# Facilitating Electronic Structure Computations on GPU based Exascale Platforms


Jean-Luc Fattebert

Computational Sciences and Engineering Division, Oak Ridge National Laboratory

**Team:**
Los Alamos National Laboratory: *Christian F. A. Negre, Michael E. Wall, Jamal Mohd-Yusof, Joshua Finkelstein, Yu Zhang*
Lawrence Livermore National Laboratory: *Daniel Osei-Kuffuor*
External: *Nick Bock* (Canonical)



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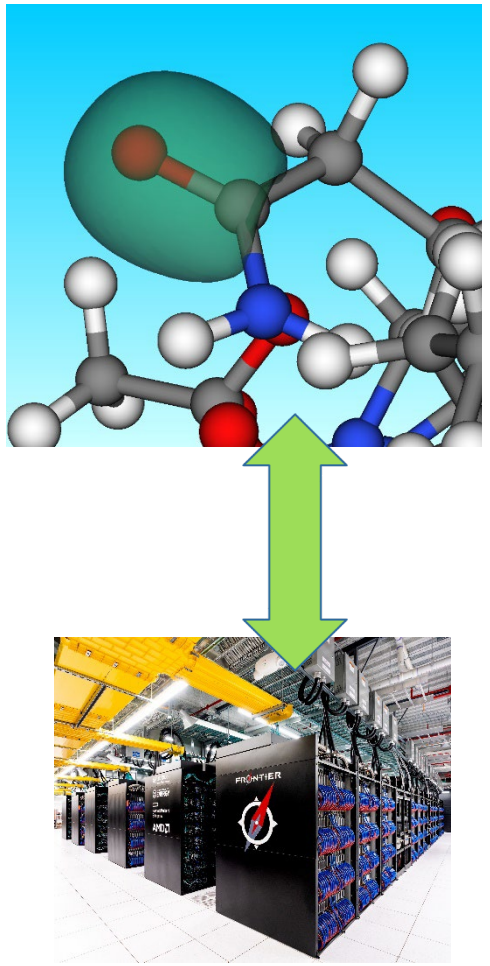
**The Exascale Computing Project (ECP)**
**Project Number: 17-SC-20-SC**


# Outline

- Motivations
- Computational strategy for Exascale hardware
  - OpenMP offload
  - Vendor libraries (cuSparse, RocSparse, MKL,…) and others (MAGMA,…)
- Solvers
  - Chebyshev dense solver on GPU
  - Distributed
- Some lessons learned

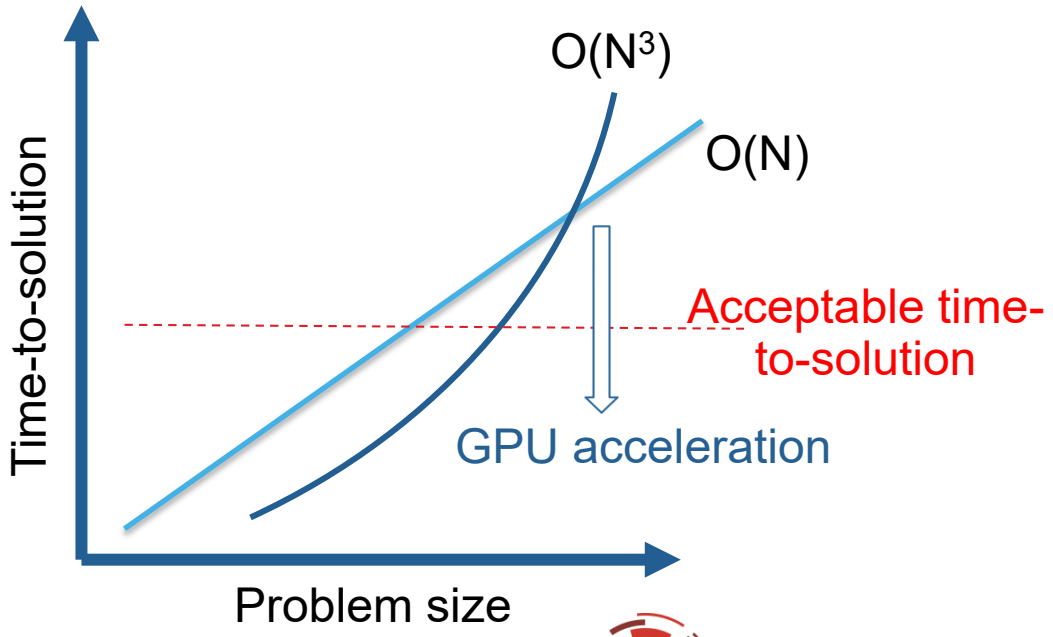
# Algorithms and performance portability for electronic structure

- Provide a library to handle the most expensive part of (some) electronic structure codes
  - Computation of single particle Density Matrix – Projector onto subspace associated with lowest eigenvalues of Hamiltonian
- Provide a library that can handle various matrix formats (dense, sparse, distributed) on various hardware (multi-core CPUs, GPUs, multi-nodes)
  - Users can explore algorithms with various matrix formats
  - Users don’t need to worry about implementation



# Speeding up electronic structure calculations to enable larger molecular dynamics (MD) simulations

- Time-to-solution is the limiting factor in *ab initio* molecular dynamics
  - How long are we willing to wait for tens of thousands of steps to complete?
- Using the power of GPUs to accelerate these simulations is not an easy task
  - We need enough concurrent operations to use GPU efficiently
  - Larger problems can use GPU resources better, but may lead to time-to-solution that is too long…



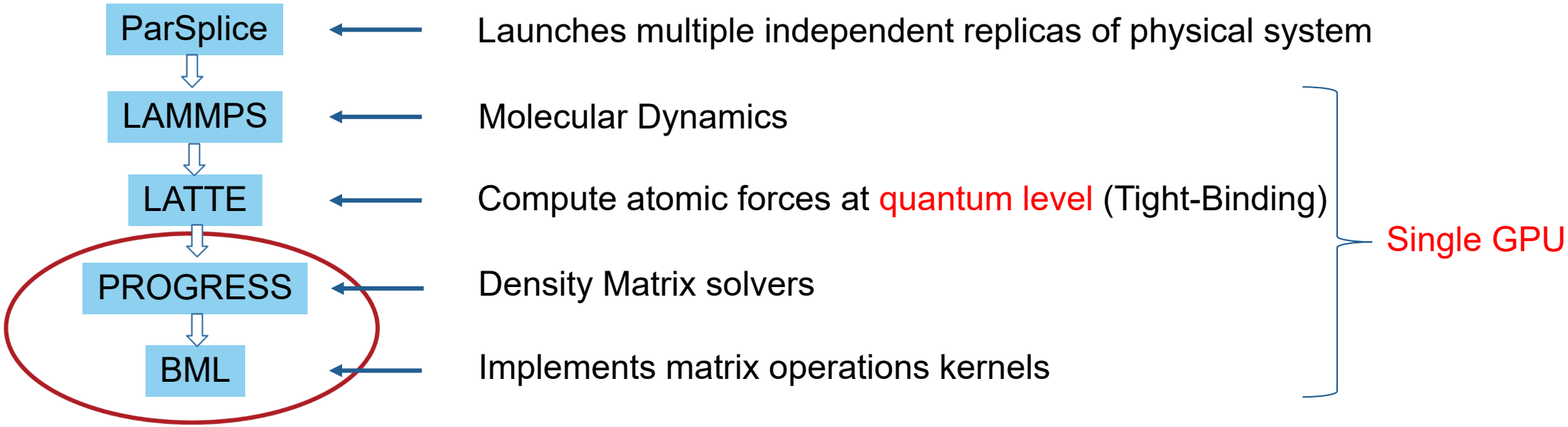
# Distributing work on several GPUs

- Needs very large problems
  - Each GPU needs enough work to be well utilized
- Time-to-solution in large problems may be too long for MD…

It is difficult to take advantages of multiple-GPUs to speedup Quantum MD

# Running MD on exascale platforms

- ECP Application Exascale Atomistic Capability for Accuracy, Length, and Time (EXAALT)
  - Running many MD simulations concurrently



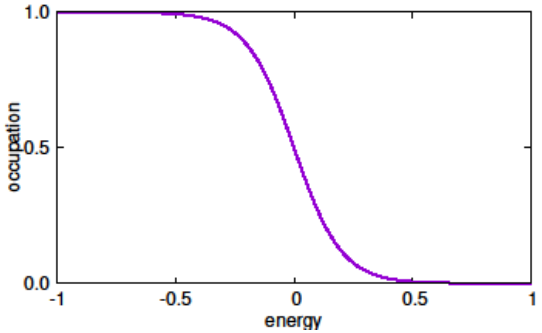
# Main numerical kernels for electronic structure calculations

- Eigensolver (Dense)
  - Eigenvectors of Hamiltonian corresponding to lowest eigenvalues
  - (For insulators) → projector onto space of occupied orbitals

Hamiltonian H (symmetric/Hermitian) → Eigenvalues/ eigenvectors $Hv_i = \varepsilon_i v_i$ → $(\varepsilon_i, v_i)$ → $P = VFV^T$

$$F = \begin{pmatrix} f(\varepsilon_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & f(\varepsilon_N) \end{pmatrix}$$

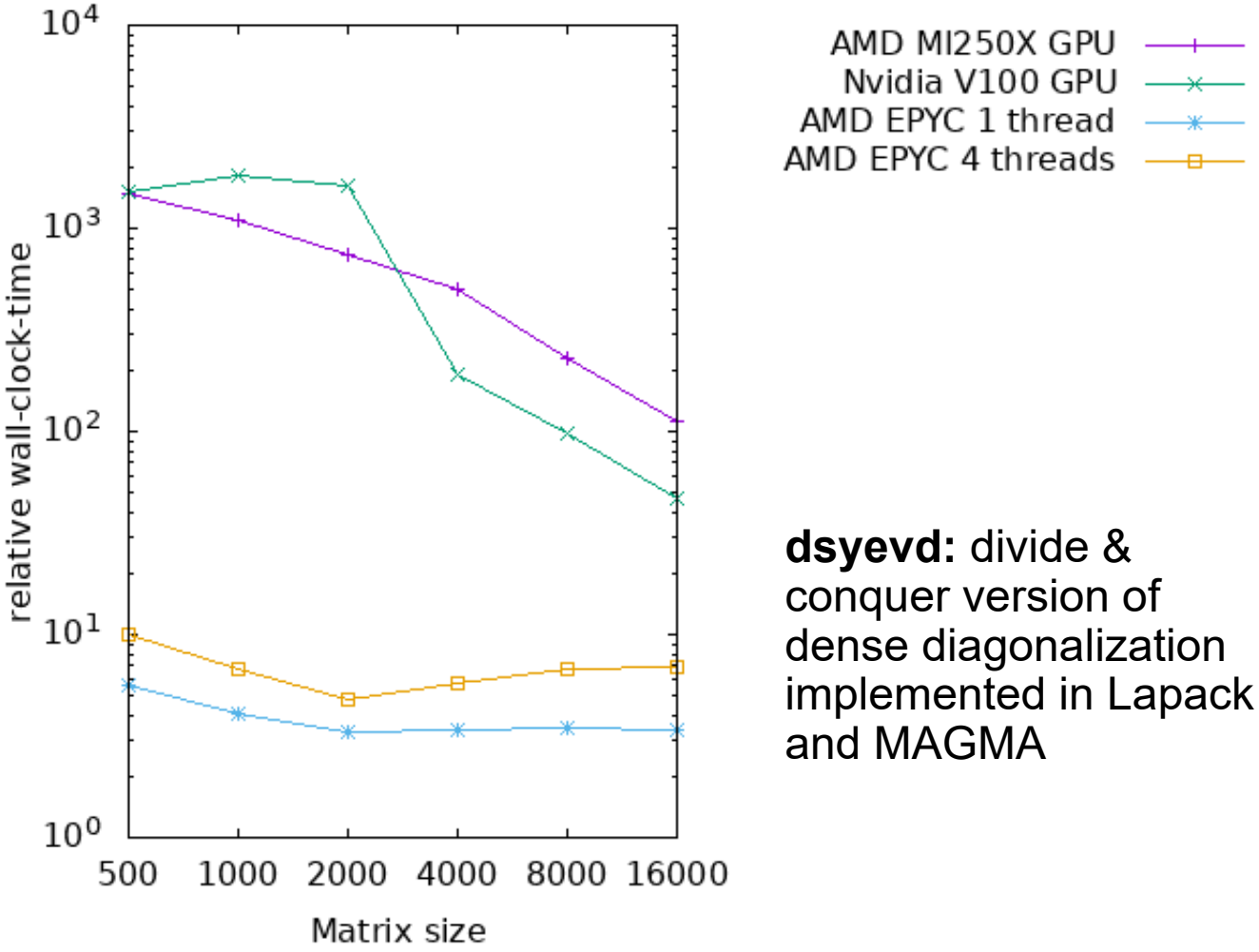
$$f(\varepsilon_i) = \frac{1}{1 + e^{\beta(\varepsilon_i - \mu)}}$$




  - P is a symmetric matrix with eigenvalues in [0,1]
  - Special case (insulators): $\varepsilon_{HOMO} < \mu < \varepsilon_{LUMO}$
    - P is a projector on subspace spanned by eigenvectors associated with lowest eigenvalues

# Underwhelming performance of dense diagonalization on GPU…

- Relative time-to-solution compared to dense matrix-matrix multiplication (dgemm) performance
  - Using Lapack dsyevd on CPU
  - Using MAGMA dsyevd_gpu on GPU
- Similar number of flops but large differences in time-to-solution, specifically for GPUs!




**dsyevd:** divide & conquer version of dense diagonalization implemented in Lapack and MAGMA

# Developing alternative solvers based on polynomials of matrices

- Iterative solver SP2 for systems with band gap

$$X_{n+1} = \begin{cases} X_n^2, & Tr(X_n) > N_e \\ 2X_n - X_n^2, & Tr(X_n) < N_e \end{cases}$$

with initial guess $X_0 = \dfrac{\epsilon_{max} I - H}{\epsilon_{max} - \epsilon_{min}}$

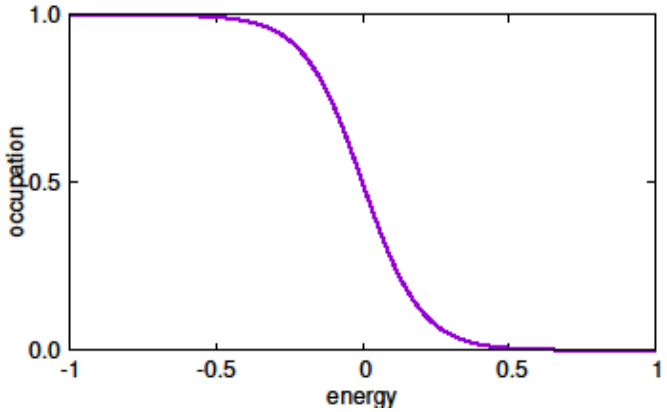
[Niklasson, Phys. Rev. B (2002)]

- Chebyshev polynomial expansion of density matrix for metals

Fermi-Dirac function

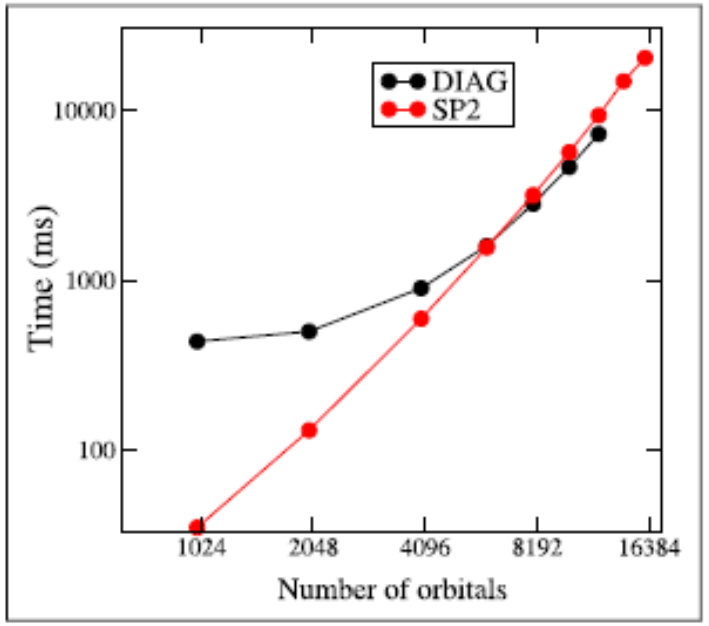
$$f(\varepsilon) = \frac{1}{1 + e^{\beta(\varepsilon - \mu)}} \longrightarrow f_H(H) = \left(I + e^{\beta(H - \mu I)}\right)^{-1} \approx \sum_{i=1}^{N} c_i T_i(H)$$

[Goedecker and Teter, Phys. Rev. B (1995)]



# Many of these ideas were introduced to reduce complexity from $O(N^3)$ to $O(N)$

- Full diagonalization in $O(N^3)$
- "Sparse matrix × sparse matrix" multiplication is O(N)
  - O(N) solver provided one can drop off "small" off-diagonal terms that creep in at every iteration
- On GPUs, dense versions of these solvers are competitive with direct diagonalization




SP2 vs. cuSolver on Nvidia V100
[Mniszewski et al., IJHPCA, 2021]

Fastest algorithm on GPU may not be the fastest on CPU

# PROGRESS and BML libraries

# Implementation divided into two libraries

- **BML**: Basic Matrix Library
  - Linear algebra matrix operations used in solvers
  - https://github.com/lanl/bml
- **PROGRESS**: Parallel, Rapid O(N) and Graph-based Recursive Electronic Structure Solvers
  - Solvers: SP2, Chebyshev, …
  - https://github.com/lanl/qmd-progress

# Using OpenMP for GPU offloading

- OpenMP, an implementation of multithreading
  - simple and flexible interface for developing parallel (shared memory) applications
- Usage
  - Add pragmas to C/C++/Fortran loop
- OpenMP 4.5 and beyond
  - Support for offloading to GPU
- Portable
  - Supported by many compilers
  - Turned on with compiler option

```
#pragma omp target map(from: b) map(to:a)
#pragma omp teams distribute parallel for
for (int i = 0; i < 1000; i++){
    b[i] = 2 * a[i];
}
```

# GPU Offload strategy in BML

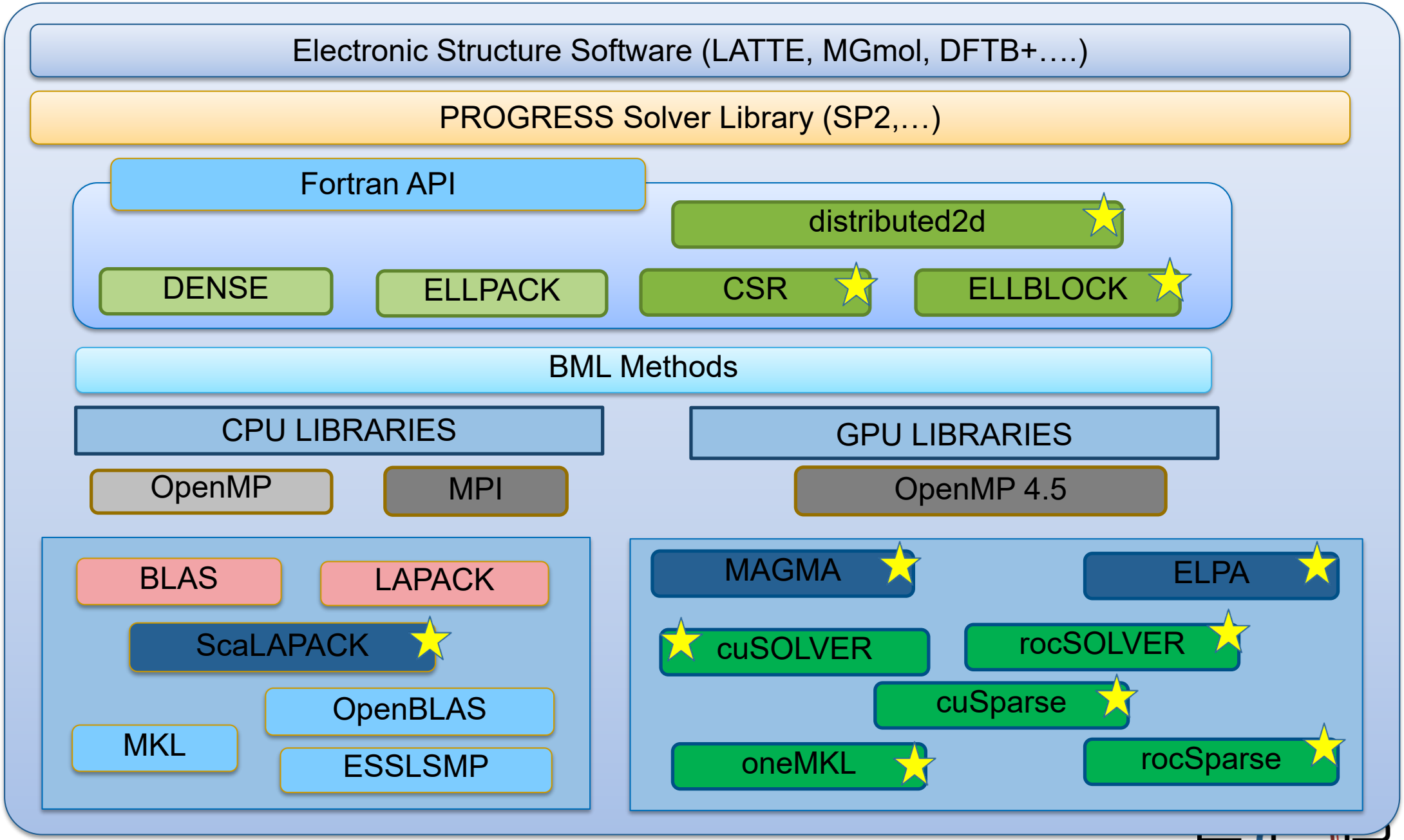
- Initial plan was to use ‘pure’ OpenMP offload
- Experience
  - Poor performance on critical kernels (sparse-sparse multiply)
  - Do not expect OpenMP to allow fine-grain tuning needed any time soon…
- Current strategy is a hybrid offload programming model
  - OpenMP offload semantics for memory management, data motion
  - Vendor/hardware-specific libraries for critical kernels
  - Some OpenMP native code for non-critical kernels

# General implementation strategy

- CPU
  - C + OpenMP + MPI + BLAS/Lapack/ScaLapack
- GPU
  - OpenMP offload (OpenMP4.5)
  - Rely on MAGMA, ELPA and vendor libraries for performance critical kernels

# Computer Science challenges

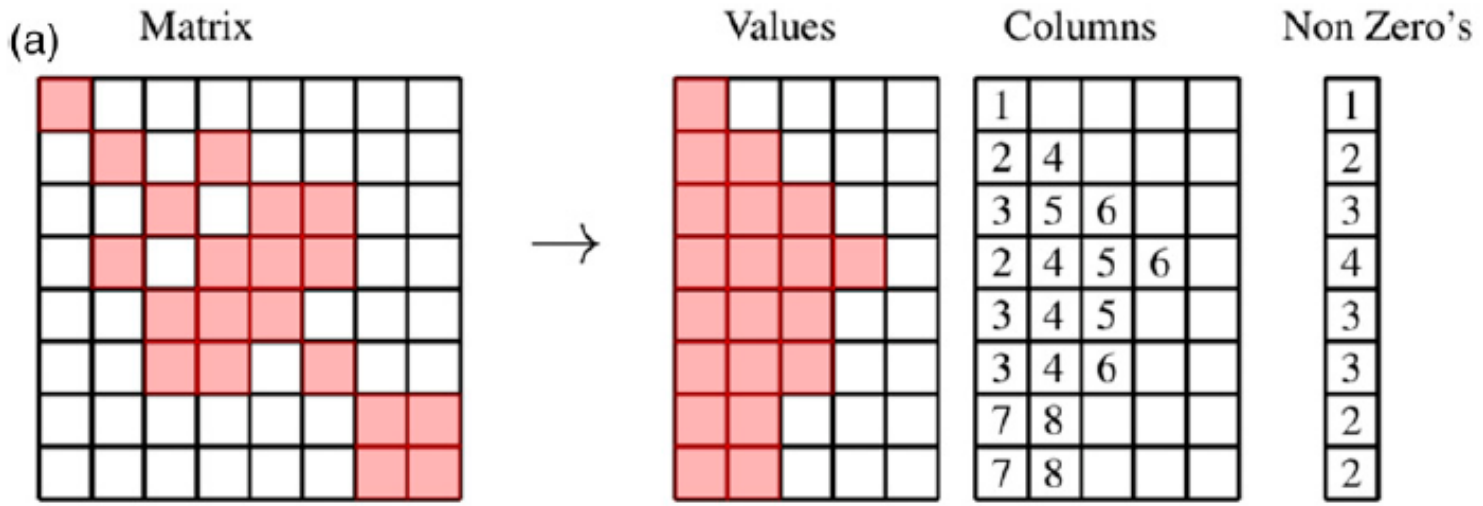
- Support various architectures
  - GPU: NVIDIA, AMD, Intel
  - no portable library for sparse × sparse matrix multiplication
- Interfaces with various vendor libraries
  - cuSparse, cuSolver, rocSparse, rocSolver, MAGMA, MKL, ScaLapack, ELPA,…
  - We do the work so that users don’t need to understand interfaces to these packages…
- Make OpenMP offload and various libraries coexist
  - Deal with changes in software stack, compiler versions,…



# BML: supported (shared memory) matrix formats

- Dense
- ELLPACK
- CSR
- ELLBLOCK

Focus for GPU offload



# BML: Supporting multiple data types in a C code

- Single precision
- Double precision
- Optional:
  - Single-precision complex
  - Double-precision complex

"k-points" calculations for periodic systems

- Strategy
  - Compile (mostly) same C code several times with different C macros

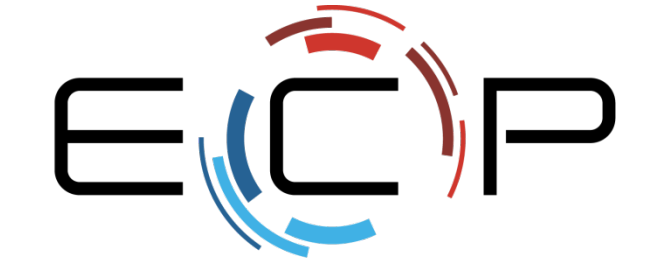
# BML: Fortran interface is important for targeted application codes

- Hand-coded wrapper functions
- Not “automatic,” but low overhead in code writing
- Interface relatively stable

# BML: Unit test/Continuous integration

- Over 1,000 unit tests
  - including four different data types and five matrix formats
  - Ctest for developers
- Continuous Integration
  - Pull Requests tested on CPUs with github
  - on GPU using Ascent @ Oak Ridge Leadership Computing Facility (OLCF)
    - Currently testing dense format using MAGMA
- Tracking “issues” on github

# Offloading to GPU



# Offloading strategy

- Dense format on Nvidia and AMD
  - Rely on MAGMA
  - Use some vendor libraries when better performing (example: dense diagonalization in cuSolver)
- Dense format on Intel and Sparse formats on Nvidia, and AMD
  - OpenMP for memory allocation, CPU-GPU data transfer and various other operations
  - Use vendor libraries for performance critical kernels

# GPU offloading with OpenMP

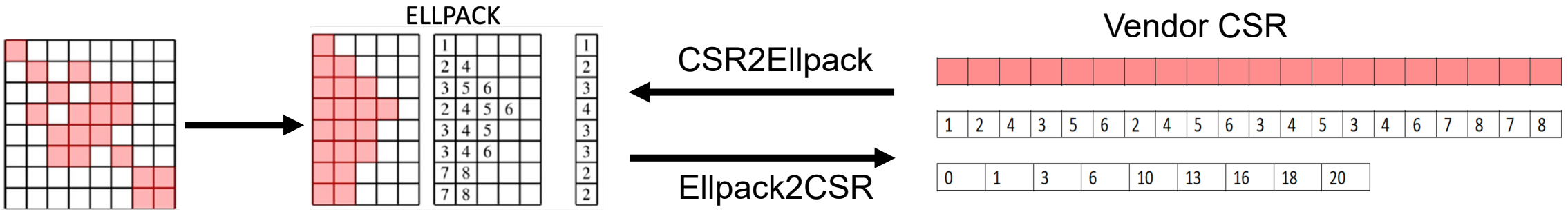
- Matrices are “C struct”
- Mapping to GPU matrix data only, not the whole struct
  - Pointer to datatype

```
REAL_T *A_matrix = (REAL_T*)A->matrix;
#pragma omp target enter data map(alloc:A_matrix[0,sizea])
#pragma omp target update to (A_matrix[0:sizea])
```

  - Full control of data movement between CPU and GPU

# Challenges in interfacing with optimized vendor libraries

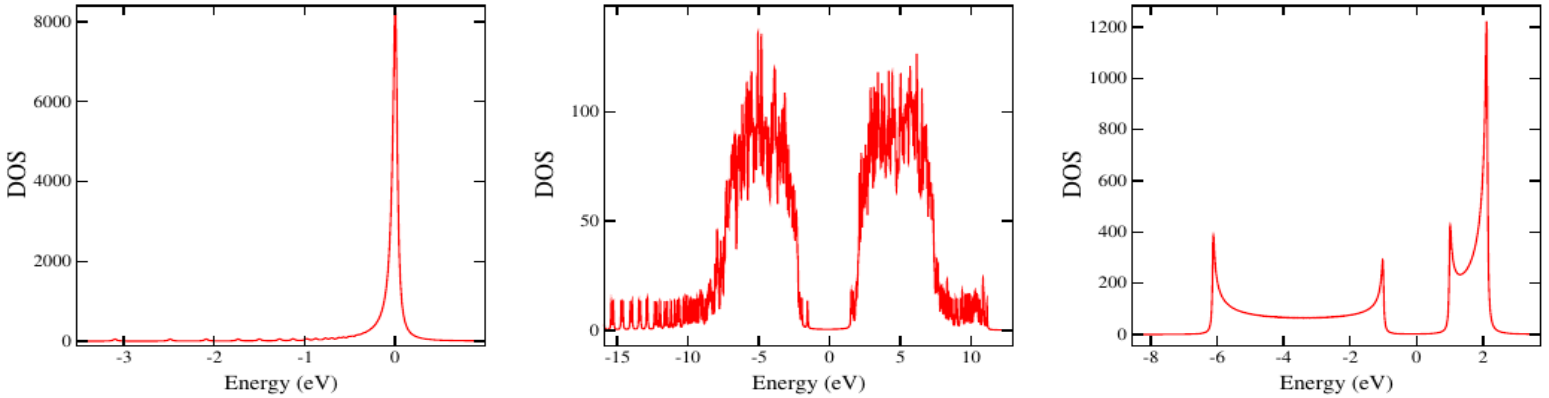
- Data mapping between BML ELLPACK and vendor sparse formats (CSR) on device




- Some functions in libraries require data to be “ordered” in each row
- cuSparse
  - Workspace required is so large, makes it not practical (CUDA11)
  - implementation of: C’ = $\alpha$A*B + $\beta$C expects sparsity pattern of C and A*B to be consistent with each other

# Using a synthetic Hamiltonian matrix for Performance Benchmarking

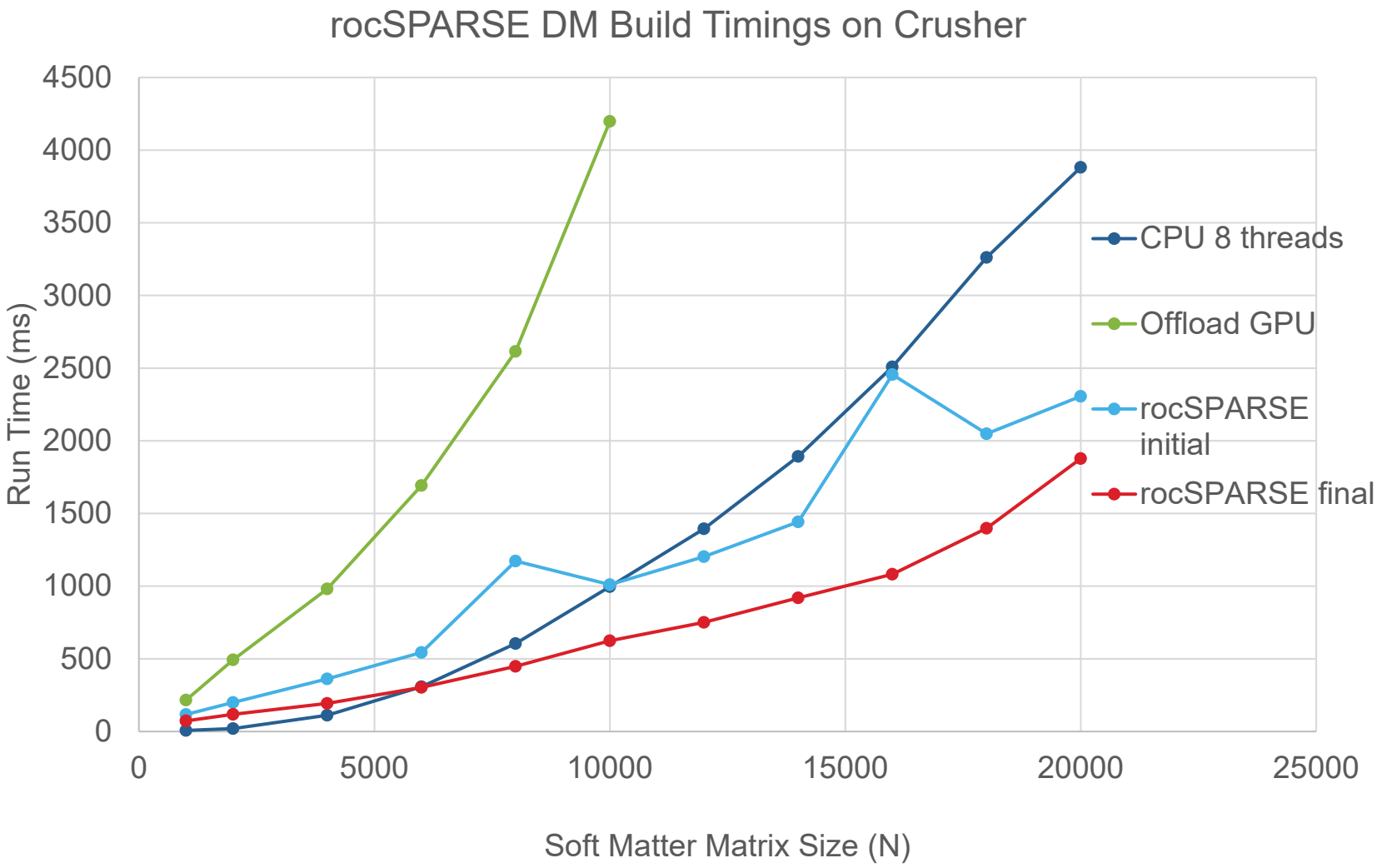
- Typical benchmarking requires storing large matrices
- There are no good standard benchmark suite for performance in electronic structure
- We use a synthetic Hamiltonian based on a simple two-orbitals/atom Tight-Binding model
  - Parameters for coupling, onsite energies, distance exponential decay, random noise factor






EXASCALE COMPUTING PROJECT

# rocSPARSE performance on Crusher @ OLCF




Profiling, fixing implementation issues

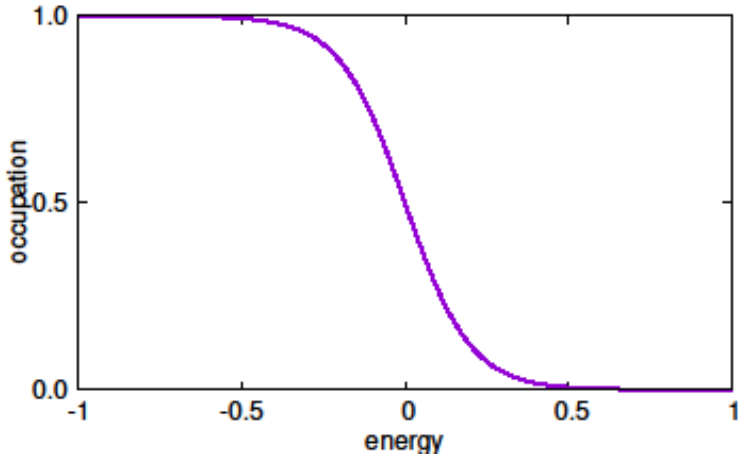
# Chebyshev expansions for modest matrix sizes (metals)

# Chebyshev expansion of Density Matrix

- An alternative to inefficient dense diagonalization on GPU is to use a Chebyshev polynomial expansion

$$D = (I + e^{\beta(H-\mu I)})^{-1} = f(H)$$

$$\sum_n c_n T_n(H) \approx f(H)$$




- Problem
  - Expansion can involve over 100 terms and be computationally very costly too

# Patterson and Stockmeyer trick [SIAM J. Sci. Comput. 1973]

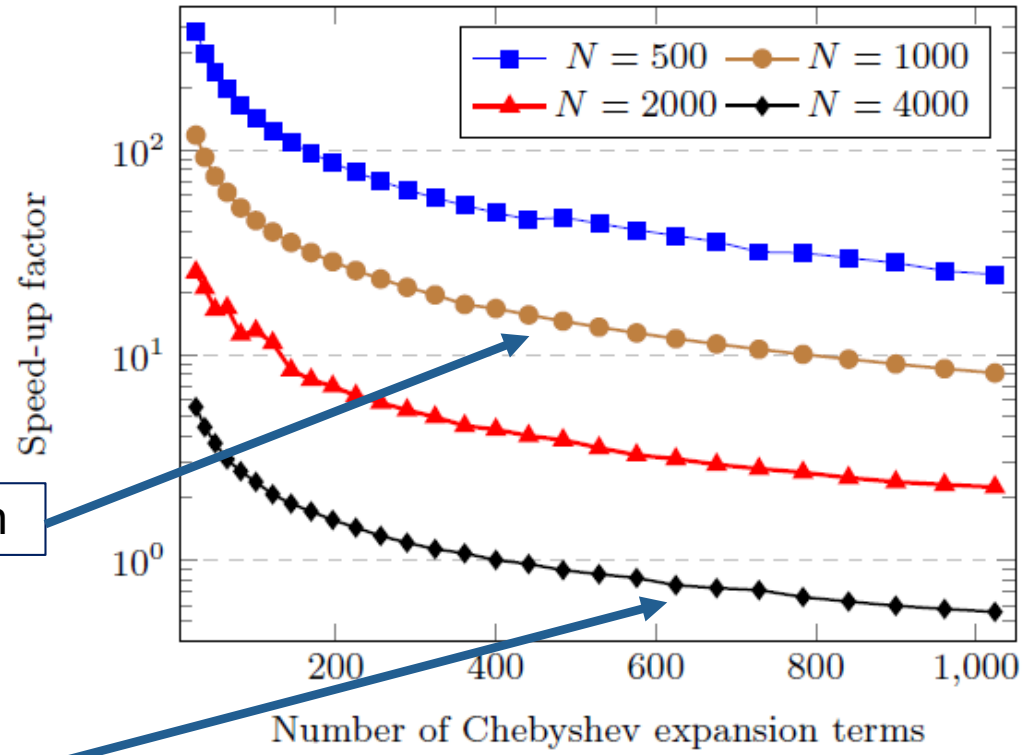
- For $km$ number of terms, $k-1+m-2$ multiplications for $x$ needed
- So, for $K$ terms in an expansion, only need ~$2\sqrt{K}$ multiplications of $H$
- Substantial savings when x is a matrix and cost dominated by matrix multiplications!
- Adapted for Chebyshev and DM calculation

$$
\begin{aligned}
&a_{km-1}x^{km-1} + \cdots + a_1 x + a_0 \\
&= (\cdots\cdots(((\underbrace{a_{km-1}x^{k-1} + \cdots + a_{k(m-1)+1}x + a_{k(m-1)}}_{\text{sum}_{m-1}})x^k \\
&\quad + \underbrace{a_{k(m-1)-1}x^{k-1} + \cdots + a_{k(m-2)+1}x + a_{k(m-2)}}_{\text{sum}_{m-2}})x^k \\
&\quad \vdots \\
&\quad + \underbrace{a_{2k-1}x^{k-1} + \cdots + a_{k+1}x + a_k}_{\text{sum}_2})x^k \\
&\quad + \underbrace{a_{k-1}x^{k-1} + \cdots + a_1 x + a_0}_{\text{sum}_1}
\end{aligned}
$$

[Liang, Baer, Saravanan, Shao, Bell, Head-Gordon, J. Comput. Phys. (2004)]

# Chebyshev expansion compared to direct diagonalization

- Time-to-solution on Nvidia V100
  - Baseline is cuSolver
  - Speedup more important for smaller matrices

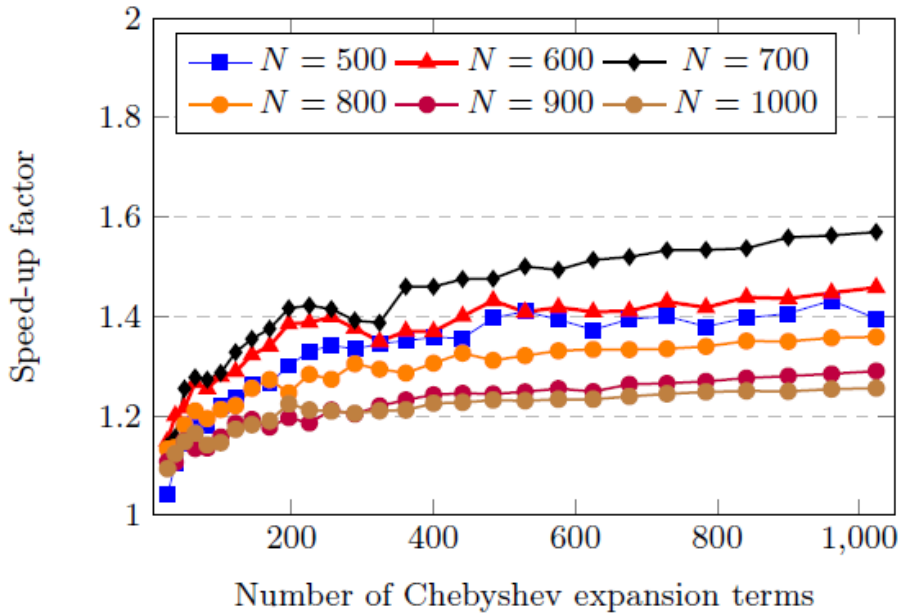


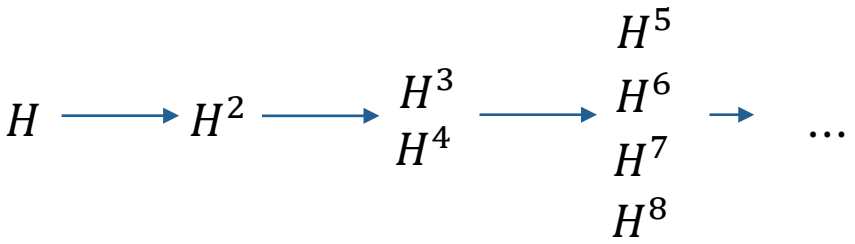

Chebyshev much faster than Diagonalization

Diagonalization faster than Chebyshev

# Exploiting GPU concurrency in calculating Chebyshev terms

- For “small” matrices, a single matrix-matrix multiplication does not fully utilize a GPU
- Several Chebyshev terms can be computed concurrently and use GPU streams for an additional speedup



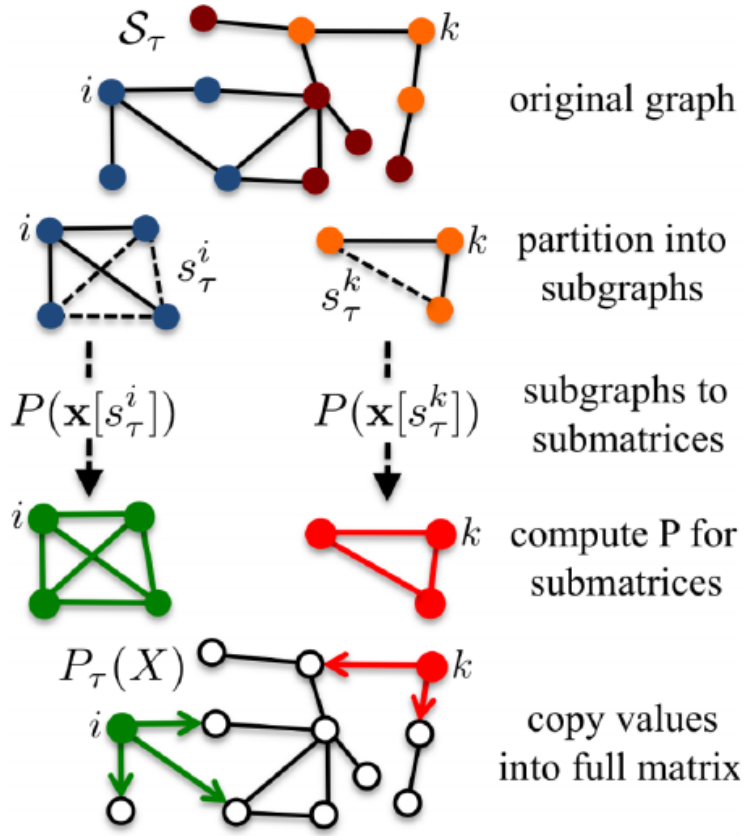




# Distributing computation

1. D&C based on matrix elements
2. Distributed Linear Algebra

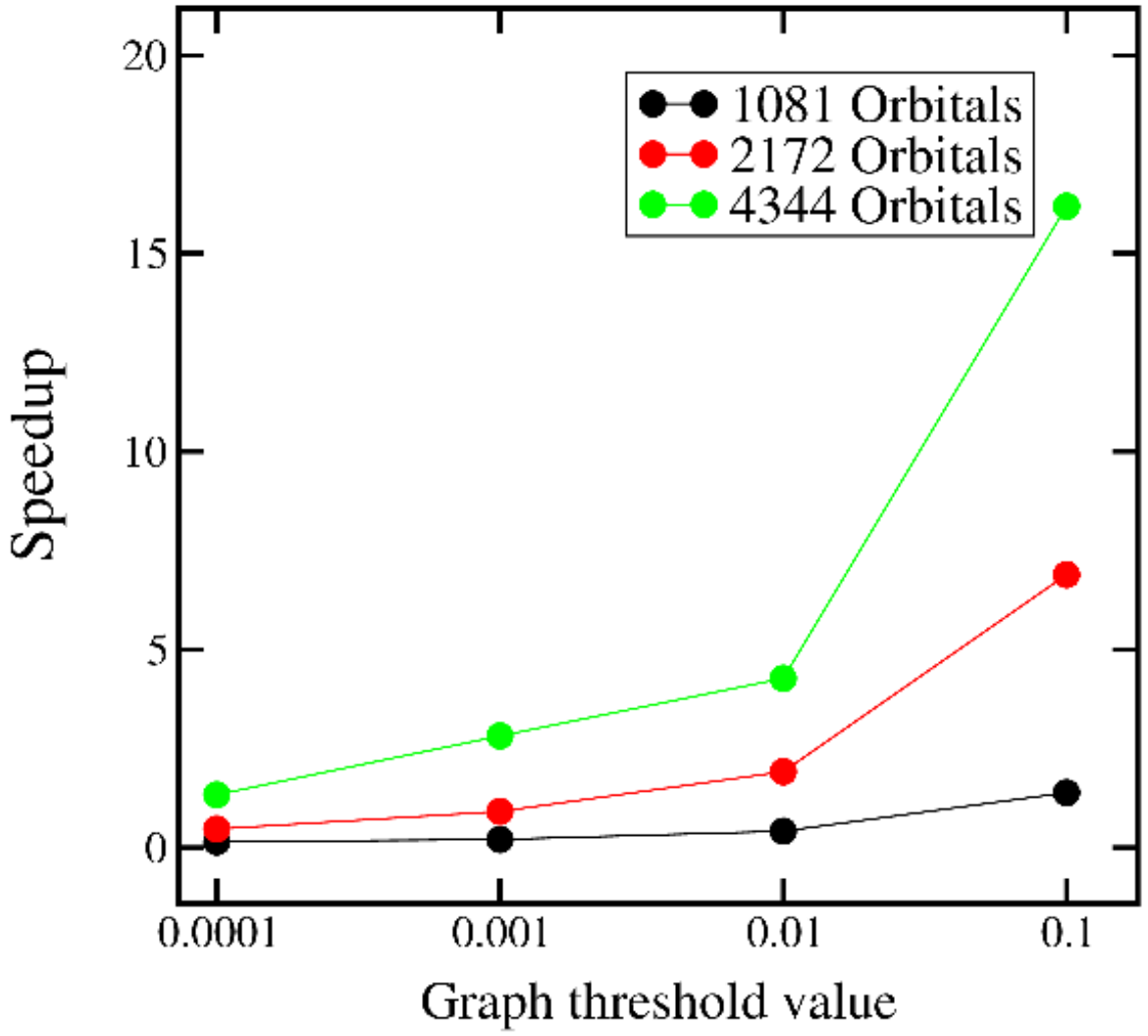
# Graph-based distributed solver implemented in PROGRESS

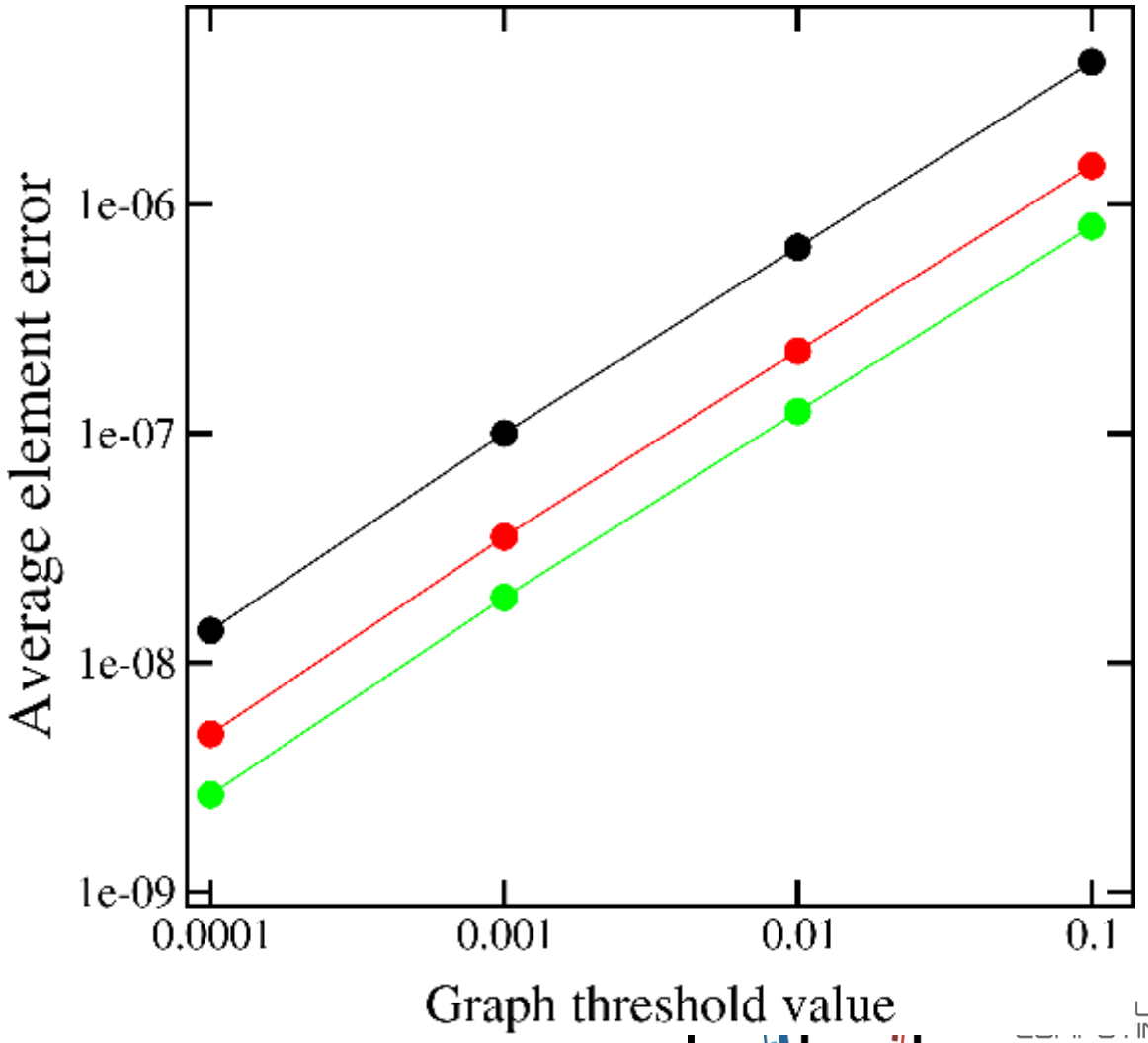
- Computations are distributed following a divide and conquer (D&C) approach
- Automatic and adaptive partitioning of matrix using graph-based thresholding
- Sub-systems solved concurrently using single-node solvers developed in project
- O(N) for given threshold/subsystem size




[Niklasson, Anders M. N., Susan M. Mniszewski, Christian F. A. Negre, Marc J. Cawkwell, Pieter J. Swart, Jamal Mohd-Yusof, Timothy C. Germann, et al. 2016. "Graph-Based Linear Scaling Electronic Structure Theory." *The Journal of Chemical Physics* 144 (23): 234101.]

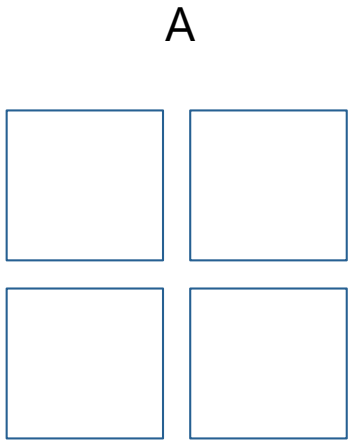
# Balancing computational cost and accuracy with matrix thresholding



# Distributed BML format: “distributed2d”

- 2D matrix decomposition using MPI
  - P x P tasks layout
  - Square submatrices
- Each submatrix is a “shared memory” BML matrix
  - Leverage developments for shared memory formats




```
struct bml_matrix_distributed2d_t
{
   bml_matrix_t *matrix;
   MPI_Comm comm;
   int ntasks;
   int nprows;
   int npcols;
   int myprow;
   int mypcol;
   int mpitask;
   …
}
```

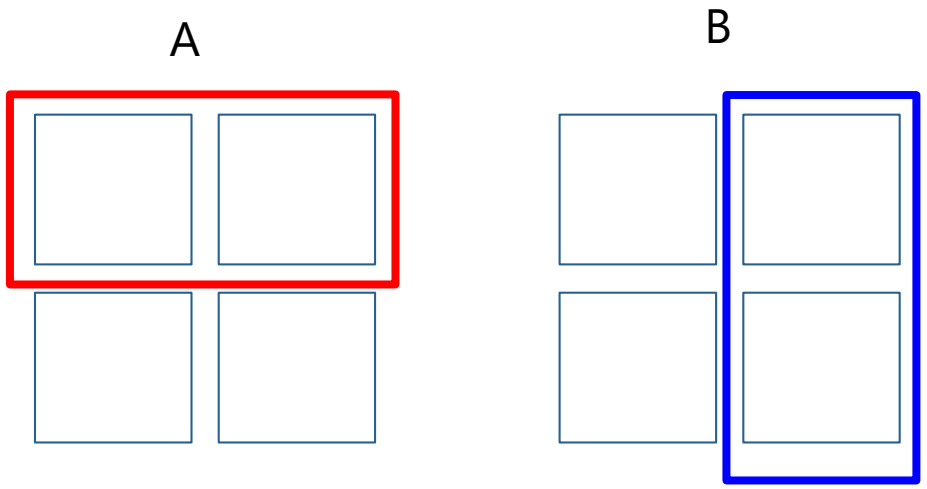
Local sub-matrix in dense, ellpack, csr, ellblock format

# A non-intrusive implementation

- “Wrapper” calling sub-matrix operations when possible
  - “distributed2d” operations combinations of “shared memory” matrix operations
  - Shared memory code untouched
- Some operations simply need reduction at the end
  - Frobenius norm,…
- Some operations require substantial communications
  - multiplication, transpose,…
- Some operation are more intrusive
  - Bounds on eigenvalues using Gershgorin circles
- Some operations are beyond scope
  - Eigensolver: interface with existing solver (ScaLapack and ELPA)

# Distributed BML format: matrix-matrix multiplication

- Implemented Cannon's algorithm for matrix-matrix multiplication
  - P-length loop over matrix blocks
  - 2 point-to-point communications at each step
    - "shift" blocks to enable computation of local block in product

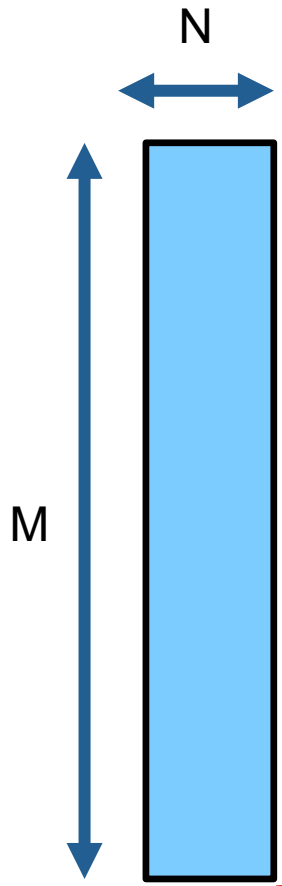



C01 = A00 x B01 + A10 x B11

# What about wavefunction-based solver? (Planewaves…)

# Numerical Discretization of DFT problem

- Plane-Waves or Finite Differences
  - Large number of degrees of freedom (DOF) / electronic wave function
- Solution
  - M x N “tall-and-skinny” matrix of coefficients
  - Number of DOF/ wave function M ~1,000 x number of wave functions N
- Hamiltonian very sparse, but very large!



# Eigenvalue problem in wavefunction-based solver (Plane Waves,…)

- Project eigenvalue problem into smaller dimension to compute Density Matrix
  - Solve eigenvalue problem

$$\Psi^T H \Psi V = \Psi^T \Psi V \Lambda$$

Wavefunctions define smaller dimension space

Generalized dense eigenvalue problem

$$\rightarrow AV = SV\Lambda$$

Small problem compared to basis set size!

- Build new trial eigenvectors of H

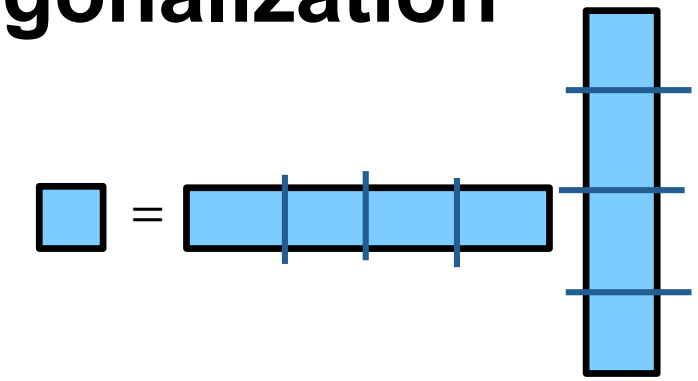
$$\Psi \rightarrow \Psi V$$

- Update wave functions using preconditioned gradient

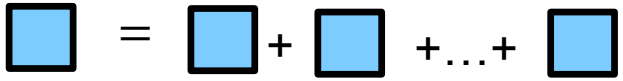
$$\Psi \rightarrow \Psi - \square KR$$

# Proxy-app: Loewdin orthogonalization

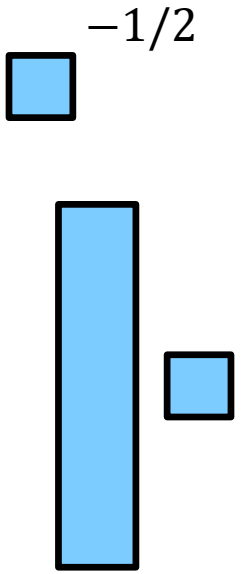
- Distributed computation of Gram matrix S = $\Psi^T\Psi$



- Accumulate S on each GPU (communication)



- compute $S^{-1/2}$ on each GPU (replicated computation)

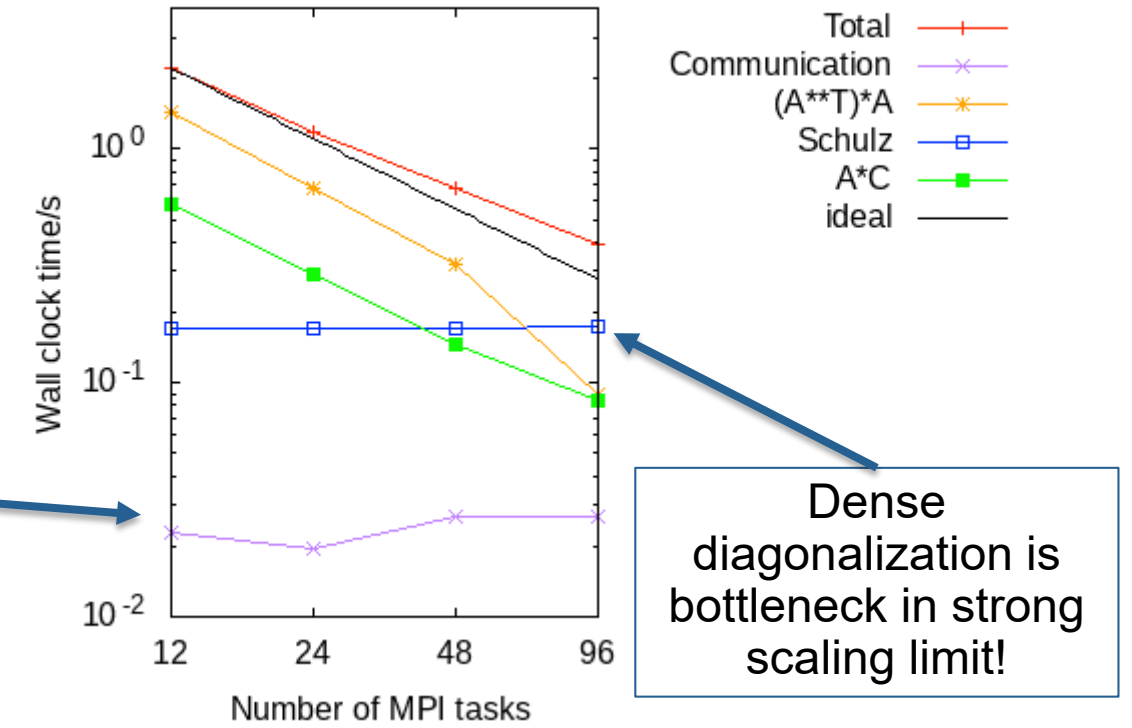


- Apply $S^{-1/2}$ to $\Psi$

Diagonalization would involve the same operations!

# Parallel scaling/performance on Summit

- Matrix 3,000,000 x 3,000
- Dense iterative solver converges in 7 iterations
- Time-to-solution better than 1 s
- Collective communications using NCCL library




[Lupo Pasini, Turcksin, Ge, Fattebert, Parallel Computing (2020)]

# Lesson learned: Efficiently using GPUs requires a lot of work!

- OpenMP alone not always sufficient to get “good” performance
- Relying on vendor libraries can help
  - requires understanding well interfaces, requirements,… for each library
- Building a software stack supporting multiple GPUs and third-party libraries is a challenging task
  - there are still a number of Computer Science challenges on exascale architectures…
- More GPU-friendly algorithms can provide substantial speedup on GPU accelerators and enable faster time-to-solution in electronic structure calculations

# Acknowledgments

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