PyMOOSE

Python module for MOOSE Simulation
Version 1.3

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This manual is for MOOSE (version 1.3), The Multiscale Object-Oriented Simulation Environment.

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Executive Summary

It contains an overview of how to use MOOSE as a Python module to setup and run simulations. It also supplements as a reference manual describing the classes of objects in MOOSE.

1 Copying this document

This manual is for MOOSE (version 1.3), The Multiscale Object-Oriented Simulation Environment.

2 Introduction to MOOSE and PyMOOSE

MOOSE is a general purpose simulation environment, and PyMOOSE its incarnation as a Python module. MOOSE stands for Multiscale Object-Oriented Simulation Environment.

The 'multiscale' comes from the fact that one can simulate systems spanning multiple scales: from a few molecules reacting with each other (Gillespie simulations) to large networks of neurons to simulate areas of the brain.

It is 'object-oriented' in the sense that it represents the simulation entities as instances of particular classes and these classes are organized in a hierarchy where a child inherits the properties of its parent.

2.1 Modeling for simulation

Computers are limited by the available memory and the speed of the electronics, whereas anything from reality has infinite complexity (if you have any doubt, see the beautiful description of the complexity of a glass of wine by Richard Feynman)[1]. Hence, when simulating any system from reality, we have to consider carefully what details are important and what to leave out.

This leads us to abstraction. We use the existing scientific knowledge to make abstract representations of entities from reality. These are called `objects`. We use `objects` as the building blocks for more complex models. An `object` in a model may be represent a real-life object or some abstract concept. How do we model the interaction between the objects in real life? Through `messages` between interacting `objects`. Also, the pieces information relevant to the situation are attached to the `objects` as `fields`. When we set up these abstractions and interactions, we have a model of the system.

As an illustration, consider modeling a simple chemical reaction, say the oxidation of Nitric oxide(NO) to Nitrogen dioxide(NO2). There are some NO molecules and some O2 molecules and depending on the concentrations they react at certain rate and form NO2. If you go too deep into reality, there is a mind boggling amount of detail: NO molecules and O2 molecules roaming around randomly inside a container at very high speed, hitting each other and the walls of the container and once in a while there will be some exchange of electrons and an atom of oxygen will stick with the NO to share them.

But we also know that as long as we are worrying only about the amount of the end product NO2 at any given time, all these details can be forgotten and a more simple law can be applied if we have some empirical information, viz., the initial concentration of each of the gases, the rate constants of the forward and backward reactions and how many molecules of each reactant gas react to produce how many molecules of the product. Given these, we can invoke the laws of chemistry to calculate the concentration of each molecule at any given time. When we compute the series of values these molecular concentrations take at a given sequence of points in time, we call that a simulation.

All this can be modeled and simulated in MOOSE as follows:

The gases will be contained in some closed volume: we represent this with a `KinCompt` object (the name is a programmers' abbreviation for COMPartmenT for chemical KINetics). We set the `volume` field of the `KinCompt` object.

[1] Feynman Lectures on Physics, Volume I, pp 3-10, The relation of Physics to other sciences

The pool of NO molecules will be modeled as *a* `Molecule` object and we set the number of molecules by setting the the field `n` of the Molecule object. Similarly, the pools of O2 and NO2 molecules will be modeled as `Molecule` objects (If initially there is no NO2, we set `n = 0` for it). When we set the number of molecules, the concentration is computed automatically from the volume of the `KinCompt` object. Alternatively, we can set the concentrations directly in the `conc` field of the `Molecule` objects.

Now the reaction itself is determined by the forward and backward rate constants. The `Reaction` class is precisely for this. We create a `Reaction` object and set its `Kf` and `Kb` fields to the forward and backward rate constants.

Now to implement the interaction between these, we set some messages between particular fields of different objects. We have to setup the substrate and product relationships of the `Molecules` with the `Reaction`. This is done by connecting the `'reac'` field of the O2 and NO `Molecule` objects with `'sub'` field of the `Reaction` object and connecting the `'reac'` field of the NO2 `Molecule` with the `'prd'` field of the `Reaction` object.

There are bunch of `Clock` objects that tick at some specified intervals. Each object is associated with some clock which controls the update interval of its state variables. Once the model is set up we can do a 'reset' to bring everything to an initial condition and then 'run' the simulation. Running the simulation causes the clocks to start. As each clock progresses, the `conc` field of the `Molecules` will be updated with the computed concentration for that time.

3 Installing (Py)MOOSE

MOOSE is available both as source code and platform-specific installer packages. However easy the platform-specific installers are to use, there may be issues with dependencies. Hence the most universal way of installing MOOSE is to build it from the sources.

3.1 Prerequisites

- GNU Make
- GNU C and C++ compiler

  gcc and g++ are required for compiling the C++ source code of MOOSE.
- Python development headers

  Python.h should be located somewhere in the include search directories. If it is in a non standard directory, you can edit pymoose/Makefile to add this directory in the include search path with −I{your_python_include_directory} argument.
- GNU Scientific Library

  GSL provides integration methods for some classes in MOOSE.
- libsbml

  The default build requires libsbml to be installed. You can download it from SBML website (`http://sbml.org`).

3.2 Configuration

Right now all configuration is done by editing the `Makefile` of MOOSE. You can have some control over what all are included in the compilation by passing commandline arguments to `make`. These options are described in the next section (Build/install).

3.3 Build/install

To build **pymoose** run make in the moose source code's top-level directory with pymoose as the targte:

make pymoose

This will do the default build. There are several options you can pass to make for customizing the build. Pass the options as key-value pairs in the make commandline as follows:

make pymoose OPTION1=value1 OPTION2=value2 OPTION3=value3

Most of the options are for enabling or disabling some feature. They are listed below:

- BUILD=release,debug (default value: release)

  BUILDTYPE can be either `debug` or `release`. Passing `debug` will build an unoptimized version with debugging symbols for gdb and will enable the built-in C++ unit tests.

  `release` will build an optimized version without debugging symbols or unit-tests.

  If unspecified, BUILD defaults to `release`.
- USE_GSL=1,0 (default value: 1) Use GNU Scientific Library for integration in kinetic simulations.

- USE_SBML=1,0 (default value: 1) Compile with support for the Systems Biology Markup Language (SBML). This allows you to read and write chemical kinetic models in the simulator-indpendent SBML format.
- USE_NEUROML=1,0 (default value: 0) Compile with support for the NeuroML. This allows you to read neuronal models in the NeuroML format. Look in external/neuroML_src/README for the extra steps needed to add the libraries & headers.
- USE_READLINE=1,0 (default value: 1) Use the readline library which provides command history and better command line editing capabilities
- USE_MPI=1,0 (default value: 0) Compile with support for parallel computing through MPICH library
- USE_MUSIC=1,0 (default value: 0) Compile with MUSIC support. The MUSIC library allows runtime exchange of information between simulators.
- USE_CURSES=1,0 (default value: 0) To compile with curses support (terminal aware printing)
- USE_GL=1,0 (default value: 0) To compile with OpenSceneGraph support to enable the MOOSE elements 'GLcell', 'GLview'.
- GENERATE_WRAPPERS=1,0 (default value: 0) Useful for python interface developers. The binary created with this option looks for a directory named 'generated' in the working directory and creates a wrapper class (one .h file and a .cpp file) for each moose class and partial code for the swig interface file (pymoose.i). These files with some modification can be used for generating the python interface using swig.

The build process for pymoose generates two final output files in the top level directory: `moose.py` and `_moose.so`. Copy these to any location in your PYTHONPATH environment variable (for Python 2.6 you can copy them to '`dist-packages`' directory inside your python installation directory (for UNIX-like systems it is: '`/usr/lib/python{version}`' or '`/usr/local/lib/python{version}`' Additionally, there is a file with some utility functions '`pymoose/pymoose.py`'. It has functions like `showmsg`, `printtree`, etc. You may copy this file along with moose.py to use these functions.

3.4 Loading

Once you have built and installed PyMOOSE, you can load it in the Python interpreter by the statement: `import moose` You should see a few informational outputs, ending with:

```
SIMPATH = .:your_home_directory
nnnn FuncVecs built for the first time
```

where *your_home_directory* stands for the full path of the user's home directory and *nnnn* stands for some number (2200 in my case).

4 Quick Start

5 In-Depth Guide to PyMOOSE

In this chapter we go through the internal details of PyMOOSE.

5.1 Overview of PyMOOSE internals

The entities in a MOOSE model are called `elements`. An `element` is an object of some MOOSE class. Elements are the basic building blocks of a model. You set the properties of the individual elements and connect them via messages to build a model.

5.1.1 Id - the unique identifier of each MOOSE object

Each element has a unique identifier, called its `id`. PyMOOSE provides Pythonic wrappers around this id. For every MOOSE class, we have a corresponding Python class provided by PyMOOSE. This class essentially creates an illusion of mirrorring the MOOSE class via a set of properties which correspond to the fields in the MOOSE class. The main data contained in instances of the PyMOOSE classes is only a copy of the `id` of the original MOOSE object. All the fields are accessed on-demand via function calls using this `id` as the handle.

5.1.2 Class hierarchy of MOOSE

MOOSE provides a class hierarchy which is closely imitated by the PyMOOSE classes. `Neutral` is at the top of the class hierarchy. So instance of any other MOOSE class is also an instance of `Neutral` class. A Neutral object is most often used as a container of other objects.

Major areas of focus in MOOSE are neuronal simulations and biochemical simulations. So many of the classes are for modeling these scenarios. Some of the commonly used classes in Neuronal models are:

- Compartment - models an isopotential fragment of a neuronal cable.
- HHChannel - Hodgkin-Huxley-type ion channel.
- SynChan - Synaptic channel.
- SpikeGen - Spike generator. This models the presynaptic terminal and is connected to the SynChan on the postsynaptic side.
- Cell - Represents a single neuron. Practically it is a container for connected compartments that constitute a neuron.

Commonly used classes in biochemistry/chemical kinetics models are:

- Molecule - A pool of molecules.
- Enzyme - An abstraction of enzymatic mechanism.
- Reaction - A general chemical reaction with forward and backward rate constants.
- KinCompt - A volume in space in which molecules exist/reactions take place.

Some classes are there to provide utilities and infrastructure for doing simulation experiments:

- Table - A versatile list-like structure which allows interpolation, data-recording, sending pre-assigned sequence of data at each time step tp some target object and saving data to file.

- AscFile - A general text(ascii) file handle.
- Random number generators - a whole bunch of them to generate samples from various distributions.

TODO: incorporate class-herarchy diagram

5.1.3 Messaging

Any complex model is composed of multiple components called `elements` which represent some well defined biological concept, like an ion-channel or an enzyme. The components of a model are connected to each other via messages. These messages allow state variables of one element to be seen by the other. For example, a synaptic channel has a conductance `g` which depends on the membrane potential `Vm` of a neuronal compartment. `Vm` on the other hand changes with change in `g`. Thus, we need a message sending `Vm` from compartment to synapse and a message sending `g` from synapse to compartment. These two messages are combined in another message, `channel`.

> Take, for example, a simple reaction: A + B <---> C. By convention, the rate of the forward reaction is represented by *Kf* and that of the backward reaction is represented by *Kb*.
>
> Now, **A**, **B** and **C** are molecular species and MOOSE provides the class Molecule to model them. The main property of a Molecule element is *n*, the number of molecules.
>
> As you will immediately recognize, just knowing the number of molecules does not help in calculating the progress of a chemical reaction with time. It is concentration that matters. But to obtain concentration from number of molecules, you need the volume of the container. This container is called a kinetic compartment, which need not be a real container, but any volume in space whithin which the molecules are homogeneously distributed. Kinetic compartments are represented by the class KinCompt in MOOSE.
>
> TODO: to be completed with an walk-through to developing the simulation.

5.2 Element Tree

All elements in MOOSE are part of a tree structure. We call this `Element Tree` or `Element Tree`. This is similar to the folder structure in the file system of your computer. Each entry in this tree is a moose object and we call it an **element**. The top level element is called the `root` element (represented as '`/`'). Every element other than `root` has a parent element. There are some predefined special elements that are used for management of the system. They are created when you startup moose (or `import` moose in Python). The following diagram shows this structure:

```
root
|
|__ shell
|  |
|  |__ sli
|  |
|  |__ BaseContext
|
|__ sched
|  |
|  |__ cj
|     |
|     |__ t0
|     |
|     |__ t1
|
|__ library
|
|__ proto
```

5.3 Id

The unique identifier for each MOOSE object is an Id. This is accessible as `id` field of pymoose objects. An Id object has two components,

- id an unsigned integer. The method `id` returns this value. The root element of the moose model tree always has the id 0.
- index an unsigned integer giving the index number of array-elements. For simple elements, it is 0. It is returned by the method `index`.

When you print an `Id` object, it is printed in the form: `id[index]`

Example:

```
>>> foo = moose.Neutral('foo') # create a Neutral object called 'foo'
>>> foo.id
<moose.Id; proxy of <Swig Object of type 'Id *' at 0x248c6f8> >
>>> print foo.id
470[0]
>>> print foo.id.id()
470
>>> print foo.id.index()
0
```

Even if you create multiple python objects wrapping the same moose element, you can always verify if the underlying moose element is the same by comparing their `id`s.

Example:

```
>>> a = moose.Neutral('my_test_object')
>>> b = moose.Neutral('my_test_object')
>>> a.id == b.id
True
```

Note that `id` is a more fundamental property than the path string of an object. The path string changes when you change the name of the object, but the `id` remains unchanged.

Example:

```
>>> a = moose.Neutral('my_test_object')
>>> print a.path
/my_test_object
>>> ii = a.id
>>> a.name = 'your_test_object'
>>> print a.path
/your_test_object
>>> ii == a.id
True
```

In addition, `Id` objects are hashable. Also, their hash is the hash of their string representation. Thus you can use them as keys in a `dict`.

5.4 Neutral

`Neutral` captures the fundamental properties of all the MOOSE elements. If you are familiar with Object Oriented Programming, you can recognize that this is the base class of all moose classes whose instances can be in the model tree.[1]

Being the base class of all other MOOSE classes, properties of Neutral class is common to all MOOSE classes. A Neutral object can wrap any valid moose object.

You can construct a Neutral object in many ways.

'`From a path string:`'

First, you can just give a path-string as the parameter to the constructor. If there is already an object with the given path, then you get a wrapper around the existing object. On the other hand, if no such object exists, it will try to create a new Neutral object with the given path.

[1] Not all classes in MOOSE are element-classes. The `Id` class, for example.

```
>>> foo_neutral = moose.Neutral('/foo')
>>> bar_neutral = moose.Neutral('/foo')
>>> foo_neutral.path
'/foo'
>>> bar_neutral.path
'/foo'
>>> bar_neutral.name = 'bar'
>>> foo_neutral.name
'bar'
```

As you can see in the above example, `bar_neutral` is just a wrapper around `foo_neutral` and thus changing a field in one of them will be reflected in the other.

Note that when you specify a path to the constructor, it has to exist up to the parent object.

'`From an Id:`'

You can wrap the Id of any existing MOOSE object inside a `Neutral`. The following example shows a common idiom used for looping through the list of children of an object.

```
>>> root = moose.Neutral('/')
>>> for child_id in root.childList:
...     child_obj = moose.Neutral(child_id)
...     print child_obj.path, 'is actually of class', child_obj.className
...
/shell is actually of class Shell
/sched is actually of class Neutral
/library is actually of class Neutral
/proto is actually of class Neutral
```

'`Specifying a parent and name:`'

You can also give the name of the objct to be created and specify the parent. You can call the constructor like this:

`>>> foo = moose.Neutral('foo', parent)` Here `parent` can be another PyMoose object or an `Id`. Thus, if the path of the parent is `'/bar'`, then path of `foo` will be: `'/bar/foo'`

'`Copy an existing object:`'

You can also make a copy of an existing object. The constructor is called like: `foo = moose.Neutral(src, new_name, parent)` or `foo = moose.Neutral(src, path)`

Here `src` can be another `Neutral` object or the `Id` thereof. `new_name` is a string specifying the name of the duplicate and parent is any PyMoose object or an Id. `path` is a string specifying the path of the duplicate object.

The following fields are available in Neutral class and hence in all element classes:

'`className`'
: The name of the MOOSE class this object belongs to. The object-oriented design of MOOSE enables you to work with an element as if it was an instance of its superclass. You can wrap any element in a `Neutral` object but of course later you may need to find out the actual MOOSE class it belongs to. `className` is the way to go.

  What about the `__class__` property in Python? The reason for having a separate `className` field is that MOOSE has its own system for class hierarchy. This is not necessarily visible to Python. Similarly, if you extend a MOOSE class in Python, it does not reach the underlying MOOSE class system. Extending MOOSE classes in Python is only useful for attaching additional information to it, but not for changing the underlying behaviour. For that you have to edit the C++ source code of MOOSE and recompile it, a task suited for the brave.

'`name`'
: Name of the element. Two different objects may have the same name but siblings in the model tree should have different names. You can change the name of an object by assigning a new string value to this field.

'`index`'
: MOOSE has two flavours of element: `simple element` and `array element`. A single entity is represented by a `simple element` whereas an `array element` represents a bunch of elements of the same kind. The `index` field indicates the position of this `Neutral` object in an `array element`. For `simple element`s it is `0`.

'`parent`'
: The `Id` of the parent element of this object in the model tree.

'`node`'
: This is the CPU node no. of on which this element is located. This is relevant only for parallel computers and PyMOOSE is yet to be adapted to such systems.

'`fieldList`'
: Vector listing the fields in the MOOSE object. You can traverse it like a Python `list`. If you add a Python attribute to the object later, that will not be visible in this. Nor will that visible to MOOSE. The way to add a field to the underlying MOOSE object is to use the `addField` function of the `PyMooseContext`.

'`cpu`'
: Reports the cost of one clock tick, very roughly # of FLOPs.

'`dataMem`'
: Memory used by data part of object

'`msgMem`'
: Memory used by messaging (Element) part of object.

'`childList`'
: Vector of `Id`s of the children of this object. This is also available via `children()` method, which is retained for backward compatibility.

5.5 PyMooseContext

One global object that provides access to global functions in PyMOOSE is the instance of PyMooseContext. It is available from the abstract base class of all PyMOOSE classes, PyMooseBase (which, being abstract, cannot be instantiated, but whose public properties are inherited throughout the class hierarchy).

PyMooseContext should be considered a singleton. There should be only one instance of it at any given time. And usually this instamce is created at startup (when moose is imported for the first time).

```
The standard way to access the context is:
context = PyMooseBase.getContext()
```

The context object provides quite low level access to MOOSE. So you should be discriminate about using the functions available. There are some functions to control simulation which are very common and must accessed via the context object.

'`setClock(clockNo, dt, stage=0)`'
: set the clock no. specified by `clockNo` with time step `dt` and stage `stage`.

'`useClock(clockNo, path, func='process')`'
: use clock specified by `clockNo` on `path`, which can be a wildcard path, calling the internal function `func` of the element class at each time step. The internal function is by default 'process', which calculates the state of the object at the end of the timestep.

'`reset()`'
: reset the simulation. This clears all recording Table objects that have been scheduled on some clock, and usually sets things back to initial values.

'`step(time)`'
: Run the simulation. If `time` is a `float`, it is taken as the length of time to be simulated. Each clock in the simulation proceeds by its `dt` until its `currentTime` reaches or exceeds `time`.

  If `time` is an integer, then it is taken as the number of steps for the fastest clock in the system. Thus, if the fastest clock in the system has `dt = 0.01` and `time = 10`, then this will run the simulation for 0.1 time units.

'`readCell`'
'`readSBML,`'
'`readNeuroML,`'
'`getCurrentTime,`'
'`addField.`'
'`loadG`'

'`runG`'

'`move`'

'`exists`'

The following are more advanced methods and should be used with caution. Usually for each of them there is a more accessible counterpart as a member of the PyMooseBase object or its derivative. The methods in PyMooseContext are required only when there is no such counterpart.

'`getField`'
'`setField`'
'`getParent`'
'`getPath`'

'`getName`'

‘getChildren’
‘copy’

5.6 Messaging

5.6.1 Source and Destination fields

Elements in a MOOSE model communicate with each other at runtime via messages. For example, to set up a constant current injection into a neuronal compartment, you want to connect a `PulseGen` object `pulsegen` to the `Compartment` object `comp`. In the definition of `PulseGen` class you have predefined source fields which tell what are the fields that can be transmitted out of the `pulsegen` object. Similarly, `Compartment` has a destination field where it can receive a current injection value. By connecting the source and the destination fields we set up communication between these two components.

The syntax for connecting source and destination messages is simple: `{source-object}.connect({source-field}, {target-object}, {target-field})`

With the current example, it will be:

```
pulsegen.connect('outputSrc', comp, 'injectMsg')
```

A very common yet confusing scenario is when you want to record the value of some state variable periodically. This is achieved by using `Table` objects. The confusing bit here is that the table object is used as a source, not a destination. The relevant source-field is `inputRequest` and the destination-field is the field to be recorded. This is a special case as the fields to be recorded are not destination fields, but value fields, which do not usually participate in messaging. Also, to use the Table object as an output buffer, you have to set the stepMode field to `TAB_BUF`.

Thus, to record the membrane potential Vm from our compartment, we can issue the following statements:

```
table = moose.Table('/Vm_tbl')
table.stepMode = 3
table.connect('inputRequest', comp, 'Vm')
```

5.7 Running GENESIS scripts in Python

There are two commands in PyMOOSE that allows you to run legacy GENESIS commands inside Python. These are `loadG` and `runG`. If you have a file `script.g` containing a GENESIS script, then you can execute the contents of it by invoking:

```
context.loadG(script.g)
```

where context is the singleton PyMooseContext object (can be obtained via: `context = moose.PyMooseBase.getContext()`).

Sometimes it is useful to access the MOOSE objects via the GENESIS commands. This is because for some classes, the Python wrappers may not be up to date, or it may just be ease of use. In those cases, just to carry out a single command, you can use `context.runG('{genesis-command}')`.

For example, to display the messages on an element specified by the path `/my_element`, you can use:

```
context.runG('showmsg /my_element')
```

6 Frequently Asked Questions

6.1 How do I load a model?

There are various formats that a model can be in. MOOSE recognizes GENESIS cell prototypes ('.p' files), SBML and neuroML files. Moreover, a GENESIS script ('.g' file) can be loaded in PyMOOSE. Here is a small description of these:

6.1.1 How do I load GENESIS prototype file?

There is a text file format used by GENESIS to define prototypes for neuronal models. The details of this format can be found in GENESIS documentation for `readcell`.

Briefly, the main content of files in this format is a sequence of rows corresponding to compartments that constitute the cell model. In each row, you have the compartment name, its parent compartment's name, position of the starting point the compartment (optionally the end point), diameter of the compartment (the spatial dimensions are in microns for position and diameter), followed by a list of channels and their conductance densities(in SI unit, Siemens/m^2).

The channels are recognized by their names and the actual channel prototype definitions must be loaded under `/lib` before loading the prototype file. Otherwise that channel will not be inserted on the compartments.

Once you have created prototypes for the channels, the `readCell` function in `PyMooseContext` can be called to load the cell prototype. For instance,

```
moose.context.readCell('/usr/share/doc/moose/DEMOS/axon/axon.p', '/axon')
```

will load read the prototype described in the file `/usr/share/doc/moose/DEMOS/axon/axon.p` as the cell `/axon`.

6.1.2 How do I load an SBML file?

SBML stands for systems biology markup language. This is an XML based file format for defining computational models in systems biology. More information can be found at the official website: http://sbml.org/.

You can load SBML models using the `readSBML(filepath, elementpath)` function in `PyMooseContext` class.

For example,

```
moose.context.readSBML('/usr/share/moose/DEMOS/sbml_Reader/acc88.xml', '/acc88')
```

will load the model defined in acc88.xml file under a container `/acc88`.

6.1.3 How do I load a neuroML file?

neuroML is an XML-based format for defining neuronal models. You can find out more about neuroML at its website: http://www.neuroml.org/. MOOSE is capable of reading some levels of neuroML model definition. You can use the `readNeuroML` function in PyMooseContext to load a neuroML model in MOOSE:

```
moose.context.readNeuroML('/usr/share/moose/DEMOS/NeuroML_Reader/CA1/Ca1.xml', '/ca1')
```

to load the model defined in Ca1.xml into a Cell object '/ca1'.

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0. PREAMBLE

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