Large-Scale GW Calculations on Pre-Exascale HPC Systems

BerkeleyGW: Method Developments and Code Optimization

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The *GW* Method

Solve Dyson's equation:

$$\left[-\frac{1}{2}\nabla^2 + V_{\rm loc} + \Sigma(E_n)\right]\phi_n = E_n\phi_n, \quad (1)$$

$\Sigma(E_n) \rightarrow$ self-energy (non-Hermitian, non-local, energy-dependent operator)

- Perturbative expansion on the screened Coulomb interaction W
- First approximation $\Sigma = iGW$
- W obtained from Inverse Dielectric Matrix ϵ^{-1} of the system

In `BerkeleyGW` [1]:

- `Epsilon` code $\rightarrow$ Compute ϵ^{-1}
- `Sigma` code $\rightarrow$ Compute W from ϵ^{-1} and solve eq.1

`Epsilon` code: Inverse Dielectric Matrix ϵ^{-1}

Input: $\psi_{m\mathbf{k}}$, $\epsilon_{m\mathbf{k}}$, $\{\mathbf{q}\text{-points}\}$, $\{\omega_i\}$

1. Calculate plane-waves matrix elements (FFT's): $O(N_v N_c N_G \log N_G)$

$$M^G_{ja\mathbf{k}}(\mathbf{q}) = \langle\psi_{j\mathbf{k}+\mathbf{q}}|\, e^{i(\mathbf{G}+\mathbf{q})\cdot\mathbf{r}}\,|\psi_{a\mathbf{k}}\rangle$$

2. Calculate RPA polarizability (Matrix-Multiplication): $O(N_\omega N_v N_c N_G^2)$

$$\chi(\mathbf{q},\omega_i) = \mathbf{M}(\mathbf{q})^\dagger \mathbf{\Delta}_{ja\mathbf{k}}(\epsilon_{j\mathbf{k}}, \epsilon_{a\mathbf{k}}, \mathbf{q}, \omega_i)\mathbf{M}(\mathbf{q})$$

$\mathbf{\Delta}$ diagonal matrix containing the frequency dependence

3. Dielectric matrix ϵ and inversion: $O(N_\omega N_G^3)$

$$\epsilon_{GG'}(\mathbf{q},\omega_i) = \delta_{GG'} - v(\mathbf{q}+\mathbf{G})\chi_{GG'}(\mathbf{q},\omega_i)$$
$$\epsilon^{-1}(\mathbf{q},\omega_i) = (I - v\chi(\mathbf{q},\omega_i))^{-1}$$

Parameters: N_v number of valence bands, N_c number of conduction (empty) bands, N_G PW basis set size, N_ω number of frequencies.

Static Subspace Approximation [2]: Speed-Up the Calculation of $\epsilon^{-1}(\omega_i)$ for $\omega_i \neq 0$

- For $\omega_i = 0$: Standard calculation of $\bar{\chi}(0) = v^{\frac{1}{2}}\chi(0)v^{\frac{1}{2}}$

$$\chi(0) = \mathbf{M}^\dagger \mathbf{\Delta}_{ja\mathbf{k}}(0)\mathbf{M}$$

  Eigendecomposition $\bar{\chi}(0) = \mathbf{C}^{0\dagger}\mathbf{x}\mathbf{C}^0$, define $\mathbf{C}^0_s$ according to threshold $t_{\rm eigen}$
- Projection of $\mathbf{M}$ into the subspace spanned by $\mathbf{C}^0_s$

$$\overline{\mathbf{M}}^0_s = \mathbf{M}v^{\frac{1}{2}}\mathbf{C}^0_s$$

- For $\omega_i \neq 0$: direct computation of $\bar{\chi}_s(\omega_i)$

$$\bar{\chi}_s(\omega_i) = \overline{\mathbf{M}}^{0\dagger}_s \mathbf{\Delta}_{ja\mathbf{k}}(\omega_i)\overline{\mathbf{M}}^0_s$$

- Final evaluation of $\epsilon^{-1}(\omega_i)$ from $\bar{\chi}_s(\omega_i)$

	Execution	Memory
Matrix Element	$O(N_v N_c N_G \log N_G)$	$O(N_v N_c N_G)$
Polarizability $\omega = 0$	$O(N_v N_c N_G^2)$	$O(N_G^2)$
Eigendecomposition: $\mathbf{C}^0_s$	$O(N_G^3)$	$O(N_G^2)$
$\overline{\mathbf{M}}^0_s$	$O(N_b N_v N_c N_G)$	$O(N_v N_c N_b)$
Polarizability $\omega \neq 0$	$O(N_\omega N_v N_c N_b^2)$	$O(N_\omega N_b^2)$
Inversion	$O(N_\omega N_b^3)$	$O(N_\omega N_b^2)$
I/O	$O(N_G N_b + N_\omega N_b^2)$	$O(N_G N_b + N_\omega N_b^2)$
Evaluation of $\epsilon^{-1}(\omega_i)$	$O(N_\omega N_b N_G^2)$	$O(N_\omega N_G^2)$

References

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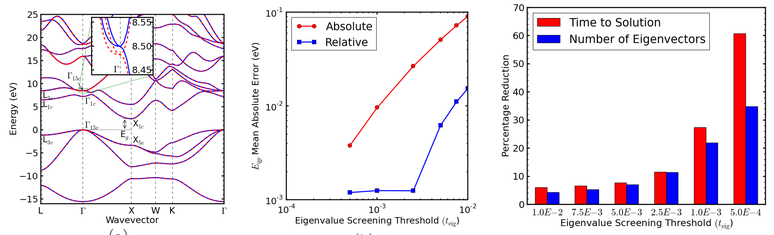
2. M. Govoni and G. Galli, J. Chem. Theory Comput. 11, 2680 (2015) ; T.A. Pham, H.V. Nguyen, D. Rocca, and G. Galli, Phys. Rev. B 87, 155148 (2013) ; H.-V. Nguyen, T. A. Pham, D. Rocca, and G. Galli, Phys. Rev. B 85, 081101 (2012) ; H. F. Wilson, D. Lu, F. Gygi, and G. Galli, Phys. Rev. B 79, 245106 (2009) ; H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).
3. P. Umari, Geoffrey Stenuit, and Stefano Baroni, Phys. Rev. B 79, 201104-R (2009)
4. M. Del Ben, F.H. da Jornada, A. Canning, N. Wichmann, K. Raman, R. Sasanka, C. Yang, S.G. Louie and J. Deslippe, In Preparation

Benchmark Calculations

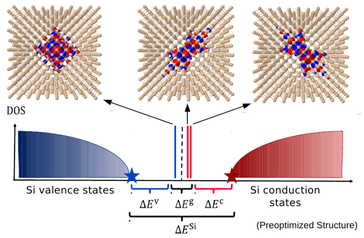
Silicon Carbide (β−SiC):



(a) (b) (c)

Figure: (a) band structure as obtained without (solid blue) and with the static subspace approximation (red dotted $t_{\rm eig} = 0.01$); (b) mean absolute error between the reference and approximate results (196 $E_{\rm QP}$ calculated); (c) percentage reduction in time to solution (red) and number of eigenvectors (blue) for the evaluation of ϵ^{-1}.

Single Vacancy V^0_1 (1000-Si Atoms Benchmark)



	ΔE^v	ΔE^g	ΔE^c	$\Delta E^{\rm Si}$	#Nodes	Time (min)
LDA	0.29	0.07	0.23	0.60	-	-
G_0W_0 (6Ry)	0.41	0.27	0.46	1.15	480	73
G_0W_0 (12Ry)	0.42	0.26	0.49	1.18	2048	157

Energies in eV
G_0W_0 = Full-Frequency Contour Deformation
Calculations Performed on Edison@NERSC (CRAY-XC30)

- Approximation tested for Insulators, Semiconductors, Metals, Clusters, Slabs
- Direct correlation between accuracy and $t_{\rm eigen}$ (5-25% of the eigenstates $\rightarrow\sim$ 1 meV accuracy)

`Sigma` code: Calculate $\Sigma_{lm}(\omega)$ and Solve Dyson's Equation

1. Calculate plane-waves matrix elements (FFT's): $O(N_\Sigma N_n N_G \log N_G)$

$$M^{-G}_{nm} = \langle\phi_n|\, e^{-i\mathbf{G}\cdot\mathbf{r}}\,|\phi_m\rangle$$

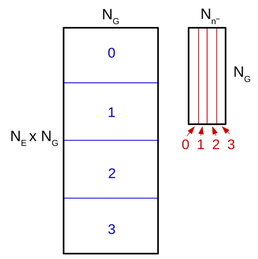
2. For any given pair of orbital functions $\{\phi_l, \phi_m\}$ calculate:

$$\Sigma_{lm}(E) = \frac{i}{2\pi}\int_0^\infty d\omega \sum_n \sum_{GG'} M^{-G}_{nl} \frac{\epsilon^{-1}_{GG'}(\omega)\cdot v(G')}{E - E_n - \omega} M^{-G'}_{nm}$$

Matrix-Multiplication + 2D Dot-Product $O(N_\Sigma N_\omega N_n N_G^2)$

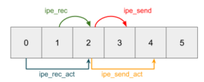
Parallelization Strategy

$\Sigma_{lm}(\omega)$ matrix elements distributed over Pools of processes. For each Pool:



Data distribution layout
$N_G \simeq 10^5$; $N_n \simeq 10^4$; $N_E \simeq 10^2$

- Left Matrix: $\epsilon^{-1}(\omega)$ distributed over rows ($N_G \times N_\omega$ combined index)
- Right Matrix: M^G_{nl} distributed over columns (FFT performed locally)
- At each cycle the matrix contraction is performed locally (ZGEMM)
- Ring communication restricted to contiguous MPI tasks



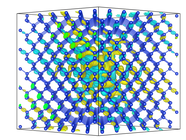
Non-blocking cyclic communication layout

- Communication can be performed over blocks of processes:
  - $N_{n''}$ size roughly constant independent on the ration OMP×MPI
  - Good ZGEMM performance independent on the number of MPI tasks employed

Same algorithm is used in the low-rank approximation case: matrix size $N_G \rightarrow N_b$

- Speed-up proportional to $(N_G/N_b)^2$
- Good performance achieved by using smaller pool sizes

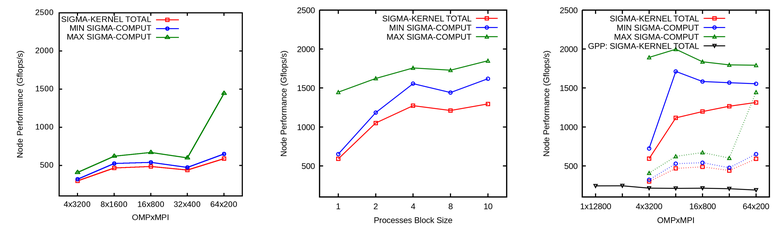
Performance Measurement on Cori-KNL@NERSC



Systems: Divacancy states in Silicon supercells containing 998 and 1726 atoms.

- FLOPs per node
- Best/worst performing node
- Strong Scaling
- Time to solution
- Comparison to peak performance

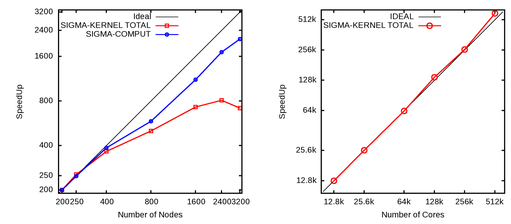
Single Pool Performance: 200 KNL Nodes



(a) (b) (c)

(a) Poor performance due to small Comput./Commun. ratio (different OMPxMPI ratio, no message blocking) (b) Improved performance for 64-OMPxMPI by using different processes block size (c) Different OMPxMPI ratio and process block size adjusted to give roughly constant n''.

Strong Scaling: Individual Pool and Full `Sigma`



(d) (e)

(a) Individual Pool scaling, total execution (red squares) and computationally intense part (blue circles), (b) Full `Sigma`, 200-NKL nodes per Pool.

Full `Sigma`: Best Performance

	998 Si	1726 Si
Number KNL Nodes	9600	9500
Number of Cores	633,600	627,000
Number $E_{\rm qp}$ Evaluated	48	38
Time to solution (s)	160	201
PetaFLOP/s	11.8	11.3
% Peak Performance	47	46

- `Sigma` kernel capable to scale to full-Cori
- `Sigma` achieves high fraction of peak performance
- Excellent time to solution (∼100 seconds) for systems made of thousands of atoms

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