



Efficient Eigensolvers for SciDAC Applications

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Rensselaer



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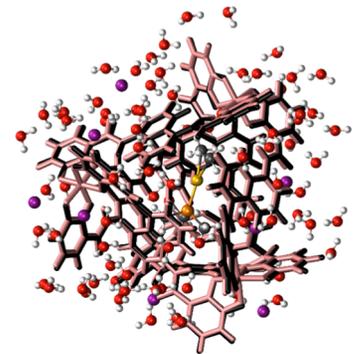


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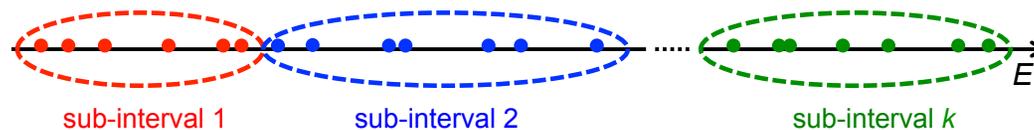
Overview

- **Technology Area: Eigensolver**
- **FASTMath Tasks**
 - Solving nonlinear eigenvalues from DFT based electronic structure calculations
 - Solving tensor eigenvalue problems
 - finite dimensional spin models with disorder
 - infinite dimensional spin models with translational invariance
 - Greedy algorithm for nuclear configuration interaction calculations
 - Model order reduction for linear response eigenvalue problem
- **Applications Impacted**
 - Enable computational chemist to study electronic properties of catalytic materials
 - Enable EFRC researchers to study localization and thermalization properties of quantum materials that depend on the interplay between many-body interaction and disorder
 - Enable material scientists to study thermodynamic limit of quantum materials
 - Enable nuclear physicists to have a better understanding of light nuclei
 - Enable chemists to simulate/predict optical properties of molecules/materials

Eigensolver for density functional theory based electronic structure calculations



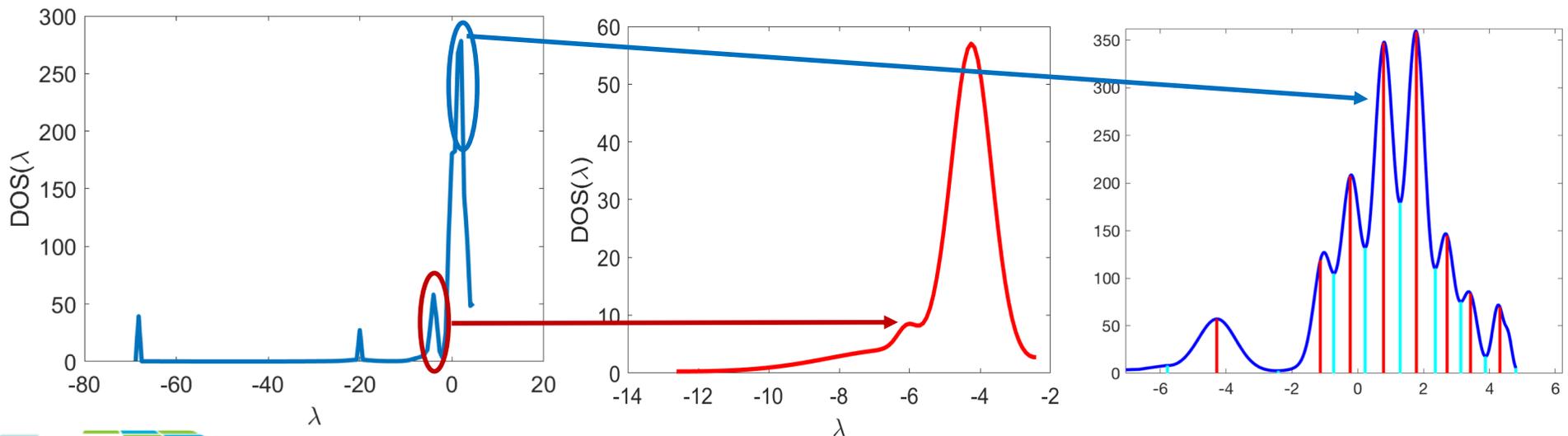
- Important for catalysis materials simulation
- $H(X)X = X\Lambda$, $X^T X = I$, $X \in \mathbb{C}^{n \times n_e}$
- Challenges
 - Need to compute many eigenpairs for large systems ($n_e \ll n$, but can still be large ($>10^5$), Rayleigh-Ritz becomes a bottleneck)
 - Be able to handle hybrid functionals (H is not sparse but has structure)
- Strategies
 - Break the spectrum into slices (spectrum slicing)



- Reformulate as unconstrained minimization
- Use low rank approximation

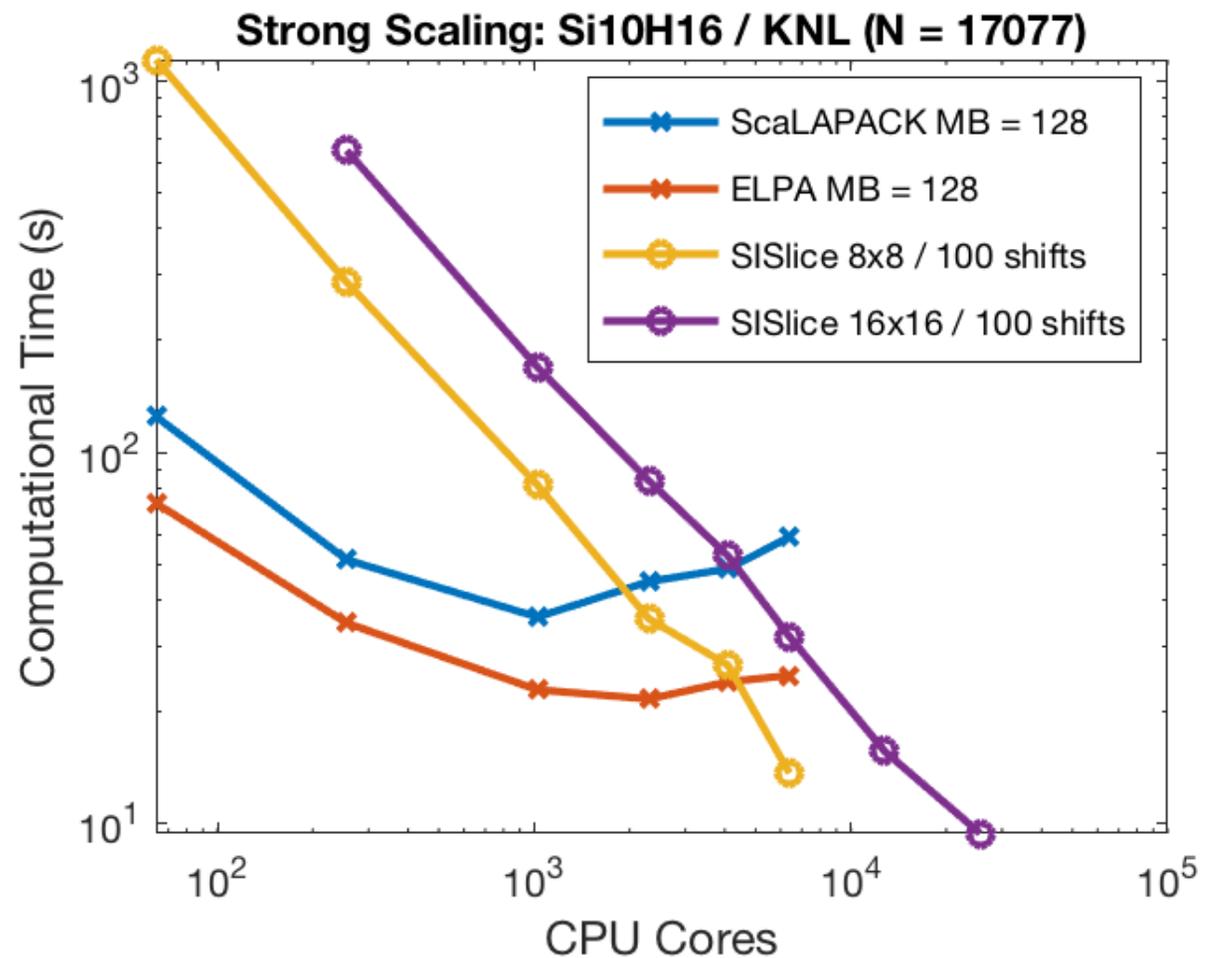
Spectrum partition for spectrum slicing

- How to partition the spectrum optimally when the spectrum is unknown?
 - Initial partition based on multi-resolution Lanczos density of state estimation
- How to adjust the partition when the matrix changes in a nonlinear (SCF) outer iteration
 - Subsequent partition based on K-means clustering



Spectrum Slicing Performance

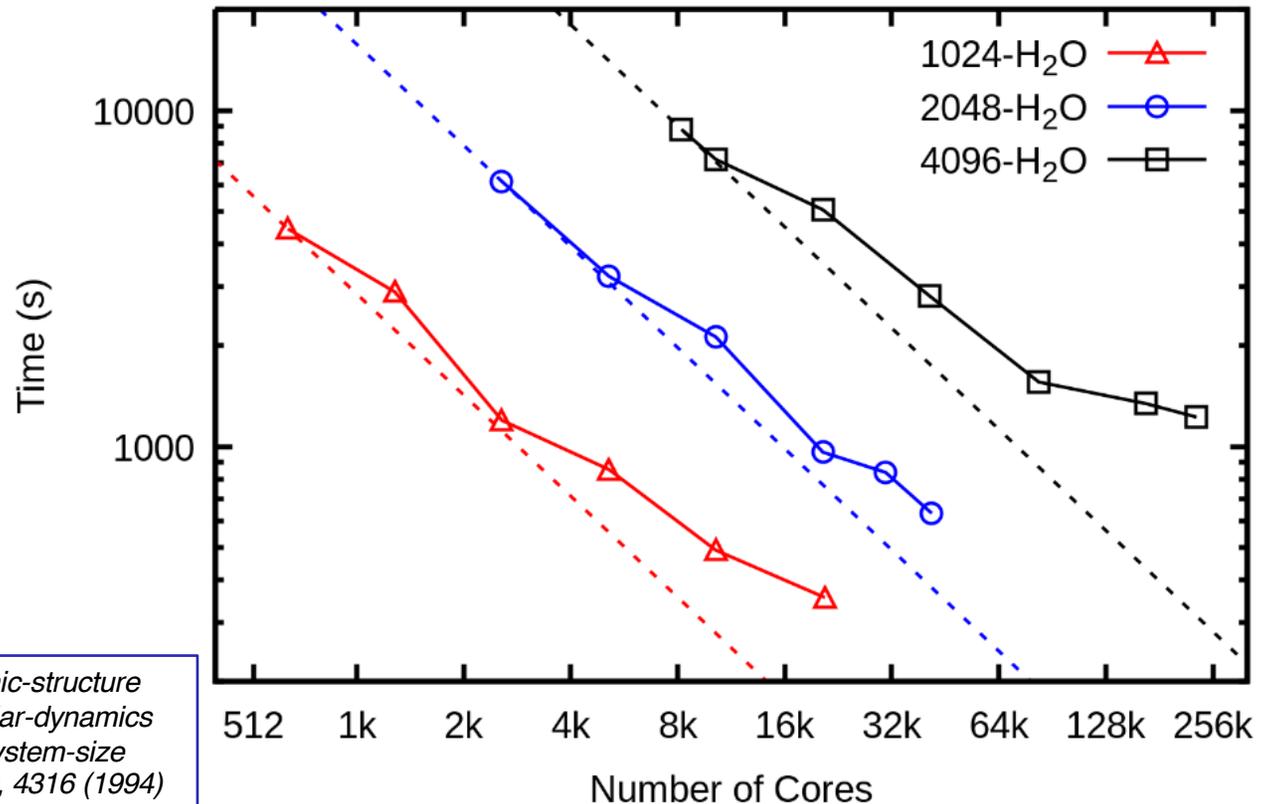
- Standard EVP
- $n = 17,077$
- Dense
- Compute all eigenpairs



Unconstrained CG-based eigensolver

- $\min_{\mathbf{X}} \text{Tr} [S^{-1} \mathbf{X}^T \mathbf{H} \mathbf{X}]$, $S = \mathbf{X}^T \mathbf{X}$, $\Psi = \mathbf{X} S^{-\frac{1}{2}}$
- Functional has same minimum as constrained functional, trial eigenvectors orthogonal at minimum

Strong scaling for bulk liquid water with 1024, 2048 and 4096 molecules, with the preconditioner that leads to the fastest time to solution (38% of the full machine for the largest system).



Mauri and Galli, Electronic-structure calculations and molecular-dynamics simulations with linear system-size scaling, Phys. Rev. B 50, 4316 (1994)

Tensor Eigenvalue Problem

- Many-body eigenvalue problem formulated in Fock (tensor product) space via second quantization

$$\mathcal{H} = \sum_{p,p'} h(p,p') a_p^\dagger a_{p'} + \frac{1}{2} \sum_{p,q,p',q'} \langle pq || p'q' \rangle a_p^\dagger a_q^\dagger a_{p'} a_{q'}$$

- Natural formulation for quantum computing
- Allow compact representation of the operator and the eigenvector in tensor product space
- Efficient algorithms such as density matrix renormalization group (DMRG) can be used to compute desired eigenpairs

Eigenvalues of a disordered spin chain

- Heisenberg Spin model with random disorder h_i :

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


The diagram shows a horizontal line representing a 1D spin chain with several light blue circular sites. Two sites are specifically labeled 'i' and 'i+1' below the line. A light blue arrow points from the text $h_i S_i^z$ in the equation above to the site labeled 'i'.

- Tensor Eigenvalue Problem $H\psi = \lambda\psi$,

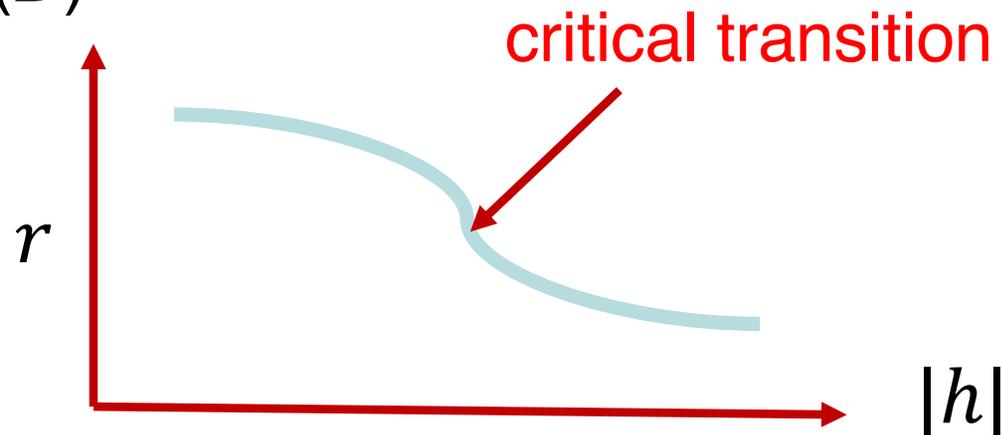
$$H = \left[\sum_{i=1}^{L-1} I \otimes \dots \otimes I \otimes M_i \otimes I \otimes \dots \otimes I \right] + D$$

- Need to compute many eigenvalues many times for different realizations of h_i (D)

Adjacent gap ratio:

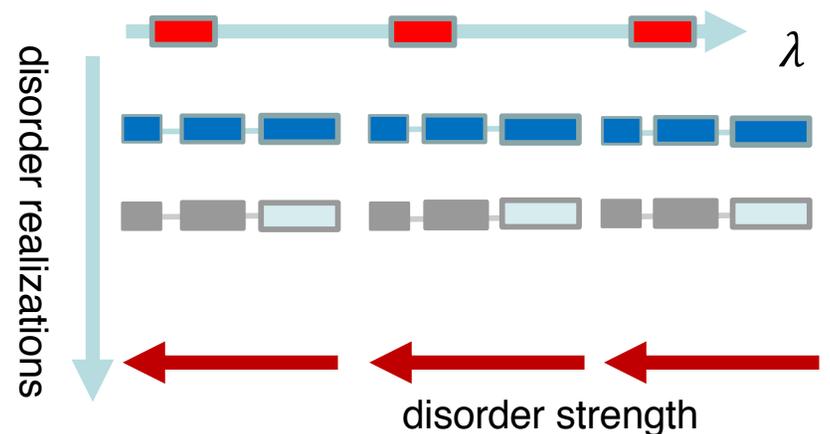
$$r^n = \frac{\min(\Delta^n, \Delta^{n+1})}{\max(\Delta^n, \Delta^{n+1})}$$

$$\Delta^n = \lambda_n - \lambda_{n-1}$$



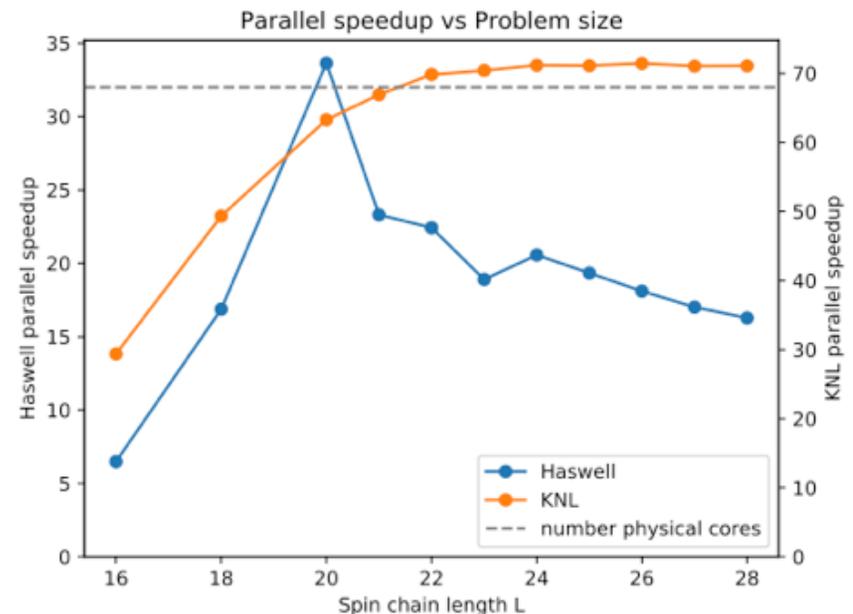
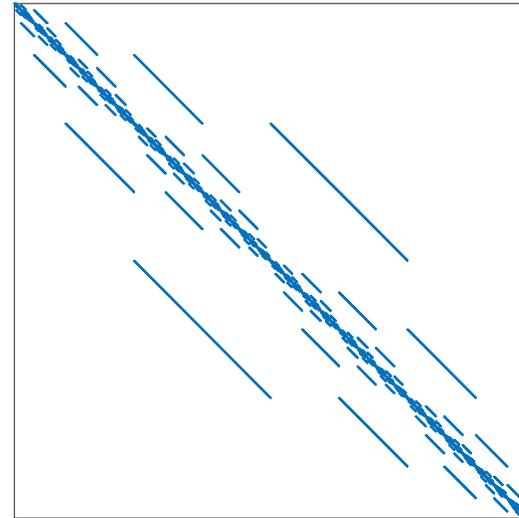
Iterative solution of tensor eigenvalue problem

- Problem dimension: $\binom{L}{L/2}$, e.g. $L = 34$ yields 2.3×10^9
- The larger the problem, the more clustered interior eigenvalues are
- New approach:
 - Use LOBPCG to compute the largest eigenvalues of $(H - \sigma_i I)^2$
 - Precondition by solving $(H - \sigma_i I)^2 x = b$ with PCG
 - Multiple linear systems solved simultaneously
 - Matrix-free Hx block-matvec
 - Multiple levels of concurrency



Results and performance

- Can perform each calculation (one realization of one disorder strength for one eigenvalue region with 32 eigenvalues) on a single node for up to $L = 28$
- Cori single KNL node:
 - 68 cores @ 1.4 GHz
- Typically 10-100 iterations of LOBPCG (depending on number of PCG iterations) to reach 10^{-6} accuracy in eigenvalue
- For larger L , vectors need to be distributed among different nodes (in progress)



Infinite dimensional tensor eigenvalue problem

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



- Solve $Hx = \lambda x$, where

$$H = \sum_{i=-\infty}^{\infty} \cdots \otimes I \otimes M_i \otimes I \otimes \cdots$$

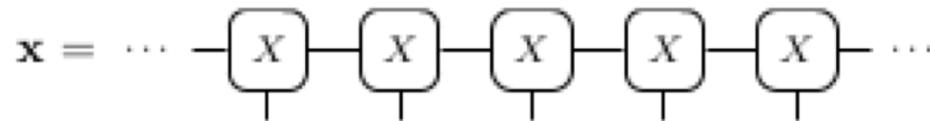
- Interested in the lowest eigenvalue (in average sense)
- Enable scientists to understand the thermodynamic limit of many-body models
- Can start with a finite model with L spins and gradually increase L , but limited to modest L (<100)
- Better to take the translational invariance nature of H

Tensor ring representation of eigenvector

- Eigenvector x is an infinite dimensional tensor
- Take advantage of translational invariance by using compact representation: each element can be approximated by

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

where $X(i_k)$ is an $r \times r$ matrix, where r is the rank.



- Related to tensor train

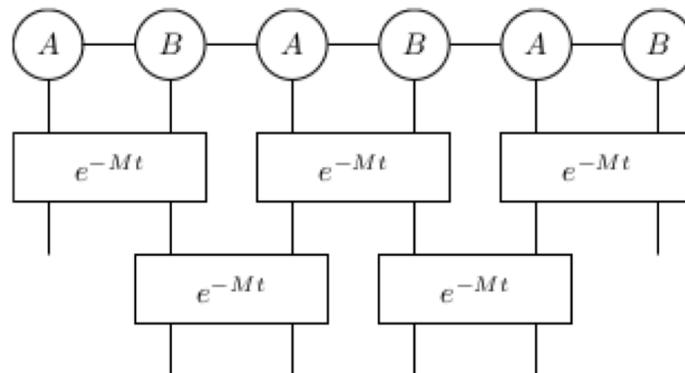
Matrix exponential and flexible power iteration

- Compute the smallest eigenvalue (ground state) of H by computing the largest eigenvalue of e^{-Ht} for some “small” t using the power method
- Need to multiply e^{-Ht} with a tensor ring approximation of x efficiently and preserve the tensor ring structure
 - Use Trotter splitting to approximate

$$e^{-Ht} \approx \prod_{k=-\infty}^{\infty} e^{-H_k t}$$

where $H_k = \dots I \otimes M \otimes I \dots$ and $e^{-H_k t} = \dots I \otimes e^{-Mt} \otimes I \dots$

- Separate the even/odd terms in $\prod_{k=-\infty}^{\infty} e^{-H_k t}$



contraction diagram

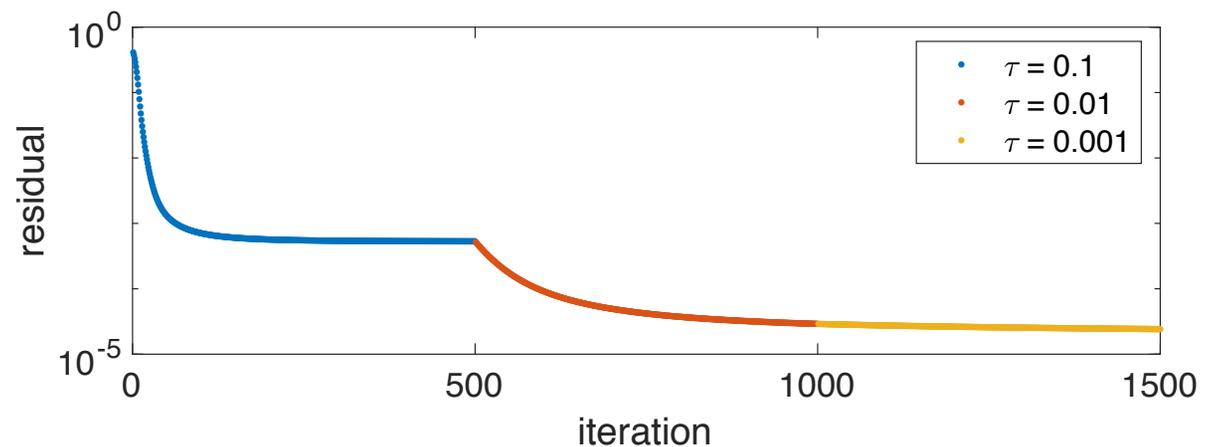
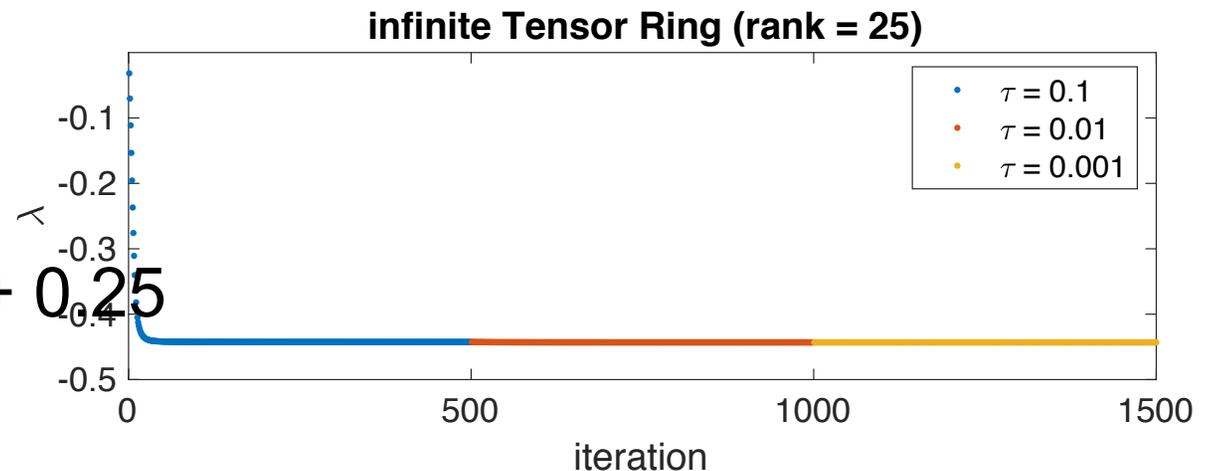
Convergence

- Heisenberg spin model

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

- Exact solution:

$$\lambda = -\log(2) + 0.25$$

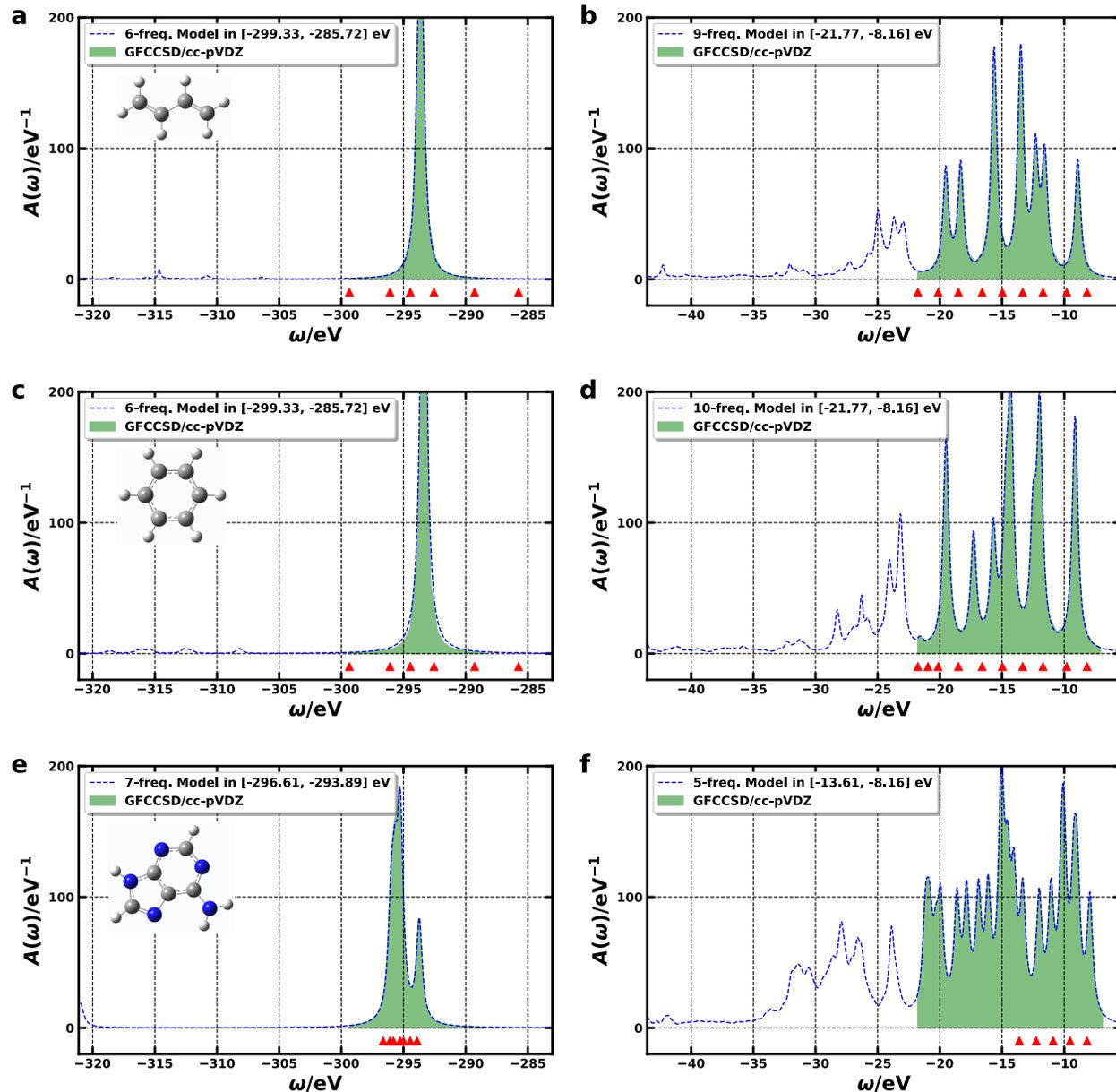


Model Order Reduction for Linear Response Eigenvalue Problem

- Green's Function Coupled Cluster Method
 - Powerful many-body tool for computing and analyzing the electronic structure of molecules
 - Avoid solving large eigenvalue problems
 - Require many different large linear system solves
- Model Order Reduction
 - Construct linear dynamical system s.t. transfer function corresponds to Green's function
 - Project large system onto subspace
 - Building subspace only requires a few large system solves

Model Order Reduction for Linear Response Eigenvalue Problem

Spectral functions of the 1,3-butadiene, benzene, and adenine molecules in the core and valence energy regimes directly computed by the conventional GFCCSD method (green shadow) and interpolated and extrapolated by their reduced order models (blue dashed line) with $\eta = 0.027$ eV and $\Delta\omega \leq 0.027$ eV.



Collaboration with applications

- SciDAC Partnership

- BES SciDAC on catalysis simulation (electronic structure calculations, nonlinear eigenvalue problem)
- NP SciDAC on light nuclei structure: large-scale configuration interaction calculation (many-body eigenvalue problem)

- Non-SciDAC

- BES EFRC (J. Moore): tensor eigenvalue problem (many-body localization, tensor ring approximation)
- BES Computational Materials Science (S. Louie): linear response eigenvalue problem
- BES Computational Chemical Science (X. Sortiris): linear response eigenvalue, model order reduction



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Spectrum estimation by Lanczos

- Regularize the DOS to make it smooth:

$$f(t) = \sum_{i=1}^n \delta(t - \lambda_i) \approx \frac{1}{\gamma} \sum_{i=1}^n e^{-(t-\lambda_i)^2/\sigma_i^2}$$

- k-step Lanczos tridiagonalization ($k \ll n$)

$$HV_k = V_k T + f e_k^T, \quad V_k^T V_k = I, \quad V_k^T f = 0$$

- Solve a small dimensional eigenvalue problem $T q_j = \theta_j q_j$
- Approximate DOS:

$$f(t) = \sum_{j=1}^k \tau_j^2 e^{-(t-\theta_j)^2/\sigma_j^2}, \quad \text{where } \tau_j = e_1^T q_j$$

- Cumulative DOS (CODS):

$$g(t) = \int_{-\infty}^t f(s) ds = \frac{\sqrt{\pi}}{2} \sum_{j=1}^k \zeta_j^2 \sigma_j \left[\operatorname{erf} \left(\frac{t-\theta_j}{\sigma_j} \right) + 1 \right]$$