ESR-3 Mid-Term Progress Report

Massively Parallel Quantum Mechanical / Molecular Mechanical Interface

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Background

University background:

University: Ural Federal University, Yekaterinburg, Russia

Field of study: Experimental detector physics

Qualification: Engineer-physicist

Programming Experience:

6 years of programming experience

2 years of team-leading experience

Experience with Java, C++

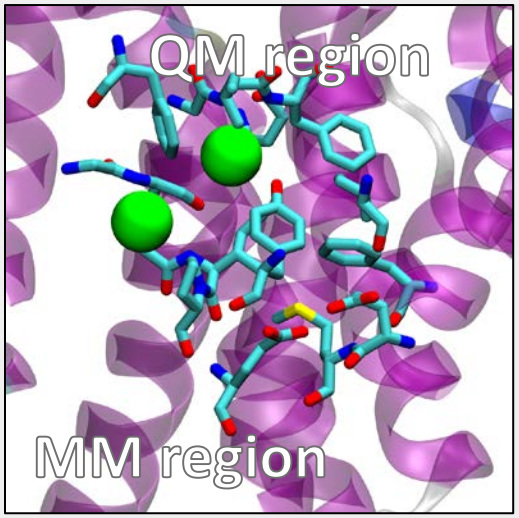
Interests:

Computational physics, biophysical simulations, massively parallel applications

Training in the Network

- 4 general HPC-LEAP workshops
- 1 thematic HPC-LEAP workshop in Computational Biology
- 1 full-semester course in Density Functional Theory at RWTH Aachen
- Advanced Fortran Topics workshop at Leibniz Research Center
- CECAM workshop “Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments” in SNS, Pisa
- EUROHACK 2017 GPU Hackathon in Jülich Supercomputing Center

QM/MM Simulations

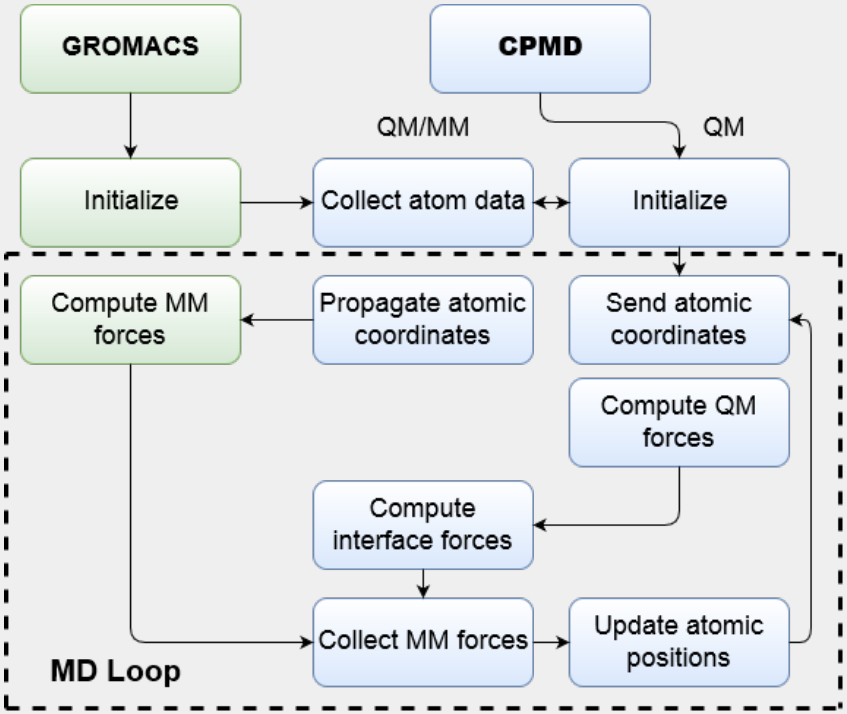


Able to describe certain processes (e.g enzymatic reactions) and properties (e.g. spectral characteristics) which are not accessible by classical means on a large systems which are typically not possible to simulate using fully quantum description (>10000 atoms).

Problems:

- Poor scalability – does not allow us to get sampling which is good enough – not truly an HPC application
- Limited number of available force-fields
- Proprietary GROMOS96 license

New HPC-based Approach

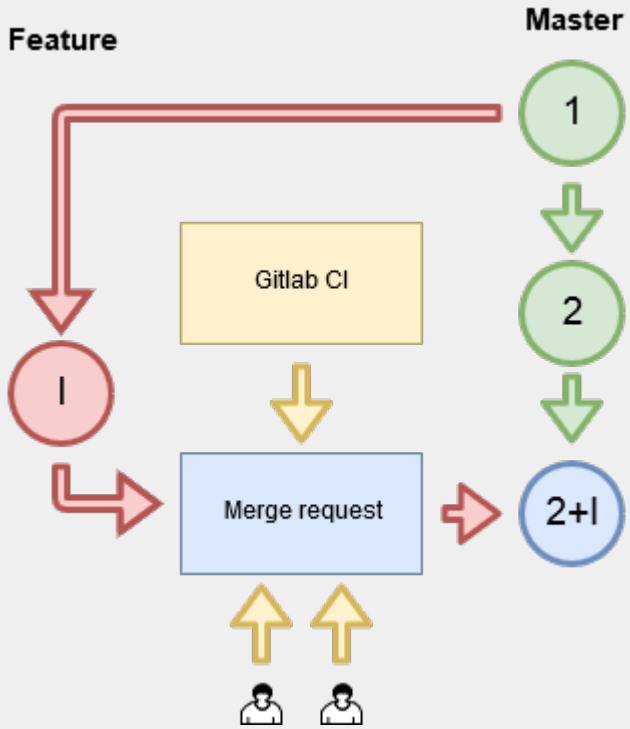


- Multiple-Program Multiple-Data approach using the ad-hoc communication library
- Fully exploits the efficient parallel architecture of both CPMD and the MM code
- Allows coupling to virtually any MM code

Improving the scaling performance allows getting better sampling, thus we obtain more meaningful results

Technology stack

- Coupling based on the development version of CPMD
- Communication library written in C++ using MPI 2.0 functionality
- Using Fortran2003 standard for the interface
- Unit testing using pFUnit framework
- Git VCS
- Gitlab CI with a number of build servers
- Merge-based GitHub workflow



Project status

- ✓ Design the architecture of an interface
- ✓ Design the protocol for data movement
- ✓ Develop the communication library
- ✓ Develop the QM/MM interface
- ⚠ Coupling to GROMACS (http://www.gromacs.org/)
- ✓ Writing the contributor manual
- ✓ Going open-source
- ✓ Performance and scaling optimizations
- ✓ Adopting different model for electrostatics treatment

Dissemination

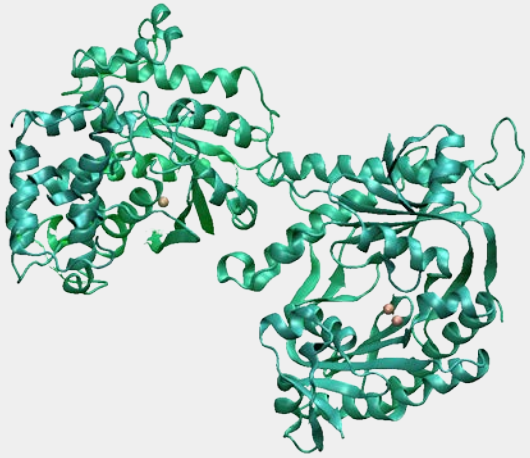
1. May 2016, SNS, Pisa, Italy – Poster, abstract, spotlight talk
2. July 2016, Jülich, Germany – Poster, abstract
3. December 2016, Jülich, Germany – Poster, abstract, spotlight talk
4. April 2017, Cagliari, Italy – Talk on the hybrid methods in biological simulations

Secondments

1. 1.10.2016 – 1.03.2017 Jülich – development of the QM/MM interface
2. Planned 2017 – IBM Research Zürich – parallel performance optimization

Expected impact

- Massively parallel QM/MM framework based on GROMACS should enable us to achieve better sampling on large-scale biological applications (Adenylyl Cyclase within the Human Brain Project)
- Publishing the interface and the GROMACS coupling in a high-impact journal is expected to result in a highly cited papers



The Network

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