Optimization of new algorithms in OCTOPUS for methods to calculate the photosynthesis

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Introduction

An overview of our experience with PRACE and RES resources, showing a real case

Outline

Background

Problems

Solutions

Results

Conclusions

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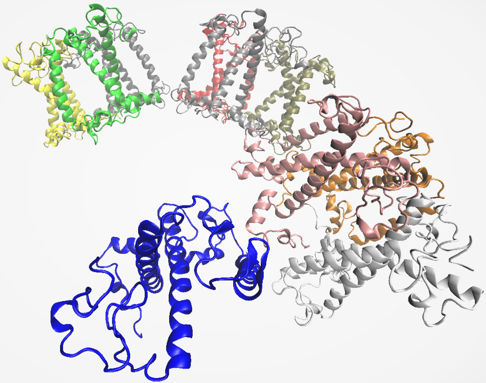
General objective

- Simulation of the light absorption in plants quantum mechanically with TDDFT[1]



- Light is absorbed by photosynthesis
- In more than 50% of the plants is done in LHCII[2] molecule

[1]MAL Marques et al. - Fundamentals of TDDFT, Springer - 2012

[2]MA Palacios et al. - J. of Physical Chemistry B - 2012

OCTOPUS

- OCTOPUS[3] is a scientific software package
- Real space ab initio virtual experimentation
  - Research of new materials, using TDDFT approach
- GPL license
- Mainly written in Fortran 90/95
  - Highly parallel by using MPI, OpenMP and OpenCL

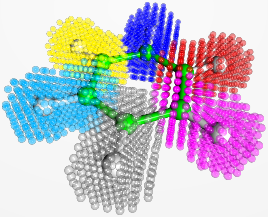


Figure: OCTOPUS simulation grid

[3] X. Andrade et al. - J. of Physics: Condensed Matter - 2012

OCTOPUS *calculation modes*

- Ground state (GS)
- Time dependent (TD)
- Both are iterative processes
- Both use Poisson solver during executions
    - Not exclusive of this two type of calculations
    - Also valid for many codes of physics, chemistry, astrophysics...

LHCII

- Light-Harvesting Complex II
- LHCII is a trimeric protein assembly with three fold symmetry
- Contains
  - 14 chlorophylls molecules
  - 4 xanthophylls molecules
    - lutein, neoxanthin and violoxanthin

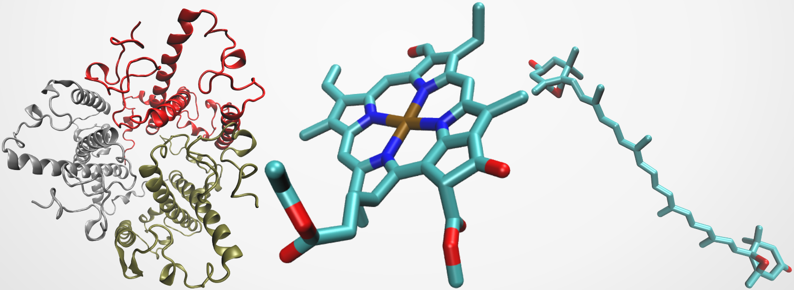


Figure: Trimer, chlorophyll and xanthophyll

LHCII computationally

- LHCII has around 16,700 atoms
  - Huge simulation grid
  - More than 32 million of grid points; more than **50 TiB** to store the wavefunctions
  - Long runs are needed to converge. For LHCII:
    - GS: 200 iterations $\times$ 25 min/iter = **3.5 days** (almost 2 million core-hours) using 24,576 CPU cores
    - TD: 6,000 iterations $\times$ 2.4 min/iter = **10 days** (almost 4 million core-hours) using 16,384 CPU cores

PRACE HPC resources

- Jugene (Blue Gene/P)
  - 294,912 “PowerPC 450” processor cores
  - 0.5 GiB RAM memory per core
  - 5 communication networks
- Juqueen (Blue Gene/Q)
  - 458,752 “PowerPC A2” processor cores
  - 1 GiB RAM memory per core
  - 5D torus communication network
- Curie fat nodes (x86-64)
  - 11,520 “Intel X7560” processor cores
  - 4 GiB RAM memory per core

Courtesy of Forschungszentrum Jülich


Courtesy of CEA

RES HPC resources

- MareNostrum III (x86-64)
  - 48,896 "Intel E5-2670" processor cores
  - 2 GiB RAM memory per core
- Magerit
  - 3,920 "Power7" processors cores
  - 2 GiB RAM memory per core

Courtesy of BSC

Courtesy of Cesvima

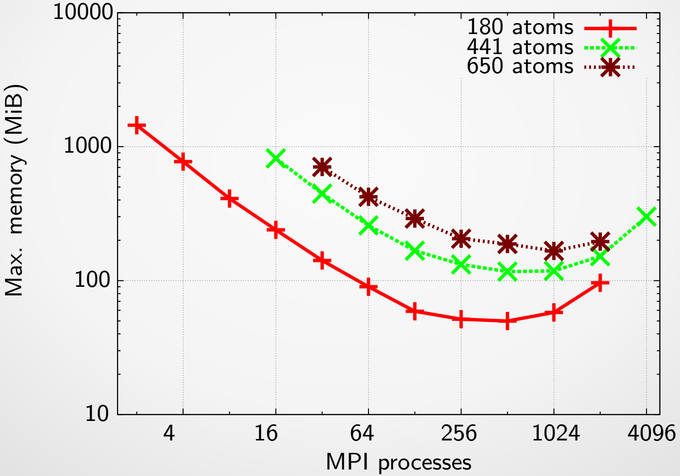
PRACE calls

- Three PRACE preparatory calls
  - 2010PA0415
    - Jugene (Blue Gene/P)
    - From 2 of May to 31 of October of 2011
    - 250,000 core-hours
    - Type C — (support from one PRACE expert)
  - 2010PA0660
    - Curie FN
    - From 1 of January to 31 of March of 2012
    - 50,000 core-hours
    - Type A — code scalability testing
  - 2010PA0763
    - Jugene at the beginning, Juqueen (BG/Q) then
    - From 25 of April to 30 of November 2012
    - 250,000 core-hours
    - Type B — Code development and optimization
- One RES call
  - FI-2013-1-0010

Outline

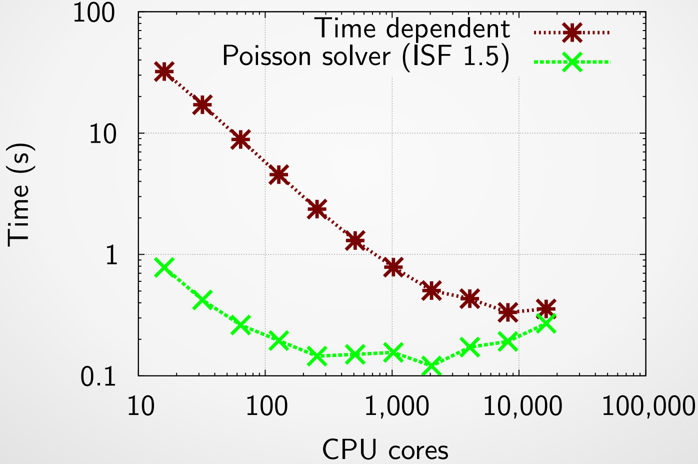
Memory limitations

- The amount of memory per processors is a limitation
- The maximum amount of memory is shown



Poisson solver did not scale

- Time dependent runs did not scale ideally [4]
- Blue Gene/P



[4] J. Alberdi-Rodriguez - LAP LAMBERT - 2012

Outline

Solutions to the memory

Use a more efficient memory scheme

- Identification of large or increasing matrices
- Delete some data structures
- Reorganisation of the code

Solutions to the scalability

Change to a new scalable Poisson solver. Implementation of

- **FMM**: fast multipole method[5] , using SCAFACOS[6]
- **PFFT**: new FFT implementation, using parallel fast Fourier transform[7]
- **ISF**: new interpolating scaling functions implementation[8], included in BIGDFT[9]

[5] I. Kabadshow, H. Dachsel, Forschungszentrum Jülich - 2010
[6] M. Bolten et al. - http://scafacos.github.com - 2013
[7] M. Pippig - SIAM J. Sci. Comput. - 2013
[8] L. Genovese et al. - J. Chem. Phys. - 2006
[9] L. Genovese et al. - J. Chem. Phys. - 2008

Parallel fast Fourier transform

Based on previous serial FFT

- Works with parallelepiped grid shapes only
- Padding from OCTOPUS grid needed
  - Done with `MPI_Gather` and `MPI_Scatter`
  - Never better than constant time.

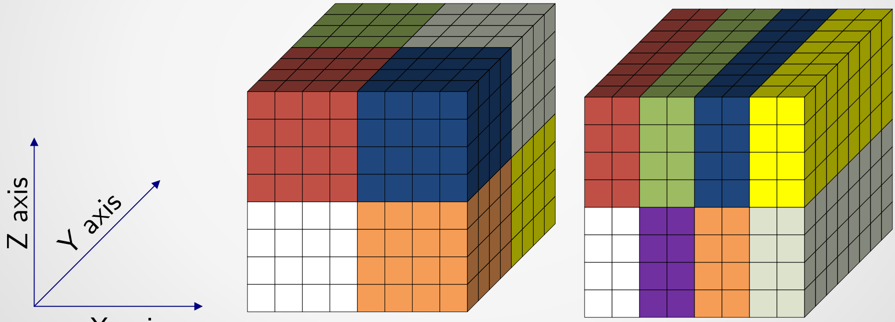
PFFT implementation

- Also, parallelepiped grid shape
- But, with a new grid partitioning (next slide)
- Implemented highly parallel data-movement, using `MPI_Alltoall`

PFFT grid partitioning

Simplified domain decomposition of the simulation grids.

- A) OCTOPUS grid with a 3D domain decomposition
- B) PFFT grid with a 2D decomposition.



A) Octopus grid

B) PFFT grid

Fast multipole method

- Usage of an external library, developed in JSC
- Use of the adaptive grid shape of OCTOPUS
- Implementation of a correction term
- $\mathcal{O}(N)$ complexity

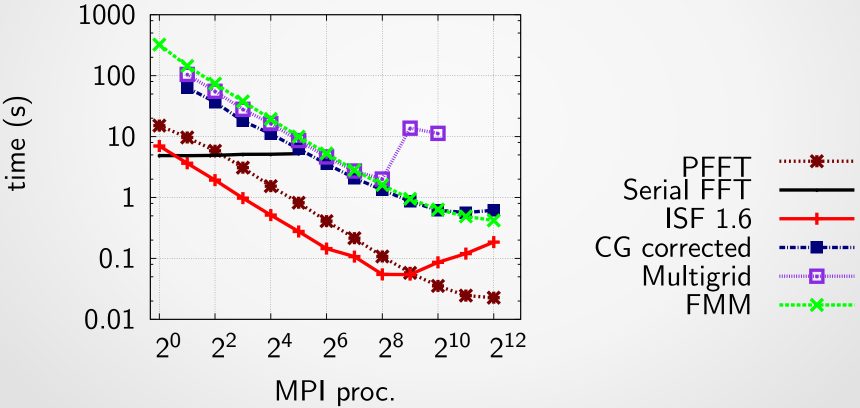
Outline

Performance

- We have used 3 different architectures
    - x86-64
        - Curie
        - Corvo (a local cluster)
    - Blue Gene/P
        - Jugene
        - Genius
    - Blue Gene/Q
        - Juqueen
- We have run hartree test and measured the time of the Poisson solver

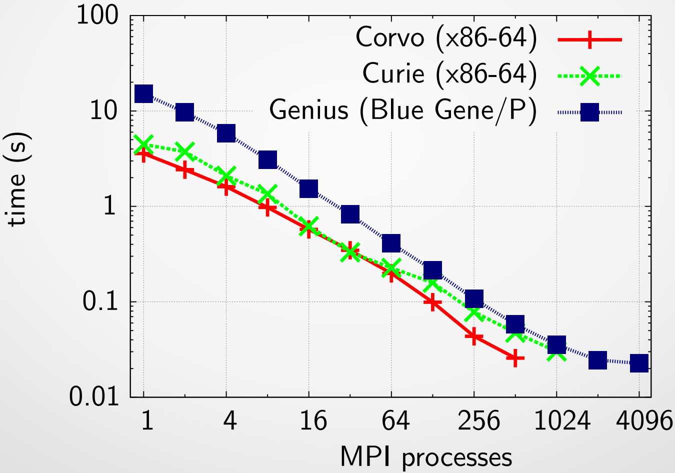
Poisson solver execution times

Hartree potential on a Blue Gene/P of a system of size $L_e = 15.8$ (4,019,679 grid points)

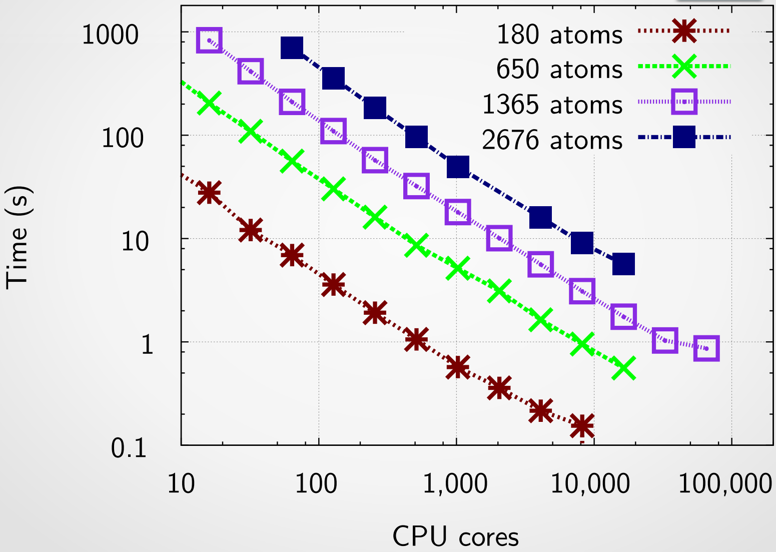


Poisson solver execution times (II)

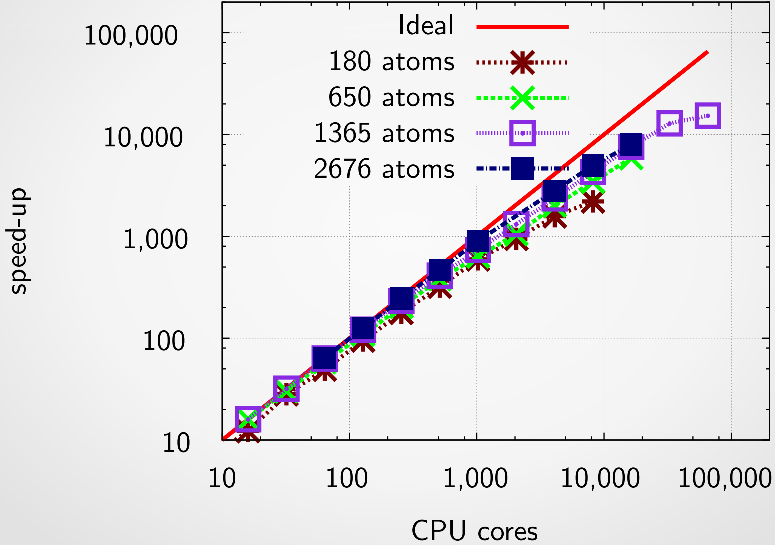
PFFT solver in several machines. The same system size of $L_e = 15.8$ (4,019,679 grid points)



TD execution-time



Speed-up of the TD



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PRACE and RES allow us to:

- Test our code
- Find the bottlenecks
- Improve the weaknesses

and, iterate over the previous three steps

So, after a deep benchmarking

- Project 2013081486 is running in PRACE Tier-0, with 21,560,000 core-hours on MareNostrum @ BSC

Acknowledgements

- PRACE research infrastructure
- RES infrastructure
- Scholarship of the University of the Basque Country UPV/EHU.

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[9] Michael Pippig. PFFT - An extension of FFTW to massively parallel architectures. *SIAM J. Sci. Comput.*, 35:C213 – C236, 2013.

"En la escuela del mundo al revés, el plomo aprende a flotar y el corcho, a hundirse. Las víboras aprenden a volar y las nubes aprenden a arrastrarse por los caminos.[10]"

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[10] E. Galeano - Patas arriba. La escuela del mundo al revés - Siglo XXI - 1998

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Algorithms
Data Mining
and Parallelism
ALDAPA

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

nano-bio spectroscopy group