Richard and the JAHA group
(**J**orge – **A**ndrea – **H**agoss - **A**lexander)

Molecular Dynamics
Fortran with Python interface
git://github.com/rbberger/ljmd-f.git

**Workshop on Computer Programming and Advanced Tools for Scientific Research Work
March 2013, Trieste, Italy**

Try to understand the code

- Simulating liquid argon for a set of particles using only Lennard-Jones potential

- It needs input files with the main parameters and initial positions and velocities

- After MD-simulation it creates an output file with a new positions and velocities

Splitting the tasks

FORTRAN

1. Separate each module and subroutine to the separate file
2. Develop of interface: Fortran to Python
3. Create a Fortran library
4. Add Morse potential

PYTHON

1. Develop the python code that reads data from input file and create output file with MD result
2. Develop the main python code that uses Fortran library

PROBLEMS

- First task splitting inefficient

- Merging files while working on the same file at the same time

- Compiling the Fortran using f2py (creating the library)

SOLUTIONS

- Well organized by the team leader

- New splitting strategy

- Every day discussion of what to do

- We used GIT COMMIT and PUSH&PULL very often

- Pair programming
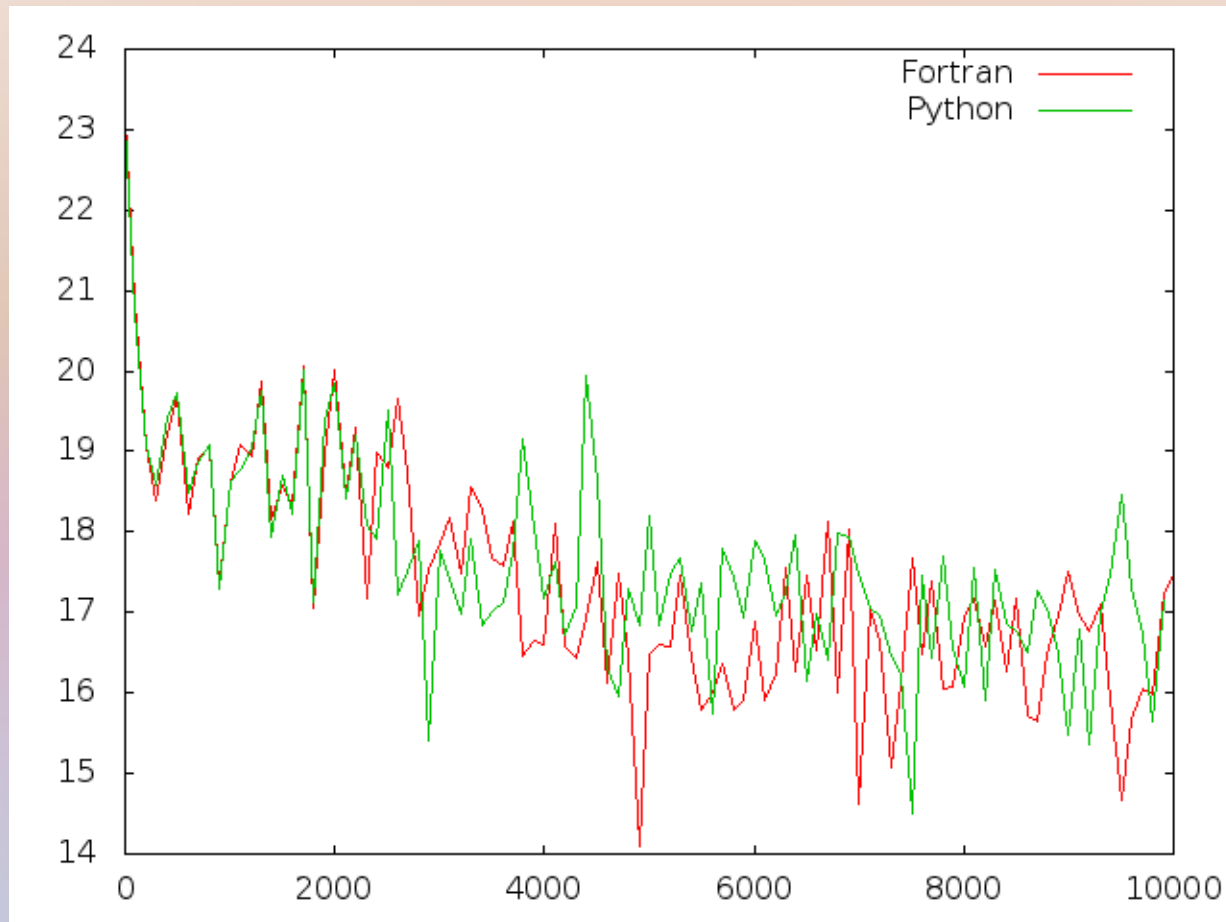
Some results

# New input parameters for the Morse potential

```
108                          # natoms
39.948                       # mass in AMU
0.2379                       # epsilon in kcal/mol
3.405                        # sigma in angstrom
8.5                          # rcut in angstrom
17.1580                      # box length (in angstrom)
argon_108.rest              # restart
argon_108.xyz               # trajectory
argon_108.dat               # energies
10000                        # nr MD steps
5.0                          # MD time step (in fs)
100                          # output print frequency
2                            # iflag 1 = LJ potential, else = Morse.
1.2379                       # D parameter for Morse
1.623                        # Alpha parameter for Morse
0.405                        # Re parameter for Morse
```
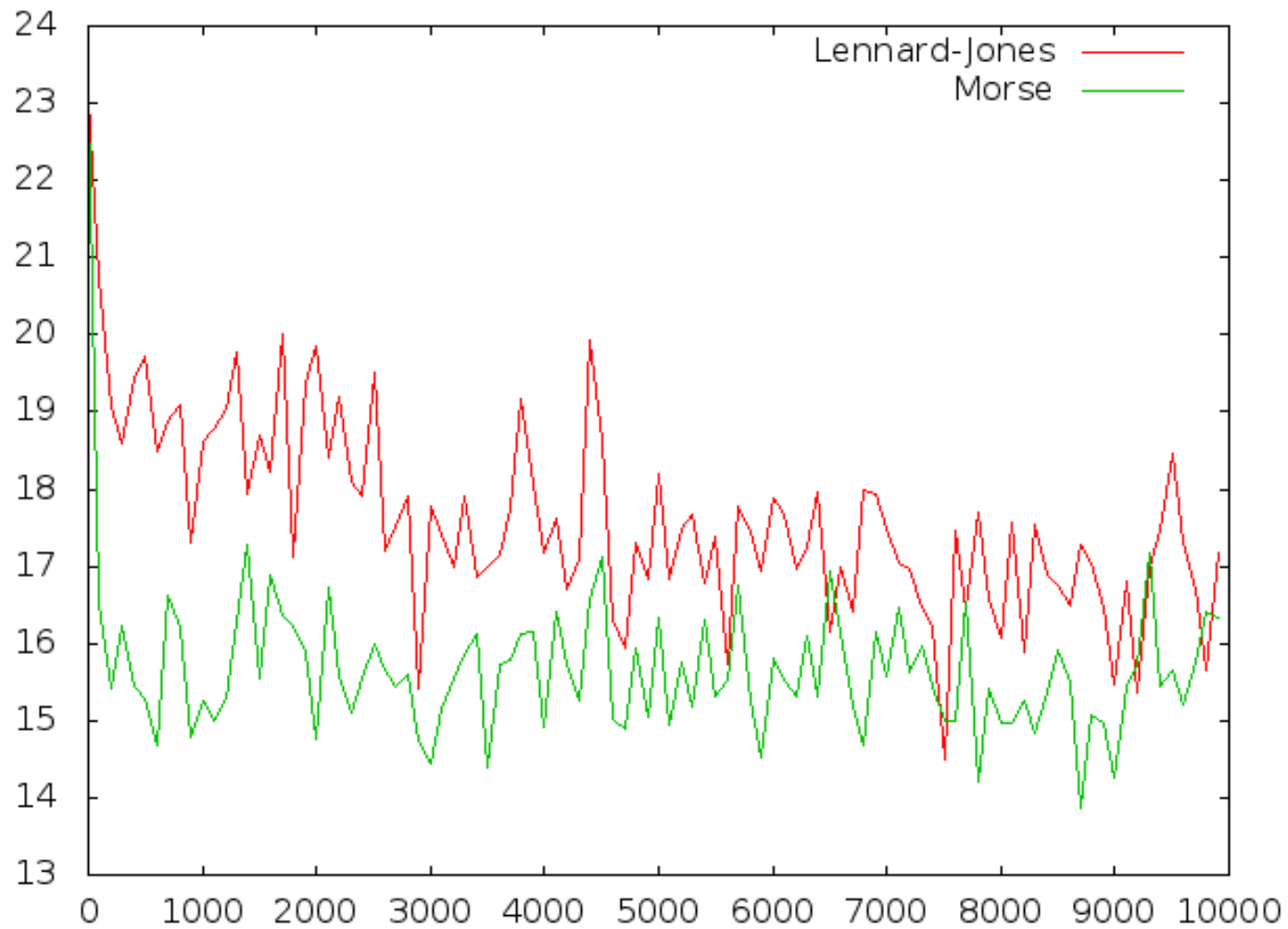
More results

Potential improvements

- Using NumPy arrays

- Write a documentation

- Include other type of atoms

- Option parsing

Conclusion

- We enjoyed the project and team work.

- We learned how to use new tools, Python, Git, f2py, Makefile