



BigDFT
project

Wavelets

CPU code

GPU code

Perspectives

Prix Bull - Joseph Fourier 2009

Forum Ter@tec 2009 – SUPELEC

*The BigDFT project:
High Performance Computing for nanosciences*

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30 june 2009

The BigDFT project: Wavelets for nanosciences



(2005-2008) – Postdoc at CEA Grenoble

STREP European project: BigDFT

Coordinator: CEA-INAC Grenoble (T. Deutsch):

Four partners, 15 contributors

(U. Basel, U. Louvain-la-Neuve, U. Kiel)



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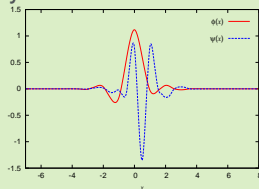
Perspectives

Objective: to develop a simulation tool for nanosciences

A new code for quantum properties of systems at nanoscale
based on **wavelets**

Optimal properties for nanosciences

- Precise, Mathematically rigorous
- Flexible, easy to optimise



2008 – BigDFT 1.0: Robust, excellent performances

Principal contributor – Maintainer of the code

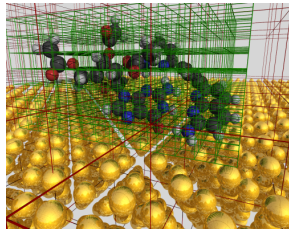
A versatile formalism, conceived for HPC



Optimal for high optimisation

“Simple” numerical operations

- Short convolutions
- Linear algebra (BLAS)

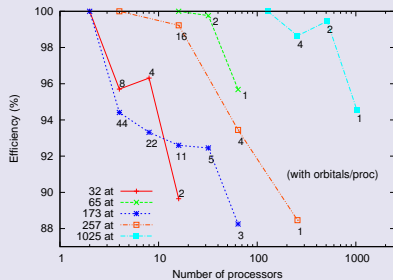


Optimal for massive parallel environment

Excellent efficiency
($\sim 90\%$), up to thousands
of processors

(Platine, CCRT \rightarrow)

- ✓ The overall time for a computation can be sensibly reduced
 \Rightarrow bigger systems



HPC for Hybrid architectures with BigDFT code



BigDFT code is suitable for GPU calculation (ESRF, '08)

with M. Ospici, J.-F. Méhaut, LIG - INRIA - UJF - Bull, Grenoble

- Moderate cost for porting
- Fully compatible with CPU parallelisation
- Allows multi-GPU computation



Wavelets

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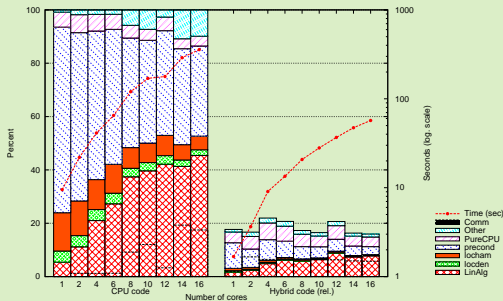
GPU code

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Tested on Multi-GPU
platforms:

- CINES - Iblis
48 GPU, Prototype
calculations
- CCRT - Titane
Up to 196 GPU
(Grand challenge
2009)

5 to 10 times faster (and improving...)



Summary



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BigDFT code: a modern approach for nanosciences

- ✓ Flexible, reliable formalism (wavelet properties)
- ✓ Conceived for massive parallel architecture
- ✓ Open a path toward the diffusion of Hybrid architectures

Now: BigDFT version 1.3 – a rapidly evolving code

Available under GNU-GPL license

Lots of applications & developments with BigDFT team:
D. Caliste, T. Deutsch ([L_Sim - CEA INAC Grenoble](#))
S. Goedecker ([U. Basel](#))
M. Ospici, J-F. Méhaut ([LIG INRIA UJF Bull Grenoble](#))

Reference paper(s):

CPU : L. Genovese *et al.*, J. Chem. Phys. 129, 014109 (08)
Hybrid : L. Genovese *et al.*, J. Chem. Phys., in press

Acknowledgements



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