LARGE SCALE ELECTRONIC STRUCTURE COMPUTATIONS FOR PLASMA DEVICES

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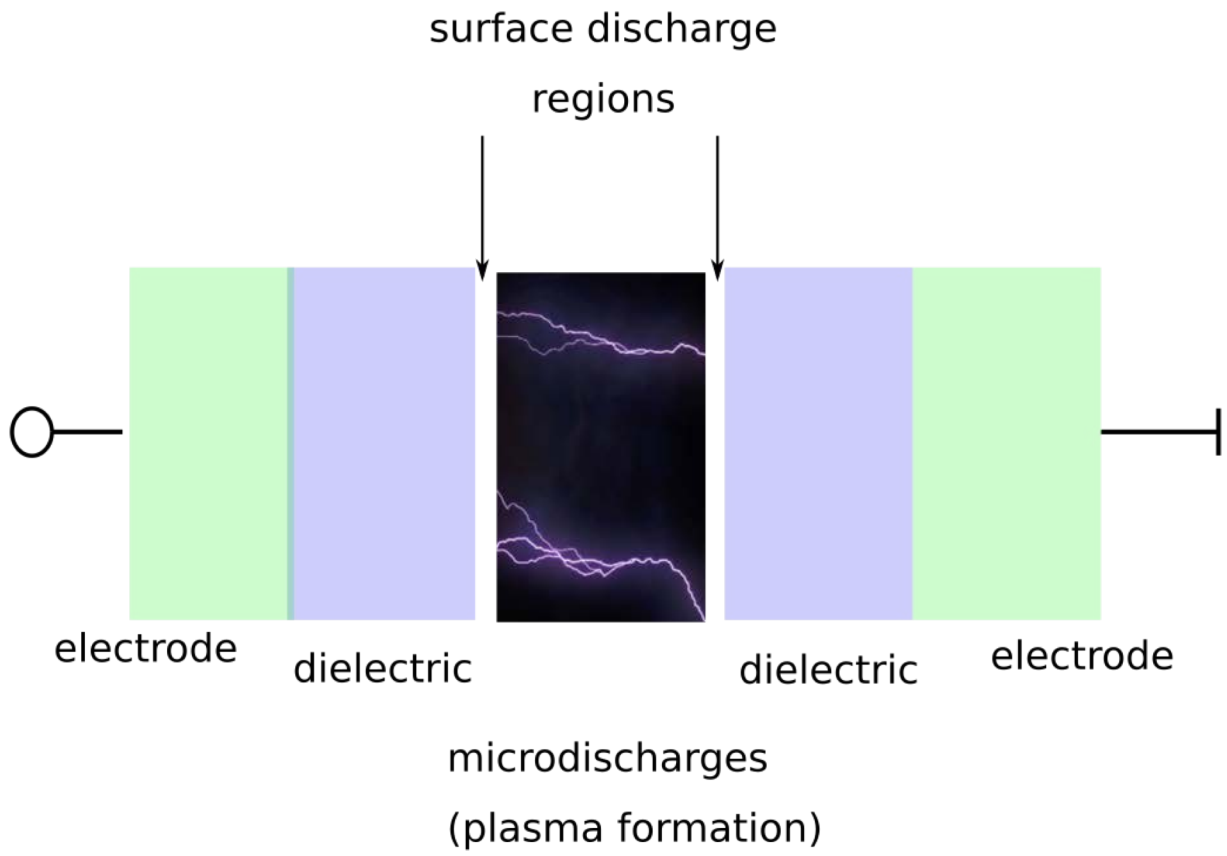
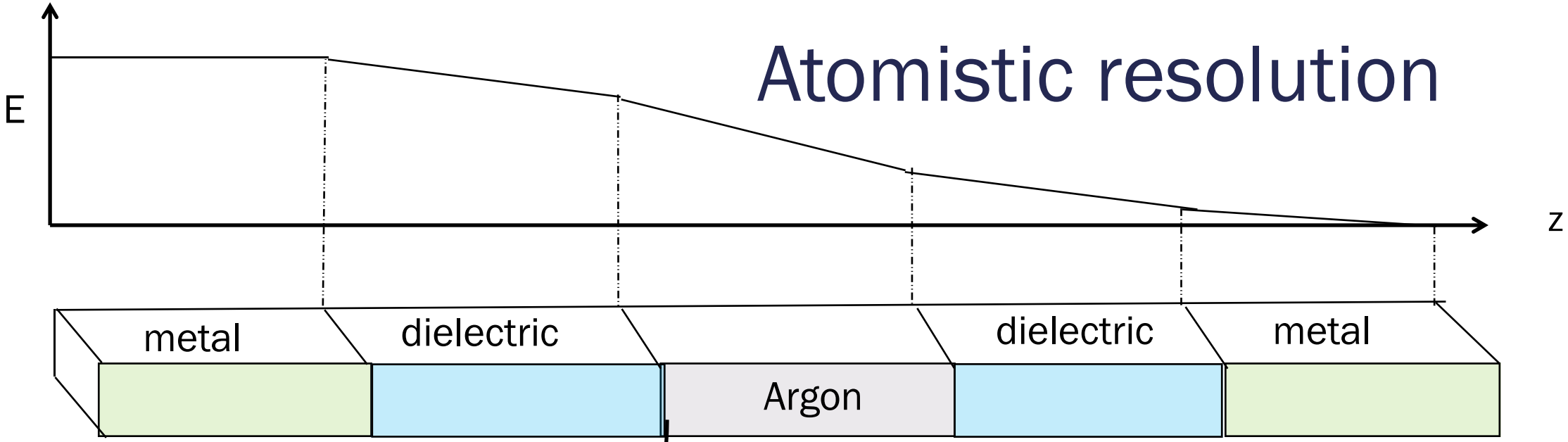
We use Blue Waters to …

- Develop large scale electronic structure calculations
- Investigate nano and microscale dielectric barrier discharges
- Technological applications in microcombustion, chemical processing

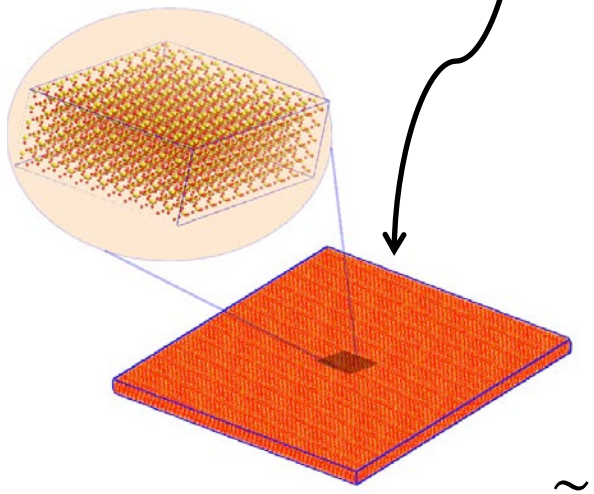


Dielectric barrier discharge, first reported by Siemens, 1857.

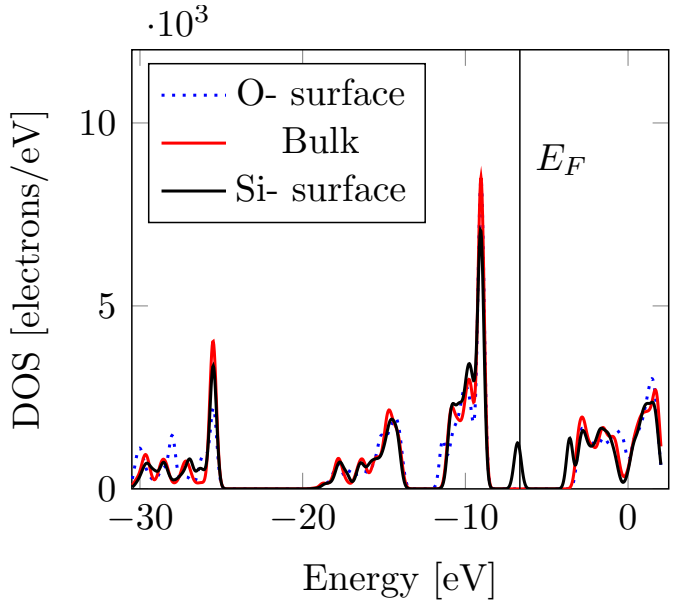
Atomistic resolution



$\sim 10^8$ atoms

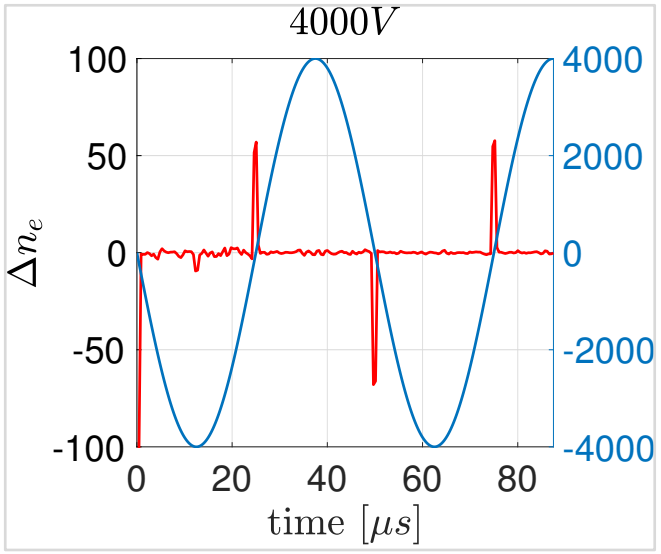


$\sim 10^6$ atoms



Of interest:

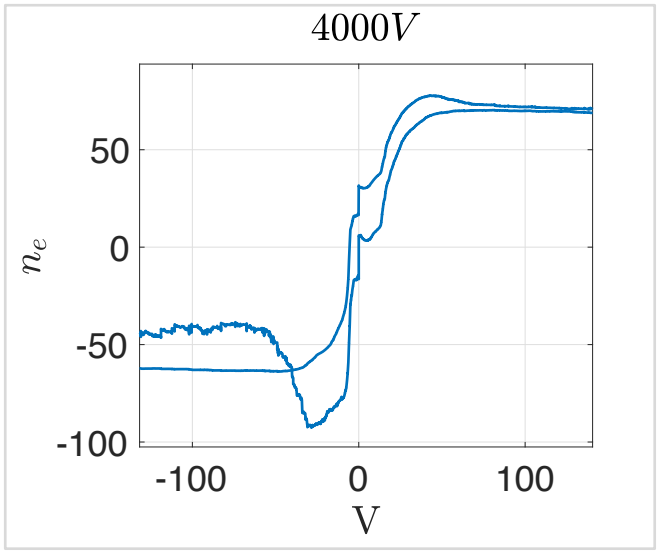
- A microscopic understanding of DBD devices
- So far, qualitative agreement with experiments



Current as a function of time

Red: Rate of electron emission from the dielectric

Blue: AC voltage. 4000V, f = 20kHz

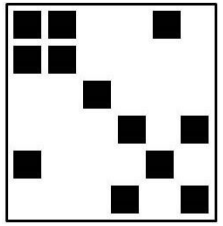


Lissajous plot under AC voltage

Surface charge on the dielectric under AC voltage.

[Ghale and Johnson, *Phys. Rev. B*, 2019]

Overview of methods



$(\vec{r}, \vec{p})$

Quantum Monte Carlo
~ 100 atoms

DFT
$\sim 1{,}000$

Tight-binding
$\sim 100{,}000$

Classical
Potentials
$\sim 10^6$

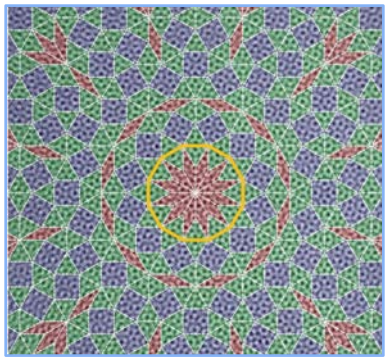
Coarse-grained
Models
?

Continuum
Models
?

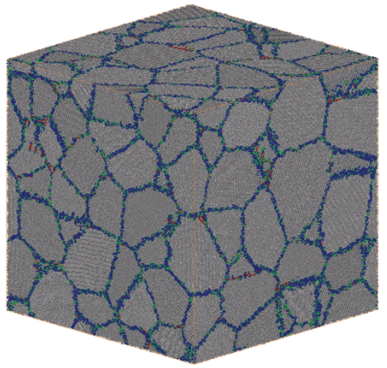
Tight-binding is the least expensive method that can still give us quantum-mechanical information about electrons at the atomistic level (bandgaps, transport, charge-density)

Possible Computations

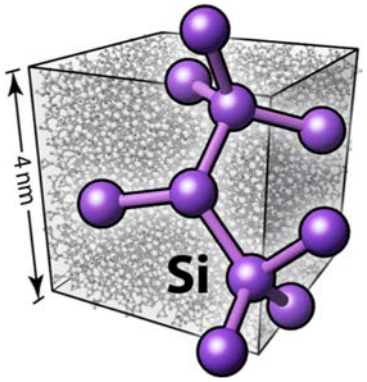
- Systems for which classical molecular dynamics have been done
- Disordered systems
- Systems without translational symmetry
- Glasses and liquids



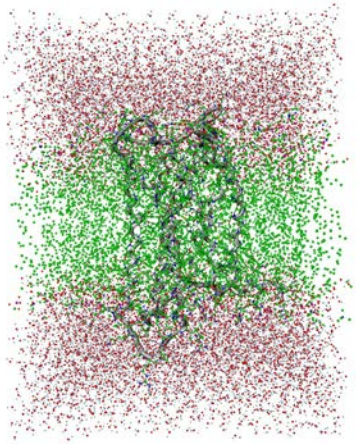
Carbon quasi-crystal
Ahn et. al. Science, 2018



Polycrystalline Ni
Swygenhoven,
Science, 2002



Quenched amorphous-Si
Deringer, et al.,
J. Phys. Chem. Lett., 2018



Protein, lipid bi-layer, water
Zuse Institute Berlin

Background

$$\left(\sum_i \frac{\nabla_i^2}{2m} + V_{ext} + \frac{1}{2}\sum_{i\neq j} \frac{1}{|x_i - x_j|}\right)\ \Psi(x_1, \dots, x_N) = E\ \Psi(x_1, \dots, x_N)$$

$$\sum_i \underbrace{\left(\frac{\nabla_i^2}{2m} + V_{eff,i}\right)}_{\widehat{H}_i} \Psi(\mathrm{x}_1, \dots, x_N) = E\ \ \Psi(\mathrm{x}_1, \dots, x_N)$$

$$\left(\widehat{H_1} + \widehat{H_2} + \cdots \widehat{H_N}\right)\Psi = (E_1 + E_2 \dots E_N\ )\Psi$$

Separation of variables : $\frac{\widehat{H_1}}{\psi_1}\psi_1 + \frac{\widehat{H_2}}{\psi_2}\psi_2 + \cdots = E_1 + E_2 + \cdots E_N$

Indistinguishability/anti-symmetry

$$\widehat{H}\ \psi_i(x_i) = \epsilon_i \psi_i(x_i)$$

$$H\vec{v}_i = \epsilon_i\ \overrightarrow{v_i}$$

Computation

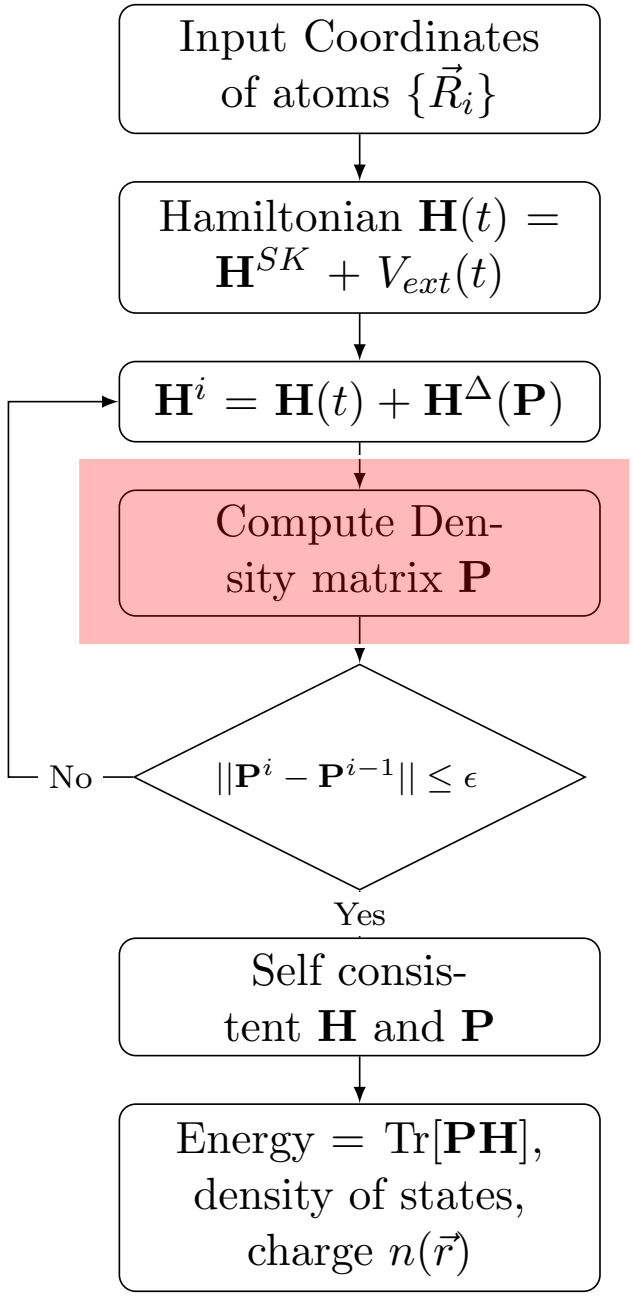
- Given matrix H, compute P where

$$H\overrightarrow{v_i} = \epsilon_i \overrightarrow{v_i}$$

$$P = \sum_i \overrightarrow{v_i} \ \overrightarrow{v_i}^T$$

$$P^2 = P$$

- Each rank of P represents an electron
- Large eigenspace problem

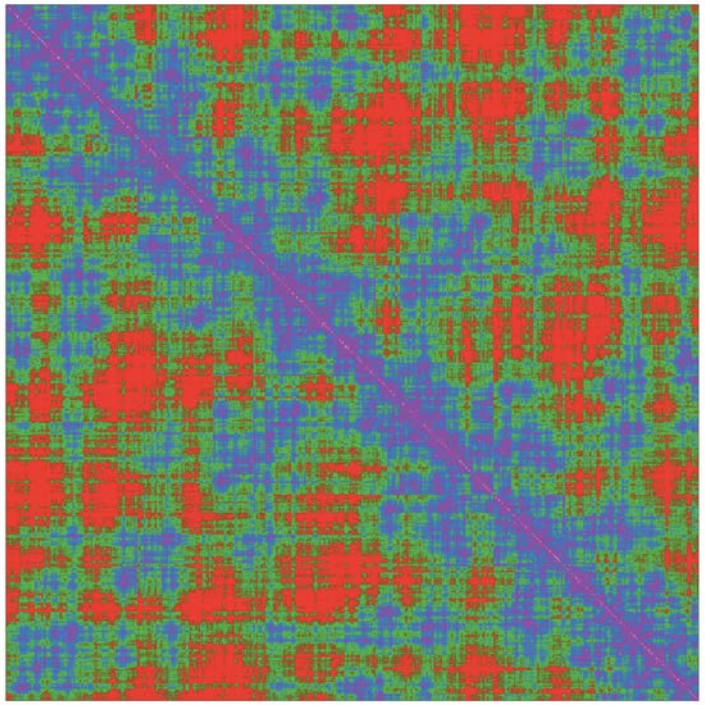


Algorithms

- O(N) in terms of FLOPS
- Rely on localization of solution matrix
- Expect P to be sparse
- Sparse matrix-matrix multiplication (SpMM)

Red 10^{-8}
Green 10^{-6}
Blue 10^{-2}
Violet 1

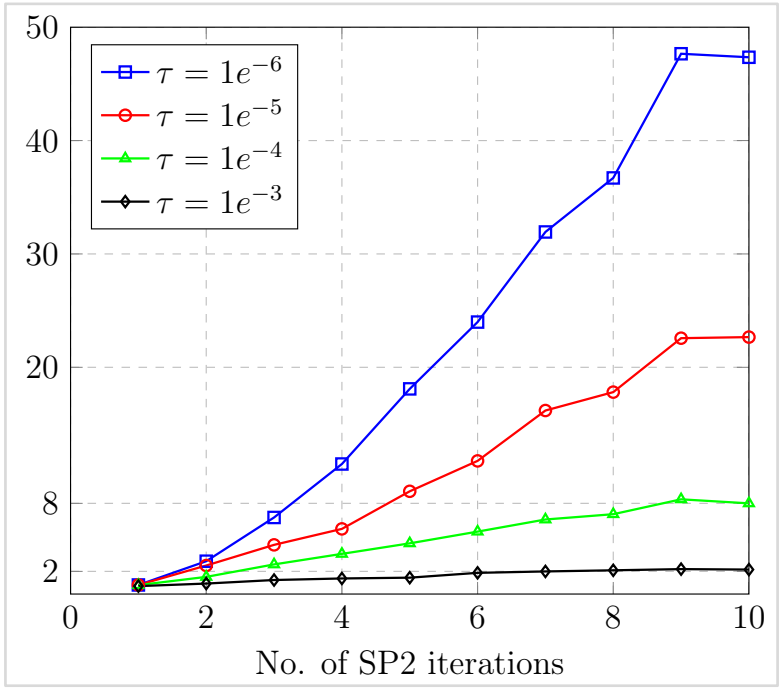
Sparsity



Density matrix (matrix size = 7500)
(Water) Bock and Challacombe *SIAM J. Sci. Comput.*, 2013

Challenge:

- Memory and communication
- Even for a moderate threshold, the % of non-zeros grows fast.
- Sparse matrix-matrix multiplications (SpMM)



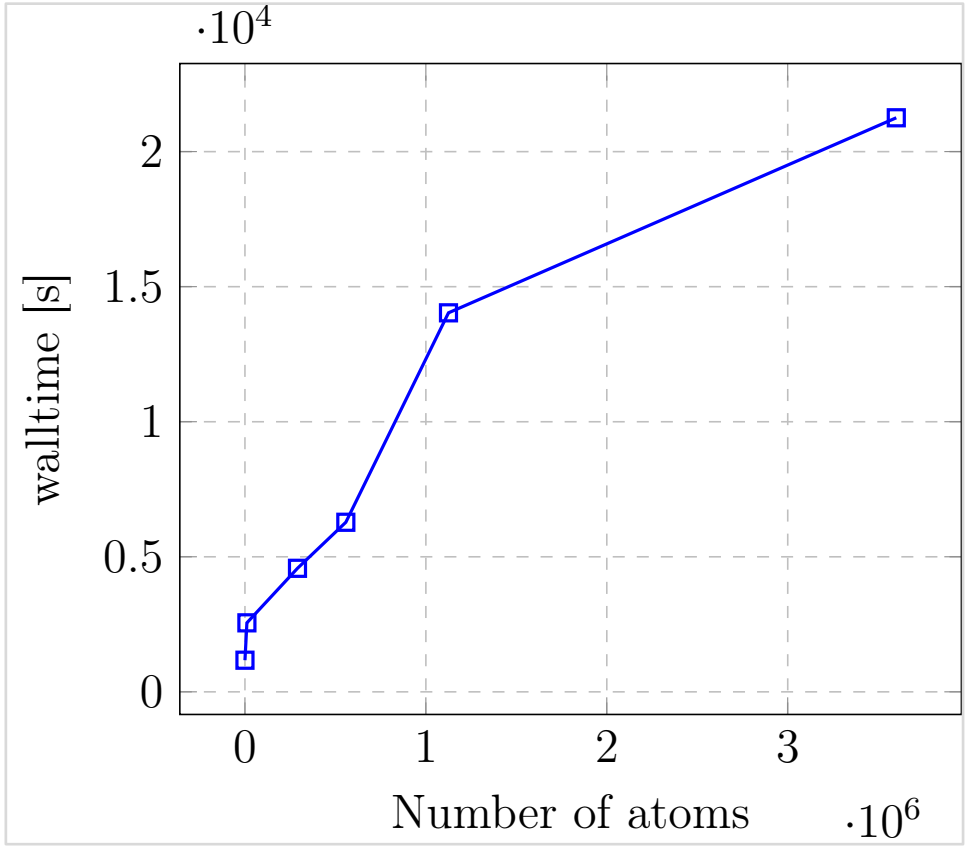
With the threshold parameter $\tau = 10^{-4}$, the memory required increases by a factor of 4.

Increase in % of non-zeros in density matrix

(Silica) Ghale and Johnson, *Comput. Phys. Comm.*, 2018

Our solution

- Memory-aware
- Based on Sparse-matrix-vector multiplications (SpMVs)
- Construct implicit solution (P)
- Sampled via random vectors

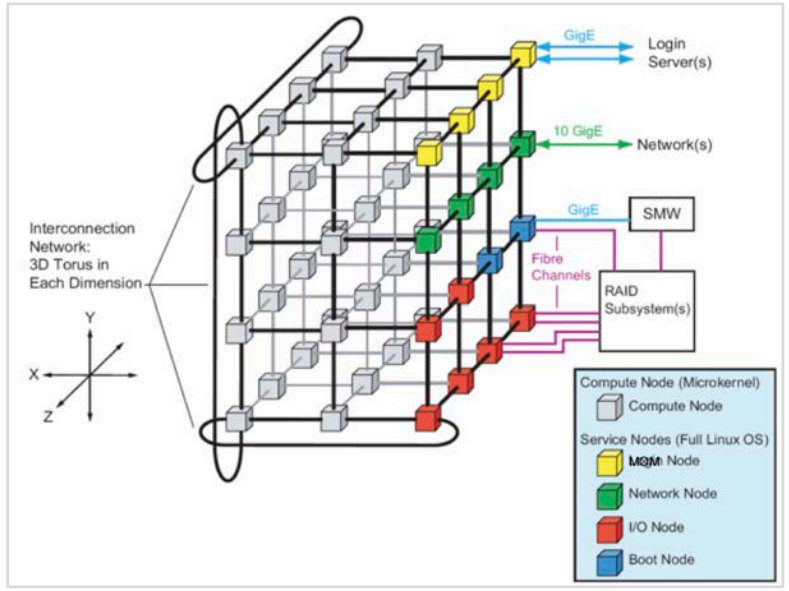


Simulation of 3.6 million atoms on a single large memory node. ~6 hours
Ghale and Johnson, Comput. Phys. Comm., 2018

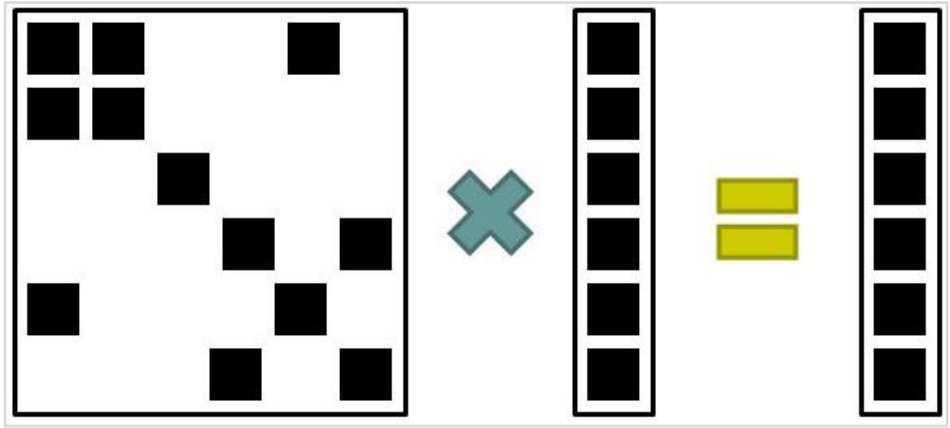
Role of Blue Waters:

- Scale of hardware
- Optimized libraries

Availability of fast, distributed, optimized SpMV kernels through PETSC



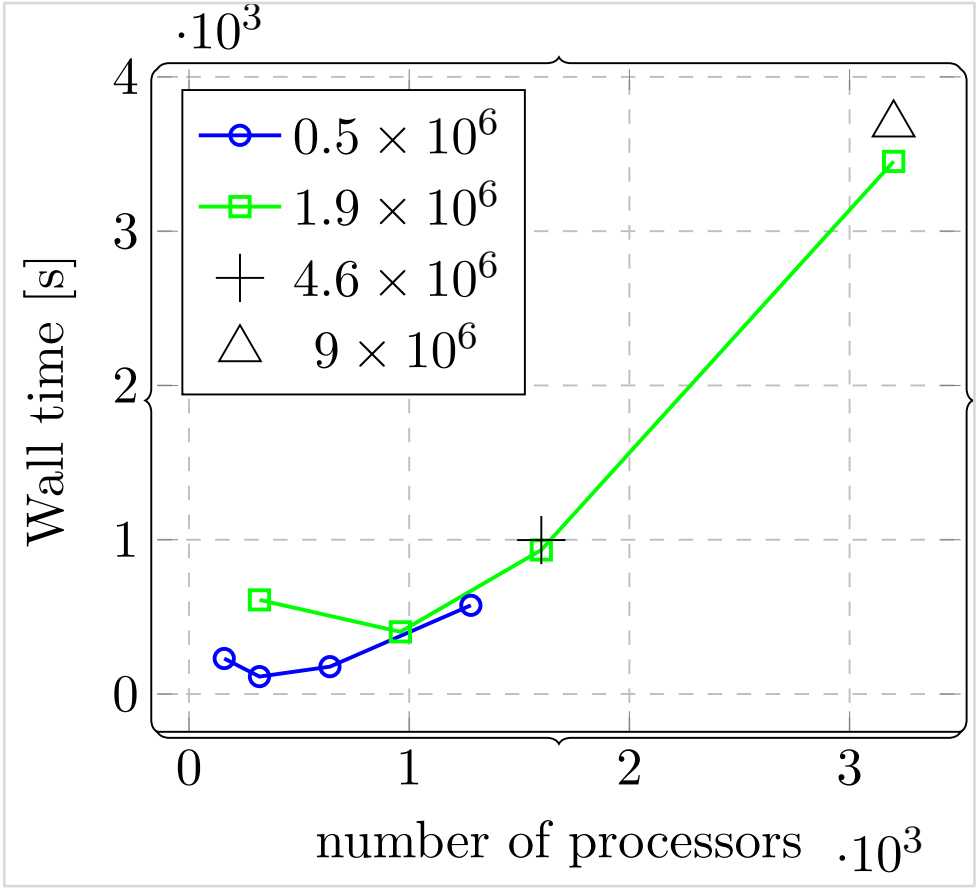
x 10,000 nodes (some testing)



Tested 10^7 atoms

Impact of Blue Waters

- Scaling up to 10^8 atoms
- Time-dependent simulations
- Essential electron emission data
- Current allocation: bawi



Scaling data (Exploratory allocation, baoq)

Future work/other impacts:

- Technical impact within area
  - *Ability to solve large systems self-consistently*
  - *Rates of electron transfer for plasma devices*
- Outside materials science
  - *fast, implicit, accurate, projection matrices*
- Future
  - *Time-dependent Hamiltonian (AC voltage)*

Acknowledgements

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- Numerous discussions within XPACC (Center for Exascale Simulation of Plasma Coupled Combustion)