C34.6

APS MARCH MEETING

MARCH 05, 2018

TEXAS
The University of Texas at Austin

USING SPECTRUM SLICING METHOD TO SOLVE THE KOHN-SHAM PROBLEMS FOR LARGE SYSTEMS

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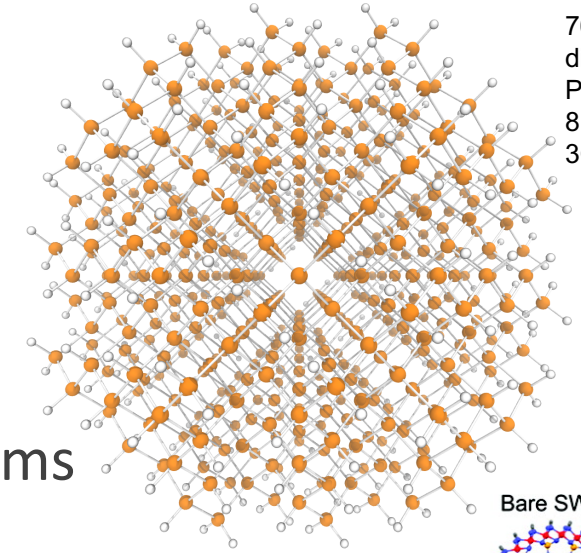
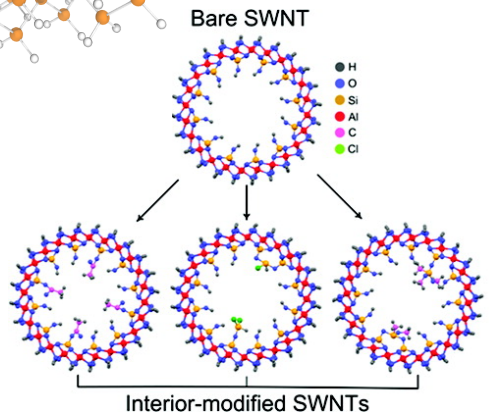
Motivation

- Silicon nanocrystals
  - Optoelectronics
  - 10 nm in diameter ~ 30,000 atoms
- Inorganic nanotubes
  - Catalysis
  - Water desalination
  - 20 nm in length ~ 5,000 atoms



765 atoms
dim. of H = 351,195
PARSEC
8 cores of Intel Xeon 3GHz, ~ 1 hour

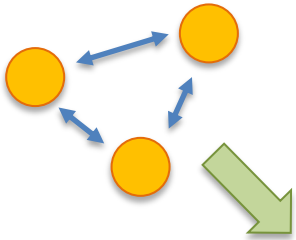


[1] D.-Y. Kang, J. Zang, C. Jones, S. Nair, Single-Walled Aluminosilicate Nanotubes with Organic-Modified Interiors, *J Phys Chem C* **115**, 7676–7685 (2011).

PARSEC

http://parsec.ices.utexas.edu

Pseudopotential
Algorithm for
Real-
Space
Electronic Structure
Calculation

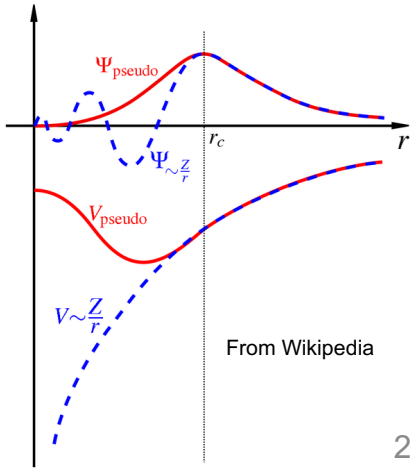


1. Kohn–Sham Density Functional Theory
   - *N* interacting electrons -> *N* independent e's

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{eff}}(r)\right]\varphi_i(\boldsymbol{r}) = \varepsilon_i\varphi_i(\boldsymbol{r})$$

$$V_{\text{eff}}(\boldsymbol{r}) = V_{\text{ext}}(\boldsymbol{r}) + V_{\text{Hartree}}[n] + V_{\text{XC}}[n] \qquad n(r) = \sum_i f_i|\varphi_i(r)|^2$$

2. Pseudopotential Theory
   - All electrons -> Only valence electrons



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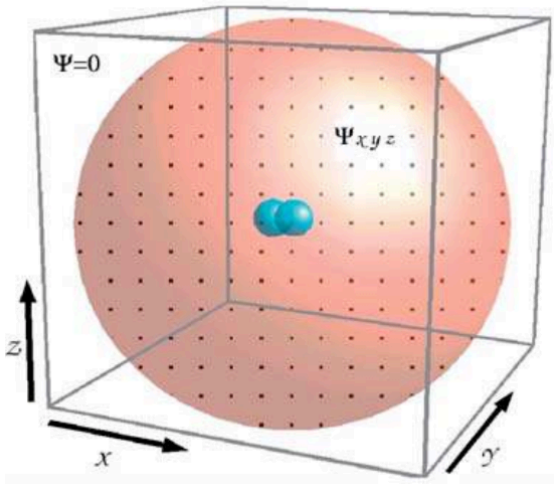


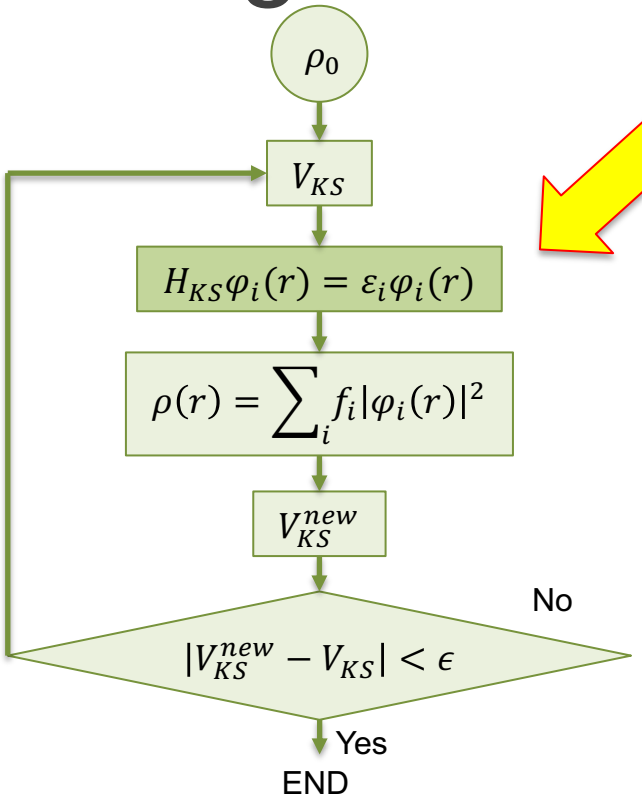
3. Real grids as the basis for wave functions
   - Finite difference method
   - Ease of implementation
   - Suitable for confined systems (defects, charged)

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{eff}}(r)\right]\varphi_i(\boldsymbol{r}) = \varepsilon_i\varphi_i(\boldsymbol{r})$$

$$\left(\frac{\partial^2\varphi_i}{\partial x^2}\right)_{x_0} \approx \sum_{n=-N}^{N} C_i\varphi_i(x_0 + nh, y, z)$$

[1] L. Kronik *et al.*, PARSEC – the pseudopotential algorithm for real-space electronic structure calculations: recent advances and novel applications to nano-structures, *Phys Status Solidi B* **243**, 1063–1079 (2006).

Solving the Kohn-Sham Equations



Key to large systems:
An efficient eigensolver

Chebyshev-filtered Subspace Iteration

- **Filtering**
- **(Distributed) Rayleigh-Ritz Procedure**

Filtering

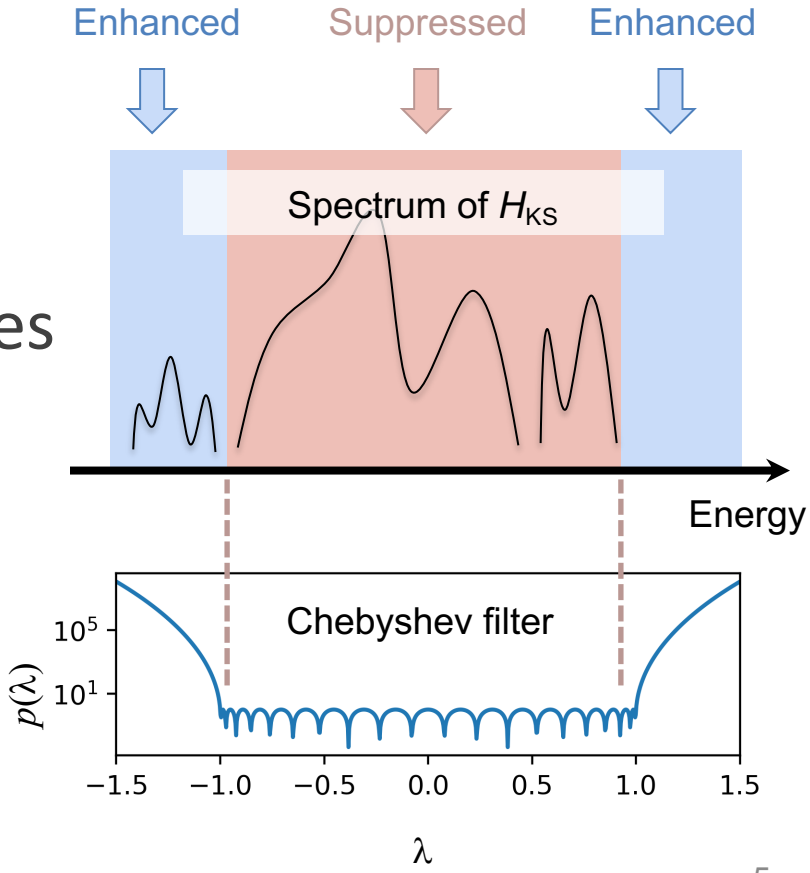
- Enhance the subspace constituting the occupied states

$\tilde{p}(H_{\mathrm{KS}})$: Chebyshev polynomial of H_{KS}
v: a state
u_i: eigenstates
λ_i: eigenvalues

$$\tilde{p}(H_{\mathrm{KS}})v = \tilde{p}(H_{\mathrm{KS}})\sum_{i=1}^{n} c_i u_i = \sum_{i=1}^{n} c_i \tilde{p}(H_{KS})u_i = \sum_{i=1}^{n} p(\lambda_i)c_i u_i$$

Expand v in terms of eigenstates

Operate the polynomial of H_{KS} to each eigenstate



(Distributed) Rayleigh-Ritz Procedure

- Generate approximate eigenpairs from a subspace

Algorithm 1: The Rayleigh–Ritz method

Input: Orthonormal basis, $V \in \mathbb{C}^{N\times m}$, and the Hamiltonian matrix, $H \in \mathbb{C}^{N\times N}$
Output: Approximate eigenpairs (ψ_i, λ_i) and their Ritz residuals, σ_i

$R = V^{\mathrm{H}} H V$; // form Rayleigh quotient matrix, $O(Nm^2)$
$Q^{\mathrm{H}} \Lambda Q = R$; // diagonalize R, $O(m^3)$
$\Psi = V Q$; // form Ritz vectors, $O(Nm^2)$
for $i = 1$ **to** m **do** // compute each residual, $O(Nm)$
  $\sigma_i = \|H\psi_i - \lambda_i \psi_i\|_2$
end

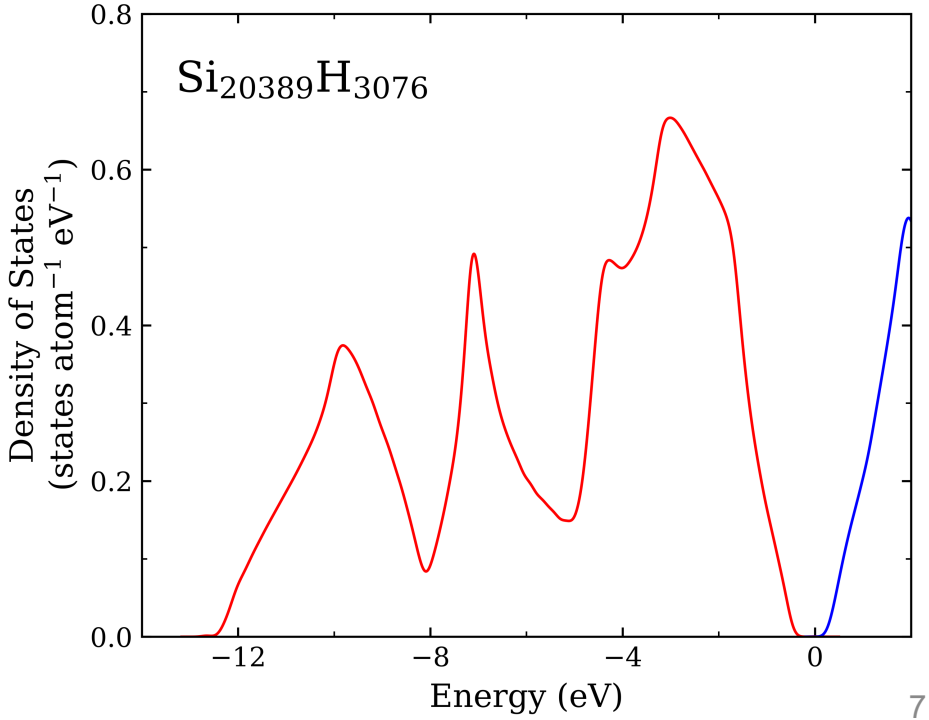
V and *R* are distributed to accommodate the increasing need for memory

Still need to diagonalize a smaller matrix

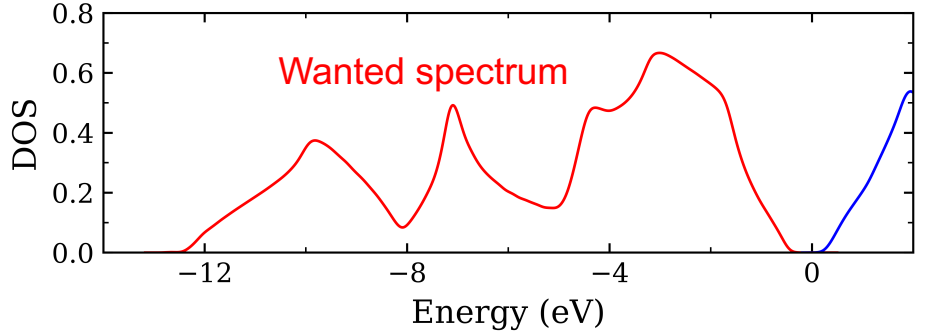
[1] G. Schofield, J. Chelikowsky, Y. Saad, A spectrum slicing method for the Kohn–Sham problem, *Comput Phys Commun* **183**, 497–505 (2012).

Results

- Electronic structure over 20,000 atoms
- Dim. of H = 5,353,944
- # of occ. states = 42,316
- Stampede2
  - Intel KNL
  - 17,408 cores



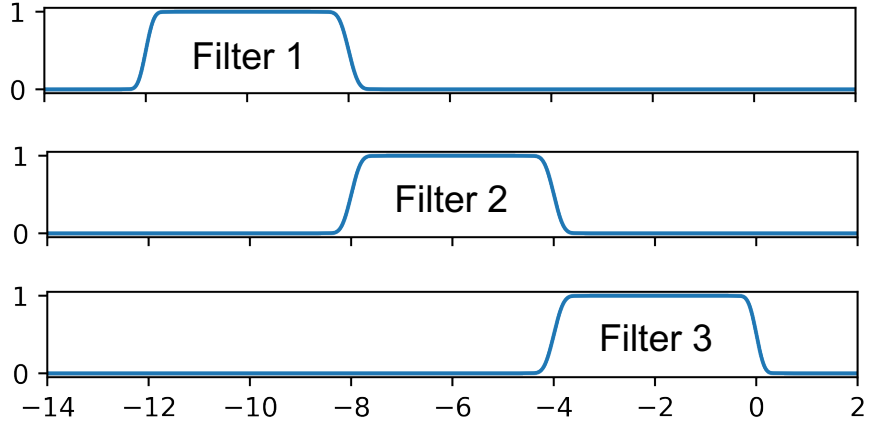
Spectrum Slicing Method



Slice 1

Slice 2

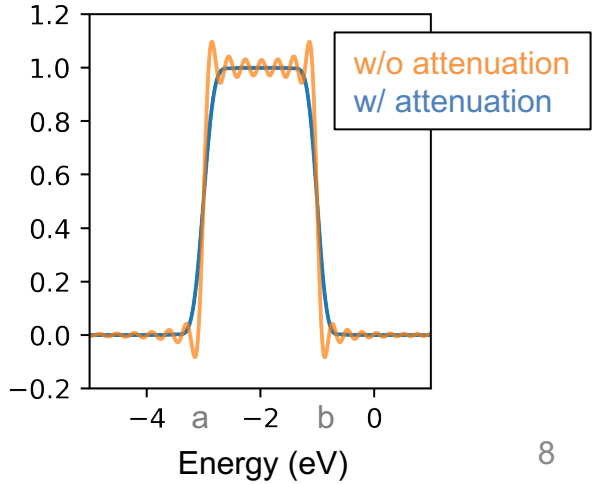
Slice 3



Chebyshev-Jackson filter

$$\tilde{p}(H_{\mathrm{KS}}) = \sum_{i=0}^{k} \gamma_i(a,b) g_i(k)\, T_i(H_{\mathrm{KS}})$$

$g_i(k)$: attenuation coefficient



Spectrum Slicing Method

1. Dividing the wanted spectrum into slices
2. Filtering out the spectrum individually
3. Solving eigenpairs individually

} Could be parallelized!

- Shifting the burden of diag. to cheaper filtering.
  - Diagonalization in Rayleigh-Ritz is $O(m^3) \sim O(N^3)$
  - Filtering is $O(Nmk) \sim O(N^2)$

N: # of grid points
m: # of states
k: degrees of filters

Identifying Duplicate Eigenpairs

- Approximate eigenpairs from Rayleigh-Ritz procedure

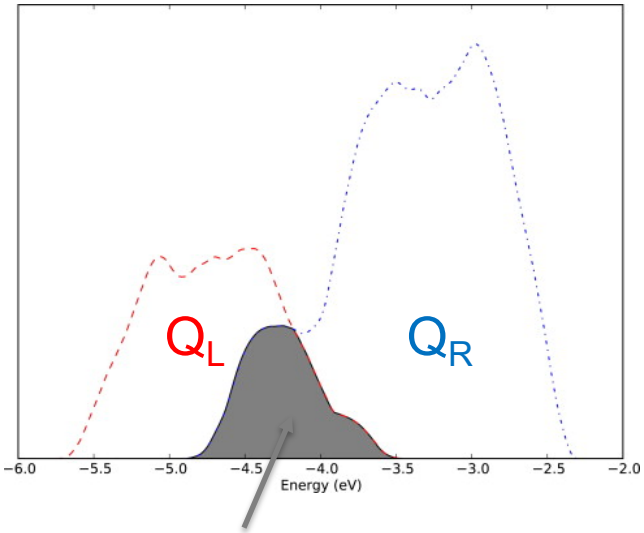
  Ritz value $\mu_i = \varphi_i^H H_{KS} \varphi_i$

  Residual $\sigma_i = \|H_{KS}\varphi_i - \mu_i \varphi_i\|_2$

  Eigenpair location $(\mu_i - \sigma_i, \mu_i + \sigma_i)$

- Singular Value Decomposition

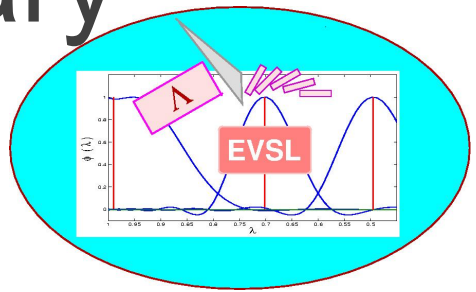
$$Q_L^H Q_R = U \Sigma V^H$$



[1] G. Schofield, J. Chelikowsky, Y. Saad, A spectrum slicing method for the Kohn–Sham problem, *Comput Phys Commun* **183**, 497–505 (2012).

EigenValues Slicing Library

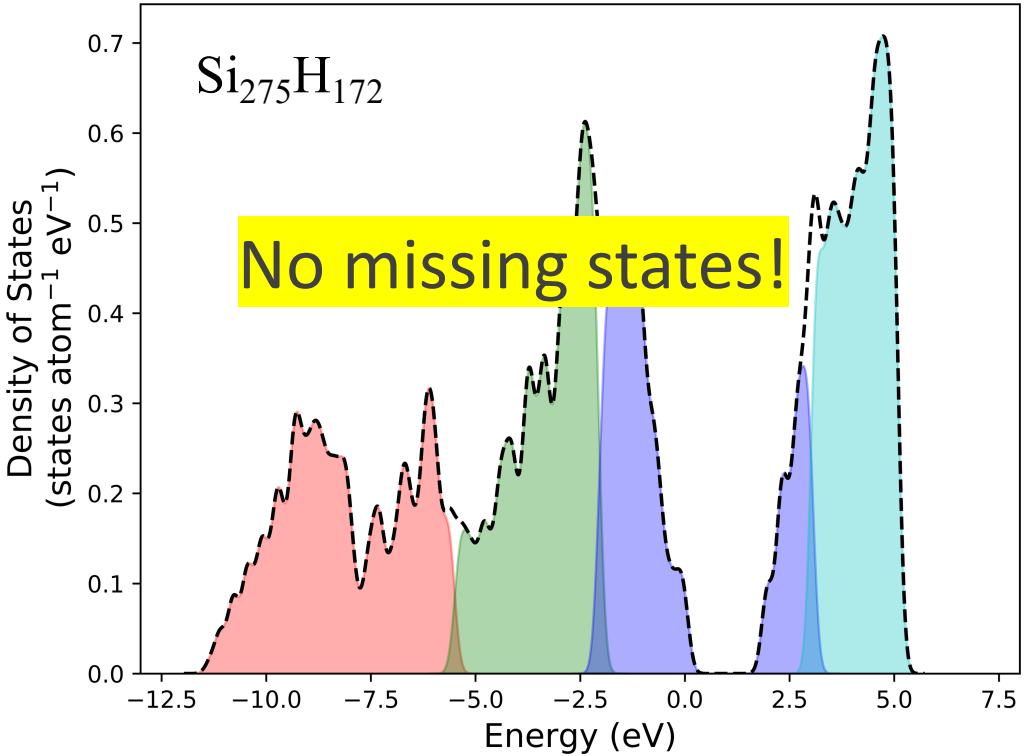
http://www-users.cs.umn.edu/~saad/software/EVSL/



- Spectrum slicing methods
  - Polynomial filtered subspace iteration
  - Polynomial filtered Lanczos with/without thick restart
  - Rational filtered Lanczos with/without thick restart
- Interfaces to various direct solvers
- Both standard and generalized eigenvalue problems
- Matrix-free format (user provides own matvec)

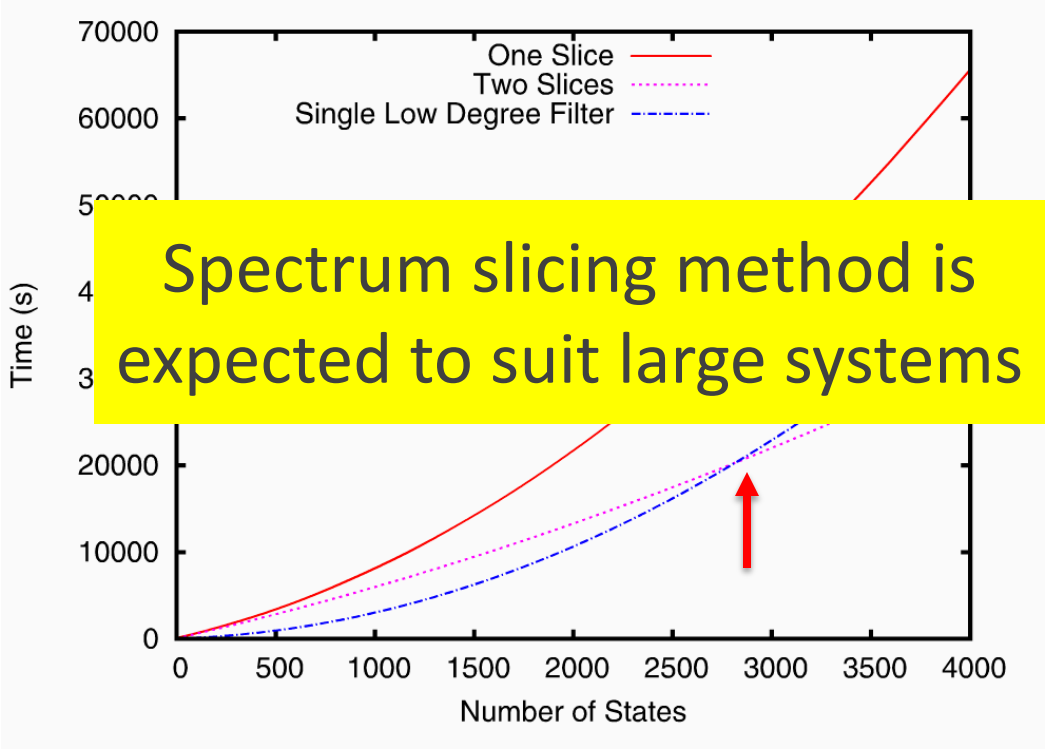
Results

Using EVSL, 1112 states, 4 slices



Results

Projection of the performance



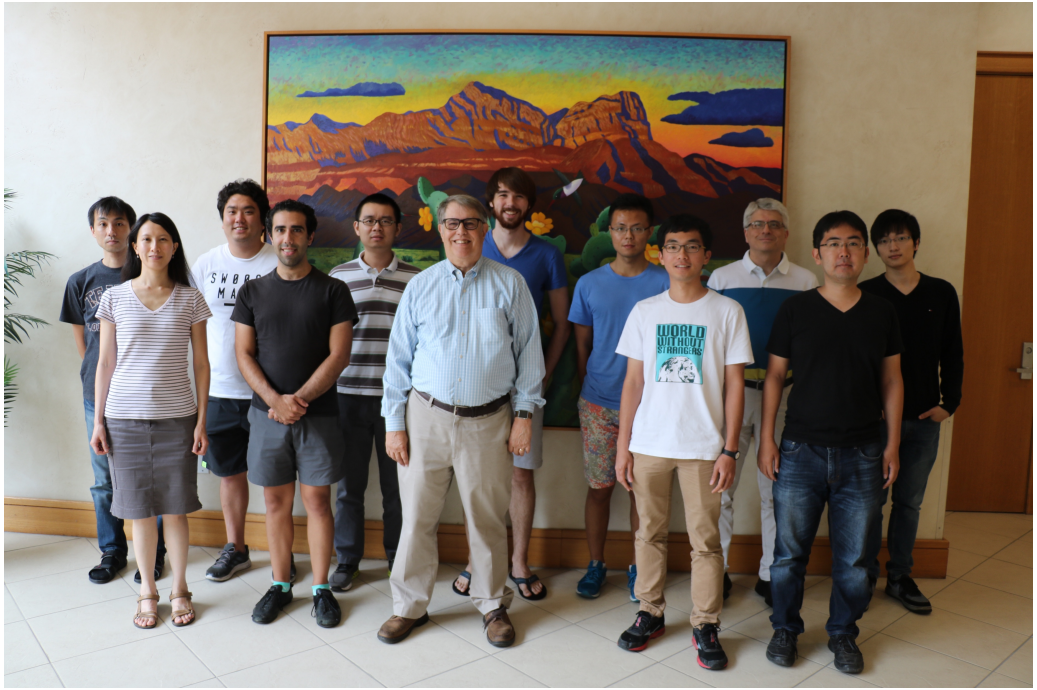
Spectrum slicing method is expected to suit large systems

[1] G. Schofield, J. Chelikowsky, Y. Saad, A spectrum slicing method for the Kohn–Sham problem, *Comput Phys Commun* **183**, 497–505 (2012).

Summary

- Electronic structure of a confined system with over 20,000 atoms was solved by Chebyshev-filtered subspace iteration (filtering + (distributed) Rayleigh-Ritz method)
- A spectrum slicing method is proposed for large electronic structure calculation

Acknowledgement



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