Multi Scale Design of nanomaterials with simulations on hybrid architectures: (the muscade project)

Pascal Pochet
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2009-2012
Chair of excellence for **Normand Mousseau**

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http://inac.cea.fr/L_sim
Methods for simulation in nanosciences?

**Used Methods**

- Ab initio, Monte Carlo
- or Molecular dynamics

**Applications**

« simple systems »

**Today**

- Ab initio + MC or MD

« User Hopping »

**Large scale Ab initio + ART methods**

**Point defect diffusion in semiconductors**

- Graphene sheet on SiC
- Au droplet on Si

**Surface science**

**Growth science**

http://inac.cea.fr/L_sim
Muscade synopsis

WP1: Software engineering

- Boost \textit{ab initio} package
- Algorithms for rare event \textit{ab initio} based exploration

\textit{Simulation tools for growth study in nanosciences}
Normand Mousseau

WP2: Application targets

- Ge QD on Si
- Si Nanowire
- Graphene on SiC

Experimental validation

http://inac.cea.fr/L_sim
GPU acceleration of simulation package (WP1 task 1)

Hybrid parallelization of BigDFT awarded in 2009

BigDFT x 7 (GPU/CPU)

We are ready to use the CCRT hybrid computing nodes!

S_GPU: Integration of GPU in parallel computations (done on Titane)

- **Increase** the speed-up
- Hybrid parallelization of **other softwares** (Abinit, Siesta, Vasp)
- Software developments and first evaluations on a **local hybrid platform**
- Large scale simulations on National computing center (Genci)

**200 k€ were asked to buy such a hybrid computer**

CEA-INRIA-UJF team: Appl. Mathematicians + Computer scientists + Physicists

Luigi Genovese

http://inac.cea.fr/L_sim
The ART package (WP1 task 2)

Empirical vs ab initio description?

BigDFT already tested with Minima Hopping

Kinetic ART: An off-lattice on-the-fly kinetic Monte-Carlo algorithm

Off-Lattice: i/ Events are classified using a topological description, allowing geometric deformation ii/ Relevant barriers are relaxed at each step, allowing for elastic deformation.

On-the-Fly: i/ Events are generated with ART nouveau and kept in the catalog associated with each topology ii/ New search is performed when a new topology is met.
**Ge QD on Si:**
Prototype for 0D nanos

What are the mechanisms that drive the shape change?

**Silicon Nanowires:**
Prototype for 1D nanos

What are the mechanisms that drive the NW growth from the droplet?

**Graphene on SiC:**
Prototype for 2D nanos

What is the structure of graphene resulting from the growth mechanisms on the SiC substrate?
Initial vs granted funding

Initial request for a cost of ~ 650 k€

- Funding of the Chair of Excellence for Normand Mousseau
- 84 postdoc's months with 1/3 for WP1 and 2/3 for WP2
- 200 k€ for a local hybrid platform @ CIMENT

Attributed Grant: 280 k€

- Chair of Excellence granted
- 51 months granted (80% of WP1, 50% of WP2)
- CIMENT platform not funded

kART + BigDFT and Ge QD:

- 21 postdoc's months (starts 7\textsuperscript{th} of December)
- 12 postdoc's months (spring 2010)
- 6 postdoc's months (spring 2011)
- 12 postdoc's months (spring 2011)

--> Application target will be partially postponed ...
Side funding

The Canadian support
WP2 task 1 using empirical potentials
3 years postdoc grant (2010-2012 thanks to FQRNT)
3 years PhD grant (2010-2012 thanks to NSERC)

The French support
WP1 task 1
ANR, ProHMPT 4 years postdoc grant (2009-2012)
WP2 task 2 and 3
ANR, Graph_Sim 2 years postdoc grant (2010-2012)
CIBLE, PhD grant (2009-2011)
CEA, CFR PhD grant (2009-2011)
G-INP, Menrt PhD grant (2011-2013)

The “France-Vietnam” support
PhD grant (2009-2012) on WP2 task3

The plateform support ?
GPU-based hybrid plateform 350 k€ needed in 2010
INRIA, CIRA, CEA, G-INP will fund 250k€, 100 k€ will be missing (RTRA 2010 call ?)
Muscade schedule

Year 1: WP1 (ART-BigDFT, GPU)

Year 2: WP2 (Ge QD, Si NW, Graphene)

Year 3: WP2 (Ge QD, Si NW, Graphene) side funding only!

Main awaited results from the Muscade project

- Collaboration of the Grenoble teams with Normand Mousseau
- Strong collaboration between the main Grenoble simulation teams
- Software developments for growth science (ART methods)
- Apply these methods to the three application targets