined by a velocity \mathbf{u}_i . Let \mathbf{q} and \mathbf{u} collect configurations and velocities of all bodies. If the time history of velocity is known, the configuration time history can be computed as

$$\mathbf{q}(t) = \mathbf{q}(0) + \int_{0}^{t} \mathbf{u} dt \tag{1.1}$$

The velocity is determined by integrating Newton's law

$$\mathbf{u}(t) = \mathbf{u}(0) + \mathbf{M}^{-1} \int_{0}^{t} (\mathbf{f} + \mathbf{H}^{T} \mathbf{R}) dt$$
(1.2)

where \mathbf{M} is an inertia operator (assumed constant here), \mathbf{f} is an out of balance force, \mathbf{H} is a linear operator, and \mathbf{R} collects some point forces \mathbf{R}_{α} . While integrating the motion of bodies, we keep track of a number of local coordinate systems (local frames). There are four of them in the above figure. Each local frame is related to a pair of points, usually belonging to two distinct bodies. An observer embedded at a local frame calculates the local relative velocity \mathbf{U}_{α} of one of the points, viewed from the perspective of the other point. Let \mathbf{U} collect all local velocities. Then, we can find a linear transformation \mathbf{H} , such that

$$\mathbf{U} = \mathbf{H}\mathbf{u} \tag{1.3}$$

In our case local frames correspond to *constraints*. We influence the local relative velocities by applying local forces \mathbf{R}_{α} . This can be collectively described by an implicit relation

$$\mathbf{C}\left(\mathbf{U},\mathbf{R}\right) = \mathbf{0}\tag{1.4}$$

Hence, in order to integrate equations (1.1) and (1.2), at every instant of time we need to solve the implicit relation (1.4). Here is an example of a numerical approximation of such procedure

$$\mathbf{q}^{t+\frac{h}{2}} = \mathbf{q}^t + \frac{h}{2}\mathbf{u}^t \tag{1.5}$$

$$\mathbf{u}^{t+h} = \mathbf{u}^t + \mathbf{M}^{-1}h\mathbf{f}^{t+\frac{h}{2}} + \mathbf{M}^{-1}\mathbf{H}^T\mathbf{R}$$
(1.6)

$$\mathbf{q}^{t+h} = \mathbf{q}^{t+\frac{h}{2}} + \frac{h}{2}\mathbf{u}^{t+h} \tag{1.7}$$

where h is a discrete time step. As the time step h does not appear by $\mathbf{M}^{-1}\mathbf{H}^{T}\mathbf{R}$, \mathbf{R} should now be interpreted as an impulse (an *integral* of reactions over [t, t+h]). At a start we have

$$\mathbf{q}^0$$
 and \mathbf{u}^0 as prescribed initial conditions. (1.8)

The out of balance force

$$\mathbf{f}^{t+\frac{h}{2}} = \mathbf{f}\left(\mathbf{q}^{t+\frac{h}{2}}, t + \frac{h}{2}\right) \tag{1.9}$$

incorporates both internal and external forces. The symmetric and positive-definite inertia operator

$$\mathbf{M} = \mathbf{M} \left(\mathbf{q}^0 \right) \tag{1.10}$$

is computed once. The linear operator

$$\mathbf{H} = \mathbf{H} \left(\mathbf{q}^{t + \frac{h}{2}} \right) \tag{1.11}$$

is computed at every time step. The number of rows of ${\bf H}$ depends on the number of constraints, while its rank is related to their linear independence. We then compute

$$\mathbf{B} = \mathbf{H} \left(\mathbf{u}^t + \mathbf{M}^{-1} h \mathbf{f}^{t + \frac{h}{2}} \right) \tag{1.12}$$

and

$$\mathbf{W} = \mathbf{H}\mathbf{M}^{-1}\mathbf{H}^{T} \tag{1.13}$$

which is symmetric and semi-positive definite. The linear transformation

$$\mathbf{U} = \mathbf{B} + \mathbf{WR} \tag{1.14}$$

maps constraint reactions **R** into local relative velocities $\mathbf{U} = \mathbf{H}\mathbf{u}^{t+h}$ at time t+h. Relation (1.14) will be here referred to as the *local dynamics*. Finally

$$\mathbf{R}$$
 is such that $\mathbf{C}(\mathbf{U}, \mathbf{R}) = \mathbf{C}(\mathbf{B} + \mathbf{W}\mathbf{R}, \mathbf{R}) = \mathbf{C}(\mathbf{R}) = \mathbf{0}$ (1.15)

where \mathbf{C} is a nonlinear and usually nonsmooth operator. A basic Contact Dynamics algorithm can be summarised as follows:

- 1. Perform first half-step $\mathbf{q}^{t+\frac{h}{2}} = \mathbf{q}^t + \frac{h}{2}\mathbf{u}^t$.
- 2. Update existing constraints and detect new contact points.
- 3. Compute W, B.
- 4. Solve $C(\mathbf{R}) = \mathbf{0}$.
- 5. Update velocity $\mathbf{u}^{t+h} = \mathbf{u}^t + \mathbf{M}^{-1}h\mathbf{f}^{t+\frac{h}{2}} + \mathbf{M}^{-1}\mathbf{H}^T\mathbf{R}$.
- 6. Perform second half-step $\mathbf{q}^{t+h} = \mathbf{q}^{t+\frac{h}{2}} + \frac{h}{2}\mathbf{u}^{t+h}$.

It should be stressed that the above presentation exemplifies only a particular instance of Contact Dynamics. Let us refer the reader to [12, 14, 3, 13, 7, 6, 1, 11, 15, 9] for more details.

Chapter 2

Installation

Although there will be perpetual releases of Solfec with some fixed version numbers, it is best to use the most recent development version of the code. This is because Solfec is in an active "beta" stage of development for the moment. In order to download the most recent sources, you first need to install *Mercurial*. Have a look at http://mercurial.selenic.com/ for instructions. Once the hg command is available on your command line, type

```
hg clone https://solfec.googlecode.com/hg/ solfec
```

This will create the directory solfec in your current directory. The next thing you need is an ANSI C development environment at your command line. Users of UNIX-like systems (Linux, FreeBSD, Mac OS X, etc.) are in privileged position here. Windows users can cope by installing Cygwin from http://www.cygwin.com/ or Mingw from http://www.mingw.org/.

Solfec is written in C and it uses a simple makefile to get compiled. The file solfec/Config.mak needs to be modified on a new machine so that to set up library paths and compilation flags. Let us have a look at the file solfec/Config.mak

```
#
# Operating System (WIN32, SOLARIS, LINUX, AIX, IRIX, OSX)
#
OS = OSX
#
# Specify C compiler here
#
CCC = cc
#
# Specify C++ compiler
#
CXX = g++
#
# Specify FORTRAN95 compiler and FORTRAN runtime library
#
FC = g95
FCLIB = -L/opt/local/lib/g95/i386-apple-darwin9/4.0.4/ -lf95
#
# Debug or optimized version switch (yes/no)
#
DEBUG = yes
PROFILE = no
```

```
MEMDEBUG = no
GEOMDEBUG = no
PARDEBUG = no
NOTHROW = no
# TIMERS (enable/disable detailed solver timings)
TIMERS = yes
# POSIX
POSIX = yes
# XDR
XDR = no
XDRINC =
XDRLIB =
# BLAS
BLAS = -L/usr/lib - lblas
# LAPACK
LAPACK = -L/usr/lib -llapack
# Python
PYTHON = -I/usr/include/python2.5
PYTHONLIB = -L/usr/lib -lpython2.5
# OpenGL (yes/no)
OPENGL = yes
GLINC =
{\tt GLLIB = -framework \ GLUT - framework \ OpenGL}
# VBO (OPENGL == yes)
VBO = yes
# MPI (yes/no)
MPI = yes
MPICC = mpicc
# Zoltan (MPI == yes)
ZOLTANINC = -I/Users/tomek/Devel/lib/zoltan/include
ZOLTANLIB = -L/Users/tomek/Devel/lib/zoltan/lib -lzoltan
```

The above configuration works on Mac OS X. Examples for Linux and Cygwin can be found in solfec/cfg. What you need is:

- C, C++, FORTRAN 95 compilers
- XDR (standard part of RPC on all Unix-like systems; on MinGW you will need PortableXDR version 4.9.1 with this patch)
- BLAS and LAPACK libraries (standard on most systems; available from http://www.netlib.org/lapack/)
- Python together with development files and libraries
- OpenGL libraries and developments files
- VBO (Vertex Buffer Object extension of OpenGL for faster rendering; optional)
- MPI libraries and development files
- Zoltan load balancing library

All of them, but Zoltan, should be already installed on your system or are quite easy to install otherwise. Zoltan on the other hand can be obtained from http://www.cs.sandia.gov/Zoltan/. In case of troubles - use the Solfec mailing list at http://groups.google.com/group/solfec.

Use "DEBUG = yes" most of the time (this is slower but outputs more information in case you would encounter a bug), but for "proper computations" compile optimized code by selecting "DEBUG = no". After you edit the Config.mak file, the first compilation should look like

```
cd solfec make all
```

This will create files solfec/solfec and solec/solfec-mpi, that is the serial and the parallel versions of the code. For every subsequent code update and compilation you will like to do the following

• Back up your *Config.mak* file. For example

```
cd solfec
cp Config.mak ..
```

• Now update the sources

```
hg pull
hg update -C
```

• Recover your Config.mak file

```
cp ../Congig.mak ./
```

• And finally compile again

```
make clean make all
```

The solfec/inp directory contains example input files. If you haven't used the "POSIX = yes" flag, you will need to create all output directories yourself. Normally though this should be done automatically. If you wish to move solfec, solfec-mpi and the input files to some other directory - you need to do it by hand. I recommend setting the PATH variable so that the solfec directory is included. This way some computations not related to development can be done "outside".

Chapter 3

Running Solfec

Solfec is a command line program. It can be run sequentially (command: solfec) or in parallel using the MPI runtime environment (command: solfec-mpi). Running it without parameters

```
./solfec
```

results in the hint

```
SYNOPSIS: solfec [-v] [-w] [-f] [-g WIDTHxHEIGHT] [-s sub-directory] path
```

The -v switch opens the interactive graphical viewer (cf. Figure 3.1). In this mode the user can view the geometrical mode, run or step through analysis, and view results. The right mouse click on the viewer window expands the menu. The -w switch forces the computation (write) mode: if some results are present, they will be overwritten. The -f switch, together with -v, opens the viewer in the wire-frame mode, which requires substantially less memory and can be used to visualize large models. The -g switch allows to specify the initial width and height of the viewer window (512 by default). The -s switch allows to output or read the results from a sub-directory. This option is useful when one wishes to output results of similar analyses to different sub-directories of a common root directory specified when creating a SOLFEC object (cf. Section 4.1.4). For example, the bellow commands would run a parallel example and output the results into different sub-directories denoted by the number of processors involved in the analysis

```
mpirun -np 4 solfec-mpi -s 4 inp/cubes.py
mpirun -np 16 solfec-mpi -s 16 inp/cubes.py
```

Because the directory out/cubes is specified when creating the SOLFEC obejet in the inp/cubes.py input file, the above commands result in creation of two output directories: out/cubes/4 and out/cubes/16. One can then view a specific set of results by running

```
./solfec -v -s 16 inp/cubes.py
```

During a parallel run Solfec updates a file named STATE, placed in the output directory of a simulation. It contains statistics relevant to the run, including an estimated time until the end of the simulation. The output directory contains as well a copy of the input file, which makes reading results more self-contained (it is harder to mismatch input and output files this way).



Figure 3.1: Solfec viewer window.

Chapter 4

Input language

Solfec input file is essentially a Python source code. Python interpreter is embedded in Solfec. At the same time Solfec extends Python by adding a number of objects and routines. There are few general principles to remember:

- Zero based indexing is observed in routine arguments.
- Parameters after the bar | are optional. For example FUNCTION (a, b/c, d) has two optional parameters c, d.
- Passing Solfec objects to some routines *empties* them. This means that a variable, that was passed as an argument, no longer stores data. For example: let x = CREATE1 () create an object x, and let y = CREATE2 (x) create an object y, using x. If CREATE2 (x) empties x, then after the call x becomes an empty placeholder. One can use it to assign value, x = CREATE1 (), but using it as an argument, z = CREATE2 (x), will cause an abnormal termination. One can create a copy of an object by calling z = COPY (x), hence using y = CREATE2 (x) leaves x intact.

Sections below document Solfec objects and routines used for their manipulation.

4.1 Solfec objects

4.1.1 CONVEX

An object of type CONVEX is either an arbitrary convex polyhedron, or it is a collection of such polyhedrons.

obj = CONVEX (vertices, faces, volid | convex)

This routine creates a CONVEX object from a detailed input data.

- obj created CONVEX object
- vertices list of vertices: [x0, y0, z0, x1, y1, z1, ...]
- faces list of faces: [n1, v1, v2, ..., vn1, s1, n2, v1, v2, ..., vn2, s2, ...], where n1 is the number of vertices of the first face, v1, v2, ..., vn1 enumerate the vertices in the CCW order when looking from the outside, and s1 is the surface identifier of the face. Similarly for the second face and so on.
- volid volume identifier
- convex (emptied) collection of CONVEX objects appending obj

Some parameters can also be accessed as members and methods of a CONVEX object. These are

Read-only members and methods

obj.nver - number of convex vertices

obj.vertex (n) - returns a (x, y, z) tuple storing coordinates of nth vertex

obj = HULL (points, volid, surfid | convex)

This routine creates a CONVEX object as a convex hull of a point set.

- obj created CONVEX object
- **points** list of points: [x0, y0, z0, x1, y1, z1, ...]
- volid volume identifier
- surfid surface identifier common to all faces
- convex (emptied) collection of CONVEX objects appending obj

4.1.2 MESH

An object of type MESH describes an arbitrary volumetric mesh, comprising tetrahedrons, pyramids, wedges, and hexahedrons (Figure 4.1). First order elements are currently supported.



Figure 4.1: Element types in Solfec.

obj = MESH (nodes, elements, surfids)

This routine creates a MESH object from a detailed input data.

- ullet obj created MESH object
- nodes list of nodes: [x0, y0, z0, x1, y1, z1, ...]
- elements list of elements: [e1, n1, n2, ..., ne1, v1, e2, n1, n2, ..., ne2, v2, ...], where e1 is the number of nodes of the first element, n1, n2, ..., ne1 enumerate the element nodes, and v1 is the volume identifier of the element. Similarly for the second element and so on.
- surfids list of surface identifiers: [gid, f1, n1, n2, ..., nf1, s1, f2, n1, n2, ..., nf2, s2, ...], where gid is the global surface identifier for all not specified faces, f1 is the number of nodes in the first specified face, n1, n2, ..., nf1 enumerate the face nodes, and s1 is the surface identifier of the face. Similarly for other specified faces. If only the gid is given, this can be done either as [gid] or as gid alone.

Some parameters can also be accessed as members and methods of a MESH object. These are

Read-only members and methods

obj.nnod - number of mesh nodes

obj.node (n) - returns a (x, y, z) tuple storing coordinates of nth node

obj = HEX (nodes, i, j, k, volid, surfids | dx, dy, dz)

This routine creates a MESH object corresponding to a hexahedral shape (hexahedral elements are used).

- obj created MESH object
- nodes list of 8 nodes: [x0, y0, z0, x1, y1, z1, ..., x7, y7, z7]. The hexahedral shape will be stretched between those nodes using a linear interpolation.
- i, j, k numbers of subdivisions along the local x, y, z directions.
- volid volume identifier
- surfids list of six surface identifiers: [s1, s2, ..., s6], corresponding to the faces of the hexahedral shape
- dx, dy, dz lists of subdivision schemes along local x, y, z directions. By default a subdivision is uniform. When dx = [1, 1, 5, 5, 1, 1] is present, then this scheme will be normalised (actual numbers do not matter, but their ratios) and applied to the local x direction of the generated shape.

$obj = ROUGH_HEX$ (shape, i, j, k | dx, dy, dz)

This routine creates a hexahedral MESH object corresponding to a given shape. The resultant mesh properly contains the input shape and with its orientation (which is based on the inertia properties of the shape).

- obj created MESH object
- **shape** an input shape defined by a collection of CONVEX objects; a list of CONVEX objects (or their collections) [cvx1, cvx2, cvx3,] is as well accepted.
- i, j, k numbers of subdivisions along the local x, y, z directions of the principal inertia axes
- dx, dy, dz lists of subdivision schemes along local x, y, z directions. By default a subdivision is uniform. When dx = [1, 1, 5, 5, 1, 1] is present, then this scheme will be normalised (actual numbers do not matter, but their ratios) and applied to the local x direction of the generated shape.

obj = PIPE (pnt, dir, rin, thi, ndir, nrad, nthi, volid, surfids)

This routine creates a MESH object corresponding to a pipe (hexahedral elements are used).

- obj created MESH object
- pnt base point tuple (x, y, z)
- dir direction tuple (dx, dy, dz); length of the pipe equals to the length of the direction
- rin inner radius
- thi thickness
- ndir, nrad, nthi number of subdivisions along the direction, radius and thickness
- volid volume identifier
- surfids list of six surface identifiers: [s1, s2, ..., s6], corresponding to the faces of the hexahedral shape

obj = TETRAHEDRALIZE (shape, path | volume, quality, volid, surfid)

This routine creates a tetrahedral mesh. Tetgen is invoked internally, http://tetgen.berlios.de/.

- obj created MESH object
- shape an input shape can be:
 - another MESH object
 - a path (e.g. 'path/to/file.stl') to an input file supported by Tetgen (e.g. http://tetgen.berlios.de/fformats.html)
- path path to the output file that will store the mesh; when called again and this file is found the mesh will be red from the file rather than generated
- volume maximum element volume (default: not enforced)
- quality value > 1.0 indicating element quality (default: not enforced); values close to 1.0 result in better mesh quality (mesh generation may fail for small values)
- volid volume identifier (default: 0); if only possible it is inherited from the input
- surfid surface identifier (default: 0); if only possible it is inherited from the input

4.1.3 SPHERE

An object of type SPHERE is either a sphere, or it is a collections of spheres.

obj = SPHERE (center, radius, volid, surfid | sphere)

This routine creates a SPHERE object.

- obj created SPHERE object
- center tuple (x, y, z) defining the center
- radius sphere radius
- volid volume identifier
- surfid surface identifier
- sphere (emptied) collection of SPHERE objects appending obj

Some parameters can also be accessed as members of a MESH object. These are

Read-only members and methods
obj.center, obj.radius

4.1.4 **SOLFEC**

An object of type SOLFEC represents the Solfec algorithm. One can use several SOLFEC objects to run several analyses from a single input file.

obj = SOLFEC (analysis, step, output)

This routine creates a SOLFEC object.

- obj created SOLFEC object
- analysis 'DYNAMIC' or 'QUASI STATIC' analysis kind
- step initially assumed time step, regarded as an upper bound
- output defines the output directory path (Important note: if this directory exists and contains valid output data SOLFEC is created in 'READ' mode, otherwise SOLFEC is created in 'WRITE' mode)

Some parameters can also be accessed as members of a SOLFEC object. These are

Read-only members	
obj.analysis	
obj.time - current time	
obj.mode - either 'READ' or 'WRITE' as described above	
obj.constraints - list of constraints (cf. Section 4.1.12)	
obj.ncon - number of constraints	
obj.bodies - list of bodies (cf. Section 4.1.7)	
obj.nbod - number of bodies	

Read/write members
obj.step
obj.verbose - either 'ON' or 'OFF' enabling or disabling writing to standard output
(default: 'ON')

4.1.5 SURFACE MATERIAL

An object of type SURFACE_MATERIAL represents material properties on the interface between two surfaces. Surfaces identifiers were included in definitions of all geometric objects.

obj = SURFACE_MATERIAL (solfec | surf1, surf2, model, label, friction, cohesion, restitution, spring, dashpot)

This routine creates a SURFACE MATERIAL object.

- obj created SURFACE MATERIAL object
- solfec obj is created for this SOLFEC object
- surf1 first surface identifier (default: 0)
- **surf2** second surface identifier (default: 0). If **surf1** or **surf2** (or both) are not specified, a *default* surface material is being defined (one used when a specific surface pairing cannot be found for a new contact point).
- model material model name (default: 'SIGNORINI_COULOMB'), see Table 4.1 and Chapter 7
- label label string (default: 'SURFACE_MATERIAL_i', where i is incremented for each call)
- friction friction coefficient (default: 0.0)
- cohesion cohesion per unit area (default: 0.0)

Model name	Employs variables
'SIGNORINI_COULOMB'	friction, cohesion, restitution (cf. Section
	7.1.1)
'SPRING_DASHPOT'	spring, dashpot, friction, cohesion (cf.
	Section 7.1.2)

Table 4.1: Surface material models.

- restitution velocity restitution (default: 0.0)
- spring spring stiffness (default: 0.0)
- dashpot dashpot stiffness (default: 0.0)

Some parameters can also be accessed as members of a SURFACE_MATERIAL object. These are

Read-only members	
obj.surf1, obj.surf2, obj.label	
Read/write members	
obj.model,obj.friction, obj.cohesion, obj.restitution, obj.spring, obj.dashpot	

4.1.6 BULK MATERIAL

An object of type BULK MATERIAL represents material properties of a volume.

obj = BULK MATERIAL (solfec model, label, young, poisson, density)

This routine creates a BULK_MATERIAL object.

- obj created BULK MATERIAL object
- solfec obj is created for this SOLFEC object
- ullet model material model name (default: 'KIRCHHOFF'), see Table 4.2 and Chapter 7
- label label string (default: 'BULK MATERIAL i', where i is incremented for each call)
- young Young's modulus (default: 1E6)
- poisson Poisson's coefficient (default: 0.25)
- density material density (default: 1E3)

Some parameters can also be accessed as members of a BULK MATERIAL object. These are

Read-only members	
obj.model, obj.label	
Read/write members	
obi.young. obi.poisson. obi.density	

4.1.7 BODY

An object of type BODY represents a solid body.

Model name	Employs variables
'KIRCHHOFF'	young, poisson, density (cf. Section 7.2.1)

Table 4.2: Bulk material models.

obj = BODY (solfec, kind, shape, material | label, form, mesh)

This routine creates a body.

- obj created BODY object
- solfec obj is created for this SOLFEC object
- kind a string: 'RIGID', 'PSEUDO_RIGID', 'FINITE_ELEMENT' or 'OBSTACLE' describing the kinematic model
- **shape** (emptied) this is can be a CONVEX/MESH/SPHERE object, or a list [obj1, obj2, ...], where each object is of type CONVEX/MESH/SPHERE. If the **kind** is 'FINITE_ELEMENT', then two cases are possible:
 - **shape** is a single MESH object: the mesh describes both the shape and the discretisation of the motion of a body
 - shape is solely composed of CONVEX objects: here a separate mesh must be given to discretise motion of a body (see the mesh argument below)
- material a BULK_MATERIAL object or a label of a bulk material (specifies an initial body-wise material, see also the MATERIAL (...) routine in Section 4.5)
- \bullet label a label string (no label is assigned by default)
- form valid when kind equals 'FINITE_ELEMENT', ignored otherwise (default: 'TL'). This argument specifies a formulation of the finite element method. See Table 4.3.
- mesh optional when kind equals 'FINITE_ELEMENT', ignored otherwise. This variable must be a MESH object describing a finite element mesh properly containing the shape composed solely of CONVEX objects. This way the 'FINITE_ELEMENT' model allows to handle complicated shapes with less finite elements, e.g. an arbitrary shape could be contained in just one hexahedron.

Some parameters can also be accessed as members of a BODY object. These are

Read-only members		
obj.kind, obj.label		
obj.conf - tuple (q1, q2,, qN) storing configuration of the body. See Table 4.4.		
obj.velo - tuple $(u1, u2,, uN)$ storing velocity of the body. See Table 4.5.		
obj.mass - referential mass of the body		
obj.volume - referential volume of the body		
obj.center - referential mass center of the body		
obj.tensor - referential Euler (pseudo-rigid, finite element kinematics) or inertia tensor		
(rigid kinematics) of the body		
obj.constraints - list of constraints attached to the body (cf. Section 4.1.12)		
obj.ncon - number of constraints attached to the body		

Formulation	Remarks
'TL'	Total Lagrangian (default)
'BC'	Body Co-rotational (one co-rotated frame per body,
	suitable for stiff bodies)

Table 4.3: Finite element formulations

Read/write members		
obj.selfcontact - self-contact detection flag (default: 'OFF") taking values 'ON' or		
'OFF'.		
obj.nodecontact - node based contact detection flag (default: 'OFF") taking values		
'ON' or 'OFF'.		
obj.scheme - time integration scheme (default: 'DEFAULT') used to integrate motion.		
See Table 4.6.		
obj.damping - stiffness proportional damping coefficient (default: 0.0) for the dynamic		
case (ignored for rigid bodies).		

Body kind	Configuration description
'RIGID'	Column-wise rotation matrix followed by the current
	mass center.
'PSEUDO_RIGID'	Column-wise deformation gradient followed by the
	current mass center.
'FINITE_ELEMENT'	Current coordinates x, y, z of mesh nodes.
'OBSTACLE'	Python None object.

Table 4.4: Types of configurations.

Body kind	Velocity description
'RIGID'	Referential angular velocity followed by the spatial
	velocity of mass center.
'PSEUDO_RIGID'	Deformation gradient velocity followed by the spatial
	velocity of mass center.
'FINITE_ELEMENT'	Components x, y, z of spatial velocities of mesh nodes.
'OBSTACLE'	Python None object.

Table 4.5: Types of velocities.

4.1.8 TIME_SERIES

An object of type TIME_SERIES is a linear spline based on a series of 2-points.

$obj = TIME_SERIES (points)$

This routine creates a TIME_SERIES object.

- $\bullet~\mathbf{obj}$ created TIME_SERIES object
- **points** either a list [t0, v0, t1, v1,] of points (where ti < tj, when i < j), or a path to a file storing times and values pairs in format:

Scheme	Kinematics	Remarks
'DEFAULT'	all	Use a default time integrator regardless of underlying
		kinematics.
'RIG_POS'	rigid	NEW1 in [10]: explicit, positive energy drift, no
		momentum conservation
'RIG_NEG'	rigid	NEW2 in [10]: explicit, negative energy drift, exact
		momentum conservation; default for rigid kinematics
'RIG_IMP'	rigid	NEW3 in [10]: semi-explicit, no energy drift and exact
		momentum conservation
'DEF_EXP'	pseudo-rigid, finite	Explicit scheme described in Chapter 5 of [9]; default
	element	for deformable kinematics, energy and momentum
		conserving, conditionally stable
'DEF_LIM'	pseudo-rigid, finite	Linearly implicit scheme similar to [17]; energy and
	element	momentum conserving, stable for moderate steps
'DEF_LIM2'	pseudo-rigid, finite	Linearly implicit scheme similar to [5]; strong
	element	numerical dissipation, stable for large steps
'DEF_IMP'	pseudo-rigid, finite	Implicit scheme similar to [16]; energy and momentum
	element	conserving, stable for large steps

Table 4.6: Time integration schema.

t0 v0 t1 v1

4.1.9 GAUSS SEIDEL SOLVER

An object of type GAUSS_SEIDEL_SOLVER represents a nonlinear block Gauss-Seidel solver, employed for the calculation of constraint reactions (cd. Section 9.1).

obj = GAUSS_SEIDEL_SOLVER (epsilon, maxiter | meritval, failure, diagepsilon, diagmaxiter, diagsolver, data, callback)

This routine creates a GAUSS SEIDEL SOLVER object.

- \bullet \mathbf{obj} created GAUSS_SEIDEL_SOLVER object
- epsilon relative accuracy of constraint reactions sufficient for termination
- maxiter maximal number of iterations before termination
- meritval constraints satisfaction merit function value sufficient for termination (default: 1E-3), cf. Chapter 8 for more details.
- failure failure (lack of convergence) action (default: 'CONTINUE'). Available failure actions are: 'CONTINUE' (simulation is continued), 'EXIT' (simulation is stopped and Solfec exits), 'CALLBACK' (a callback function is called if it was set or otherwise the 'EXIT' scenario is executed). In all cases *obj.error* variable is set up, cf. Table 4.7.
- diagepsilon diagonal block solver relative accuracy of constraint reactions (default: min (epsilon, meritval, 1E-4) / 100)
- diagmaxiter diagonal block solver maximal number of iterations (default: max (100, maxiter / 100))

- diagsolver diagonal block solver kind (default: 'SEMISMOOTH_NEWTON'). Available diagonal solvers are 'SEMISMOOTH_NEWTON', 'PROJECTED_GRADIENT', 'DE_SAXCE_FENG', 'PROJECTED_NEWTON', cf. Chapter 9.
- data data passed to the failure callback function (if this is a tuple it will accordingly expand the parameter list of the callback routine)
- callback failure callback function of form: value = callback (obj, data), where for the returned value equal zero Solfec run is stopped

Some parameters can also be accessed as members of a GAUSS_SEIDEL_SOLVER object. These are

Read-only members	
obj.failure	
obj.error - current error code, cf. Table 4.7	
obj.iters - number of iterations during a last run of solver	
obj.rerhist - a list of relative error values for each iteration of the last run	
obj.merhist - a list of merit function values for each iteration of the last run	

Read/write members

obj.epsilon, obj.maxiter, obj.meritval, obj.diagepsilon, obj.diagmaxiter, obj.diagsolver

obj.reverse - 'ON' or 'OFF' flag switching iteration reversion modes (whether to alternate backward and forward or not, default is 'OFF')

obj.variant - variant of parallel Gauss-Seidel update (default: 'FULL'), cf. Table 4.8. Ignored in sequential mode.

obj.innerloops - number of inner Gauss-Seidel loops per one global step during a parallel run (default: 1). Ignored in sequential mode.

'OK'	No error has occurred
'DIVERGED'	Global iteration loop divergence
'DIAGONAL_DIVERGED'	Diagonal solver iteration loop divergence
'DIAGONAL_FAILED'	Failure of a diagonal solver (e.g. singularity)

Table 4.7: Error codes of GAUSS_SEIDEL_SOLVER object.

4.1.10 PENALTY_SOLVER

An object of type PENALTY_SOLVER represents a penalty based constraint solver (cf. Section 9.2). When in use, all 'SIGNORONI_COULOMB' type contact interfaces are regarded as 'SPRING_DASHPOT' ones. One should then remember about specifying the *spring* value for those.

obj = PENALTY SOLVER (| variant)

- obj created PENALTY SOLVER object
- variant 'IMPLICIT' or 'EXPLICIT' normal force computation variant (default: 'IMPLICIT')

4.1.11 NEWTON SOLVER (Under development)

Object of type NEWTON SOLVER represents a projected quasi-Newton constraints solver.

'FULL'	Full Gauss-Seidel update as in sequential case. Although the
	slowest, it works in all cases. It should be noted, that all of the
	below variants will usually fail for all-rigid-body models.
'MIDDLE_JACOBI'	Jacobi update for off-processor data of W matrix blocks
	communicating with processors of higher and lower colors. Of use
	for deformable kinematics, where off-diagonal interactions are
	weaker. The Gauss-Seidel run-time should be halved for large
	numbers of processors.
'BOUNDARY_JACOBI'	Use Jacobi update for all off-processor data. This approach will
	fail in most cases. It servers as illustration.
'SIMPLIFIED'	A single sweep over contacts is done with previous values of
	off-processor data. This is followed by local Gauss-Seidel
	iterations for all non-contact constraints. This is the fastest and
	least consistent approach, of use for deformable kinematics
	dominated models.

Table 4.8: Variants of parallel Gauss-Seidel update.

obj = NEWTON_SOLVER (| meritval, maxiter, locdyn, theta, epsilon, presmooth)

- obj created NEWTON SOLVER object
- meritval value of merit function sufficient for termination (default: 1E-8), cf. Chapter 8 for more details
- maxiter iterations bound (default: 100)
- locdyn 'ON' or 'OFF' deciding whether to fully assemble local dynamics (default: 'ON')
- theta relaxation parameter greater than 0 and not greater than 1 (default: 0.25); theta is automatically decreased in case of numerical instability; smaller initial theta may improve overall convergence behavior
- epsilon non-negative smoothing epsilon (default: 1E-9)
- **smooth** number of Gauss-Seidel (pre- and post-) smoothing steps (default: 0); smoothing is only performed when **locdyn** value is 'ON'

Some parameters can also be accessed as members of a NEWTON SOLVER object. These are

Read-only members	
obj.iters - number of iterations during a last run of solver	
obj.merhist - a list of merit function values for each iteration of the last run	

Read/write members	
obj.meritval, obj.maxiter, obj.locdyn, obj.theta, obj.epsilon, obj.smooth	

4.1.12 CONSTRAINT

An object of type CONSTRAINT represents a constraint and some of its associated data (e.g. constraint reaction). Both user prescribed constraints and contact constraints are represented by an object of the same type.

obj = FIX POINT (body, point)

This routine creates a fixed point constraint.

- obj created CONSTRAINT object
- body BODY object whose motion is constrained
- point (x, y, z) tuple with referential point coordinates

obj = FIX_DIRECTION (body, point, direction)

This routine fixes the motion of a referential point along a specified spatial direction.

- obj created CONSTRAINT object
- body BODY object whose motion is constrained
- point (x, y, z) tuple with referential point coordinates
- direction (vx, vy, vz) tuple with spatial direction components

$obj = SET_DISPLACEMENT (body, point, direction, tms)$

This routine prescribes a displacement history of a referential point along a specified spacial direction.

- obj created CONSTRAINT object
- body BODY object whose motion is constrained
- **point** (x, y, z) tuple with referential point coordinates
- direction (vx, vy, vz) tuple with spatial direction components
- tms TIME SERIES object with the displacement history

obj = SET VELOCITY (body, point, direction, value)

This routine prescribes a velocity history of a referential point along a specified spacial direction.

- obj created CONSTRAINT object
- body BODY object whose motion is constrained
- \mathbf{point} (x, y, z) tuple with referential point coordinates
- direction (vx, vy, vz) tuple with spatial direction components
- value a constant value or a TIME SERIES object with the velocity history

obj = SET ACCELERATION (body, point, direction, tms)

This routine prescribes an acceleration history of a referential point along a specified spacial direction.

- ullet obj created CONSTRAINT object
- body BODY object whose motion is constrained
- **point** (x, y, z) tuple with referential point coordinates
- direction (vx, vy, vz) tuple with spatial direction components
- tms TIME SERIES object with the acceleration history

obj = PUT RIGID LINK (body1, body2, point1, point2)

This routine creates a rigid link constraints between two referential points of two distinct bodies.

- obj created CONSTRAINT object
- **body1** BODY object one whose motion is constrained (could be *None* when **body2** is not *None* then one of the points is fixed "in the air")
- body2 BODY object two whose motion is constrained (could be *None* when body1 is not *None*)
- point1 (x1, y1, z1) tuple with the first referential point coordinates
- point2 (x2, y2, z2) tuple with the second referential point coordinates

Some parameters can also be accessed as members of a CONSTRAINT object. These are

Read-only members obj.kind - kind of constraint: 'CONTACT', 'FIXPNT' (fixed point), 'FIXDIR' (fixed direction), 'VELODIR' (prescribed velocity; note that prescribed displacement and acceleration are converted into this case), 'RIGLNK' (rigid link) **obj.** R - current average (over time step [t, t+h]) constraint reaction in a form of a tuple: (RT1, RT2, RN) given with respect to a local base stored at obj.base obj.base - current spatial coordinate system in a form of a tuple: (eT1x, eT2x, eNx, eT1y, eT2y, eNy, eT1z, eT2z, eNz) where x, y, z components are global **obj. point** - current spatial point where the constraint force acts. This is a (x, y, z) tuple for all constraint types, but 'RIGLNK' for which this is a (x1, y1, z1, x2, y2, z2) tuple. obj.area - current area for contact constraints or zero otherwise obj.gap - current gap for contact constraints or zero otherwise obj.merit - current value of the per-constraint merit function obj.adjbod - adjacent bodies. This is a tuple (body1, body2) of BODY objects for 'CONTACT' and 'RIGLNK' or a single BODY object otherwise. obj.matlab - surface material label for constraints of kind 'CONTACT', or a None object otherwise.

4.2 Applying loads

Routines listed in this section apply loads.

GRAVITY (solfec, vector)

This routine sets up the gravitational acceleration.

- solfec SOLFEC object for which the acceleration is set up
- **vector** (vx, vy, vz) tuple defining the gravity acceleration. Each entry is a number or a TIME_SERIES object defining the value of the acceleration component.

FORCE (body, kind, point, direction, value data)

This routine applies a point force to a body.

- body BODY object to which the force is applied
- kind either 'SPATIAL' or 'CONVECTED'; the *spatial* direction remains fixed, while the *convected* one follows deformation

- point (x, y, z) tuple with the referential point where the force is applied
- direction (vx, vy, vz) tuple defining the direction of force
- value a number, a TIME_SERIES object or a callback routine defining the value of the applied force. In case of a callback routine, the following format is assumed:

$force = value_callback\ (data,\ q,\ u,\ time,\ step)$

where: **data** is the optional user data passed to **FORCE** routine (if **data** is a tuple it will expand the list of parameters to the callback), **q** is the configuration of the body passed to the callback, **u** is the velocity of the body passed to the callback, **time** is the current time passed to the callback and **step** is the current time step passed to the callback. The callback returnes a **force** tuple. For rigid body the force reads (spatial force, spatial torque, referential torque), while for other hinds of bodies this is a generalised force of the same dimension as the velocity **u** (power conjugate to it).

• data - callback routine user data

TORQUE (body, kind, direction, value)

This routine applies a torque to a *rigid* body.

- body BODY object of kind 'RIGID' to which the torque is applied
- kind either 'SPATIAL' or 'CONVECTED'; the *spatial* direction remains fixed, while the *convected* one follows deformation
- direction (vx, vy, vz) tuple defining the direction of torque
- value a number or a TIME SERIES object defining the value of the applied torque

PRESSURE (body, surfid, value)

This routine applies a constant surface pressure to MESH based bodies.

- body BODY object to which the pressure is applied (the shape has to be composed of a single MESH)
- surfid the integer surface identifier
- value a number or a TIME SERIES object defining the value of the applied load

4.3 Fragmentation (Under development)

Routines listed in this section control fragmentation of bodies.

SIMPLIFIED_CRACK (body, point, normal, surfid, criterion | ft, Gf) (Under development)

This routine prescribes a potential body-wise planar cracks together with a cracking criterion. Creation of a simplified crack results in splitting of the body in two parts.

- body a pseudo-rigid or FEM based BODY object
- **point** crack plane referential point (x, y, z)

Criterion	Parameters	Description
'TENSILE'	ft, Gf	Tensile stress at any point of the the crack plane is
		larger than the tensile strength.

Table 4.9: Cracking criteria.

- **normal** crack plane referential normal (n_x, n_y, n_z)
- surfid crack surface identifier
- criterion cracking criterion, cf. Table 4.9
- ft tensile strength (default: 0.0)
- **Gf** fracture energy (default: 0.0)

4.4 Running simulations

Routines listed in this section control the solution process.

RUN (solfec, solver, duration)

This routine runs a simulation.

- solfec SOLFEC object
- solver constraint solver object (e.g. GAUSS SEIDEL SOLVER, PENALTY SOLVER)
- duration duration of analysis. Note: this parameter is ignored when an analysis is run in the viewer mode (with -v switch).

OUTPUT (solfec, interval | compression)

This routine specifies the frequency of writing to the output file.

- solfec SOLFEC object
- interval length of the time interval elapsing before consecutive output file writes
- **compression** output compression mode: 'OFF' (default) or 'ON'. Compressed output files are smaller, although they might not be portable between hardware platforms.

EXTENTS (solfec, extents)

This routine bounds the simulation space. Bodies falling outside of the extents are deleted from the simulation.

- solfec SOLFEC object
- extents (xmin, ymin, zmin, xmax, ymax, zmax) tuple

CALLBACK (solfec, interval, data, callback)

This routine defines a callback function, invoked during a run of Solfec every interval of time. A callback routine can interrupt the course of **RUN** command by returning 0.

- ullet solfec SOLFEC object
- interval length of the time interval elapsing before consecutive callback calls
- data data passed to the callback function
- callback callback function of form: $value = callback \ (data)$, where for the returned value equal zero Solfec run is stopped

UNPHYSICAL PENETRATION (solfec, depth)

This routine sets a depth of an unphysical interpenetration. Once it is exceeded, the simulation is stopped and a suitable error message printed out.

- solfec SOLFEC object
- **depth** interpenetration depth bound (default: ∞)

GEOMETRIC EPSILON (epsilon)

This routine sets a numerical tolerance for geometric tests performed within Solfec. The tolerance is a characteristic distance between two distinct points below which they can be regarded as one.

• epsilon - geometrical tolerance (default: 1E-6)

WARNINGS (state)

This routine disables or enables Solfec warnings. It is a good practice to have the warnings enabled and only switch them off after making sure, that they can be ignored.

• state - 'ON' or 'OFF' (default: 'ON')

INITIALIZE STATE (solfec, path, time)

This routine initializes the state of a Solfec object with the state red from an output directory at a given time. It is ignored in the 'READ' mode.

- solfec Solfec object in the 'WRITE' mode
- path path to the output directory containing matching analysis results
- time time at which the state should be red from the output files

4.5 Utilities

Various utility routines are listed below.

IMBALANCE TOLERANCE (solfec, tolerance | weightfactor)

This routine sets the imbalance tolerance for parallel balancing of Solfec data. A ratio of maximal to minimal per processor count of objects used. Hence, 1.0 indicates perfect balance, while any ratio > 1.0 indicates an imbalance. Initially imbalance tolerances are all set to 1.3. This routine is ignored during sequential runs.

- solfec SOLFEC object
- tolerance data imbalance tolerance (default: 1.3)
- weightfactor a local dynamics weight factor between 0.0 and 1.0 (default: 1.0). Computational load of local dynamics assembling is best balanced when weightfactor equals 1.0. This however can sometimes result in a poor load balance for contact detection or time integration. Making it smaller than 1.0 can improve the overall balance in such cases.

num = RANK()

This routine returns the rank of the CPU that runs the current copy of Solfec.

• num - the CPU rank

BARRIER ()

This routine sets up a parallel barrier in the MPI mode (all processes need to meet at it before they can continue). It is ignored in the serial mode.

num = NCPU (solfec)

This routine returns the number CPUs used in the analysis.

- num the number of CPUs
- solfec SOLFEC object

ret = HERE (solfec, object)

This routine tests whether an object is located on the current processor. During parallel runs objects migrate between processors. When calling a function (or a member) for an object not present on the current processor, the call will usually return None or be ignored. Hence, it is convenient to check whether an object resides on the current processor.

- ret True or False
- solfec SOLFEC object
- \bullet ${\bf object}$ BODY or CONSTRAINT object

obj = VIEWER ()

This routine tests whether the viewer is enabled.

• obj - True or False depending on whether the viewer (-v command line option) was enabled

BODY CHARS (body, mass, volume, center, tensor)

This routine overwrites referential characteristics of a body.

- body BODY object
- mass body mass
- volume body volume
- center (x, y, z) mass center
- tensor $(t_{11}, t_{21}, \dots, t_{33})$ column-wise inertia tensor for a rigid body or Euler tensor otherwise

INITIAL VELOCITY (body, linear, angular)

This routine applies initial (at time zero) linear and angular (in the sense of rigid motion) velocity to a body.

- body BODY object
- linear linear velocity (v_x, v_y, v_z)
- angular angular velocity $(\omega_x, \omega_y, \omega_z)$

MATERIAL (solfec, body, volid, material)

This routine applies material to a subset of geometric objects with the given volume identifier.

- solfec SOLFEC object
- body BODY object
- volid volume identifier
- material MATERIAL object or material label

DELETE (solfec, object)

This routine deletes a BODY object or a CONSTRAINT object from a SOLFEC object.

- solfec SOLFEC object
- object (emptied) BODY or CONSTRAINT object

obj = SCALE (shape, coefs)

This routine scales a geometrical object or a collection of such objects.

- **obj** when **shape** is not (x, y, z) tuple: same as **shape**, returned for convenience. Otherwise the $(x \cdot coefs[0], y \cdot coefs[1], z \cdot coefs[2])$ tuple.
- **shape** object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE. Alternately this can be a single (x, y, z) tuple, but then one must use **point** = **SCALE** (**point**, **coefs**) in order to modify the **point** (Python tuples are immutable they cannot be modified "in place" after creation).
- coefs (cx, cy, cz) tuple of scaling factors along each axis

obj = TRANSLATE (shape, vector)

This routine translates a geometrical object or a collection of such objects.

- **obj** when **shape** is not (x, y, z) tuple: same as **shape**, returned for convenience. Otherwise the (x + vector[0], y + vector[1], z + vector[2]) tuple.
- **shape** object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE. Alternately this can be a single (x, y, z) tuple, but then one must use **point** = **TRANSLATE** (**point**, **vector**) in order to modify the **point** (Python tuples are immutable they cannot be modified "in place" after creation).
- vector (vx, vy, vz) tuple defining the translation

obj = ROTATE (shape, point, vector, angle)

This routine rotates a geometrical object or a collection of such objects.

- **obj** when **shape** is not (x, y, z) tuple: same as **shape**, returned for convenience. Otherwise the rotated (x1, y1, z1) image of (x, y, z).
- shape object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE. Alternately this can be a single (x, y, z) tuple, but then one must use **point1** = **ROTATE** (**point1**, **point2**, **vector**, **angle**) in order to modify **point1** (Python tuples are immutable they cannot be modified "in place" after creation).
- point (px, py, pz) tuple defining a point passed by the rotation axis
- vector (vx, vy, vz) tuple defining a direction of the rotation axis
- angle rotation angle in degrees

(one, two) = SPLIT (shape, point, normal | surfid)

This routine splits a geometrical object (or a collection of objects) by a plane passing by a point.

- one objects placed below the splitting plane (None if no objects were placed below)
- two objects placed above the splitting plane (*None* if no objects were placed above)
- **shape** (emptied) object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, SPHERE or MESH
- point (px, py, pz) tuple defining a point passed by the splitting plane
- **normal** (nx, ny, nz) tuple defining the splitting plane normal
- surfid surface identidier of a newly created surface (default: 0)

WARNING: Mesh splitting generates tetrahedral mesh in place of the input one. The meshing is randomized and it may generate different results for the same input. Use TETRAHEDRALIZE in order to refine and save the generated mesh parts. Otherwie you may encounter input/output erros.

obj = COPY (shape)

This routine makes a copy of input objects.

- obj created collection of copied objects
- shape object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE

obj = BEND (shape, point, direction, angle)

This routine bends a shape around an axis. The bending is performed from the section of the shape closest to the axis onward. The orientation of the axis direction determines the orientation of the bending according to the right hand rule. Let \mathbf{q} be the closest to the axis mesh node. Then $\mathbf{v} = \mathbf{d} \times (\mathbf{q} - \operatorname{proj}(\mathbf{q}))$, where \mathbf{d} is the axis direction and $\operatorname{proj}[\cdot]$ projects a point onto the axis. Bending starts from the section containing \mathbf{q} and proceeds in the direction of \mathbf{v} .

- obj same as shape
- shape object of type MESH
- point axis point
- direction axis direction
- angle positive bending angle in degrees

obj = BYLABEL (solfec, kind, label)

This routine finds a labelled object inside of a SOLFEC object.

- **obj** returned object (*None* if a labelled object was not found)
- solfec SOLFEC object
- kind labelled object: 'SURFACE MATERIAL', 'BULK MATERIAL', 'BODY'
- label the label string

$obj = MASS_CENTER$ (shape)

This routine calculates the mass center of a geometrical object or a collection of such objects.

- \mathbf{obj} (x, y, z) tuple storing the mass center
- **shape** object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE. Alternately this can be a single BODY object.

CONTACT EXCLUDE BODIES (body1, body2)

This routine disables contact detection for a specific pair of bodies. By default contact detection is enabled for all possible body pairs. **NOTE:** must be invoked on all processors during a parallel run (do not use from within a callback).

- body1 first BODY object
- body2 second BODY object

CONTACT EXCLUDE SURFACES (solfec, surf1, surf2)

This routine disables contact detection for a specific pair of surfaces. By default contact detection is enabled for all possible surface pairs. **NOTE:** must be invoked on all processors during a parallel run (do not use from within a callback).

- solfec SOLFEC object
- surf1 first BODY object
- surf2 second BODY object

CONTACT EXCLUDE OBJECTS (body1, point1, body2, point2)

This routine disables contact detection for a specific pair of geometric objects (e.g. elements, convices, sheres). By default, between different bodies, contact detection is enabled for all possible object pairs. **NOTE:** must be invoked on all processors during a parallel run (do not use from within a callback).

- body1 first BODY object
- point1 referential point properly contained in the 1st geometric object
- bod2 second BODY object
- point2 referential point properly contained in the 2nd geometric object

CONTACT SPARSIFY (solfec, threshold | minarea, mindist)

This routine modifies contact filtering (sparsification) behaviour. Generally speaking, some contact points are filtered out in order to avoid unnecessary dense contact point clusters. If a pair of bodies is connected by two or more contact points, one of the points generated by topologically adjacent entities (elements, convices) will be removed (sparsified) if the ratio of contact areas of is smaller than the prescribed threshold (cf. Section 6.2).

- solfec SOLFEC object
- threshold sparsification threshold (default: 0.01) from within the interval [0, 1]. Zero corresponds to the lack of sparsification.
- minarea minimal contact area (default: 0.0). Contact points with area smaller then minarea are dropped.
- mindist minimal distance between distinct contact points (default: GEOMETRIC EPSILON).

LOCDYN DUMP (solfec, path)

This routine dumps into a file the most recent state of local dynamics. It is meant for debugging and test purposes, e.g. comparing local dynamics between runs on various processor counts.

- ullet solfec Solfec object
- path file path

obj = PARTITION (body, parts)

This routine partitions a finite element body into parts glued by compatibility constraints. This allows to improve parallel scalability of simulations with large FE meshes. Metis [8] is employed as the partitioner.

- **obj** list of bodies obtained as a result of partitioning. If the label of an input body was 'BOD', then the partitioned bodies have labels 'BOD_PART1', 'BOD_PART2', etc.
- **body** (emptied) a finite element body (cannot have "rough mesh"). After partitioning the input body is removed from the domain and replaced by the glued parts.
- parts number of partitions

obj = OVERLAPPING (obstacles, shapes | not, gap)

This routine looks for shapes (not) overlapping the obstacles.

- obj list of shapes (not) ovrelapping the obstacles.
- **obstacles** object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE.
- **shapes** (emptied) object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE.
- not 'NOT' string.
- gap maximal negative gap.

MBFCP EXPORT (solfec, path)

This routine exports Solfec model into the MBFCP problem definition format. See http://code.google.com/p/mbfcp/for details.

- solfec Solfec object
- path output path

4.6 Results access

Results can be accessed either in the 'READ' mode of a SOLFEC object, or in the 'WRITE' mode once some analysis has been run.

value = DURATION (solfec)

This routine returns the duration of a simulation in SOLFEC's 'READ' mode, or **solfec.time** in the 'WRITE' mode.

- value (t0, t1) duration limits of the simulation in 'READ' mode or current time in 'WRITE' mode
- solfec SOLFEC object

FORWARD (solfec, steps)

This routine steps forward within the simulation output file. Ignored in SOLFEC's 'WRITE' mode.

- solfec SOLFEC object
- steps numbers of steps forward

BACKWARD (solfec, steps)

This routine steps backward within the simulation output file. Ignored in SOLFEC's 'WRITE' mode.

- solfec SOLFEC object
- steps number of steps backward

SEEK (solfec, time)

This routine to a specific time within the simulation output file. Ignored in SOLFEC's 'WRITE' mode.

- solfec SOLFEC object
- time time to start reading at

disp = DISPLACEMENT (body, point)

This routine outputs the displacement of a referential point.

- disp (dx, dy, dz) tuple storing the displacement
- body BODY object
- point (x, y, z) tuple storing the referential point

velo = VELOCITY (body, point)

This routine outputs the velocity of a referential point.

- velo (vx, vy, vz) tuple storing the velocity
- body BODY object
- **point** (x, y, z) tuple storing the referential point

stre = STRESS (body, point)

This routine outputs the Cauchy stress of a referential point.

- stre (sx, sy, sz, sxy, sxz, syz, mises) tuple storing the Cauchy stress and the von Mises norm of it
- body BODY object
- **point** (x, y, z) tuple storing the referential point

$ene = ENERGY (solfec \mid object)$

The routine outputs the value of energy of a specific object.

- ene (kinetic, internal, external, contact, friction) tuple of energy values; internal energy corresponds to the work of internal forces, external energy corresponds to the work of external forces (including constraint reactions), contact energy corresponds to the work of normal contact reactions, friction energy corresponds to the work of tangential contact reactions
- solfec SOLFEC object
- object SOLFEC object, BODY object or a list of BODY objects

tim = TIMING (solfec, kind)

The routine outputs the value of a specific action timing per time step.

- $\bullet~$ \mathbf{tim} value of timing
- solfec SOLFEC object
- kind this is one of: 'TIMINT' (time integration), 'CONUPD' (constraints update), 'CONDET' (contact detection), 'LOCDYN' (local dynamics setup), 'CONSOL' (constraints solution), 'PARBAL' (parallel load balancing). The load balancing timing is non-zero only for parallel runs.

hist = HISTORY (solfec, list, t0, t1 | skip, progress)

This routine outputs time histories of entities.

- hist a tuple of list objects storing the histories: (times, values1, values2, ..., valuesN)
- solfec SOLFEC object
- list list of objects [object1, object2, ..., objectN] indicating requested values. The valid objects are:
 - a tuple (body, point, entity) where body is a BODY object, point is a (x, y, z) tuple storing the referential point, and entity is one of: 'DX', 'DY', 'DZ' (displacement), 'VX', 'VY', 'VZ' (velocity), 'SX', 'SY', 'SZ', 'SXY', 'SXZ', 'SYZ' (stress), 'MISES' (von Mises norm of stress)
 - a tuple (object, kind) where object is a SOLFEC object, a BODY object or a list of BODY objects, and kind is a string 'KINETIC', 'INTERNAL', 'EXTERNAL', 'CONTACT', 'FRICTION' and it corresponds to the energy kind
 - a string 'TIMINT', 'CONUPD', 'CONDET', 'LOCDYN', 'CONSOL', 'PARBAL' for timing histories
 - a string 'STEP' for time step history
 - a string 'CONS', 'BODS' for constraint and body number histories
 - a string 'DELBODS', 'NEWBODS' for deleted and inserted (after time 0) body number histories (nonzero only for uncompressed outputs)
 - a string 'GSITERS' (Gauss-Seidel iterations count), 'GSCOLORS' (Gauss-Seidel processor colors count), 'GSBOT', 'GSMID', 'GSTOP', 'GSINN' (Gauss-Seidel bottom, middle, top and inner set sizes), 'GSINIT' (Gauss-Seidel setup time), 'GSRUN' (Gauss-Seidel computations time), 'GSCOM' (Gauss-Seidel communication time, except the middle set), 'GSMCOM' (Gauss-Seidel middle set communication time); values other than 'GSITERS' are non-zero only for parallel runs
 - a string 'MERIT' for the time history of the constraints satisfaction merit function
 - a string 'NTITERS' for the NEWTON SOLVER iterations count
 - a tuple (object, entity) or (object, direction, pair, entity) where object is a SOLFEC object, a BODY object or a list of BODY objects, direction is a tuple (d_x, d_y, d_z) storing a direction (use **None** if the normal direction is preferred), pair is a tuple (surf1, surf2) defining a surface pair (use **None** if no surface pair is preferred), and entity is:
 - * 'GAP' for the time history of the minimal contact gap among constraints attached to given bodies (negative gap corresponds to the penetration depth)
 - * 'R' for the time history of the resultant (and average over time step [t, t + h]) constraint reactions along the directions: normal or given by the direction
 - * 'U' for the time history of the average constraint velocities along the directions: normal or given by the *direction*
 - * 'CR' for time histories like in the 'R' case, but for contact constraints only
 - * 'CU' for time histories like in the 'U' case, but for contact constraints only
- \bullet **t0** time interval start
- **t1** time interval end
- skip number of steps to skip between two time instants
- progress 'ON' or 'OFF'; print out a percentage based progress bar (default: 'OFF'); useful for large output files and slow hard disks

Chapter 5

Tutorials

5.1 Three basic geometric objects

This example illustrates the three basic geometric objects: CONVEX, MESH and SPHERE. We are going to construct a simple structure and hit it with a ball. Let us first create a horizontal floor.

We simply created a convex hull about eight points. This is only a geometric object for the moment. It exists only in Python interpreter, but not yet inside of a Solfec model. In order to insert it into a model, we need first to create a SOLFEC object, a BULK_MATERIAL object, and finally a BODY object having the shape described by the *floor*. Here we go.

Note, that the floor is simply an obstacle - it does not move. Before creating the floor body we had to create a SOLFEC object. This object gather all necessary data for an individual simulation. In our case this will be a dynamic simulation, pursued with the time step at least as small as the specified one. The time step can be automatically decreased during a simulation due to stability requirements. The result files of this tutorial will

be written to the specified path - relative to from there the 'solfec' command was involved. Once a body has been inserted into a model, we can view the effect as follows

```
> ./solfec -v inp/tutorial/three-basic-geometric-objects.py
```

This will create a Solfec viewer, which should result in the following picture

t=0



Le us now construct a stack made of two bodies. The first one comprises four juxtaposed convex objects.

```
a = 2
b = 2
c = 2
brick\_vid = 2
brick\_sid = 2
brick = CONVEX ([0, 0, 0,
                 a/2, 0, 0,
                 a/2, b/2, 0,
                 0, b/2, 0,
                 0, 0, c/2,
                 a/2, 0, c/2,
                 a/2, b/2, c/2,
                 0, b/2, c/2],
                 [4, 0, 3, 2, 1, brick_sid,
                 4, 1, 2, 6, 5, brick_sid,
                 4, 2, 3, 7, 6, brick_sid,
                 4, 3, 0, 4, 7, brick_sid,
                 4, 0, 1, 5, 4, brick_sid,
                 4, 4, 5, 6, 7, brick_sid], brick_vid)
b1 = COPY (brick)
b2 = TRANSLATE (COPY (brick), (a, 0, 0))
b3 = TRANSLATE (COPY (brick), (0, b, 0))
```

```
b4 = TRANSLATE (COPY (brick), (a, b, 0))
shape = [b1, b2, b3, b4]
TRANSLATE (shape, (-a, -b, 0))
BODY (solfec, 'RIGID', shape, bulk)
```

Note, that a base brick was created first. Then this brick was copied and manipulated into four different objects: b1,b2, ..., b4. The list of those objects was passed as a shape when creating the first rigid body. The second body will be pseudo-rigid and will have its shape defined by a mesh.

The hexahedral mesh is spanned on eight nodes and has an inclined shape due to z level slope. Note, that we have specified the "dy" argument of the HEX command, so to illustrate non-uniform meshing along one of the directions. The mesh is translated to rest on top of the previous body. Then a pseudo-rigid body is created. Now, let us create the sphere.

```
sphere = SPHERE ((0, 0, 5), 1, 1, 1)
body = BODY (solfec, 'RIGID', sphere, bulk)
INITIAL_VELOCITY (body, (0, 0, -10), (0, 0, 0))
```

When creating the rigid body corresponding to the sphere, we have now retrieved the *body* object. It is needed in order to prescribe the initial velocity. The sphere has the initial linear velocity $v_z = -10$ m/s. Let us have a look at the model so far.





Now, in order to be able to control contact behaviour, we need to define a surface material. This will be a default material, hence we shall not specify a surface pairing (int this example surface identifiers are not used). Whenever a contact is detected, the following Signorini-Coulomb model is employed

It will be also of use to apply some gravity loading.

```
GRAVITY (solfec, (0, 0, -10))
```

Before running the actual simulation, it remains to create a solver object. We use the Gauss-Seidel solver here.

```
gs = GAUSS_SEIDEL_SOLVER (1E-3, 1000)
```

The relative constraint reaction accuracy was set to 1E-3, while the maximal the maximal number of iterations is 1000. It remains to run the simulation.

```
RUN (solfec, gs, 1.0)
```

And then actually run solfec from the command line

```
./solfec inp/tutorial/three-basic-geometric-objects.py
```

One second of the simulation was computed. Let us have a look at the displacement along z at the end of this time



5.2 Ball impact

This example illustrates using multiple SOLFEC objects, application of the PENALTY_SOLVER, and using HISTORY to retrieve and then plot time histories. First we define a Python function that will create a model of ball impacting a plate for a specific set of parameters.

```
def ball_impact (step, stop, spring_value, dashpot_value, output):
  w = 2
 1 = 2
 h = 1
  floor_vid = 1
  floor_sid = 1
  floor = HULL ([-w/2, -1/2, -h],
                  w/2, -1/2, -h,
                  w/2, 1/2, -h,
                 -w/2, 1/2, -h,
                 -w/2, -1/2, 0,
                  w/2, -1/2, 0,
                  w/2, 1/2, 0,
                 -w/2, 1/2, 0], floor_vid, floor_sid)
  solfec = SOLFEC ('DYNAMIC', step, output)
  bulk = BULK_MATERIAL (solfec, model = 'KIRCHHOFF',
                        young = 15E9, poisson = 0.3, density = 2E3)
  BODY (solfec, 'OBSTACLE', floor, bulk)
  sphere = SPHERE ((0, 0, 1.0), 1, 1, 1)
  body = BODY (solfec, 'RIGID', sphere, bulk)
  INITIAL_VELOCITY (body, (0, 0, -5), (0, 0, 0))
  SURFACE_MATERIAL (solfec, model = 'SPRING_DASHPOT', friction = 0.0,
                    spring = spring_value, dashpot = dashpot_value)
  GRAVITY (solfec, (0, 0, -10))
  xs = PENALTY_SOLVER ()
  RUN (solfec, xs, stop)
  return solfec
```

The above code is similar to the previous example. Here though the complete model is created inside of a Python function called <code>ball_impact</code>. By itself this will not run any simulation - this function needs to be called from the main module of the input file (we remind that Python uses indentation to decide upon code blocking - in our case no indentation indicates the main module). Above the 'SPRING_DASHPOT' material model is used for the contact interface. The parameters of the spring and damper are passed as arguments of the <code>ball_impact</code> function. It should be noted, that the SOLFEC object is returned from the routine. Now, here is the main module

```
step = 1E-3
stop = 2.0
spring = 1E+9
sol1 = ball_impact (step, stop, spring, 0E0, 'out/tutorial/ball-impact-1')
sol2 = ball_impact (step, stop, spring, 1E6, 'out/tutorial/ball-impact-2')
sol3 = ball_impact (step, stop, spring, 1E7, 'out/tutorial/ball-impact-3')
```

We simply run three different simulations for three values of the dashpot parameter. We can now view the three models by typing

./solfec -v ./inp/tutorial/ball-impact.py

The viewer allows change the current model by using '<' and '>' keyboard shortcuts, or using the right-mouse click for the drop-down menu and then selecting *menu: domain: previous* or *menu: domain: next*. In this example the three models do not visibly differ.



We could now run each model in the viewer mode (menu: analysis: run), but it will be more useful to plot kinetic energy and compare it for all the three values of the dashpot parameter. The code below does the job

```
if not VIEWER() and sol1.mode == 'READ':
   import matplotlib.pyplot as plt
   th = HISTORY (sol1, (sol1, 'KINETIC'), 0, stop)
   plt.plot (th [0], th [1], lw = 2, label='kin (0)')
   th = HISTORY (sol2, (sol2, 'KINETIC'), 0, stop)
   plt.plot (th [0], th [1], lw = 2, label='kin (1E6)')
   th = HISTORY (sol3, (sol3, 'KINETIC'), 0, stop)
   plt.plot (th [0], th [1], lw = 2, label='kin (1E7)')
   plt.axis (xmin = 0, xmax = 2, ymin=-10000, ymax=110000)
   plt.legend(loc = 'upper right')
   plt.savefig ('doc/figures/ball-impact.eps')
```

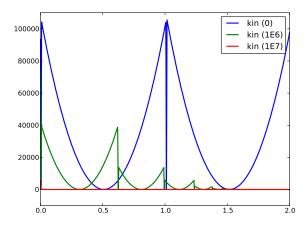
First, we check whether Solfec is not run with the -v option and whether it is in 'READ' mode. This is the case, when after running the complete analysis

```
./solfec ./inp/tutorial/ball-impact.py we again run
```

```
./solfec ./inp/tutorial/ball-impact.py
```

Now, Solfec will find out that the output files in out/tutorial/ball-impact-(1,2,3) are present. It will open in 'READ' mode. In order to create the plot we are going to use the matplotlib Python package - please refer to

http://matplotlib.sourceforge.net/index.html in order to learn how to install it. We next use the HISTORY command in order to retrieve the time histories of the kinetic energy for all three created SOLFEC objects. The result in plotted into an EPS file, visible below.



We can see that the dashpot=0 results in a fully elastic impact (energy conserving behaviour), dahspot=1E6 introduces some fractional energy restitution after impacts, while dashpot=1E7 results in a nearly plastic impact.

Contact points

6.1 Contacts from overlaps

Body shapes are juxtapositions of convex objects (Sections 4.1.1, 4.1.2, 4.1.3). A contact point and normal direction result from an overlap of two convex objects (Figure 6.1). This is motivated by two factors. Firstly, the point and the normal direction derived from an overlap are well defined for nonsmooth geometry. Secondly, we wish to use as few contact points as possible, but still be able to control the accuracy of contact resolution by mesh refinement. A non-positive gap function is suitably derived from such overlap. We refer the reader to Chapter 9 of [9] for more details.



Figure 6.1: A contact point and normal direction extracted from an intersection of two convex objects.

6.2 Contact sparsification

Let us have a look at an arch in Figure 6.2. The detail of two bricks shows narrow meshing near the inner and outer boundaries. This will allow to better reproduce the hinging mechanism of arch collapse. A single brick is composed of six elements: the two large middle elements and the four narrow inner and outer elements. If we now apply contact detection algorithm, all possible volumetric overlaps will be detected. Because identically meshed bodies are perfectly adjacent to each other we shall end up with a clutter of contact points, generated by all of the adjacent element volumes. This is visible on the left in Figure 6.3. If one would have to generate contact points by hand, they would probably look like those on the right in Figure 6.3. A heuristic sparsification algorithm filters out redundant contact points (cf. Algorithm 6.1).

Algorithm 6.1 Contact sparsification algorithm.

```
SPARSIFY ()
for each contact1 do
for each body adjacent to contact1 do
for each contact2 adjacent to body do
if contact1 = contact2 skip
if area\left(contact1\right) < threshold \cdot area\left(contact2\right) and
topologically\_adjacent\left(contact1,contact2\right) then remove contact1
else if point\left(contact1\right) = point\left(contact2\right) then remove contact1
```

We walk over all contact points and compare each of them with other contacts adjacent through common bodies. If the area of a contact is a smaller than an area of a topologically adjacent neighbouring contact, then we remove it. The same happens if the two contact points coincide. Topological adjacency of contact points indicates that they have been created between the mesh elements that are topologically adjacent. We know then, that next to a contact point with a small supporting area there is another one with a suitably larger contact area. The Solfec command CONTACT_SPARSIFY sets the *threshold* value (cf. Section 4.5).



Figure 6.2: An arch and a detail of two bricks. Note the narrow meshing near the edge of inner and outer boundaries.



Figure 6.3: A detail of the arch from Figure 6.2. Contact points on the left are not sparsified. Contact points on the right are sparsified.

Materials

7.1 Surface materials

A surface material is assigned to a pairing of surfaces. See Section 4.1.5 for the input syntax.

7.1.1 Signorini-Coulomb

The velocity Signorini condition reads

$$\bar{U}_N \ge 0 \ R_N \ge 0 \ \bar{U}_N R_N = 0$$
 (7.1)

where $\bar{U}_N = U_N^{t+h} + \eta \min{(0, U_N^t)}$, η is the velocity restitution coefficient, U_N is the the normal relative velocity, and R_N is the normal reaction. The normal direction is consistent with the positive gap velocity so that (7.1) states, that any violation of the non-penetration results in a reactive force or velocity driving at the penetration-free configuration. Using \bar{U}_N allows to account for the Newton impact law. Only restitution = 0 or 1 is energy consistent TODO (cf. Section 10.5 of [9]). The Coulomb's friction law reads

$$\begin{cases}
\|\mathbf{R}_T\| \le \mu R_N \\
\|\mathbf{R}_T\| < \mu R_N \Rightarrow \mathbf{U}_T = \mathbf{0} \\
\|\mathbf{R}_T\| = \mu R_N \Rightarrow \exists_{\lambda \ge 0} \mathbf{U}_T = -\lambda \mathbf{R}_T
\end{cases}$$
(7.2)

A friction force smaller than μR_N implies sticking, while sliding occurs with the force of value μR_N and direction opposite to the slip velocity. The two laws can expressed in a compact from $\mathbf{C}(\mathbf{U}, \mathbf{R}) = \mathbf{0}$. An examples is

$$\mathbf{C}(\mathbf{U}, \mathbf{R}) = \begin{bmatrix} \max(\mu d_N, \|\mathbf{d}_T\|) \mathbf{R}_T - \mu \max(0, d_N) \mathbf{d}_T \\ R_N - \max(0, d_N) \end{bmatrix}$$
(7.3)

where

$$d_N = R_N - \rho \bar{U}_N \tag{7.4}$$

$$\mathbf{d}_T = \mathbf{R}_T - \rho \mathbf{U}_T \tag{7.5}$$

and $\rho > 0$. We refer the reader to Chapter 10 of [9] for more details.

7.1.2 Spring-dashpot

Let

$$s = spring \text{ and } d = dashpot \text{ and } g = gap$$
 (7.6)

The normal reaction is computed as follows

$$R_N = -s \cdot \frac{g^{t+h} + g^t}{2} - d \cdot \frac{U_N^{t+h} + U_N^t}{2}$$
 (7.7)

where U_N is the normal relative velocity. Recall, that the gap function is computed for the configuration $\mathbf{q}^t + \frac{h}{2}\mathbf{u}^t$, so that the gap function value computed during geometrical contact detection reads

$$g = g^t + \frac{h}{2}U_N^t \tag{7.8}$$

We then have

$$g^{t+h} = g^t + \frac{h}{2} \left(U_N^{t+h} + U_N^t \right) = g + \frac{h}{2} U_N^{t+h} \tag{7.9}$$

and since $g^t = g - \frac{h}{2}U_N^t$ we can estimate

$$R_N = -s \cdot \left(g + \frac{h}{4} \left(U_N^{t+h} - U_N^t \right) \right) - \frac{d}{2} \cdot \left(U_N^{t+h} + U_N^t \right)$$
 (7.10)

We then use the diagonal block of local dynamics

$$\mathbf{U}^{t+h} = \mathbf{B} + \mathbf{WR} \tag{7.11}$$

in order to estimate U_N^{t+h} as follows

$$U_N^{t+h} = B_N + \mathbf{W}_{NT} \mathbf{R}_T + W_{NN} R_N \tag{7.12}$$

where a previous tangential reaction \mathbf{R}_T is employed. Inserting this it into (7.10) results in

$$\bar{B}_N = B_N + \mathbf{W}_{NT} \mathbf{R}_T \tag{7.13}$$

$$R_N = \left[-s \cdot \left(g + \frac{h}{4} \left(\bar{B}_N - U_N^t \right) \right) - \frac{d}{2} \cdot \left(\bar{B}_N + U_N^t \right) \right] / \left[1 + \left(s \cdot \frac{h}{4} + \frac{d}{2} \right) \cdot W_{NN} \right]$$
 (7.14)

The reason for using the above, rather than the classical $R_N = -s \cdot g - d \cdot U_N^t$ is in an increased stability of the current approach. Assuming $\mathbf{U}_T^{t+h} = 0$ we then estimate the tangential stick reaction

$$\mathbf{R}_T = -\mathbf{W}_{TT}^{-1} \left(\mathbf{B}_T + \mathbf{W}_{TN} R_N \right) \tag{7.15}$$

The complete interface law is expressed in Algorithm 7.1 (μ refers there to the coefficient of friction). We refer the reader to Chapter 7 of [9] for more details on local dynamics.

Algorithm 7.1 Spring-dashpot reaction calculation.

SPRING_DASHPOT $(h, g, s, d, \mu, cohesion, cohesive)$

$$\bar{B}_N = B_N + \mathbf{W}_{NT} \mathbf{R}_T$$

$$R_N = \left[-s \cdot \left(g + \frac{h}{4} \left(\bar{B}_N - U_N^t \right) \right) - \frac{d}{2} \cdot \left(\bar{B}_N + U_N^t \right) \right] / \left[1 + \left(s \cdot \frac{h}{4} + \frac{d}{2} \right) \cdot W_{NN} \right]$$
 if not $cohesive$ and $R_N < 0$ then $\mathbf{R} = 0$ return

$$\mathbf{R}_T = -\mathbf{W}_{TT}^{-1} \left(\mathbf{B}_T + \mathbf{W}_{TN} R_N \right)$$

if cohesive and $R_N < -cohesion$ then cohesive = false and $R_N = -cohesion$

if
$$\|\mathbf{R}_T\| > \mu |R_N|$$
 then

$$\mathbf{R}_T = \mu R_N \mathbf{R}_T / \|\mathbf{R}_T\|$$

if cohesive then cohesive = false

7.2 Bulk materials

A bulk material is assigned to a volume. See Section 4.1.6 for the input syntax.

7.2.1 Kirchhoff - Saint Venant

This is a simple extension of the linearly elastic material to the large deformation regime. Suitable for large rotation, small strain problems. The strain energy function Ψ of the Kirchhoff - Saint Venant materials reads

$$\Psi = \frac{1}{4} \left[\mathbf{F}^T \mathbf{F} - \mathbf{I} \right] : \mathbf{C} : \left[\mathbf{F}^T \mathbf{F} - \mathbf{I} \right]$$
 (7.16)

where

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu \left[\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right]$$
(7.17)

In the above λ and μ are Lamé constants, while δ_{ij} is the Kronecker delta. The Lamé constants can be expressed in terms of the Young modulus E and the Poisson ratio ν as

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}\tag{7.18}$$

$$\mu = \frac{E}{2 + 2\nu} \tag{7.19}$$

The first Piola stress tensor is computed as a gradient of the hyperelastic potential Ψ

$$\mathbf{P} = \partial_{\mathbf{F}} \Psi \left(\mathbf{F} \right) \tag{7.20}$$

where \mathbf{F} is the deformation gradient.

Constraints accuracy

As explained in Chapter 1, at every time step an implicit equation $\mathbf{C}(\mathbf{R}) = \mathbf{0}$ is solved. Ideally, when for some \mathbf{R} there holds $\mathbf{C}(\mathbf{R}) = \mathbf{0}$ we have an exact solution. Of course, in numerical terms this is not possible. For very large problems, and especially for problems where the amount of constraints exceeds the amount of kinematic freedom, obtaining very accurate solutions is hard and often impractical. In any case, it is useful to have an accuracy measure that has some physical interpretation. In order to compute constraints accuracy, we formulate $\mathbf{C}(\mathbf{R})$ in terms of velocity (cf. Section 8.1 for the Signorini-Coulomb law) and use

$$g(\mathbf{R}) = \sum_{\alpha} \langle \mathbf{W}_{\alpha\alpha}^{-1} \mathbf{C}_{\alpha} (\mathbf{R}), \mathbf{C}_{\alpha} (\mathbf{R}) \rangle / \sum_{\alpha} \langle \mathbf{W}_{\alpha\alpha}^{-1} \mathbf{B}_{\alpha}, \mathbf{B}_{\alpha} \rangle$$
(8.1)

in order to approximately measure the relative amount of spurious energy, due to an inexact satisfaction of constraints. The denominator corresponds to the kinetic energy of the relative free motion, hence $g(\mathbf{R})$ is the ratio of the spurious energy over the nominal amount of the energy available at the constraints. Since inverting \mathbf{W} would be unpractical or impossible due to singularity, we only use the diagonal blocks, which are always positive definite.

8.1 Signorini-Coulomb revisited

We express the Signorini-Coulomb law defined in Section 7.1.1 in the form suitable for (8.1). The friction cone FC_{α} is defined as

$$FC_{\alpha} = \{ \mathbf{R}_{\alpha} : \| \mathbf{R}_{\alpha T} \| \le \mu_{\alpha} R_{\alpha N}, R_{\alpha N} \ge 0 \}$$

$$(8.2)$$

where μ_{α} is the coefficient of friction. It has been shown by De Saxcé and Feng [4], that the Signorini-Coulomb law can be expressed in a compact form

$$-\begin{bmatrix} \mathbf{U}_{\alpha T} \\ \bar{U}_{\alpha N} + \mu_{\alpha} \|\mathbf{U}_{\alpha T}\| \end{bmatrix} \in N_{FC_{\alpha}} (\mathbf{R}_{\alpha})$$
(8.3)

where $N_{FC_{\alpha}}$ stands for the normal cone of the set FC_{α} . For a convex set A the normal cone $N_A(\mathbf{R})$ at point $\mathbf{R} \in A$ is defined as the set of all vectors \mathbf{V} such that $\langle \mathbf{V}, \mathbf{S} - \mathbf{R} \rangle \leq 0$ for all $\mathbf{S} \in A$. Let

$$\mathbf{F}(\mathbf{R}) = \begin{bmatrix} \dots \\ \mathbf{U}_{\alpha T}(\mathbf{R}) \\ \bar{U}_{\alpha N}(\mathbf{R}) + \mu_{\alpha} \|\mathbf{U}_{\alpha T}(\mathbf{R})\| \\ \dots \end{bmatrix}$$
(8.4)

and

$$FC = \bigcup_{\alpha} FC_{\alpha} \tag{8.5}$$

where the dependence $\mathbf{U}_{\alpha}(\mathbf{R})$ is defined in (1.14). Formula (8.3) states, that the frictional contact constraints are satisfied if $-\mathbf{F}(\mathbf{R})$ belongs to the normal cone of the friction cone at \mathbf{R} . Hence

$$-\mathbf{F}(\mathbf{R}) = \mathbf{R} - \mathbf{F}(\mathbf{R}) - \operatorname{proj}_{FC}(\mathbf{R} - \mathbf{F}(\mathbf{R}))$$
(8.6)

which can be reduced to the usual projection formula $\mathbf{R} = \operatorname{proj}_{FC}(\mathbf{R} - \mathbf{F}(\mathbf{R}))$. Let us not do it though, but rather define a vector field

$$\mathbf{m}(\mathbf{S}) = \mathbf{S} - \operatorname{proj}_{FC}(\mathbf{S}) = \mathbf{n}(\mathbf{S}) \langle \mathbf{n}(\mathbf{S}), \mathbf{S} \rangle$$
 (8.7)

where

$$\mathbf{n}_{\alpha}\left(\mathbf{S}_{\alpha}\right) = \begin{cases} \mathbf{0} & \text{if } \|\mathbf{S}_{\alpha T}\| - \mu_{\alpha} S_{\alpha N} \leq 0\\ \mathbf{S}_{\alpha} / \|\mathbf{S}_{\alpha}\| & \text{if } \mu_{\alpha} \|\mathbf{S}_{\alpha T}\| + S_{\alpha N} < 0\\ \frac{1}{\sqrt{1 + \mu_{\alpha}^{2}}} \begin{bmatrix} \mathbf{S}_{\alpha T} / \|\mathbf{S}_{\alpha T}\| \\ -\mu_{\alpha} \end{bmatrix} & \text{otherwise} \end{cases}$$
(8.8)

We can rewrite (8.3) as

$$C(R) = F(R) + m(R - F(R)) = 0 \text{ and } R \in FC$$
 (8.9)

Note, that $\mathbf{F}(\mathbf{R})$ is expressed in terms of velocity, and so is $\mathbf{C}(\mathbf{R})$.

Solvers

Development of solvers for unilateral dynamics is one of the main driving forces behind Solfec. The two solvers described in Sections 9.1 and 9.2 are the classical Gauss-Seidel approach of Contact Dynamics and a somewhat modified penalty solver of the Discrete Element Method.

9.1 Gauss-Seidel solver

The equations of local dynamics (1.14) read

$$\mathbf{U}_{\alpha} = \mathbf{B}_{\alpha} + \sum_{\beta} \mathbf{W}_{\alpha\beta} \mathbf{R}_{\beta} \tag{9.1}$$

where \mathbf{U}_{α} are relative velocities and \mathbf{R}_{α} are reactions at constraint points. $\mathbf{U}_{\alpha}, \mathbf{R}_{\alpha}, \mathbf{B}_{\alpha}$ are 3-vectors, while $\mathbf{W}_{\alpha\beta}$ are 3×3 matrix blocks. Each constraint equation can be formulated as

$$\mathbf{C}_{\alpha}\left(\mathbf{U}_{\alpha}, \mathbf{R}_{\alpha}\right) = \mathbf{0} \tag{9.2}$$

or in other words

$$\mathbf{C}_{\alpha} \left(\mathbf{B}_{\alpha} + \sum_{\beta} \mathbf{W}_{\alpha\beta} \mathbf{R}_{\beta}, \mathbf{R}_{\alpha} \right) = \mathbf{0}$$
(9.3)

Algorithm 9.1 is quite simple: diagonal block problems are solved until reaction change is small enough. The Gauss-Seidel paradigm corresponds to the fact, that the most recent off-diagonal reactions are used when solving the diagonal problem. Of course, because of that, a perfectly parallel implementation is not possible. After all, reactions are updated in a sequence. We can nevertheless relax the need for sequential processing. Perhaps the most scalable Gauss-Seidel approach to date was devised by Adams [2]. Although originally it was

Algorithm 9.1 Serial Gauss-Seidel algorithm

```
SERIAL_GAUSS_SEIDEL (Constraints, \epsilon, \gamma)
1 do
2 for each \alpha in Constraints do
3 \mathbf{S}_{\alpha} = \mathbf{R}_{\alpha}
4 find \mathbf{R}_{\alpha} such that \mathbf{C}_{\alpha} \left( \mathbf{B}_{\alpha} + \sum_{\beta} \mathbf{W}_{\alpha\beta} \mathbf{R}_{\beta}, \mathbf{R}_{\alpha} \right) = \mathbf{0}
5 assuming \mathbf{R}_{\beta} = \text{constant for } \beta \neq \alpha
6 while \|\mathbf{S} - \mathbf{R}\| / \|\mathbf{R}\| > \epsilon and g(\mathbf{R}) > \gamma
```

Algorithm 9.2 Simple processor coloring.

```
COLOR ()  \begin{array}{lll} \text{1} & \text{for } i=1,...,n \text{ do } color\left[i\right]=0 \\ \text{2} & \text{for } i=1,...,n \text{ do} \\ \text{3} & \text{do} \\ \text{4} & & color\left[i\right]=color\left[i\right]+1 \\ \text{5} & \text{while for any } j\in adj\left(i\right) \text{ there holds } color\left[i\right]=color\left[j\right] \\ \end{array}
```

used as a multi-grid smoother, the core idea can be as well applied in our context. Each processor owes a subset of (internal) constraints Q_i , where i = 1, 2, ..., n are the processors indices. Therefore the local velocity update can be rewritten as

$$\mathbf{U}_{\alpha} = \mathbf{B}_{\alpha} + \sum_{\beta \in Q_i} \mathbf{W}_{\alpha\beta} \mathbf{R}_{\beta} + \sum_{\beta \notin Q_i} \mathbf{W}_{\alpha\beta} \mathbf{R}_{\beta}$$
(9.4)

Some of the $\mathbf{W}_{\alpha\beta}$ blocks and reactions \mathbf{R}_{β} correspond to the (external) constraints stored on other processors $(\beta \notin Q_i)$. Let us denote the set of corresponding reaction indices by P_i . That is

$$P_i = \{ \beta : \exists \mathbf{W}_{\alpha\beta} \neq \mathbf{0} \text{ and } \alpha \in Q_i \text{ and } \beta \notin Q_i \}$$

$$(9.5)$$

For each $\beta \in P_i$ we know an index of processor $cpu(\beta)$ storing the constraint with index β . For processor i we can then define a set of adjacent processors as follows

$$adj(i) = \{cpu(\beta) : \beta \in P_i\}$$

$$(9.6)$$

When updating reactions, a processor needs to communicate only with other adjacent processors. We are going to optimise a pattern of this communication by *coloring* the processors. We shall then assign to each processor a color, such that no two adjacent processors have the same color. A simple coloring method is summarised in Algorithm 9.2. We try to assign as few colors as possible. We then split the index sets Q_i as follows

$$Top_{i} = \{\alpha : \forall \mathbf{W}_{\alpha\beta} : \beta \in P_{i} \land color [cpu (\beta)] < color [i]\}$$

$$(9.7)$$

$$Bottom_{i} = \{\alpha : \forall \mathbf{W}_{\alpha\beta} : \beta \in P_{i} \land color \left[cpu\left(\beta\right)\right] > color \left[i\right]\}$$

$$(9.8)$$

$$Middle_i = \{\alpha : \forall \mathbf{W}_{\alpha\beta} : \beta \in P_i \land \alpha \notin Top_i \cup Bottom_i\}$$
 (9.9)

$$Inner_i = Q_i \setminus \{Top_i \cup Bottom_i \cup Middle_i\}$$

$$(9.10)$$

The top constraints require communication only with processors of lower colors. The bottom constraints require communication only with processors of higher colors. The middle constraints require communication with either. The inner constraints require no communication. The inner reactions are further split in two sets

$$Inner_i = Inner1_i \cup Inner2_i \tag{9.11}$$

so that

$$|Bottom_i| + |Inner2_i| = |Top_i| + |Inner1_i|$$

$$(9.12)$$

The parallel Gauss-Seidel scheme is summarised in Algorithm 9.3. The presented version is simplified in the respect, that alternate forward and backward runs are not accounted for (in terms of constraints ordering). We first process the Top_i set: a single sweep over the corresponding diagonal block problems is performed

Algorithm 9.3 Parallel Gauss-Seidel algorithm.

```
SWEEP (Set)
1 for each \alpha \in Set do
          find \mathbf{R}_{lpha} such that \mathbf{C}_{lpha}\left(\mathbf{B}_{lpha}+\sum_{eta}\mathbf{W}_{lphaeta}\mathbf{R}_{eta},\mathbf{R}_{lpha}\right)=\mathbf{0} assuming \mathbf{R}_{eta}= constant for eta
eq lpha
3
LOOP (Set)
1 descending sort of \alpha \in Set based on \max(color[cpu(\beta)]) where \exists \mathbf{W}_{\alpha\beta}
      for each ordered \alpha in Set\ {\rm do}
          for each \beta such that \exists \mathbf{W}_{\alpha\beta} and color\left[cpu\left(\alpha\right)\right] < color\left[cpu\left(\beta\right)\right] do
3
              if not received (\mathbf{R}_{eta}) then receive (\mathbf{R}_{eta})
4
          find \mathbf{R}_{\alpha} such that \mathbf{C}_{\alpha}\left(\mathbf{B}_{\alpha}+\sum_{\beta}\mathbf{W}_{\alpha\beta}\mathbf{R}_{\beta},\mathbf{R}_{\alpha}\right)=\mathbf{0} assuming \mathbf{R}_{\beta}= constant for \beta\neq\alpha
5
6
7
          send (\mathbf{R}_{lpha})
     receive all remaining \mathbf{R}_{eta}
PARALLEL_GAUSS_SEIDEL (\epsilon, \gamma)
        COLOR ()
1
2
        do
3
            SWEEP (Top_i)
            send (Top_i)
4
            SWEEP (Inner2_i)
6
            receive (Top_i)
7
            LOOP (Middle_i)
8
            SWEEP (Bottom_i)
            send (Bottom_i)
9
            SWEEP (Inner1_i)
10
            receive (Bottom_i)
11
12 while \|\mathbf{S} - \mathbf{R}\| / \|\mathbf{R}\| > \epsilon and g(\mathbf{R}) > \gamma
```

in line 3. Then we send the computed top reactions to the processors with lower colors. We try to overlap communication and computation, hence we sweep over the $Inner2_i$ set (line 5) while sending. We then receive the top reactions. It should be noted that all communication is asynchronous - we only wait to receive reactions immediately necessary for computations. In line 7 we enter the loop processing the $Middle_i$ set. This is the location of the computational bottleneck. Middle nodes communicate with processors of higher and lower colors and hence, they need to be processed in a sequence. The sequential processing is still relaxed by using processor coloring. In the LOOP algorithm we first sort the constraints according to the descending order of maximal colors of their adjacent processors (line 1). We then maintain this ordering while processing constraints. As the top reactions were already sent, some of the constraints from the middle set will have their external reactions from higher colors fully updated. These will be processed first in line 5 of LOOP and then sent to lower and higher (by color) processors in line 7. This way some processors with lower colors will have their higher color off-diagonal reactions of middle set constraints fully updated and they will proceed next. And so on. At the end (line 8), we need to receive all remaining reactions that have been sent in line 7 of LOOP. Coming back to PARALLEL_GAUSS_SEIDEL, after the bottleneck of the LOOP, in lines 8-11 we process the $Bottom_i$ and $Inner1_i$ sets in the same way as we did with the Top_i and $Inner2_i$ sets. The condition (9.12) attempts to balance the amount of computations needed to hide the communication (e.g. the larger the Top_i set is, the larger the $Inner2_i$ set becomes). It should be noted that the convergence criterion in line 12 is global across all processors.

In Section 4.1.9 several variants of the parallel algorithm are listed. Algorithm 9.3 corresponds to the FULL variant. We might like to relax the bottleneck of LOOP in line 7 of Algorithm 9.3 by replacing it with

```
7.1 SWEEP (Middle_i)
7.2 send (Middle_i)
7.3 receive (Middle_i)
```

so that the middle nodes are processed in an inconsistent manner: the off-processor information corresponds to the previous iteration (just like in the Jacobi method). Usually the $Middle_i$ sets are small and hence this inconsistency does not have to lead to divergence (especially for deformable kinematics, where constraint interactions are weak, while \mathbf{W} is diagonally dominant). This is the MIDDLE_JACOBI variant of the algorithm. The last variant corresponds to a rather gross inconsistency: something usually called "a processor Gauss-Seidel method". Let us define the set

$$All_i = Top_i \cup Bottom_i \cup Middle_i \cup Inner_i$$

$$(9.13)$$

In this case, lines 3-11 of PARALLEL GAUSS SEIDEL from Algorithm 9.3 need to be replaced with

```
3 SWEEP (All_i)
4 send (All_i)
5 receive (All_i)
```

Although this kind of approach does work as a multi-grid smoother, it has little use in our context. Nevertheless, we use for illustration sake and name the BOUNDARY_JACOBI. The final and crudest variant of the solver is called SIMPLIFIED. This variant is devised with soft deformable models in mind. We split constraints into $Contacts_i$ and $Others_i$, hence we separate contact constraints from bilateral ones. We then do the following

```
 \begin{array}{lll} & \text{SWEEP } (Contacts_i) \\ & \text{send } (Contacts_i) \\ & \text{send } (Contacts_i) \\ & \text{do} \\ & \text{SWEEP } (Others_i) \\ & \text{6} & \text{while } \|\mathbf{S}-\mathbf{R}\|/\|\mathbf{R}\| > \epsilon \text{ and } g\left(\mathbf{R}\right) > \gamma \\ \end{array}
```

A single sweep over contacts is followed by the Gauss-Seidel loop over bilateral constraints. This is possible because bilateral constraints migrate together with bodies and hence are local to the processor (an exception is for the rigid link constraint, for which this approach might break down **TODO**).

Algorithm 9.4 Parallel penalty solver.

```
\begin{array}{lll} \operatorname{PARALLEL\_PENALTY\_SOLVER} & (\epsilon) \\ 1 & \operatorname{for\ all} \ \alpha \ \operatorname{in\ } Contacts_i \ \operatorname{do} \\ 2 & \operatorname{SPRING\_DASHPOT} \ (h, gap_\alpha, spring_\alpha, dashpot_\alpha, friction_\alpha, cohesion_\alpha, cohesive_\alpha) \\ 3 & \operatorname{send} \ (Contacts_i) \\ 4 & \operatorname{receive} \ (Contacts_i) \\ 5 & \operatorname{SERIAL\_GAUSS\_SEIDEL} \ (Others_i, \epsilon) \\ 6 & \operatorname{send} \ (Others_i) \\ 7 & \operatorname{receive} \ (Others_i) \end{array}
```

9.2 Penalty solver

The penalty solver is quite straightforward. On each processor we split the constraints into $Contacts_i$ and $Others_i$, hence we separate contact constraints from bilateral ones. We then update the contacts using the spring-dashpot model and calculate reactions of bilateral constraints using a local Gauss-Seidel solver. We use the Gauss-Seidel approach for non-contacts because in this case it is quite fast, while it avoids issues related to penalisation of bilateral constraints. Using Gauss-Seidel is possible because bilateral constraints migrate together with bodies and hence are local to the processor (an exception is for the rigid link constraint, for which this approach might break down **TODO**). Algorithm 9.4 summarises the method.

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