Using Python in LAMMPS

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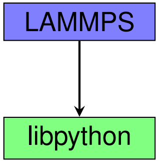
LAMMPS Workshop 2017

Outline

Modes

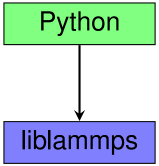
Embedded Python

- LAMMPS binary launches embedded Python interpreter
- executes Python code on demand



Python as Driver

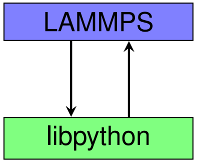
- Python starts LAMMPS as library
- controls LAMMPS through library calls



Modes

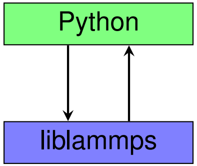
Hybrid (Embedded)

- Python code lauched from LAMMPS can control/access it like a library



Hybrid (Python as Driver)

- LAMMPS can call Python code defined in driver and has access to all global objects



Requirements

- PYTHON package must be installed
- LAMMPS must be compiled as **shared-library**
- (Optional) `-DLAMMPS_EXCEPTIONS` for better error handling
- LAMMPS Python module (lammps.py) must be installed

```
---------------------------------------------------------------------------
Exception                                 Traceback (most recent call last)
<ipython-input-3-6bfbbfdb2363> in <module>()
----> 1 L.test()

~/GitHub/lammps/lammps/build_py3/myenv3/lib/python3.6/site-packages/lammps.py in handler(*args, **kwargs)
    810
    811         with OutputCapture() as capture:
--> 812           self.command(' '.join(cmd_args))
    813           output = capture.output
    814

~/GitHub/lammps/lammps/build_py3/myenv3/lib/python3.6/site-packages/lammps.py in command(self, cmd)
    625
    626   def command(self,cmd):
--> 627     self.lmp.command(cmd)
    628     self._cmd_history.append(cmd)
    629

~/GitHub/lammps/lammps/build_py3/myenv3/lib/python3.6/site-packages/lammps.py in command(self, cmd)
    193         if error_type == 2:
    194           raise MPIAbortException(error_msg)
--> 195         raise Exception(error_msg)
    196
    197   # send a list of commands

Exception: ERROR: Unknown command: test (/home/richard/GitHub/lammps/lammps/src/input.cpp:315)
```

Step 1: Building LAMMPS as a shared library

```
cd $LAMMPS_DIR/src

make yes-PYTHON

# compile shared library
make mpi mode=shlib LMP_INC="-DLAMMPS_EXCEPTIONS"
```

Step 2: Installing the LAMMPS Python package

```
cd $LAMMPS_DIR/python
python install.py
```

Warning!

Recompiling the shared library requires reinstaling the Python package.

CMake (*soon*)

```
cd $LAMMPS_DIR/src

mkdir build
cd build
cmake ../cmake -DENABLE_PYTHON=on \
               -DBUILD_SHARED_LIBS=on \
               -DLAMMPS_EXCEPTIONS=on \
               -DCMAKE_INSTALL_PREFIX=...
make
make install
```

Adding Python code within a LAMMPS input script

Embed Python code

```
python simple here """
def simple():
    print("Inside simple function")
"""

python simple invoke
```

Calling existing Python code

```
python simple file my_funcs.py
python simple invoke
```

Computes: Call Python function and save result in variable

```
python      factorial &
            input 1 v_n &
            return v_fact &
            format ii &
            here """
def factorial(n):
    if n == 1: return 1
    return n*factorial(n-1)
"""

variable    fact python factorial
```

- Evaluation of the variable calls the function

Computes: Call Python function and save result in variable

```
variable n string 10
print    "Factorial of $n = ${fact}"

variable n string 20
print    "Factorial of $n = ${fact}"
```

Pair Python

```
pair_style  python 2.5
pair_coeff  * * py_pot.LJCutMelt lj
```

- (created by Dr. Axel Kohlmeyer)
- for defining simple additive pair potentials in Python
- PYTHONPATH and LAMMPS_POTENTIALS in module search path
- loads class `LJCutMelt` from user-defined `py_pot` module
- Python class implements `compute_force` and `compute_energy` functions
- many examples, including hybrid usage in examples/python folder

Python

```
class LJCutMelt(LAMMPSPairPotential):
    def __init__(self):
        super(LJCutMelt, self).__init__()
        # set coeffs: 48*eps*sig**12, 24*eps*sig**6,
        #              4*eps*sig**12,  4*eps*sig**6
        self.units = 'lj'
        self.coeff = {'lj'  : {'lj'  : (48.0,24.0,4.0,4.0)}}

    def compute_force(self, rsq, itype, jtype):
        coeff = self.coeff[self.pmap[itype]][self.pmap[jtype]]
        r2inv  = 1.0/rsq
        r6inv  = r2inv*r2inv*r2inv
        lj1 = coeff[0]
        lj2 = coeff[1]
        return (r6inv * (lj1*r6inv - lj2))*r2inv
```

Why do this?

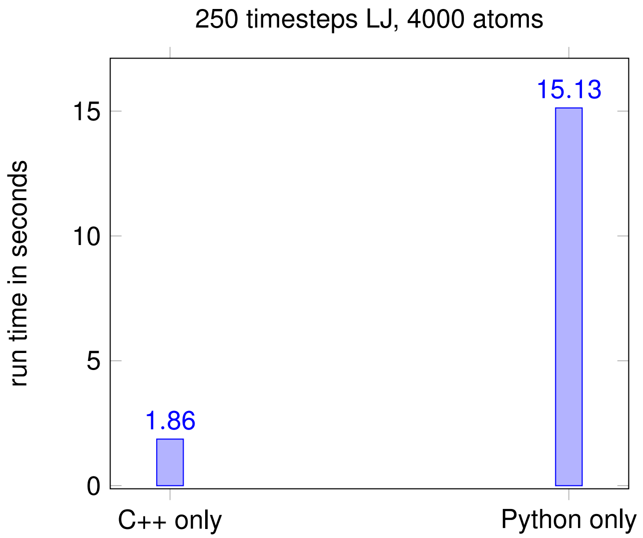
Why do this?

Because Python is Awesome!

Why do this?

But Python is slow. . .

Performance hit



Why do this?

- $\Rightarrow$ **Quick prototyping**
- You don’t have to recompile LAMMPS to test it
- You don’t have to work in C++
- And you gain the flexibility / simplicity of the Python language to test new things

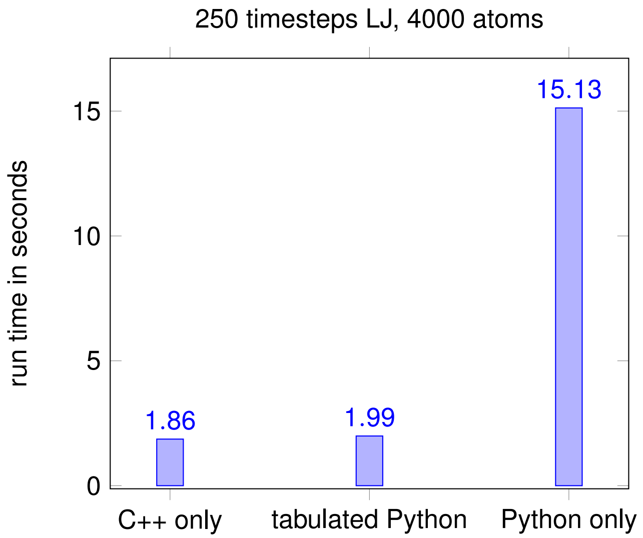
Workaround: Create a tabulated version

```
# use python pair style
pair_style  python 2.5
pair_coeff  * * py_pot.LJCutMelt lj

# generate tabulated potential from python variant
pair_write     1 1 2000 rsq 0.01 2.5 lj_1_1.table LJ

# switch pair style to tabulated potential
pair_style     table linear 2000
pair_coeff     1 1 lj_1_1.table LJ
```

Performance hit



Fix Python

- like any other fix it implements callback functions for certain events in integration loop
- executed every N time steps
- currently limited to `post_force` and `end_of_step`

```
fix       1 all nve
fix       2 all python 50 end_of_step end_of_step_callback
fix       3 all python 50 post_force post_force_callback
```

Accessing LAMMPS from Python

```
from lammps import lammps

def end_of_step_callback(lmp):
  L = lammps(ptr=lmp)
  t = L.extract_global("ntimestep", 0)
  print("### END OF STEP ###", t)

def post_force_callback(lmp, v):
  L = lammps(ptr=lmp)
  t = L.extract_global("ntimestep", 0)
  print("### POST_FORCE ###", t)
```

Python Interfaces

lammps.lammps

- uses C-Types
- direct memory access to native C++ data
- provides functions to send and receive data to LAMMPS
- requires knowledge of how LAMMPS works

lammps.PyLammps

- higher-level abstraction built on top of original C-Types interface
- manipulation of Python objects
- communication with LAMMPS is hidden from API user
- shorter, more concise Python code

PyLammps

Motivation

- Create a simpler, Python-like interface to LAMMPS
- API should be discoverable (no knowlege of the C++ code necessary)
- IPython notebook integration

Usage

```
from lammps import PyLammps
L = PyLammps()
```

Commands

LAMMPS Input Script

```
region box block 0 10 0 5 -0.5 0.5
```

Original Python Interface

```
L.command("region box block 0 10 0 5 -0.5 0.5")
```

PyLammps

```
L.region("box block", 0, 10, 0, 5, -0.5, 0.5)
```

Commands - Easier parametrization

Original Python Interface

```
L.command( \
    "region box block %f %f %f %f %f %f" % \
    (xlo, xh ylo, yhi, zlo, zhi) \
)
```

PyLammps

```
L.region("box block", xlo, xhi, ylo, yhi, zlo, zhi)
```

PyLammps interface Example

Live Demo: python/examples/pylammps/interface_usage.ipynb

Validating a Dihedral potential

Live Demo: python/examples/pylammps/dihedrals/dihedral.ipynb

Summary & Outlook

Ways to call Python from LAMMPS

- compute function mapped to variable
- invoke function
- pairwise potentials (pair python & pair_write)
- fix python for end_of_step and post_force

Ways to access/control LAMMPS from Python

- lammps.lammps
- lammps.PyLammps (Jupyter Notebooks)

Coming soon

- fix python/integrate (implement fix nve in Python)
- read and write access to atom properties as numpy arrays

References

Documentation

- http://lammps.sandia.gov/doc/Section_python.html
- http://lammps.sandia.gov/doc/tutorial_pylammps.html

Example Folders

- (Pair Python Fix Python): examples/python
- (PyLammps and Python Interface): python/examples

Questions?