MuPIF.org Platform User Manual

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2. Introduction

MuPIF (www.mupif.org) is an integration framework, that facilitates the implementation of multi-physic and multi-level simulation workflows, built from independently developed components. MuPIF is open source, distributed under LGPL license.

The approach followed in the MuPIF is based on an system of distributed, interacting objects designed to solve given problem. The individual objects represent entities in the problem domain, including individual simulation packages, but also the data, such as fields and properties. The abstract classes are introduced for all entities in the model space [1]. They define a common interface, called API, that needs to be implemented by any derived class, representing particular implementation of specific component. Such interface concept allows using any derived class on a very abstract level, using common services defined by abstract class, without being concerned with the implementation details of an individual software component. The APIs have been developed not only for individual models, but also for simulation data, like spatial fields, properties, etc.

The complex simulation pipeline developed in MuPIF-platform consists of top-level script in Python language [3] (called scenario) enriched by newly introduced classes. Later in the project, the top level script will be generated using a graphical tool. In principle, any control script can be recasted into a class implementing Application class interface, so that it could itself represent an application in MuPIF platform. Such an approach would allow building a hierarchy of nested applications. The application steering and data exchange will be realized in a standard way by calling individual services (methods). In case of distributed environments, a transparent communication layer is provided, as described in the subsection on Distributed environments. The software design of the platform has been described in [5,6,7].

Even though the platform can be used locally on a single computer orchestrating installed applications, the real strength of the MuPIF platform is its distributed design, allowing to execute simulation scenarios involving remote applications. The concept of so called proxy object that represent remote objects allows to hide all the details of remote data exchange and execution to the user. In turn, only minimal change of local simulation scenarios is required when distributed resources are included. The distributed model is described in Section Distributed Model.

3. Platform installation

3.1. Prerequisites

3.1.1. Windows platforms

- We suggest to install Anaconda scientific python package, which includes Python ≥3.4, https://store.continuum.io/cshop/anaconda/
- Ssh client: putty.exe is recommended, http://www.putty.org/
- Optionally ssh key generator: puttygen.exe is recommended, http://www.putty.org/

- Optionally ssh server if you need to accept SSH incoming connections and allowing others to be on your system. FreeSSHd server is recommended, http://www.freesshd.com/

3.1.2. Linux / Unix (*nix) platforms

- The Python (Python ≥3.4) installation is required.
- You can download the python installation package from https://www.python.org/downloads/. Just pick up the latest version in the 3.x series (tested version 3.5.2).
- We recommend to install *pip* - a tool for installing and managing Python packages. If not already installed as a part of your python distribution, the installation instructions can be found here.
- Ssh client (normally included in standard distributions)
- Optionally ssh server (required for application server installation)
- VPN server or VPN client if VPN connection is preferred, e.g. https://openvpn.net/index.php/open-source/downloads.html

3.1.3. General requirements

- MuPIF platform depends/requires, besides others, Pyro4 and numpy modules. They can be installed separately for a particular system or using *pip*. If you install the whole MuPIF package, it takes care automatically for all dependencies. However, using *git* repository requires those Python modules to installed separately. For example, to install Pyro4 version 4.54:

```
pip install Pyro4==4.54
```

- MuPIF platform requires pyvtk (tested 0.4.85) python module. To install this module using *pip*:

```
pip install pyvtk
```

- MuPIF requires enum34 module, which can be installed also using *pip*:

```
pip install enum34
```

3.1.4. Other recommended packages/softwares

- Paraview (tested 4.2.0), visualization application for vtu data files, http://www.paraview.org/
- Windows: Notepad++ (tested 6.6.9), http://notepad-plus-plus.org/
- Windows: conEmu, windows terminal emulator, https://code.google.com/p/conemu-maximus5/

3.2. Installing the MuPIF platform

The recommended procedure is to install platform as a python module using *pip*:

```
pip install mupif
```

This type of installation automatically satisfies all the dependencies.

Alternatively, the development version of the platform can be installed from *git* repository:

- We recommend to install git, a open source revision control tool. You can install git using your package management tool or download installation package directly from git website.
- Once you have git installed, just clone the MuPIF platform repository into a directory "mupif-code":

```
git clone https://github.com/mupif/mupif.git mupif
```

3.3. Verifying platform installation

3.3.1. Running unit tests

MuPIF platform comes with unit tests. To run unit tests we recommend to install *nose* python module, which facilitates automatic discovery and execution of individual tests. To install node module using pip:

```
pip install nose
```

This will install the nose libraries, as well as the *nosetests* script, which can be used to execute the unit tests. From top level MuPIF installation directory enter:

```
cd tests
nosetests -v
```

You should see output something like this:

```
test_containsPoint (mupif.tests.test_BBox.BBox_TestCase) ... ok
test_intersects (mupif.tests.test_BBox.BBox_TestCase) ... ok
test_merge (mupif.tests.test_BBox.BBox_TestCase) ... ok
test_containsPoint (mupif.tests.test_Cell.Triangle_2d_lin_TestCase) ... ok
test_geometryType (mupif.tests.test_Cell.Triangle_2d_lin_TestCase) ... ok
test_glob2loc (mupif.tests.test_Cell.Triangle_2d_lin_TestCase) ... ok
test_interpolate (mupif.tests.test_Cell.Triangle_2d_lin_TestCase) ... ok
…..
testOctreeNotPickled (mupif.tests.test_saveload.TestSaveLoad) ... ok
----------------------------------------------------------------------
Ran 82 tests in 2.166s

OK
```

Indicating that *nose* found and ran listed tests successfully.

3.3.2. Running examples

In addition, the platform installation comes with many examples, that can be used to verify the successful installation as well, but they also serve as an educational examples illustrating how to use the platform. The examples are located in examples subfolder. For example, to run Example01:

```
cd examples/Example01
python Example01.py
```

4. Platform operations

The complex simulation pipeline developed in MuPIF-platform consists of top-level script in Python language (called scenario) enriched by newly introduced classes. These classes represent fundamental entities in the model space (such as simulation tools, properties, fields, solution steps, interpolation cells, units, etc). The top level classes are defined for these entities, defining a common interface allowing to manipulate individual representations using a single common interface. The top level classes and their interface is described in platform Interface Specification document [1].

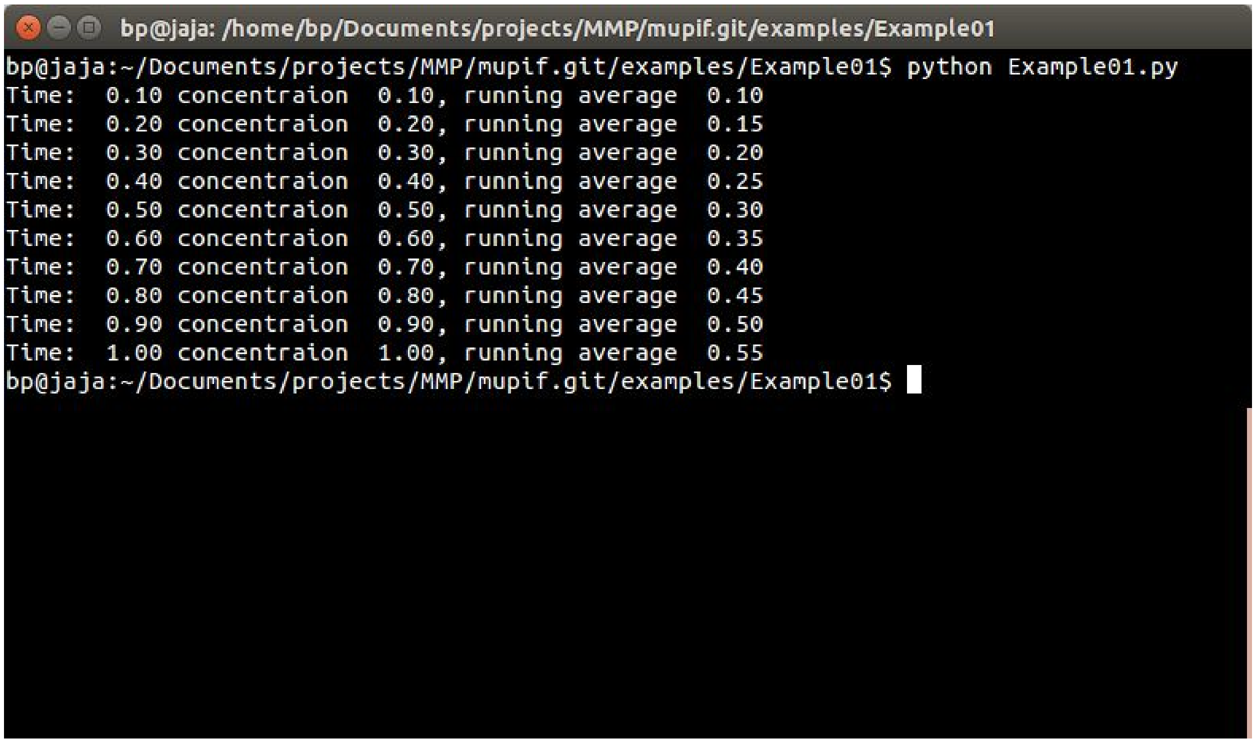
In this document, we present a simple, minimum working example, illustrating the basic concept. The example presented in this section is assumed to be executed locally. How to extend these examples into distributed version is discussed in the section 8. Distributed Model.

The presented example in Listing 1 illustrates an example of so called weak-coupling, where for each solution step, the first application (Application1) evaluates the value of concentration that is passed to the second application (Application2) which, based on provided concentration values (PropertyID.PID_Concentration), evaluates the average cumulative concentration (PropertyID.PID_CumulativeConcentration). This is repeated for each solution step. The example also illustrates, how solution steps can be generated in order to satisfy time step stability requirements of individual applications.

```
from mupif import *
import application1
import application2

time  = 0
timestepnumber=0
targetTime = 1.0

app1 = application1.application1(None) # create an instance of application #1
app2 = application2.application2(None) # create an instance of application #2
```

```
# loop over time steps
while (abs(time -targetTime) > 1.e-6):
       #determine critical time step
       dt2 = app2.getCriticalTimeStep()
       dt = min(app1.getCriticalTimeStep(), dt2)
       #update time
       time = time+dt
       if (time > targetTime):
              #make sure we reach targetTime at the end
              time = targetTime
       timestepnumber = timestepnumber+1

       # create a time step
       istep = TimeStep.TimeStep(time, dt, timestepnumber)

       try:
              #solve problem 1
              app1.solveStep(istep)
              #request temperature field from app1
              c = app1.getProperty(PropertyID.PID_Concentration, istep)
              # register temperature field in app2
              app2.setProperty (c)
              # solve second sub-problem
              app2.solveStep(istep)
              prop = app2.getProperty(PropertyID.PID_CumulativeConcentration, istep)
              print ("Time: %5.2f concentraion %5.2f, running average %5.2f" %
                     (istep.getTime(), c.getValue(), prop.getValue()))

       except APIError.APIError as e:
              logger.error("Following API error occurred: %s" % e )
              break

# terminate
app1.terminate();
app2.terminate();
```
Listing 1: Simple example illustrating simulation scenario

The full listing of this example can be found in examples/Example01. The output is illustrated in Fig. 1.


bp@jaja: /home/bp/Documents/projects/MMP/mupif.git/examples/Example01

```
bp@jaja:~/Documents/projects/MMP/mupif.git/examples/Example01$ python Example01.py
Time:  0.10 concentraion  0.10, running average  0.10
Time:  0.20 concentraion  0.20, running average  0.15
Time:  0.30 concentraion  0.30, running average  0.20
Time:  0.40 concentraion  0.40, running average  0.25
Time:  0.50 concentraion  0.50, running average  0.30
Time:  0.60 concentraion  0.60, running average  0.35
Time:  0.70 concentraion  0.70, running average  0.40
Time:  0.80 concentraion  0.80, running average  0.45
Time:  0.90 concentraion  0.90, running average  0.50
Time:  1.00 concentraion  1.00, running average  0.55
bp@jaja:~/Documents/projects/MMP/mupif.git/examples/Example01$
```

Fig. 1: Output from Example01.py

The platform installation comes with many examples, located in *examples* subdirectory of platform installation and also accessible online in the platform repository. They illustrate various aspects, including field mapping, vtk output, etc.

5. Platform APIs

In this chapter are presented the abstract interfaces (APIs) of abstract classes that have been designed to represent basic building blocks of the complex multi-physics simulations, including individual simulation packages, but also the high level complex data (such as spatial fields and properties). The abstract base classes are defined for all relevant entities. Their primary role is to define abstract interfaces (APIs), which allow manipulating individual objects using generic interface without being concerned by internal details of individual instances. One of the key and distinct features of the MuPIF platform is that such an abstraction (defined by top level classes) is not only developed for individual models, but also defined for the simulation data themselves. The focus is on services provided by objects and not on underlying data. The object representation of data encapsulates the data themselves, related metadata, and related algorithms. Individual models then do not have to interpret the complex data themselves; they receive data and algorithms in one consistent package. This also allows the platform to be independent of particular data format, without requiring any changes on the model side to work with new format.

In the rest of this section, the individual abstract classes and their interfaces are described in detail. For each class a table is provided, where on the left column the individual services and their arguments are presented, following the Pydoc [7] syntax. In the right column, the description of individual service is given, input arguments are described (denoted by ARGS) including their type (in parenthesis). The return values are described in a similar way (denoted by Returns). More extensive documentation of MuPIF abstract classes exist in MuPIF documentation [8].

5.1. Application class

This abstract class represents an external application and defines its interface. The interface is defined in terms of abstract services for data exchange and steering. Derived classes represent individual simulation tools. The data exchange services consist of methods for getting and registering external properties, fields, and functions, which are represented using corresponding, newly introduced classes. Steering services allow invoking (execute) solution for a specific solution step, update solution state, terminate the application, etc.

Service	**Description**
`__init__ (self, file)`	`Constructor. Initializes the application.` **ARGS:** - `file (str): path to application initialization file.`

getField(self,fieldID, time)	Returns the requested field at given time. Field is identified by fieldID. **ARGS**: - fieldID (FieldID): identifier - Time (double): target time **Returns**: Returns requested field (Field).
setField(self, field)	Registers the given (remote) field in application. **ARGS**: - field (Field): remote field to be registered by the application **Returns**: None
getProperty(self,propID, time, objectID=0)	Returns property identified by its ID evaluated at given time. **ARGS**: - propID (PropertyID): property ID - time (double): time when property to be evaluated - objectID (int): identifies object/submesh on which property is evaluated (optional) **Returns**: Returns representation of requested property (Property).
setProperty(self, property, objectID=0)	Register given property in the application **ARGS**: - property (Property): the property class - objectID (int): identifies object/submesh on which property is evaluated (optional) **Returns**: None
getFunction(self,funcID, objectID=0)	Returns function identified by its ID **ARGS**: - funcID (FunctionID): function ID - objectID (int): identifies optional object/submesh **Returns**: Returns requested function(Function)
setFunction(self,func, objectID=0)	Register given function in the application **ARGS**: - func(Function): function to register - objectID (int): identifies optional object/submesh

getMesh (self, tstep)	Returns the computational mesh for given solution step. **ARGS**: - tstep(TimeStep): solution step **Returns**: Returns the representation of mesh (Mesh)
solveStep(self, tstep, stageID=0, runInBackground=False)	Solves the problem for a given time step. Evaluates the solution from actual state to given time. The actual state should not be updated at the end, as this method could be called multiple times for the same solution step until the global convergence is reached. When global convergence is reached, finishStep is called and then the actual state has to be updated. Solution can be split into individual stages identified by optional stageID parameter. In between the stages, the additional data exchange can be performed. See also wait and isSolved services. **ARGS**: - tstep(TimeStep): solution step - stageID(int): optional argument identifying solution stage - runInBackground(bool): if set to True, the solution will run in background (in separate thread), if supported. **Returns**: None
wait(self)	Wait until solve is completed when executed in background. **Returns**: None
isSolved(self)	Returns true or false depending whether solve has completed when executed in background. **Returns**: (Boolean)
finishStep(self, tstep)	Called after a global convergence within a time step. **ARGS**: - tstep(TimeStep): solution step **Returns**: None
getCriticalTimeStep(self)	Returns the actual (related to the current state) critical time step increment (double). **Returns**: Critical time step (double)

getAssemblyTime(self, tstep)	Returns the assembly time related to a given time step. The registered fields (inputs) should be evaluated in this time. **ARGS**: - tstep (TimeStep): solution step **Returns**: Assembly time (double)
storeState(self, tstep)	Store the solution state of an application. **ARGS**: - tstep(TimeStep): solution step **Returns**: None
restoreState(self, tstep)	Restore the saved state of an application. **ARGS**: - tstep(TimeStep): solution step **Returns**: None
terminate(self)	Terminates the application. **Returns**: None
getAPIVersion(self)	Returns the supported API version. **Returns**: API version (int)

5.2. Property class

Property is a characteristic value of a problem, which has no spatial variation. Property is identified by *PropertyID*, which is an enumeration determining its physical meaning. It can represent any quantity of a scalar, vector, or tensorial type. Property keeps its value, type, associated time and an optional *objectID*, identifying related component/subdomain.

Service	**Description**
__init__(self, value, propID, valueType, time, objectID=0)	Constructor, initializes the property. **ARGS**: - value (tuple): value of a property. Scalar value is represented as array of size 1. Vector is represented as values packed in a tuple. Tensor is represented as 3D tensor stored in a tuple, column by column. - propId (PropertyID): property ID - valueType (ValueType): type of property value - time (double): time

	- objectID (int): optional ID of problem object / subdomain to which property is related.
getValue(self)	Returns the value of property in a tuple. **Returns:** Property value as array (tuple)
getPropertID(self)	Returns type of property. **Returns:** Receiver property ID (PropertyID)
getObjectID(self)	Returns property objectID. **Returns:** ID of related object (int)

5.3. Field class

Representation of field. *Field* is a scalar, vector, or tensorial quantity defined on a spatial domain (represented by the *Mesh* class). The field provides interpolation services in space, but is assumed to be fixed in time (the application interface allows to request field at specific time). The fields are usually created by the individual applications (sources) and being passed to target applications. The field can be evaluated in any spatial point belonging to underlying domain. Derived classes will implement fields defined on common discretizations, like fields defined on structured or unstructured FE meshes, finite difference grids, etc. Basic services provided by the field class include a method for evaluating the field at any spatial position and a method to support graphical export (creation of VTK dataset).

Service	**Description**
__init__(self, mesh, fieldID, valueType, time, values=None)	Constructor. Initializes the field instance. **ARGS:** - mesh (Mesh): Instance of Mesh class representing underlying discretization. - fieldID (FieldID): field type - valueType (ValueType): type of field values - time (double): time - values (tuple): field values, usually at mesh vertices (format dependent of particular field type)
getMesh(self)	Returns representation of underlying discretization. **Returns:** Reference to associated mesh (Mesh)

getValueType(self)	Returns type of field values (ValueType) of the receiver. **Returns**: (ValueType)
getFieldID(self)	**Returns**:Field ID (FieldID)
evaluate(self, position, eps=0.001)	Evaluates the receiver at given spatial position. **ARGS**: - position (tuple, list of tuples): 3D position vector or list of position vectors - eps(double): Optional tolerance **Returns**: Receiver value or list of values evaluated at given position(s) (tuple, list of tuples)
getValue(self, componentID)	Returns the value associated to given component (vertex or cell IP, implementation dependent). **ARGS**: - componentID (tuple): identifies the component (vertexID) or (CellID, IPID) **Returns**: component value (tuple)
setValue(self, componentID, value)	Sets the value associated to given component (vertex or cell IP). Note, that the field values are updated after a commit method is invoked. **ARGS**: - componentID (tuple): The componentID is a tuple: (vertexID) or (CellID, IPID) - value(tuple): Component value **Returns**: None
commit(self)	Commits the recorded changes (via setValue method). **Returns**: None
merge(self, field)	Merges the receiver with a given field together. Both fields should be on different parts of the domain (can also overlap), but should be of the same type and refer to the same underlying discretization. **ARGS**: - field (Field): field to merge **Returns**: None
field2VTKData (self)	Returns VTK representation of the receiver. **Returns**: VTK dataset (VTKDataSource)

5.4. Function class

Represents a user defined function. Function is an object defined by mathematical expression and can be a function of spatial position, time, and other variables. Derived classes should implement evaluate service by providing a corresponding expression. The function arguments are packed into a dictionary, consisting of pairs (called items) of keys and their corresponding values.

Service	**Description**
`__init__(self,funcID, objectID=0)`	Constructor. Initializes the function. **ARGS**: - funcID (FunctionID): function ID - objectID (int): optional ID of associated subdomain.
`evaluate (self, d)`	Evaluates the function for given parameters packed as a dictionary. A dictionary is container type that can store any number of Python objects, including other container types. Dictionaries consist of pairs (called items) of keys and their corresponding values. Example: d={'x':(1,2,3), 't':0.005} initializes dictionary containing tuple (vector) under 'x' key, double value 0.005 under 't' key. Some common keys: - 'x': position vector - 't': time **ARGS**: - d (dictionary): dictionary containing function arguments (number and type depends on particular function) **RETURNS**: function value (tuple) evaluated for given parameters
`getID (self)`	Returns receiver's ID. **Returns**: id (FunctionID)
`getObjectID(self)`	**Returns**: returns receiver's object ID (int)

5.5. TimeStep class

Class representing solution time step. The time step manages its number, target time, and time increment.

Service	Description
`__init__(self, t, dt, n=1)`	Constructor. Initializes the new time step. **ARGS**: - t (double): time - dt (double): step length (time increment) - n (int): time step numbeR
getTime(self)	**Returns**: Time step time (double)
getTimeIncrement(self)	**Returns**: time increment (double)
getNumber(self)	**Returns**: receiver's number (int)

5.6. Mesh class

Mesh class is an abstract representation of a computational domain and its spatial discretization. The mesh geometry is described using computational cells (representing finite elements, finite difference stencils, etc.) and vertices (defining cell geometry). Derived classes represent structured, unstructured FE grids, FV grids, etc. Mesh is assumed to provide a suitable instance of cell and vertex localizers. In general, the mesh services provide different ways how to access the underlying interpolation cells and vertices, based on their numbers, or spatial location.

Service	Description
`__init__(self)`	Constructor, creates an empty mesh.
copy(self)	This will return a copy of the receiver. Note, that DeepCopy will not work, as individual cells contain mesh link attributes, leading to underlying mesh duplication in every cell. **Returns**: Copy of receiver (Mesh)
getNumberOfVertices(self)	**Returns**: Number of Vertices (int)
getNumberOfCells(self)	**Returns**: Number of Cells

getVertex(self, i)	Returns i-th vertex (i corresponds to a vertex number, not a label). **Returns**: vertex (Vertex)
getCell(self, i)	Returns i-th cell (identified by cell number, not label). **Returns**: cell (Cell)
vertexLabel2Number(self, label)	Returns local vertex number corresponding to given label. If no label corresponds, throws an exception. **Returns**: vertex number (int)
cellLabel2Number(self, label)	Returns local cell number corresponding to a given label. If no label corresponds, it throws an exception. **Returns**: cell number (int)
getVerticesInBBox (self, bbox):	Returns the list of all vertices which are inside given bounding Box **ARGS**: - bbox (BoundingBox): bounding box **Returns**: list of vertices inside bbox (list)
getCellsInBBox (self, bbox):	Returns the list of cells which bbox intersects with given bounding box **ARGS**: - bbox (BoundingBox): bounding box **Returns**: list of cells at least partially in bbox (list)
evaluateVertices(self, functor):	Returns the list of all vertices for which the functor is satisfied. The functor is a user defined class with two methods: *giveBBox*() which returns an initial functor bbox, and *evaluate* (obj) which should return true if functor is satisfied for a given object. **ARGS**: - functor: functor class **Returns**:list of all vertices for which the functor is satisfied (list)
evaluateCells(self, functor):	Returns the list of all cells for which the functor is satisfied. The functor is user defined class with two methods:*getBBox*() which returns an initial functor bbox, and *evaluate* (obj) which should return true if functor is satisfied for given object. **ARGS**:

	- functor: functor class **Returns:**List of all cells for which the functor is satisfied (list)

5.7. Cell class

Representation of a computational cell (finite element). The solution domain is composed of cells, whose geometry is defined using vertices. Cells provide interpolation over their associated volume, based on given vertex values. Derived classes will be implemented to support common interpolation cells (finite elements, FD stencils, etc.)

Service	**Description**
`__init__(self, mesh, number, label, vertices)`	Constructor. Creates the new cell. **ARGS:** - mesh(Mesh): the mesh to which cell belongs. - number(int): local cell number - label(int): cell label - vertices(tuple): cell vertices (local numbers)
copy(self)	This will copy the receiver, making deep copy of all attributes EXCEPT mesh attribute **Returns:** the copy of receiver (Cell)
getVertices(self)	**Returns:** the list of cell vertices (tuple of Vertex instances)
containsPoint(self, point)	**Returns:** True if cell contains given point, False otherwise
getGeometryType(self)	**Returns:** geometry type of receiver (CellGeometryType)
getBBox(self)	**Returns:** bounding box of the receiver (BBox)

5.8. Vertex class

Represents a vertex. In general, a set of vertices defines the geometry of interpolation cells. A vertex is characterized by its position, number and label. Vertex number is locally assigned number (by *Mesh* class), while a label is a unique number defined by application.

Service	**Description**
`__init__(self, number, label, coords=None)`	Constructor. Creates the new vertex instance. **ARGS**: - number(int): local vertex number - label(int): vertex label - coords(tuple): 3D position vector of verteX
`getCoordinates(self)`	**Returns**: receiver coordinates (tuple)
`getNumber(self)`	**Returns**: receiver number (int)
`getLabel(self)`	**Returns**: receiver label (int)

5.9. BoundingBox

Represents an axis aligned bounding box - a rectangle in 2d and a prism in 3d. Its geometry is described using two points - lover left and upper right. The bounding box class provides fast and efficient methods for testing whether point is inside and whether an intersection with another bounding box exists.

Service	**Description**
`__init__(self, coords_ll, coords_ur)`	Constructor. Creates the new Bounding box instance. **ARGS**: - coords_ll (tuple): coordinates of lower left corner - coords_ur (tuple): coordinates of upper right corner
`containsPoint (self, point)`	Returns true if point inside receiver. **ARGS**: - point (tuple): point coordinates **Returns**: True if point is inside receiver, false otherwise (Bool)
`intersects (self, bbox)`	**Returns**: Returns true if receiver intersects given bounding box (Bool)

merge (self, entity)	Merges (expands) receiver with given entity (position or bbox) **ARGS**: - entity (tuple or BoundingBox): position vector (tuple) or bounding box. **Returns**: None

5.10. APIError

This class serves as a base class for exceptions thrown by the framework. Raising an exception is a way to signal that a routine could not execute normally - for example, when an input argument is invalid (e.g. value is outside of the domain of a function) or when a resource is unavailable (like a missing file, a hard disk error, or out-of-memory errors). A hierarchy of specialized exceptions can be developed, derived from the *APIError* class.

Exceptions provide a way to react to exceptional circumstances (like runtime errors) in programs by transferring control to special functions called handlers. To catch exceptions, a portion of code is placed under exception inspection. This is done by enclosing that portion of code in a try-block. When an exceptional circumstance arises within that block, an exception is thrown that transfers the control to the exception handler. If no exception is thrown, the code continues normally and all handlers are ignored.

An exception is thrown by using the throw keyword from inside the try-block. Exception handlers are declared with the keyword "except", which must be placed immediately after the try block.

Service	**Description**
__init__(self,msg)	Constructor. Initializes the exception. **ARGS**: - msg (string) Error message
__str__(self)	**Returns**: string representation of the exception, ie. error message (string).

6. Developing Application Program Interface (API)

In order to establish an interface between the platform and external application, one has to implement an Application class. This class defines a generic interface in terms of general purpose, problem independent, methods that are designed to steer and communicate with the application. The Table 2 presents an overview of application interface, the full details with complete specification can be found in 5.1. Application class specification.

Method	Description
__init__(self, file)	Constructor. Initializes the application.
getMesh (self, tstep)	Returns the computational mesh for given solution step.
getField(self, fieldID, time)	Returns the requested field at given time. Field is identified by fieldID.
setField(field)	Registers the given (remote) field in application.
getProperty(self, propID, time, objectID=0)	Returns property identified by its ID evaluated at given time.
setProperty(self, property, objectID=0)	Register given property in the application
setFunction(self, func,objectID=0)	Register given function in the application
solveStep(self, tstep)	Solves the problem for given time step.
finishStep(self, tstep)	Called after a global convergence within a time step.
getCriticalTimeStep()	Returns the actual critical time step increment.
getApplicationSignature()	Returns the application identification
terminate()	Terminates the application.

Table 2: Application interface: an overview of basic methods.

From the perspective of individual simulation tool, the interface implementation can be achieved by means of either direct (native) or indirect implementation.

- **Native implementation** requires a simulation tool written in Python, or a tool with Python interface. In this case the Application services will be implemented directly using direct calls to suitable application's functions and procedures, including necessary internal data conversions. In general, each application (in the form of a dynamically linked library) can be loaded and called, but care must be taken to convert Python data types into target application data types. More convenient is to use a wrapping tool (such as Swig [5] or Boost [6]) that can generate a Python interface to the application, generally taking care of data conversions for the basic types. The result of wrapping is a set of Python functions or classes, representing their application counterparts. The user calls an automatically generated Python function which performs data conversion and calls the corresponding native equivalent.
- **Indirect implementation** is based on wrapper class implementing Application interface that implements the interface indirectly, using, for example, simulation tool scripting or I/O capabilities. In this case the application is typically standalone application, executed by the wrapper in each solution step. For the typical solution step, the wrapper class has to cache all input data internally (by overloading corresponding set methods), execute the application from previously stored state, passing input data, and parsing its output(s) to collect return data (requested using get methods).

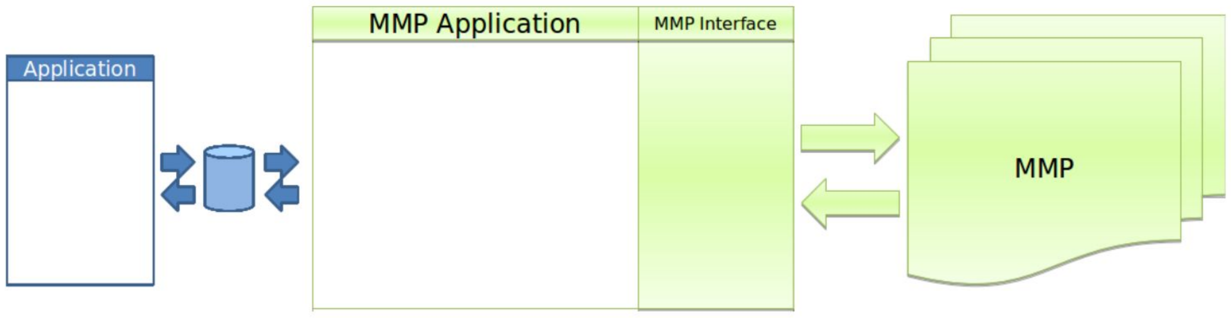
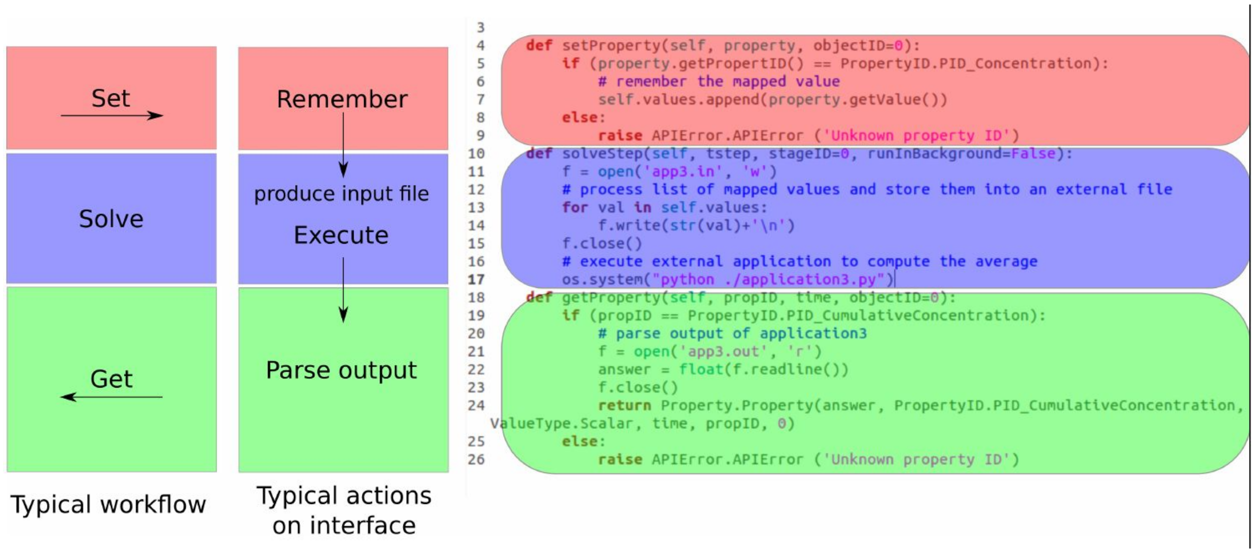


Fig. 2: Illustration of indirect approach

The example illustrating the indirect implementation is available from MuPIF distribution, located in *examples/Example03* directory. Typically, this is a three-phase procedure. In the first step, when external properties and fields are being set, the application interface has to remember all these values. In the second step, when the application is to be executed, the input file is to be modified to include the mapped values. After the input file(s) are generated, the application itself is executed. In the last, third step, the computed properties/fields are requested. They are typically obtained by parsing application output and returned. This three-step procedure is illustrated in the following example listing taken from Example03. In this example, the application should compute the average value from mapped values of concentrations over the time. The external application is available, that can compute an average value from the input values given in a file. The application interface accumulates the mapped values of concentrations in a list data structure, this is done is setProperty method. During the solution step in a solveStep method, the accumulated values of concentrations over the time are written into a file, the external application is invoked taking the created file as input and producing an output file containing the computed average. The output file is parsed when the average value is requested using getProperty method.



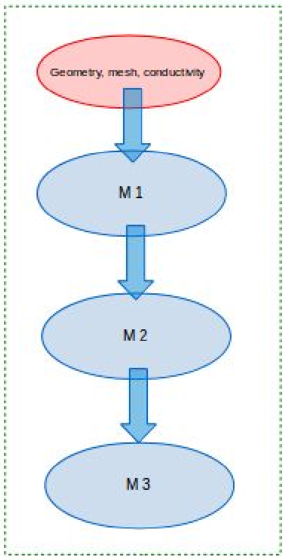
```python
def setProperty(self, property, objectID=0):
    if (property.getPropertID() == PropertyID.PID_Concentration):
        # remember the mapped value
        self.values.append(property.getValue())
    else:
        raise APIError.APIError ('Unknown property ID')
def solveStep(self, tstep, stageID=0, runInBackground=False):
    f = open('app3.in', 'w')
    # process list of mapped values and store them into an external file
    for val in self.values:
        f.write(str(val)+'\n')
    f.close()
    # execute external application to compute the average
    os.system("python ./application3.py")
def getProperty(self, propID, time, objectID=0):
    if (propID == PropertyID.PID_CumulativeConcentration):
        # parse output of application3
        f = open('app3.out', 'r')
        answer = float(f.readline())
        f.close()
        return Property.Property(answer, PropertyID.PID_CumulativeConcentration,
ValueType.Scalar, time, propID, 0)
    else:
        raise APIError.APIError ('Unknown property ID')
```

Fig. 3: Typical workflow in indirect approach for API implementation

7. Developing user workflows

Multiscale/multiphysics simulations are natively supported in MuPIF, allowing easy data passing from one model to another one, synchronizing and steering all models. Simulation workflow of multiscale/multiphysics simulations, called also a simulation scenario, defines data flow among various models and their steering. Natively, the workflow in MuPIF is represented as Python script combining MuPIF components into workflow. However, a many benefits can be further gained by implementing a workflow as class derived from abstract *Workflow* class. The benefits and example are discussed in chapter “Workflow as a class”.

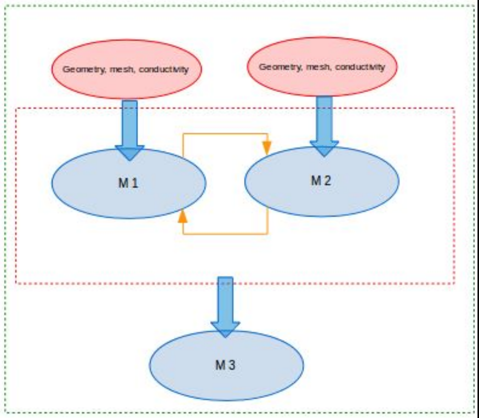
7.2 Workflow templates



```
time  = 0
timeStepNumber = 0
targetTime = 10

while (abs(time-targetTime) > 1.e-6):
    dt=min(m1.getCriticalTimeStep(),
                                 m2.getCriticalStep(),
                           m3.getCriticalStep())
    time = time+dt
    if (time>targetTime): time=targetTime

    timeStepNumber = timeStepNumber+1
    istep=TimeStep.TimeStep(time, td, timeStepNumber)
    try:
        m1.solveStep(istep)
        p = m1.getProperty()
        m2.setProperty(p)
        m2.solveStep(istep)
        ...
        m3.solveStep(istep)
    except APIError.APIError as e:
        print ("Appi Error occured:",e)
        break

m1.terminate()
m2.terminate()
m3.terminate()
```

Time loop

Sequential workflow template



```
time  = 0
timeStepNumber = 0
targetTime = 10

while (abs(time-targetTime) > 1.e-6):
    dt=min(m1.getCriticalTimeStep(), m2.getCriticalStep(),
                m3.getCriticalStep())
    time = time+dt
    if (time>targetTime): time=targetTime
    timeStepNumber = timeStepNumber+1
    istep=TimeStep.TimeStep(time, td, timestep)

    try:
        convergedFlag = False
        while not covergedFlag:
            m1.solveStep(istep)
            m2.setProperty(m1.getProperty(id))
            m2.solveStep(istep)
            m1.setProperty(m2.getProperty(id2))

            #check for convergence
            convergedFlag=checkConvergence()

        m3.solveStep()

    except APIError.APIError as e:
        print ("Appi Error occured:",e)
        break

m1.terminate()
m2.terminate()
m3.terminate()
```

Coupling loop

Time loop

Loosely coupled workflow template

7.3 Workflow example

A thermo-mechanical, multiphysical example *Demo13.local.py* explains linking and steering in greater detail. The example presents a local (non-distributed) version and can be found under *examples/Example13-thermoMechanicalNonStat* directory of MuPIF installation.

A cantilever, clamped on the left hand side edge, is subjected to nonstationary temperature loading, see Figure 4. Heat convection is prescribed on the top edge with ambient temperature 10°C. Left and bottom edges have prescribed temperature 0°C, the right edge has no boundary condition. Initial temperature is set to 0°C, heat conductivity is 1 W/m/K, heat capacity 1.0 J/kg/K, material density 1.0 kg/m^3. The material has assigned Young's modulus as 30 GPa, Poisson's ratio 0.25 and coefficient of linear thermal expansion 12e-6°C^{-1}. Integration time step is constant as 1 s, 10 steps are executed in total.

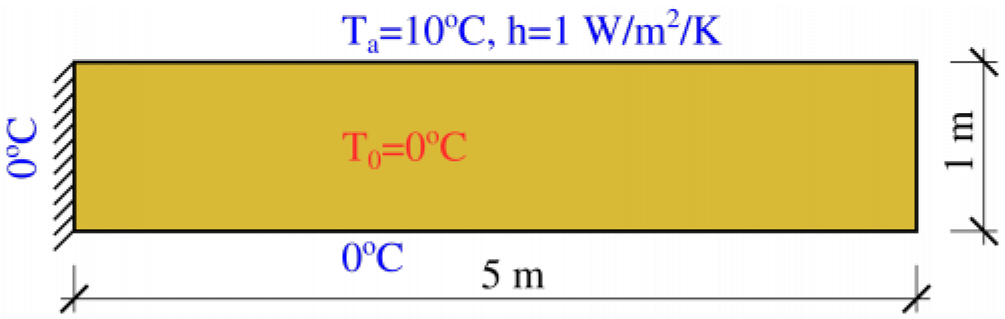


Fig. 4: Elastic cantilever subjected to thermal boundary conditions.

First, the temperature distribution has to be solved in the whole domain from the given initial and boundary conditions. The temperature field is passed afterwards to the mechanical analysis, which evaluates the corresponding displacement field. Such simulation flow is depicted in Figure 5, linking two models in discretized time steps. The thermal model implements *getField(T)* and *solveStep(istep)* methods. In addition, the mechanical model needs to set up an initial thermal field *setField(T)* prior to execution in each time step. Steering occurs in 1s increments, calling thermal and mechanical models.

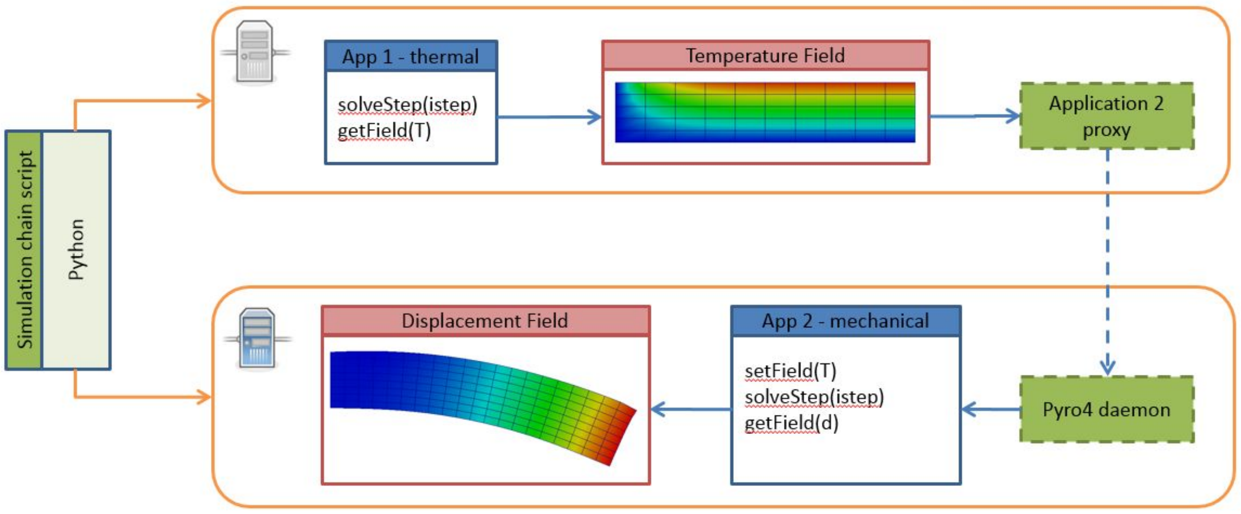


Fig. 5: Thermo-mechanical simulation flow

The discretizations for thermal and mechanical problems are in this particular case different and the platform takes care of field interpolation. The mesh for thermal problem consist of 50 linear elements with linear approximation and 55 nodes. The mesh for mechanical analysis consist of 168 nodes and 160 elements with linear approximation. Results for 10 s are shown in Figure 6.

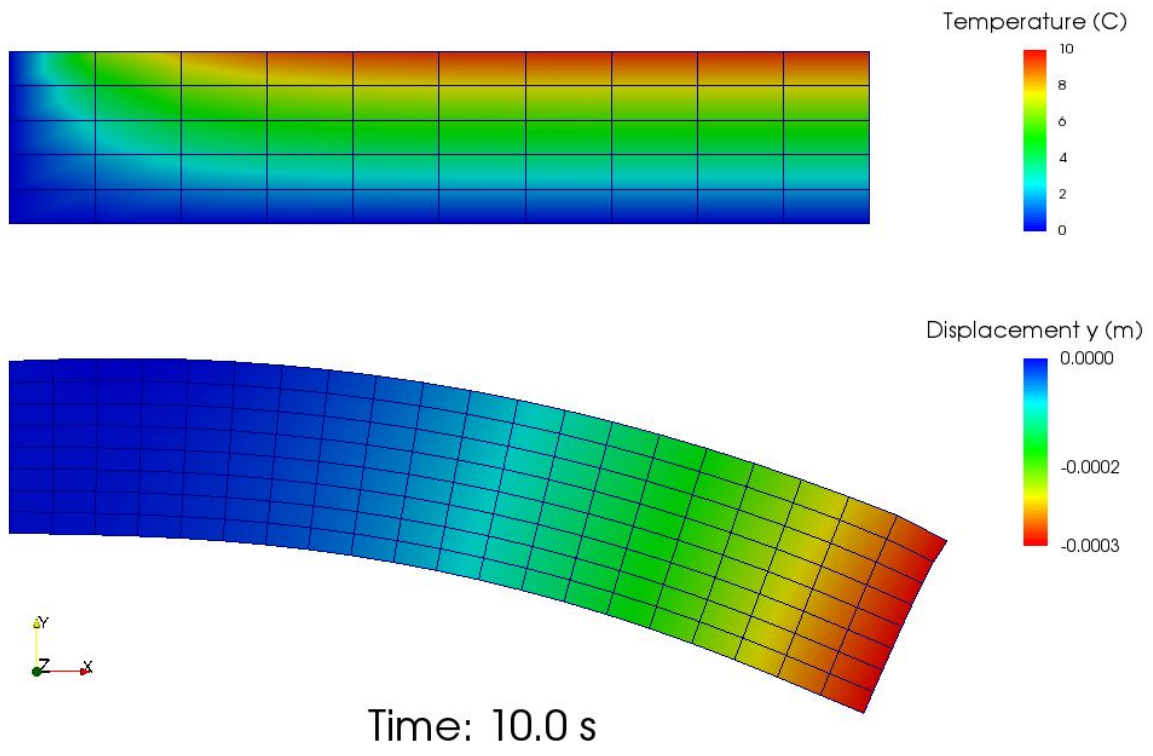


Fig. 6: Results of thermo-mechanical simulation at 10 s

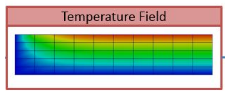
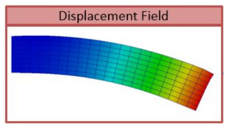
A code below shows a thermo-mechanical simulation in *Example13*. Thermal and mechanical solvers are implemented as *demoapp* module and loaded from *Example10* directory. It is straightforward to extend this workflow for distributed version which needs in addition a nameserver and VPN/ssh tunnels, as described in subsequent chapters.

```
from __future__ import print_function
import sys
sys.path.append('../../..')
from mupif import *
from mupif import logger
sys.path.append('../Example10')
import demoapp

time  = 0.
dt = 0.
timestepnumber = 0
targetTime = 10.0

thermal = demoapp.thermal_nonstat('inputT13.in','.')
mechanical = demoapp.mechanical('inputM13.in', '.')

while (abs(time - targetTime) > 1.e-6):

      logger.debug("Step: %g %g %g"%(timestepnumber,time,dt))
```

```
        istep = TimeStep.TimeStep(time, dt, timestepnumber)

        try:
        thermal.solveStep(istep)
        f = thermal.getField(FieldID.FID_Temperature, istep.getTime())
        data = f.field2VTKData().tofile('T_%s'%str(timestepnumber))

        mechanical.setField(f)
        sol = mechanical.solveStep(istep)
        f = mechanical.getField(FieldID.FID_Displacement, istep.getTime())
        data = f.field2VTKData().tofile('M_%s'%str(timestepnumber))

        thermal.finishStep(istep)
        mechanical.finishStep(istep)

        dt = min (thermal.getCriticalTimeStep(), mechanical.getCriticalTimeStep())

        # update time
        time = time+dt
        if (time > targetTime):
               time = targetTime
        timestepnumber = timestepnumber+1

        except APIError.APIError as e:
        logger.error("Following API error occurred:",e)
        break

thermal.terminate();
mechanical.terminate();
```

Listing 2: *Example13* showing a thermo-mechanical simulation

As already mentioned, the thermo-mechanical simulation chain can run in various configurations, composed of a steering script, nameserver, thermal and mechanical applications. Table 3 shows MuPIF examples of thermo-mechanical configuration. In principle, each component can run on different computer, except a steering script.

	Steering script	Nameserver	Thermal application 	Mechanical application 
Example13 local	Local	-	Local	Local
Example14 VPN	Local	Remote	Remote	Remote
Example15 ssh JobMan	Local	Remote	Remote JobMan	Local

Example16 VPN JobMan	Local	Remote	Remote JobMan	Local

Table 3: Examples of thermo-mechanical simulation on local and various distributed configurations.

7.4 Workflow as a class

The object oriented design of MuPIF allows to build a hierarchy of workflows, where the top level workflow may utilise the components, which may be again workflows. From this point of view, any workflow can be regarded as an application, composed from individual components, implementing itself an application interface. The application interface, as introduced in Chapter on Platform APIs, allows to perform any data and steering operation, i.e. to get and set any data, update response for the given solution step, etc.

Another important advantage of having workflow represented as a class is that the individual workflows can be allocated and executed by a jobManager on remote resources in a same way as individual applications.

MuPIF comes with abstract *Workflow* class, derived from *Application* class, supposed to be a parent class for any workflow represented as a class. It extends the *Application* interface by defining *solve* method, which implements a time loop over the individual time steps, solved by *solveStep* method defined already in *Application* interface.

The default implementation of Workflow solve method is shown in a listing below. It generates a sequence of time steps satisfying the stability requirements till reaching the target time. If the default implementation does not fit, the method can be overloaded.

```
class Workflow(Application.Application):
        def solve(self, runInBackground=False):
            time = 0.
            timeStepNumber = 0

            while (abs(time-self.targetTime) > 1.e-6):
                dt = self.getCriticalTimeStep()
                time=time+dt
                if (time > self.targetTime):
                    time = targetTime
                timeStepNumber = timeStepNumber+1
                istep=TimeStep.TimeStep(time,dt, timeStepNumber)

                self.solveStep(istep)
                self.finishStep(istep)
            self.terminate()
```

The subsequent code snippet illustrates the concept on coupled, steady-state thermo-mechanical workflow. The implementation should be extending by implementing the get/set methods to interact with other components. The working example of workflow defined as a class can be found in examples/Example18 directory of MuPIF installation (Available since MuPIF version 2.0)

```
class Demo18(Workflow.Workflow):
    def __init__ (self, targetTime=0.):
        super(Demo18, self).__init__(file='', workdir='', targetTime=targetTime)
        # initialize / connect to individual applications
        locate nameserver
        ns = PyroUtil.connectNameServer(nshost, nsport, hkey)
        #connect to JobManager running on (remote) server and create a tunnel to it
        self.thermalJobMan = PyroUtil.connectJobManager(ns, cfg.jobManName)
        #allocate the thermal server
        self.thermal = PyroUtil.allocateApplicationWithJobManager( ns,self.thermalJobMan,
                        jobNatport, PyroUtil.SSHContext(userName, sshClient))
        # connect to standalone mechanical server;
        self.mechanical = PyroUtil.connectApp(ns, 'mechanical')

    def solveStep(self, istep, stageID=0, runInBackground=False):
        self.thermal.solveStep(istep)
        f = self.thermal.getField(FieldID.FID_Temperature, istep.getTime())
        self.mechanical.setField(f)
        self.mechanical.solveStep(istep)
        f = self.mechanical.getField(FieldID.FID_Displacement, istep.getTime())
        data = f.field2VTKData().tofile('M_%s'%str(istep.getNumber()))
        self.thermal.finishStep(istep)
        self.mechanical.finishStep(istep)

    def getCriticalTimeStep(self):
        # determine critical time step
        return min
(self.thermal.getCriticalTimeStep(),self.mechanical.getCriticalTimeStep())

    def terminate(self):
         self.thermalAppRec.terminateAll()
         self.mechanical.terminate()
        super(Demo18, self).terminate()

    def getApplicationSignature(self):
        return "Demo18 workflow 1.0"
```

8. Distributed Model

Common feature of parallel and distributed environments is a distributed data structure and concurrent processing on distributed processing nodes. This brings in an additional level of complexity that needs to be addressed. To facilitate execution and development of the simulation workflows, the platform provides the transparent communication mechanism that will take care of the network communication between the objects. An important feature is the transparency, which hides the details of remote communication to the user and allows to work with local and remote objects in the same way.

The communication layer is built on Pyro library [4], which provides a transparent distributed object system fully integrated into Python. It takes care of the network communication between the objects when they are distributed over different machines on the network. One just calls a method on a remote object as if it were a local object – the use of remote objects is (almost) transparent. This is achieved by the introduction of so-called proxies. A proxy is a special kind of object that acts as if it were the actual object. Proxies forward the calls to the remote objects, and pass the results back to the calling code. In this way, there is no difference between simulation script for local or distributed case, except for the initialization, where, instead of creating local object, one has to connect to the remote object.

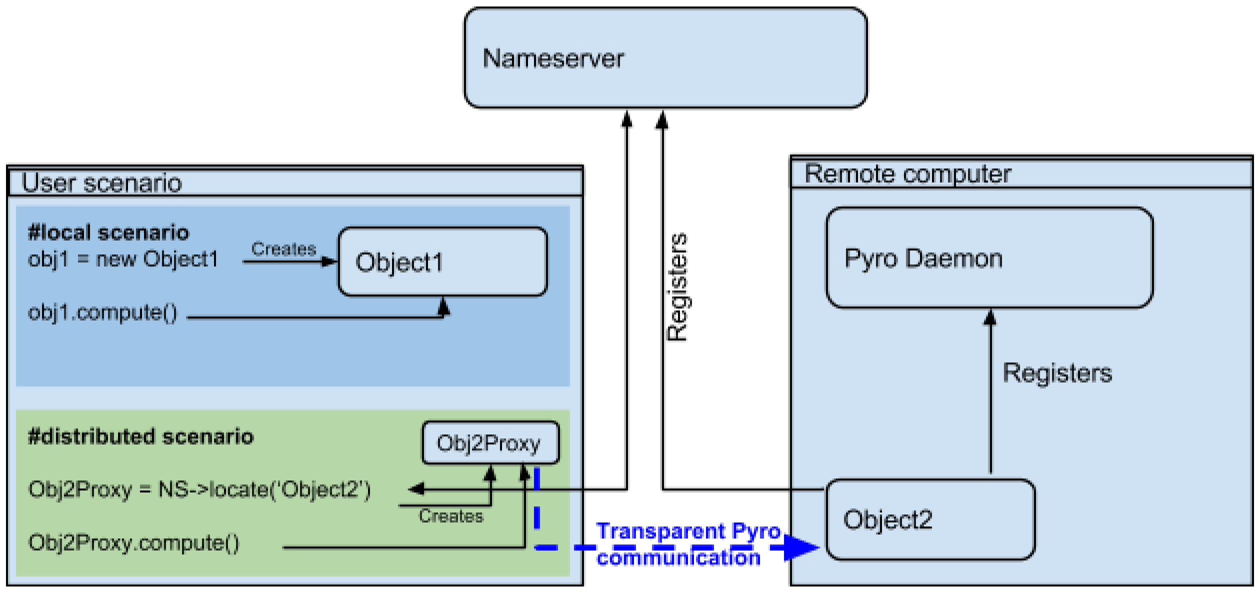


Fig. 7: Comparison of local vs. remote object communication scenarios

To make an object remotely accessible, it has to be registered with the daemon, a special object containing server side logic which dispatches incoming remote method calls to the appropriate objects. To enable runtime discovery of the registered objects, the name server is provided, offering a phone book for Pyro objects, allowing to search for objects based on logical name. The name server provides a mapping between logical name and exact location of the object in the network, so called uniform resource identifier (URI). The process of object registration and of communication with remote objects (compared to local objects) is illustrated in Fig. 7.

8.1. Distributed aspects of the API

One of the important aspect in distributed model is how the data are exchanged between applications running at different locations. The Pyro4 communication layer allows to exchange data in terms of get and set API methods in two ways. The communication layer automatically takes care of any object that is passed around through remote method calls. The receiving side of a call can receive either a local copy of the remote data or the representation of the remote data (Proxy).

- The communication in terms of exchanging local object copies can be less efficient than communication with remote objects directly, and should be used for objects with low memory footprint. One potential advantage is that the receiving side receives the copy of the data, so any modification of the local copy will not affect the source, remote data. Also multiple method invocation on local objects is much more efficient, compared to costly communication with a remote object.
- On the other hand, the data exchange using proxies (references to remote data) does not involves the overhead of creating the object copies, which could be prohibitively large for complex data structures. Also, when references to the remote objects are passed around, the communication channel must be established between receiving side

and remote computer owning the actual object, while passing local objects requires only communication between caller and receiver.

Both approaches have their pros and cons and their relative efficiency depends on actual problem, the size of underlying data structures, frequency of operations on remote data, etc.

Pyro4 will automatically take care of any Pyro4 objects that you pass around through remote method calls. If the autoproxying is set to on (AUTOPROXY = True by default), Pyro4 will replace objects by a proxy automatically, so the receiving side can call methods on it and be sure to talk to the remote object instead of to a local copy. There is no need to create a proxy object manually, a user just has to register the new object with the appropriate daemon. This is a very flexible mechanism, however, it does not allow explicit control on the type of passed objects (local versus remote).

Typically, one wants to have explicit control whether objects are passed as proxies or local copies. The get methods (such as *getProperty*, *getField*) should not register the returned object at the Pyro4 daemon. When used, the remote receiving side obtains the local copy of the object. To obtain the remote proxy, one should use *getFieldURI* API method, which calls getField method, registers the object at the server daemon and returns its URI. The receiving side then can obtain a proxy object from URI. This is illustrated in the following code snippet:

```
field_uri = Solver.getFieldURI(FieldID.FID_Temperature, 0.0)
field_proxy = Pyro4.Proxy(uri)
```

8.2. Requirements for distributed computing

To enable the discovery of remote objects a nameserver service is required, allowing to keep track of individual objects in network. It is also allows to use readable uniform resource identifiers (URI) instead of the need to always know the exact object id and its location.

The platform is designed to work on virtually any distributed platform, including grid and cloud infrastructure. For the purpose of performing simulations within a project, it is assumed that individual simulations and therefore the individual simulation packages will be distributed over the network, running on dedicated servers provided by individual partners, forming grid-like infrastructure.

According to requirements specified in D1.2 Software Requirements Specification Document for Cloud Computing [2], different functional requirements have been defined, with different levels of priorities. Typical requirements include services for resource allocation, access and license control, etc. In the project, we decided to follow two different strategies, how to fulfill these defined requirements. The first one is based on developing custom solution for resource allocation combined with access control based on standardized SSH technology based on public key cryptography for both connection and authentication. It uses platform distributed object technology and this allows its full integration in the platform. This solution is intended to satisfy only the minimum requirements, but its setup and operation is easy. It setup does not requires administrative rights and can be set up and run using user credentials. The second approach is based on established condor middleware. This solution provides more finer control over all aspects. On the other hand, its setup is more demanding. The vision is to allow the combination of both approaches. Both approaches and their requirements are described in following sections.

8.3. Internal platform solution - JobManager resource allocation

This solution has been developed from a scratch targeting fulfilment of minimal requirements only while providing simple setup. The resource allocation is controlled by *JobManager*. Each computational server within a platform should run an instance of JobManager, which provides services for allocation of application instances based on user request and monitoring services.

The *JobManager* is implemented as python object like any other platform components and is part of platform source code. It is necessary to create an instance of *JobManager* on each application server and register it on the platform nameserver to make it accessible for clients running simulation scenarios. This allows to access *JobManager* services using the same Pyro technology, which makes the resource allocation to be part of the the simulation scenario. Typically, the simulation scenario script first establishes connection to the platform nameserver, which is used to query and create proxies of individual *JobManagers*. The individual *JobManagers* are subsequently requested to create the individual application instances (using *allocateJob* service) and locally represented by corresponding proxy objects. Finally, the communication with remote application instances can be established using proxies created in the previous step, see Fig. 8 illustrating typical work flow in the distributed case.

The job manager has only limited capability to control allocated resources. In the present implementation, the server administrator can impose the limit on number of allocated applications. The configuration of the jobmanager requires only simple editing of configuration file. The individual applications are spawned under new process to enable true concurrency of running processes and avoid limitations of Python related to concurrent thread processing.

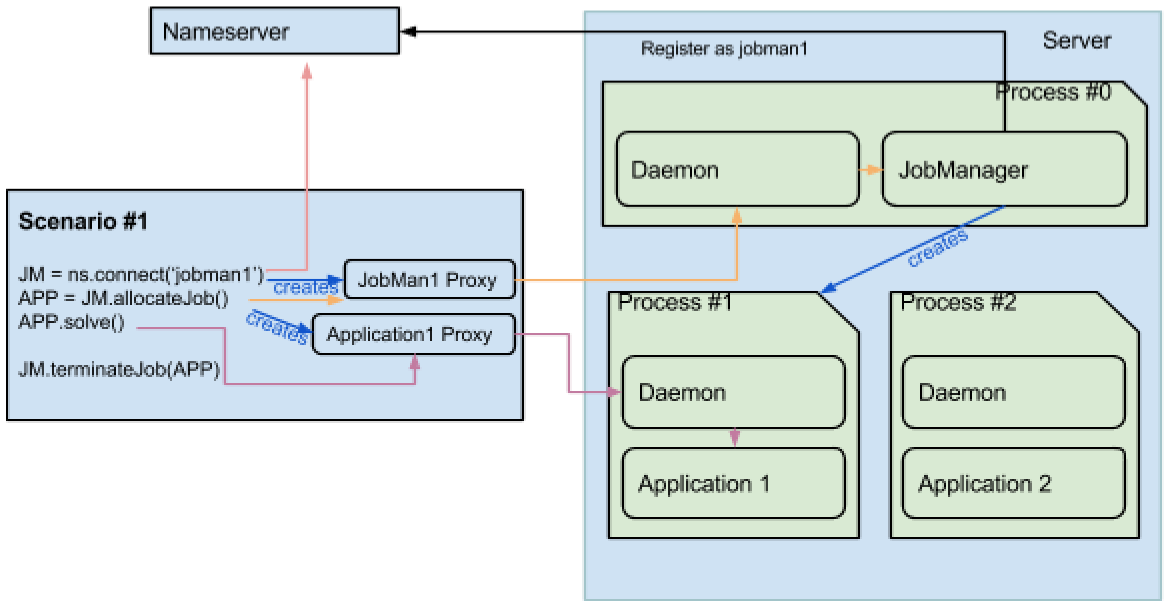
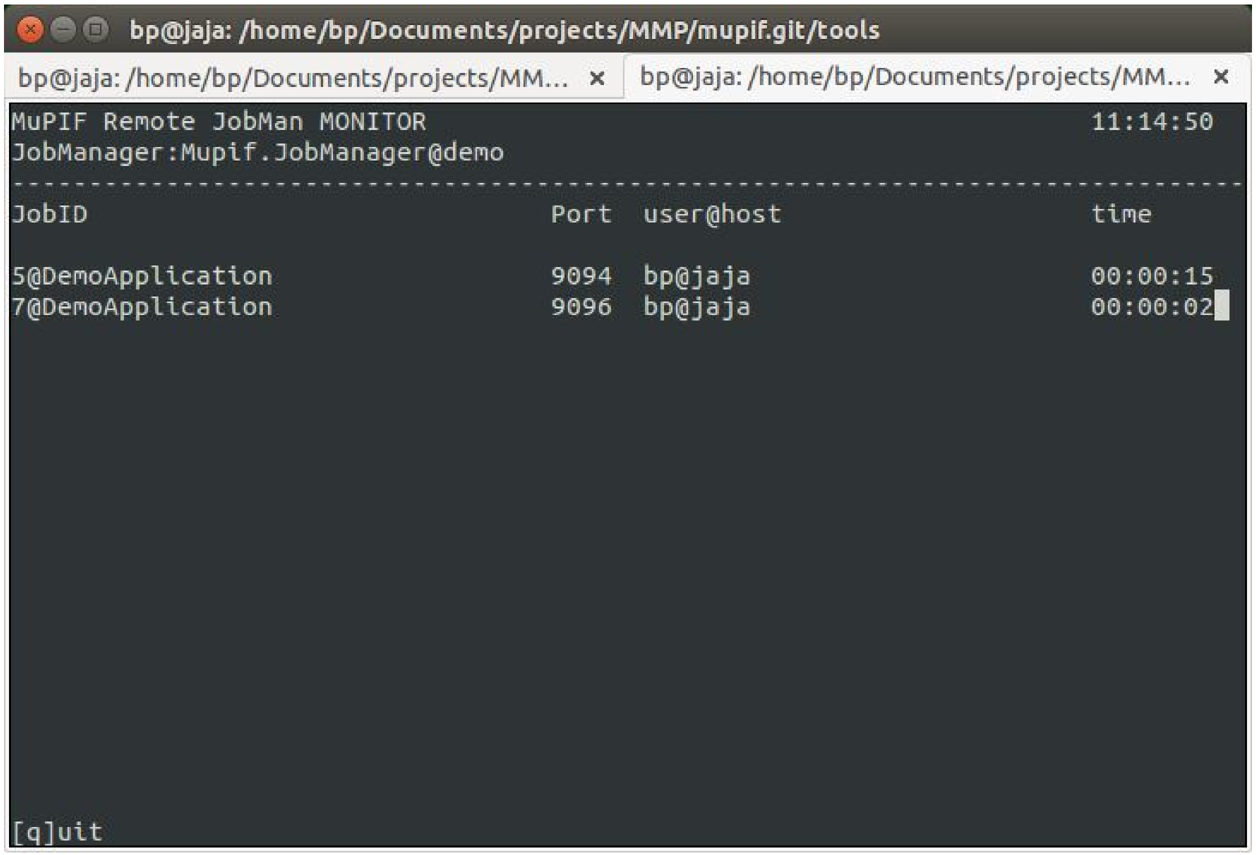


Fig. 8: Typical control flow with resource allocation using JobManager.

The status of individual job managers can be monitored with the jobManStatus.py script, located in tools subdirectory of the platform distribution. This script displays the status of individual jobs currently running, including their run time and user information. The information displayed is continuously refreshed, see Fig. 9.


bp@jaja: /home/bp/Documents/projects/MMP/mupif.git/tools
bp@jaja: /home/bp/Documents/projects/MM...
bp@jaja: /home/bp/Documents/projects/MM...

```
MuPIF Remote JobMan MONITOR                                  11:14:50
JobManager:Mupif.JobManager@demo
--------------------------------------------------------------------------------
JobID                              Port  user@host                    time

5@DemoApplication                  9094  bp@jaja                      00:00:15
7@DemoApplication                  9096  bp@jaja                      00:00:02

[q]uit
```

Fig. 9: Screenshot of Job Manager monitoring tool

The internal jobManager does not provide any user authentication service at the moment. The user access is assumed to be controlled externally, using ssh authorization. For example, to establish the authorized connection to a remote server and platform services (jobManager) using a ssh tunnel, a valid user credentials for the server are required. The secured, authenticated connection is realized using setting up ssh tunnel establishing a secure and trusted connection to a server. The ssh connections can be authorized by traditional user/passwords or by accepting public ssh keys generated by individual clients and send to server administrators. More details are given in a Section on SSH tunneling.

The status of individual computational servers can be monitored online using the provided monitoring tool. A simple ping test can be executed, verifying the connection to the particular server and/or allocated application instance.

8.3.1. Setting up a Job Manager

The skeleton for application server is distributed with the platform and is located in *examples/Example06-JobMan*. The following files are provided:

- server.py: The implementation of application server. It starts JobManager instance and corresponding daemon. Most likely, no changes are required.
- serverConfig.py: configuration file for the server. The individual entries have to be customized for particular server. Follow the comments in the configuration file. In the example, the server is configured to run on Unix-based system.
- JobMan2cmd.py: python script that is started in a new process to start the application instance and corresponding daemon. Its behaviour can be customized by Config.py.
- test.py: Python script to verify the jobManager functionality.
- clientConfig.py: configuration file for client code (simulation scenarios). The client can run on both Unix / Windows systems, configuring correctly ssh client.

The setup requires to install the platform, as described in 3. Platform installation. Also, the functional application API class is needed. Fig. 10 shows the flowchart with a JobManager using ssh tunnels.

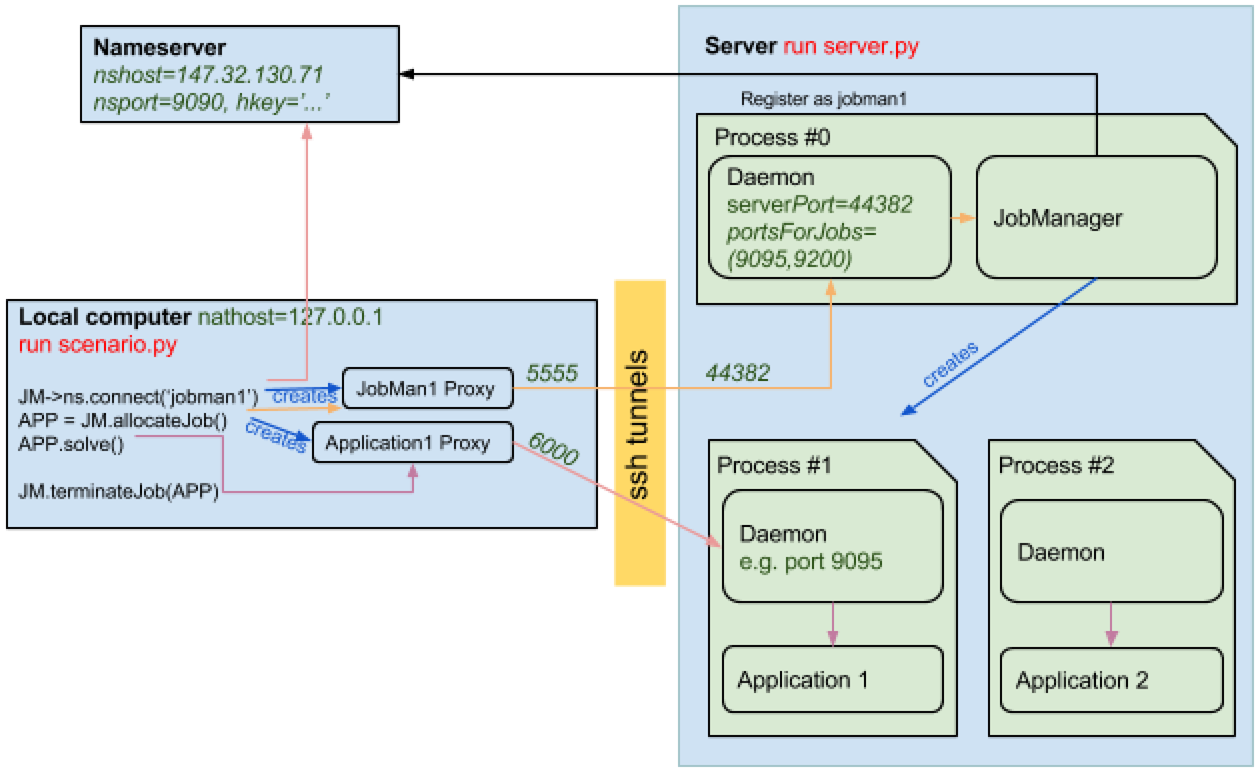


Fig. 10: *Example06-JobMan* displaying ports and tunnels in a distributed setup using ssh tunnels.

The recommended procedure to set up job manager for your server is to create a separate directory, where you will copy the server.py and serverConfig.py files from *examples/Example06-JobMan* directory and customize settings in serverConfig.py.

Simpler situation exists for VPN network setup where no ssh tunnels needs to be allocated and all communication runs on a local-like network.

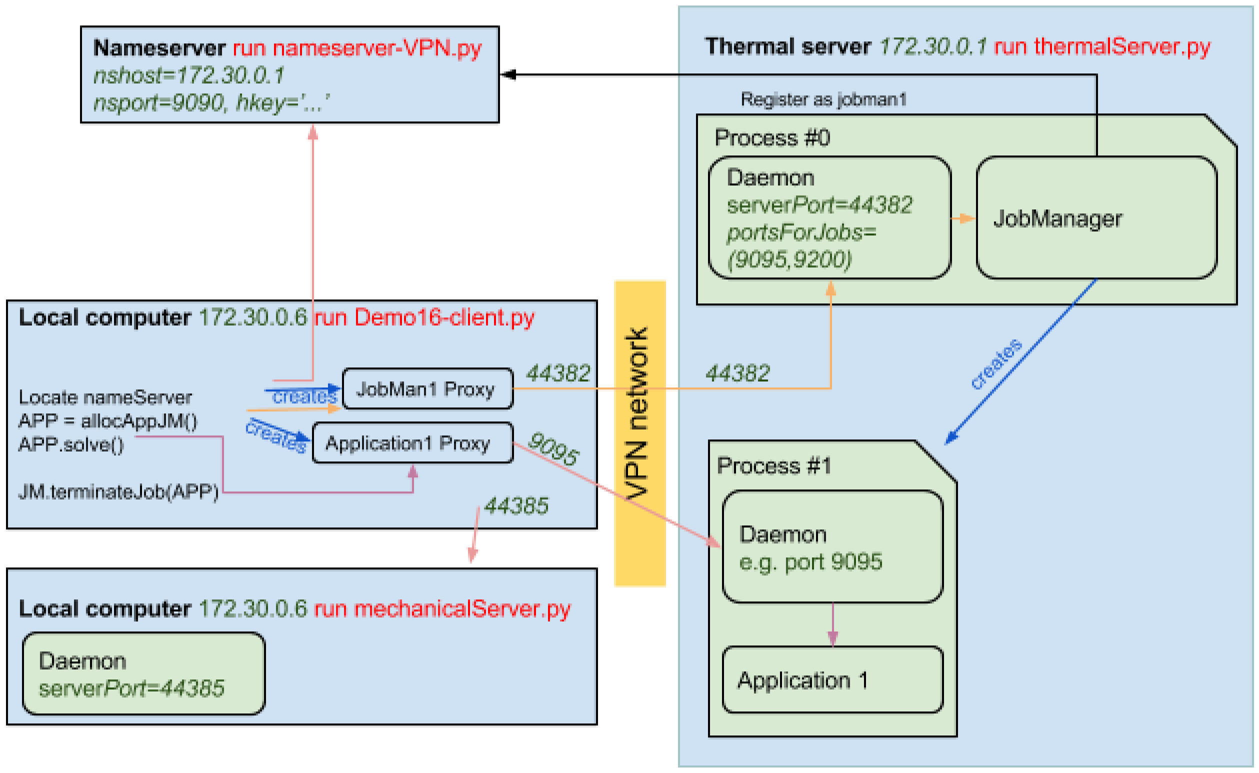


Fig. 11: *Example16* thermo-mechanical analysis displaying ports and tunnels in a distributed setup using VPN.

8.3.2. Configuration

The configuration of the job manager consists of editing the configuration file (serverConfig.py). The following variables can be used to customize the server settings:

Variable	Description
deamonHost	hostname or IP address of the application server, i.e. daemonHost='147.32.130.137'
hostUserName	user name to establish ssh connection to server, i.e. hostUserName='mmp'
jobManPort	Server port where job manager daemon listens, i.e., jobManPort=44361.

jobManNatport	Port reported by nameserver used to establish tunnel to destination JobManager port (jobManPort), i.e. jobManNatport=5555
jobManName	Name used to register jobManager at nameserver, i.e, jobManName='Mupif.JobManager@micress'
jobManPortsForJobs	List of dedicated ports to be assigned to application processes (recommended to provide more ports than maximum number of application instances, as the ports are not relesead immediately by operating system, see jobManMaxJobs) Example: jobManPortsForJobs=(9091, 9092, 9093, 9094)
jobManMaxJobs	Maximum number of jobs that can be running at the same time. jobManMaxJobs=4
jobManWorkDir	Path to JobManager working directory. In this directory, the subdirectories for individual jobs will be created and these will become working directories for individual applications. Users can upload/download files into these job working directories. Note: the user running job manager should have corresponding I/O (read/write/create) permissions.
applicationClass	Class name of the application API class. The instance of this class will be created when new application instance is allocated by job manager. The corresponding python file with application API definition need to be imported.

The individual ports can be selected by the server administrator, the ports from range 1024-49152 can be used by users / see IANA (Internet Assigned Numbers Authority).

To start application server run:

```
$ python server.py
```

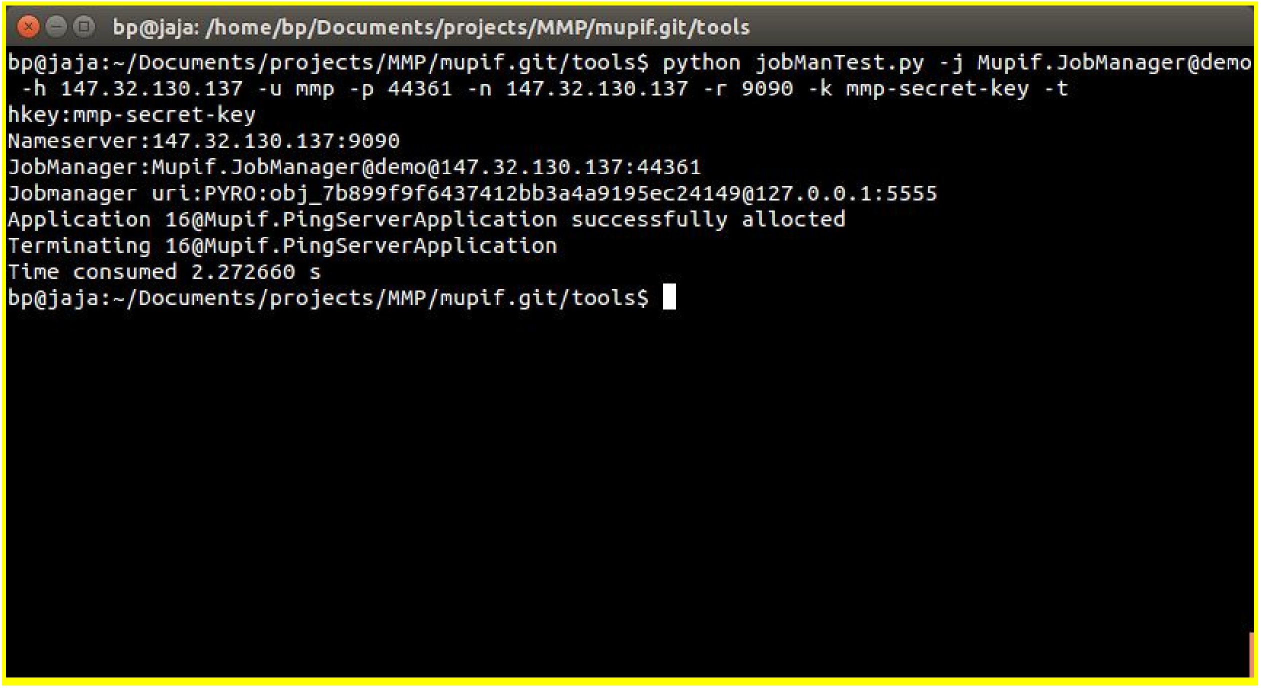
The command logs on screen and also in the server.log logfile the individual requests.

The status of the application server can be monitored on-line from any computer (provided you have established ssh connection to server) using tools/jobManStatus.py monitor. To start monitoring, run the following command:

```
$ python jobManStatus.py -j Mupif.JobManager@demo -h 147.32.130.137 -u mmp -p 44361 -n
147.32.130.137 -r 9090 -k mmp-secret-key -t
```

The -j option specifies the jobmanager name (as registered in pyro nameserver), -h determines the hostname where jobmanager runs, -p determines the port where jobmanager is listening, -n is hostname of the nameserver, -r is the nameserver port, -k allows to set PYRO hkey, -t enforces the ssh tunnelling, and -u determines the username to use to establish ssh connection on the server, see Fig. 12.

There is also a simple test script (tools/jobManTest.py), that can be used to verify that the installation procedure was successful. It contact the application server and asks for new application instance.



```
bp@jaja: /home/bp/Documents/projects/MMP/mupif.git/tools
bp@jaja:~/Documents/projects/MMP/mupif.git/tools$ python jobManTest.py -j Mupif.JobManager@demo
 -h 147.32.130.137 -u mmp -p 44361 -n 147.32.130.137 -r 9090 -k mmp-secret-key -t
hkey:mmp-secret-key
Nameserver:147.32.130.137:9090
JobManager:Mupif.JobManager@demo@147.32.130.137:44361
Jobmanager uri:PYRO:obj_7b899f9f6437412bb3a4a9195ec24149@127.0.0.1:5555
Application 16@Mupif.PingServerApplication successfully allocted
Terminating 16@Mupif.PingServerApplication
Time consumed 2.272660 s
bp@jaja:~/Documents/projects/MMP/mupif.git/tools$
```

Fig. 12: Testing job manager in a simple setup

8.4. Securing the communication using SSH tunnels

8.4.1. Setting up ssh server

SSH server provides functionalities which generally allows to

- Securely transfer encrypted data / streams
- Securely transfer encrypted files (SFTP)

- Set up port forwarding via open ports, so called tunneling, allowing to get access to dedicated ports through a firewall in between
- Remote command execution
- Forwarding or tunneling a port
- Securely mounting a directory on a remote server (SSHFS)

Ssh server is the most common on Unix systems, *freeSSHd* server can be used on Windows free of charge. The server usually requires root privileges for running. Ssh TCP/UDP protocol uses port 22 and uses encrypted communication by default.
Connection to a ssh server can be carried out by two ways. A user can authenticate by typing username and password. However, MuPIF prefers authentication using asymmetric private-public key pairs since the connection can be established without user's interaction and password typing every time. Fig. 13 shows both cases.

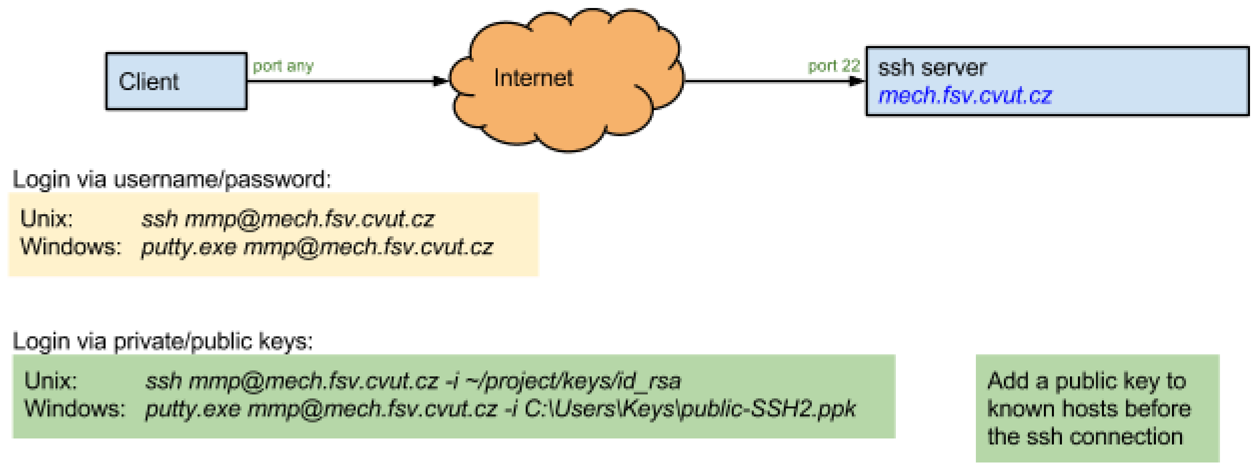

Client
port any
Internet
port 22
ssh server
mech.fsv.cvut.cz
Login via username/password:
Unix: ssh mmp@mech.fsv.cvut.cz
Windows: putty.exe mmp@mech.fsv.cvut.cz
Login via private/public keys:
Unix: ssh mmp@mech.fsv.cvut.cz -i ~/project/keys/id_rsa
Windows: putty.exe mmp@mech.fsv.cvut.cz -i C:\Users\Keys\public-SSH2.ppk
Add a public key to known hosts before the ssh connection

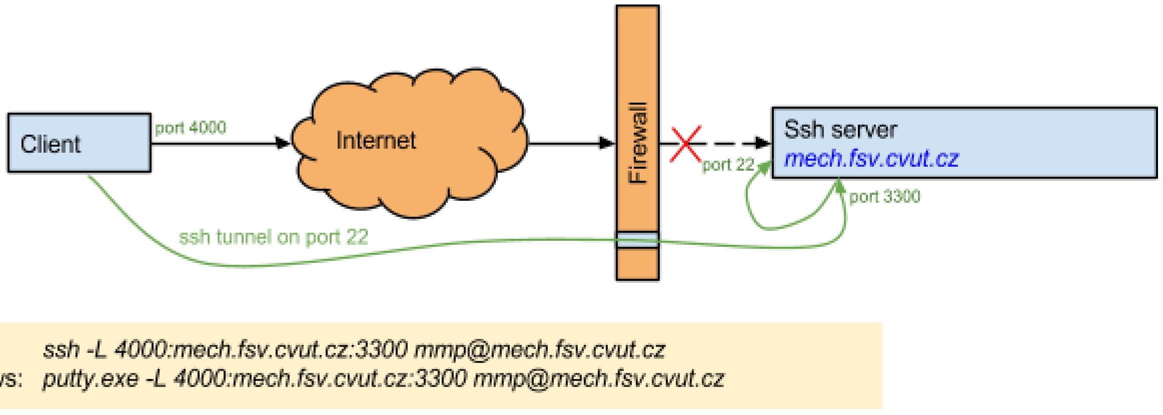
Fig. 13: Connection to a ssh server using username/password and private/public keys

Private and public keys can be generated using commands *ssh-keygen* for Unix and *puttygen.exe* for Windows. Ssh2-RSA is the preferred key type, no password should be set up since it would require user interaction. Keys should be stored in ssh2 format (they can be converted from existing openSSH format using *ssh-keygen* or *puttygen.exe*). Two files are created for private and public keys; Unix *id_rsa* and *id_rsa.pub* files and Windows *id_rsa.ppk* and *id_rsa* files. Private key is a secret key which remains on a client only.

Authentication with the keys requires appending a public key to the ssh server. On Unix ssh server, the public key is appended to e.g. *mech.fsv.cvut.cz:/home/user/.ssh/ authorized_keys*. The user from a Unix machine can log in without any password using a ssh client through the command

```
ssh user@mech.fsv.cvut.cz -i ~/project/keys/id_rsa
```

Ssh protocol allow setting up port forwarding via port 22, so called tunneling. Such scenario is sketched in Fig. 14, getting through a firewall in between. Since the communication in distributed computers uses always some computer ports, data can be easily and securely transmitted over the tunnel.



```
Unix:      ssh -L 4000:mech.fsv.cvut.cz:3300 mmp@mech.fsv.cvut.cz
Windows:   putty.exe -L 4000:mech.fsv.cvut.cz:3300 mmp@mech.fsv.cvut.cz
```

Fig. 14: Creating a ssh forward tunnel

8.4.2. Example of distributed scenario with ssh tunneling

The process of allocating a new instance of remote application is illustrated on adapted version of the local thermo-mechanical scenario, already presented in 7. Developing user workflows. First, the configuration file is created containing all the relevant connection information, see Listing 3.

```
#Network setup configuration
import sys, os, os.path
import Pyro4
# Pyro config
Pyro4.config.SERIALIZER="pickle"
Pyro4.config.PICKLE_PROTOCOL_VERSION=2 #to work with python 2.x and 3.x
Pyro4.config.SERIALIZERS_ACCEPTED={'pickle'}
Pyro4.config.SERVERTYPE="multiplex"

#Absolute path to mupif directory - used in JobMan2cmd
mupif_dir = os.path.abspath(os.path.join(os.getcwd(), "../../.."))
sys.path.append(mupif_dir)

import logging

#NAME SERVER
nshost = '147.32.130.71' #IP/name of a name server
nsport = 9090 #Port of name server
hkey = 'mmp-secret-key' #Password for accessing nameServer and applications

#Remote server settings
server = '147.32.130.71' #IP/name of a server's daemon
serverPort = 44382 #Port of server's daemon
serverNathost = '127.0.0.1' #Nat IP/name (necessary for ssh tunnel)
serverNatport = 5555 #Nat port (necessary for ssh tunnel)

jobManName='Mupif.JobManager@Example' #Name of job manager
```

```
appName = 'MuPIFServer' #Name of application

#JobManager setup
portsForJobs=( 9095, 9200 ) #Range of ports to be assigned on the server to jobs
jobNatPorts = list(range(6000, 6050)) #NAT client ports used to establish ssh
connections
maxJobs=4 #Maximum number of jobs
#Auxiliary port used to communicate with application daemons on a local computer
socketApps=10000 jobManWorkDir='.' #Main directory for transmitting files

jobMan2CmdPath = "../../tools/JobMan2cmd.py" #Path to JobMan2cmd.py

#CLIENT
erverUserName = os.getenv('USER')

#ssh client params to establish ssh tunnels
if(sys.platform.lower().startswith('win')):#Windows ssh client
       sshClient = 'C:\\Program Files\\Putty\\putty.exe'
       options = '-i L:\\.ssh\\mech\id_rsa.ppk'
       sshHost = ''
else:#Unix ssh client
       sshClient = 'ssh'
       options = '-oStrictHostKeyChecking=no'
       sshHost = ''
```
Listing 3: Simple example illustrating simulation scenario

The adapted simulation scenario is presented in Listing 4. This example assumes that the nameserver and thermal solver run on remote server, while the mechanical solver is executed locally on the same computer as simulation scenario. First, the simulation scenario connects to the nameserver and subsequently the handle to thermal solver allocated by the corresponding job manager is created using *PyroUtil.allocateApplicationWithJobManager service.* This service first obtains the remote handle of the job manager for thermal application, requests allocation of a new instance of thermal solver, returning an instance of RemoteAppRecord class, which encapsulate all the details of opened connections, established ssh tunnels, etc. It provides two useful methods: *getApplication()* returning application Proxy and *terminate()* that can be used to correctly terminate the application and close all connections.

The listing shows the complete distributed scenario, with the required modifications highlighted by the blue color. Note that the differences are only in the setup and terminating part, the core logic of the scenario remains the same for local as well as distributed case.
This example is available in MuPIF distribution under *examples/Example15-thermoMechanicalNonStat-ssh-JobMan* directory.

```
import sys
sys.path.extend(['..', '../../..'])
from mupif import *
```

```
import mupif
import conf as cfg

import time as timeTime
start = timeTime.time()
mupif.log.info('Timer started')

#locate nameserver
ns = PyroUtil.connectNameServer(nshost=cfg.nshost, nsport=cfg.nsport,
hkey=cfg.hkey)
#localize JobManager running on (remote) server and create a tunnel to it
#allocate the thermal server
solverJobManRec = (cfg.serverPort, cfg.serverNatport, cfg.server,
cfg.serverUserName, cfg.jobManName)


jobNatport = cfg.jobNatPorts.pop(0)

try:
	appRec = PyroUtil.allocateApplicationWithJobManager( ns, solverJobManRec,
jobNatport, cfg.sshClient, cfg.options, cfg.sshHost )
	thermal = appRec.getApplication()
except Exception as e:
	mupif.log.exception(e)
else:
	if thermal is not None:
	appsig=thermal.getApplicationSignature()
	mupif.log.info("Working thermalServer " + appsig)
	mechanical = PyroUtil.connectApp(ns, 'mechanical')

	time  = 0.
	dt = 0.
	timestepnumber = 0
	targetTime = 10.0

	while (abs(time - targetTime) > 1.e-6):

		mupif.log.debug("Step: %g %g %g"%(timestepnumber,time,dt))
		# create a time step
		istep = TimeStep.TimeStep(time, dt, timestepnumber)

		try:
		thermal.solveStep(istep)
		f = thermal.getField(FieldID.FID_Temperature, istep.getTime())
		data = f.field2VTKData().tofile('T_%s'%str(timestepnumber))

		mechanical.setField(f)
		sol = mechanical.solveStep(istep)
		f = mechanical.getField(FieldID.FID_Displacement, istep.getTime())
		data = f.field2VTKData().tofile('M_%s'%str(timestepnumber))

		thermal.finishStep(istep)
		mechanical.finishStep(istep)
```

```
              # determine critical time step
              dt = min (thermal.getCriticalTimeStep(),
                        mechanical.getCriticalTimeStep())

              # update time
              time = time+dt
              if (time > targetTime):
                    # make sure we reach targetTime at the end
                    time = targetTime
              timestepnumber = timestepnumber+1

              except APIError.APIError as e:
              log.error("Following API error occurred:",e)
              break
       mechanical.terminate();

       else:
       mupif.log.debug("Connection to thermal server failed, exiting")

finally:
       if appRec: appRec.terminateAll()
```
Listing 4: Simple example illustrating simulation scenario

8.4.3. Advanced SSH setting

When a secure communication over ssh is used, then typically a steering computer (a computer executing top level simulation script/workflow) creates connections to individual application servers. However, when objects are passed as proxies, there is no direct communication link established between individual servers. **This is quite common situation, as it is primarily the steering computer and its user, who has necessary ssh-keys or credentials to establish the ssh tunnels from its side, but typically is not allowed to establish a direct ssh link between application servers.** The solution is to establish such a communication channel transparently via a steering computer, using forward and reverse ssh tunnels. The platform provides handy methods to establish needed communication patterns (see *PyroUtil.connectApplications* method and refer to *example10* for an example).

As an example, consider the simulation scenario composed of two applications running on two remote computers as depicted in Fig. 15. The Pyro4 daemon on server 1 listens on communication port 3300, but the nameserver reports the remote objects registered there as listening on local ports 5555 (so called NAT port). This mapping is established by ssh tunnel between client and the server1. Now consider a case, when application2 receives a proxy of object located on server1. To operate on that object the communication between server 1 and server 2 needs to be established, again mapping the local port 5555 to target port 3300 on server1. Assuming that steering computer already has an established communication link from itself to Application1 (realized by ssh tunnel from local NAT port 5555 to target port 3300 on the server1), an additional communication channel from server2 to steering computer has to be established (by ssh tunnel connecting ports 5555 on both sides). In this way, the application2 can directly work with remote objects at server 1 (listening on true port 3300) using proxies with NAT port 5555.

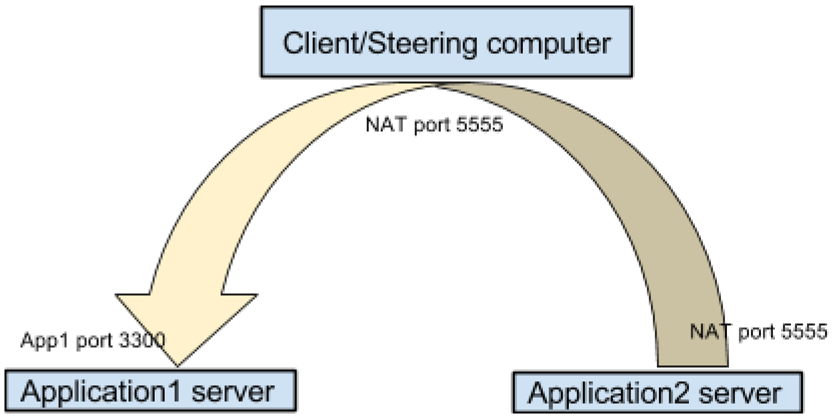


Fig. 15: Establishing a communication link between two application servers via SSH tunnels.

8.4.4. Troubleshooting SSH setup

- Verify that the connection to nameserver host works:
    - ping name_server_hostname
- Run the jobManTest.py with additional option “-d” to turn on debugging output, examine the output (logged also in mupif.log file)
- Examine the output of server messages printed on screen and/or in file *server.log*

8.5. Using Virtual Private Network (VPN)

8.5.1. Generalities

This section only provides background for VPN and can be skipped. The standard way of node communication in MuPIF is to use SSH tunnels. SSH tunnels have the following advantages:

- No need for administrator privileges.
- Often the way for remotely accessing computers which are already in use.
- Easy traversal of network firewalls (as long as the standard port 22 is open/tunneled to the destination).

They also have some disadvantages:

- Non-persistence: the tunnel has to be set up every time again; if connection is interrupted, explicit reconnection is needed, unless automatic restart happens, e.g. autossh.

The tunnel is only bi-directional and does no routing; thus is A-B is connected and B-C is connected, it does not imply C is reachable from A. Though, it is possible to create a multi-hop tunnel by chaining *ssh* commands.
VPN is an alternative to SSH tunnels, providing the encryption and authorization services. The VPNs work on a lower level of communication (OSI Layer 2/3) by establishing “virtual” (existing

on the top of other networks) network, where all nodes have the illusion of direct communication with other nodes through TCP or UDP, which have IP addresses assigned in the virtual network space, see Fig. 16. The VPN itself communicates through existing underlying networks, but this aspect is not visible to the nodes; it includes data encryption, compression, routing, but also authentication of clients which may connect to the VPN. OpenVPN is a major implementation of VPN, and is supported on many platforms, including Linux, Windows, Android and others.

Using VPN with MuPIF is a trade-off where the infrastructure (certificates, VPN server, …) is more difficult to set up, but clients can communicate in a secure manner without any additional provisions - it is thus safe to pass unencrypted data over the VPN, as authentication has been done already; in particular, there is no need for SSH tunnels

Note that all traffic exchanged between VPN clients will go through the OpenVPN server instance; the connection of this computer should be fast enough to accommodate all communication between clients combined.

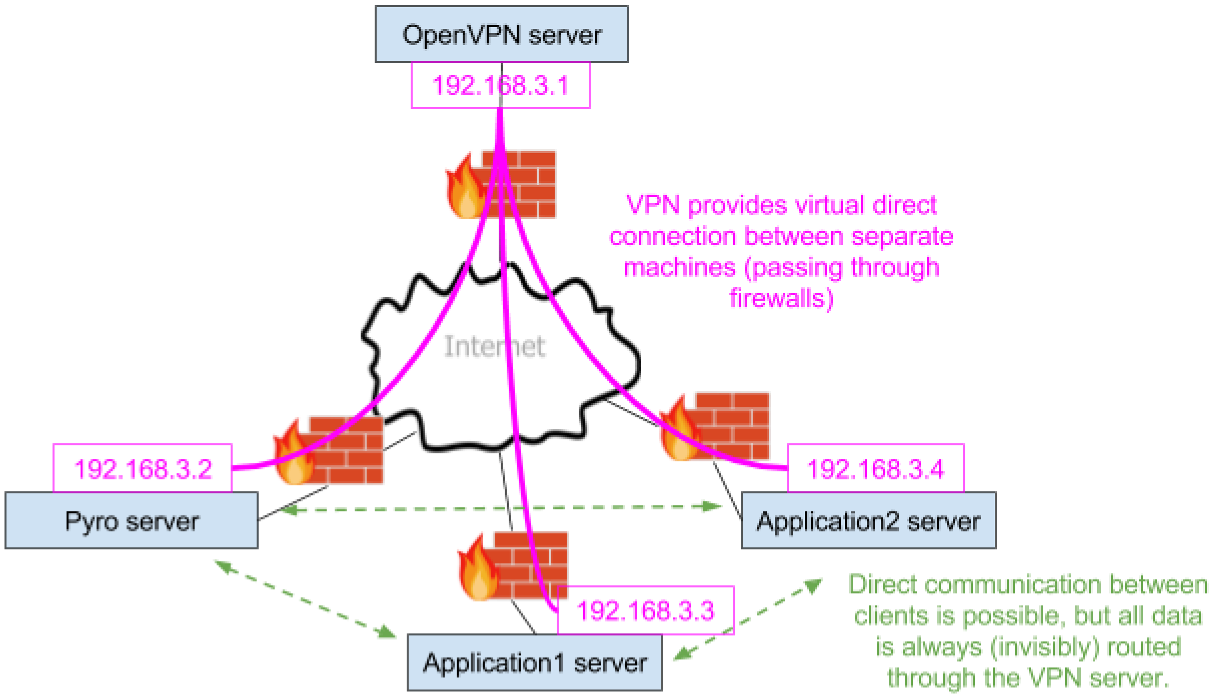

OpenVPN server
192.168.3.1
VPN provides virtual direct connection between separate machines (passing through firewalls)
Internet
192.168.3.2
Pyro server
192.168.3.4
Application2 server
192.168.3.3
Application1 server
Direct communication between clients is possible, but all data is always (invisibly) routed through the VPN server.

Fig. 16: VPN architecture

8.5.2. Setup

Setting up the VPN is generally more difficult than ssh tunnels. It comprises the following:

- Communication ports reachable by all clients must be set up as a part of the infrastructure (usually on a static & public IP address); this involves opening ports in firewalls, and most network administrators are not very keen to do that. While these are configurable, the default is UDP 1194 for client access; often TCP 443 is also (ab)used (it is commonly and by standard used for HTTPS).

- Running the OpenVPN daemon on the server; server configuration is not overly complicated, there are in fact many good tutorials available.
- Distributing OpenVPN configuration files (usually ending .ovpn) to the clients.
- Clients have to connect to the VPN whenever they want to communicate with the network - this can be done from the command-line or using graphical interfaces.

Whenever a client connects to the OpenVPN server, the following happens:

1. The client is authenticated, either via username/password or certificate.
2. The client is handed an IP address from the VPN range, as specified by ifconfig-pool configuration option, or assigned a fixed IP based on the client configuration (client-config-dir), see OpenVPN Addressing.
3. The client's OS assigns the IP address to a virtual network adapter (tun0, tun1 etc in Linux) and sets IP routing accordingly. Depending on server configuration, all non-local traffic (such as to public internet hosts) may be routed through the VPN, or only traffic for VPN will go through the VPN. At this moment, other clients of the VPN become visible to the new client, and vice versa (it is client's responsibility to firewall the VPN interface, if desired).

There are example scripts to generate OpenVPN configuration for MuPIF in *tools/vpn*. The script generates certificate authority and keys used for authentication of server and clients, and also for traffic encryption; those files must be slightly hand-adjusted for real use afterwards. The recommended configuration for MuPIF is the following (non-exhaustive; the tutorial from digitalocean (www.digitalocean.com/…..) explains most of the procedure).

1. Use the usual "subnet" network topology.
2. IP addresses within the VPN may be assigned from the address pool, but at least some machines should have fixed IP - this can be done using the client-config-dir option. In particular, the Pyro nameserver should have a well-known and stable IP address so that the client configuration does not have to change; the best is to run the OpenVPN server on the same computer where Pyro runs, then the IP address will be stable.
3. Only in-VPN traffic should be routed through the VPN (thus the redirect-gateway option should not be used); communication of clients with Internet will go through the usual ISP route of each client.
4. Firewall facing internet should allow UDP traffic on port 1194. Optionally, other port can be used (even non-OpenVPN port, like TCP/443, which is normally used for HTTPS). All traffic on the tun0 (or other number) interfaces should be allowed; one can use the "-i tun+" option of iptables to apply a rule to any interface of which name starts with tun.
5. Keepalive option can be used to increase network reliability (functions as both heart-beat & keep-alive).
6. Authentication can be done using username & password, but key-based authentication (client keys must be distributed to clients) is recommended.

7. The server is started either as a daemon (through init.d or systemd) or from the commandline, in which case “Initialization Sequence Completed” will be shown when ready to serve clients.

Client configuration:

1. If the configuration is distributed as .ovpn file with embedded keys, the VPN can be activated from command-line by issuing sudo openvpn --config client.ovpn. The client will say Initialization Sequence Completed after successful connection to the VPN. Use Ctrl-C to terminate the client and disconnect from the VPN.
2. The GUI of NetworkManager can import the configuration and use it, but not in all cases (embedded keys seem to be the problem), in which case the .ovpn file can only contain filenames where the keys/certs are stored, or the configuration can be created by hand through the NetworkManager GUI.
3. Connection to the VPN can be verified by issuing “ip addr show” which should show the tun0 (or similar) interface with an IP assigned from the OpenVPN server pool.

8.5.3. Example of simulation scenario using VPN

The process of allocating a new instance of remote application is illustrated on adapted version of the local thermo-mechanical scenario, already presented in 7. Developing user workflows. First, the configuration file is created containing all the relevant connection information, see Listing 5.

```
#Common configuration for examples
import sys, os, os.path
import Pyro4
Pyro4.config.SERIALIZER="pickle"
Pyro4.config.PICKLE_PROTOCOL_VERSION=2 #to work with python 2.x and 3.x
Pyro4.config.SERIALIZERS_ACCEPTED={'pickle'}
Pyro4.config.SERVERTYPE="multiplex"

#Absolute path to mupif directory - used in JobMan2cmd
mupif_dir = os.path.abspath(os.path.join(os.getcwd(), "../../.."))
sys.path.append(mupif_dir)

#from mupif import logging

#NAME SERVER and SERVER
nshost = '172.30.0.1'#IP/name of a name server
nsport = 9090 #Port of name server
hkey = 'mmp-secret-key'#Password for accessing nameServer and applications

#SERVER for a single job or for JobManager
server = '172.30.0.1' #IP/name of a server's daemon
serverPort = 44382 #Port of server's daemon
jobManName='Mupif.JobManager@Example'#Name of job manager
appName = 'MuPIFServer'#Name of application
```

```
#Jobs in JobManager
portsForJobs=( 9095, 9200 )#Range of ports to be assigned on the server to jobs
maxJobs=4 #Maximum number of jobs
#Auxiliary port used to communicate with application daemons on a local computer
socketApps=10000
jobManWorkDir='.' #Main directory for transmitting files
jobMan2CmdPath = "../../tools/JobMan2cmd.py" #Path to JobMan2cmd.py

#Name of the application
appName = 'MuPIFServer'
```

Listing 5: Simple example illustrating simulation scenario

The adapted simulation scenario is presented in Listing 6. This example assumes that the nameserver and individual application servers (job managers) run on different computers. The main difference now is that there is no need to create any ssh tunnels so there is also no need to set ssh related parameters in config file. The listing shows the complete distributed scenario, with the required modifications highlighted by the blue color. This example is available in MuPIF distribution under
examples/Example16-thermoMechanicalNonStat-VPN-JobMan directory.

```
import sys
sys.path.extend(['..', '../../..'])
from mupif import *
import mupif
import conf_vpn as cfg

import time as timeTime
start = timeTime.time()
mupif.log.info('Timer started')

#locate nameserver
ns = PyroUtil.connectNameServer(nshost=cfg.nshost, nsport=cfg.nsport,
hkey=cfg.hkey)
#localize JobManager running on (remote) server and create a tunnel to it
#allocate the thermal server
solverJobManRecNoSSH = (cfg.serverPort, cfg.serverPort, cfg.server, '',
cfg.jobManName)

jobNatport = -1

try:
      appRec = PyroUtil.allocateApplicationWithJobManager( ns,
solverJobManRecNoSSH, jobNatport, sshClient='manual', options='', sshHost = '' )
      mupif.log.info("Applocated application %s" % appRec)
      thermal = appRec.getApplication()
except Exception as e:
      mupif.log.exception(e)
else:
      if thermal is not None:
      appsig=thermal.getApplicationSignature()
      mupif.log.info("Working thermalServer " + appsig)
      mechanical = PyroUtil.connectApp(ns, 'mechanical')

      time  = 0.
      dt = 0.
      timestepnumber = 0
      targetTime = 10.0

      while (abs(time - targetTime) > 1.e-6):

              mupif.log.debug("Step: %g %g %g"%(timestepnumber,time,dt))
              # create a time step
              istep = TimeStep.TimeStep(time, dt, timestepnumber)

              try:
              thermal.solveStep(istep)
              f = thermal.getField(FieldID.FID_Temperature, istep.getTime())
              data = f.field2VTKData().tofile('T_%s'%str(timestepnumber))

              mechanical.setField(f)
              sol = mechanical.solveStep(istep)
              f = mechanical.getField(FieldID.FID_Displacement, istep.getTime())
              data = f.field2VTKData().tofile('M_%s'%str(timestepnumber))

              thermal.finishStep(istep)
              mechanical.finishStep(istep)

              # determine critical time step
              dt = min (thermal.getCriticalTimeStep(),
mechanical.getCriticalTimeStep())

              # update time
              time = time+dt
              if (time > targetTime):
                      # make sure we reach targetTime at the end
                      time = targetTime
              timestepnumber = timestepnumber+1

              except APIError.APIError as e:
              log.error("Following API error occurred:",e)
              break
      mechanical.terminate();

      else:
      mupif.log.debug("Connection to thermal server failed, exiting")

finally:
      if appRec: appRec.terminateAll()
```
Listing 6: Simple example illustrating simulation scenario

9. Acknowledgements

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The authors would like to acknowledge the EU support from Horizon 2020 Project Composelector, Contract N°: 721105

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ChangeLog

- **V1.1 (05/2017):** Expanded section on workflow implementation, added subsections on workflow templates and workflow as a class. Already describes some concept to be introduced in ver. 2.0 (transparent ssh tunnel handling using decorator classes). Added acknowledgement to EU via Composelector project.

ToDo

- Description of metadata support missing