Atomistic Simulations of Materials Strength on BG/L

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Outline

- Background
- Workload and storage estimates on BlueGene/L – our vision
- Programming models

  Domain decomposition

  I/O

  Communication schemes
- Conclusion and future work

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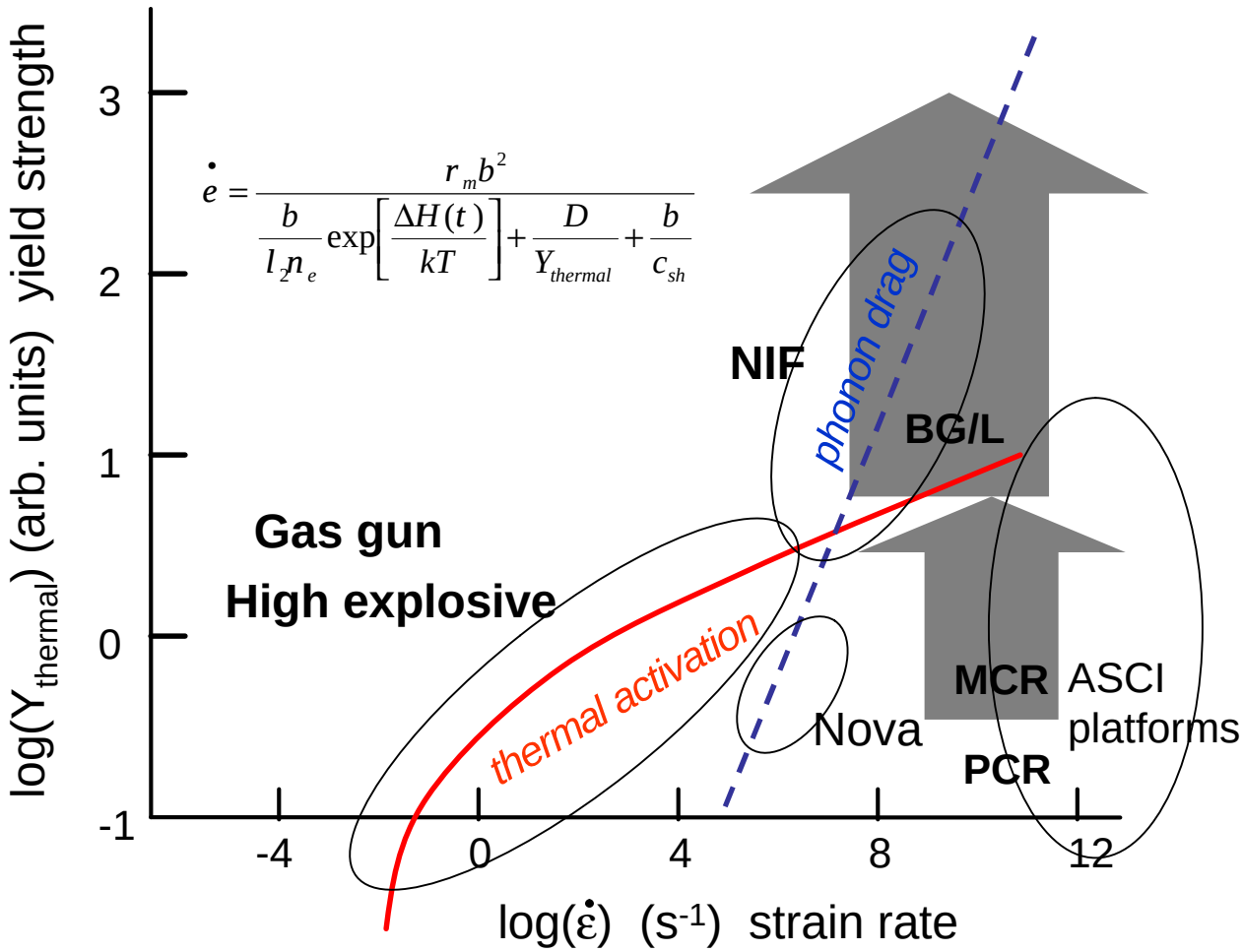
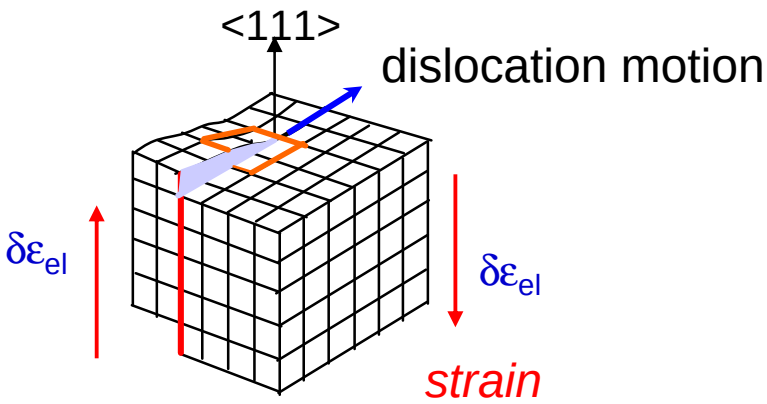
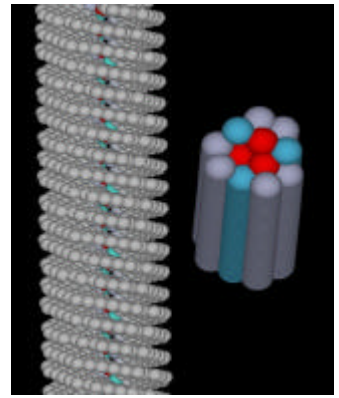
Materials strength is described by physics-based constitutive models

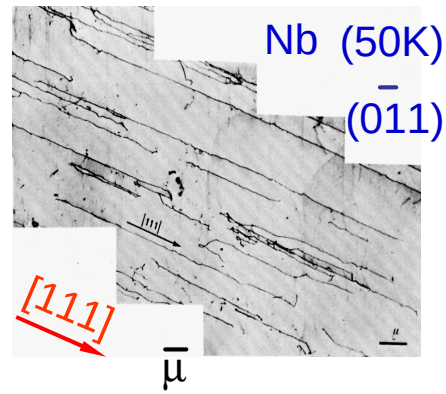


The gaps between simulations and experiments are narrowing in space and time

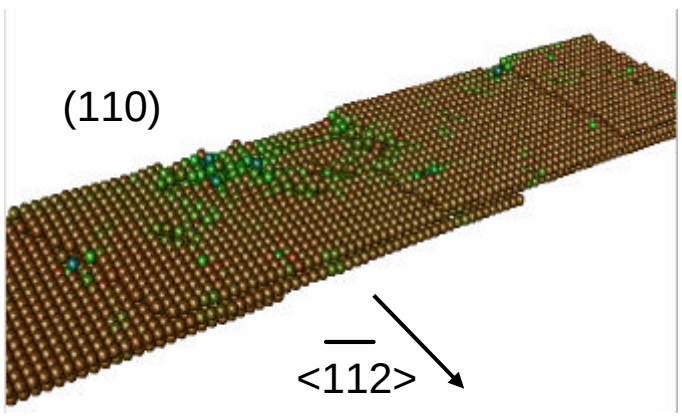
Physics-based properties are controlled by dislocation motion



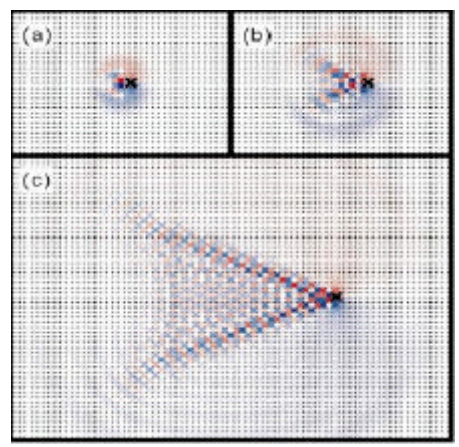




Dislocations are line defects in materials

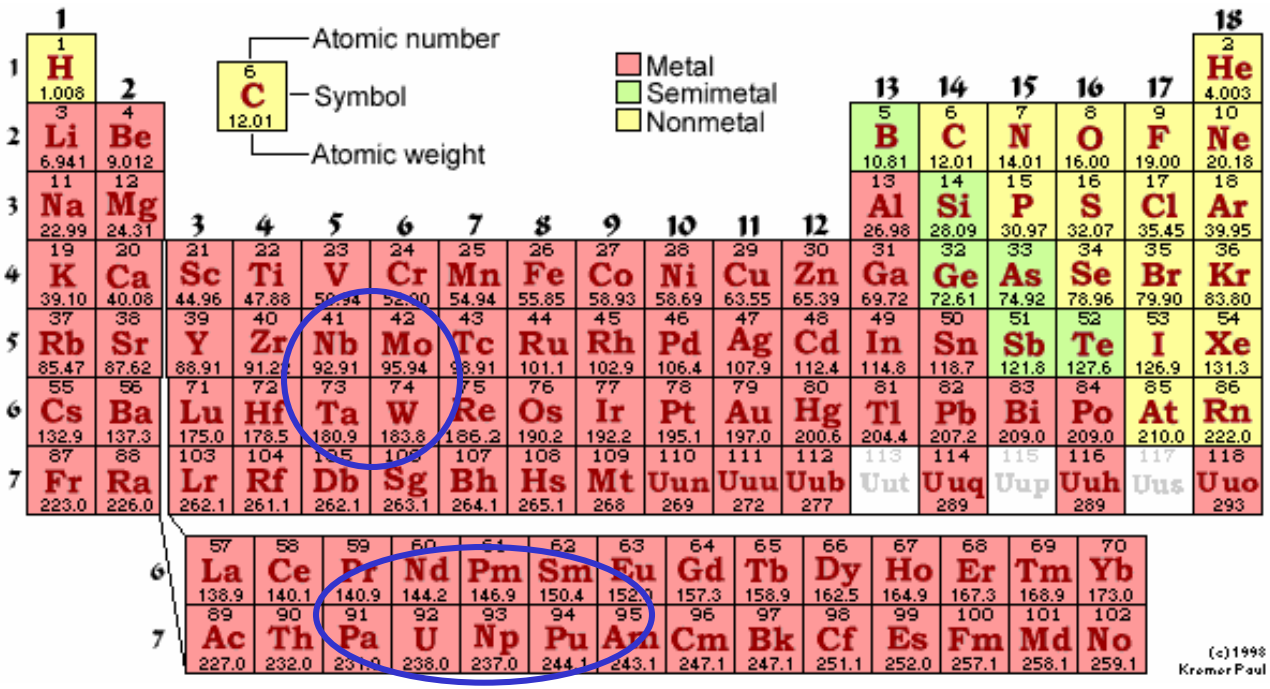


Thermal–activation region
(low temperatures and strain rates)



Phonon-drag region
(high temperatures and strain rates)

Materials strength involving *d- and f*-electrons



Important issues:

Energy functional

Boundary conditions

Energy functional involving mid-range interactions (far beyond the nearest neighbors)

$$E_{tot}(R_1 .....R_N) = E_{vol}(\Omega) + \frac{1}{2}\sum_{i,j}{}' v_2(ij;\Omega) + \frac{1}{6}\sum_{i,j,k}{}' v_3(ijk;\Omega) + \frac{1}{24}\sum_{i,j,k,l}{}' v_4(ijkl;\Omega)$$

$$v_2(r;\Omega) = v_2^{sp}(r;\Omega) + v_2^{hc}(r;\Omega) + v_2^{d}(r;\Omega)$$

$$v_2^{d}(r;\Omega) = v_a(\Omega)[f(r)]^4 - v_b(\Omega)[f(r)]^2$$

$$f(r) = \begin{cases} \left(\frac{r_0}{r}\right)^p, r \le R_0 \\ \left(\frac{r_0}{r}\right)^p \left[1 + a\left(\frac{r}{R_0} - 1\right)^2\right] \exp\left[-a\left(\left(\frac{r}{R_0} - 1\right)^2\right]\right., r > R_0 \end{cases}$$

$$v_3(r_1, r_2, r_3;\Omega) = v_c(\Omega) f(r_1) f(r_2) f(r_3) L(q_1, q_2, q_3) + v_d(\Omega)\{ [f(r_1) f(r_2)]^2 P(q_3) + [f(r_2) f(r_3)]^2 P(q_1) + [f(r_3) f(r_1)]^2 P(q_2)\}$$

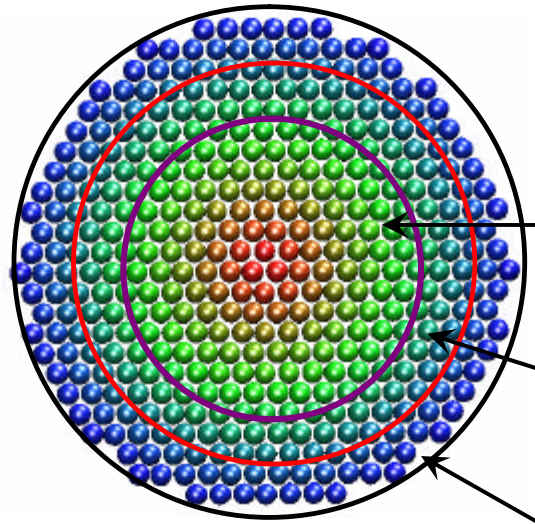
$$\begin{aligned} v_4(r_1, r_2, r_3, r_4, r_5, r_6;\Omega) = v_e(\Omega)\{ & f(r_1) f(r_2) f(r_4) f(r_5) M(q_1, q_2, q_3, q_4, q_5, q_6) \\ & + f(r_3) f(r_2) f(r_6) f(r_5) M(q_7, q_8, q_9, q_{10}, q_5, q_2) \\ & + f(r_1) f(r_6) f(r_4) f(r_3) M(q_{11}, q_{12}, q_5, q_6, q_3, q_4) \} \end{aligned}$$

Computational efforts:

Including 1st and 2nd order derivatives

Matrix-matrix, matrix-vector and matrix-scalar operations

Green's function molecular dynamics (GFMD) simulation method – multi-resolution in space and time



$$m\ddot{u}_a(R_m,t) = f_a(R_m,t) + \sum G_{ab}(R_{mn}) f_b^{II}(R_n)$$

Atomistic region

$$u_a^I(R_m,t+?t) = u_a^I(R_m,t) + v_a^I(R_m,t)?t + \frac{1}{2m} f_a^I(R_m,t)\,?t^2 + \sum G_{ab}(R_{mn}) f_b^{II}(R_n)$$

$$kT^I = \sum m v_a^I(R_m,t)^2 \Big/ (\sum f^I)$$

Green's function region

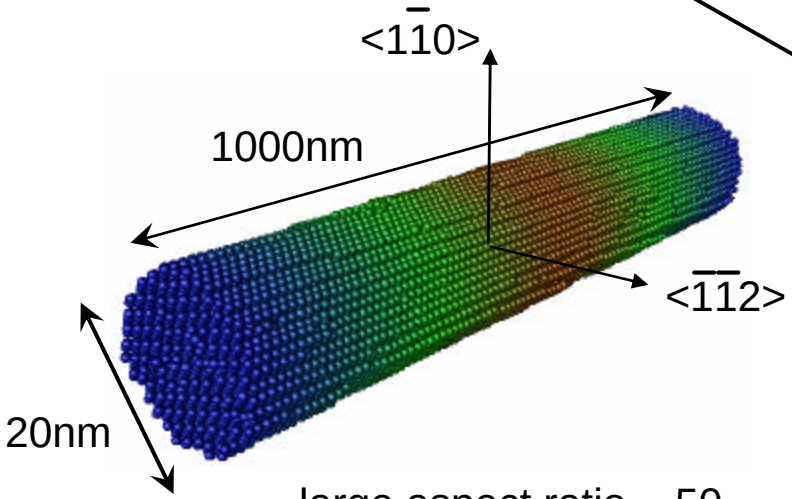
$$u_a^{II}(R_m,t+?t) = u_a^{II}(R_m,t) + v_a^{II}(R_m,t)?t + \sum G_{ab}(R_{mn}) f_b^{II}(R_n)$$

$$kT^{II} = \sum m v_a^{II}(R_m,t)^2 \Big/ (\sum f^{II})$$

Continuum region

$$u_a^{III}(R_m,t+?t) = u_a^{III}(R_m,t) + v_a^{III}(R_m,t)?t + \sum G_{ab}(R_{mn}) f_b^{II}(R_n)$$

$$kT^{III} = \sum m v_a^{III}(R_m,t)^2 \Big/ (\sum f^{III})$$

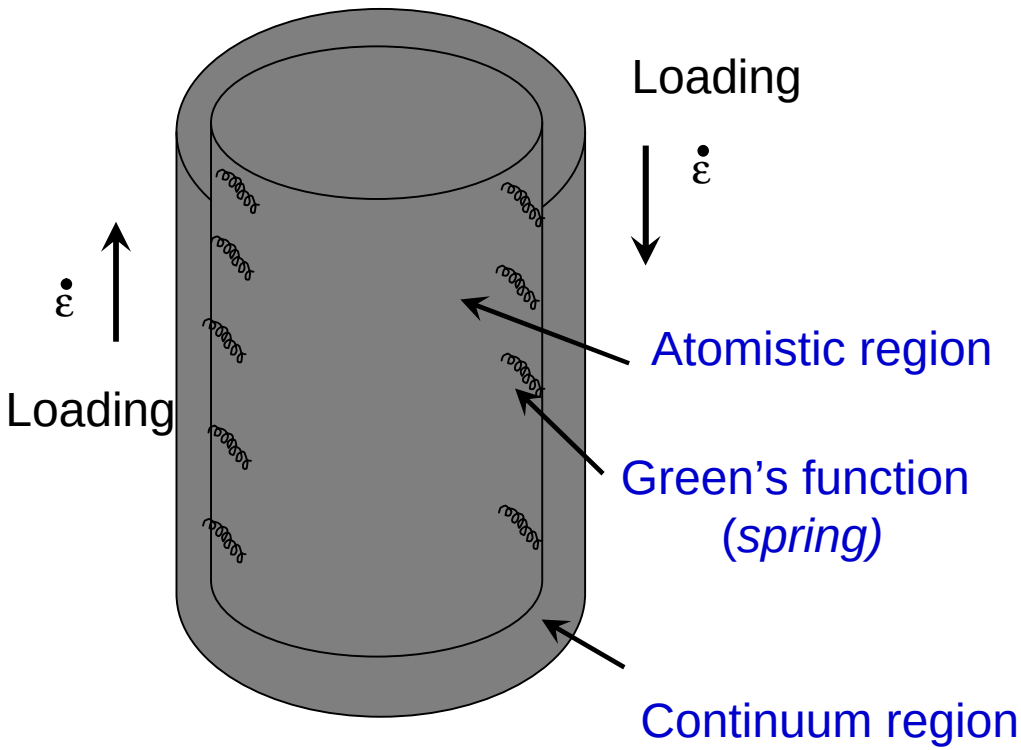


large aspect ratio ~ 50

Summary of GFMD method

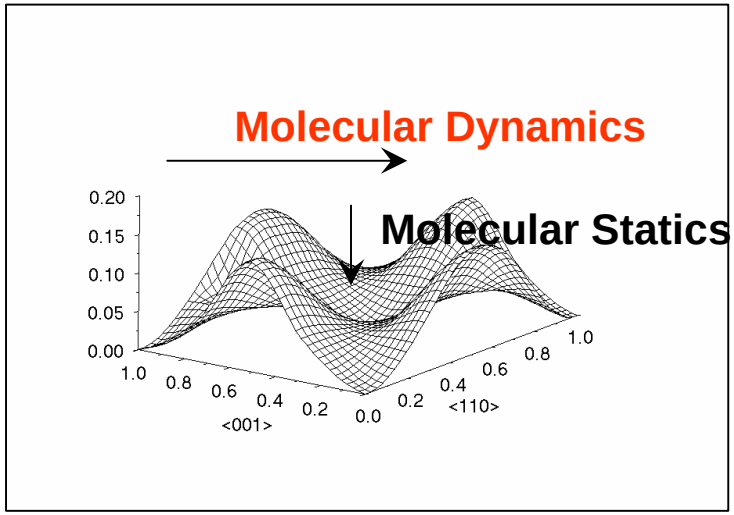
- A saving of 95% in size as compared to the traditional MD method

Simulation box



Goal:

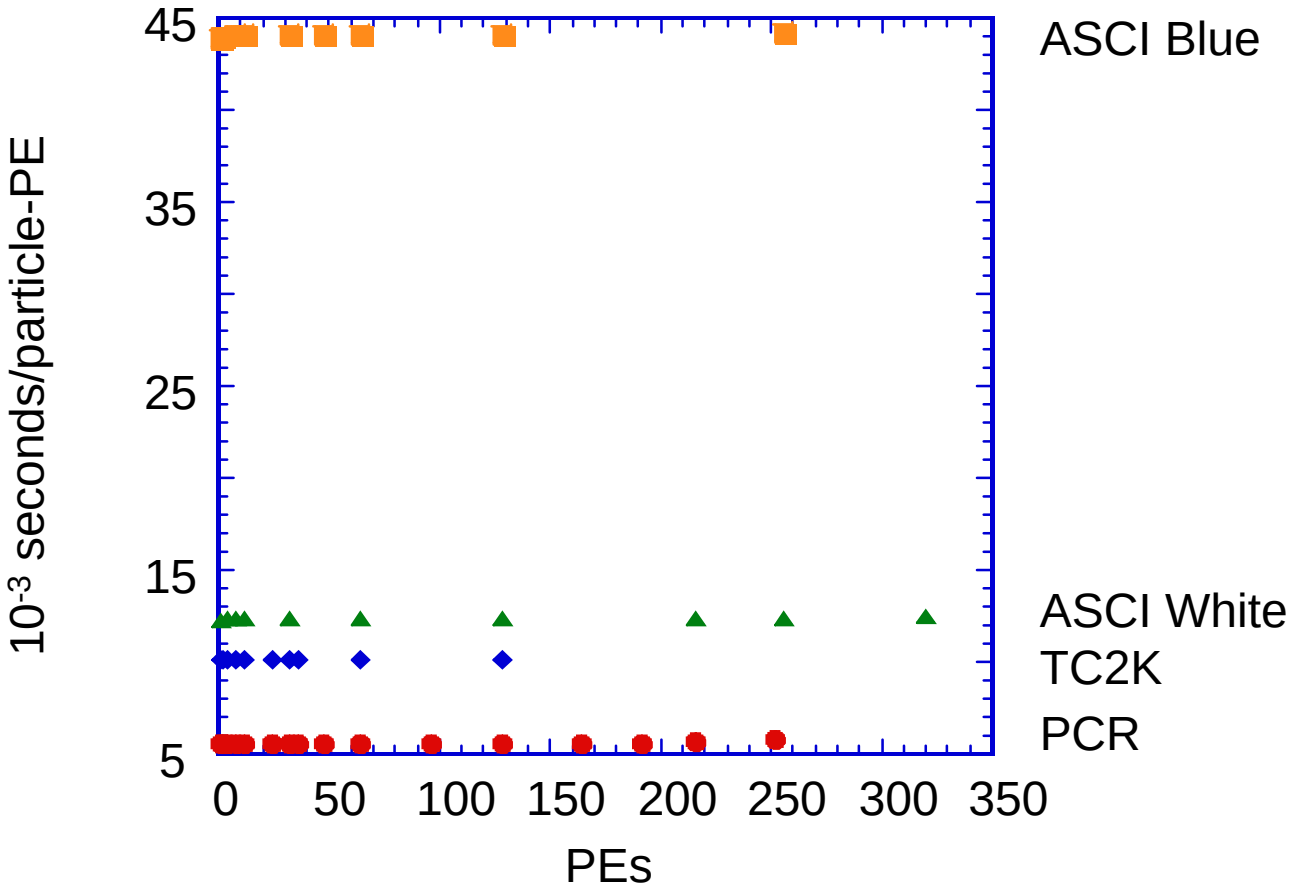
Probe the energy landscape



physical time X size = constant

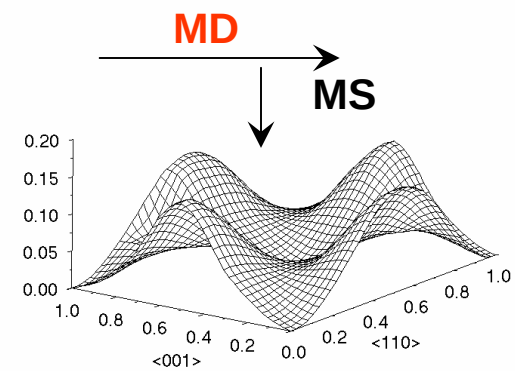
GFMD simulation is a compute-bound application

- 4000 atoms per PE



Our vision of GFMD simulations on BG/L – an estimate of workload

- Physical time for simulations **10^{-8}** seconds
- Typical time step size 10^{-15} seconds
- Number of MD time steps **10^{7}**
- Number of MS steps 10^{4}



Compute-bound applications

- Number of atoms **3×10^{7}** (500/node, <200MB/node)
- Number of interactions in force calculations 192×10^{7}/time step
- Machine instructions per force calculations 5,000
- Total number of machine instructions (40 runs) **40×10^{20}**

assume 75% usage

Estimated total wall-clock time 230 / 0.75 = **307** days

Use virtual node mode (200 TF)

Our vision of GFMD simulations on BG/L – an estimate of storage requirement

• Bytes per atom	92
• Number of atoms	**3×10^7**
• Number of MD time steps	**10^7**
• Interval for MD data storage (time steps)	200
• Total storage (TB)	**1,380**
• Data quantization (integers)	50%
• Data compression	40% (?)

Data redundancy
I/O failures

Estimated total storage requirement (TB) 40 x 276 x 0.5 = 5520

Number of MD runs

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Programming models

✓ Based on our experiences learned from LLNL's PCR Linux cluster and (hopefully) *incoming* MCR platform

✓ *Providing that BG/L shares similar design philosophy*

- Initialization
- Computation
- Data management
- Communication

Initialization

MPI_Init()

MPI_Comm_size()

MPI_Comm_rank()

……

GFMD_Init()

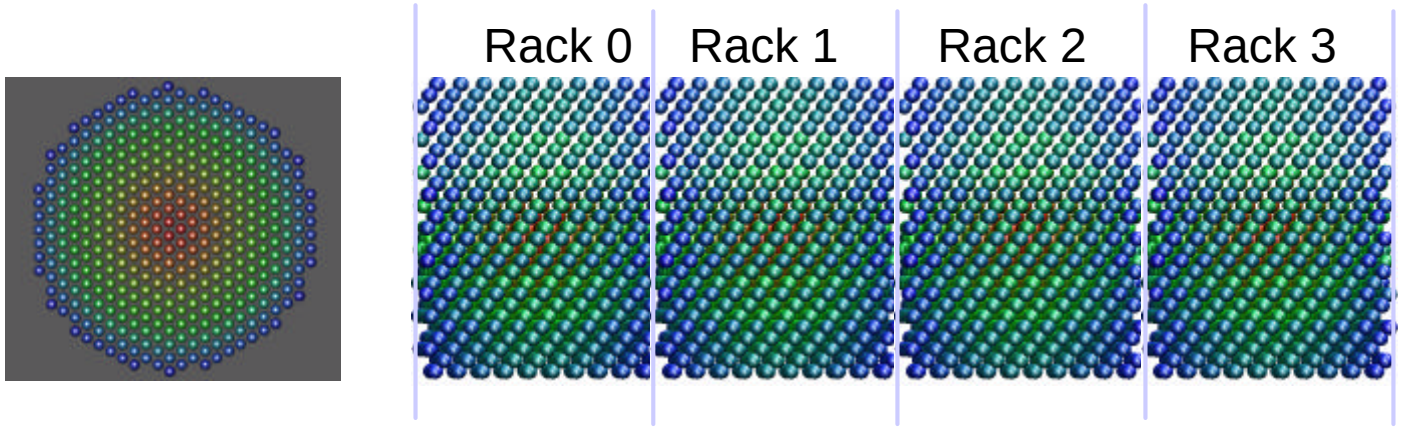
- Start from t-Δt – check data consistency
- MPI_Cart_create() – mapping from domain decomposition to processor topology
- Check I/O – file creation and write

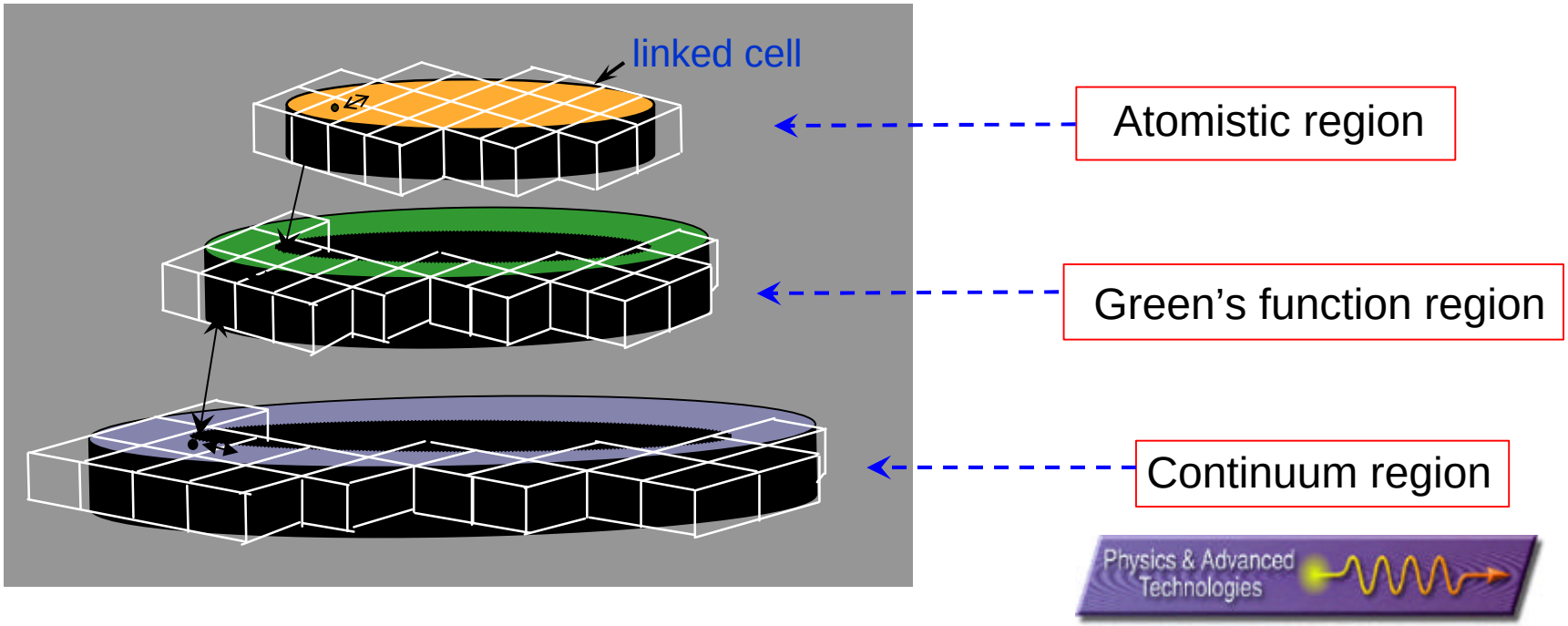
→ MPI_Abort()

or

Continue

Layered-cake domain decomposition





Unix-like interface for parallel I/O

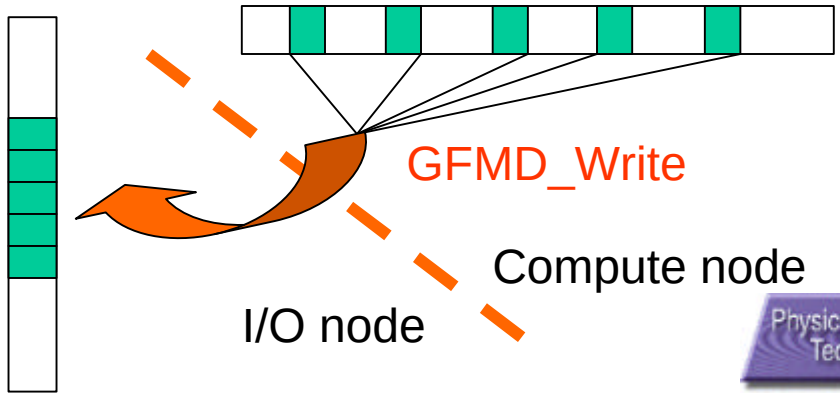
- Compute nodes calculate offsets and sizes of data to be transmitted
- Each compute nodes combine all overlapping or consecutive I/O requests into one single I/O call
- Use MPI derived data type
- Global synchronization file creation

FILE *GFMD_Create(char *filename) { Single file creation / Multiple file creation

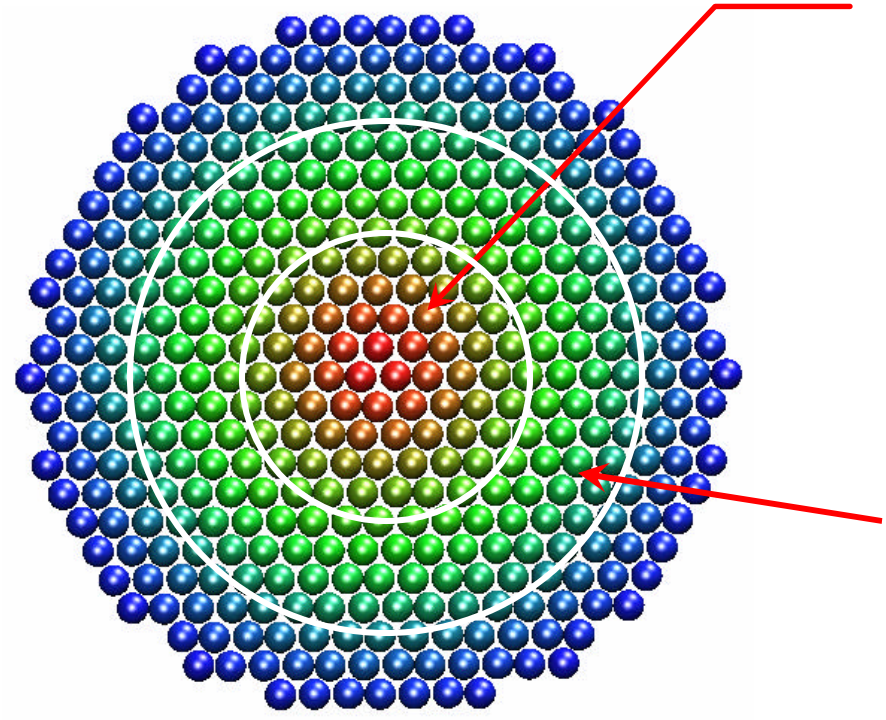
- Non-blocking I/O

GFMD_Read(FILE *f, long offset, MPI_Datatype *data, unsigned long size)

GFMD_Write(FILE *f, long offset, MPI_Datatype *data, unsigned long size)



Communication schemes



Short- and mid-range communications

- Required for every time step
- MPI derived data type
- MPI_Sendrecv()

  (MPI_Sendrecv_replace()?)

- Fixed communication patterns

Global

- Required for every 10 time steps
- MPI derived data type
- MPI_Allreduce()
- MPI_Scatterv()

Conclusion and future work

- BG/L can bring atomistic simulations of materials strength one step closer to the experiments designed for NIF

- The incoming LLNL's MCR Linux cluster can provide a great opportunity to test and modify our programming models for BG/L

- Data compression scheme designed for MD simulations

- Optimization of I/O performance

- Domain decomposition based on computational and I/O requirements

Collaborators

H Division, PAT, LLNL

- Jim Glosli
- John A. Moriarty
- Per Soderlind