



The Abdus Salam
**International Centre
for Theoretical Physics**

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

The screenshot shows a web browser window titled "MyMD: Class List - Mozilla Firefox". The address bar displays the file path: `file:///afs/ictp.it/home/m/mproissl/Projects/workspace/ljmd-c/DOC/html/annotat`. The browser's menu bar includes File, Edit, View, History, Bookmarks, Tools, and Help. The toolbar shows a search bar with "Google" and a home button. Below the toolbar, a "Most Visited" section lists several links: ICP, Library, Computer Services, Diploma Website, Diploma Lectures, and webmail.

The main content area features the "MyMD" logo and a navigation menu with tabs: Main Page, Classes (selected), and Files. A search bar is located to the right of the navigation menu. Below the navigation menu, there are sub-tabs: Class List (selected), Class Index, and Class Members.

The "Class List" section is titled "Class List" and contains the text: "Here are the classes, structs, unions and interfaces with brief descriptions:". Below this text is a table listing the classes and their descriptions.

_cell	
_mdsys	
Atoms	This class provides an abstract summary of all atoms in the system
Force	This class provides force calculations
Integrator	This class provides integration methods and allows to calculate kinetic energies, velocities and performs cell updates of the MD system
MyMD	
Pair	This class provides what is needed to compute pair forces
Pair_LJ	This class provides what is needed to compute pair forces of Lennard-Jones type

At the bottom of the page, a footer indicates: "Generated on Thu Mar 21 2013 18:57:17 for MyMD by doxygen 1.7.6.1".

MYMD VALIDATION

- Simple validation using reference data and gdb.

The screenshot shows a Vim diff window titled `~/Projects/workspace/ljmd-c/examples : vimdiff`. The window displays a side-by-side comparison of two data files. The left pane shows `argon 78732 NEW.dat` and the right pane shows `../reference/argon 78732.dat`. Both panes show a table of data with 11 columns. The first column contains line numbers (0, 5, 10, 15, 20). The subsequent columns contain numerical values. The data in both files appears to be identical. The status bar at the bottom of the window shows `~/Projects/workspace/ljmd-c/examples : vimdiff`.

Line	Column 1	Column 2	Column 3	Column 4	Column 5	Column 6	Column 7	Column 8	Column 9	Column 10	Column 11
0	71.96990686	16890.05291324	-122097.78543738	-105207.7325	0	71.96990686	16890.05291324	-122097.78543738	-105207.7325		
5	70.75285384	16604.43228639	-121809.07486243	-105204.6425	5	70.75285384	16604.43228639	-121809.07486243	-105204.6425		
10	68.54614858	16086.55793729	-121291.84036391	-105205.2824	10	68.54614858	16086.55793729	-121291.84036391	-105205.2824		
15	66.28981949	15557.03776251	-120761.98955692	-105204.9517	15	66.28981949	15557.03776251	-120761.98955692	-105204.9517		
20	64.75450416	15196.72665073	-120405.58768951	-105208.8610	20	64.75450416	15196.72665073	-120405.58768951	-105208.8610		

- It WORKS!!! (most likely..)