Massively Parallel Eigensolvers based on Unconstrained Energy Functionals Methods

Osnir Marques, Mauro Del Ben and Andrew Canning

Lawrence Berkeley National Laboratory

Overview
- The implementation and performance of a preconditioned conjugate gradient based iterative eigensolver using an unconstrained energy functional minimization scheme avoiding explicit reorthogonalization is studied.
- This approach shows improved parallel efficiency over standard methods.
- We have developed a set of preconditioner techniques that fix the known flaw of slow convergence of the unconstrained minimization.
- Large scale electronic structure calculations, with thousands of atoms, can then be performed with excellent time to solution, running at scale on hundreds of thousands of cores at HPC facilities.
- The unconstrained formulation was implemented in the first-principles materials and chemistry CP2K code, which performs electronic structure calculations through a density functional theory approximation to the solution of the many-body Schrödinger equation.

Strategies for Preconditioned CG
- Path 1: Hessian $A$ of the unconstrained functional as preconditioner for the gradient, $A^{-1}G$ (quasi-Newton step) solve $A^P = G$ iteratively
- $S^{-1}$ or $\tilde{A}^{-1}$ as preconditioner for the inner solver (with $K$ iterations) $A = \tilde{A}$
- Path 2: $S^{-1}$ or $\tilde{A}^{-1}$ as preconditioner for the unconstrained functional minimization

Formalism

$$H\psi_f(r) = e\psi_f(r) \rightarrow HC = SE$$ (for non-orthonormal basis)

Direct Methods
- ScalAPACK, EigenExa, ELPA

Iterative Methods
- Davidson, Lanczos, LOBPCG
- attractive when a small fraction (2-10%) of the many-body Schrödinger equation
- Convergence of the charge density and potential field.

Initial Guess $\{ \psi_0 \}$

Calculate Density $\rho(r) = \sum_{i} |\psi_i|^2$

New Set $\{ \psi_i \}$

Update $H$

Solve: $H\psi_f(r) = e\psi_f(r)$

Self-consistency

$H\psi_f(r) = e\psi_f(r) \rightarrow HC = SE$ (for non-orthonormal basis)

Basic physical and computational parameters of the systems employed in the numerical experiments. $N$ is the basis set size (the dimension of the Hamiltonian matrix that needs to be diagonalized at each SCF step), $N_o$ the number of eigenvectors to be computed (number of wavefunctions needed to build the electronic density), and $\gamma$ is the energy difference between eigenvalues $N_o$ and $N_o + 1$ in atomic units (AU), the unit employed to express $\gamma$. The number of atoms range from 2,247 to 12,288.

CG-based constrained eigensolver
- $\min Tr[C^THC]$ with $C^T = C$

CG-based unconstrained eigensolver
- $\min Tr[C^THX]$ with $C^T = I$

Path 1: Hessian $A$ of the unconstrained functional as preconditioner for the gradient, $A^{-1}G$ (quasi-Newton step) solve $A^P = G$ iteratively
- $S^{-1}$ or $\tilde{A}^{-1}$ as preconditioner for the inner solver (with $K$ iterations) $A = \tilde{A}$
- Path 2: $S^{-1}$ or $\tilde{A}^{-1}$ as preconditioner for the unconstrained functional minimization

Numerical Results

Convergence of the energy (unconstrained objective function) for a single unconstrained functional diagonalization (unconstrained subspace minimization). Five setups, the time for a single unconstrained-PCG iteration is given in parenthesis. Left: Complex. Right: SiDivac.

Convergence of the SCF procedure. Four setups; the average time for a single SCF step is given in parenthesis. Left: Complex. Right: SiDivac.

Systems Studied

- Bulk liquid water
- Solvated catalyst complex
- MoS$_2$-WSe$_2$, bilayer
- Divacancy defect in silicon

Time to solution for full SCF convergence compared to direct solvers (ScalAPACK and ELPA). (a) Water-1024, (b) Complex, (c) Bilayer and (d) SiDivac. Actual times are given in parenthesis. For SiDivac, $8^*$ and $D^*$ are times obtained with a larger basis (about 1.7 times larger than in $B$ and $D$, with 160 KNL nodes).

Computational Environment
- Cray XC40 system (cori @ NERSC)
- MPI$+\text{OpenMP}$ implementation
- Intel compiler, MKL, ELPA, and LBXSM (latest available releases)

References

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Authors’ e-mails: {osmarques, mdelben, acanning}@lbl.gov