

SIAM PP 2022
February 23rd – 26th

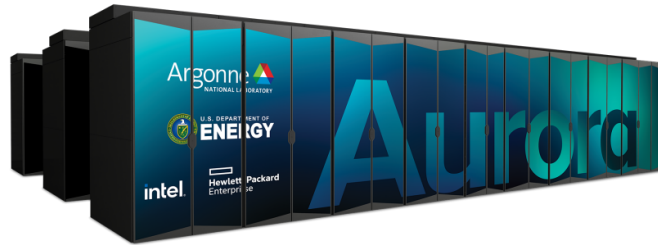
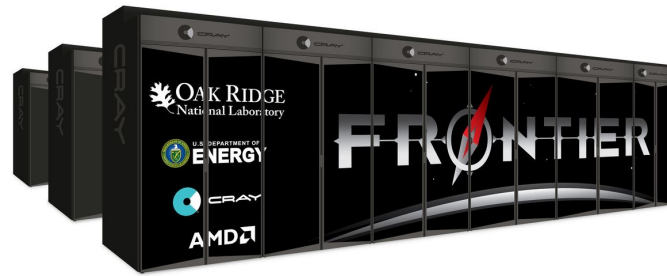
Beyond 2D Parallelization of Multi-Dimensional FFTs

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Current Hardware Trends in the Exascale Era

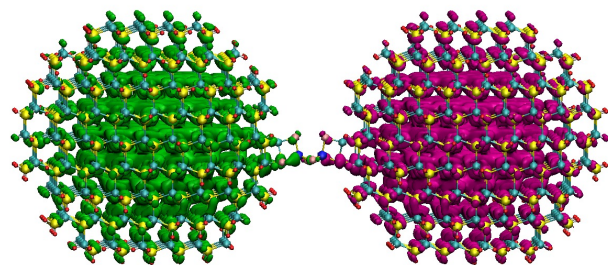


Thousands
of
Compute
Nodes

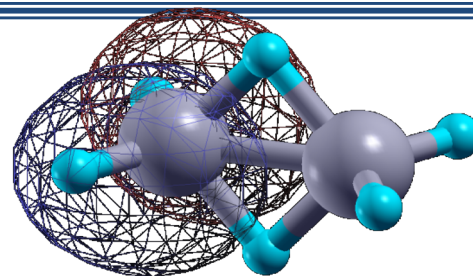
Computation Needs to Scale on these Systems



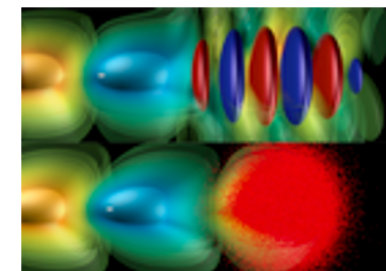
Fourier Transforms Ubiquitous in Scientific Applications



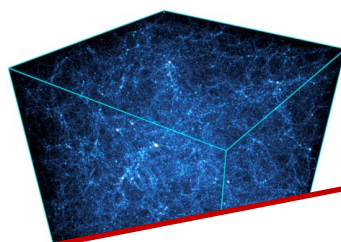
Molecular Dynamics



Density Functional Theory



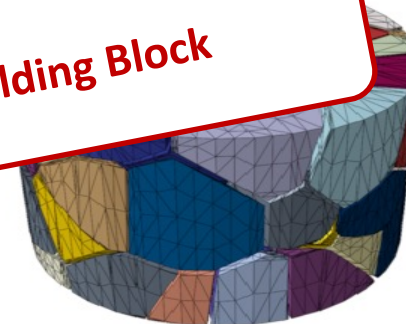
Modeling Particle Accelerators



Simulation

Discrete
Fourier
Transform

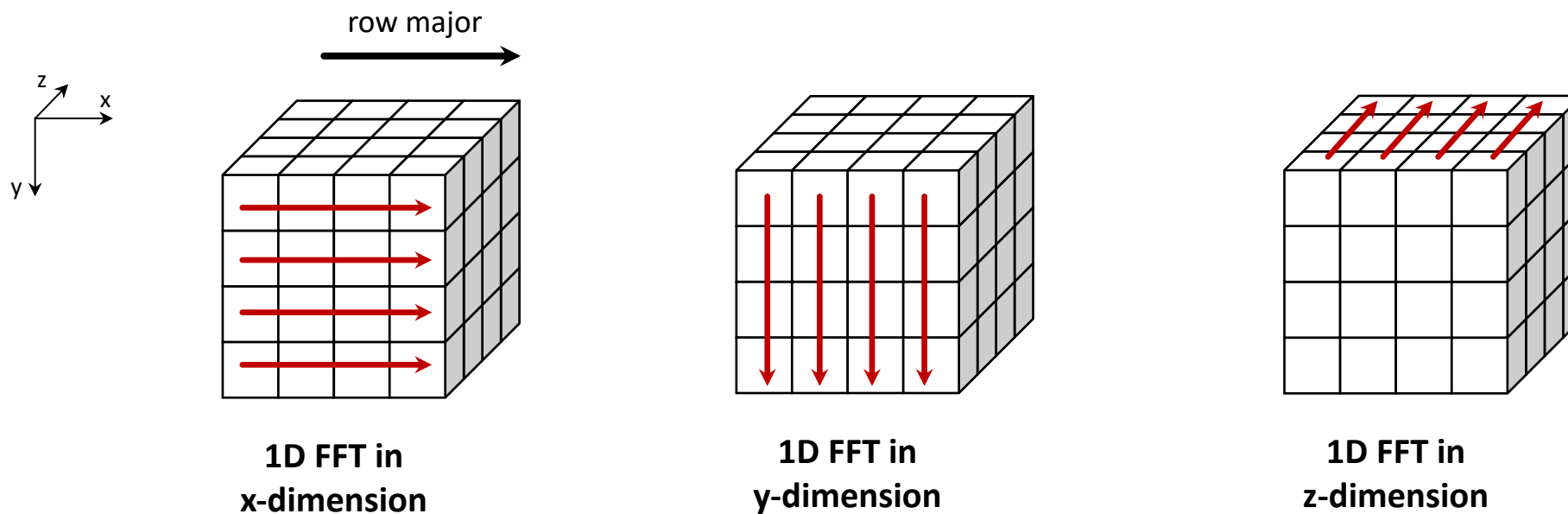
The Discrete Fourier Transform Appears as a Building Block



Material Sciences

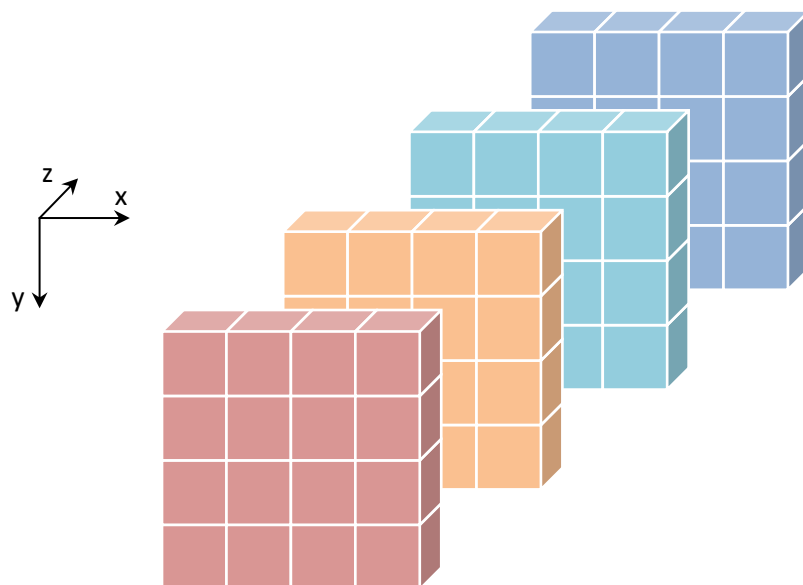
Computing the 3D FFT

3D FFTs **are usually decomposed** as 1D FFTs applied in each dimension



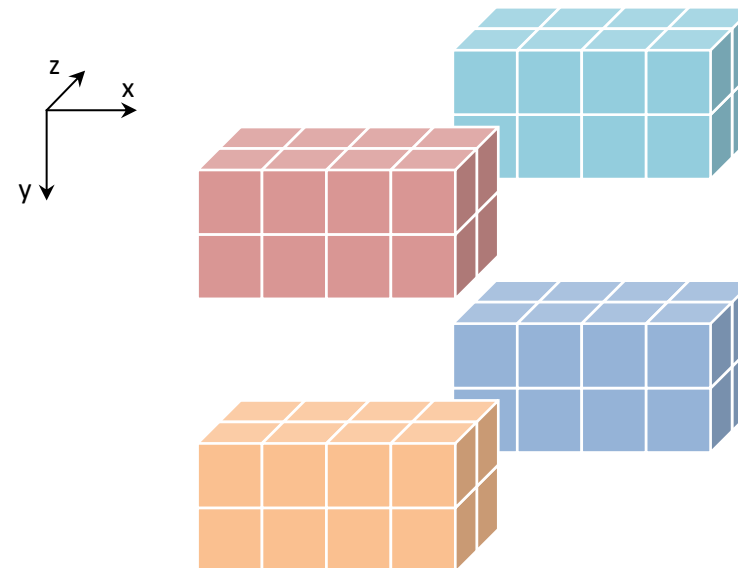
Classical Approaches for Computing 3D FFTs

Slab Pencil Decomposition



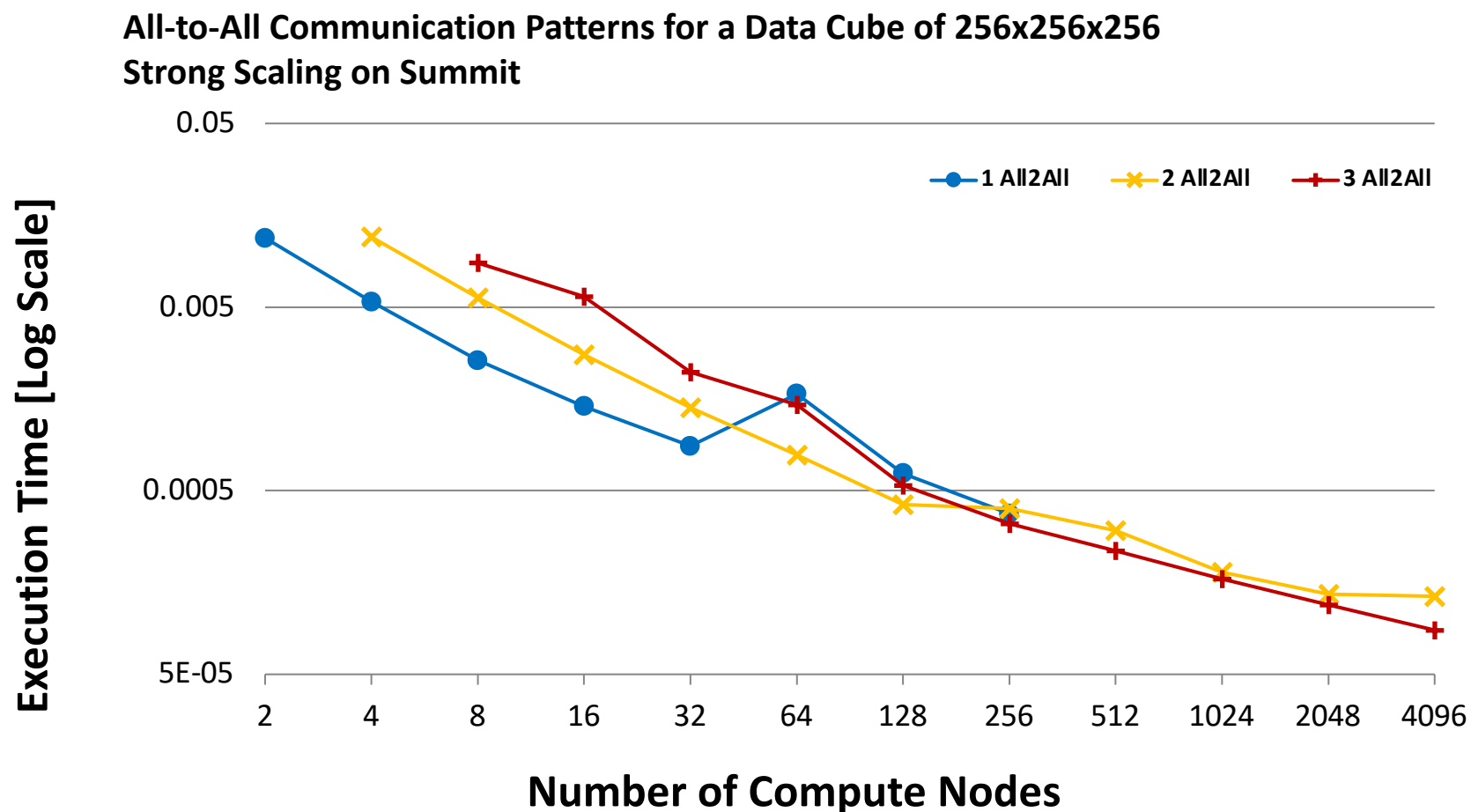
Parallelism and
communication only in the
z-dimension

Pencil Pencil Decomposition



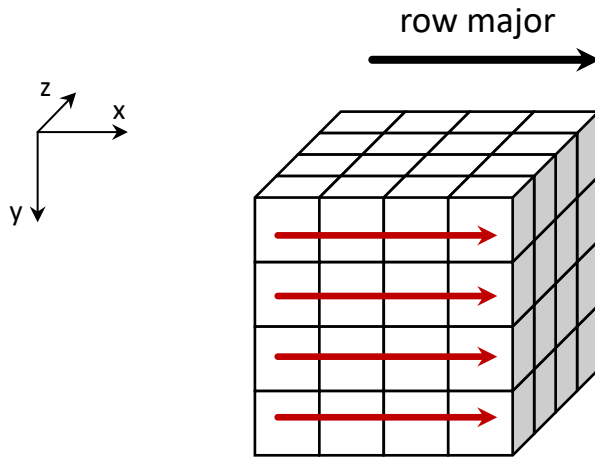
Parallelism and
communication in the **y-** and
z-dimensions

Looking at the Data Movement



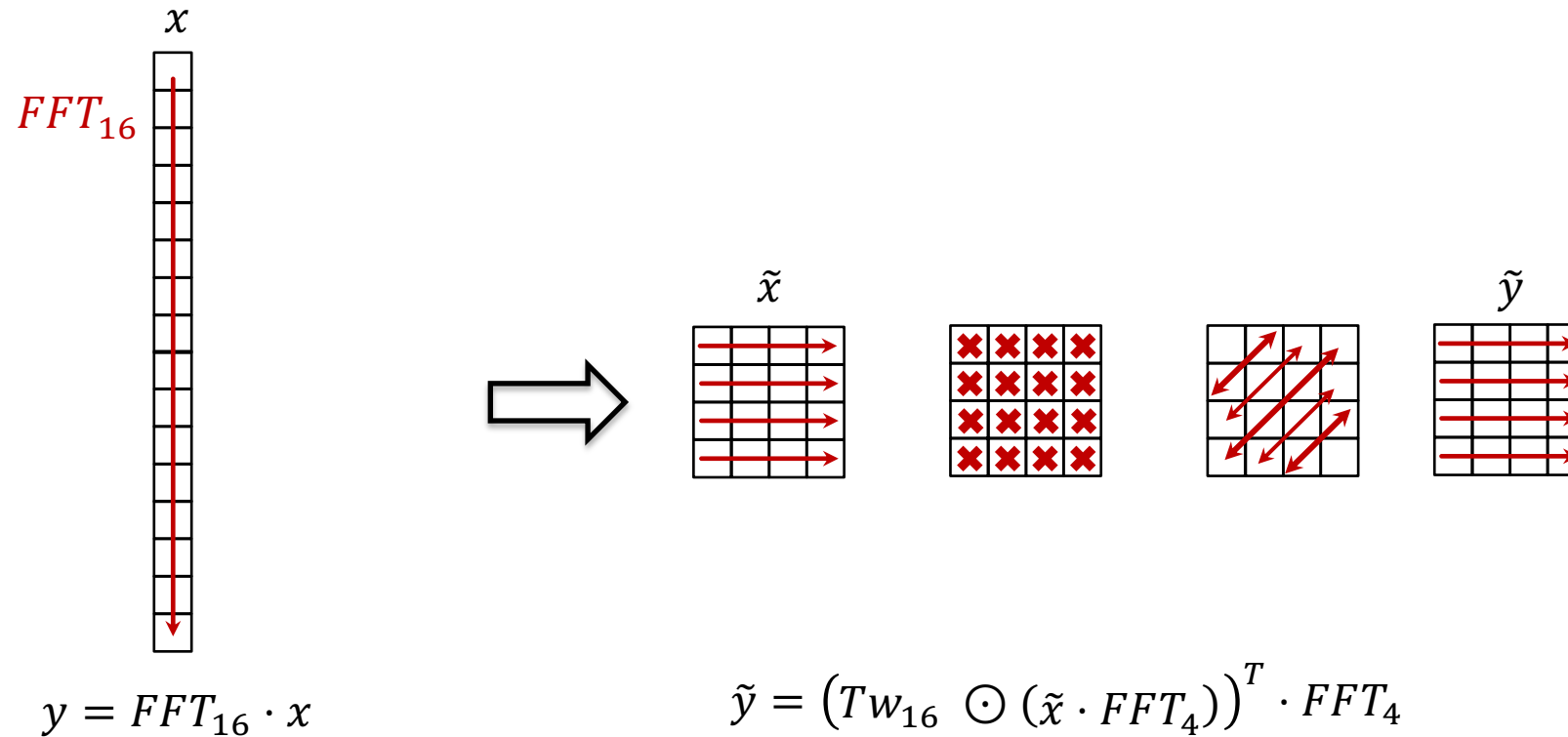
Beyond 2D Decompositions

3D FFTs **are usually decomposed** as 1D FFTs applied in each dimension



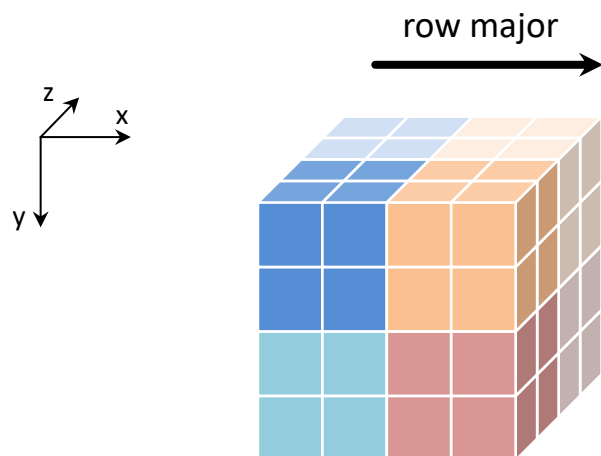
- The 1D FFT can **further be decomposed**

Decompose the 1D FFT as Linear Algebra Operations



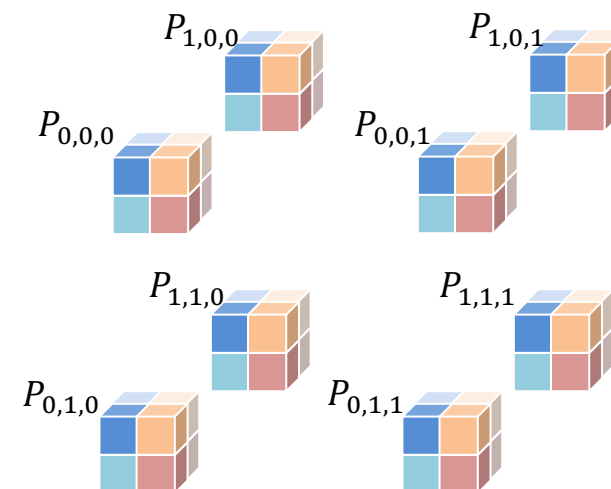
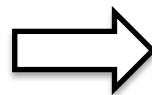
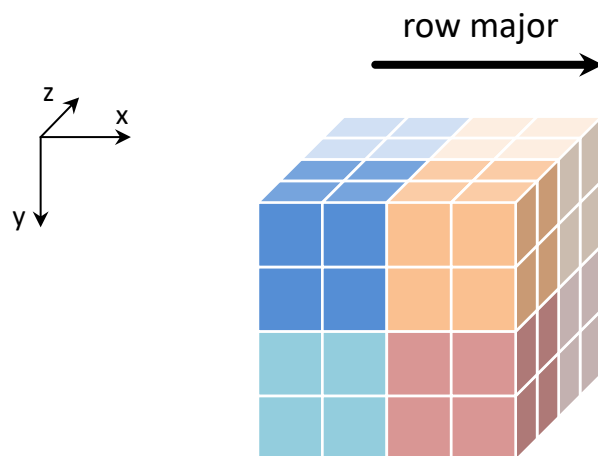
Decompose the Domain into Bricks

Parallelize the computation in all **three dimensions**

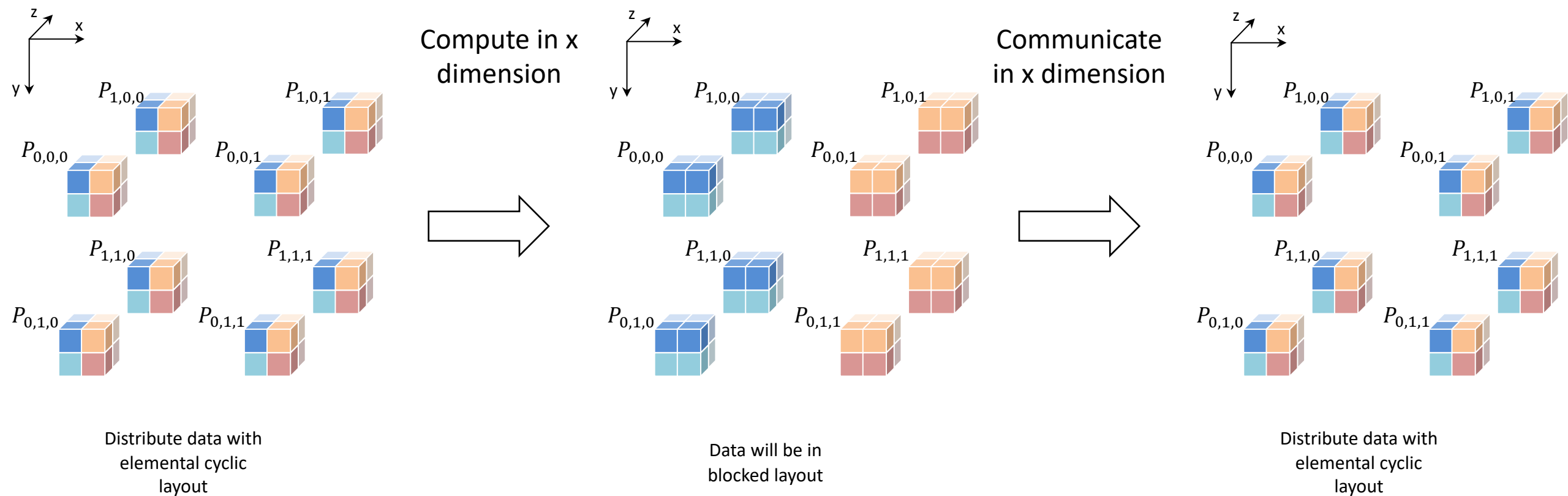


Elemental Cyclic Distribution

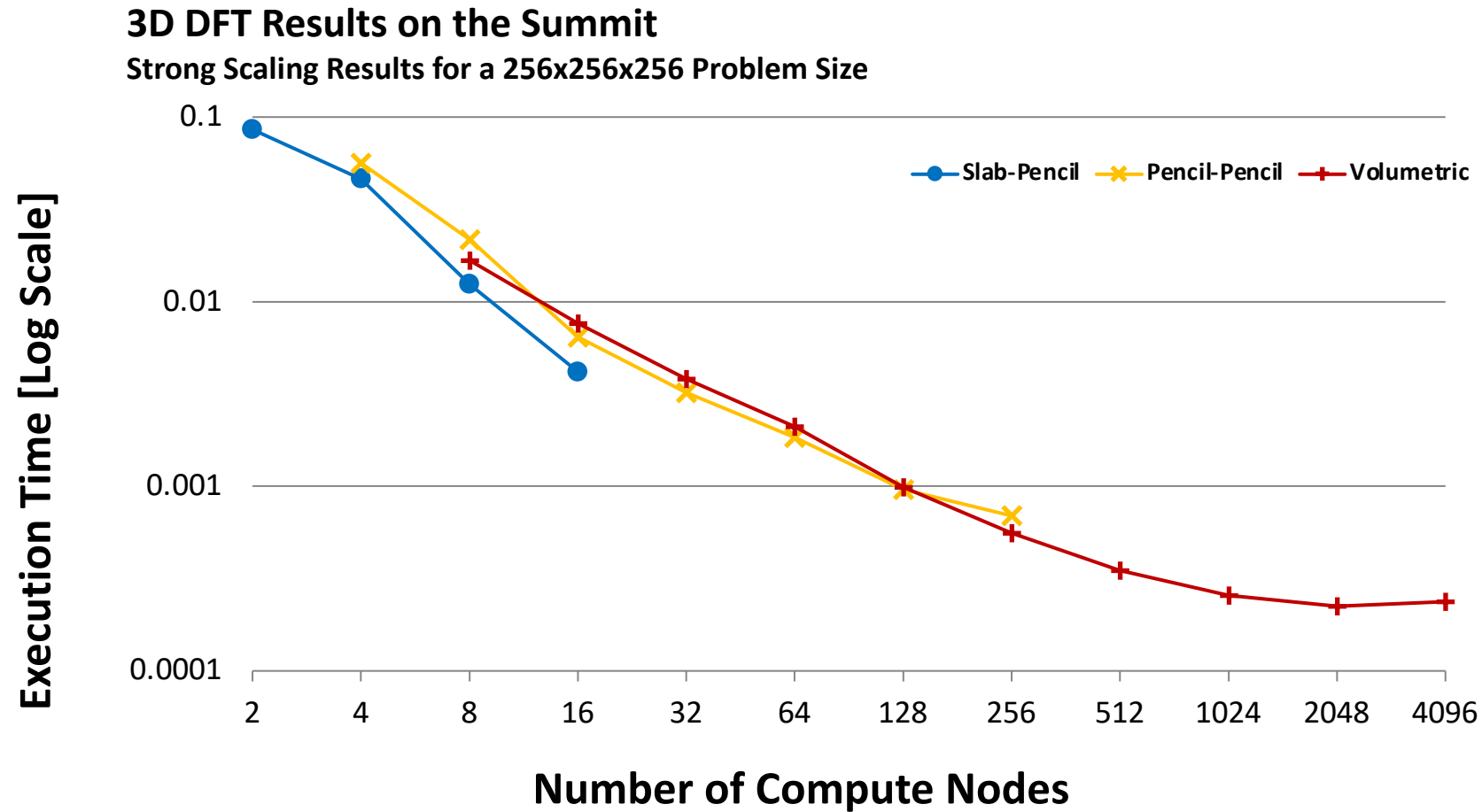
Parallelize the computation in all **three dimensions**



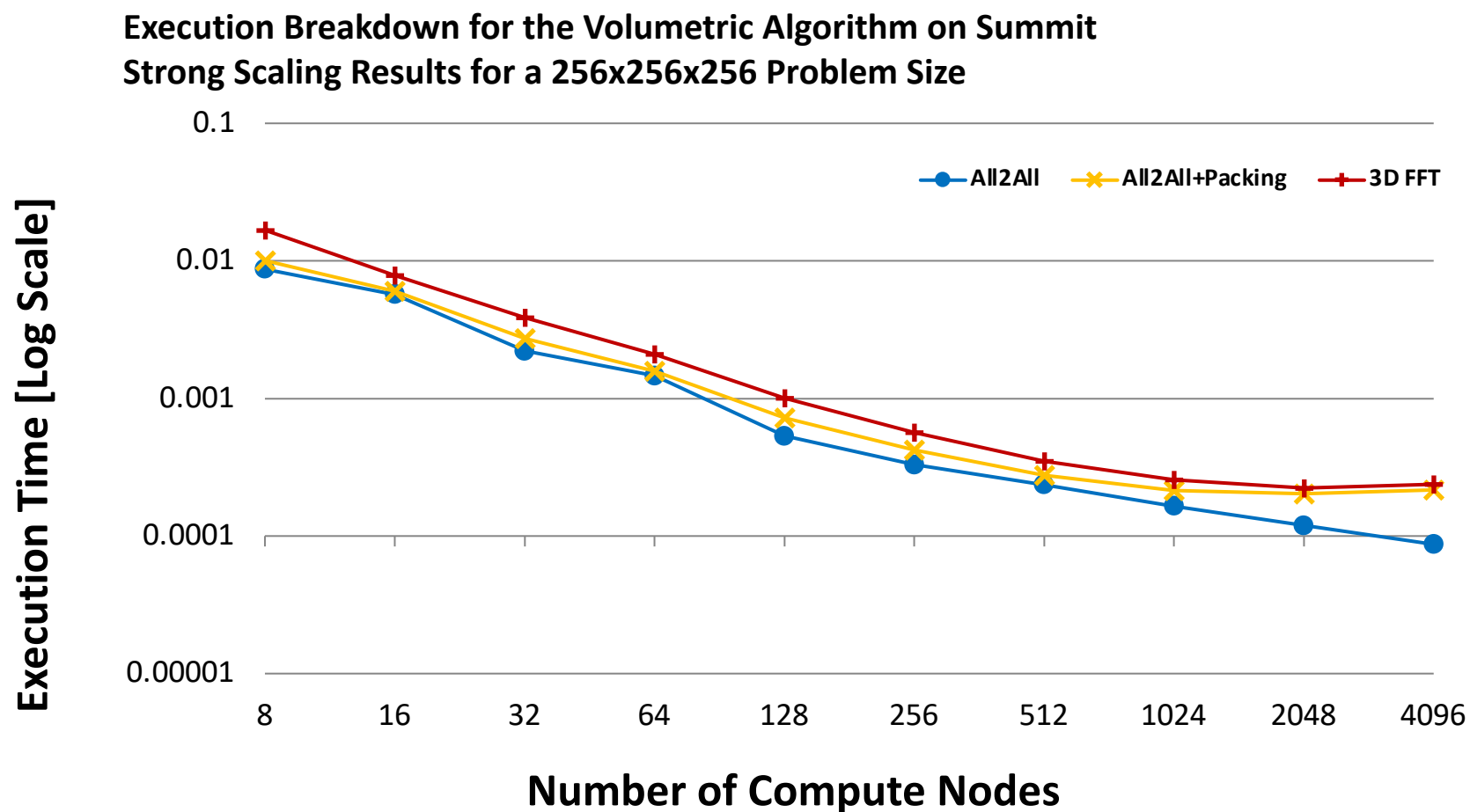
Elemental Cyclic Distribution + Partial Computation



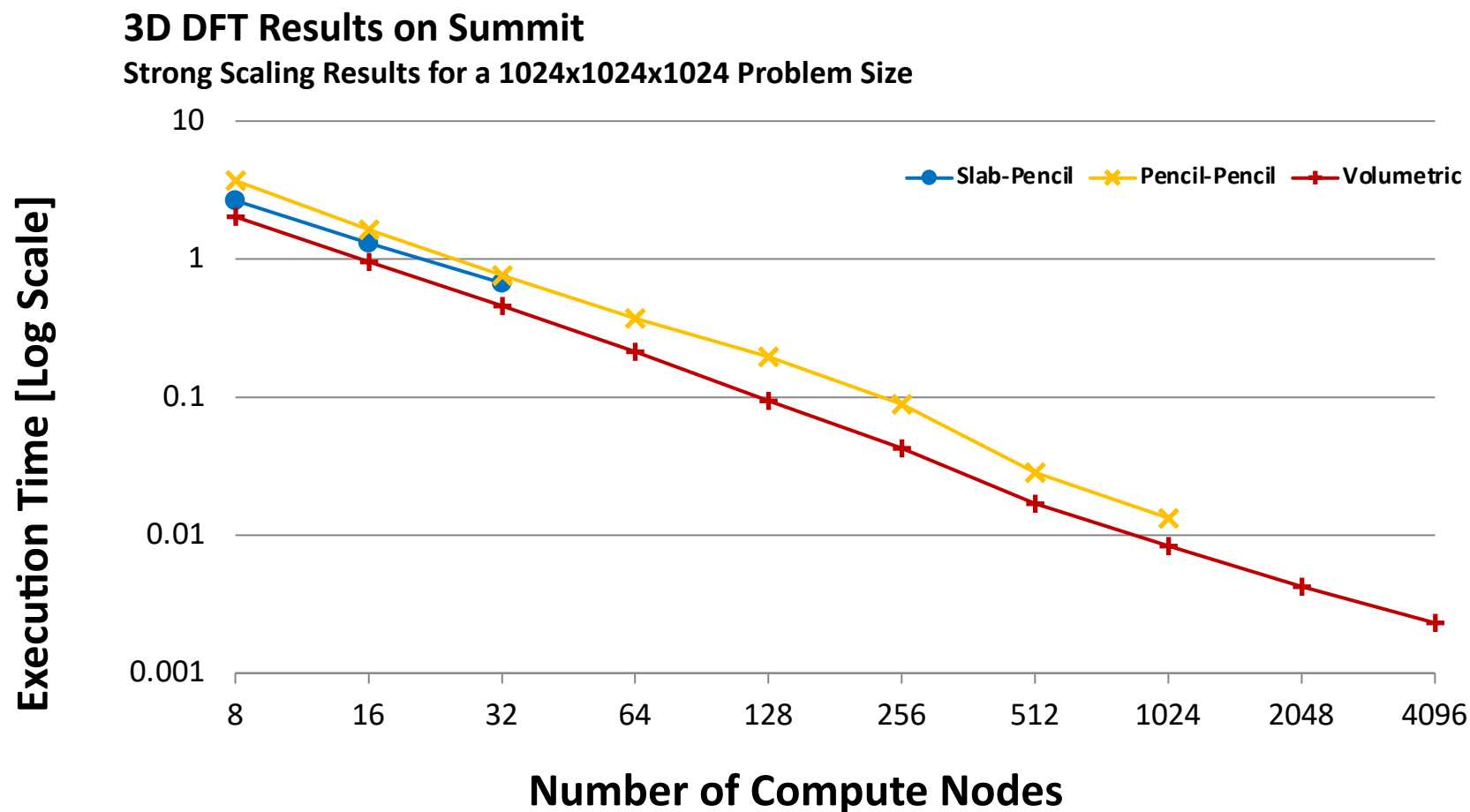
Strong Scaling Results



Strong Scaling Results



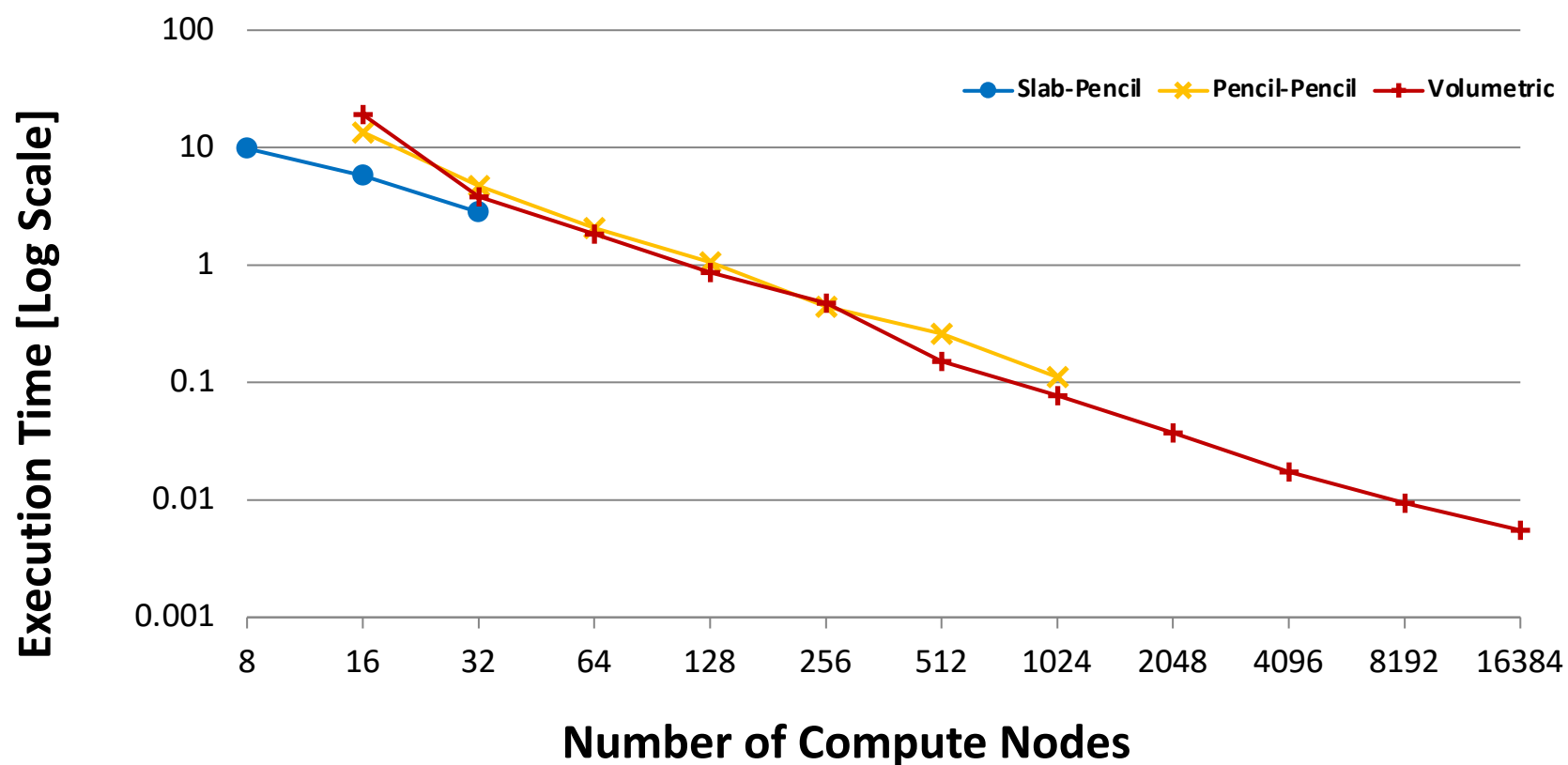
Strong Scaling Results



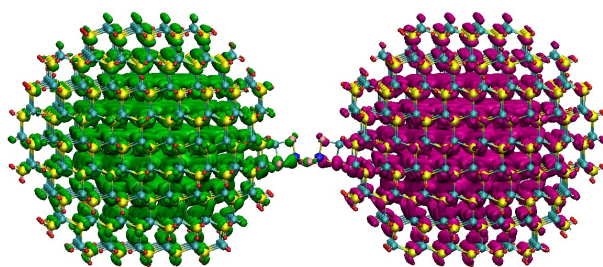
Strong Scaling Results

3D DFT Results on the K-Computer

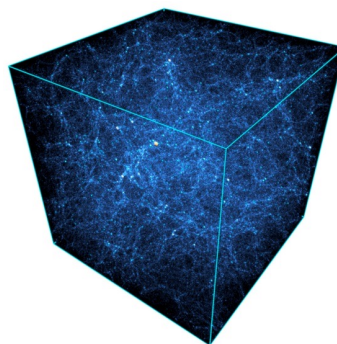
Strong Scaling Results for a 1024x1024x1024 Problem Size



Summary



Molecular Dynamics



Particle in Cell Simulations

Discrete
Fourier
Transform

