Multiple Time Stepping

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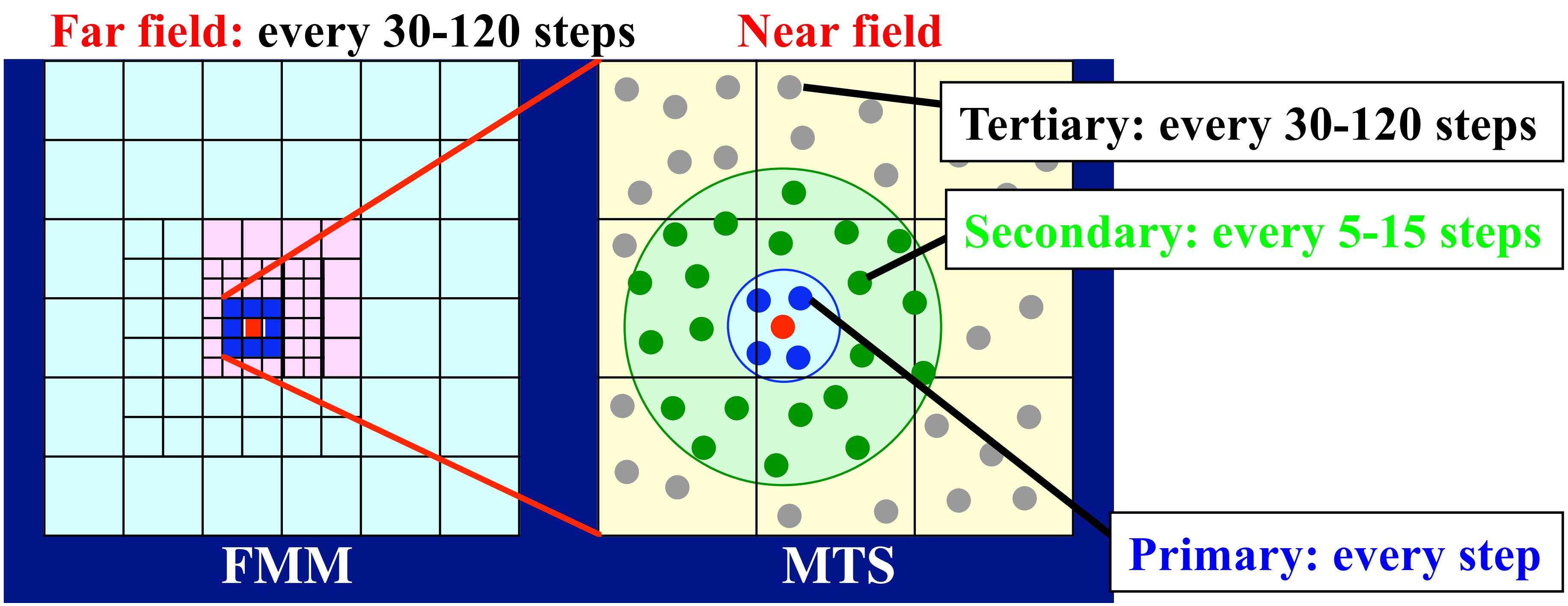
Objectives: Space-time multiresolution algorithms
> Tree codes: fast multipole method
> Multiple time stepping

Temporal Locality: Multiple Time Stepping

- Different force-update schedules for different force components
  → i) Reduced computation
    ii) Enhanced data locality & parallel efficiency



A. Nakano *et al.*, *Comput. Phys. Commun.* **83**, 197 ('94)

https://aiichironakano.github.io/cs653/Nakano-MRMD-CPC94.pdf

Loop Invariant for Long-time Stability

Reversible symplectic integrator *via* split-operator method

$$\Gamma(t+n\Delta t) = e^{iL_{\text{long}} n\Delta t/2}\left(e^{iL_{\text{short}}\Delta t}\right)^n e^{iL_{\text{long}} n\Delta t/2}\Gamma(t)$$

SYMPLECTIC-MTS(positions $\mathbf{r}^N$, velocities $\mathbf{v}^N$)

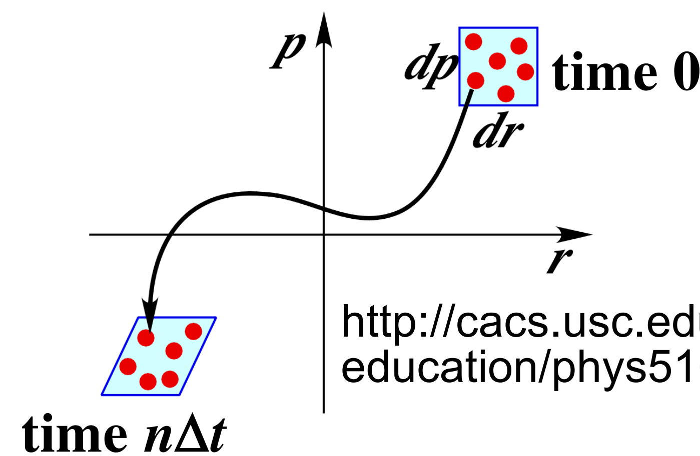
initialize long-range accelerations, $\mathbf{a}_{\text{long}}{}^N(\mathbf{r}^N)$
for outer_step ← 1 **to** Max_outer
    $\mathbf{v}^N \leftarrow \mathbf{v}^N + \mathbf{a}_{\text{long}}{}^N \times$Max_inner$\times\Delta t/2$
    initialize short-range
    accelerations, $\mathbf{a}_{\text{short}}{}^N(\mathbf{r}^N)$
    for inner_step ← 1 **to** Max_inner
        $\mathbf{v}^N \leftarrow \mathbf{v}^N + \mathbf{a}_{\text{short}}{}^N\Delta t/2$
        $\mathbf{r}^N \leftarrow \mathbf{r}^N + \mathbf{v}^N\Delta t$
        update $\mathbf{a}_{\text{short}}{}^N(\mathbf{r}^N)$
        $\mathbf{v}^N \leftarrow \mathbf{v}^N + \mathbf{a}_{\text{short}}{}^N\Delta t/2$
    update $\mathbf{a}_{\text{long}}{}^N(\mathbf{r}^N)$
    $\mathbf{v}^N \leftarrow \mathbf{v}^N + \mathbf{a}_{\text{long}}{}^N \times$Max_inner$\times\Delta t/2$

Phase-space volume is a simulation-loop invariant

↓

Long-time stability

$$\frac{\partial(p_{n\Delta t}^N, r_{n\Delta t}^N)}{\partial(p_0^N, r_0^N)}^T \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix} \frac{\partial(p_{n\Delta t}^N, r_{n\Delta t}^N)}{\partial(p_0^N, r_0^N)} = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}$$

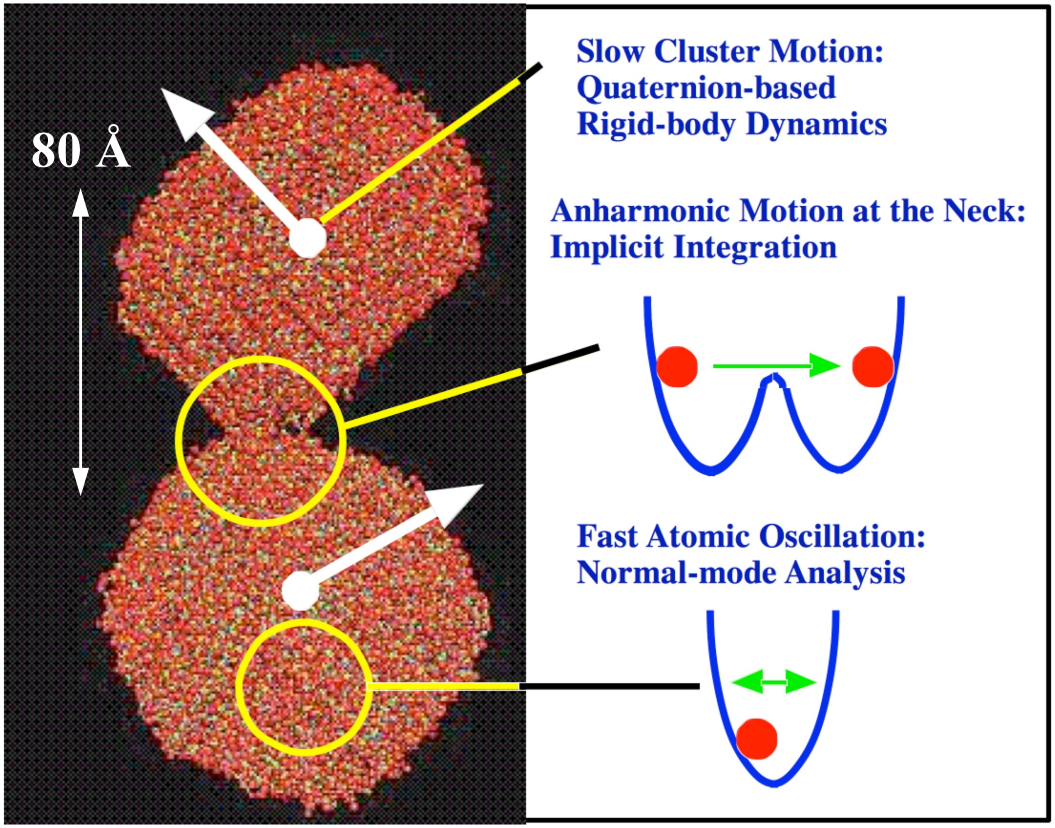


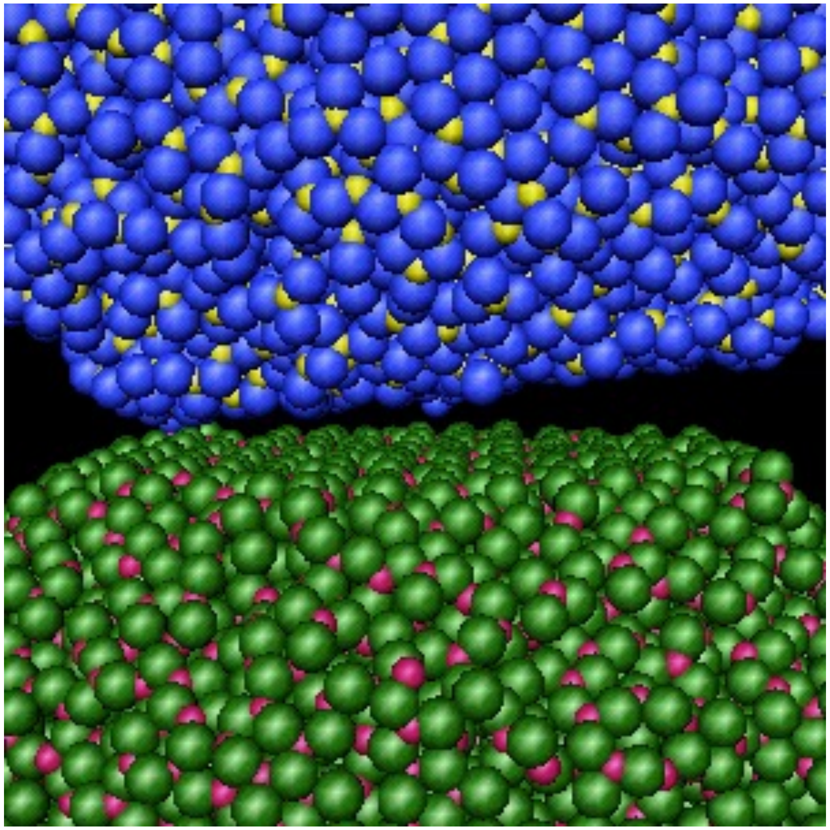
http://cacs.usc.edu/education/phys516.html

M. Tuckerman, B.J. Berne & G.J. Martyna, *J. Chem. Phys*. **97**, 1990 ('92)
https://aiichironakano.github.io/cs653/Tuckerman-RESPA-JCP92.pdf

Clustering-based Hierarchical Dynamics

10^{-6} sec simulation requires 10^9 iterations ($\Delta t = 10^{-15}$ sec): 1,000-fold increase of Δt?



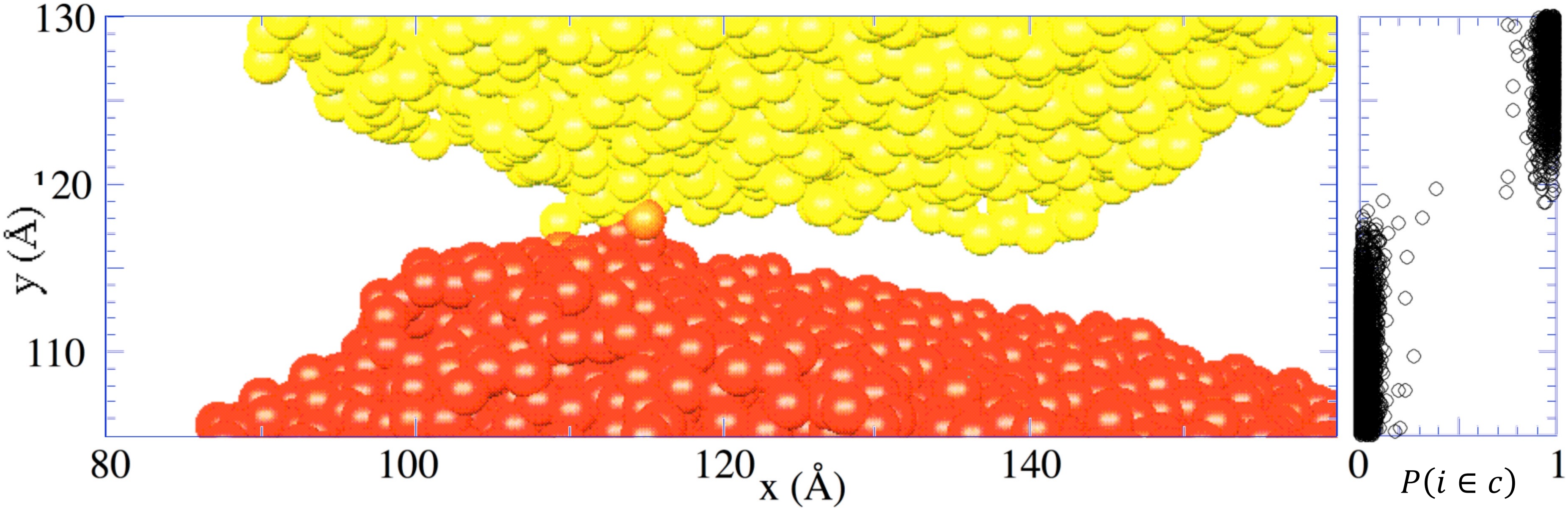


Rigid-body/implicit-integration/normal-mode approach achieves 28-fold speedup over a conventional MD

$$m_i \frac{d^2 \mathbf{z}_i}{dt^2} = \mathbf{F}_i\left(\{\mathbf{z}_i + \mathbf{r}_i^{\mathrm{RigidBody}}\}\right) - \mathbf{F}_i\left(\{\mathbf{r}_i^{\mathrm{RigidBody}}\}\right) + \frac{\partial^2 V}{\partial \mathbf{r}_{\min,i}^2}\left(\mathbf{r}_i^{\mathrm{NormalMode}} - \mathbf{r}_{\min,i}\right)$$

Fuzzy Clustering Facilitates Seamless Integration of Hierarchical Abstraction

Fractional membership function: $P(i \in c)$



Clustering based on chemical cohesion, v_{ij}

[*cf*. fuzzy c-means algorithm, Bezdek]

$$E_c(i) = \frac{1}{2} \sum_{j(\neq i)} P(j \in c) v_{ij}\left(\left|\vec{r}_i - \vec{r}_j\right|\right)$$

A. Nakano, *Comput. Phys. Commun*. **105**, 139 ('97)

https://aiichironakano.github.io/cs653/Nakano-fuzzy-CPC97.pdf

Fuzzy Clustering Improves the Numerical Accuracy of Hierarchical Dynamics

Maximum entropy principle

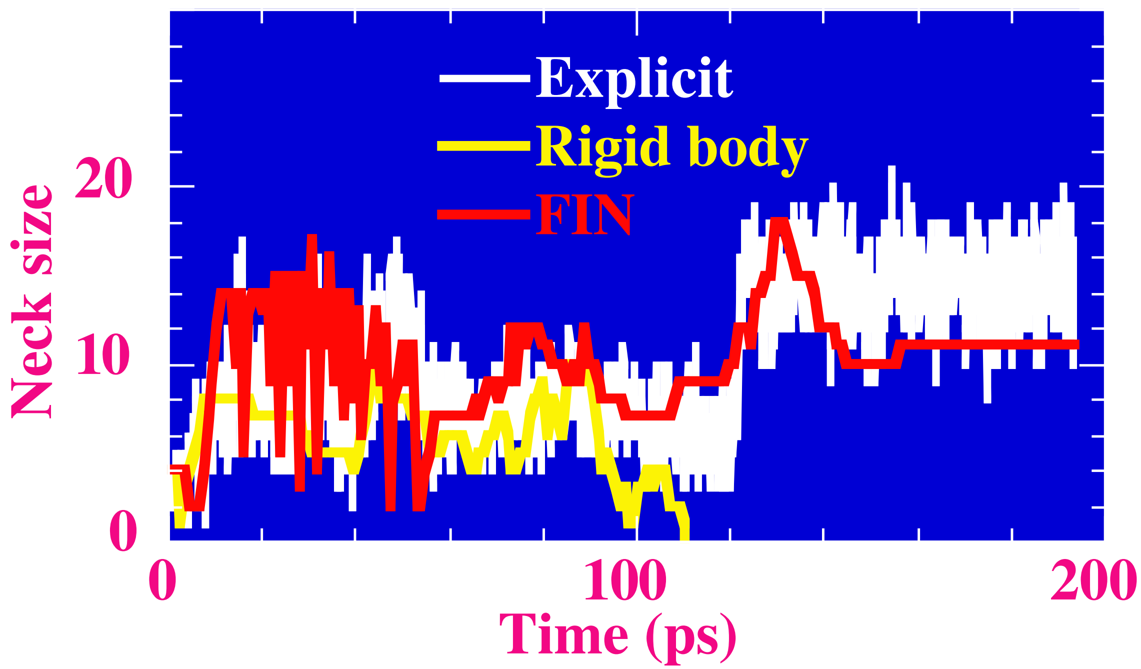
Constrained maximization: $S_i = -\sum_c P(i \in c) \log P(i \in c)$

$$\sum_c P(i \in c) = 1; \ \sum_c E_c(i) P(i \in c) = \text{const.}$$

↓

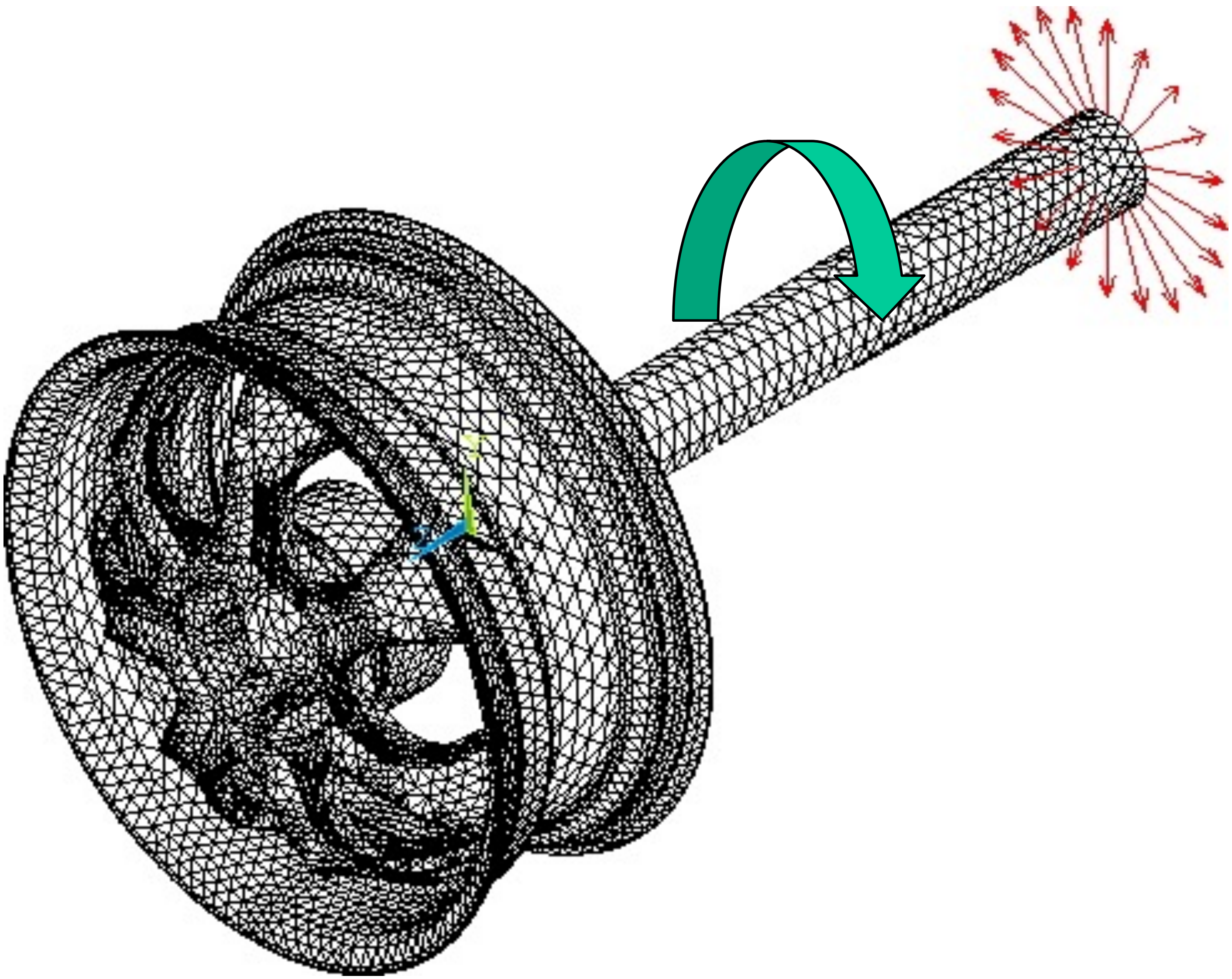
$$P(i \in c) = \exp[-E_c(i)/k_\mathrm{B}T] / \sum_{c'} \exp[-E_{c'}(i)/k_\mathrm{B}T]$$

Fixed-point iteration to determine *P*



Lesson

Use the right representation at each length/time scale



Multiscale MD/QD/FD Simulation

- **Hybrid atoms (molecular dynamics, MD)-electrons (quantum dynamics, QD)-electromagnetic field (field dynamics, FD) simulations**
- **Multiple time-scales: atoms, Δt_{MD} (10^{-15} s) > electrons, Δt_{QD} (10^{-18} s) > electromagnetic field ($e^2/\hbar c \times \Delta t_{QD} = \Delta t_{QD}/136$)**
- **Split-operator formulation:**

$$\exp\left(\frac{iL_{\mathrm{MD}}\Delta t_{\mathrm{MD}}}{2}\right) \times \left[\exp\left(\frac{iH_{\mathrm{QD}}\Delta t_{\mathrm{QD}}}{2}\right) \exp(iL_{\mathrm{FD}}\Delta t_{\mathrm{FD}})^{N_{\mathrm{FD}}} \exp\left(\frac{iH_{\mathrm{QD}}\Delta t_{\mathrm{QD}}}{2}\right)\right]^{N_{\mathrm{QD}}} \times \exp\left(\frac{iL_{\mathrm{MD}}\Delta t_{\mathrm{MD}}}{2}\right)$$

- **Divide-&-conquer Maxwell-Ehrenfest-surface hopping (DC-MESH) code implemented on heterogeneous CPU (central processing unit)-GPU (graphics processing unit) parallel computers**

cf. T. Linker *et al*., *Science Adv.* **8**, eabk2625 ('22)

What We Have Learned So Far

- **Molecular dynamics (MD) represents the dynamic, irregular dwarf (*i.e.*, interaction among spatially-distributed entities).**
- **Data locality (*e.g.*, finite interaction range) is essential to achieve high scalability, which in turn should be expressed using appropriate data structures (*e.g.*, linked-list cells).**
- **If there is no obvious locality, consider divide-conquer-"recombine (*e.g.*, interactive cells in fast multipole method)" —multiresolution in space.**
- **Different subtasks may require different update schedules; consider divide-&-conquer or multiresolution in time.**

Q: Any spatiotemporal multiresolution in "your" application? Any interesting papers?

Tip: Learn a new concept by applying it to what you know well.