A Concurrent Parallel Multiscale Algorithm for Large 3D Continuum/Atomistic Simulations at Finite Temperature Using LAMMPS

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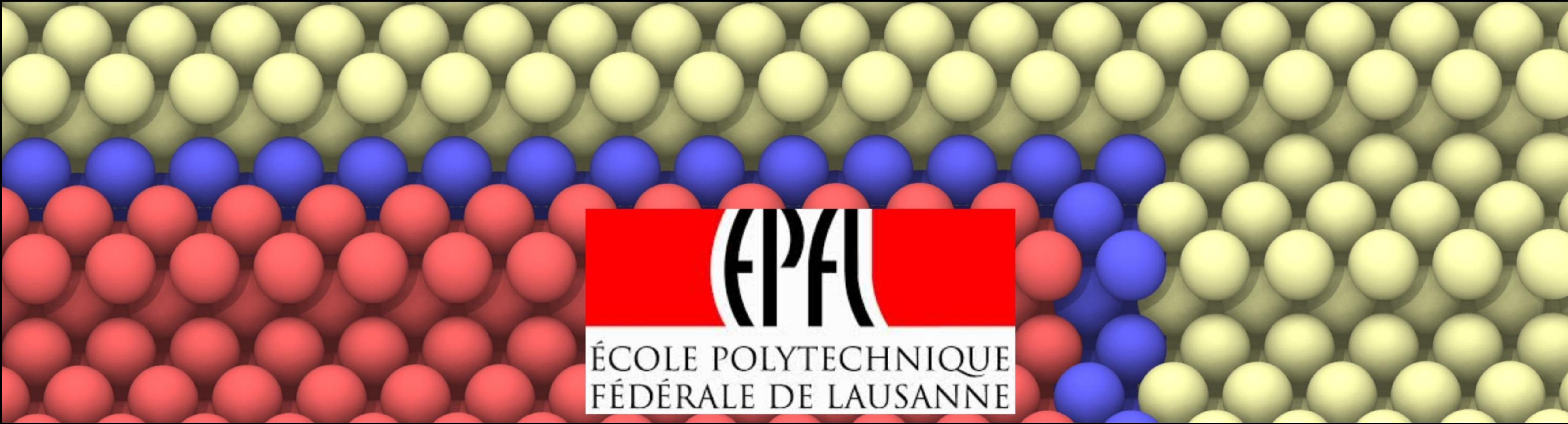

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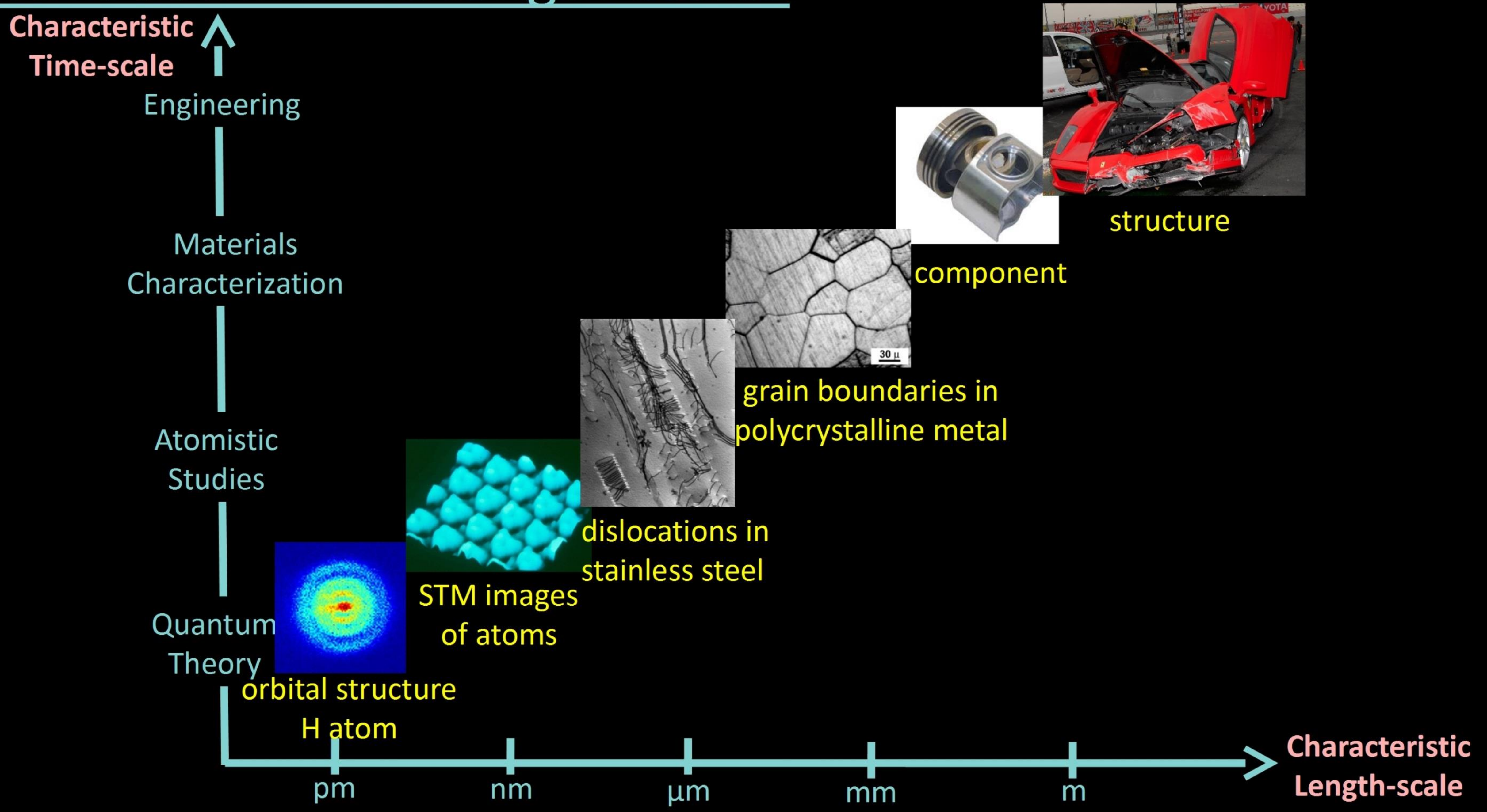
Outline

- Background
- Implementations
- Applications to Dislocations in Aluminum
- Summary

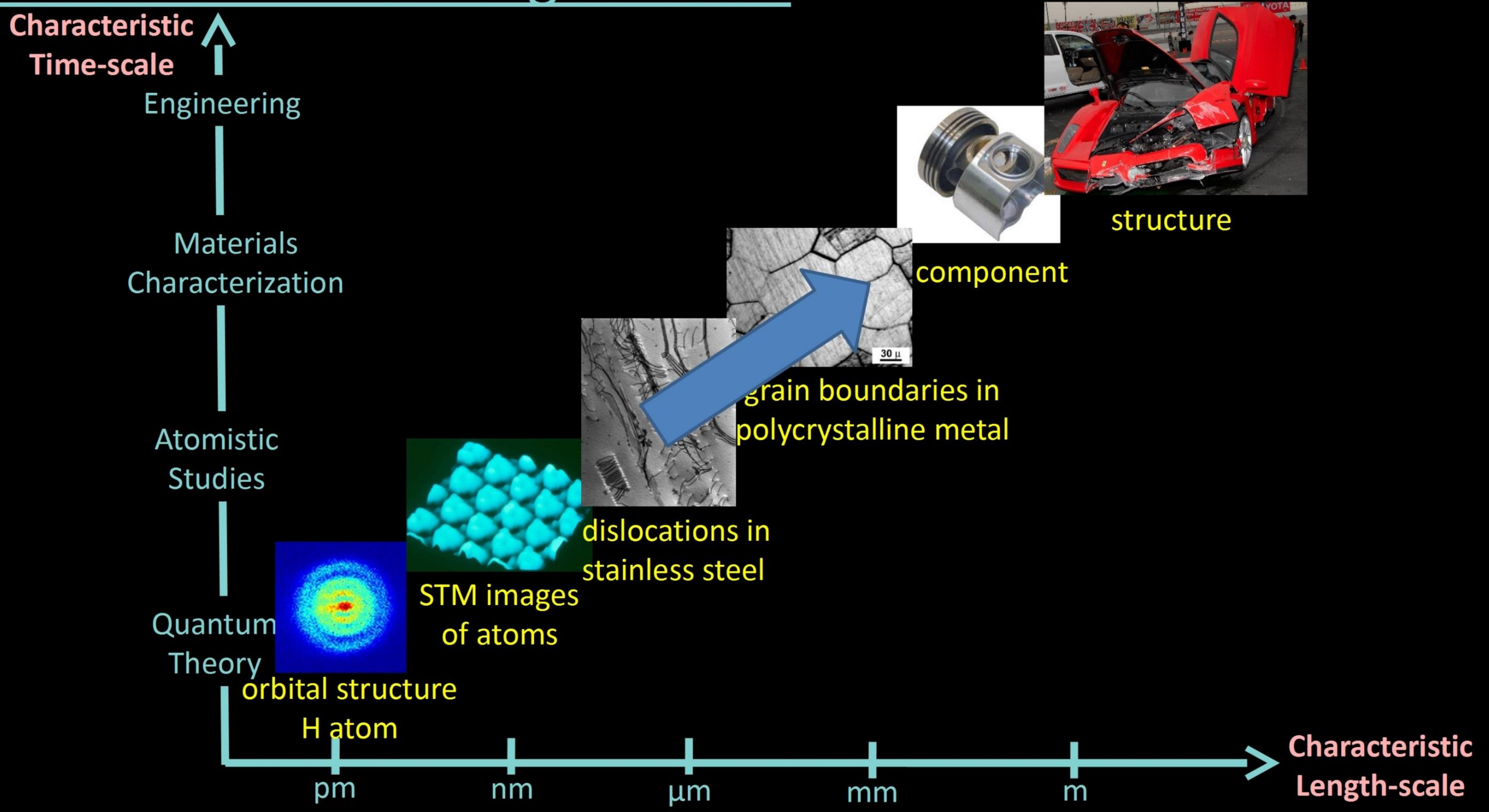
The "Need for (Computational) Speed…"

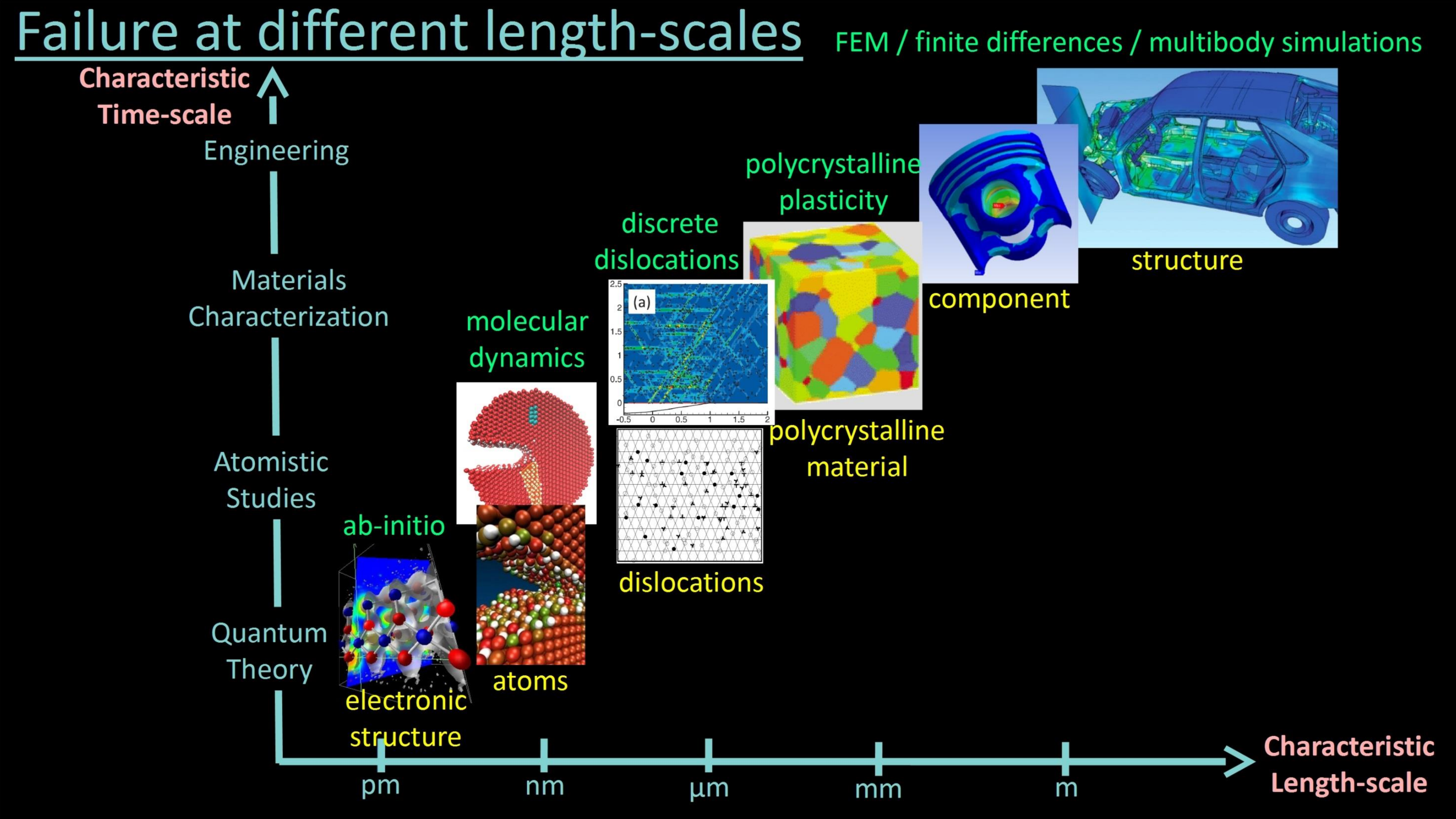
…A Beautiful Example of Failure

Failure at different length-scales



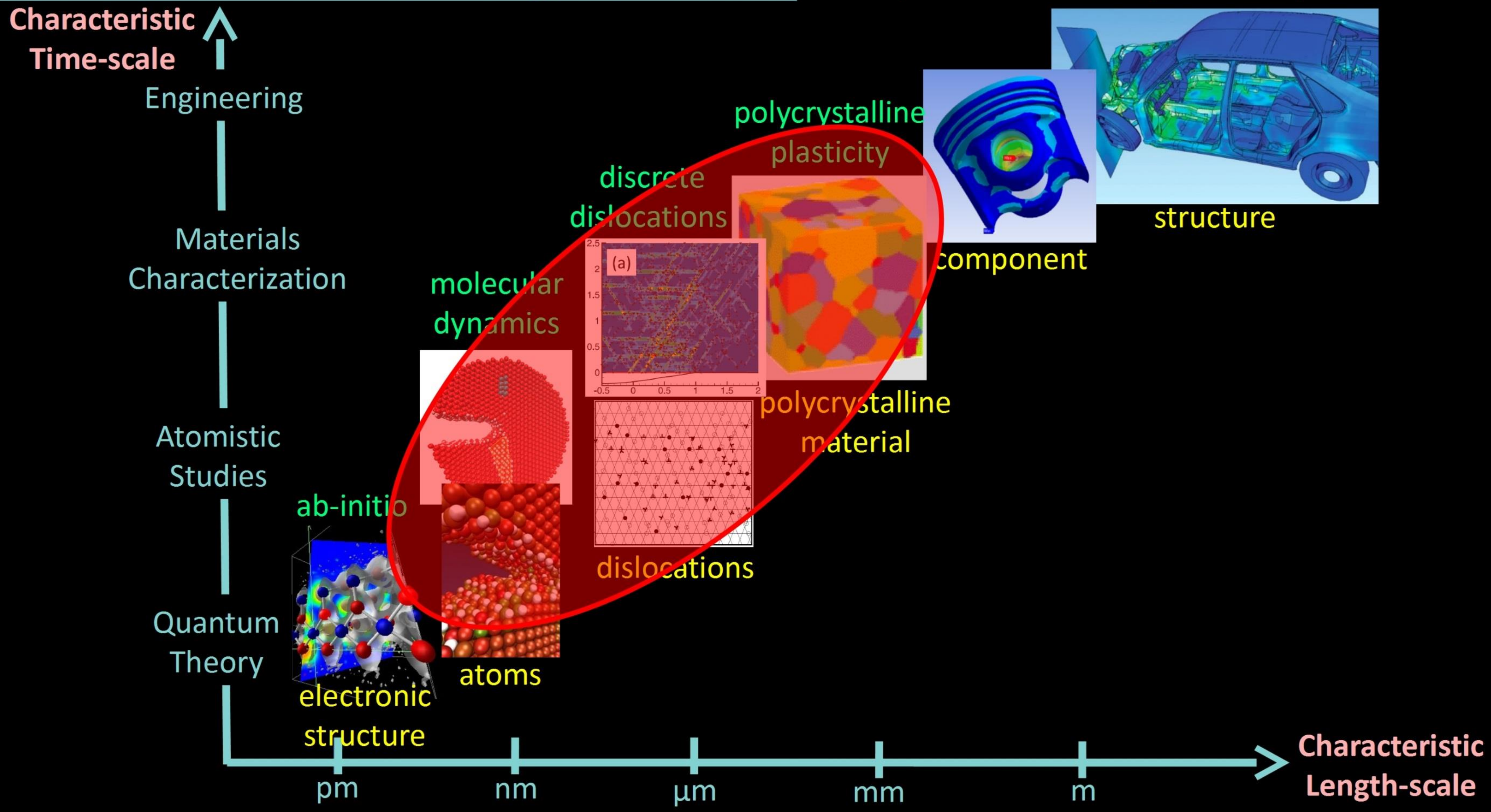
Failure at different length-scales





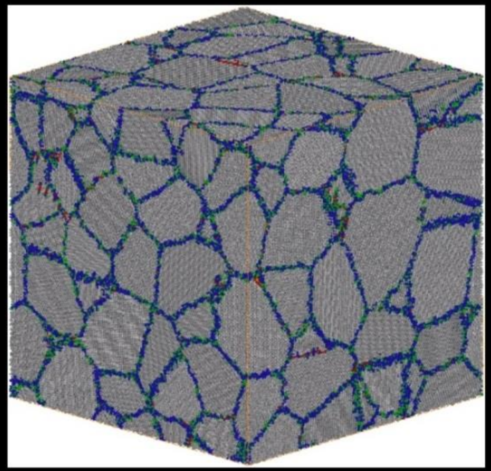
Failure at different length-scales
FEM / finite differences / multibody simulations
Characteristic Time-scale
Engineering
Materials Characterization
Atomistic Studies
Quantum Theory
ab-initio
electronic structure
molecular dynamics
atoms
discrete dislocations
dislocations
polycrystalline plasticity
polycrystalline material
component
structure
Characteristic Length-scale
pm
nm
µm
mm
m

Failure at different length-scales

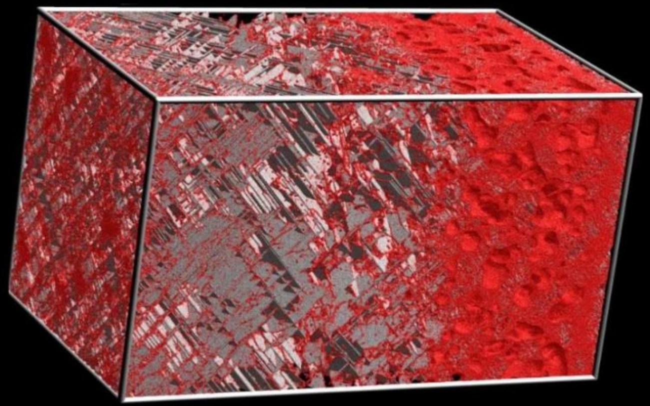


Possible Strategies

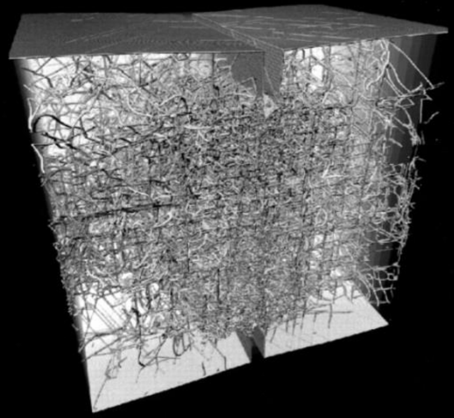
(1) Very large atomic models



Van Swygenhoven H., Weertman J. R., Materials Today 2006



Germann T. C., Kadauy K., Lomdahl P. S., Gordon Bell Performance Prize 2005



Abraham et al., PNAS 2001

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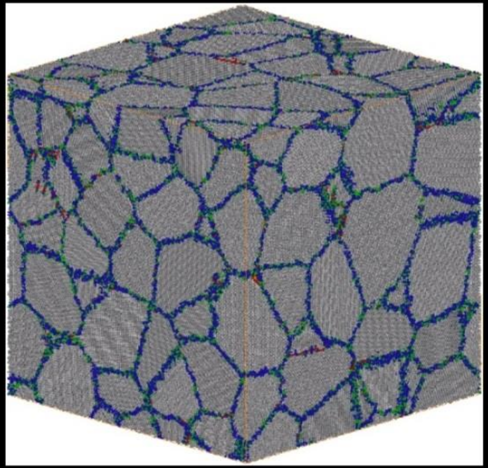
(1) Very large atomic models



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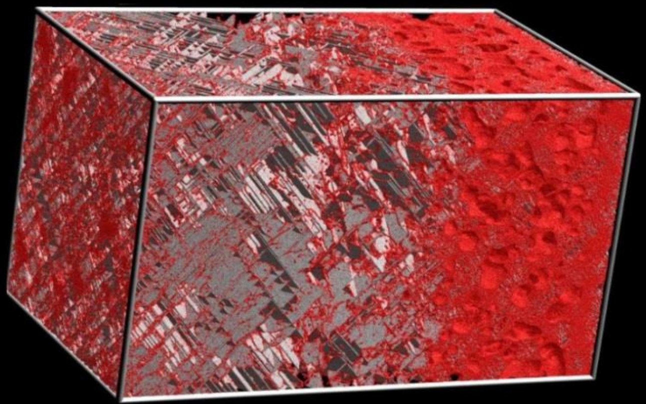

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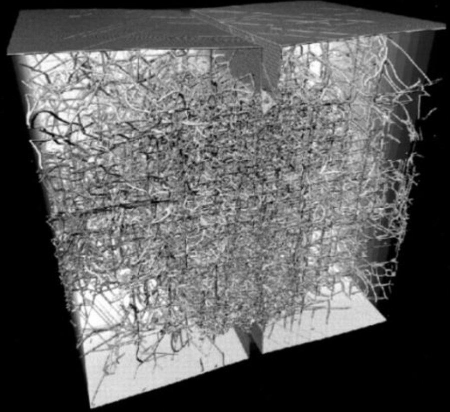

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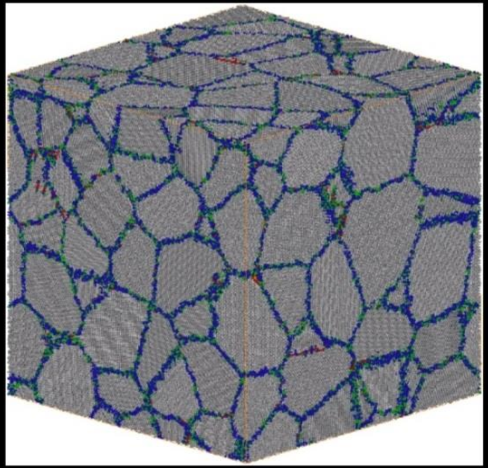
(2) Hierarchical / Sequential Multiscale Models → weak coupling between scales

Possible Strategies

(1) Very large atomic models



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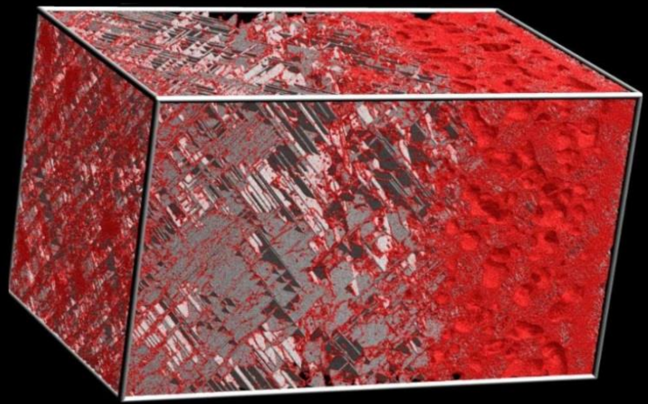

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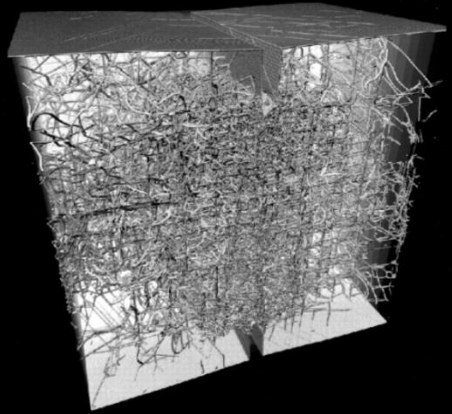


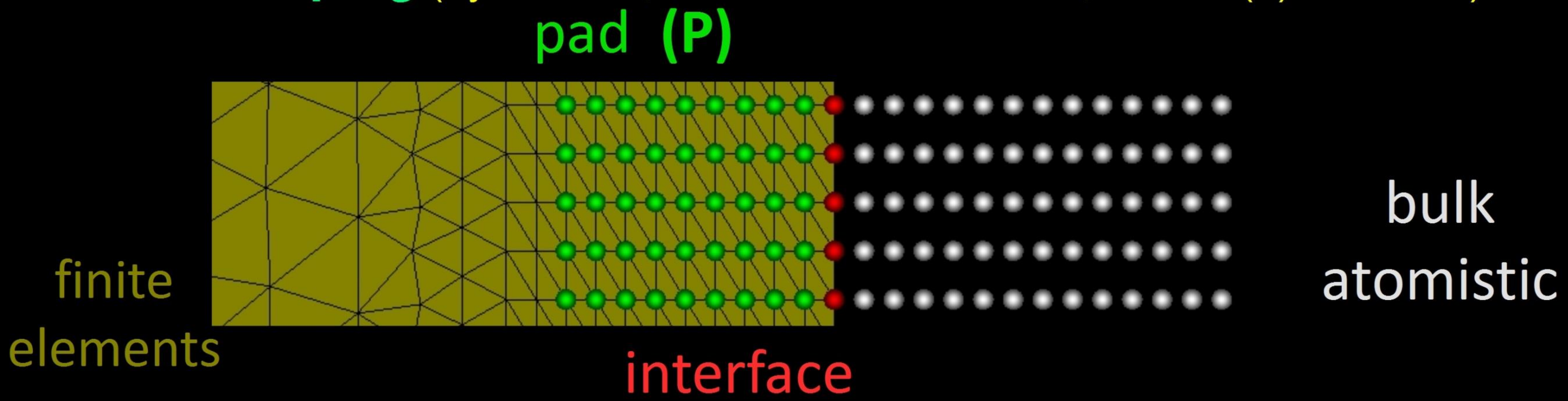
Abraham et al., PNAS 2001

(2) Hierarchical / Sequential Multiscale Models → weak coupling between scales

(3) Concurrent Multiscale Models → strong coupling between scales

Our Multiscale Approach

CADD-*like* Coupling (by Shilkrot, Miller and Curtin 2002, *PRL* 89(2) #025501) **in 3D**



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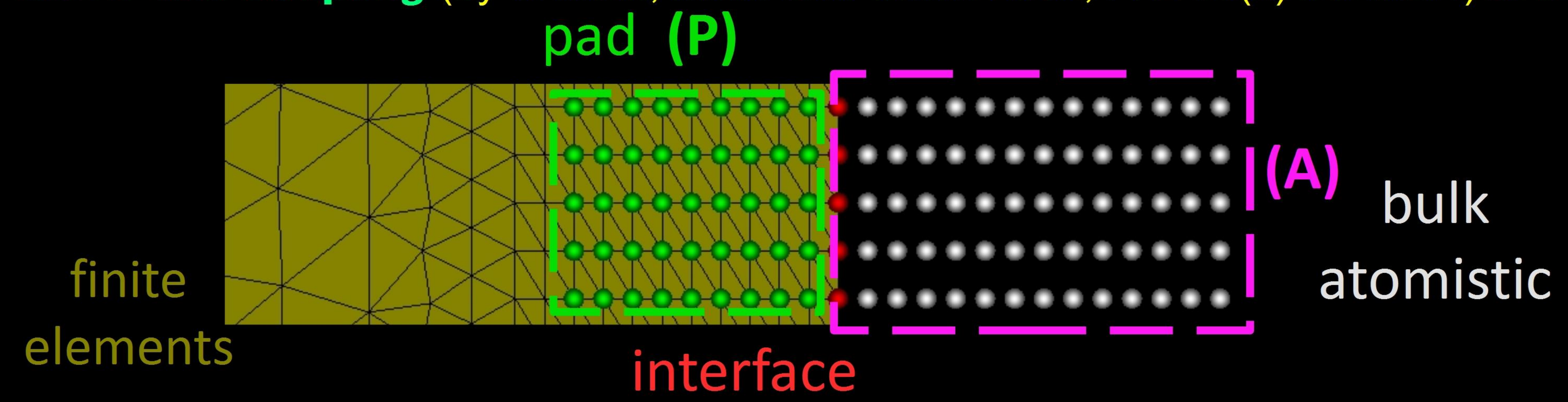

Energy → Forces

Atoms

$$W^{A+P} = \sum_{i \in \Omega^A, \Omega^P} E^i \quad \longrightarrow \quad \mathbf{F}^i = -\frac{\partial}{\partial \mathbf{r}^i}\left(W^{A+P}\right) \quad i \in \Omega^A$$

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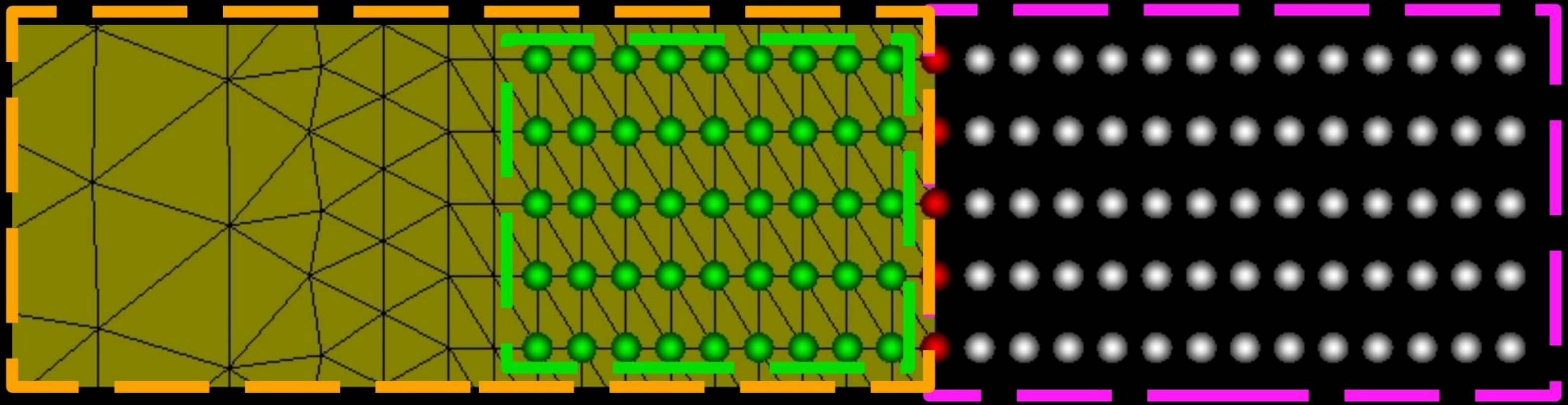
pad **(P)**, forces from (C)

(C)



(A)

bulk atomistic

finite elements

interface, disp. BCs from (A) to (C)

Energy — Forces

Atoms

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Nodes

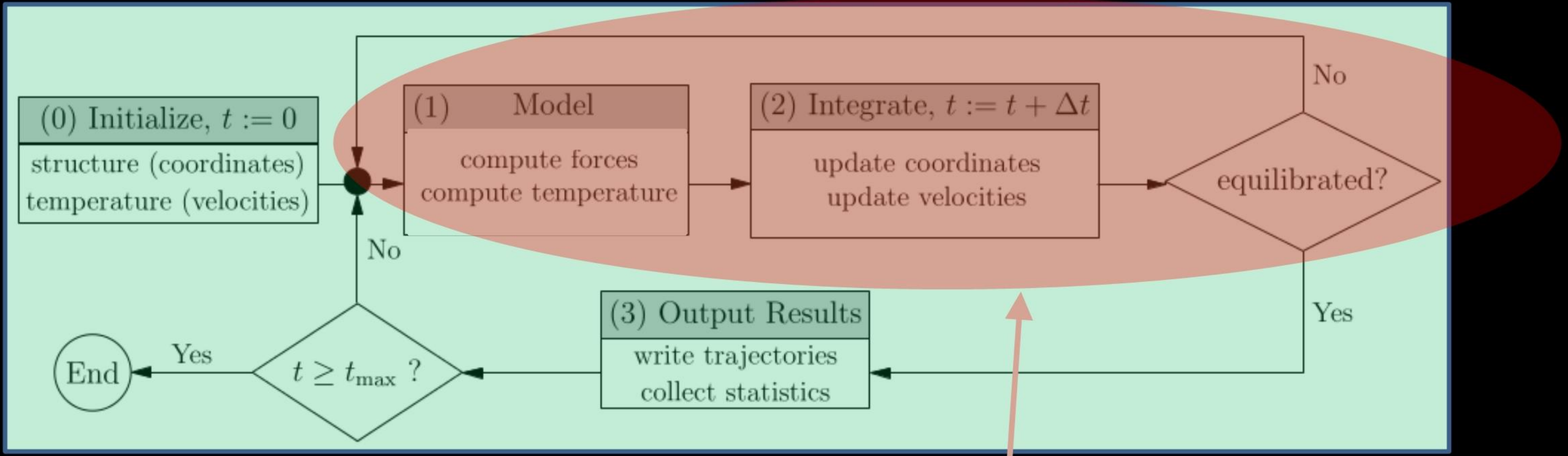
$$W^{C+P} = \int_{\Omega^{C+P}} W(\mathbf{r}) d\Omega$$

$$W(\mathbf{r}) = \frac{1}{2}\epsilon_{ij}(\mathbf{r})\epsilon_{kl}(\mathbf{r})C_{ijkl}$$

$$\longrightarrow \mathbf{F}^i = -\frac{\partial}{\partial \mathbf{r}^i}\left(W^{C+P}\right) \quad i \in \Omega^{C+P} \longrightarrow \mathbf{F} = \sum_{e=1}^{n_{elem}} \int_{V_e} \mathbb{B}^T \mathbb{D} \mathbb{B} \mathbf{U}_e dV$$

Our Multiscale Approach

Explicit Dynamics (**Velocity Verlet** + **Langevin**) for both MD and FE regions



while $t \leq t_{\text{final}}$ **do**

$$\boldsymbol{r}_{t+\Delta t} := \boldsymbol{r}_t + \boldsymbol{v}_t \Delta t + \widehat{\boldsymbol{f}}_t \frac{(\Delta t)^2}{2m}$$ ← positions end of step

$$\boldsymbol{v}_{t+\Delta t/2} := \boldsymbol{v}_t + \frac{\widehat{\boldsymbol{f}}_t}{2m} \Delta t$$ ← velocities half of step

$$\widehat{\boldsymbol{f}}_{t+\Delta t} := \boldsymbol{f}^{\mathrm{L}}(\boldsymbol{r}_{t+\Delta t}, \boldsymbol{v}_{t+\Delta t/2})$$ ← forces end of step

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$$t := t + \Delta t$$

end while

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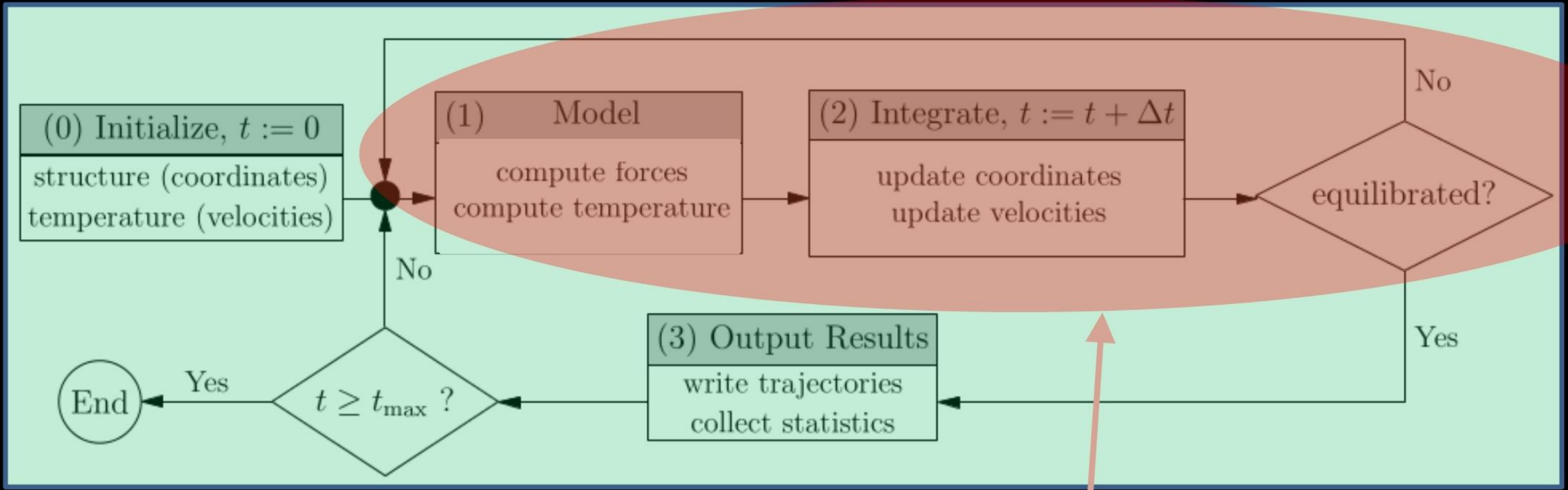

Absorb reflected waves from atomistic region

Langevin equation:

$$\boldsymbol{f}^{\mathrm{L}}(\boldsymbol{r}, \boldsymbol{v}) = \boldsymbol{f} - \gamma m \dot{\boldsymbol{r}} + \boldsymbol{G},$$

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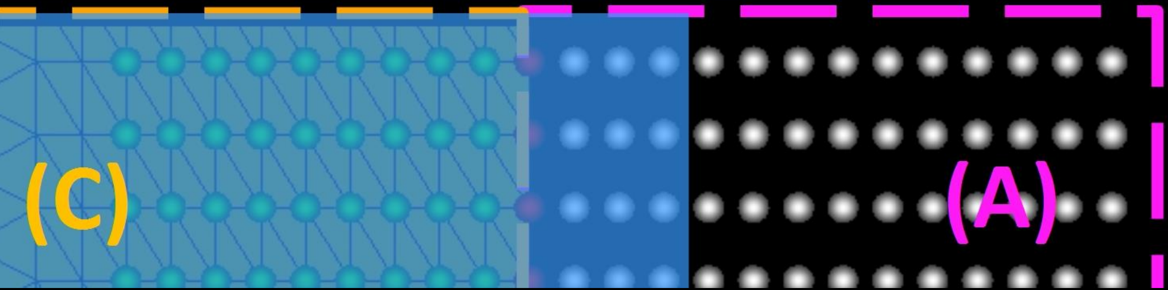

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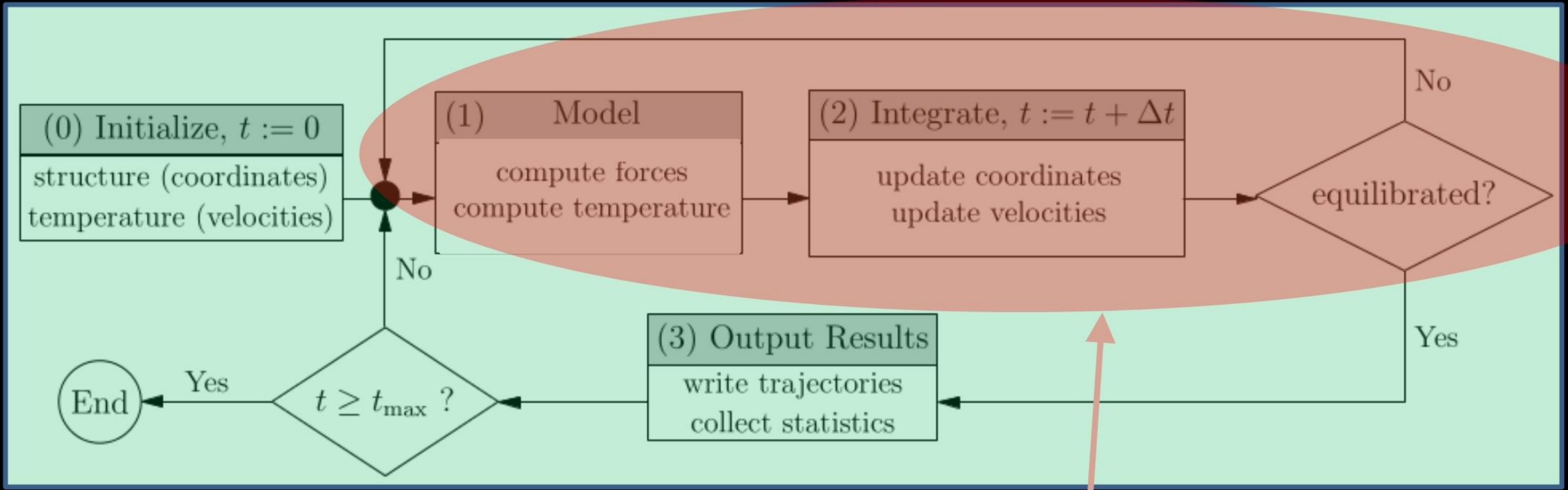

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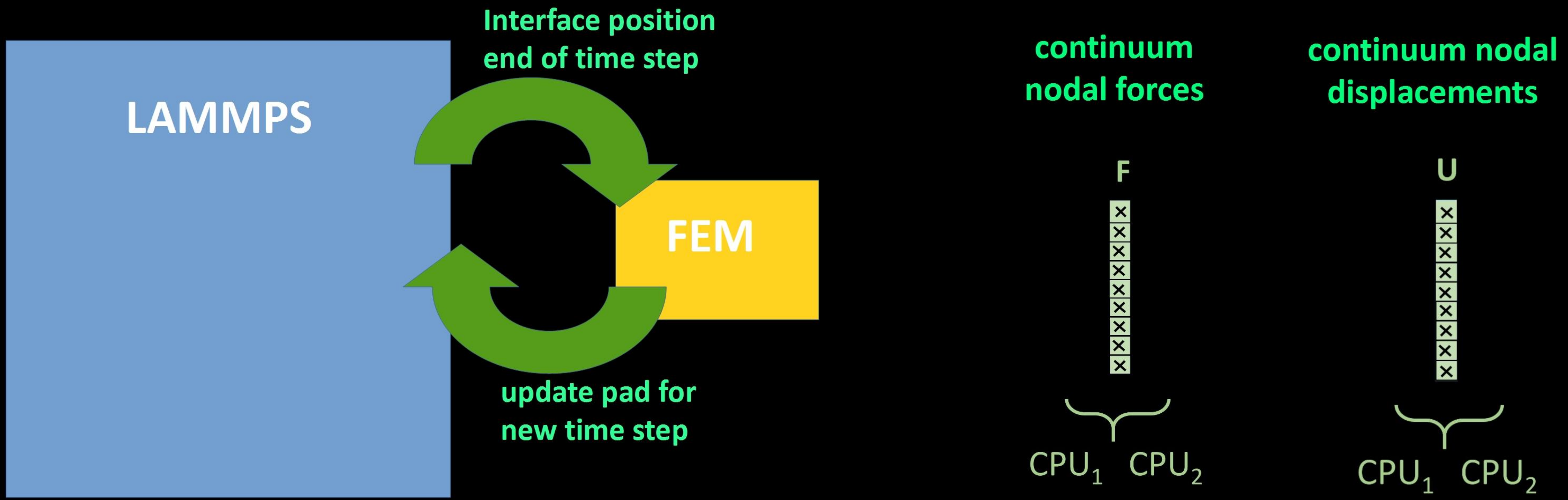
end while

Use LAMMPS for the parallel coupling with the forces on pad from FE

Our Multiscale Approach - LAMMPS

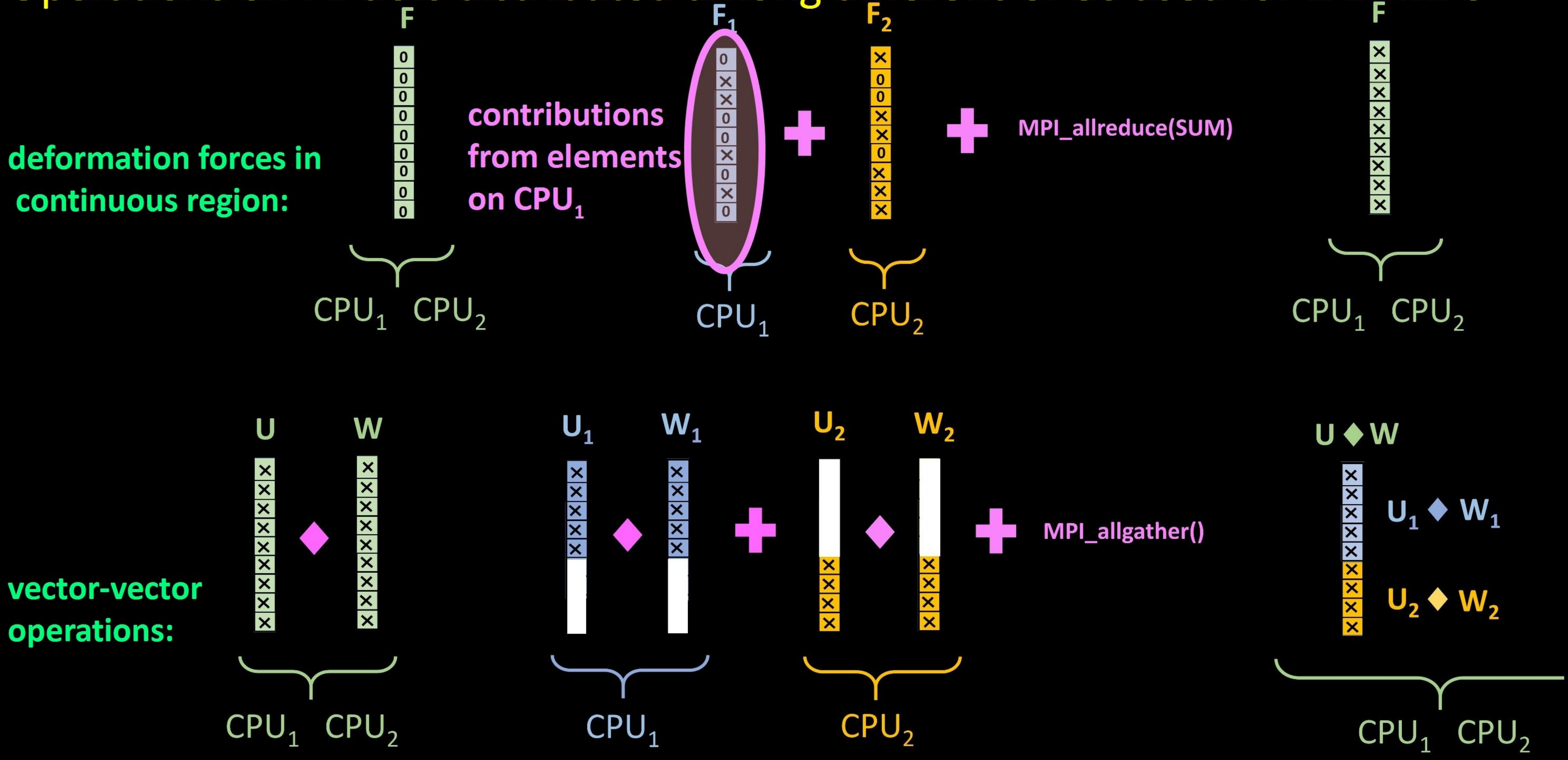
LAMMPS as main driver code, calling the FEM subroutines (C++) when needed



Additional FE dofs (nodal values) stored in global arrays, while tables of finite elements distributed among the CPUs

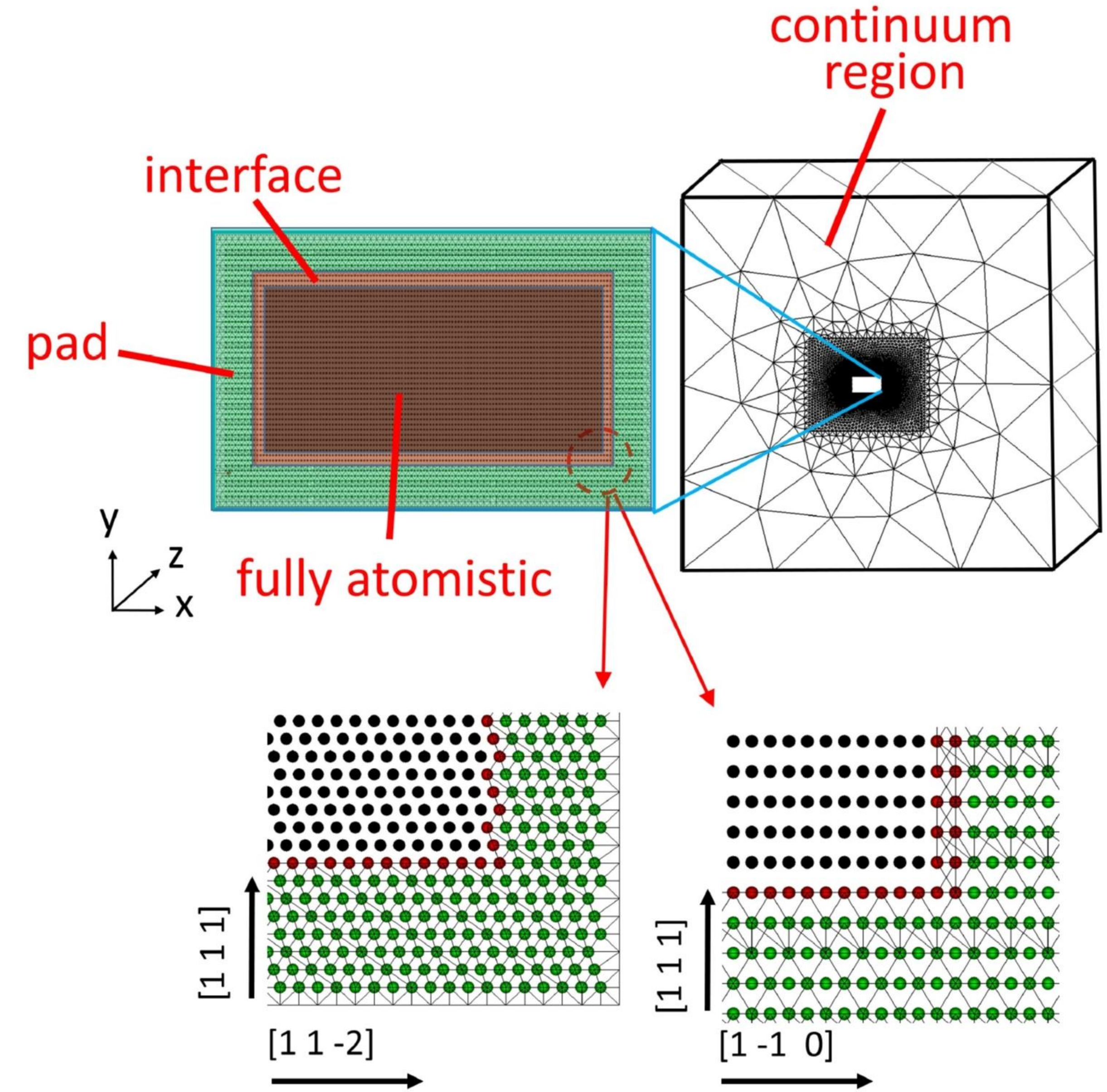
Our Multiscale Approach - Parallelization

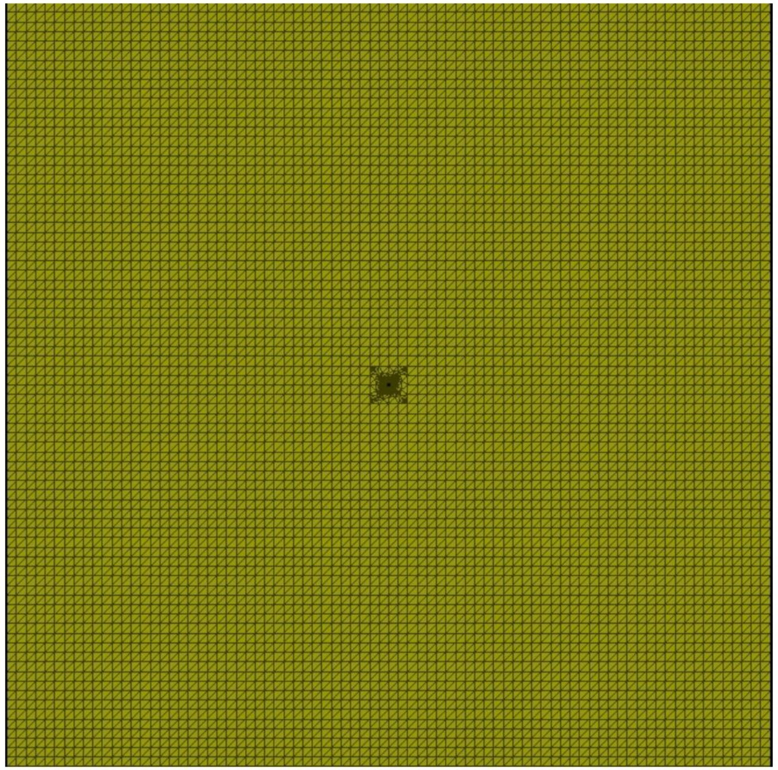
Operations on FE dofs distributed among different CPUs used for LAMMPS

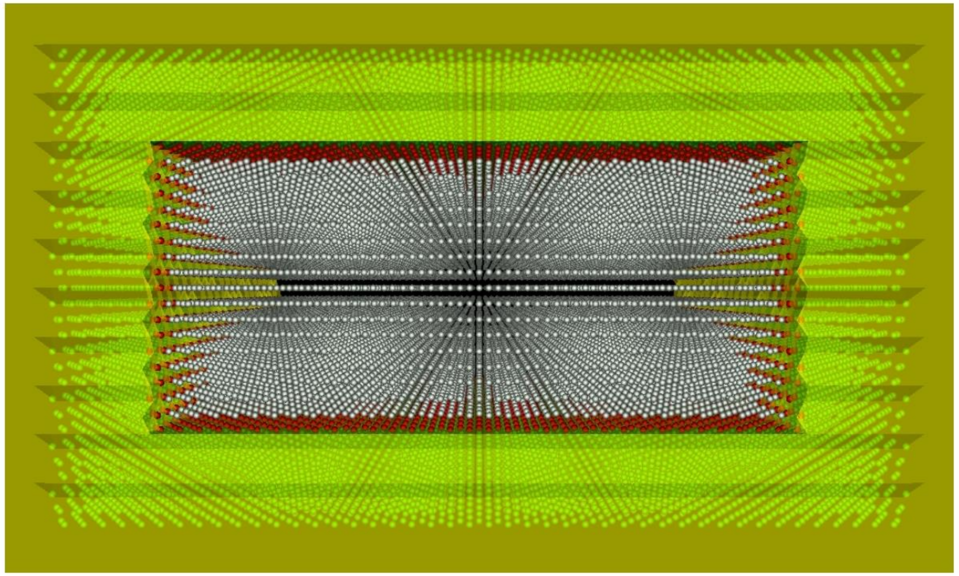


A Multiscale Thin Plate

Modeling a block of aluminum at finite temperature

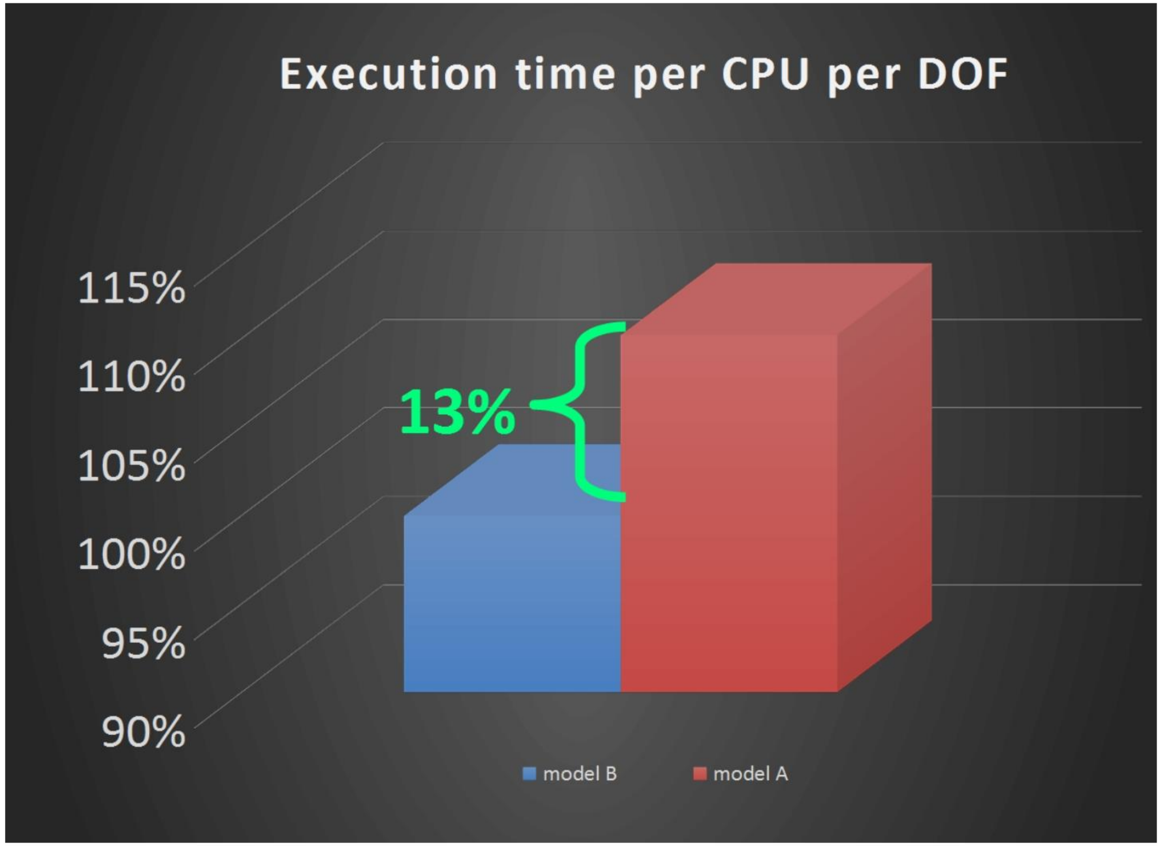






A Multiscale Thin Plate - Benchmark

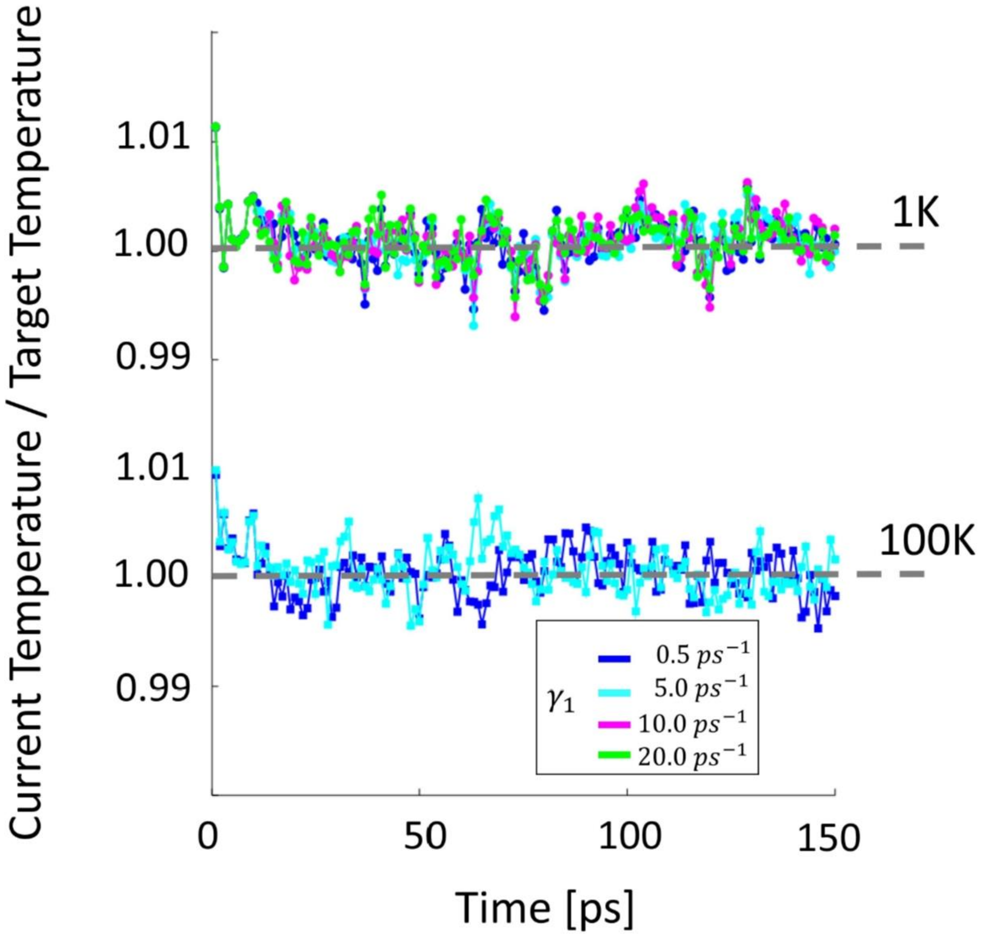
MODEL A (big)	MODEL B (small)
Continuum:	
4000x4000x52nm	4000x4000x11nm
2864134 nodes	278337 nodes
17170903 elements	1575678 elements
Atomistic:	
16x9x52nm	9x4x11nm
458850 atoms	55170 atoms
239400 pad-atoms	29349 pad-at
9968952 DOF 128 CPUs	**1000521 DOF 64 CPUs**



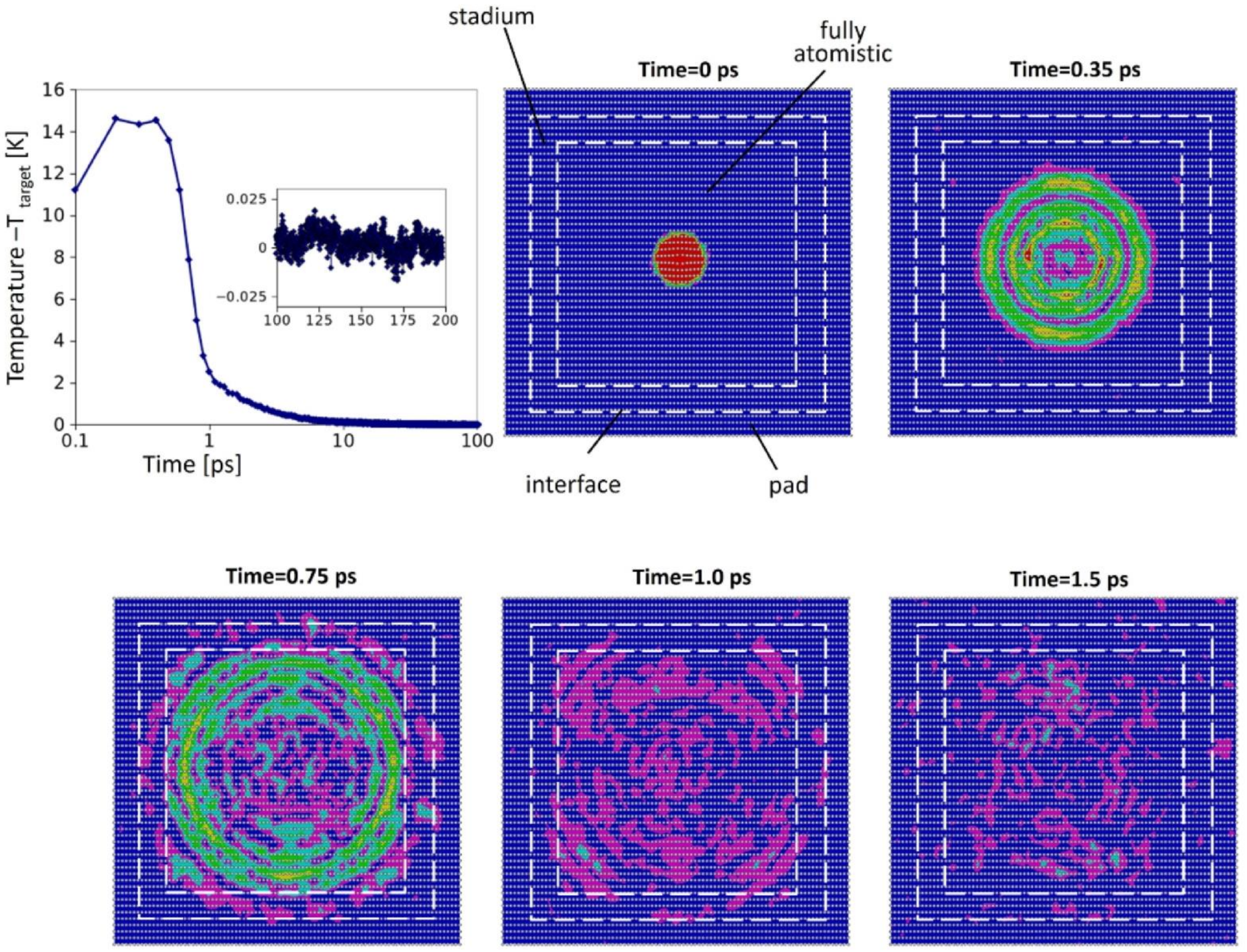
This is how the code scales….

A Multiscale Thin Plate – Temperature Control

Different damping values for the continuum region with fixed damping in the atomistic



Transient Test – Pulse of Radial Displacement

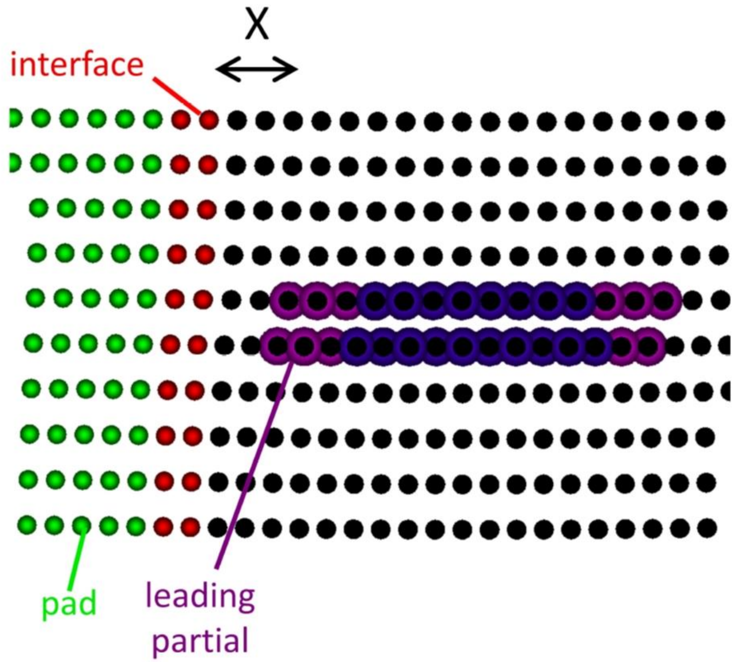


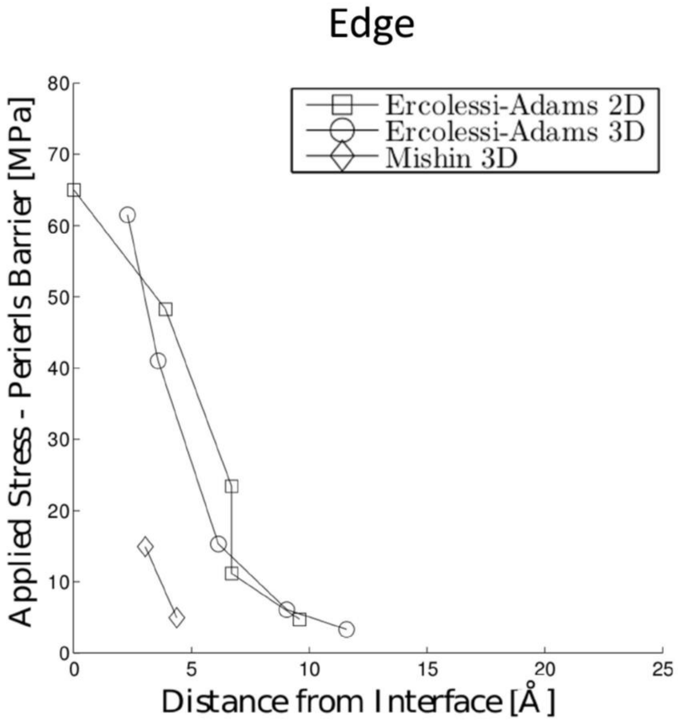
Testing the thermostat….

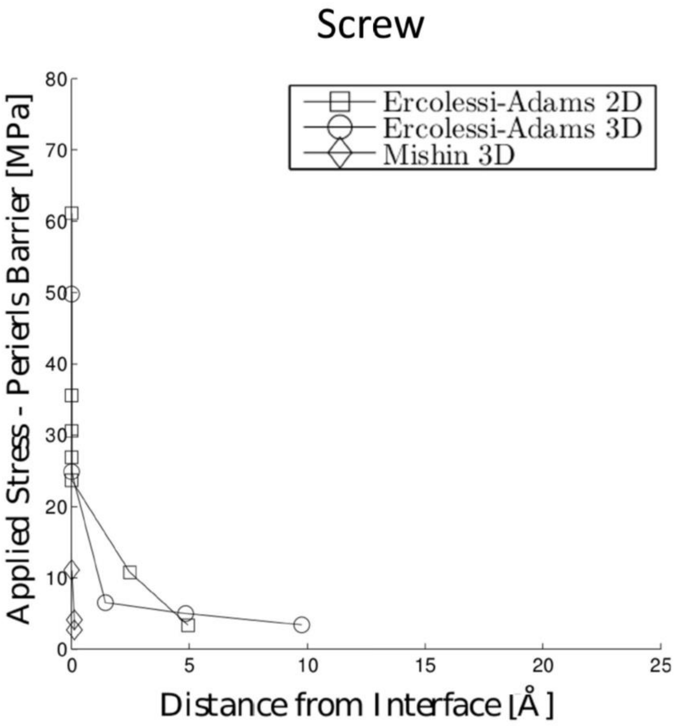
A Multiscale Thin Plate – Insert a Dislocation and Apply Shear

Insert a dislocation (a defect) in the atomistic region and apply uniform shear strain

Continuum discontinuities in the displacements fields treated analytically



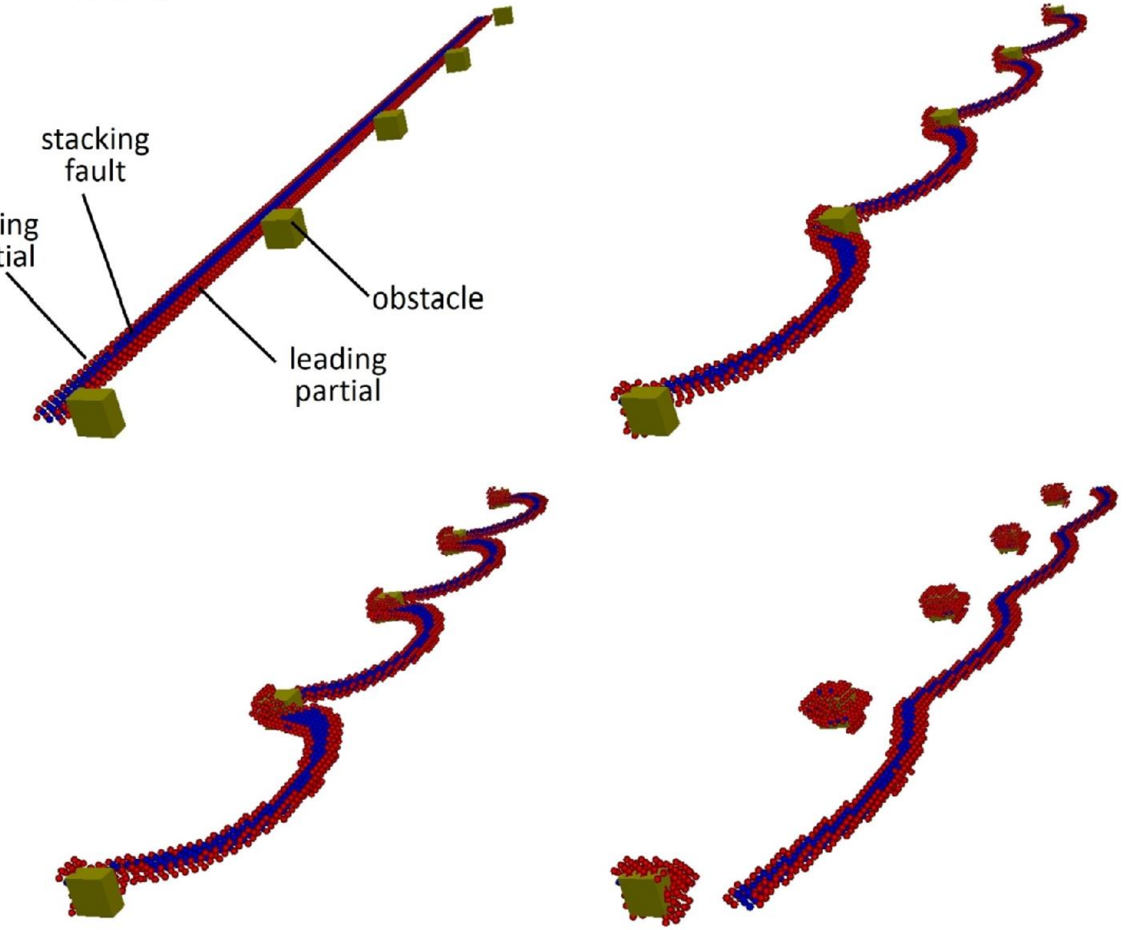


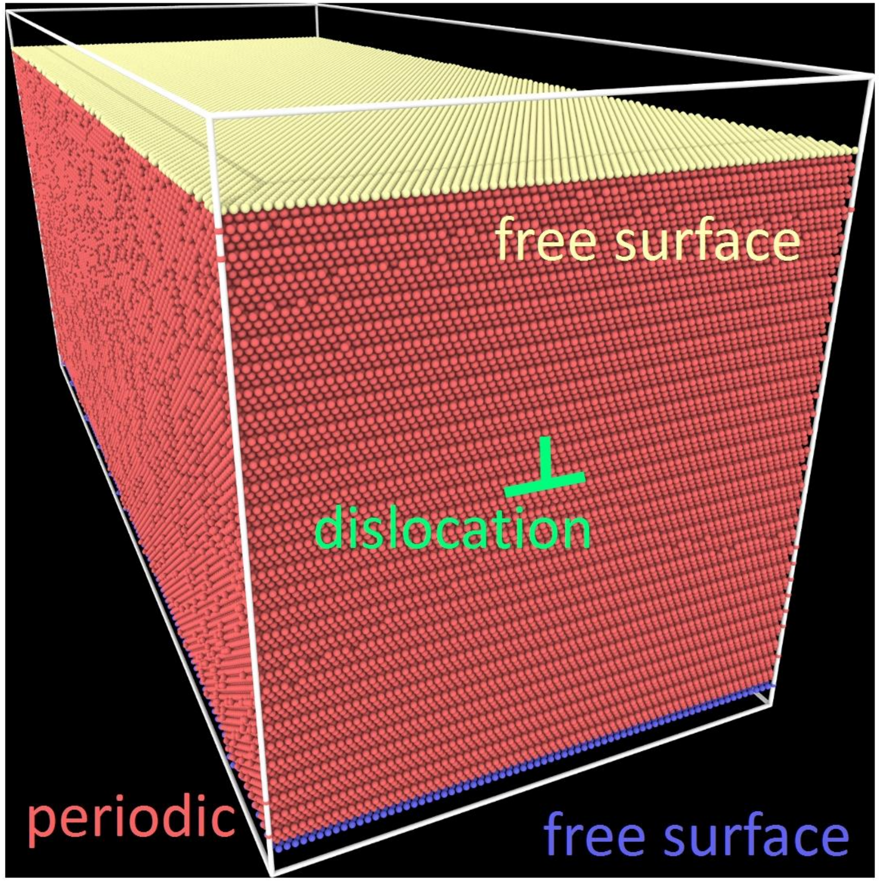


Spurious forces stops the dislocation **before** the interface with continuum region, **high deformation at the dislocation core**

A Multiscale Thin Plate – Disl. Bowout and Finite Size Effects

Create a field of rigid obstacles in the atomistic region to make the dislocation bowout

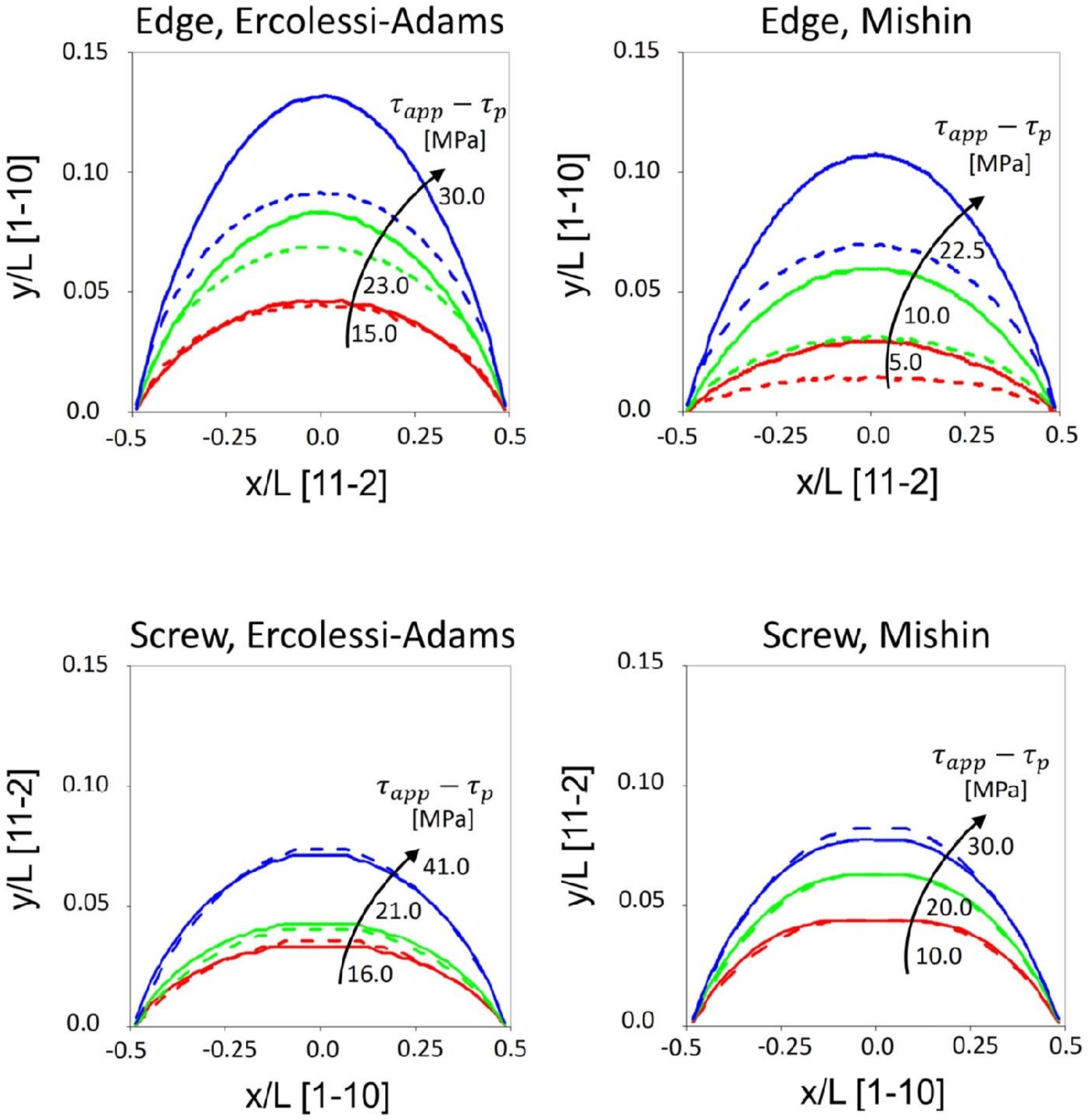




21x21x52nm 1370250 atoms
(Osetsky and Rodney)

Deformed shapes from multiscale simulations compared to smaller finite size only atomistic results (full atomistic box of 4000x4000x52nm requires 62 billions atoms!)

A Multiscale Thin Plate – Disl. Bowout and Finite Size Effects



Infinite vs. finite size with image forces (free surfaces and periodic images)

Image forces reduced on screw dislocations for this particular configurations

Edge disl. bow out approximately twice as much then screw disl., continuum model of line tension normally uses a value close to 1/4

Summary

MD/FE in LAMMPS with a *fix*

Easy to implement and customize

Parallel with good scaling

Accurate - dislocations get to ≈10Å from interface with essentially zero spurious forces

Mesh generation (it is hard in 3D!) for edge and screw disl., atomic mesh resolution with this methodology

Thank you for your attention!