Accelerating Large-Scale GW Calculations on Hybrid CPU-GPU Architectures

BerkeleyGW: Algorithm Development and Code Optimization

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The *GW* Method

BerkeleyGW is a massively parallel software package for studying the electron excited-state properties of materials employing the GW and Bethe-Salpeter equation approach and beyond. The dynamical properties of the electron are obtained as solution of the Solve Dyson's equation:

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

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

- Perturbative expansion on the screened Coulomb interaction $W \rightarrow$ At first order $\Sigma = iGW$
- W obtained from the inverse dielectric matrix ϵ^{-1} of the system

In `BerkeleyGW` [1]:

- `Epsilon` code $\rightarrow$ Compute ϵ^{-1}, $O(N^4)$
- `Sigma` code $\rightarrow$ Compute W from ϵ^{-1} and solve Eq.1, $O(N^4)$

`Epsilon` code: Inverse Dielectric Matrix ϵ^{-1} and its Frequency Dependence

Static Dielectric Matrix $\epsilon^{-1}(\omega = 0)$, input: $\psi_{m\mathbf{k}}$ wavefunctions and $\epsilon_{m\mathbf{k}}$ energies

1. Calculate plane-waves matrix elements: $O(N_v N_c N_G \log N_G) \rightarrow$ `MTXEL` kernel.
   Matrix elements are calculated by many node-local fast Fourier transforms (FFTs), matrix elements are distributed in a tall and skinny matrix **M**.
2. Static polarizability $\chi(\omega = 0)$: $O(N_v N_c N_G^2) \rightarrow$ `CHI-0` kernel.
   Large distributed matrix-multiplication between tall and skinny matrices.
3. Dielectric matrix ϵ and inversion: $O(N_G^3) \rightarrow$ `Inv` (ScaLAPACK)
   Algebraic inversion (LU factorization + triangular inversion) of a square complex matrix

Frequency Dependence $\epsilon^{-1}(\omega_i)$ **for** $\omega_i \neq 0$ within the static subspace approximation [2,3,4], input: **M** from step 1 and $\chi(\omega = 0)$ from step 2

1. Eigendecomposition $\bar{\chi}(0) = \mathbf{C}^{0\dagger}\mathbf{x}\mathbf{C}^0$, define define new subspace basis $\mathbf{C}_s^0$ of size N_{eig} according $t_{\rm eigen}$ threshold $O(N_G^3) \rightarrow$ `Diag` (ScaLAPACK, ELPA)
2. Basis transormation of **M** into the subspace spanned by $\mathbf{C}_s^0$ $O(N_v N_c N_{eig} N_G) \rightarrow$ `Transf` kernel
   Distribute matrix multiplication: $\overline{\mathbf{M}}_s^0 = \mathbf{M} v^{\frac{1}{2}} \mathbf{C}_s^0$ ($\mathbf{v}^{\frac{1}{2}}$ diagonal)
3. For $\omega_i \neq 0$: direct computation of $\bar{\chi}_s(\omega_i)$ $O(N_\omega N_v N_c N_{eig}^2) \rightarrow$ `CHI-freq` kernel
   Distribute matrix multiplication at multiple frequency: $\bar{\chi}_s(\omega_i) = \overline{\mathbf{M}}_s^{0\dagger} \mathbf{\Delta}(\omega_i) \overline{\mathbf{M}}_s^0$ with $\mathbf{\Delta}$ diagonal matrix containing the band energy/frequency dependence
4. Final evaluation of $\bar{\epsilon}^{-1}(\omega_i)$ from $\bar{\chi}_s(\omega_i)$ in the subspace basis $O(N_\omega N_{eig}^3) \rightarrow$ `Inv-Sub` (ScaLAPACK)

	Execution	Memory
Matrix Element (`MTXEL`)	$O(N_v N_c N_G \log N_G)$	$O(N_v N_c N_G)$
Polarizability $\omega = 0$ (`CHI-0`)	$O(N_v N_c N_G^2)$	$O(N_G^2)$
$\mathbf{C}_s^0$ or ϵ^{-1} (`Diag` / `Inv`)	$O(N_G^3)$	$O(N_G^2)$
Basis transformation: $\overline{\mathbf{M}}_s^0$ (`Transf`)	$O(N_{eig} N_v N_c N_G)$	$O(N_v N_c N_{eig})$
Polarizability $\omega \neq 0$ (`CHI-freq`)	$O(N_\omega N_v N_c N_{eig}^2)$	$O(N_\omega N_{eig}^2)$
Inversion (`Inv-Sub`)	$O(N_\omega N_{eig}^3)$	$O(N_\omega N_{eig}^2)$
I/O	$O(N_G N_{eig} + N_\omega N_{eig}^2)$	$O(N_G N_{eig} + N_\omega N_{eig}^2)$

Table: (1) Computational cost associated with each of the kernels of the `epsilon` code. The parameters in the table are N_v number of valence bands, N_c number of conduction (empty) bands, N_G plane waves basis set size, N_{eig} subspace basis size, and N_ω number of frequencies.

References

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3. M. Del Ben, H. Felipe, G. Antonius, T. Rangel, S.G. Louie, J. Deslippe and A. Canning, Phys. Rev. B 99 (12), 125128 (2019).
4. M. Govoni and G. Galli, J. Chem. Theory Comput. 11, 2680 (2015).

GPU Support for Computational Kernels

Matrix Elements Kernel $\rightarrow$ `MTXEL`

- Double loop over valence (outer) and conduction (inner) wavefunctions/bands

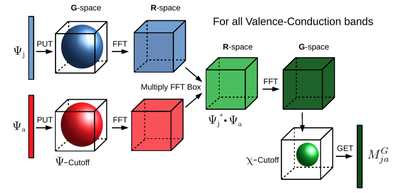


Figure: Schematic representation of the operations performed in the inner loop of the `MTXEL` kernel.

- Use cuFFT library to perform the fast Fourier transforms.
- Use data streams and host pinned memory, one stream for each conduction wavefunction (inner loop index) $\rightarrow$ asynchronous memory transfer + high concurrency on device .
- Conduction bands (FFT boxes) offloaded to device over batches to avoid out of memory.
- CUDA kernels for Put/Multiply/Get to keep intermediates on device.

Static Polarizability Kernel $\rightarrow$ `CHI-0`

- Large distributed matrix multiplication

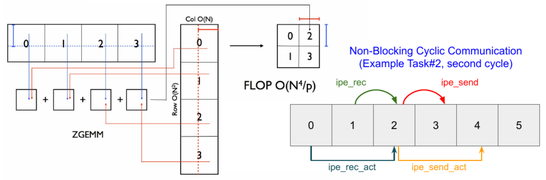


Figure: Schematic representation of the data layout and communication scheme for the `CHI-0` kernel.

- Use cuBLAS to perform the local ZGEMM
- Data stream and host pinned memory for the matrix buffers $\rightarrow$ asynchronous memory transfer and calls to cuBLAS
- Non-blocking cyclic communication scheme: communication is finalized before stream is synchronized $\rightarrow$ overlap communication (CPU) computation (GPU)
- Batch over conduction wavefunction index to control memory usage on device

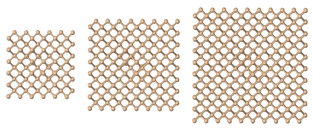
Basis Transformation $\rightarrow$ `Transf`

- Similar communication scheme as `CHI-0`, potential memory bottlenecks for both host/device $\rightarrow$ all eigenvectors need to be communicated to all MPI tasks
- Batch communication over eigenvector index $\rightarrow$ control host memory usage
- Batch computation over (valence) wavefunction index $\rightarrow$ control device memory usage

Frequency-dependent Polarizability Kernel $\rightarrow$ `CHI-freq`

- Similar communication scheme as `CHI-0`
- Many matrix multiplication at multiple frequencies, matrices smaller than `CHI-0` ($N_G/N_{eig} \simeq 5-10$)
- Data streams over frequency index $\rightarrow$ concurrent cuZGEMM execution on device
- Batch over (conduction) wavefunction index to control memory usage on device

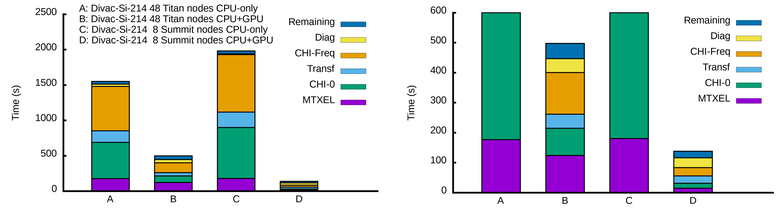
Benchmarks for Performance Measurement



	Dvac-Si-214	Dvac-Si-510	Dvac-Si-998
N_G^ψ	31,463	74,653	145,837
N_G	11,075	26,529	51,627
N_b	6,397	15,045	29,346
N_v	428	1,020	1,996
N_c	5,969	14,025	27,350
N_{eig}	3,500	7,000	14,000
N_ω	10	10	10
Epsilon Min PFlops	5.8	157.9	2335.7
Epsilon Min Memory (Tb)	0.6	7.7	57.5

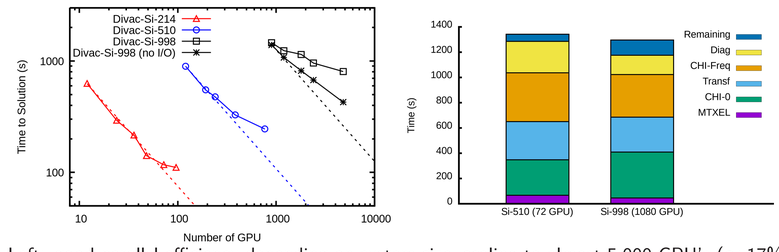
Benchmark systems for performance measurement. The benchmarks are based on a silicon divacancy defect in silicon (a prototype of a solid state qbit). The table shows the computational characteristics for each benchmark, see Table (1) for the actual computational cost.

CPU-Only vs CPU+GPU



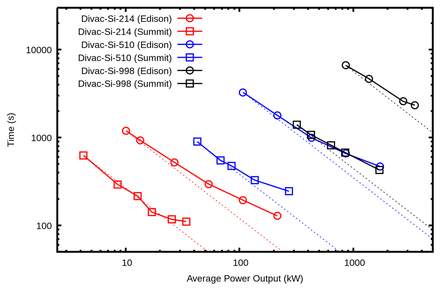
Comparison between the CPU-only and CPU+GPU executions measured on Titan and Summit (OLCF). The right plot is the zoom-in version of the left. All optimized kernels show great acceleration from GPU support, with a 14x speedup for the overall execution on Summit.

Strong and Weak Scaling on Summit@OLCF



Left: good parallel efficiency depending on system size, scaling to almost 5,000 GPU's ($\simeq$ 17% of full machine). Parallel I/O issues for large scale calculation (HDF5 library). Right: good weak scaling; as problem size increases, memory grows to $O(N^3)$ and flops increases to $O(N^4) \rightarrow$ more memory available for larger systems, less communication and better parallel performance.

Comparison Across Architectures: Time vs Power



Comparing performance in term of energy efficiency between Edison@NERSC and Summit@OLCF. Ideal scaling (dotted lines) $\rightarrow$ constant energy consumption increasing power. GPUs are 16x more power efficient than CPUs consistently through all three benchmarks.

Summary

- BerkeleyGW large-scale GW calculations are moving to GPUs!
- 14x speedup obtained from GPU acceleration and lots of lessons learned during optimization!
- Excellent time to solution (minutes) is achieved for systems made of thousands of atoms!
- More efforts are needed to optimize parallel I/O and accelerate libraries for eigensolvers and matrix inversions!

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