52nd Sanibel Symposium
19-24 February 2012, St. Simons Island, Georgia, USA

Implementation of Time-Dependent Density-Functional Theory in the Wavelet Code BIGDFT: First Results

Bhaarathi Natarajan[1,2], Mark E. Casida[1,*], Luigi Genovese[2], and Thierry Deutsch[2]

[1] *Laboratoire de Chimie Théorique (LCT), Département de Chimie Moléculare (DCM, UMR CNRS/UJF 5250), Institut de Chimie Moléculaire de Grenoble (ICMG, FR-2607), Université Joseph Fourier (Grenoble I), 301 rue de la Chimie, BP 53, F-38041 Grenoble Cedex 9, FRANCE.*
[2]*UMR-E CEA/UJF-Grenoble 1, INAC, Grenoble, F-38054, FRANCE.*

[*] *corresponding author: mark.casida@ujf-grenoble.fr*

Wavelet approaches have largely replaced Fourier approaches in many engineering applications because wavelets are by nature a multiresolution basis set which allows details only when and where needed. The idea of using wavelets in quantum chemistry has evolved greatly since early propositions **[FD93,C96]**. In particular, BIGDFT is a massively parallel wavelet-based code for carrying out density-functional theory (DFT) calculations on large finite or periodic systems with large unit cells. While DFT is a ground-state theory, time-dependent DFT (TD-DFT) allows electronic excited states to be treated via linear response theory. Reference [CH12] provides a recent review of TD-DFT while Ref. **[NCGD11]** is a timely review of wavelets for DFT and TD-DFT. In this talk we will report on progress in implementing TD-DFT into BIGDFT and compare results with the Gaussian-based quantum chemistry program DEMON2K **[NCGD11,NGC+11]**. Orbital energies converge amazingly quickly to the basis set limit in the wavelet code. First TD-DFT results are reported which are quite encouraging but which also beg for a better approach to the handling (or avoidance) of continuum states.

References:

[CH12] M.E. Casida and M. Huix-Rotllant, "Progress in Time-Dependent Density-Functional Theory," *Annu. Rev. Phys. Chem.* **63**, xxxx (2012) (*in press*), arXiv:1108.0611v1

[NGC+11] B. Natarajan, L. Genovese, M.E. Casida, T. Deutsch, O.N. Burchak, C. Philouze, and M.Y. Balakirev, "Wavelet-Based Linear-Response Time-Dependent Density-Functional Theory," *Chem. Phys.*, *submitted*, arXiv:1108.3475v1

[NCGD11] B. Natarajan, M.E. Casida, L. Genovese, M.E. Casida, and T. Deutsch, "Wavelets for Density-Functional Theory and Post-Density-Functional Theory Calculations," in *Theoretical and Computational Methods in Density Functional Theory*, A.K. Roy, Editor (Nova Science Publishers: *in press*), arXiv:1110.4853v1

[C96] J.-L. Calais, "Wavelets—Something for Quantum Chemistry?", *Int. J. Quant. Chem.* **58**, 541 (1996)

[FD93] P. Fischer and M. Defraceschi, "Looking at Atomic Orbitals Through Fourier and Wavelet Transforms" *Int. J. Quant. Chem.*, **45**, 619 (1993)

BIGDFT, `http://inac.cea.fr/L_Sim/BigDFT/`

DEMON2K, `http://www.demon-software.com/public_html/index.html`