Software Integration
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Software Integration Group

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1. Create MEMOSA integration framework
2. Work with others to integrate code
3. Set up regression testing and monitor results
## Software Components

<table>
<thead>
<tr>
<th>Code</th>
<th>From</th>
<th>Lang</th>
<th>LOC</th>
<th>Purpose</th>
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</thead>
<tbody>
<tr>
<td>LAMMPS</td>
<td>Sandia</td>
<td>C++</td>
<td>118,000</td>
<td>MD simulator</td>
</tr>
<tr>
<td>FVM</td>
<td>Purdue</td>
<td>C++</td>
<td>10,000</td>
<td>Core for FVM solver</td>
</tr>
<tr>
<td>MPM</td>
<td>UNM</td>
<td>F90/F77/C</td>
<td>25,000</td>
<td>Core for MPM solver</td>
</tr>
<tr>
<td>Rar Gas Dyn</td>
<td>Purdue</td>
<td>F90</td>
<td>6,000</td>
<td>Boltzmann-ESBGK</td>
</tr>
<tr>
<td>Reactive MD</td>
<td>Purdue</td>
<td>C</td>
<td>27,500</td>
<td>Reactive force fields</td>
</tr>
<tr>
<td>Dislocations</td>
<td>Purdue</td>
<td>C/F77</td>
<td>2,000</td>
<td>Micromechanical models</td>
</tr>
<tr>
<td>Rappture</td>
<td>Purdue</td>
<td>C/C++/XML</td>
<td>60,000</td>
<td>Input/output handling</td>
</tr>
<tr>
<td>MEMOSA</td>
<td>Purdue</td>
<td>C/C++/Python</td>
<td>10,000</td>
<td>Simulation framework</td>
</tr>
<tr>
<td>Im Boundary</td>
<td>Purdue</td>
<td>C</td>
<td>5,000</td>
<td>FVM / MPM connection</td>
</tr>
<tr>
<td>Sensitivity</td>
<td>Purdue</td>
<td>C++</td>
<td>10,000</td>
<td>Sensitivity analysis</td>
</tr>
<tr>
<td>UQ drivers</td>
<td>Purdue</td>
<td>C/Python</td>
<td>5,000</td>
<td>Uncertainty quantification</td>
</tr>
<tr>
<td>Models</td>
<td>Purdue</td>
<td>C/F77</td>
<td>5,000</td>
<td>Various physical models</td>
</tr>
</tbody>
</table>
MEMOSA Architecture

Python Scripts

Solver Suite

Python Bindings

Finite Volume Method (FVM)

Material Point Method (MPM)

C/C++ Data Objects

Setup

- ANSYS
- ProE
- CUBIT

Visualization

ParaView

Compact Models

LAMMPS

Mesoscale micromechanical models
Software Infrastructure for Collocation UQ

from Parameter import *
from sweep import *

# define some parameters here
length = Parameter('length', 'Length', mean=5.0, max=5.8)
width = Parameter('width', 'Width', mean=30, max=32)

# run script 'tsolver.py' on the list of parameters
uq_sweep('./tsolver.py', [length, width], level=2)

~/memosa/uq> ./test_uq.py
Solving for width=30.000000 and length=5.000000
Solving for width=30.000000 and length=4.200000
Solving for width=30.000000 and length=5.800000
...
Object-Oriented Infrastructure

- C++/F90 core for solvers
- C++ templates for arithmetic types
- Python objects for high-level scripting
Python Bindings

.i files for 33 classes (so far)

```cpp
template<class T>
class FlowModel : public Model {
public:
    FlowModel(const GeomFields& geomFields, 
               virtual ~FlowModel();
    virtual void init();
    void advance(const int niter);
};
```

```python
fmodel = models.FlowModelA(geomFields, flowFields)
fmodel.init()
fmodel.advance(numIterations)
```

SWIG - http://www.swig.org
Regression Tests

- Nightly regression tests: 90 tests
  - 6 FVM core
  - 4 MPM core
  - 75 FVM+MPM with simple geometries
  - 5 LAMMPS

- Framework for adding new tests
- Web-based system for browsing results
Visualization: ParaView

Visualize finite elements
AND particles

Notes online at https://memshub.org/information/memosa/wiki/ParaView
Project Infrastructure

- Subversion repository
  - FVM, MPM, LAMMPS code under build/test
  - 2.7 million lines of code in total under Subversion control
- Automated build system
  - make + 1,500 lines of Python
  - Configuration files for various platforms
- Wiki for project notes
Computational Power

Steele
848 x 8 core Dell 1950
60 teraFLOPS

Coates
1,000 x 8 core HP DL165
All 10 GigE
90 teraFLOPS

LLNL Hera
New Hub for MEMS

5 online lectures

1 simulation tool

Q-factor calculator with UQ

MEMOSA project

http://memsHUB.org
Plans for This Year

Finish UQ framework: compute output PDFs

Compact Model Framework

Improve connection to ParaView run in parallel

More regression tests
Q-Factor Calculator with UQ