Computational Chemistry and Material Science Session

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Information Society and Media

Talks

- **David Reid**

  Supporting Statistical Semiconductor Device Analysis Using EGEE and OMII-UK Middleware
- **Bhalchandra Pujari**

  Exploiting Grid for Condensed Matter Applications Quantum Dots and Building Clusters Atom-by-Atom
- **Aneta Karaivanova**

  Ultra-fast Semiconductor Carrier Transport Simulation on the Grid. SALUTE: new results for the inhomogeneous case
- **Osvaldo Gervasi**

  The study of Cytochrome C oxidase on EGEE Grid

David Reid

Supporting Statistical Semiconductor Device Analysis Using EGEE and OMII-UK Middleware

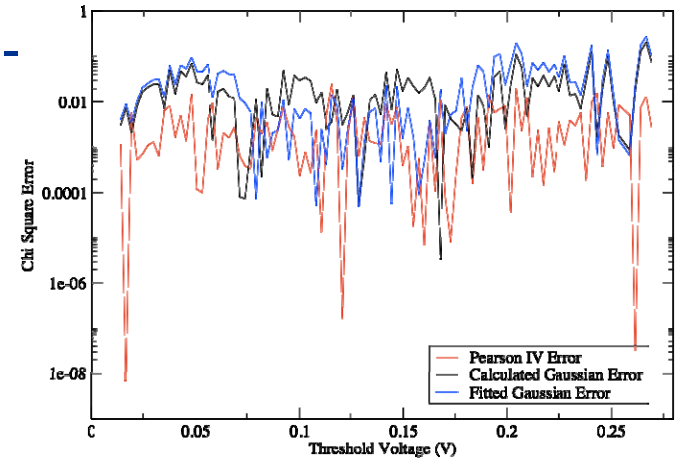
QuickTime™ and a
decompressor
are needed to see this picture.

Scientific context

Studies of CMOS devices

- **Device Simulations**
  - Voltage threshold
  - How Do Random Dopants Affect V_{th}?
  - Storage of off-current
  - Simulations done at low drain: V_d=100mV
- **Over 100,000 devices to be studied**
- **Conclusions**
  - The distribution of threshold voltage is non-gaussian
  - Histograms better fitted by Pearson IV distribution

QuickTime™ and a decompressor are needed to see this picture.



Grid Utilization

- **Difficulties:**
  - Job submission (GANGA used)

    huge number of short time jobs needs to be executed

  - Data management (Tracking 2 files per device quickly becomes problematic for huge ensembles)
- **Data obtained on SCOTGrid**
- **Research carried under NanoCMOS project (`www.nanocmos.ac.uk`)**
- **Aim:**
  - Enable device flow design to the Grid
  - Develop a methodology that allows grid resources to be used to improve designs

Talk

- **Bhalchandra Pujari**

  Exploiting Grid for Condensed Matter Applications Quantum Dots and Building Clusters Atom-by-Atom

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Scientific context

- **Point of interest**
  - Structure of the quantum dot (confined electron system)
  - Change of properties with QD size
  - Structure of atomic clusters and their evolution as the number of atoms grows
- **Application**
  - Basic Physics
  - Electronics
  - Home appliances
  - Biological Dyes
- **Computational method**
  - Density Functional Theory with local potential (no need for GGA potentials)

Computations

- **Quantum Dot computations**
  - The number of electrons vary for N =2 to 20
  - Typical dot size varies in 5 steps of lengths
  - Addition of impurity multiplies the calculation by 2!

    For 10-electron quantum dot, with 5 values of spins and 100 initial guesses → No of calculations 🖫 5000!
- **Clusters**
  - Simulated annealing at finite temperature for up to 50000 iterations (1000 iterations 🖫 3 picosec.)
  - A few hundred to a few thousand structures to be searched and quenched
  - Grid Each minimization may take up to 100-300 CPU hours on say, single Xeon processor
- **For a series of 10 clusters, with 400 geometries and 2 states: total number of jobs = 10*400*2 = 8000!**

Aneta Karaivanova

Ultra-fast Semiconductor Carrier Transport Simulation on the Grid. SALUTE: new results for the inhomogeneous case

Salute

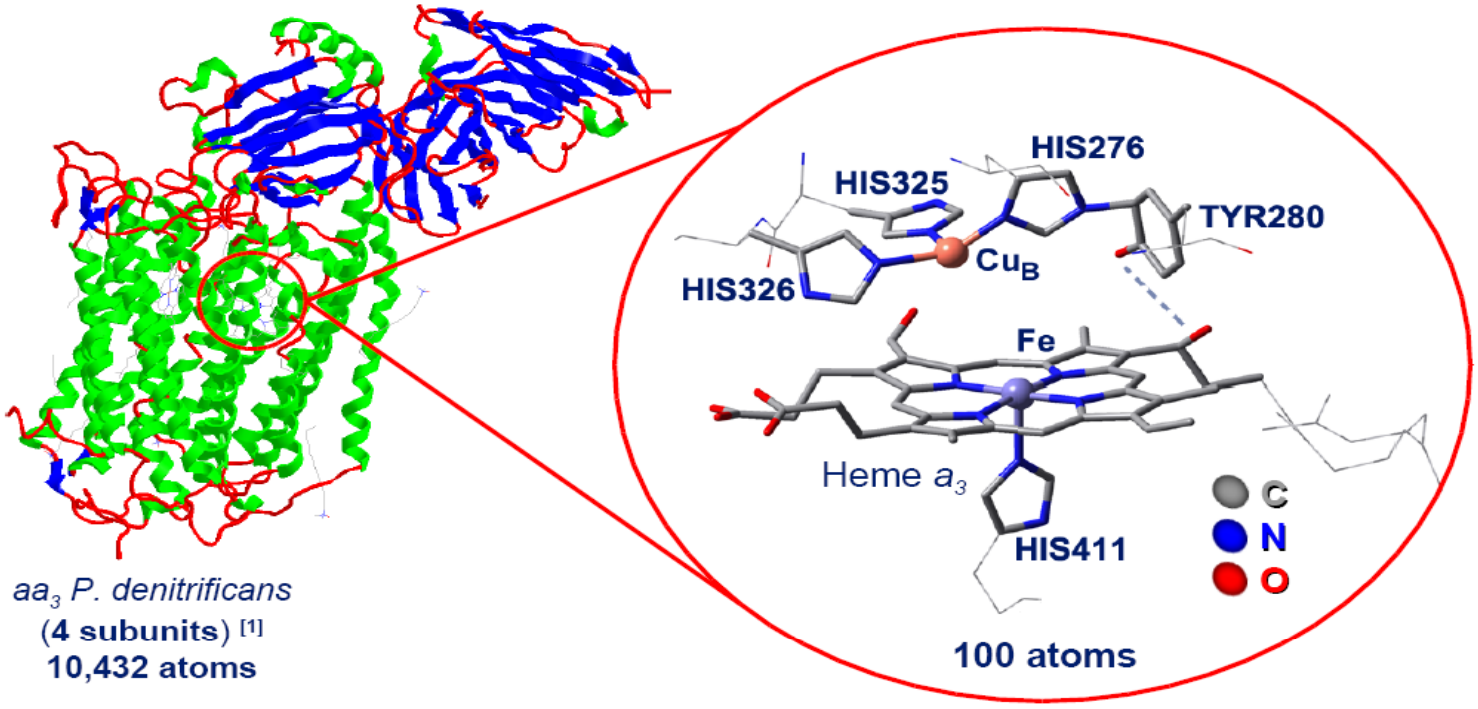
- SALUTE (**St**ochastic AL**gorithms for U**ltra-fast T**ransport in sEmiconductors**) is a grid application, which integrates a set of novel Monte Carlo and quasi-Monte Carlo algorithms for solving various computationally intensive problems which describe ultrafast carrier transport in semiconductors.
- SALUTE studies memory and quantum effects during the relaxation process due to electron-phonon interaction in semiconductors.
- The quantum kinetic model: a femtosecond relaxation process of optically excited carriers in one-band semiconductors or quantum wires. The electron-phonon interaction is switched on after a laser pulse creates an initial electron distribution. Two cases are considered – with and without applied electric field.

Achievements

- **Major achievements**
  - New results about distribution density, energy distribution and Wigner function for large evolution times
  - For the inhomogeneous case in the presence of electric field are obtained.
  - In order to solve this computationally challenging problem, we have developed two novel advanced Monte Carlo algorithms, and grid implementation scheme which allows massive production work.
- **Benefits for EGEE user community**
  - SALUTE is one of the SEEGRID2 supported application.
  - The use of the Grid provides not only CPU power but also a platform for sharing the achieved results among scientists and avoiding of duplication of efforts (the results are used by scientists from IPP-BAS, TU-Vienna, University of Glasgow, and Arizona State University).
  - SALUTE stresses the availability and scalability of the various Grid services and resources on the SEE-GRID-2 infrastructure.

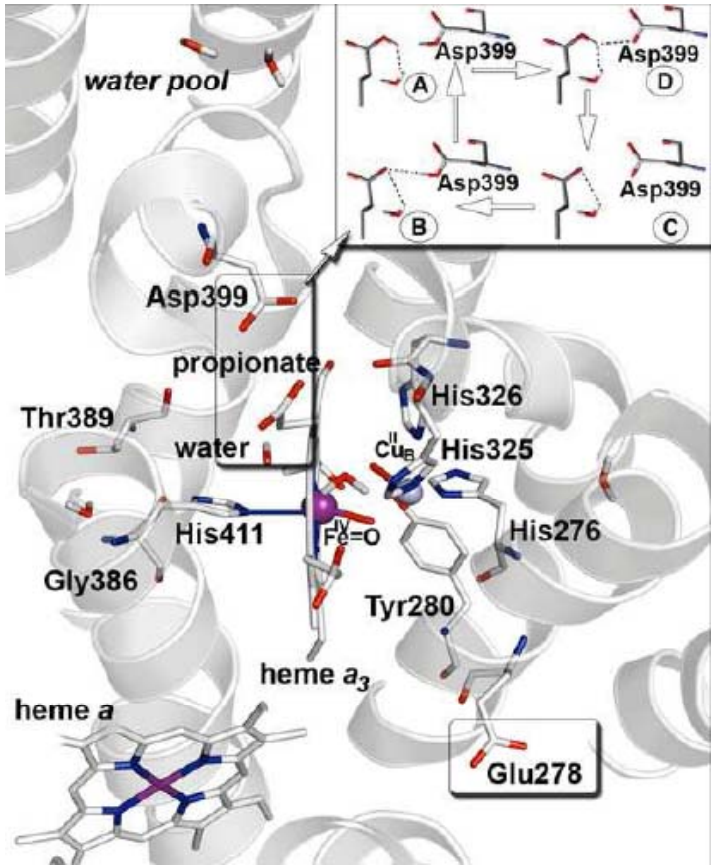
Osvaldo Gervasi

The study of Cytochrome C oxidase on EGEE Grid



The study

- Cytochrome c Oxydase (CcO) consists of approximately 10.000 atoms and the dynamics calculations are unfeasible on ordinary clusters (2.4 years are required for a simulation of 5.2 ns).
- CcO couples the four electron reduction of the Oxygen molecule to water with the pump of four protons across the inner mitochondrial membrane attributing to the electrochemical gradient that is used to synthesize ATP
- Electrons from CcO pass through a heme *a* group and are transferred to the binuclear heme a_3/Cu_B active site where the dioxygen is reduced
- We study the dynamics of the protein matrix near the active site at the ferryl-oxo oxidation level concentrating on the v(Fe-O) and the role of Glu278



Computational methods

- **Computational methods**
  - Molecular Dynamics, T=300K using Tinker with Amber99 ff
  - Density Functional Theory
- **Difficulties**
  - Job management
- **Achievements**
  - the feasibility on EGEE Grid of a very intensive computational campaign about the study of the dynamics of Cytochrome c Oxydase. This goal will be unreachable in ordinary clusters
- **Benefits from Grid usage**
  - sharing of expertise and experiences made using the large computational resources available through Compchem and SEE VOs.
  - share some techniques necessary to survive managing a large amount of submitted jobs

Thank you for your attention