

MyMD. A program with potential...

Workshop on Computer Programming and Advanced Tools for Scientific Research Work

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PROJECT MANAGEMENT

With the intention to restructure an existing C version of a MD code, we have decided to turn this into an object-oriented C++ version and applied the following class structure:

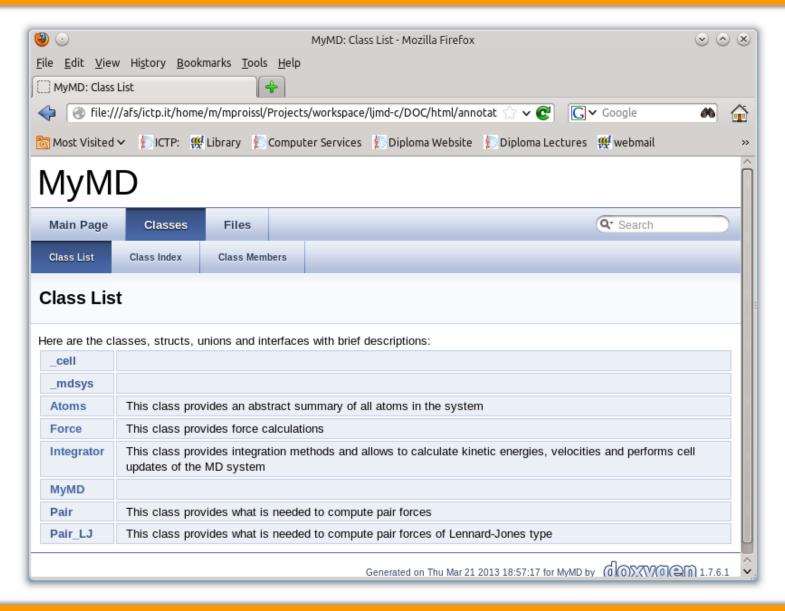
Classes	Number of group members
MyMD (main class), Helper	2
Atoms, Integrator	2
Force, Pair(_LJ)	2
Python interface	2

- In addition we have developed a flexible Python interface to run the program with different inputs.
- Working as a group in an amateur-software-company-style:
 - ✓ One main meeting to plan the program structure
 - ✓ Individual work on classes in sub-groups
 - ✓ Several meetings to debug and compile the code
 - ✓ Validating the output with reference data from original C version.

DEVELOPMENT PROBLEMS / STATUS

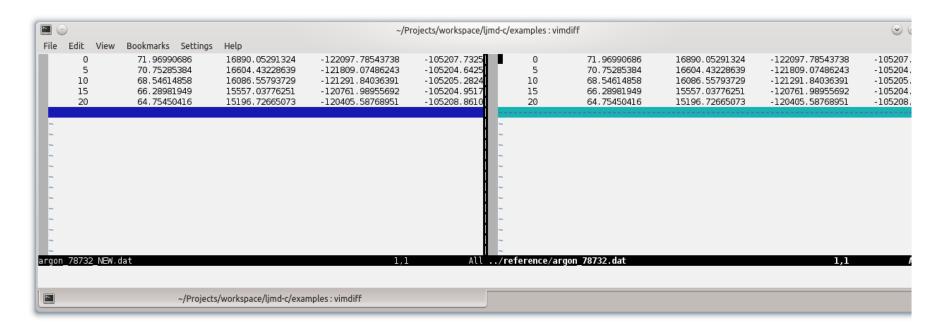
- The baseline: group members with none, a little and a lot C++ experience.
- No coding style conventions were defined.
- Code was only compiled at the end, rather than iteratively.
- Once all pieces were put together, the program "obviously" did not compile.
- Spent one day only on debugging the code and getting it into a working state.
- No improvements in terms of functionality (e.g. adding Morse potential) have been made, BUT the program structure allows now easily extensions!
- A Doxygen website has been created and mostly inline documentation provided.
- A flexible interface in Python has been developed and allows convenient config.

MYMD DOCUMENTATION



MYMD VALIDATION

Simple validation using reference data and gdb.



It WORKS!!! (most likely..)