

# Solfec User Manual

Tomasz Koziara

5th January 2010

# Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Installation</b>	<b>5</b>
<b>3</b>	<b>Input language</b>	<b>8</b>
3.1	Solfec objects . . . . .	8
3.1.1	CONVEX . . . . .	8
3.1.2	MESH . . . . .	9
3.1.3	SPHERE . . . . .	10
3.1.4	SOLFEC . . . . .	11
3.1.5	SURFACE_MATERIAL . . . . .	11
3.1.6	BULK_MATERIAL . . . . .	12
3.1.7	BODY . . . . .	13
3.1.8	TIME_SERIES . . . . .	14
3.1.9	GAUSS_SEIDEL_SOLVER . . . . .	14
3.1.10	EXPLICIT_SOLVER . . . . .	16
3.1.11	CONSTRAINT . . . . .	16
3.2	Applying loads . . . . .	19
3.3	Running simulations . . . . .	20
3.4	Utilities . . . . .	21
3.5	Results access . . . . .	25
<b>4</b>	<b>Tutorials</b>	<b>28</b>
4.1	Three basic geometric objects . . . . .	28
4.2	Ball impact . . . . .	31
<b>5</b>	<b>Contact points</b>	<b>35</b>
5.1	Contacts from overlaps . . . . .	35
5.2	Contact sparsification . . . . .	35
<b>6</b>	<b>Materials</b>	<b>37</b>
6.1	Surface materials . . . . .	37
6.1.1	Signorini-Coulomb . . . . .	37
6.1.2	Spring-dashpot . . . . .	38
6.2	Bulk materials . . . . .	38
6.2.1	Kirchhoff - Saint Venant . . . . .	38
<b>7</b>	<b>Solvers</b>	<b>40</b>
7.1	Gauss-Seidel solver . . . . .	40
7.2	Explicit solver . . . . .	40

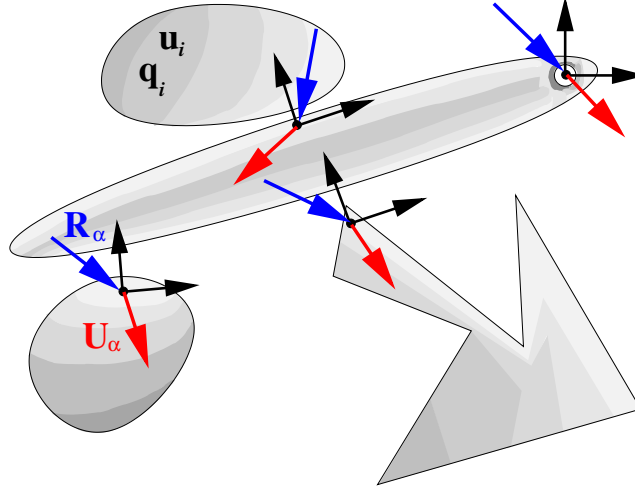
# Chapter 1

## 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 [5] and Jean [2], hence the constraints are solved 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 a figure below



There are four bodies in the figure. Placement of each point of every body is determined by the configuration  $\mathbf{q}_i$ . Velocity of each point of every body is determined by the 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 can be computed as

$$\mathbf{q}(t) = \mathbf{q}(0) + \int_0^t \mathbf{u} dt \quad (1.1)$$

The velocity is determined by integrating Newton's law

$$\mathbf{u}(t) = \mathbf{u}(0) + \mathbf{M}^{-1} \int_0^t \mathbf{f} + \mathbf{H}^T \mathbf{R} dt \quad (1.2)$$

where  $\mathbf{M}$  is an inertia operator,  $\mathbf{f}$  is an out of balance force,  $\mathbf{H}$  is a linear operator, while  $\mathbf{R}$  collects some point forces  $\mathbf{R}_\alpha$ . While integrating the motion of bodies, one keeps track of a number of local coordinate systems (local frames). There are four of them in the figure. Each local frame is related to a pair of points, belonging to two distinct bodies. An observer embedded at a local frame calculates the local relative velocity  $\mathbf{U}_\alpha$  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

$$\mathbf{U} = \mathbf{H}\mathbf{u} \quad (1.3)$$

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

$$\mathbf{C}(\mathbf{U}, \mathbf{R}) = \mathbf{0} \quad (1.4)$$

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

$$\mathbf{q}^{t+\frac{h}{2}} = \mathbf{q}^t + \frac{h}{2} \mathbf{u}^t \quad (1.5)$$

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

$$\mathbf{q}^{t+h} = \mathbf{q}^{t+\frac{h}{2}} + \frac{h}{2} \mathbf{u}^{t+h} \quad (1.7)$$

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 be interpreted as an *integral* of reactions over  $[t, t+h]$ . At a start we have

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

The out of balance force

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

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

$$\mathbf{M} = \mathbf{M}(\mathbf{q}^0) \quad (1.10)$$

is computed once. The linear operator

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

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

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

and

$$\mathbf{W} = \mathbf{H} \mathbf{M}^{-1} \mathbf{H}^T \quad (1.13)$$

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

$$\mathbf{U} = \mathbf{B} + \mathbf{W}\mathbf{R} \quad (1.14)$$

maps constraint reactions  $\mathbf{R}$  into local relative velocities  $\mathbf{U} = \mathbf{H}\mathbf{u}^{t+h}$  at time  $t + h$ . Finally

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

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  $\mathbf{W}$ ,  $\mathbf{B}$ .
4. Solve  $\mathbf{C}(\mathbf{R}) = \mathbf{0}$ .
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  $\mathbf{q}^{t+h} = \mathbf{q}^{t+\frac{h}{2}} + \frac{h}{2}\mathbf{u}^{t+h}$ .

Let us refer the reader to [3] and references therein 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 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 a directory *solfec* in your current directory. The next thing you need is an ANSI C (and prospectively also FORTRAN) 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 (tested) from <http://www.cygwin.com/> or Mingw (not tested) 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*

```
#
# Specify C compiler here
#
CC = cc
#
# Specify FORTRAN compiler here
#
FF = g95
#
# Debug or optimized version switch (yes/no)
#
DEBUG = yes
PROFILE = no
MEMDEBUG = no
GEOMDEBUG = no
PARDEBUG = no
NOTHROW = no
#
# POSIX
#
POSIX = yes
#
```

```

# 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 =
GLLIB = -framework GLUT -framework OpenGL
#
# MPI (yes/no)
#
MPI = yes
MPICC = mpicc
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 *sofec/cfg*. At the current point a FORTRAN compiler is not really needed (there will be a need for it soon though due to planned work). What you need is:

- A C compiler
- **BLAS** and **LAPACK** libraries (standard on most systems)
- **Python** together with development files and libraries
- **OpenGL** libraries and developments files
- **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 *sofec/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 ../Config.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

# 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* (*COPY* (*x*)) leaves *x* intact.

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

### 3.1 Solfec objects

#### 3.1.1 CONVEX

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

**obj** = **CONVEX** (**vertices**, **faces**, **valid** | **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.
- **valid** - 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
<i>obj.nver</i> - number of convex vertices
<i>obj.vertex</i> ( <i>n</i> ) - returns a ( <i>x</i> , <i>y</i> , <i>z</i> ) tuple storing coordinates of <i>n</i> th vertex

**obj = HULL (points, valid, 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*, ...]
- **valid** - volume identifier
- **surfid** - surface identifier common to all faces
- **convex** (emptied) - collection of CONVEX objects appending **obj**

### 3.1.2 MESH

An object of type MESH describes an arbitrary volumetric mesh, comprising tetrahedrons, pyramids, wedges, and hexahedrons (Figure 3.1).

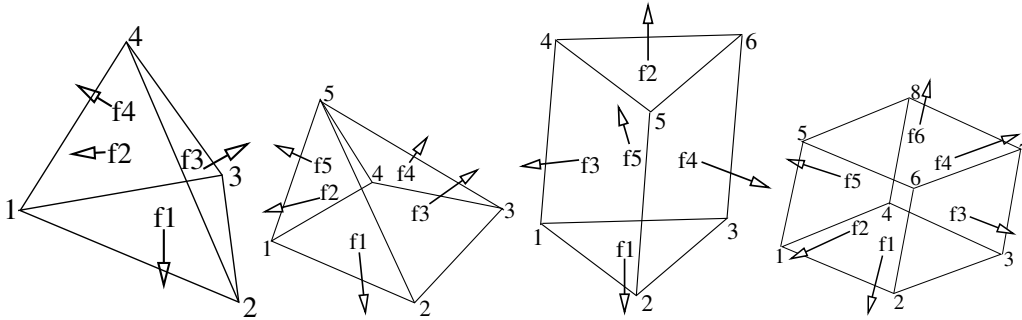


Figure 3.1: Element types in Solfec

**obj = MESH (nodes, elements, surfids)**

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

- **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

<b>Read-only</b> members and methods
<i>obj.nnod</i> - number of mesh nodes
<i>obj.node (n)</i> - returns a $(x, y, z)$ tuple storing coordinates of $n$ th 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:  $[x0, y0, z0, x1, y1, z1, \dots, x7, y7, z7]$ . 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:  $[s1, s2, \dots, s6]$ , 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)  $[cvx1, cvx2, cvx3, \dots]$  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.

### 3.1.3 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
<i>obj.center</i> , <i>obj.radius</i>

### 3.1.4 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
<i>obj.analysis</i>
<i>obj.time</i> - current time
<i>obj.mode</i> - either 'READ' or 'WRITE' as described above
<i>obj.constraints</i> - list of constraints (cf. Section 3.1.11)
<i>obj.ncon</i> - number of constraints
<i>obj.bodies</i> - list of bodies (cf. Section 3.1.7)
<i>obj.nbod</i> - number of bodies
Read/write members
<i>obj.step</i>

### 3.1.5 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)

Model name	Employs variables
'SIGNORINI_COULOMB'	friction, cohesion, restitution (cf. Section 6.1.1)
'SPRING_DASHPOT'	spring, dashpot, friction, cohesion (cf. Section 6.1.2)

Table 3.1: Surface material models.

- **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 3.1 and Chapter 6
- **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)
- **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

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

### 3.1.6 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
- **model** - material model name (default: 'KIRCHHOFF'), see Table 3.2 and Chapter 6
- **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

Model name	Employs variables
'KIRCHHOFF'	young, poisson, density (cf. Section 6.2.1)

Table 3.2: Bulk material models.

<b>Read-only</b> members
<i>obj.model, obj.label</i>
<b>Read/write</b> members
<i>obj.young, obj.poisson, obj.density</i>

### 3.1.7 BODY

An object of type BODY represents a solid body.

**obj = BODY (solfec, kind, shape, material | label, formulation, 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 3.4)
- **label** - a label string (no label is assigned by default)
- **formulation** - valid when **kind** equals 'FINITE\_ELEMENT', ignored otherwise (default: 'FEM\_O1'). This argument specifies a formulation of the finite element method. See Table 3.3.
- **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

<b>Read-only</b> members
<i>obj.kind, obj.label</i>
<b>obj.conf</b> - tuple $(q1, q2, \dots, qN)$ storing configuration of the body. See Table 3.4.
<b>obj.velo</b> - tuple $(u1, u2, \dots, uN)$ storing velocity of the body. See Table 3.5.

Formulation	Remarks
'FEM_O1'	Use first order elements
'FEM_O2'	Use second order elements <b>TODO</b>

Table 3.3: Bulk material models.

Read/write members
<b>obj.selfcontact</b> - self-contact detection flag (default: 'OFF') taking values 'ON' or 'OFF'.
<b>obj.scheme</b> - time integration scheme (default: 'DEFAULT') used to integrate motion. See Table 3.6.
<b>obj.damping</b> - mass proportional damping coefficient (default: 0.0) for the dynamic case.

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 <i>None</i> object.

Table 3.4: 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 <i>None</i> object.

Table 3.5: Types of velocities.

### 3.1.8 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.

- **obj** - created TIME\_SERIES object
- **points** - either a list  $[t0, v0, t1, v1, \dots]$  of points (where  $t_i < t_j$ , when  $i < j$ ), or a path to a file storing times and values pairs

### 3.1.9 GAUSS\_SEIDEL\_SOLVER

An object of type GAUSS\_SEIDEL\_SOLVER represents a nonlinear block Gauss-Seidel solver, employed for the calculation of constraint reactions.

Scheme	Kinematics	Remarks
'DEFAULT'	all	Use a default time integrator regardless of underlying kinematics.
'RIG_POS'	rigid	NEW1 in [4]: explicit, positive energy drift, no momentum conservation
'RIG_NEG'	rigid	NEW2 in [4]: explicit, negative energy drift, exact momentum conservation; <b>default</b> for rigid kinematics
'RIG_IMP'	rigid	NEW3 in [4]: semi-explicit, no energy drift and exact momentum conservation
'DEF_EXP'	pseudo-rigid, finite element	Explicit scheme described in Chapter 5 of [3]; <b>default</b> for deformable kinematics
'DEF_LIM'	pseudo-rigid, finite element	Linearly implicit scheme similar to [1]
'DEF_IMP'	pseudo-rigid, finite element	Implicit scheme similar to [6]

Table 3.6: Time integration schema.

**obj** = **GAUSS\_SEIDEL\_SOLVER** (epsilon, maxiter | failure, diagepsilon, diagmaxiter, diagsolver, data, callback)

This routine creates a **GAUSS\_SEIDEL\_SOLVER** object.

- **obj** - created **GAUSS\_SEIDEL\_SOLVER** object
- **epsilon** - relative accuracy of constraint reactions sufficient for termination
- **maxiter** - maximal number of iterations before termination
- **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 3.7.
- **diagepsilon** - diagonal block solver relative accuracy of constraint reactions (default:  $\epsilon / 100$ )
- **diagmaxiter** - diagonal block solver maximal number of iterations (default:  $\max(100, \text{maxiter} / 100)$ )
- **diagsolver** - diagonal block solver kind (default: 'SEMISMOOTH\_NEWTON'). Available diagonal solvers are 'SEMISMOOTH\_NEWTON', 'PROJECTED\_GRADIENT', 'DE\_SAXE\_AND\_FENG', cf. Chapter 7.
- **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:  $\text{value} = \text{callback}(\text{obj}, \text{data})$ , 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
<i>obj.failure</i>
<b>obj.error</b> - current error code, cf. Table 3.7
<b>obj.itors</b> - number of iterations during a last run of solver
<b>obj.rerhist</b> - if history recording is on, this is a list of relative error values for each iteration of the last run. Otherwise a <i>None</i> object is returned.



<b>Read/write members</b>
<i>obj.epsilon</i> , <i>obj.maxiter</i> , <i>obj.diagepsilon</i> , <i>obj.diagmaxiter</i> , <i>obj.diagsolver</i>
<b><i>obj.history</i></b> - 'ON' or 'OFF' flag switching history recording (default is 'OFF')
<b><i>obj.reverse</i></b> - 'ON' or 'OFF' flag switching iteration reversion modes (whether to alternate backward and forward or not, default is 'OFF')
<b><i>obj.variant</i></b> - variant of parallel Gauss-Seidel update (default: 'FULL'), cf. Table 3.8. 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 3.7: Error codes of GAUSS\_SEIDEL\_SOLVER object

'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 <b>W</b> 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 serves 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 3.8: Variants of parallel Gauss-Seidel update.

### 3.1.10 EXPLICIT\_SOLVER

An object of type EXPLICIT\_SOLVER represents a penalty based constraint solver. 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 = EXPLICIT\_SOLVER ()**

- **obj** - created EXPLICIT\_SOLVER object

### 3.1.11 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 (solfec, body, point)**

This routine creates a fixed point constraint.

- **obj** - created CONSTRAINT object
- **solfec** - **obj** is created for this SOLFEC object
- **body** - BODY object whose motion is constrained
- **point** -  $(x, y, z)$  tuple with referential point coordinates

**obj = FIX\_DIRECTION (solfec, body, point, direction)**

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

- **obj** - created CONSTRAINT object
- **solfec** - **obj** is created for this SOLFEC 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 = FIX\_SURFACE (solfec, body, surfid, direction) TODO**

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

- **obj** - list of created point CONSTRAINT objects
- **solfec** - **obj** is created for this SOLFEC object
- **body** - BODY object whose motion is constrained
- **surfid** - surface identifier
- **direction** -  $(vx, vy, vz)$  tuple defining the direction of load, or 'NORMAL' if load is normal to the surface, or 'TANGENT1' if load acts along the first tangent direction, or 'TANGENT2' if it acts along the second tangent direction. The normal direction ('NORMAL') is outward. The first tangent direction ('TANGENT1') is the one of the steepest descent, or a global  $x$  direction if the surface is horizontal. The second tangent direction ('TANGENT2') is such that the local ('TANGENT1', 'TANGENT2', 'NORMAL') coordinate system is right-handed.

**obj = SET\_DISPLACEMENT (solfec, body, point, direction, tms)**

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

- **obj** - created CONSTRAINT object
- **solfec** - **obj** is created for this SOLFEC 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 (solfec, body, point, direction, value)**

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

- **obj** - created CONSTRAINT object
- **solfec** - **obj** is created for this SOLFEC 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
- **value** - a constant value or a TIME\_SERIES object with the velocity history

**obj = SET\_ACCELERATION (solfec, body, point, direction, tms)**

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

- **obj** - created CONSTRAINT object
- **solfec** - **obj** is created for this SOLFEC 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 (solfec, body1, body2, point1, point2)**

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

- **obj** - created CONSTRAINT object
- **solfec** - **obj** is created for this SOLFEC 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

<b>Read-only members</b>
<b>obj.kind</b> - 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)
<b>obj.R</b> - current average constraint reaction in a form of a tuple: $(RT1, RT2, RN)$ given with respect to a local base stored at <b>obj.base</b>
<b>obj.base</b> - 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
<b>obj.point</b> - 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.
<b>obj.adjbod</b> - adjacent bodies. This is a tuple (body1, body2) of BODY objects for 'CONTACT' and 'RIGLNK' or a single BODY object otherwise.
<b>obj.matlab</b> - surface material label for constraints of kind 'CONTACT', or a <i>None</i> object otherwise.

## 3.2 Applying loads

Routines listed in this section apply loads.

### GRAVITY (solfec, direction, value)

This routine sets up the gravitational acceleration.

- **solfec** - SOLFEC object for which the acceleration is set up
- **direction** -  $(vx, vy, vz)$  tuple defining the direction
- **value** - a number or a TIME\_SERIES object defining the value of the acceleration

### 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 returns a **force** tuple. For rigid body the force reads (*spatial force, spatial torque, referential torque*), while for other kinds 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

**LOAD (body, kind, surfid, direction, value) TODO**

This routine applies a surface load.

- **body** - BODY object to which the load is applied
- **kind** - either 'SPATIAL' or 'CONVECTED'; the *spatial* direction remains fixed, while the *convected* one follows deformation
- **surfid** - the integer surface identifier
- **direction** -  $(vx, vy, vz)$  tuple defining the direction of load, or 'NORMAL' if load is normal to the surface, or 'TANGENT1' if load acts along the first tangent direction, or 'TANGENT2' if it acts along the second tangent direction. The normal direction ('NORMAL') is outward. The first tangent direction ('TANGENT1') is the one of the steepest descent, or a global  $x$  direction if the surface is horizontal. The second tangent direction ('TANGENT2') is such that the local ('TANGENT1', 'TANGENT2', 'NORMAL') coordinate system is right-handed.
- **value** - a number or a TIME\_SERIES object defining the value of the applied load

**3.3 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, EXPLICIT\_SOLVER)
- **duration** - duration of analysis

**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 'FASTLZ'. 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.

- **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:  $\infty$ )

**3.4 Utilities**

Various utility routines are listed below.

**IMBALANCE\_TOLERANCE (solfec, tolerance)**

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)

**num = NCPU ()**

This routine returns the number CPUs used in the analysis.

- **num** - the number of CPUs

**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
- **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  $(x \cdot \text{coefs}[0], y \cdot \text{coefs}[1], z \cdot \text{coefs}[2])$  tuple.
- **shape** - object, collection of objects, or a list  $[a, b, c, \dots]$  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  $(x + \text{vector}[0], y + \text{vector}[1], z + \text{vector}[2])$  tuple.
- **shape** - object, collection of objects, or a list  $[a, b, c, \dots]$  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  $[a, b, c, \dots]$  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)**

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  $[a, b, c, \dots]$  of objects of type CONVEX or SPHERE
- **point** -  $(px, py, pz)$  tuple defining a point passed by the splitting plane
- **normal** -  $(nx, ny, nz)$  tuple defining the splitting plane normal

**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  $[a, b, c, \dots]$  of objects of type CONVEX, MESH, SPHERE

**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.

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

**CONTACT\_EXCLUDE\_BODIES (solfec, 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).*

- **solfec** - SOLFEC object
- **body1** - first BODY object
- **body2** - second BODY object

**CONTACT\_EXCLUDE\_OBJECTS (solfec, 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).*

- **solfec** - SOLFEC object
- **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)**

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 5.2).

- **solfec** - SOLFEC object
- **threshold** - sparsification threshold (default: 0.01) from within the interval [0, 1]. Zero corresponds to the lack of sparsification.

**3.5 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** - ( $t_0, t_1$ ) 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 | 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.

- **tim** - value of timing
- **solfec** - SOLFEC object
- **kind** - this is one of: 'TIMINT' (time integration), 'CONDET' (contact detection), 'LOCODYN' (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)**

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', 'CONDET', 'LOCDDYN', 'CONSOL', 'PARBAL' for timing histories
- **t0** - time interval start
- **t1** - time interval end
- **skip** - number of steps to skip between two time instants

## Chapter 4

# Tutorials

### 4.1 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.

```
w = 10
l = 10
h = 1
floor_vid = 1
floor_sid = 1
floor = HULL ([-w/2, -l/2, -h,
               w/2, -l/2, -h,
               w/2,  l/2, -h,
               -w/2,  l/2, -h,
               -w/2, -l/2,  0,
               w/2, -l/2,  0,
               w/2,  l/2,  0,
               -w/2,  l/2,  0], floor_vid, floor_sid)
```

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.

```
step = 1E-3
solfec = SOLFEC ('DYNAMIC', step, 'out/tutorail/three-basic-geometric-objects')
bulk = BULK_MATERIAL (solfec,
                      model = 'KIRCHHOFF',
                      young = 15E9,s
                      poisson = 0.3,
                      density = 2E3)
BODY (solfec, 'OBSTACLE', floor, bulk)
```

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



Let 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:  $b1, b2, \dots, b4$ . 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.

```

nodes = [-1.0, -1.0, 0.0,
         1.0, -1.0, 0.0,
         1.0, 1.0, 0.0,
         -1.0, 1.0, 0.0,
         -1.0, -1.0, 2.0,
         1.0, -1.0, 2.0,
         1.0, 1.0, 1.0,
         -1.0, 1.0, 1.0]
mesh = HEX (nodes, 2, 3, 2, 3, [3, 3, 3, 3, 3, 3], dy = [1, 1, 2])
TRANSLATE (mesh, (0, 0, c))
BODY (solfec, 'PSEUDO_RIGID', mesh, bulk)

```

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.

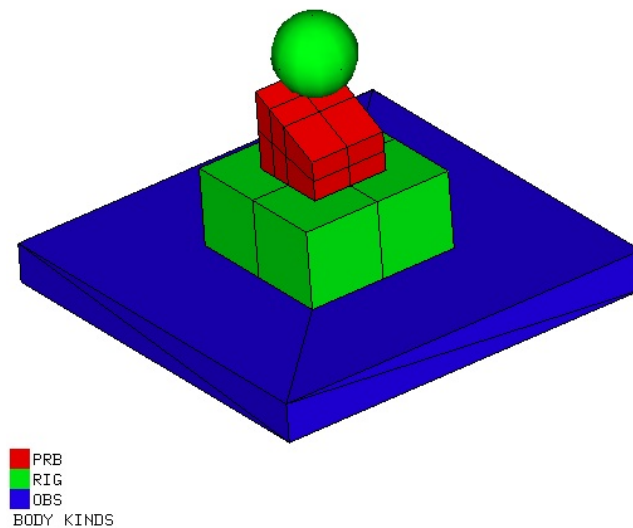
```

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.

t=0



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

```
SURFACE_MATERIAL (solfec, model = 'SIGNORINI_COULOMB',
                  friction = 0.5, restitution = 0.0)
```

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

```
GRAVITY (solfec, (0, 0, -1), 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)
```

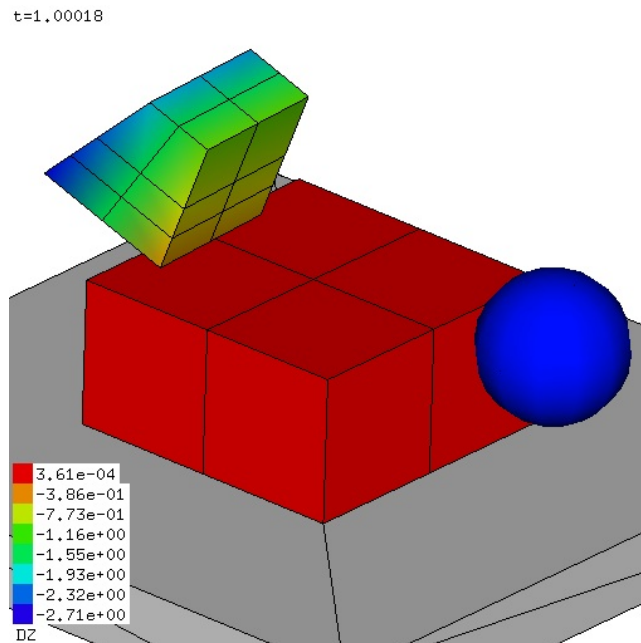
The relative constraint reaction accuracy was set to 1E-3, while the maximal the maximal number of iterations is 1000. It remains to run the simulation.

```
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.



## 4.2 Ball impact

This example illustrates using multiple SOLFEC objects, application of the EXPLICIT\_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
    l = 2
    h = 1
    floor_vid = 1
    floor_sid = 1
    floor = HULL ([-w/2, -l/2, -h,
                  w/2, -l/2, -h,
                  w/2, l/2, -h,
                  -w/2, l/2, -h,
                  -w/2, -l/2, 0,
                  w/2, -l/2, 0,
                  w/2, l/2, 0,
                  -w/2, l/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, -1), 10)

    xs = EXPLICIT_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 *sphere\_impact*. 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 *sphere\_impact* function. It should be noted, that the SOLFEC object is returned from the routine. Now, here is the main module

```

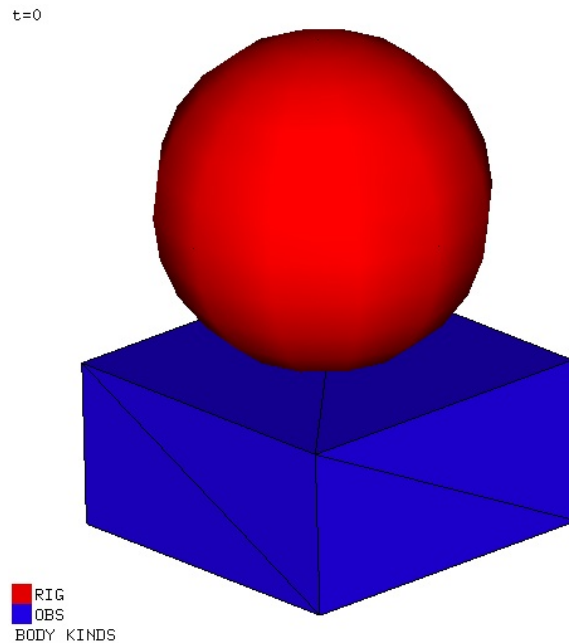
stop = 2.0
sol1 = ball_impact (1E-3, stop, 1E+9, 0E0, 'out/tutorial/sphere-impact-1')
sol2 = ball_impact (1E-3, stop, 1E+9, 1E6, 'out/tutorial/sphere-impact-2')
sol3 = ball_impact (1E-3, stop, 1E+9, 1E7, 'out/tutorial/sphere-impact-3')

```

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/ball-impact.eps', format = 'eps')
```

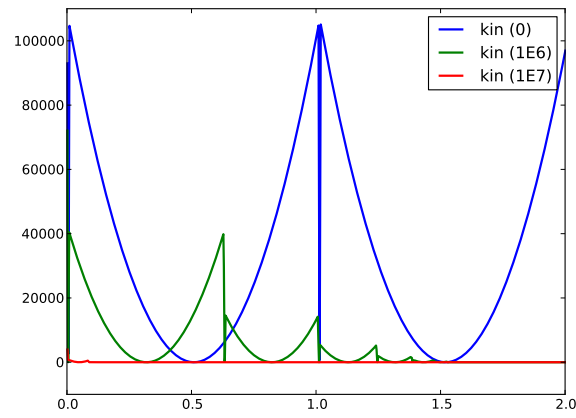
First, we check whether Solfec is not run with the *-v* option and whether it is in 'READ' mode. This is the case, when after running the complete analysis

```
./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/sphere-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 is plotted into an EPS file, visible below.



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

## Chapter 5

# Contact points

### 5.1 Contacts from overlaps

Body shapes are juxtapositions of convex objects (Sections 3.1.1, 3.1.2, 3.1.3). A contact point and normal direction result from an overlap of two convex objects (Figure 5.1). 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 [3] for more details.



Figure 5.1: A contact point and normal direction extracted from an intersection of two convex objects.

### 5.2 Contact sparsification

Let us have a look at an arch in Figure 5.2. 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 5.3. If one would have to generate contact points by hand, they would probably look like those on the right in Figure 5.3. A heuristic sparsification algorithm filters out redundant contact points.

```

for each contact1 do
  for each body adjacent to contact1 do
    for each contact2 adjacent to body do
      if contact1 = contact2 skip
      if area(contact1) < threshold · area(contact2) and
         topologically_adjacent(contact1, contact2) then remove contact1
      else if point(contact1) = point(contact2) 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 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 3.4).

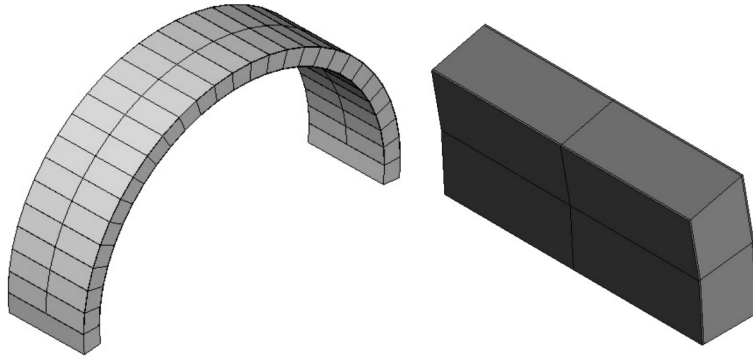


Figure 5.2: An arch and a detail of two bricks. Note the narrow meshing near the edge of inner and outer boundaries.

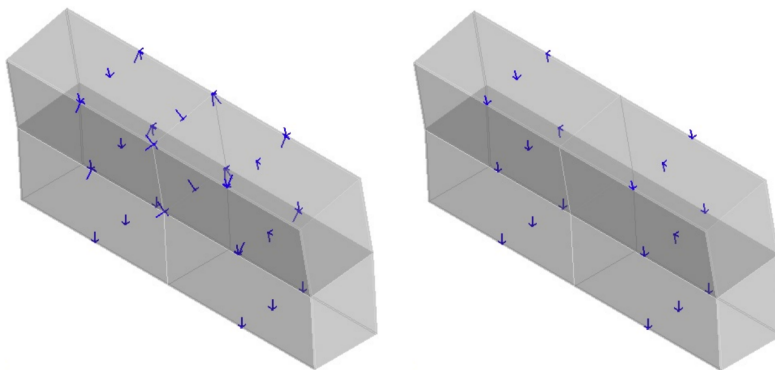


Figure 5.3: A detail of the arch from Figure 5.2. Contact points on the left are not sparsified. Contact points on the right are sparsified.

# Chapter 6

## Materials

### 6.1 Surface materials

A surface material is assigned to a pairing of surfaces. See Section 3.1.5 for the input syntax.

#### 6.1.1 Signorini-Coulomb

The velocity Signorini condition reads

$$\bar{U}_N \geq 0 \quad R_N \geq 0 \quad \bar{U}_N R_N = 0 \quad (6.1)$$

where  $\bar{U}_N = U_N^{t+h} + \eta \min(0, U_N^t)$ ,  $\eta$  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 (6.1) 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 [3]). The Coulomb's friction law reads

$$\begin{cases} \|\mathbf{R}_T\| \leq \mu R_N \\ \|\mathbf{R}_T\| < \mu R_N \Rightarrow \mathbf{U}_T = \mathbf{0} \\ \|\mathbf{R}_T\| = \mu R_N \Rightarrow \exists_{\lambda \geq 0} \mathbf{U}_T = -\lambda \mathbf{R}_T \end{cases} \quad (6.2)$$

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

$$\mathbf{C}(\mathbf{U}, \mathbf{R}) = \begin{bmatrix} \max(\mu d_N, \|\mathbf{d}_T\|) \mathbf{R}_T - \mu \max(0, d_N) \mathbf{d}_T \\ R_N - \max(0, d_N) \end{bmatrix} \quad (6.3)$$

where  $\rho > 0$  and

$$d_N = R_N - \rho \bar{U}_N \quad (6.4)$$

$$\mathbf{d}_T = \mathbf{R}_T - \rho \mathbf{U}_T \quad (6.5)$$

We refer the reader to Chapter 10 of [3] for more details.

### 6.1.2 Spring-dashpot

The normal reaction is computed as follows

$$R_N = -spring \cdot gap - dashpot \cdot \frac{U_N^{t+h} + U_N^t}{2} \quad (6.6)$$

where  $U_N$  is the normal relative velocity. We use the diagonal block of local dynamics

$$\mathbf{U}^{t+h} = \mathbf{B} + \mathbf{W}\mathbf{R} \quad (6.7)$$

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

$$U_N^{t+h} = B_N + \mathbf{W}_{NT}\mathbf{R}_T + W_{NN}R_N \quad (6.8)$$

where a previous tangential reaction  $\mathbf{R}_T$  is employed. Inserting this it into (6.6) results in

$$R_N = [-spring \cdot gap - 0.5 \cdot dashpot \cdot (B_N + \mathbf{W}_{NT}\mathbf{R}_T + U_N^t)] / [1 + 0.5 \cdot dashpot \cdot W_{NN}] \quad (6.9)$$

We then utilise the tangential part of local dynamics and assuming  $\mathbf{U}_T^{t+h} = 0$  estimate the tangential stick reaction

$$\mathbf{R}_T = -\mathbf{W}_{TT}^{-1}(\mathbf{B}_T + \mathbf{W}_{TN}R_N) \quad (6.10)$$

Let  $\mu$  stand for the coefficient of friction. The complete interface law reads

```

if not cohesive and gap ≥ 0 then R = 0
else
   $R_N = [-spring \cdot gap - 0.5 \cdot dashpot \cdot (B_N + \mathbf{W}_{NT}\mathbf{R}_T + U_N^t)] / [1 + 0.5 \cdot dashpot \cdot W_{NN}]$ 
  if not cohesive and  $R_N < 0$  then  $R_N = 0$ 
   $\mathbf{R}_T = -\mathbf{W}_{TT}^{-1}(\mathbf{B}_T + \mathbf{W}_{TN}R_N)$ 
  if cohesive and  $|R_N| > cohesion$  then cohesive = false
  if not cohesive and  $\|\mathbf{R}_T\| > \mu R_N$  then  $\mathbf{R}_T = \mu R_N \mathbf{R}_T / \|\mathbf{R}_T\|$ 

```

We refer the reader to Chapter 7 of [3] for more details on local dynamics.

## 6.2 Bulk materials

A bulk material is assigned to a volume. See Section 3.1.6 for the input syntax.

### 6.2.1 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  $\Psi$  of the Kirchhoff - Saint Venant materials reads

$$\Psi = \frac{1}{4} [\mathbf{F}^T \mathbf{F} - \mathbf{I}] : \mathbf{C} : [\mathbf{F}^T \mathbf{F} - \mathbf{I}] \quad (6.11)$$

where

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu [\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}] \quad (6.12)$$

In the above  $\lambda$  and  $\mu$  are Lamé constants, while  $\delta_{ij}$  is the Kronecker delta. The Lamé constants can be expressed in terms of the Young modulus  $E$  and the Poisson ratio  $\nu$  as

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad (6.13)$$

$$\mu = \frac{E}{2 + 2\nu} \quad (6.14)$$

The first Piola stress tensor is computed as a gradient of the hyperelastic potential  $\Psi$

$$\mathbf{P} = \partial_{\mathbf{F}} \Psi(\mathbf{F}) \quad (6.15)$$

where  $\mathbf{F}$  is the deformation gradient.



## Chapter 7

# Solvers

### 7.1 Gauss-Seidel solver

### 7.2 Explicit solver

# Bibliography

- [1] Mihai Anitescu Bogdan Gavrea Jeff Trinkle Florian A. Potra. A linearly implicit trapezoidal method for integrating stiff multibody dynamics with contact, joints, and friction. *International Journal for Numerical Methods in Engineering*, 66:1079–1124, 2006.
- [2] M. Jean. The non-smooth contact dynamics method. *Computer Methods in Applied Mechanics and Engineering*, 177(3-4):235–257, 1999.
- [3] Tomasz Koziara. *Aspects of computational contact dynamics*. PhD thesis, University of Glasgow, <http://theses.gla.ac.uk/429/>, 2008.
- [4] Tomasz Koziara and Nenad Bićanić. Simple and efficient integration of rigid rotations suitable for constraint solvers. *To appear in the International Journal for Numerical Methods in Engineering*, 2009.
- [5] J. J. Moreau. Numerical aspects of the sweeping process. *Computer Methods in Applied Mechanics and Engineering*, 177(3-4):329–349, 1999.
- [6] T. A. Laursen V. Chawla. Energy consistent algorithms for frictional contact problems. *International Journal for Numerical Methods in Engineering*, 42:799–827, 1998.