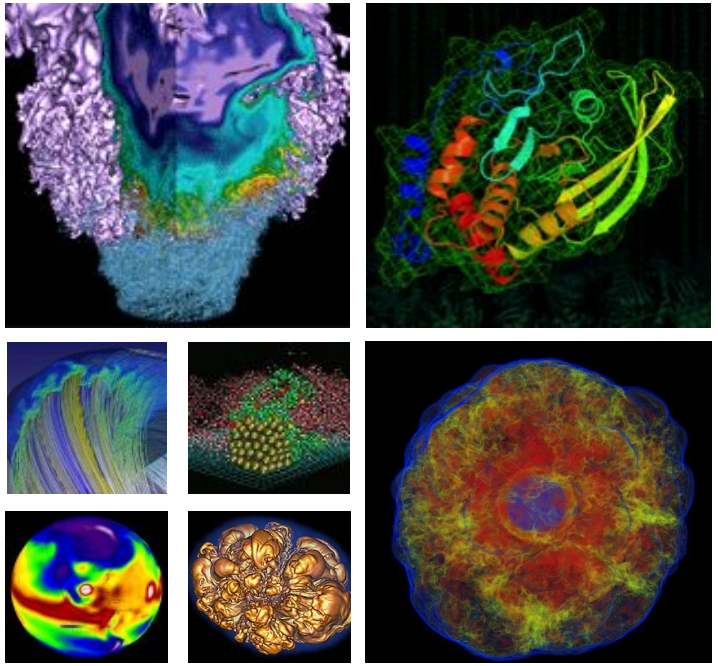
Eigenproblems in MBPT and Practical Considerations



Jack Deslippe
NERSC

U.S. DEPARTMENT OF ENERGY | Office of Science

Who am I?

Jack Deslippe

- NERSC Application Performance Group Lead
- One of Lead Developers in BerkeleyGW project (C2SEPEM)
- US Exascale Computing Project Applications (ECP) Area Lead for Materials Sci. and Chemistry

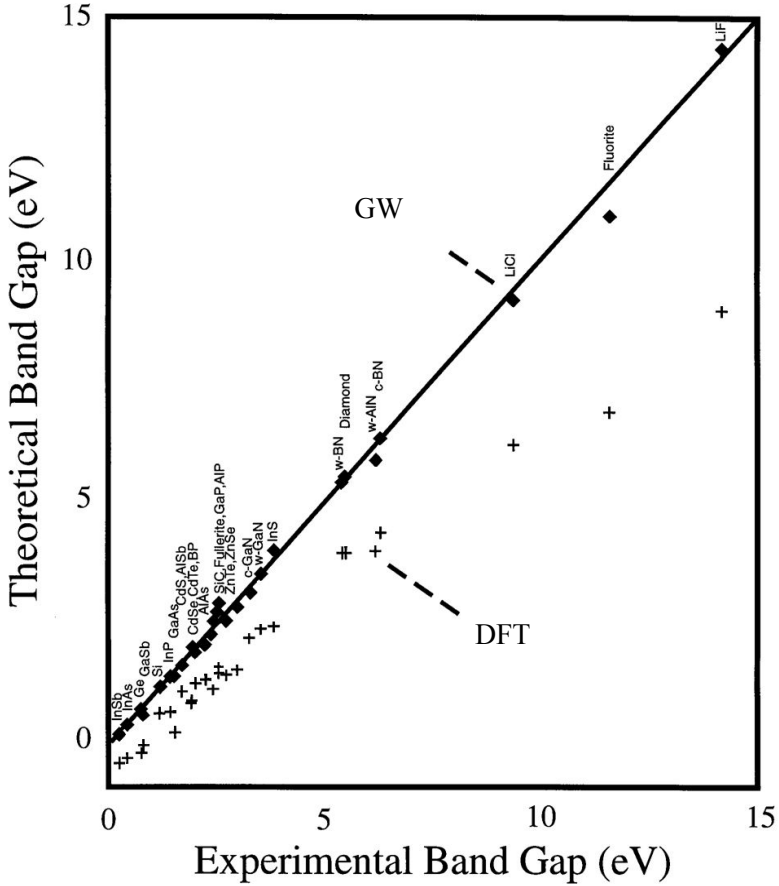
What is GW

$$[E_{n\mathbf{k}} - H_0(\mathbf{r}) - V_H(\mathbf{r})]\,\psi_{n\mathbf{k}}(\mathbf{r}) - \int \Sigma(\mathbf{r},\mathbf{r}',E_{n,\mathbf{k}})\psi_{n\mathbf{k}}(\mathbf{r}')d\mathbf{r}' = 0$$

The “GW” method is an accurate approach to compute the “**excited state**” properties of materials through Dyson equation (Σ=iGW). Examples:

- What happens when you add or remove an electron from a system
- How do electrons behave when you apply a voltage
- How does the system respond to light or x-rays

GW is complementary to the widely used density functional theory methods (DFT) which predict ground state properties of materials



GW Reputation

$$[E_{n\mathbf{k}} - H_0(\mathbf{r}) - V_H(\mathbf{r})]\,\psi_{n\mathbf{k}}(\mathbf{r}) - \int \Sigma(\mathbf{r}, \mathbf{r}', E_{n,\mathbf{k}})\psi_{n\mathbf{k}}(\mathbf{r}')d\mathbf{r}' = 0$$

The Good:

Quantitatively accurate for quasiparticle properties in a wide variety of systems.

Accurately describes dielectric screening important in excited state properties.

The Bad:

Prohibitively slow for large systems. Usually thought to cost orders of magnitude more time that DFT.

Memory intensive and scales badly. Exhausted by storage of the dielectric matrix and wavefunctions. Limited ~50 atoms.

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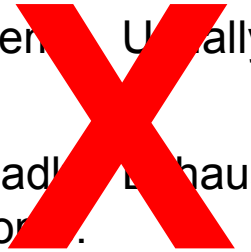


BerkeleyGW

BerkeleyGW

A massively parallel highly optimized "GW" material science

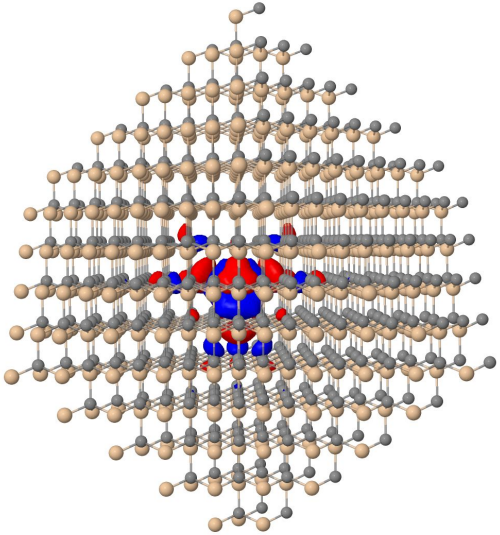
code that sits on top

of DFT codes like Quantum

ESPRESSO / PARATEC / PARSEC / SIESTA / Octopus / Abinit

Algorithms dominated by:

Dense Linear Algebra and Large Matrix/Tensor Reduction Loops, FFTs



SiC Diacancy Calculation.
Run on All of Cori

GW Example : Computational Bottlenecks

A. Compute transition probabilities for electrons between orbitals (N^3) (FFT)

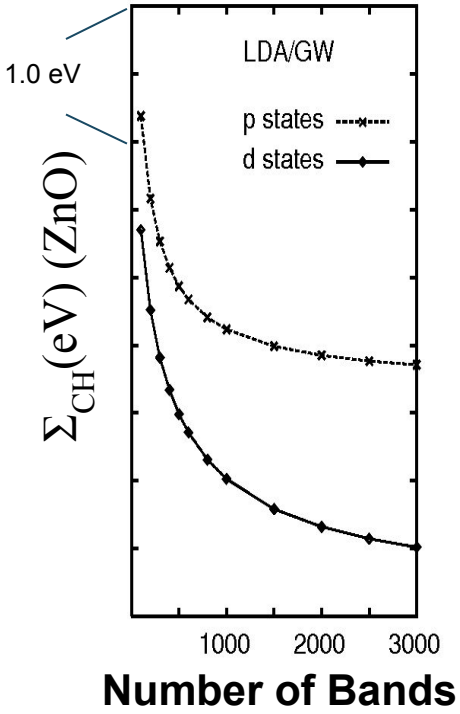
B. Sum (A) to form overall material response function (polarizability) (N^4) (ZGEMM)

C. Calculate interacting electron self energy in (N^4) (Hand Coded (GPP), ZGEMM (FF))

$$\chi^0_{\mathbf{G}\mathbf{G}'}(\omega) = \sum_{n}^{\text{occ}} \sum_{n'}^{\text{emp}} \left[M^{\mathbf{G}}_{nn'}\right]^* M^{\mathbf{G}'}_{nn'} \frac{1}{E_n - E_{n'} - \omega}$$

***M* are complex double-precision arrays representing transition probabilities between orbitals**
E_n are DFT orbital energies

Empty State Requirements



Lots of (empty) Orbitals Required. For meV accuracy 10%-100% necessary.

Typical DFT codes (QE, Abinit etc.) are not good at this! We find that when more than about 10% of eigenvalues are needed it is cheaper to use ScaLAPACK/ELPA to exactly diagonalize.

P. Zhang et al.

Empty State Requirements

Approximations We've Employed

1. Assume high-energy orbitals are just plane-waves.
   Not good. Properties of dielectric depend sensitively on orthogonality of Eigenfunctions.

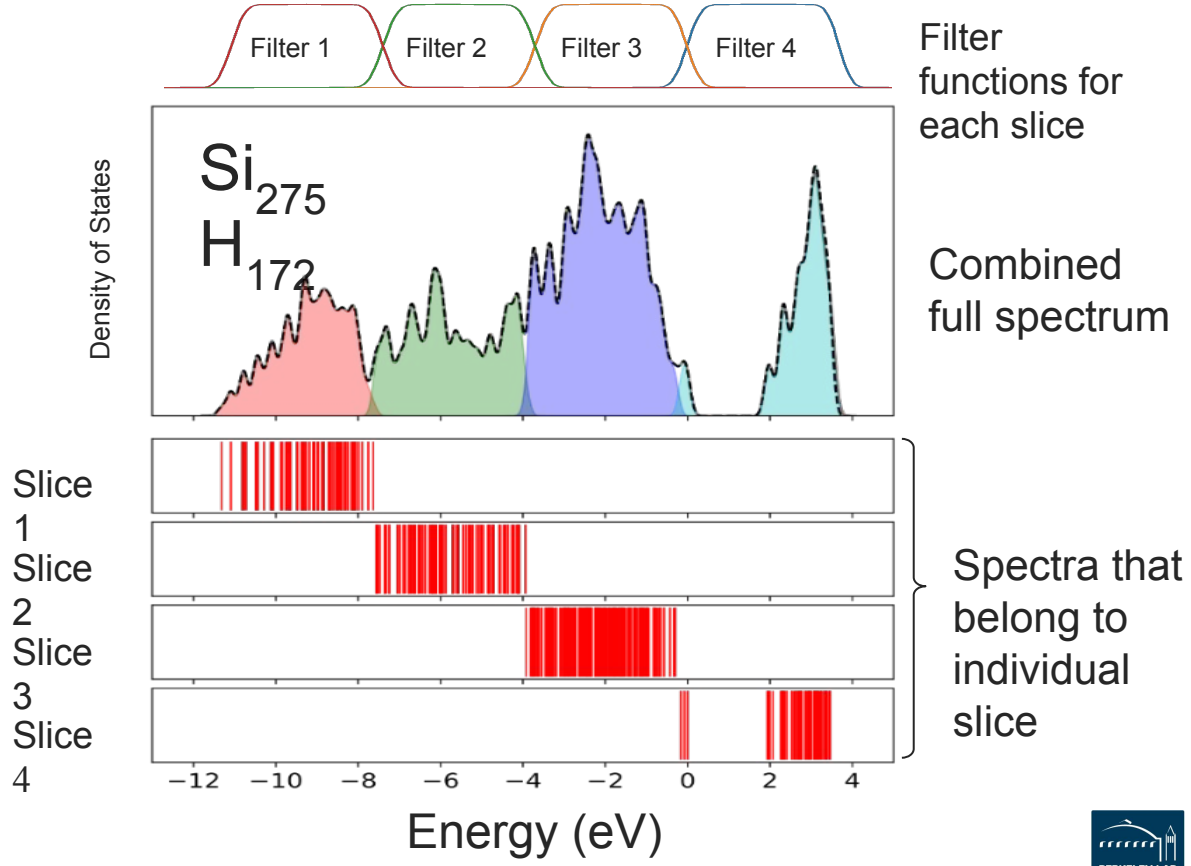
2. Form a new basis: exact low energy orbitals + orthogonalized PWs
   Is OK. Orthogonalization alone doesn't quite give meV accuracy. And diagonalization in basis not much better than just diagonalizing H in PWs.

Smarter Ways to Generate the Orbitals

Spectrum Slicing - filtering spectrum to individual slices with polynomial filter.

Adds new level of parallelism on HPC systems.

W. Gao, K. Liou, C. Yang, J. Chelikowsky, Y. Saad

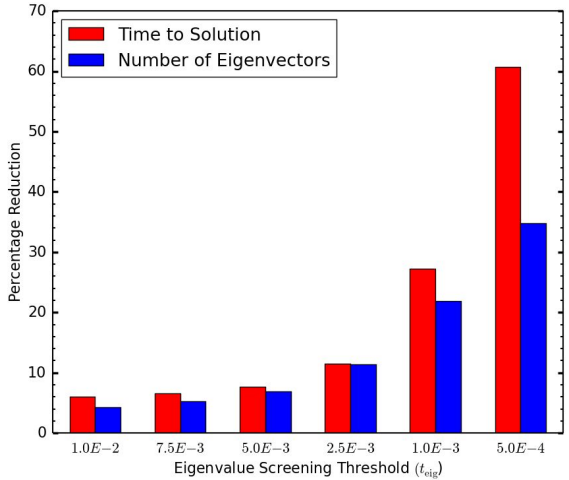


Other Eigen Problems

Polarizability

Construct low rank approximation at ω = 0 to accelerate ω != 0

$$\chi^0_{\mathbf{G}\mathbf{G}'}(\omega) = \sum_{n}^{\text{occ}} \sum_{n'}^{\text{emp}} \left[M^{\mathbf{G}}_{nn'}\right]^* M^{\mathbf{G}'}_{nn'} \frac{1}{E_n - E_{n'} - \omega}$$



M. Del Ben, F. H. da Jornada, J. Deslippe, S.G. Louie and A. Canning, *To be submitted* ; T.A. Pham, H.V. Nguyen, D. Rocca, and G. Galli, Phys. Rev. B 87, 155148 (2013) ; H.-V. Nguyen, T. A. Pham, D. Rocca, and G. Galli, Phys. Rev. B 85, 081101 (2012) ; H. F. Wilson, D. Lu, F. Gygi, and G. Galli, Phys. Rev. B 79, 245106 (2009) ; H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).

Shao, MeiYue, et al. *Science China Mathematics* 59.8 (2016): 1593-1612.

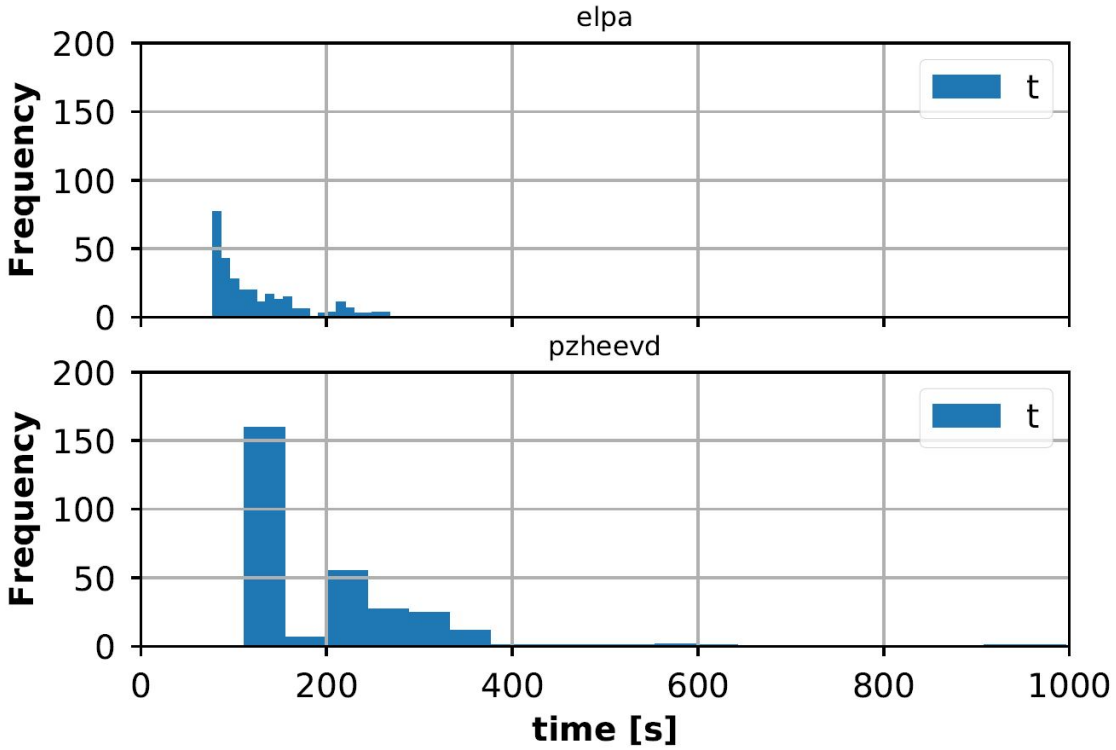
Bethe-Salpeter Equation (BSE)

Meiyue Shao, Chao Yang, Lin Lin Developed parallel solver for complex, non-Hermtian “Hamiltonian” - BSEPACK library

$$H_{\text{BSE}} = \left[\begin{array}{c|c} R & C \\ \hline -C^* & -R^* \end{array}\right]$$

Meiyue Shao, Felipe Homrich da Jornada, Chao Yang, Jack Deslippe, Steven G. Louie. Elsevier Linear Algebra and its Applications

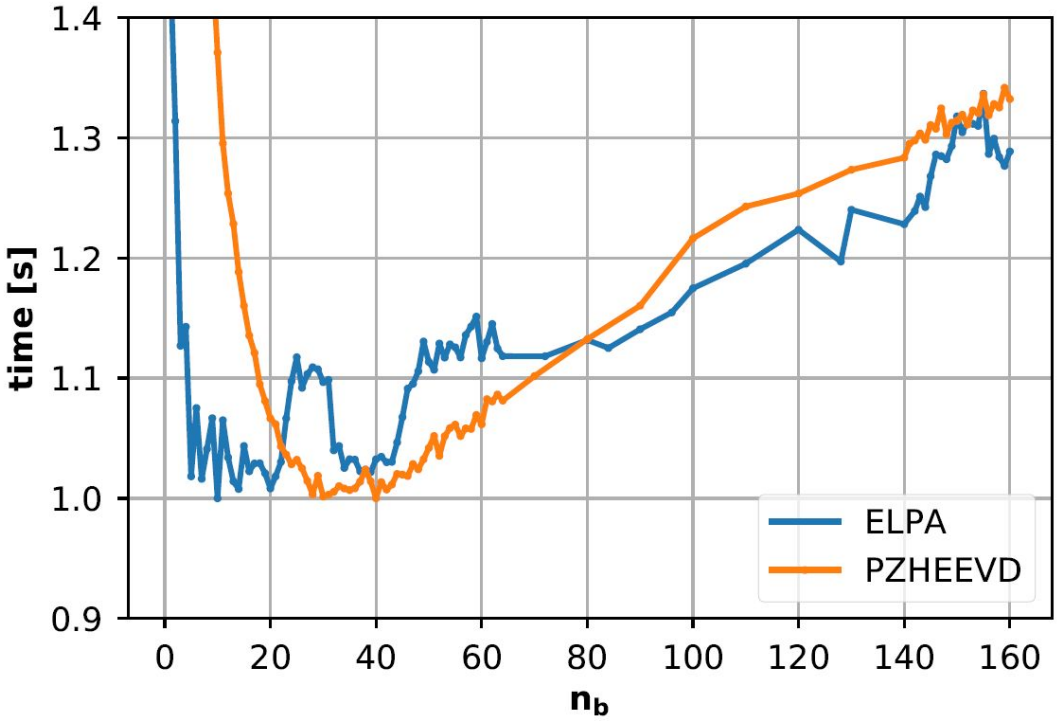
Practical Use of ScaLAPACK + ELPA



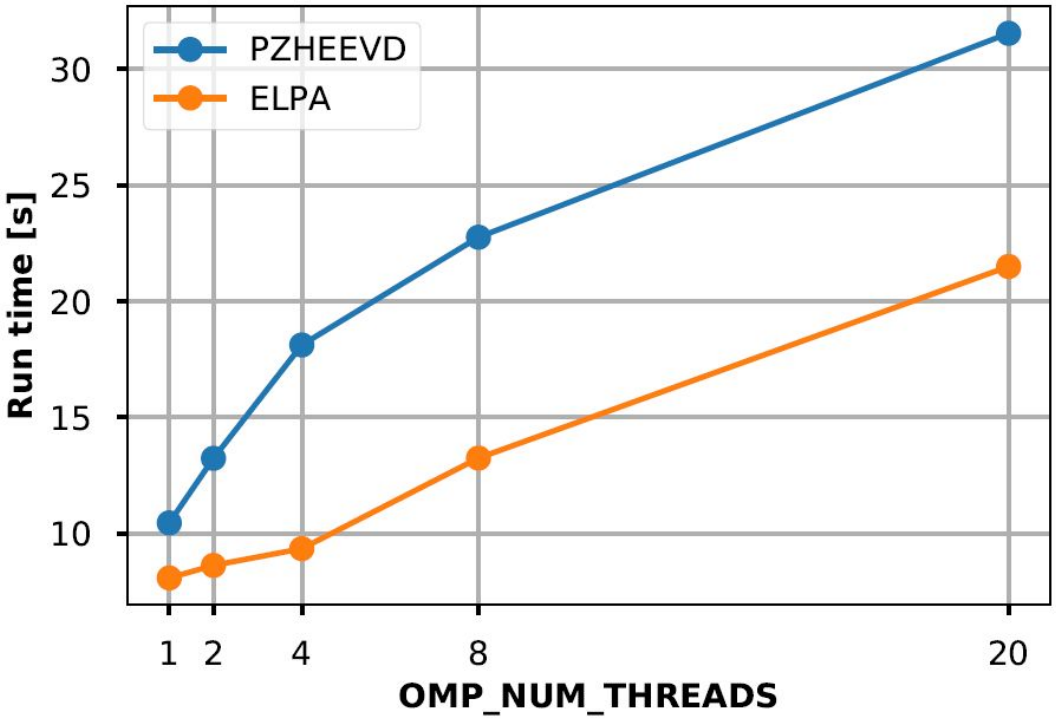
(nx,ny)	ALL
nb	1...100
N	20000
Architecture	KNL
Nodes	4

Parameter landscape - nb

(nx,ny)	(10, 32)
N	40000
Architecture	SKX
Nodes	8



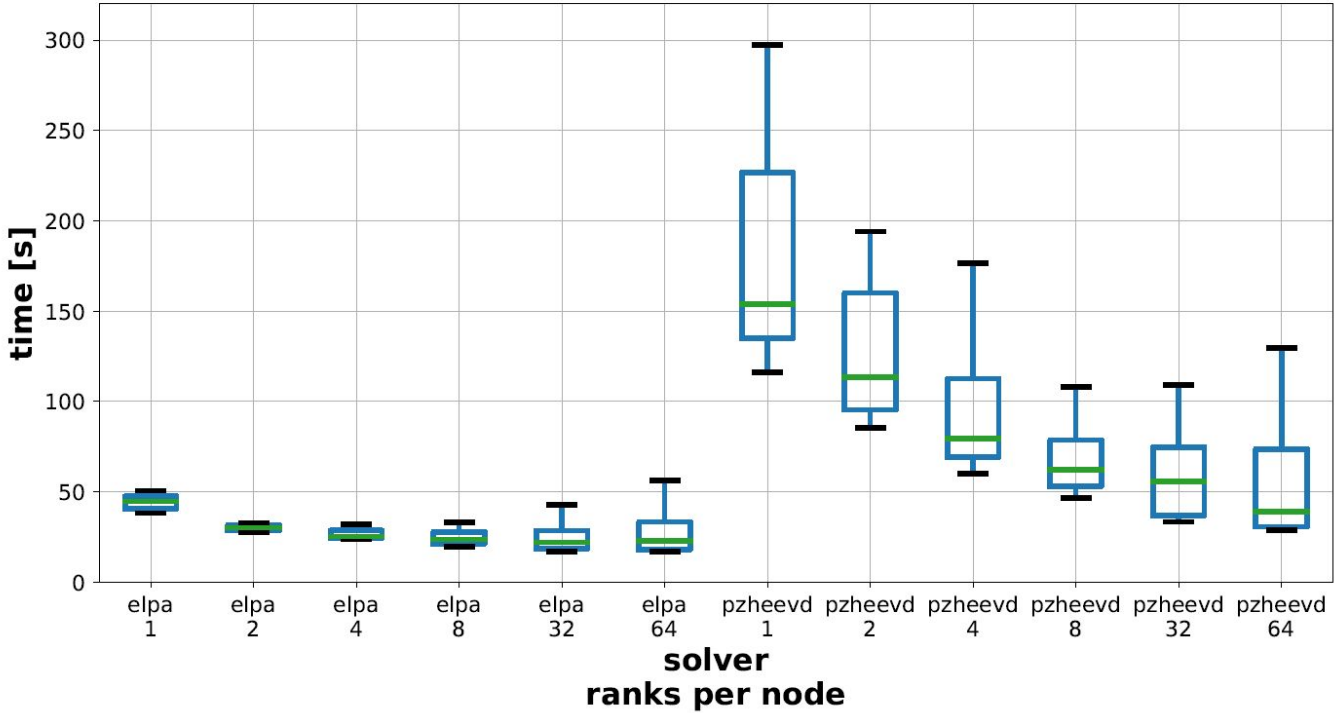
OpenMP scalability



- OMP_NUM_THREADS * MPI_Ranks kept constant
- No OpenMP penalty would be a horizontal line
- ELPA is OK up to 4 threads
- Useful for e.g. Quantum Espresso Exact Exchange simulations

(nx,ny)	best
nb	best
Architecture	SKX
nodes	4

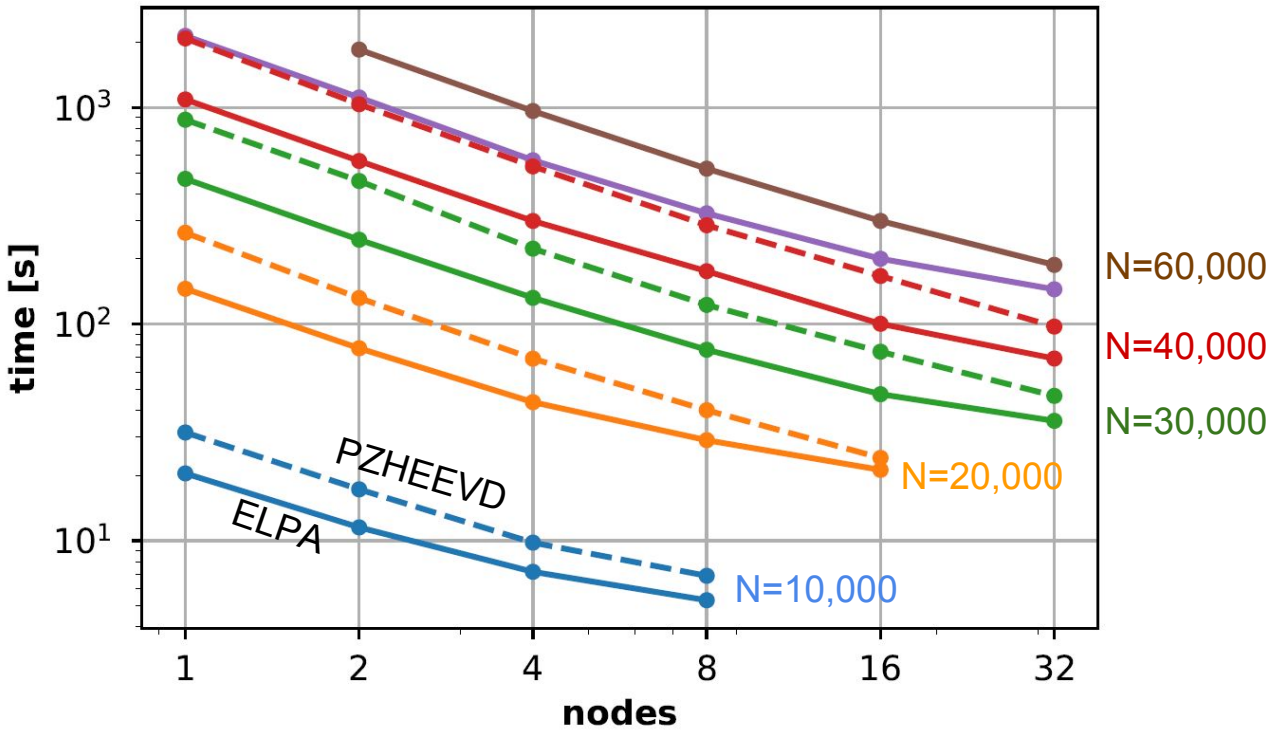
OpenMP performance



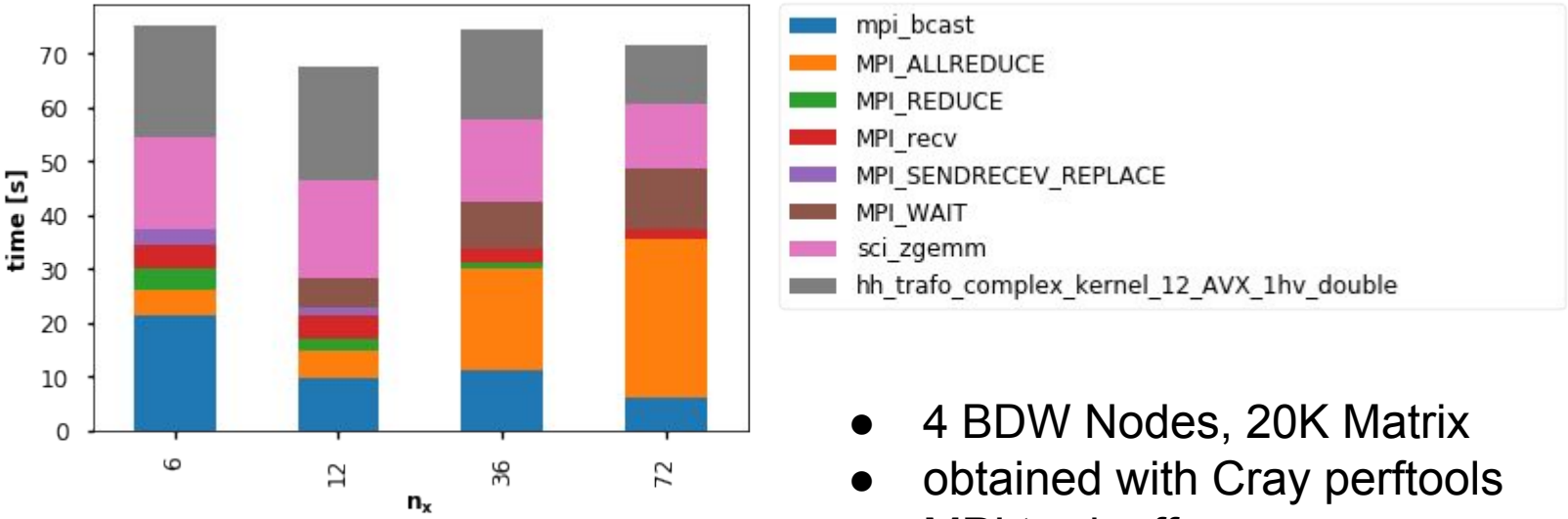
N	10000
Architecture	KNL
Nodes	4

Scaling of ELPA and PZHEEVD

(nx,ny)	best
nb	best
Architecture	SKX



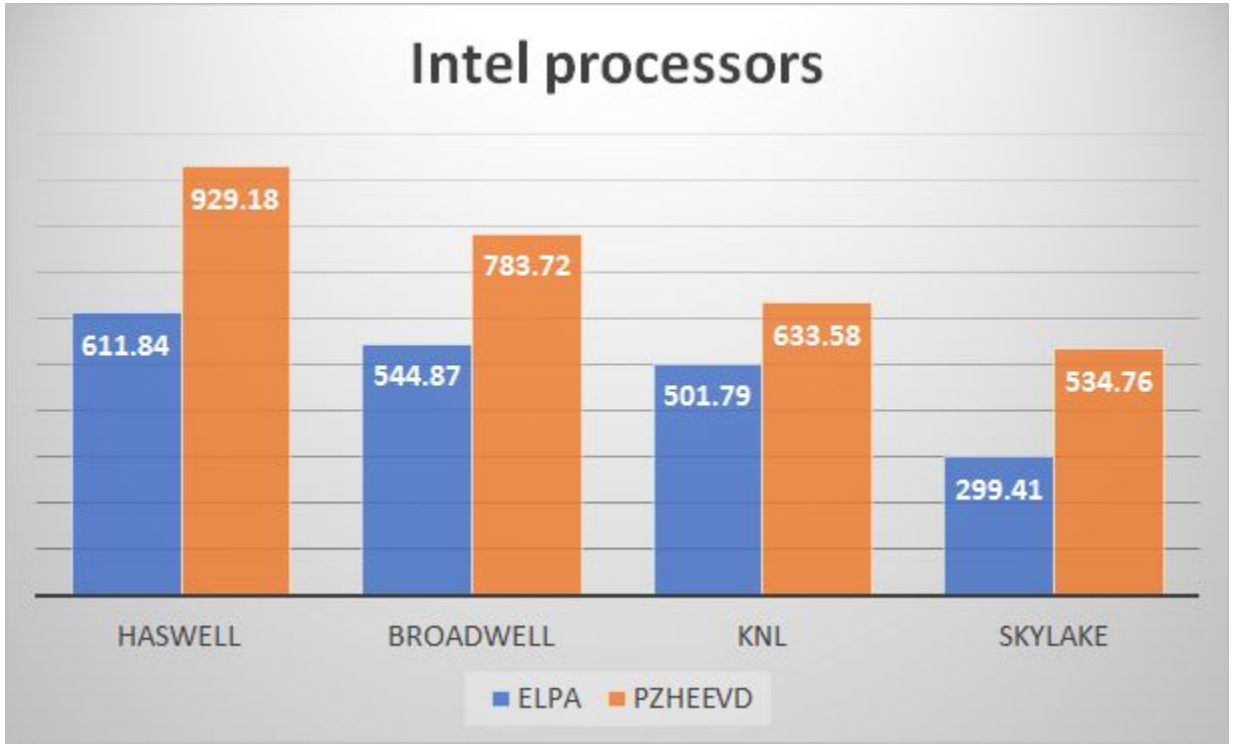
ELPA profile



- 4 BDW Nodes, 20K Matrix
- obtained with Cray perftools
- MPI tradeoff
- nx=12 is best overall time

Processor evolution

solution time on 4 nodes



Opportunity

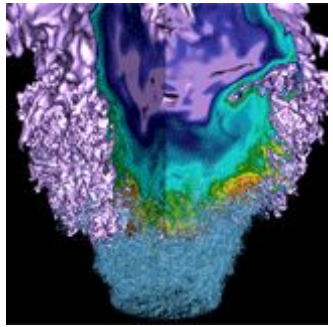
Collaborate with HPC Facilities on Supporting Vendor Upcoming Roadmaps

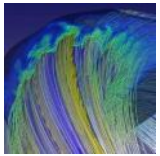
NERSC - NESAP

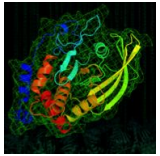
OLCF - CAAR

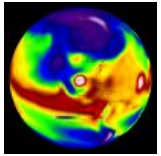
ALCF - ESP

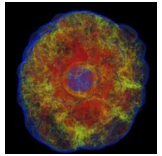
Extras

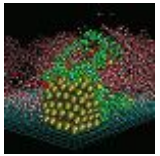












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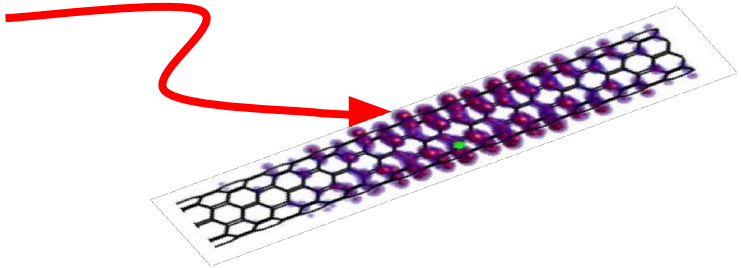
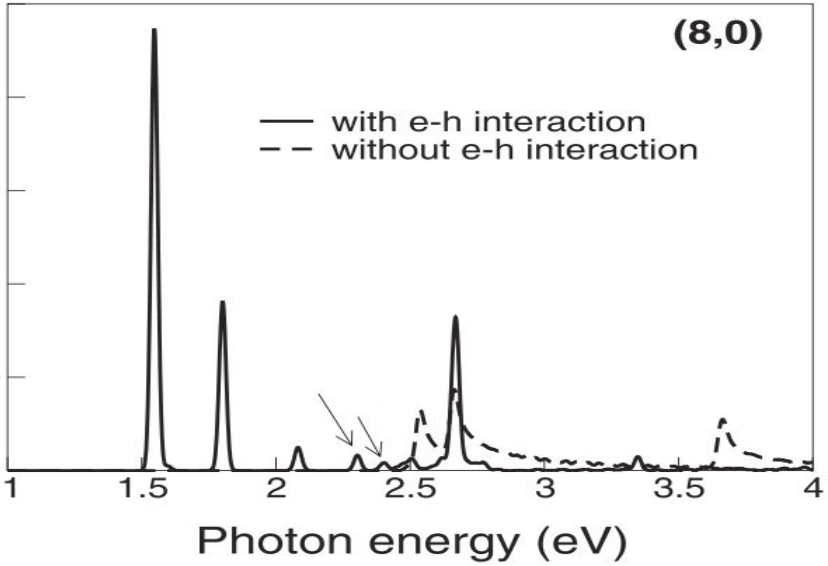
Why We Need GW



Many-body effects extremely important in **Excited-State properties** of Complex Materials.

Accurately describes properties important for:

- Photovoltaics
- LEDs
- Junctions / Interfaces
- Defect Energy Levels
- ….



*C.D. Spataru, S. Ismail-Beigi, L.X. Benedict, S.G. Louie. PRL 077402 (2004)

*J. Deslippe, C.D. Spataru, D. Prendergast, S.G Louie. Nano Letters. 7 1626 (2007)