GPU Acceleration of the WEST Code for Large-Scale Full-Frequency GW Calculations

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WEST! MICCoM

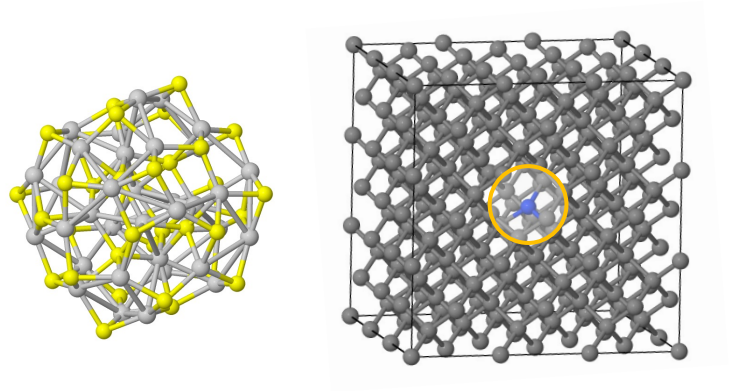
Argonne NATIONAL LABORATORY

Motivation and introduction

http://west-code.org

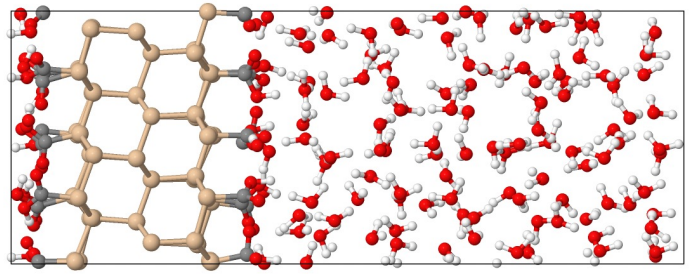
Using first-principles simulations, we study electronic structures, charged and neutral excitations of large heterogeneous systems

- Nanoparticles for energy conversion
- Solid/liquid interfaces for photocatalysis
- Spin defects in semiconductors for quantum information science

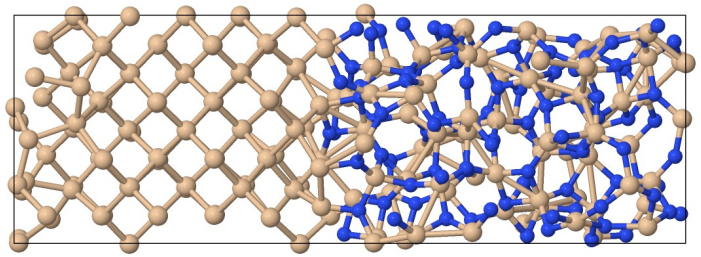


We have developed **WEST**, a massively parallel implementation of many-body perturbation theory (GW/BSE) **without empty states**

- ✓ No explicit summation over virtual orbitals
- ✓ No explicit storage or inversion of large dielectric matrices
- ✓ Full frequency integration with contour deformation

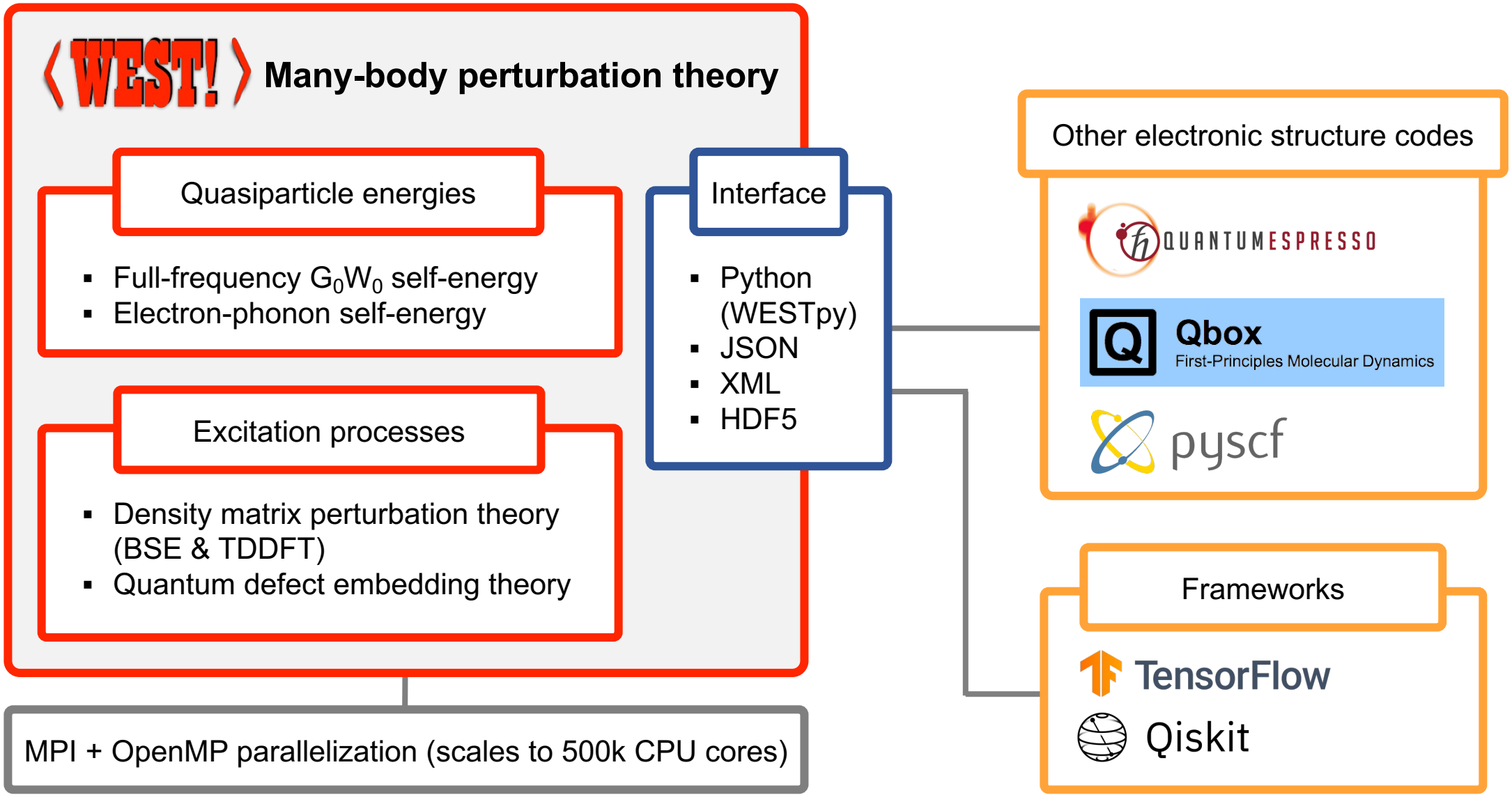


WEST has been successfully applied to large G_0W_0 calculations consisting of ~2,000 electrons on CPUs



Govoni and Galli, J. Chem. Theory Comput.11, 2680-2696 (2015)

The **WEST** code: **W**ithout **E**mpty **ST**ates



Govoni and Galli, J. Chem. Theory Comput.11, 2680-2696 (2015)

GPU acceleration in WEST

WEST has been ported to **NVIDIA GPUs**

Porting strategies

- GPU libraries for performance:
  cuFFT, cuBLAS, cuSOLVER, ...
- Directives for portability:
  CUDA Fortran → OpenACC → OpenMP

Achievements

- Significant speedup over CPU code
- Excellent strong and weak scalability demonstrated on various supercomputers
- Tractable size of full-frequency G_0W_0 pushed to **10k electrons**

✅ ⟨WEST!⟩

OLCF/Summit
200.79 PFLOP/s
NVIDIA V100 GPUs

https://www.olcf.ornl.gov/olcf-resources/compute-systems/summit

✅ ⟨WEST!⟩

NERSC/Perlmutter
93.75 PFLOP/s
NVIDIA A100 GPUs

https://www.nersc.gov/systems/perlmutter

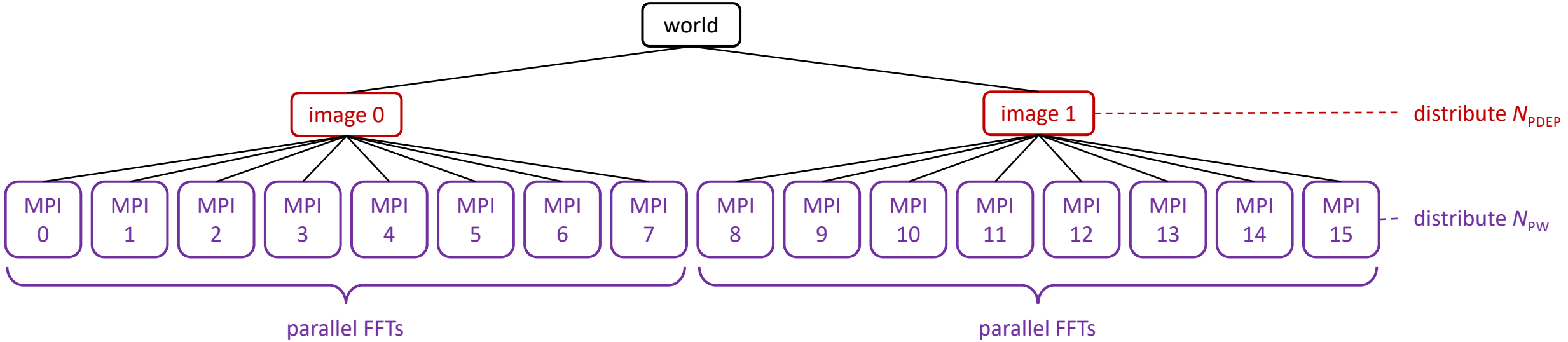
Yu and Govoni, J. Chem. Theory Comput.18, 4690-4707 (2022)

Projective dielectric eigenpotentials (PDEP)

```
davidson loop
  perturbation loop
    spin loop
      band loop
        FFT
        solve linear system
        FFT
    density
  solve eigenproblem
```

N_{PDEP} perturbations distributed across “images”

N_{PW} coefficients distributed across MPI tasks within an image



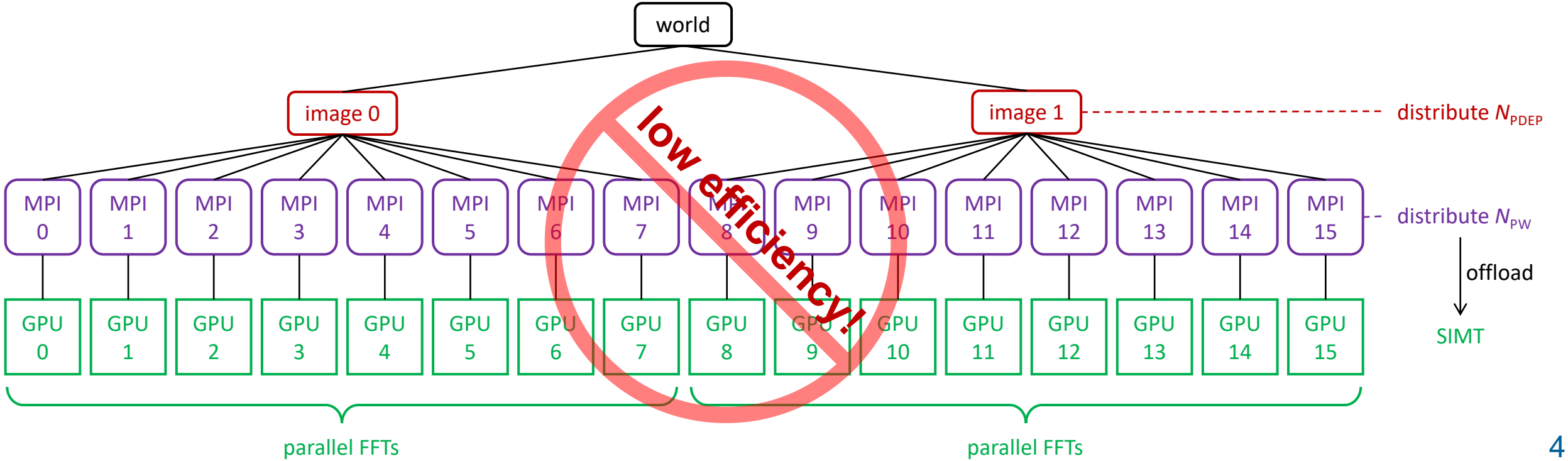
Straightforward GPU offloading?

```
davidson loop
  perturbation loop
    spin loop
      band loop
        FFT
        solve linear system
        FFT
    density
  solve eigenproblem
```

perturbation loop → N_{PDEP} perturbations distributed across "images"

FFT, solve linear system, FFT → N_{PW} coefficients distributed across MPI tasks within an image

Each MPI task offloads to a GPU



Hierarchical parallelization scheme

```
davidson loop
    perturbation loop
        spin loop
            band loop
                FFT
                solve linear system
                FFT
        density
    solve eigenproblem
```

N_{PDEP} perturbations distributed across “images”

N_{PW} coefficients distributed across MPI tasks **within an image**

The calculation of the response can be done independently for each perturbation, band, and spin channel
→ **many layers of parallelism**

```
davidson loop
    copy to GPU
    perturbation loop
        spin loop
            band loop
                GPU FFT
                GPU solve linear system
                GPU FFT
        density
    GPU solve eigenproblem
    copy from GPU
```

N_{PDEP} perturbations distributed across “images”

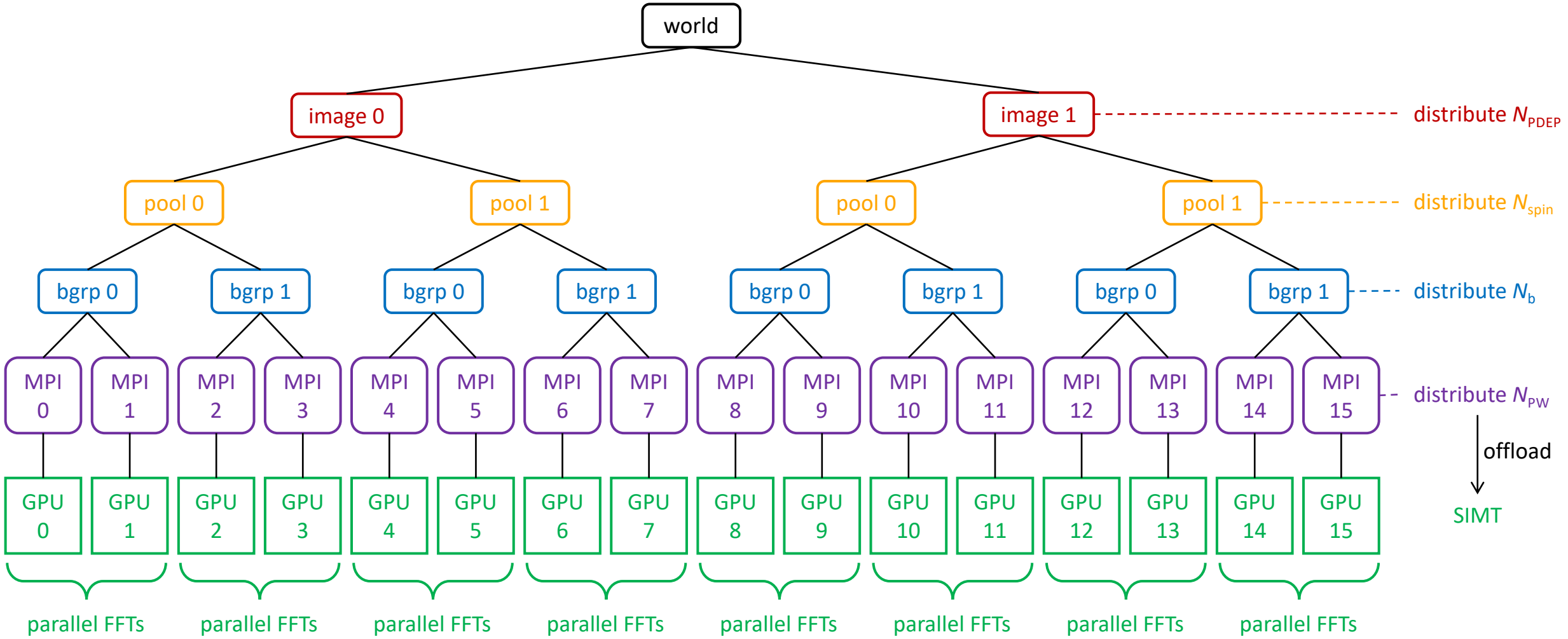
N_{spin} spin channels distributed across “pools” within an image

N_b bands distributed across “band groups” within a pool

N_{PW} coefficients distributed across MPI tasks **within a band group**

Each MPI task offloads to a GPU

Hierarchical parallelization scheme



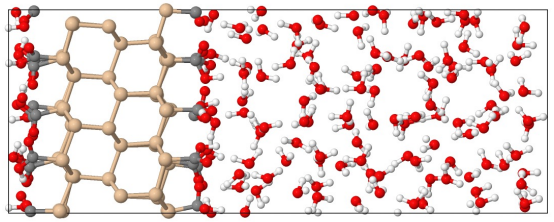
- All levels of parallelism in the PDEP algorithm are fully harnessed
- CPU-GPU and GPU-GPU communication cost is reduced

GPU porting and optimization strategies

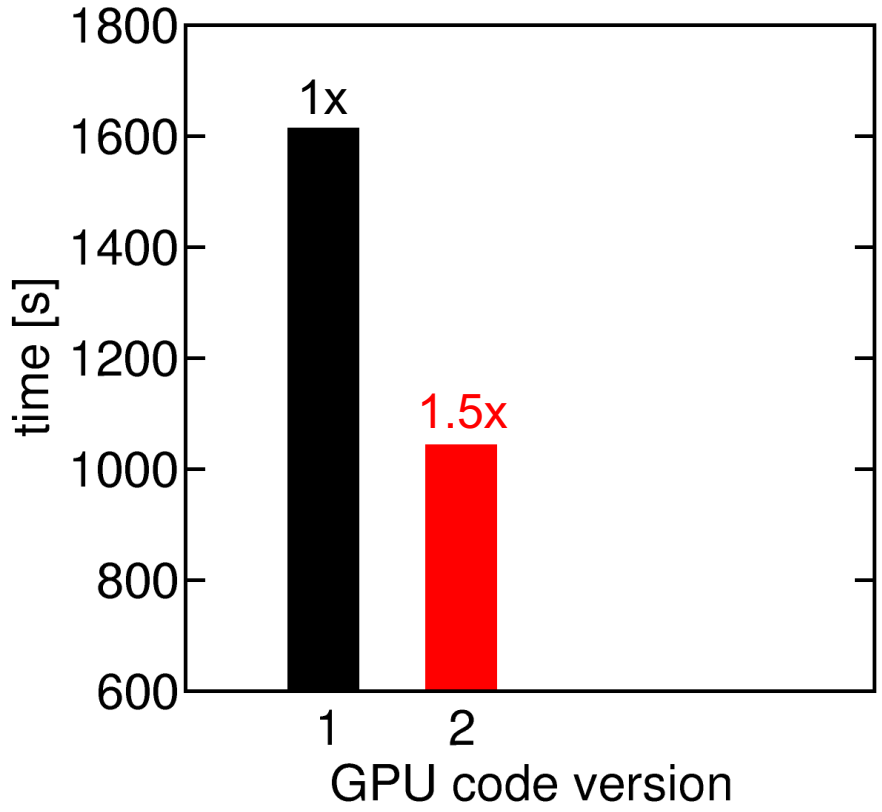
v1: Initial GPU porting (baseline)

v2: Multi-level parallelization and data distribution

- Reduced CPU-GPU and MPI communication
- Improved load balance across GPUs



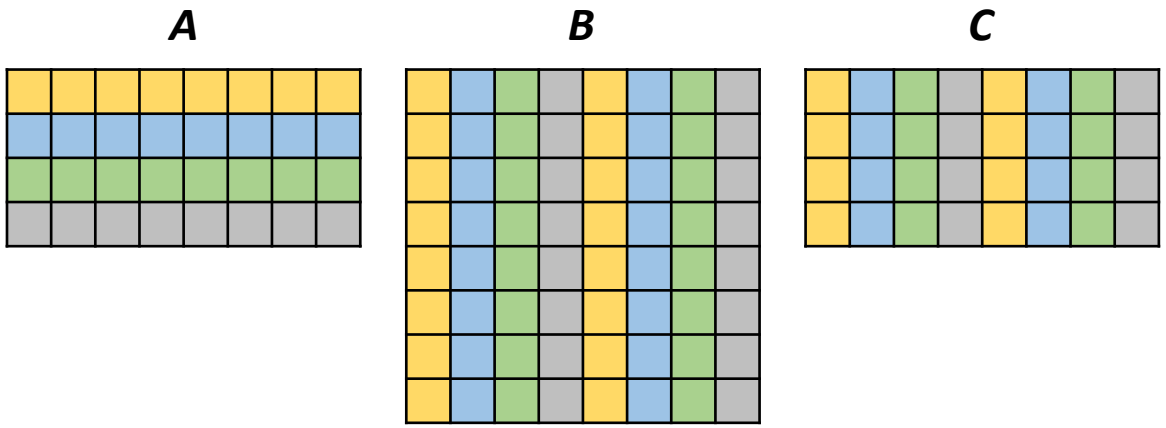
Full-frequency G_0W_0 calculation of COOH-Si/H_2O interface
1560 electrons, cutoff 60 Ry, PBE, ONCV PP
Ground state DFT with Quantum ESPRESSO



Overlapping communication and computation

CPU and GPU operations can be done asynchronously
- MPI communications
- CPU-GPU communications
- GPU computations

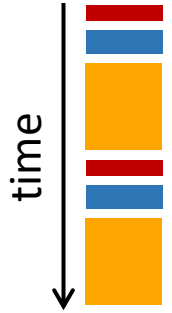
Example:
Distributed matrix multiplication ***A*** x ***B*** = ***C***



(each color represents an MPI process)

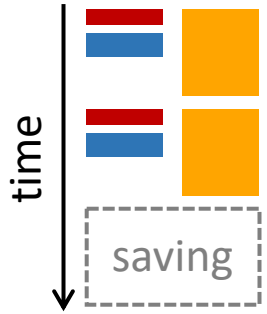
GPU v1

```
1 do i = 1, n_mpi
2   copy a_h to a_d
3   compute c_d(i) = a_d * b_d
4   circular shift a_h
5 end do
```



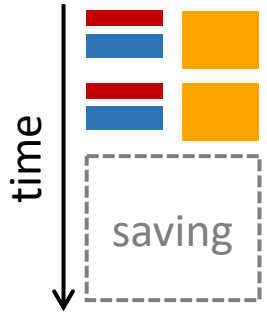
GPU v2 (async)

```
1 do i = 1, n_mpi
2   async circular shift a_h
3   copy a_h to a_d
4   compute c_d(i) = a_d * b_d
5 end do
```



GPU v3 (async + SP)

```
1 convert a_h to a_h_sp
2 do i = 1, n_mpi
3   async circular shift a_h_sp
4   copy a_h_sp to a_d_sp
5   convert a_d_sp to a_d
6   compute c_d(i) = a_d * b_d
7 end do
```



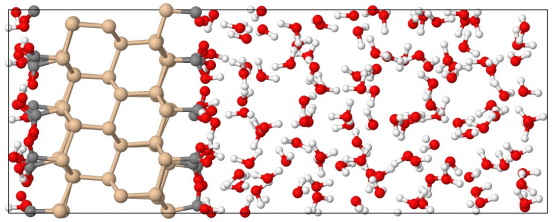
GPU porting and optimization strategies

v1: Initial GPU porting (baseline)

v2: Multi-level parallelization and data distribution
- Reduced CPU-GPU and MPI communication
- Improved load balance across GPUs

v3: Single-precision for selected operations
- Fast Fourier transforms (FFTs)
- Data communication (MPI)
- Quasiparticle energies match double-precision

v4: Additional optimizations
- Overlap between communication and computation
- GPU memory access
- MPI I/O



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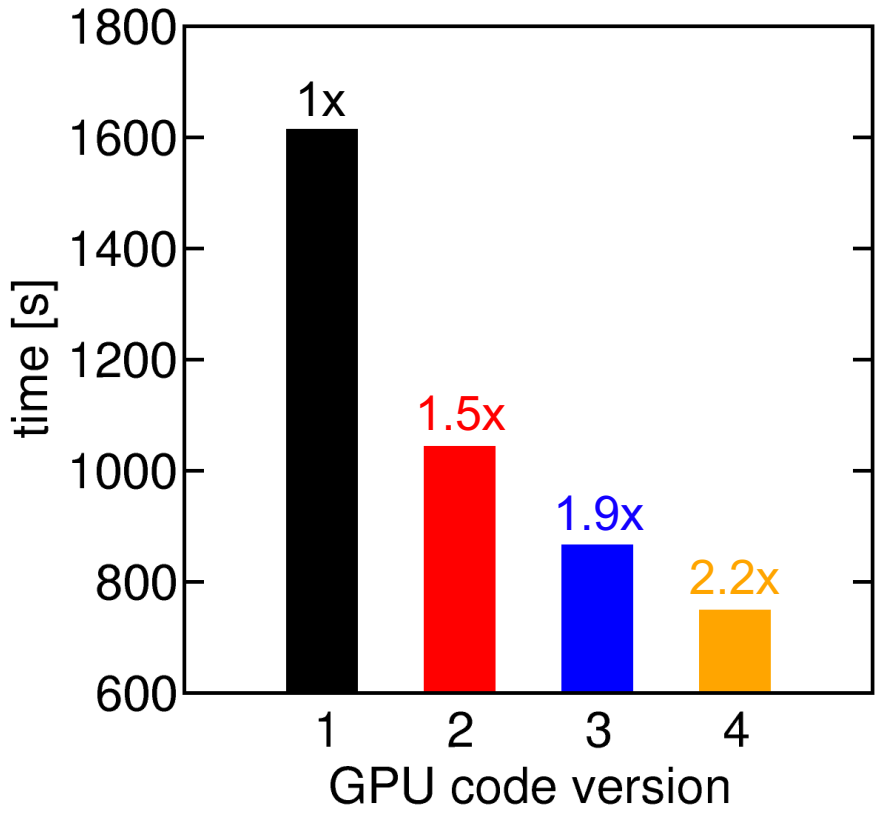
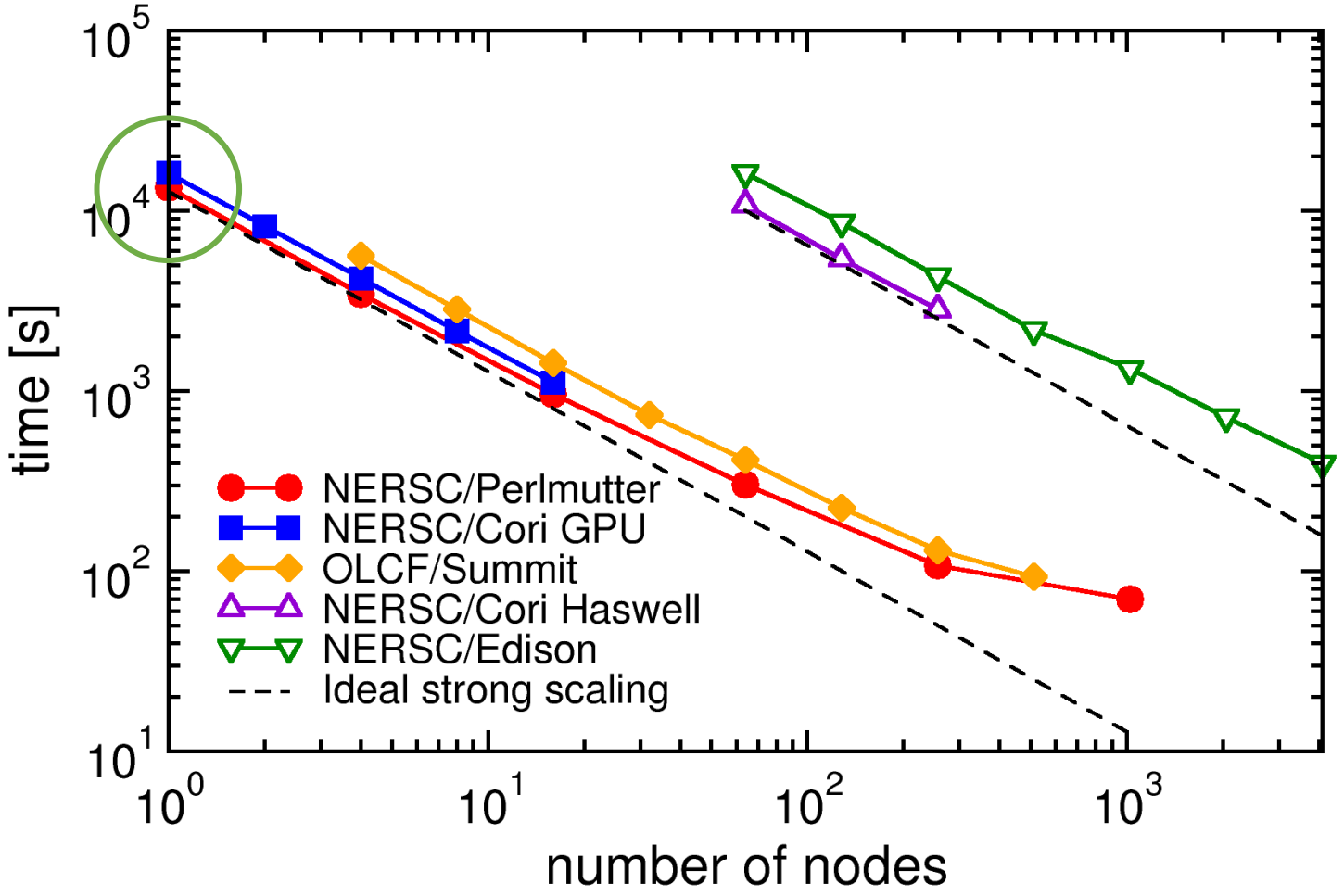
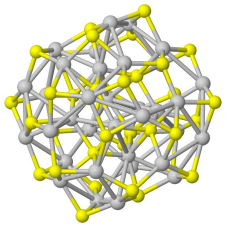


Performance benchmark



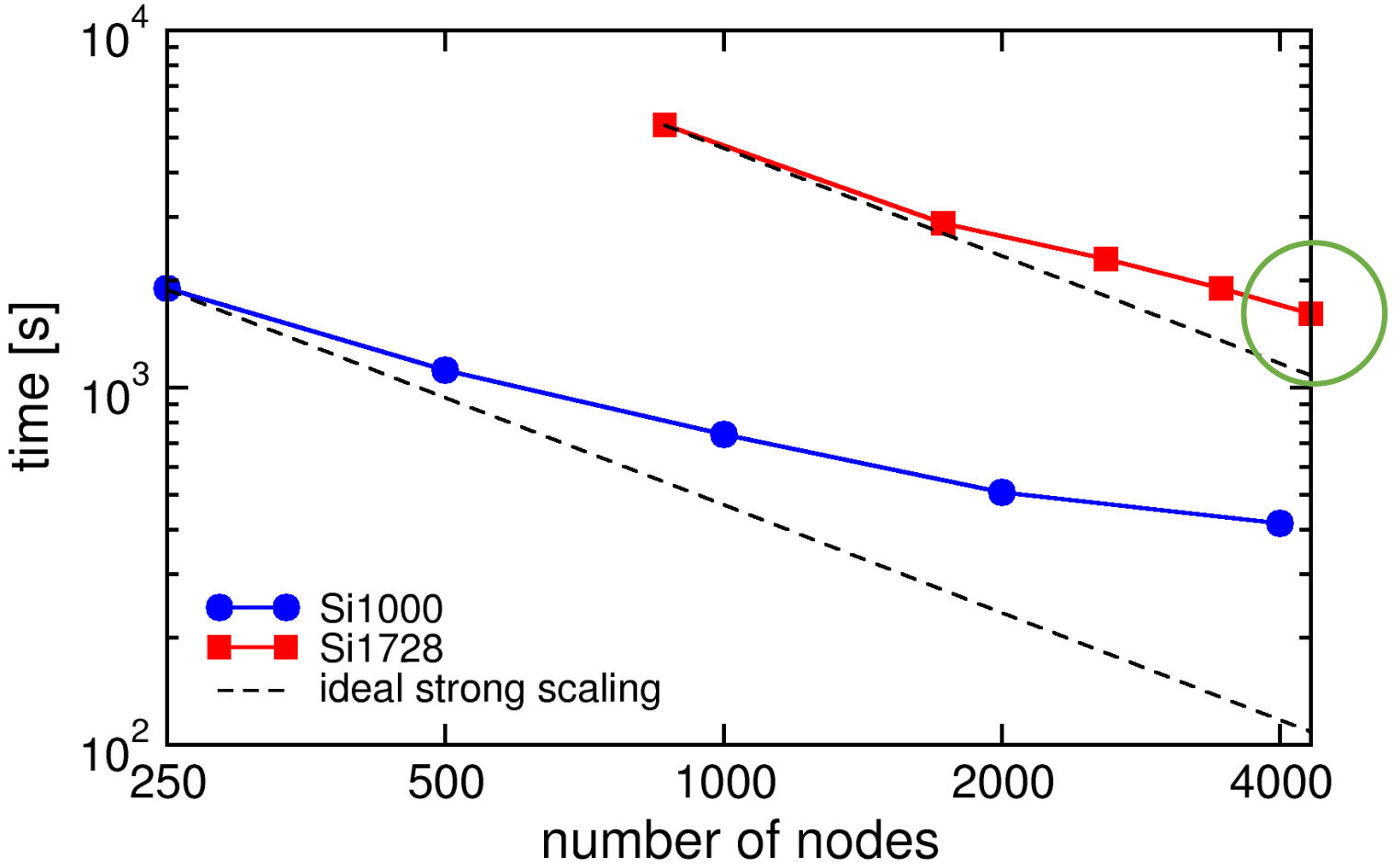
1 NERSC/Perlmutter node = 4 NVIDIA A100 GPUs
1 NERSC/CoriGPU node = 8 NVIDIA V100 GPUs
1 OLCF/Summit node = 6 NVIDIA V100 GPUs
1 NERSC/CoriHaswell node = 32 Intel Haswell CPU cores
1 NERSC/Edison node = 24 Intel Ivy Bridge CPU cores



Full-frequency G_0W_0 calculation of CdSe nanoparticle
884 electrons, cutoff 50Ry, PBE, ONCV PP
Ground state DFT with Quantum ESPRESSO

- Nearly ideal strong scaling demonstrated on various machines
- Time to solution on GPU nodes is less than **1/30** of that on CPU nodes
- **2x faster on A100** than on V100 (more memory, higher memory bandwidth, FP64 tensor cores)

Strong scaling to full Summit

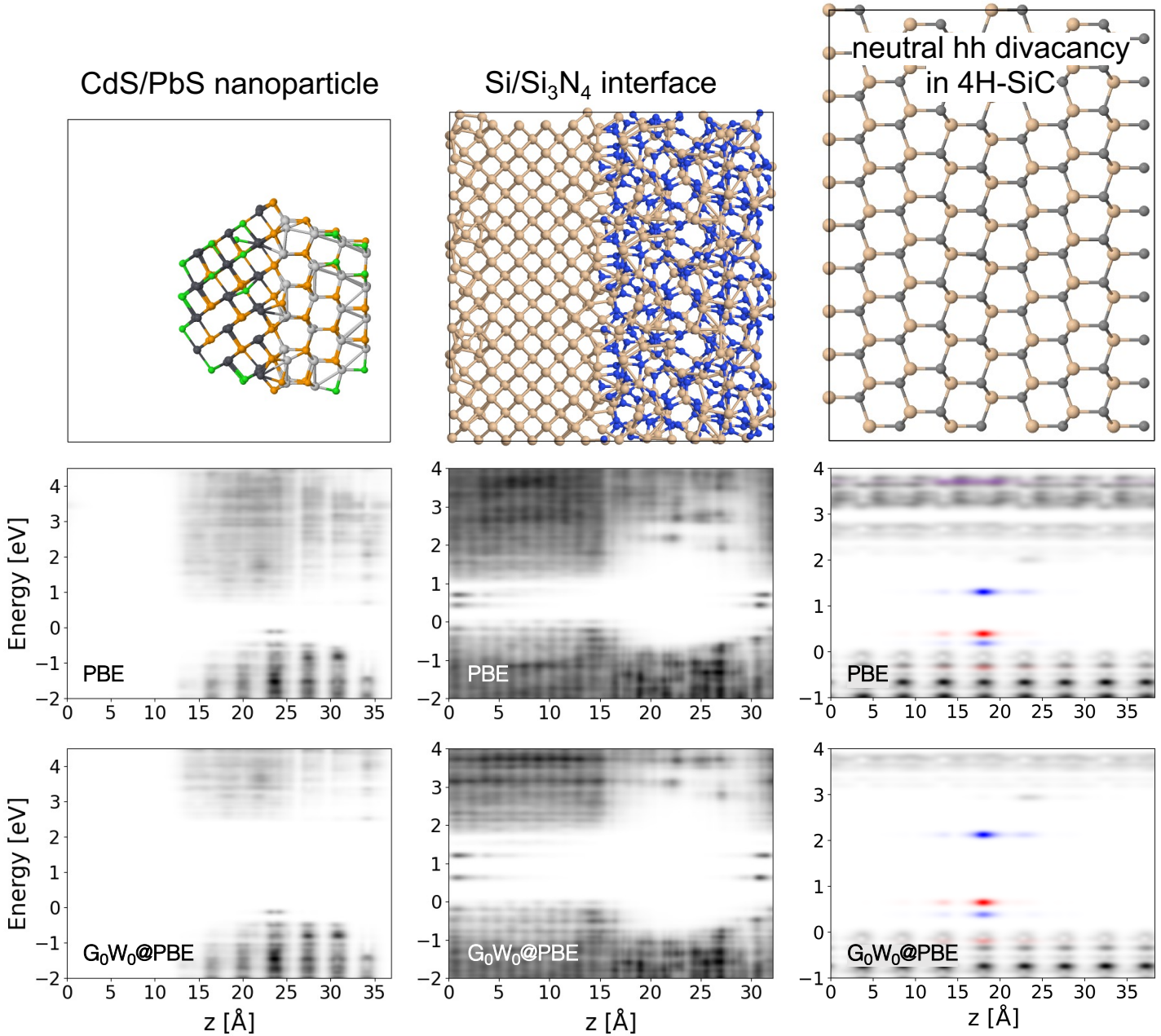


1 Summit node = 2 IBM POWER9 CPUs + 6 NVIDIA V100 GPUs

Full-frequency G_0W_0 calculation of 1000 or 1728 Si atoms
Ground state DFT with Quantum ESPRESSO

- WEST-GPU scales to the entire Summit supercomputer
- Better scalability observed for bigger system (1,728-atom silicon supercell) due to a higher computation-to-communication ratio
- 80 quasiparticle energies of the 1,728-atom silicon supercell solved in ~30 min using **25,920 V100 GPUs** (94% of Summit)

Large-scale full-frequency G_0W_0 calculations



Local density of states computed for prototypical systems representing our target applications:

- Large nanoparticles and interfaces
  → materials for energy conversion
- Defects in semiconductors
  → quantum information science (quantum computation, communication, and sensing)

system	N_{atom}	$N_{electron}$	N_{spin}	N_{PW}
CdS/PbS	301	2,816	1	948,557
Si/Si_3N_4	2,376	10,368	1	638,633
VV^0	1,598	6,392	2	314,653

Summary

The GW code in WEST has been ported to **NVIDIA GPUs**, with excellent **performance & scalability** achieved on various supercomputers including **Perlmutter**

Large-scale full-frequency G_0W_0 calculations demonstrated on OLCF/Summit

- **25k+** NVIDIA V100 GPUs
- **10k+** valence electrons

Next steps

- Demonstrate scalability to GPUs for quantum defect embedding theory (**QDET**) calculations (newly ported)
- Expand the GPU porting to cover BSE and electron-phonon **without empty states**
- Achieve performance portability targeting **exascale** systems (ALCF/Aurora, OLCF/Frontier)

http://west-code.org

Yu and Govoni, J. Chem. Theory Comput.18, 4690-4707 (2022)

Acknowledgments

NERSC NESAP Tier-1
- Dr. Brandon Cook (LBNL)
- Dr. Soham Ghosh (LBNL)
- NERSC/Cori-GPU
- NERSC/Perlmutter

Computational resources
- OLCF/Summit (ALCC and INCITE)
- ALCF/Theta-GPU (discretionary allocation)

ANL GPU Hackathon (April 2021)
- Dr. William Huhn (ANL; now Intel)
- Dr. Kristopher Keipert (NVIDIA)

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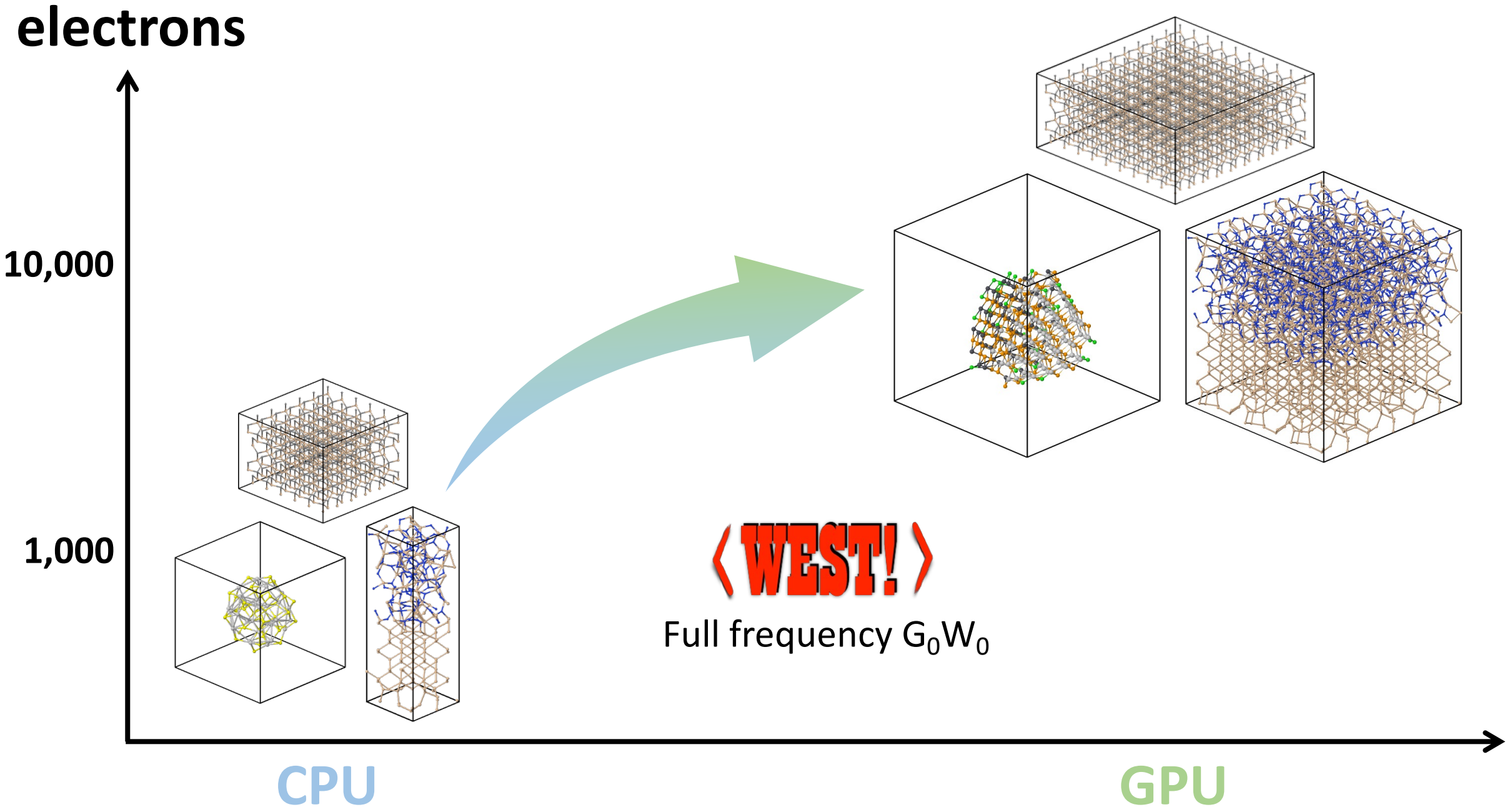
electrons
10,000
1,000
CPU
GPU
WEST!
Full frequency G_0W_0