

Abstract Submitted  
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**Real Space DFT by Locally Optimal Block Preconditioned Conjugate Gradient Method** VINCENT MICHAUD, HONG GUO, McGill University — Real space approaches solve the Kohn-Sham (KS) DFT problem as a system of partial differential equations (PDE) in real space numerical grids. In such techniques, the Hamiltonian matrix is typically much larger but sparser than the matrix arising in state-of-the-art DFT codes which are often based on directly minimizing the total energy functional. Evidence of good performance of real space methods - by Chebyshev filtered subspace iteration (CFSI) - was reported by Zhou, Saad, Tiago and Chelikowsky [1]. We found that the performance of the locally optimal block preconditioned conjugate gradient method (LOGPCG) introduced by Knyazev [2], when used in conjunction with CFSI, generally exceeds that of CFSI for solving the KS equations. We will present our implementation of the LOGPCG based real space electronic structure calculator.

[1] Y. Zhou, Y. Saad, M. L. Tiago, and J. R. Chelikowsky, “Self-consistent-field calculations using Chebyshev-filtered subspace iteration,” *J. Comput. Phys.*, vol. 219, pp. 172-184, November 2006.

[2] A. V. Knyazev, “Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method,” *SIAM J. Sci. Comput.*, vol. 23, pp. 517-541, 2001.

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