FASTMath: Eigensolver Activities

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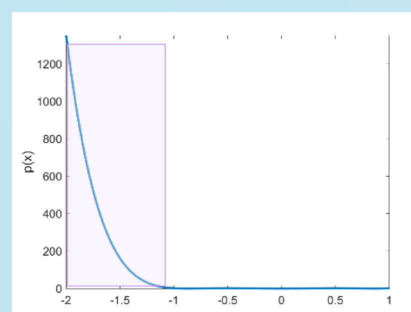
The FASTMath eigensolver team develops efficient algorithms for solving large-scale eigenvalue problems arising from a number of SciDAC applications. These algorithms exploit special structures of the application problems and use compact representations of operators and eigenfunctions. A variety of techniques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

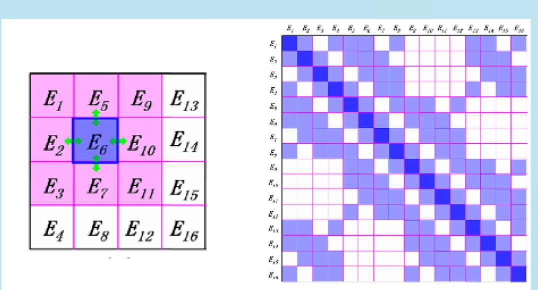
DFT electronic structure calculations

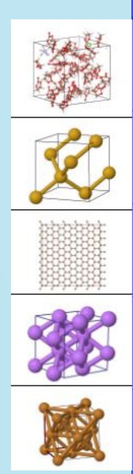
Chebyshev polynomial filtering

- Amplify low end of the spectrum
- Only requires MATVEC



- Use complementary subspace technique to reduce the Rayleigh-Ritz calculation cost
- Implemented in DGDFT

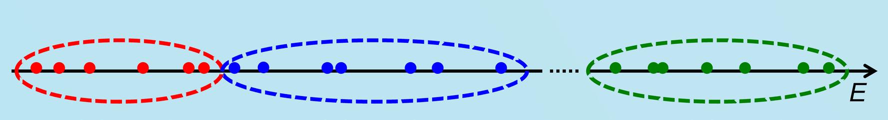




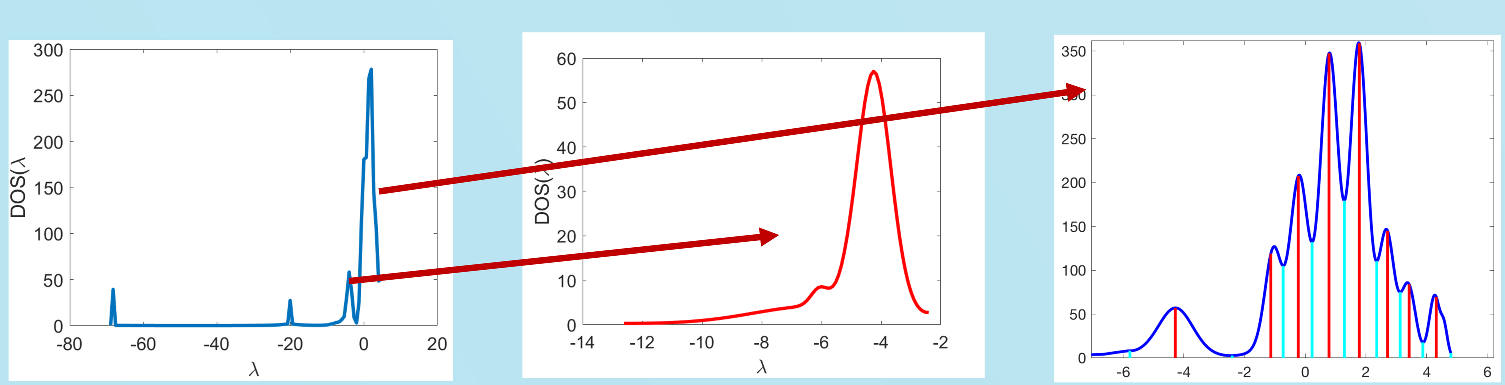
system	# of atoms	Matrix size	# of cores (in sub)	CheFSI (subspace)
Electrolyte3D	8,586 (28,808)	343,440	34,560 (3,456)	34 (19)
SiDiamond3D	8,000 (32,000)	320,000	34,560 (3,456)	40 (24)
Graphene2D	11,520 (23,040)	230,400	27,648 (4,608)	35 (27)
CuFCC3D	4,000 (44,000)	140,000	30,000 (3,000)	75 (46)
LiBCC3D	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, increase concurrency
- Strategy: Divide the spectrum into subintervals and compute eigenvalues within each interval simultaneously

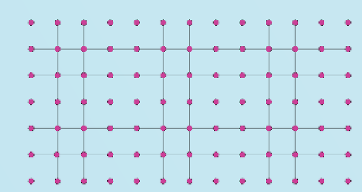


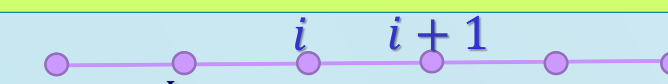
- How to split the spectrum (identify eigenvalue clusters)
  - Multi-resolution estimate distribution of eigenvalues (L. Lin, Y. Saad, C. Yang SIREV, 2016) by Lanczos
  - Apply K-means clustering to previous eigenvalue approximations
- Interior eigenvalue solver
  - Bandpass polynomial filter (Saad et al 2017)
  - Shift-invert subspace iteration



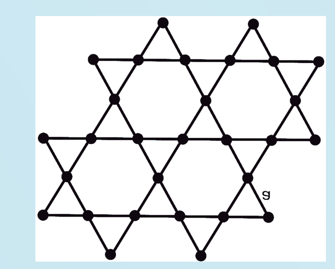
Tensor Eigenvalue Problem

Finite dimensional spin model





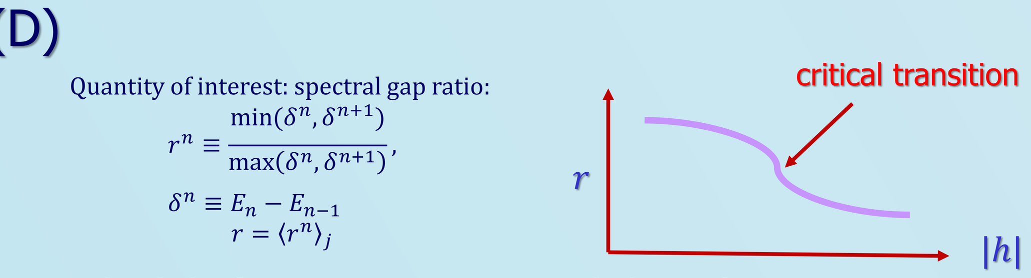
$$H = \sum_{i=1}^{L} \vec{S}_i \cdot \vec{S}_{i+1} - h_i S_i^Z$$



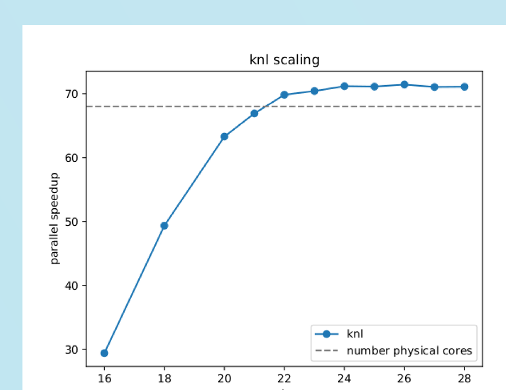
- Hamiltonian with tensor product structure

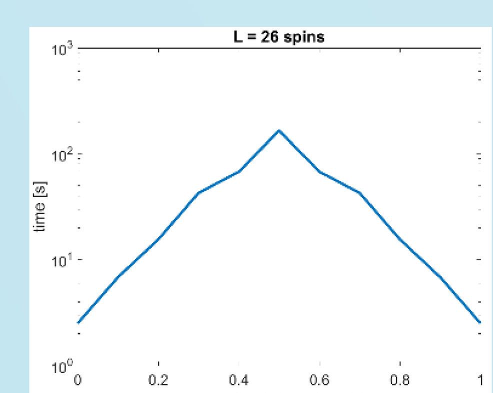
$$H = \left[\sum_{i=1}^{L} I \otimes \cdots \otimes A_{i,i+1} \otimes I \cdots\right] + D$$

- Challenge: compute many eigenvalues many times for different realizations (D)



- Previous approach (shift-invert Lanczos) has large memory footprint and poor scalability
- New iterative matrix-free solvers has excellent on-node performance on Cori KNL
  - LOBPCG applied to $(H - \sigma I)^2$
  - Block synchronous PCG preconditioner



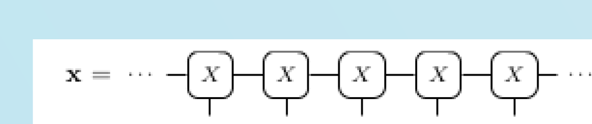


Infinite dimensional translational invariant spin model

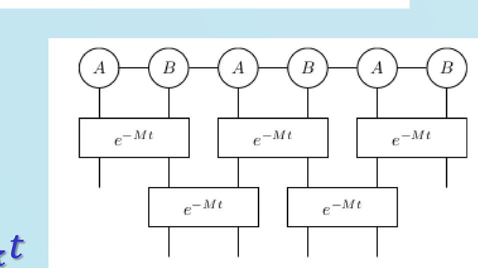
$$H = J \sum_{i=-\infty}^{\infty} \vec{S}_i \cdot \vec{S}_{i+1}$$

- Tensor ring representation (approximation) of the eigenvector

$$x(\cdots, i_{-1}, i_0, i_1, \cdots) \approx \mathrm{Trace}\left[\prod_{k=-\infty}^{\infty} X(i_k)\right]$$

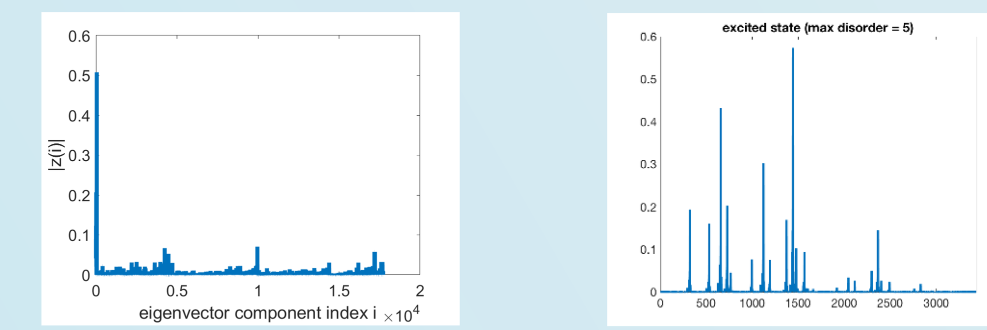


- Apply a flexible power method to e^{-Ht}
  - Use Trotter splitting to approximate e^{-Ht}
  - Separate the even/odd terms in $\prod_{k=-\infty}^{\infty} e^{-H_k t}$

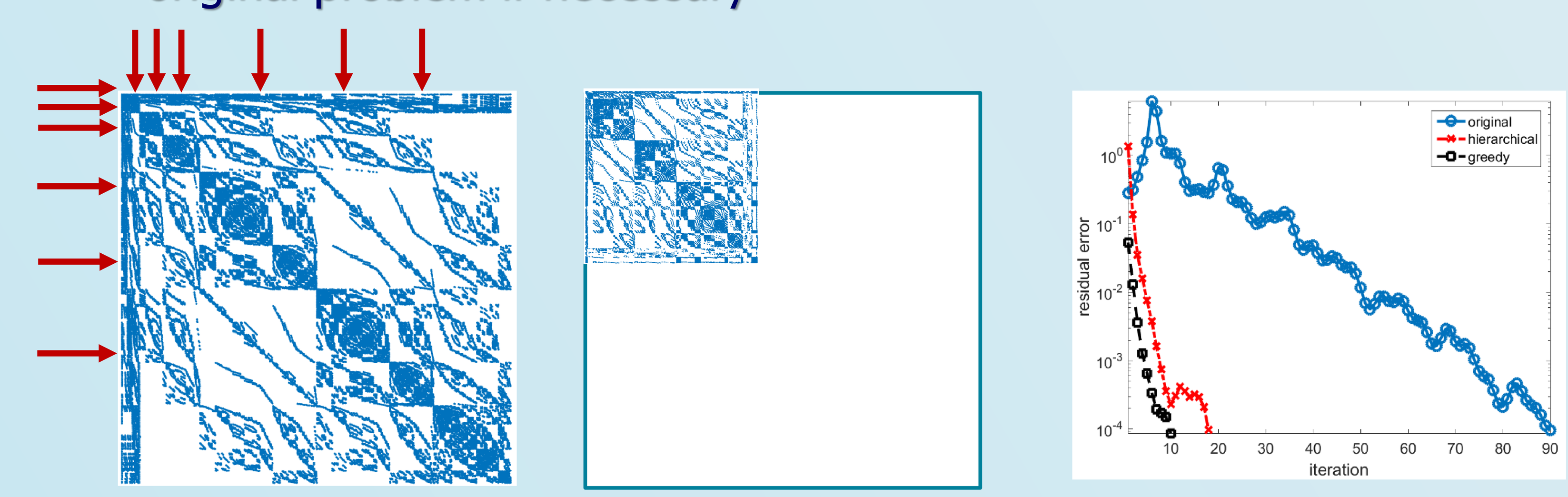


Greedy Algorithm for Localized Eigenvectors

- Eigenvectors of many large-scale eigenvalue problems exhibit localization properties (e.g. spin models with disorder, Anderson localization, configuration interaction models for molecules and nuclei)



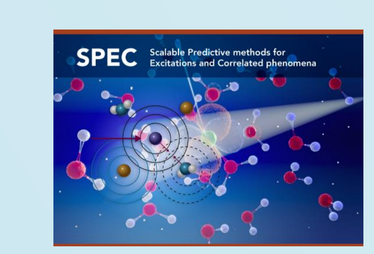
- Select "important" rows and column of the matrix to be diagonalized and solve a much smaller eigenvalue problem. The solution can be used to construct a good initial guess for the original problem if necessary.

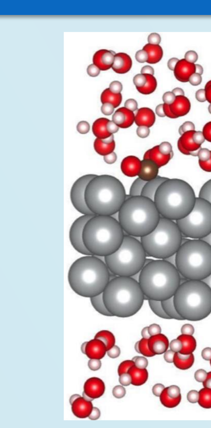


Application List

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

C2SEPEM





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