SUMA Meeting

WP 4 – Updates

November 8th, 2013

People involved in this work project

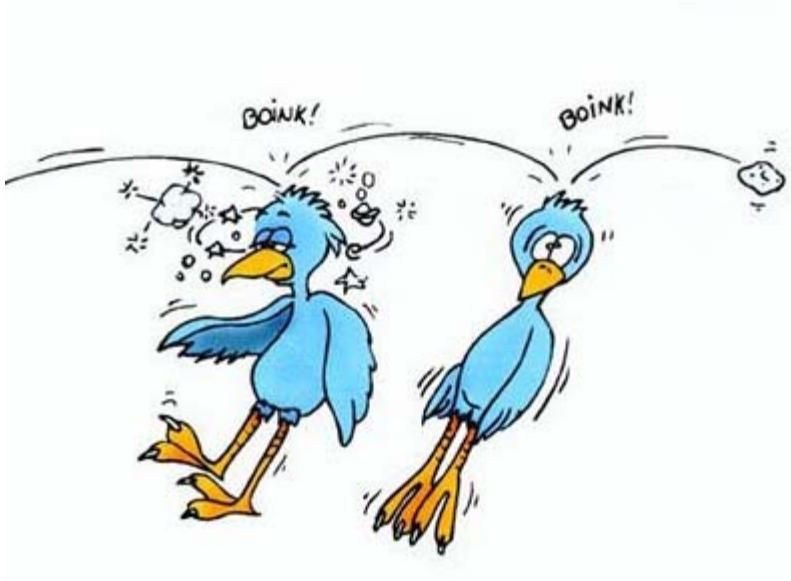
- Roberto Ammendola
- Giovanni La Penna
- Velia Minicozzi
- Silvia Morante
- Gian Carlo Rossi
- Gaetano Salina
- Francesco Stellato
- …

3 Levels of Simulations

- Quantum-mechanical simulations
  - QuantumESPRESSO
- Semi-quantistic (tight binding) simulations
  - DFTB+
- Classical mechanics simulations
  - GROMACS

Benchmarks

A properly-sized test system is needed for the benchmarks



Catch two birds with one stone

A system which is also appealing from the scientific point of view

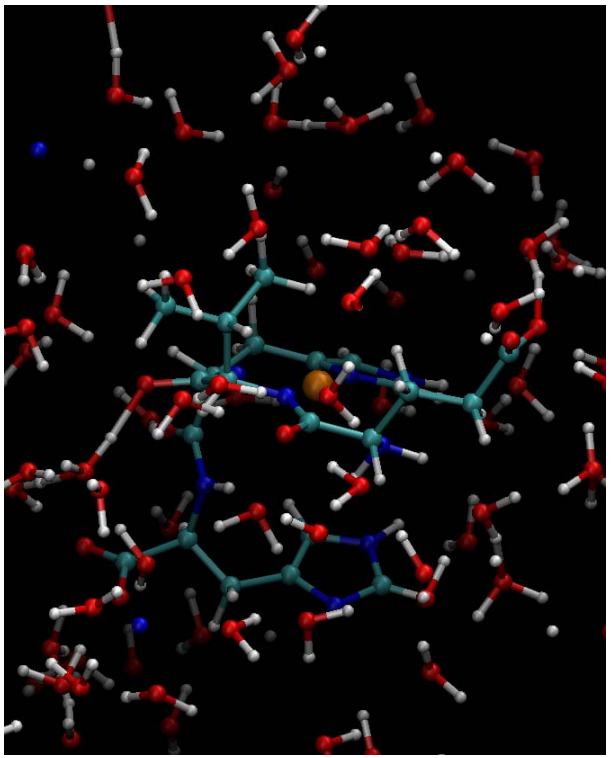
Benchmark System

A short portion of the Aβ peptide, involved in the pathogenesis of Alzheimer's disease, is used. A metal ion is bound.

Ni^{2+} –[Glu–Val–His–His]

380 Atoms

521 Electrons



Benchmark – System

1- Peptide aggregation propensity

Classical molecular dynamics

2- Effect of metal binding on aggregation

Tight-binding methods

3- Effect of metal binding on protein folding

Fully quantum-mechanical treatment

Benchmark – First Results

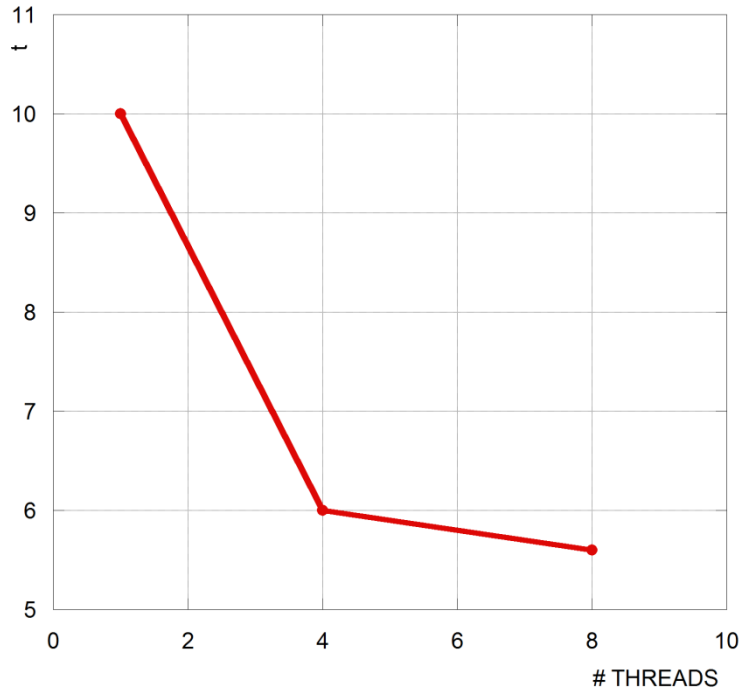
Program: DFTB+ 1.2.2

Most time-consuming step: large, sparse matrix diagonalization

Using OMP DFTB+

on Eurora

(problems with multiple CPUs)

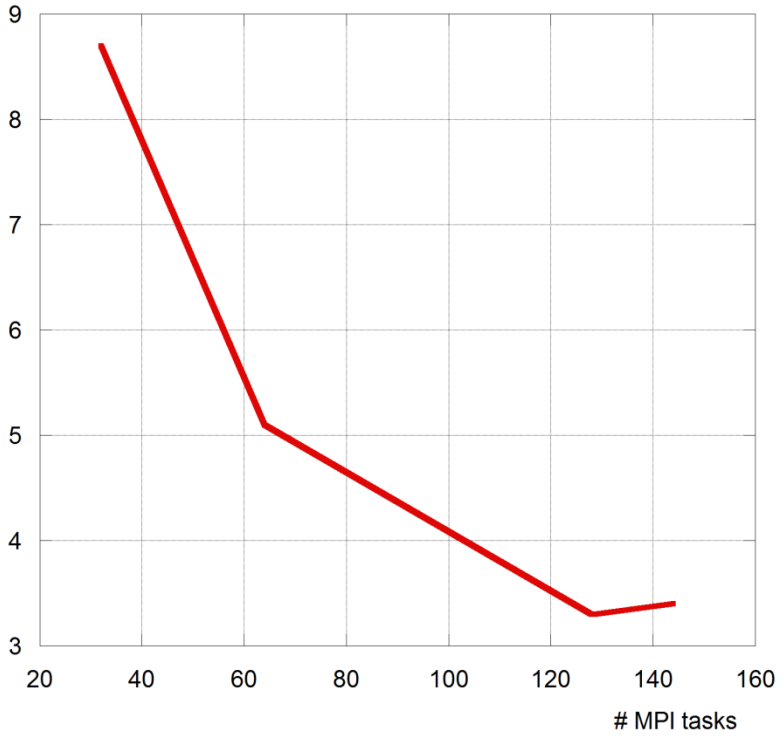


Benchmark – First Results

Program: QuantumESPRESSO 5.0.3, CP module
Most time consuming steps: linear algebra, FFT

Due to memory limitations
a smaller system
is used
$Cu[(CH_3COO)_2]_2 + 105\ H_2O$

345 atoms



Side-Project 1
Experiment related simulations
X-ray Absorption Spectroscopy

- Use Plane Wave (PW) methods to calculate X-ray Absorption cross sections

XSPECTRA package within QuantumESPRESSO

- *A useful tool for phenomenology*
- *For ensemble statistics and analysis of large systems good computing power is required*

Side-Project 2
Experiment related calculations
Serial Crystallography

- New protocols for *protein crystallography* require the analysis of up to10^6 diffraction patterns
- Easy to parallelize
- Potentially interesting for an increasingly large community of physicists, chemists and biologists

Available Machines

Eurora	@ Cineca	CPUs and GPUs
QUonG	@ Roma1	CPUs and GPUs
TheoPhys	@ Pisa	
Drum	@ Roma2	Few nodes, but fully connected

The Story So Far

1- GROMACS up and running on Eurora on CPUs and GPUs

2- QuantumESPRESSO up and running on Eurora CPUs

3- DFTB+ running on Eurora – MPI not yet working properly

4- First benchmark systems being tested

Short-Term Plans

- Compile and debug the MPI version of DFTB+ on Eurora
- Install QuantumEspresso on QUonG/CPUs and test it with infiniband and APEnet+

- Benchmark…
- Benchmark…
- Benchmark…
- Benchmark…
- Benchmark…

Mid-Term Plans

Algorithm optimization

- Optimized *FFT* on different architechtures
- Multi-dimensional *FFT*
- Find a good test program
  (e.g. QuantumESPRESSO *FFT*s)
  and use it to test various *FFT* implementations

Thanks!