Linear-scaling ab initio study of surface defects in metal oxide and carbon nanostructures

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http://www.uam.es/spmth

7th RES Users Meeting, Barcelona, 13/09/2013
Outline

1. **SPMTH Group: ab initio Forces and currents on nanostructures**

2. **PRACE Tier-0 Project Access**
   - What are Tier-0 machines and PRACE?
   - Why to apply for Tier-0 resources?
   - How?: Preparatory Access: code scalability
   - Problems during the testing stage
   - Project Access / Problems during the running stage

3. **What are we doing with these resources?**:
   - $O(N)$ vs diagonalization for total energy calculations
   - CuO: 3D STM/AFM Maps: Quantification of forces near defects only seen on the STM channel
   - Vacancies on Graphene: electronic, magnetic and mechanical properties
About us

Our work is focused on ab initio calculations amenable to forces and transport in nanostructures. We develop new capacities for the Scanning Probe Microscope use of currents and forces to visualize nanoscale.

We work, in close collaboration worldwide, in topics such as:

1. **Scanning Tunneling (STM) and Atomic Force (AFM)**
   energy dissipation mechanisms and nanomanipulation.

2. **Nanomechanics**: Fracture, Friction and Wear at the Transport properties of nanocontacts.

3. **Adsorption, reactivity, and self-organization** of fullerene on surfaces.

We use a suite of total-energy methods based in Density Functional Theory and very efficient codes based on local orbitals (like FIREBALL: MBE/PWSCF, RAPID: PWSCF, CASTEP: VASP) in the ab initio calculations.
Methodology

Ab-initio total energy methods
(based in Density Functional Theory)
both plane wave & local orbital basis:
accuracy/efficiency balance

Non-equilibrium Green’s Functions
Linked with the local orbital description

Structure + electronic properties

Electronic transport

Energy vs tip height ⇒ Forces !!

OPENMX + VASP

\[ \text{O(N) Method (Krylov subspace)} \]

+ vdW corrections:
  - semi-empirical (Grimme)
  - vdW-DF (Klimes)

“The computer is a tool for clear thinking” Freeman J. Dyson
Chemical identification with FM-AFM
Nature 446, 64 (2007).

Single-atom manipulation with FM-AFM
Science 322, 413 (2008)
Nature Nanot. 4, 803 (2009)

Forces and Currents in Carbon Nanostructures: Are We Imaging Atoms?

Martin Ondráček, Pablo Pou, Vít Rozsival, Cesar González, Pavel Jelínek, and Rubén Pérez.*

Understanding Dissipative Tip–Molecule Interactions with Submolecular Resolution on an Organic Adsorbate

Gernot Langewisch, Wojciech Kamiński, Daniel-Alexander Braun, Rolf Möller, Harald Fuchs, André Schirmeisen, and Rubén Pérez*

We use a suite of total-energy methods based in Density Functional Theory (DFT) and very efficient codes based on local orbitals (like FIREBALL and OPENMX) to more accurate
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What are Tier-0 machines and PRACE?

Tier-0: 50,000 – 460,000 cores, petaflop scale

<table>
<thead>
<tr>
<th>System Name</th>
<th>Hosting Centre</th>
<th>Launch date</th>
<th>Architecture</th>
<th>Speed</th>
</tr>
</thead>
<tbody>
<tr>
<td>CURIE</td>
<td>GENCI@CEA, France</td>
<td>Q2 2011</td>
<td>Bullx cluster</td>
<td>2 Petaflops/s</td>
</tr>
<tr>
<td>Hermit</td>
<td>GCS@HLRS, Germany</td>
<td>Q3 2011</td>
<td>Cray XE6</td>
<td>5 Petaflops/s</td>
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<tr>
<td>FERMI</td>
<td>CINECA, Italy</td>
<td>Q2 2012</td>
<td>BlueGene/Q</td>
<td>2 Petaflops/s</td>
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<tr>
<td>SuperMUC</td>
<td>GCS@LRZ, Germany</td>
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<td>iDataPlex</td>
<td>3 Petaflops/s</td>
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<tr>
<td>JUQUEEN</td>
<td>GCS@FZJ, Germany</td>
<td>Q4 2012</td>
<td>BlueGene/Q</td>
<td>5.87 Petaflops/s</td>
</tr>
<tr>
<td>MareNostrum</td>
<td>BSC, Spain</td>
<td>Q4 2012</td>
<td>iDataPlex</td>
<td>1 Petaflops/s</td>
</tr>
</tbody>
</table>

Partnership for Advanced Computing in Europe

PRACE (Partnership for Advanced Computing in Europe), the European research infrastructure for High Performance Computing (HPC), makes it possible for researchers from across Europe and the world to apply for access to Tier-0 HPC systems via a peer-review process.
Why Tier-0? (or better… Why bother?)

- It requires extra effort & different perspective from Tier-1 (typical job: from hundreds to thousands of processors)

- Many popular codes (e.g. VASP) do not have the required scalability

- Access to massive resources in terms of computer power and time

TGCC : PRACE Project 2012060986 on CURIE
PRACE Project : 2012060986
Project number : RA0986
16.250.000 core hours on standard nodes on Curie.
dates : 2012-11-01 to 2013-11-01
How?: Applying for a PRACE Tier-0 project

- Technical review
  - Scalability
- Scientific review

Project access vs Preparatory access (different calls!!)
How?: Preparatory access projects

**GOAL:** to show the scalability of your code

1.1. Proposal ID
2010PA0638  *(Type A PA project intended for code scalability testing)*

1.3. Period of access to the PRACE facilities
01/11/2011 to 31/12/2011  *(just two months !)*

1.4. Name of the PRACE facility assigned
Curie  *(why?: large memory on Curie fat nodes)*

2.1. Project name
Large-scale O(N) DFT simulations of defects in metal oxides

2.2. Research field

<table>
<thead>
<tr>
<th>Astrophysics</th>
<th>Engineering and Energy</th>
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<tbody>
<tr>
<td>Earth Sciences and Environment</td>
<td>Mathematics and Computer Science</td>
</tr>
<tr>
<td>Medicine and Life Sciences</td>
<td>Finance and Social Science</td>
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<tr>
<td>Chemistry and Materials</td>
<td>Linguistics and Encryption</td>
</tr>
<tr>
<td>Fundamental Physics</td>
<td></td>
</tr>
</tbody>
</table>


OpenMX scalability with hybrid MPI/OpenMP

# of MPI process X # of threads (1-32) = # of cores < 4096 (limitation Prep. Acc.)

Table 1: 3400 atoms, 8 thread test

<table>
<thead>
<tr>
<th># cores</th>
<th>absolute timing (s)</th>
<th>speed-up</th>
<th>ideal speed-up</th>
<th>efficiency [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>256</td>
<td>53.0</td>
<td>1.0000</td>
<td>1.0</td>
<td>100.0</td>
</tr>
<tr>
<td>512</td>
<td>31.3</td>
<td>1.6924</td>
<td>2.0</td>
<td>84.6</td>
</tr>
<tr>
<td>1024</td>
<td>15.7</td>
<td>3.3760</td>
<td>4.0</td>
<td>84.4</td>
</tr>
<tr>
<td>2048</td>
<td>9.4</td>
<td>5.6572</td>
<td>8.0</td>
<td>70.7</td>
</tr>
<tr>
<td>4096</td>
<td>7.3</td>
<td>7.3057</td>
<td>16.0</td>
<td>45.7</td>
</tr>
</tbody>
</table>

X 4
OpenMX scalability with hybrid MPI/OpenMP

Normalized Speed-up

Parallel Efficiency

a) OpenMX speed-up performance with multithreading for large test calculation sizes (normalized to the first data point)
b) corresponding parallel efficiency computed for the 3400 atom test input.
OpenMX scalability with hybrid MPI/OpenMP

Variation in computational resources with multithreading for a constant number of cores (3400 atom calculation)

Linear-scaling of computational time with test system size (128 MPI procs with multithreading)
Problems in the testing stage

- Make sure that you test the same architecture you want to apply for: tests on the CURIE fat nodes (larger memory) BUT most of the PRACE time allocated on CURIE thin nodes)

  FIX: Repeat selected tests at the beginning of the project.

- Limited resources: < 4096 cores + small time allocation (while you are really intended to go for larger production jobs…)

  FIX: We got access to a larger machine (Cray XT5 @ JAIST, Japan) + (validation of scripts for scalability tests in Curie)
Applying for a PRACE Tier-0 project

- **Technical review**
  - Scalability
  - minimum request: 5 million hours
  - minimum job size > 512 cores (system dependent)

- **Scientific review**
  - Scientific excellence, novelty and impact
  - Focus on topics of major relevance for European research
  - Suggestion of three qualified reviewers.
Problems in the running stage (I)

- Beware of changing the parameters of the calculations (errors get amplified… and you are blacklisted !!!)

- Do not trust your internal functions to estimate the memory usage; use tools like Valgrind

Mem. peak predicted by OpenMX: 1.542 Gb
Mem. peak given by ps ux tracking: 2.932 Gb
Mem. peak (real) given by Valgrind: 2.955 Gb

Memory consumption profile from Valgrind code for a test OpenMX calculation
(288 atoms, 13 orbitals, 2x2x1 grid for SCF & 10x10x1 DOS)
Problems in the running stage (II)

- Significant improvement in the performance of your code (3x for O(N), > 10x for diagonalization): you have asked for too much time…

v3.644 -O1 (lapack) vs v3.7 -O3 (elpa1 diagonalisation library)
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Cu(100)-0: An oxide ML on top of a metal
Cu tip on Cu(100)-0: O(N) vs diagonalization

Large Diagonalization calcs possible with the elpa1 library !!!
Cu(100)-0: Force contrast around the defect
Vacancies in Graphene: Magnetism??

2.58Å

2.01Å
Why do we need these large unit cells and fine k-sampling?
Why do we need these large unit cells and fine k-sampling?
Conclusions

1. Ab initio O(N) energies and forces on metallic nanostructures
   
   CuO: large scale defect structures; domain nucleation and growth, link between forces and chemical reactivity
   Vacancies on Graphene: magnetic and mechanical properties

2. PRACE Tier-0 Project Access: Key points for success
   
   Preparatory Access: demonstrate code scalability
   Project Access: World-class science project

Apply in the next PRACE call !!
SPM Theory & Nanomechanics Group

SPM-TH

- Group Leader: Prof. Rubén Pérez

- **Postdoctoral Researchers:**
  - Pablo Pou (RyC)
  - Delia Fernández
  - Milica Todorovic
  - Guilherme Vilhena

- **PhD Students:**
  - Lucía Rodrigo
  - Carlos Romero
  - Diego Rodriguez
  - Michael Ellner

- www.uam.es/spmth

- Nanotubes, graphene
- Oxides
- Molecular self-assembly
- KPFM Simulations
- Oxides
- AFM in biology
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