FASTMath: Eigensolver Activities

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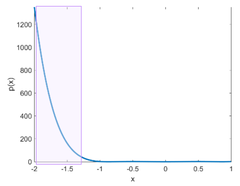
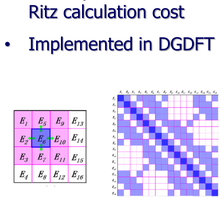
The FASTMath eigensolver team develops efficient algorithms for solving large-scale eigenvalue problems arising from a number of SciDAC applications. These algorithms exploit special structures of the application problems and use compact representations of operators and eigenfunctions. A variety of techniques are used in the implementation of these algorithms to ensure eigensolvers are scalable on DOE leadership class high performance computers.

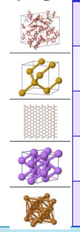
Polynomial Filtering for DFT Eigenvalue Problems

- Chebyshev polynomial
  - Amplify low end of the spectrum
  - Only requires sparse MATVEC
- Subspace iteration
  - $Y = p_k(H)X$
  - $X \leftarrow \mathrm{orth}(Y)$

  Repeat until "convergence"
- Use complementary subspace technique to reduce the Rayleigh-Ritz calculation cost
- Implemented in DGDFT





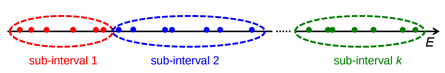


system	# of atoms (electrons)	Matrix size	# of cores (used in sub)	CheFSI (subspace)
Electrolyte3D	8,586 (28,808)	343,440	34,560 (3,456)	34 (19)
SiDiamond3D	8,000 (32,000)	320,000	34,560 (3,456)	40 (24)
Graphene2D	11,520 (23,040)	230,400	27,648 (4,608)	35 (27)
CuFCC3D	4,000 (44,000)	140,000	30,000 (3,000)	75 (46)
LiBCC3D	27,648 (82,944)	1,382,400	38,880 (12,960)	180 (165)

Spectrum slicing

Motivation: Reduce Rayleigh-Ritz calculation cost for the projected problem

Strategy: Divide the spectrum into subintervals and compute eigenvalues within each interval simultaneously



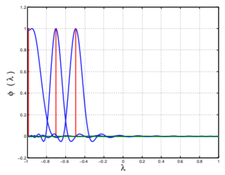
How to split the spectrum

- Estimate distribution of eigenvalues (spectral density, DOS) (L. Li 2016.)
- Depends on architecture, sparse solver efficiency

Interior eigenvalue solver

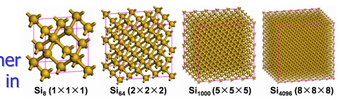
- Bandpass polynomial filter (Saad et al 2017)

Post-processing to eliminate duplicates and catch missing eigenvalues

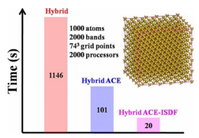


FAST Eigensolver for Hybrid Functional DFT

- Construct low rank approximation to V_X through interpolative separable density fitting (ISDF)
- Use adaptive exchange compressing (ACE) to further reduce the cost of applying V_X to occupied orbitals in an iterative diagonalization procedure
- Robust and efficient DIIS for SCF without constructing full Hamiltonian or density matrices

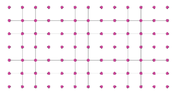


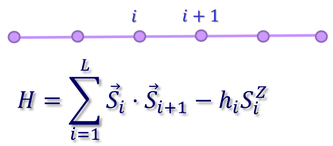
Methods / Systems	ACE HSE06 (LOBPCG) E_{HF}	ACE HSE06 (LOBPCG) E_{tot}	Conventional HSE06 (LOBPCG) E_{HF}	Conventional HSE06 (LOBPCG) E_{tot}
Si_{64}	-13.541616 (10^{-6})	1.488335	-13.541629	1.488352
Si_{216}	-45.471192 (10^{-7})	1.449790	-45.471190	1.449790
Si_{512}	-107.698011 (10^{-7})	1.324901	-107.698016	1.324902
Si_{1000}	-210.300628 (10^{-8})	1.289162	-210.300524	1.289128



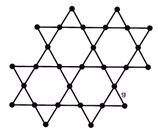
Tensor Eigenvalue Problem

- Spin model





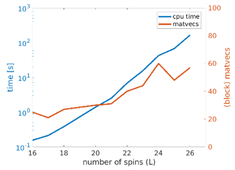
$$H = \sum_{i=1}^{L} \vec{S}_i \cdot \vec{S}_{i+1} - h_i S_i^Z$$

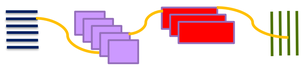


- Hamiltonian with tensor product structure

$$H = \left[\sum_{i=1}^{L} I \otimes \cdots \otimes A_{i,i+1} \otimes I \cdots\right] + D$$

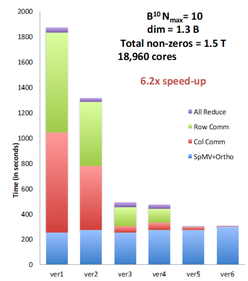
- Matrix-free solvers
  - LOBPCG
  - Polynomial filtering
- DMRG
  - Compact tensor train representation of the eigenvector
  - Alternating Energy minimization
  - Imaginary time evolution
  - Variational Monte Carlo (stochastic gradient descent)





Nuclear Configuration Interaction

- Eigenfunction approximation: $\Psi \approx \sum_a \Phi_a(r_1, r_2, \ldots, r_A)$, where Φ_a is a Slater determinant defined by a quantum number a that satisfy certain constraints
- $\hat{H}_{a,b} = \langle \Phi_a | H | \Phi_b \rangle$ is the sparse representation of Hamiltonian in the Φ_a basis
- Use iterative solver (Lanczos, LOBPCG) to compute a few lowest eigenstates of $\hat{H}$
  - Develop appropriate data distribution ($\hat{H}$ and vectors)
  - Reduce communication cost
  - Use block algorithms (e.g. locally optimal block preconditioned conjugate gradient)
  - Optimized local sparse matrix (block) vector multiplication
  - Good preconditioner
  - Hierarchical eigensolver with good starting guesses



Nonlinear Eigenvalue Problem

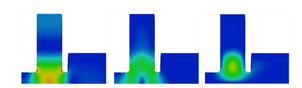
Application:

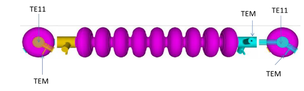
- Enable the computation of cavity resonant frequencies and damping modes for accelerator cavities with external waveguide coupling

$$\left(K - \lambda^2 M + i\sum_m \sqrt{\lambda^2 - k_{0m}^2}\, W_m^{TE} + i\sum_m \frac{\lambda^2}{\sqrt{\lambda^2 - k_{0m}^2}}\, W_m^{TM}\right) x = 0$$

Impact:

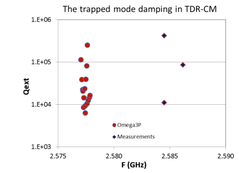
- This is the first time we are able to compute trapped modes damped in an ideal eight 9-cell SRF cavity cryomodule





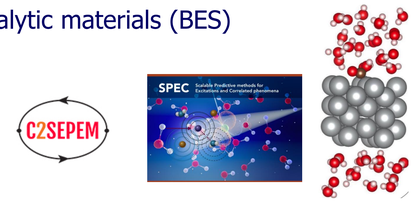
Techniques

- Rational approximation to the nonlinear terms
- Special linearization to turn the rational eigenvalue problem into a linear eigenvalue problem
- Compact scheme to represent the linearized operator and eigenvectors



Application List

- Electronic structure of catalytic materials (BES)
- Quantum materials (BES)
- NUCLEI (NP)
- C2SEPEM (CSM center)
- SPEC (CCS center)
- EFRC
- NWChemEX (ECP)



Future Plans

- Load balance in spectrum slicing
- Integration of spectrum slicing with application software (NWChemEX, PARSEC, DGDFT etc.)
- Hybrid OpenMP-MPI parallel implementation tensor eigenvalue solver
- A greedy hierarchical eigensolver for nuclear configuration interaction
- Port and optimize on KNL

More Information: http://www.fastmath-scidac.org or contact Chao Yang, LBNL, CYang@lbl.gov

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