

MMP Platform User Manual

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Table of Content

Table of Content

Introduction

Platform installation

Prerequisites

Windows platforms

Linux / Unix (*nix) platforms

General requirements

Other recommended packages/softwares

<u>Installing the MMP platform</u>

Verifying platform installation

Platform operations

Developing application API

Distributed Model

Internal platform solution - JobManager resource allocation

Installation

Setting up ssh server

Setting up Job Manager

Configuration

Troubleshooting

Simple distributed example using jobManager resource allocation

References

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Introduction

The approach followed in the MMP-project 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 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. This essentially allows to manipulate all simulation tools using the same interface. Moreover, as the simulation data are represented by objects as well, the platform is independent on particular data format(s), as the exchanged data (such as fields and properties) can be manipulated using the same abstract interface. Therefore, the focus on services is provided by objects (object interfaces) and not on underlying data itself.

The complex simulation pipeline developed in MMP-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 MMP 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 MMP 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.

Platform installation

Prerequisites

Windows platforms

- We suggest to install Anaconda scientific python package (tested version 2.1): 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/

Linux / Unix (*nix) platforms

- The Python (Python 2.x) installation is required. Some functionality depend on vtk python module, that is available in Python 2.x version only.
- You can dowload the python installation package from https://www.python.org/downloads/. Just pick up the latest version in the 2.x series (tested version 2.7.8).
- 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)

General requirements

 MMP platform depends/requires Pyro4 (tested version 4.30) and numpy (tested 1.6.2) modules. To install these modules using pip:

pip install Pyro4

• MMP platform requires pyvtk (tested 0.4.85) python module. To install this module using pip:

pip install pyvtk

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/

Installing the MMP platform

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

pip install mupif

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 MMP platform repository into a directory "mupif-code":

git clone git://git.code.sf.net/p/mupif/code mupif-code

Verifying platform installation

The platform installation comes with many examples, that can be used to verify the successful installation. The examples are located in examples subfolder. For example, to run Example01:

cd examples/Example01 python Example01.py

Platform operations

The complex simulation pipeline developed in MMP-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 Simple distributed example using JobManager.

The presented example in Table 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();
```

Table 1: Simple example illustrating simulation scenario

The full listing of this example can be found in <u>examples/Example01</u>. The output is illustrated in Figure 1.

Fig. 1: Output from Example01.py

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

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 API specificaton [1], also available online.

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).

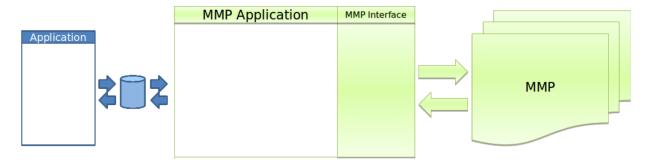


Fig. 2: Illustration of indirect approach

The example illustrating the indirect implementation is available from 2nd workshop material (located in examples/Workshop02/Demo31). 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 Demo31. 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.

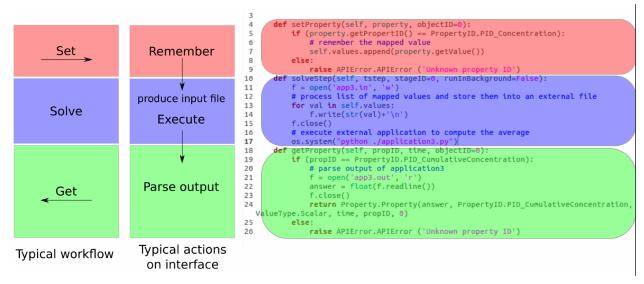


Fig. 3: Typical workflow in indirect approach to API implementation

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.

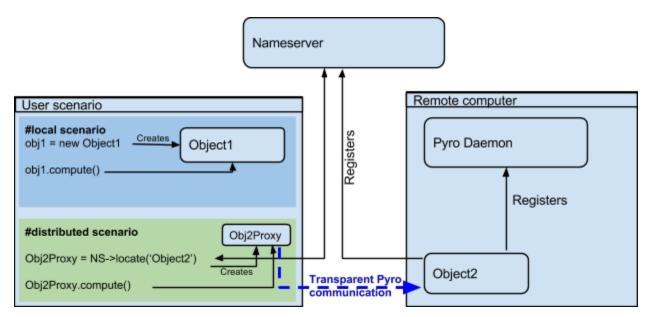


Fig.4: Local vs remote object communication scenarios compared

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 on Fig. 4.

Within the MMP project, the nameserver service is hosted at CTU infrastructure, see Table 3 for details. For the use of the platform outside the MMP project a different Pyro nameserver should be set up and used, see Pyro documentation.

nameserver hostname	nameserver IP address	port
mech.fsv.cvut.cz	147.32.130.137	9090

Table 3: MMP nameserver parameters.

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.

Internal platform solution - JobManager resource allocation

This solution has been developed from 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. 4 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.

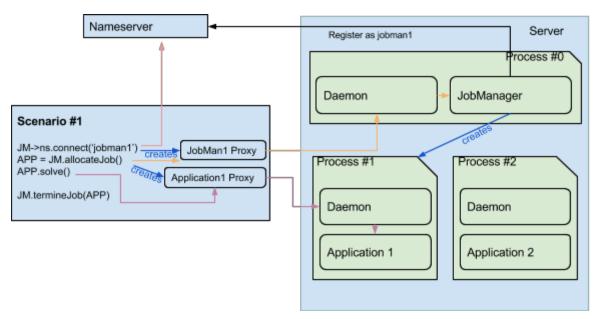


Fig. 5: Typical control flow with resource allocation using JobManager.

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. 6.

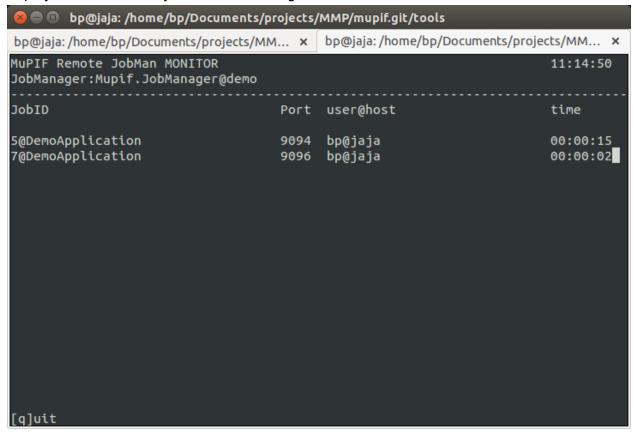


Fig. 6: Screenshot of Job Manager monitoring tool

The user and access control is controlled using ssh authorization. The individual computational servers and their platform services are assumed to run behind a firewall. To establish the connection to a remote server and platform services a secure connection has to be established. This is realized using setting up ssh tunnel, that allows client to communicate with protected communication ports on the 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.

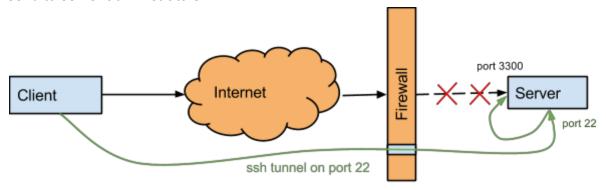


Fig. 7: Bypassing firewalls with ssh tunnels

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.

Installation

Setting up ssh server

SSH server provides functionalities which generally allows to

- Securely transfer encrypted data / streams
- Securely transfer encrypted files (SFTP)
- 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 runs on a 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. Figure 8 shows both cases.

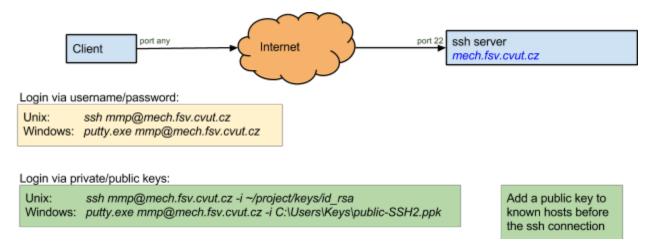


Fig. 8: Connection to a ssh server using username/password and private/public keys

Private and public keys can be generated using commands <code>ssh-keygen</code> for Unix and <code>puttygen.exe</code> 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 <code>ssh-keygen</code> or <code>puttygen.exe</code>). Two files are created for private and public keys; Unix <code>id_rsa</code> and <code>id_rsa.pub</code> files and Windows <code>id_rsa.ppk</code> and <code>id_rsa</code> 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. <code>mech.fsv.cvut.cz:/home/mmp./ssh/authorized_keys</code>. The user from a Unix machine can log in without any password using a ssh client through the command

ssh mmp@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 Figure 9, 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.

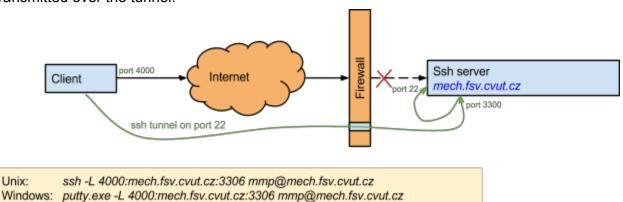


Fig. 9: Creating a ssh forward tunnel

Setting up 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 conf.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 Section <u>Platform installation</u>. Also, the functional application API class is needed. Fig. 10 shows the flowchart

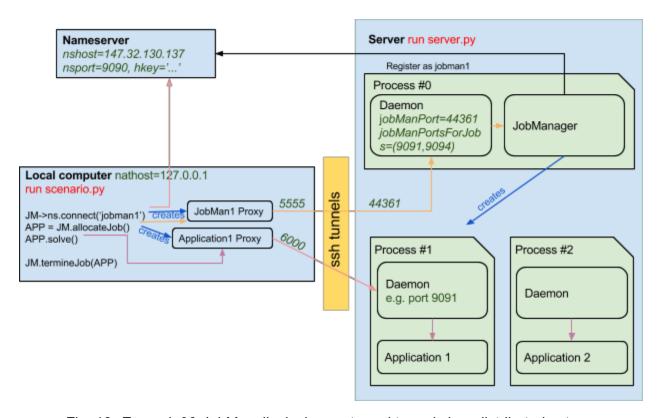


Fig. 10: Example06-JobMan displaying ports and tunnels in a distributed setup.

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.

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 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 Figure 11.

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.

Fig. 11: Testing job manager in a simple setup

Troubleshooting

- Verify that the connection to nameserver host works: ping 147.32.130.137
- 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

Simple distributed example using jobManager resource allocation

The process of allocating a new instance of remote application involves several steps, see Table 4. First, the secure connection to corresponding job manager has to be established using ssh tunnel. In the second step, the jobManager is requested to allocate a new application instance and returns corresponding URI of new application. As the application is executed in a separate process, a second secure connection to the new process pyro daemon has to be established and the proxy of application instance obtained. When the scenario is terminating, all these connections have to be correctly terminated. As this involves a lot of steps, a utility function *PyroUtil.allocateApplicationWithJobManager* is provided, returning an instance of RemoteAppRecord class, which encapsulate all the details of opened connections, 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. Here we show again the example presented in section <u>Platform operations</u>, with the potential modifications for the distributed case shown in 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.

```
from mupif import *
import application1
import application2
time = 0
timestepnumber=0
targetTime = 10.0
#locate nameserver
ns = PyroUtil.connectNameServer(nshost=conf.nshost, nsport=conf.nsport,
hkey=conf.hkey)
#establish secure tunnel to JobManager running on (remote) server
try:
      app1Rec = PyroUtil.allocateApplicationWithJobManager (ns, conf.app1JobManRec,
                                                           conf.jobNatPorts.pop())
      app2Rec = PyroUtil.allocateApplicationWithJobManager (ns, conf.app2JobManRec,
                                                           conf.jobNatPorts.pop())
      app1 = app1Rec.getApplication()
      app2 = app2Rec.getApplication()
except Exception as e:
      logger.exception(e)
      app1Rec.terminate()
      app2Rec.terminate()
      break
#establish secure tunnel to JobManager running on (remote) server
      jobMan2 = PyroUtil.connectApp(ns, conf.jobManName)
      retRec2 = jobMan.allocateJob(PyroUtil.getUserInfo(), natPort=conf.jobNatPort)
      app2 = PyroUtil.connectApp(ns, retRec2[1])
except Exeption as e:
      logger.error("Following API error occurred: %s" % e )
      break
# 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
```

```
print ("Step: %d %f %f" % (timestepnumber, time, dt) )
      # 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 ("Result: %f" % prop.getValue() )
      except APIError.APIError as e:
             logger.error("Following API error occurred: %s" % e )
             break
# terminate
app1Rec.terminate()
app2Rec.terminate()
```

Table 4: Simple example illustrating simulation scenario

References

- 1. D1.1 Application Interface Specification, MMP Project, 2014.
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- 7. B. Patzak, V. Smilauer, and G. Pacquaut, presentation & paper "Design of a Multiscale Modelling Platform" at the 15 th International Conference on Civil, Structural, and

Environmental Engineering Computing, 1st - 4th of September 2015, Prague (Czech Republic).