## Solfec User Manual

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## 1 Introduction

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.

#### 2.1 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

#### **2.2 MESH**

An object of type MESH describes an arbitrary volumetric mesh, comprising tetrahedrons, pyramids, wedges, and hexahedrons (Figure 2.1).

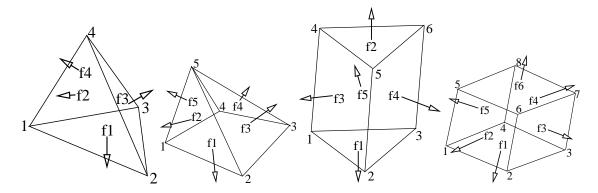


Figure 2.1: Element types in Solfec

#### 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

| Read-only members and methods  |  |  |
|--|--|--|
| obj.nnod - number of mesh nodes  |  |  |
| $oxed{obj.node\ (n)}$ - 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 inerpolation.
- $\bullet$  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 normalized (actual numbers do not matter, but their ratios) and applied to the local x direction of the generated shape.

#### 2.3 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        |  |  |

#### 2.4 SOLFEC

An object of type SOLFEC represents the Solfec algorithm. One can use several SOLFEC objects to run several analyzes 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 2.11) |  |  |
| obj.ncon - number of constraints                         |  |  |
| obj.bodies - list of bodies (cf. Section 2.7)            |  |  |
| obj.nbod - number of bodies                              |  |  |

| Read/write members |  |
|--------------------|--|
| obj.step           |  |

## 2.5 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\_COULMB'), see Table 2.1 and Chapter 4
- 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)

| Model name          | Employs variables                   |
|---------------------|-------------------------------------|
| 'SIGNORINI_COULOMB' | friction, cohesion, restitution     |
| 'SPRING_DASHPOT'    | spring, dashpot, friction, cohesion |

Table 2.1: Surface material models.

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   |  |  |

## 2.6 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 2.2 and Chapter 4
- 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 |                          |  |
|--------------------|--------------------------|--|
| obj.young,         | obj.poisson, obj.density |  |

| Model name  | Employs variables       |
|-------------|-------------------------|
| 'KIRCHHOFF' | young, poisson, density |

Table 2.2: Bulk material models.

#### **2.7 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', 'ROUGH\_FINITE\_ELEMENT', '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', only a single MESH object can be given. If the **kind** is 'ROUGH\_FINITE\_ELEMENT' then **shape** must composed of CONVEX objects.
- 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 2.14)
- label a label string (no label is assigned by default)
- formulation valid when kind equals 'FINITE\_ELEMENT' or 'ROUGH\_FINITE\_ELEMENT', ignored otherwise (default: 'HEX\_TET\_O1'). This argument specifies a formulation of the finite element method. See Table 2.3.
- mesh necessary when kind equals 'ROUGH\_FINITE\_ELEMENT', ignored otherwise. This variable must be a MESH object describing a "rough" finite element mesh properly containing the shape. The 'ROUGH\_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 2.4.  |
| obj.velo - tuple (u1, u2,, uN) storing velocity of the body. See    |
| Table 2.5.  |

| Formulation  | Remarks                            |
|--------------|------------------------------------|
| 'TET_O1'     | Use first order tetrahedrons only  |
| 'TET_O2'     | Use second order tetrahedrons only |
| 'HEX_TET_O1' | Use first order hexahedrons        |
|              | whenever possible or tetrahedrons  |
|              | otherwise                          |

Table 2.3: Bulk material models.

| Read/write members  |  |
|---|--|
| obj.selfcontact - self-contact detection flag (default: 'OFF") taking |  |
| values 'ON' or 'OFF'.   |  |
| obj.scheme - time integration scheme (default: 'DEFAULT') used to     |  |
| integrate motion. See Table 2.6.                                      |  |

| 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.                |
| 'ROUGH_FINITE_ELEMENT' | Current coordinates x, y, z of rough mesh  |
|                        | nodes.                                     |
| 'FINITE_ELEMENT'       | Current coordinates x, y, z of mesh nodes. |
| 'OBSTACLE'             | Python <i>None</i> object.                 |

Table 2.4: Types of configurations.

## 2.8 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

| 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.         |
| 'ROUGH_FINITE_ELEMENT' | Components x, y, z of spatial velocities of  |
|                        | rough mesh nodes.                            |
| 'FINITE_ELEMENT'       | Components x, y, z of spatial velocities of  |
|                        | mesh nodes.                                  |
| 'OBSTACLE'             | Python <i>None</i> object.                   |

Table 2.5: Types of velocities.

| Scheme    | Body kind | Remarks                                       |
|-----------|-----------|---|
| 'DEFAULT' | all       | Use a default time integrator regardless of   |
|           |           | underlying kinematics.                        |
| 'RIG_POS' | 'RIGID'   | NEW1 in [1]: explicit, positive energy drift, |
|           |           | no momentum conservation                      |
| 'RIG_NEG' | 'RIGID'   | NEW2 in [1]: explicit, negative energy        |
|           |           | drift, exact momentum conservation;           |
|           |           | default for rigid kinematics                  |
| 'RIG_IMP' | 'RIGID'   | NEW3 in [1]: semi-explicit, no energy drift   |
|           |           | and exact momentum conservation               |

Table 2.6: Time integration schema.

## 2.9 GAUSS SEIDEL SOLVER

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

# 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 othewise the 'EXIT' scenario is executed). In all cases *obj.error* variable is set up, cf. Table 2.7.

- diagepsilon diagonal block solver relative accuracy of constraint reactions (default: epsilon / 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 SAXE AND FENG', cf. Chapter 5.
- 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

 ${\it obj.error}$  - current error code, cf. Table 2.7

obj.iters - number of iterations during a last run of solver

**obj.rerhist** - if history recording is on, this is a list of relative error values for each iteration of the last run. Otherwise a *None* object is returned.

#### Read/write members

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

obj.history - 'ON' or 'OFF' flag switching history recording (default is 'OFF')

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

*obj.variant* - a variant of parallel algorithm (ignored during sequential runs, dafult: 'MID LOOP'), cf. Table 2.8

## 2.10 EXPLICIT\_SOLVER

An object of type EXPLICIT\_SOLVER represents a penlaty based constraint solver. When in use, all 'SIGNORONI\_COULOMB' type contact interfaces are regarded as 'SPRING\_DASHPOT' ones. One should then remember about specyfying the *spring* value for those.

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

Table 2.7: Error codes of GAUSS\_SEIDEL\_SOLVER object

| 'MID_LOOP'   | Process mid-nodes in a semi-sequential loop with processor coloring    |  |
|--------------|--|--|
| 'MID_THREAD' | Process the loop in a separate thread                                  |  |
| 'MID_TO_ALL' | Gather mid nodes at all processors                                     |  |
| 'MID_TO_ONE' | MID_TO_ONE' Gather mid nodes at one processor (with smallest load)     |  |
| 'NOB_*'      | e.g. 'NOB_MID_LOOP', etc. Use non-blocking communication when possible |  |

Table 2.8: Error codes of GAUSS SEIDEL SOLVER object

#### obj = EXPLICIT SOLVER ()

• obj - created EXPLICIT SOLVER object

#### 2.11 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 constrint.

- 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, tms)

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
- tms 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

#### 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 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.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.

### 2.12 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 *spactial* 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 *spactial* 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 *spactial* 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

### 2.13 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:  $\infty$ )

#### 2.14 Utilities

Various utility routines are listed below.

#### IMBALANCE TOLERANCES (solfec, timint, condet, locdyn)

This routine sets the imbalance tolerances 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
- timint time integration imbalance tolerance (default: 1.3)
- condet contact detection imbalance tolerance (default: 1.3)
- locdyn local dynamics imbalance tolerance (default: 1.3)

#### LOCDYN BALANCING (solfec, mode)

This routine sets the mode of local dynamics balancing for a parallel run. It is ignored in sequential mode.

- solfec SOLFEC object
- mode 'OFF' disables balancing (in this case geometrical balancing related to contact detection is inherited by local dynamics), 'GEOM' enables geometrical balancing based on spatial constraint points, 'GRAPG' enables topological balancing based on the adjacency structure of the **W** operator.

#### 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 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 sometimes 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**  $(t_{11}, t_{21}, ..., t_{33})$  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.
- 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.
- 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.
- 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, ...] 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 coppied objects
- shape object, collection of objects, or a list [a, b, c, ...] of objects of type CONVEX, MESH, SPHERE

#### obj = BYLABEL (solfec, kind, label)

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

- **obj** returned object (*None* if a labeled object was not found)
- solfec SOLFEC object
- kind labeled 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, ...] 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.

- 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.

- solfec SOLFEC object
- body1 first BODY object
- point1 referential point properly contained in the 1st geometric object
- bod2 second BODY object
- point2 referentail 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.

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

#### 2.15 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.

- $\operatorname{disp}$  (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

#### hist = HISTORY (body, point, entity, t0, t1)

This routine outputs the history of an entity at a referential point.

- hist a tuple of list objects storing the history of the entity: (times, values)
- body BODY object
- **point** (x, y, z) tuple storing the referential point
- entity this is one of: 'DX', 'DY', 'DZ' (displacement), 'VX', 'VY', 'VZ' (velocity), 'SX', 'SY', 'SZ', 'SXY', 'SXZ', 'SYZ' (stress), 'MISE' (von Mises norm of stress)
- t0 time interval start
- $\bullet$  **t1** time interval end

#### ene = ENERGY (obj, kind) TODO

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

- ene value of the energy
- obj this can be: a SOLFEC object, a BODY object, or a list of BODY objects
- **kind** this is one of: 'KINETIC', 'POTENTIAL', 'EXTWORK' (work of external forces, including friction), 'FRICWORK' (work of friction forces)

#### hist = ENERGY HISTORY (obj, kind, t0, t1) TODO

This routine outputs the history of energy for a collection of objects.

- hist a tuple of list objects storing the history of the entity: (times, values)
- obj this can be: a SOLFEC object, a BODY object, or a list of BODY objects
- kind same as kind in ENERGY routine
- $\bullet$  **t0** time interval start
- $\bullet$  **t1** time interval end

#### 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), 'LOCDYN' (local dynamics setup), 'CONSOL' (constraints solution), 'TIMBAL' (time integration balancing), 'CONBAL' (contact detection balancing), 'LOCBAL' (local dynamics balancing). The balancing timings are non-zero only for parallel runs.

### hist = TIMING HISTORY (solfec, kind, t0, t1)

This routine outputs the history of timing.

- hist a tuple of list objects storing the history of timing: (times, values)
- solfec SOLFEC object
- kind same as kind in TIMING routine
- t0 time interval start
- $\bullet$  **t1** time interval end

## 3 Parallelism

## 4 Material models

## 5 Solvers

# 6 Examples

## Bibliography

[1] 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.