Maxwell Equations Molecular Dynamics (MEMD)

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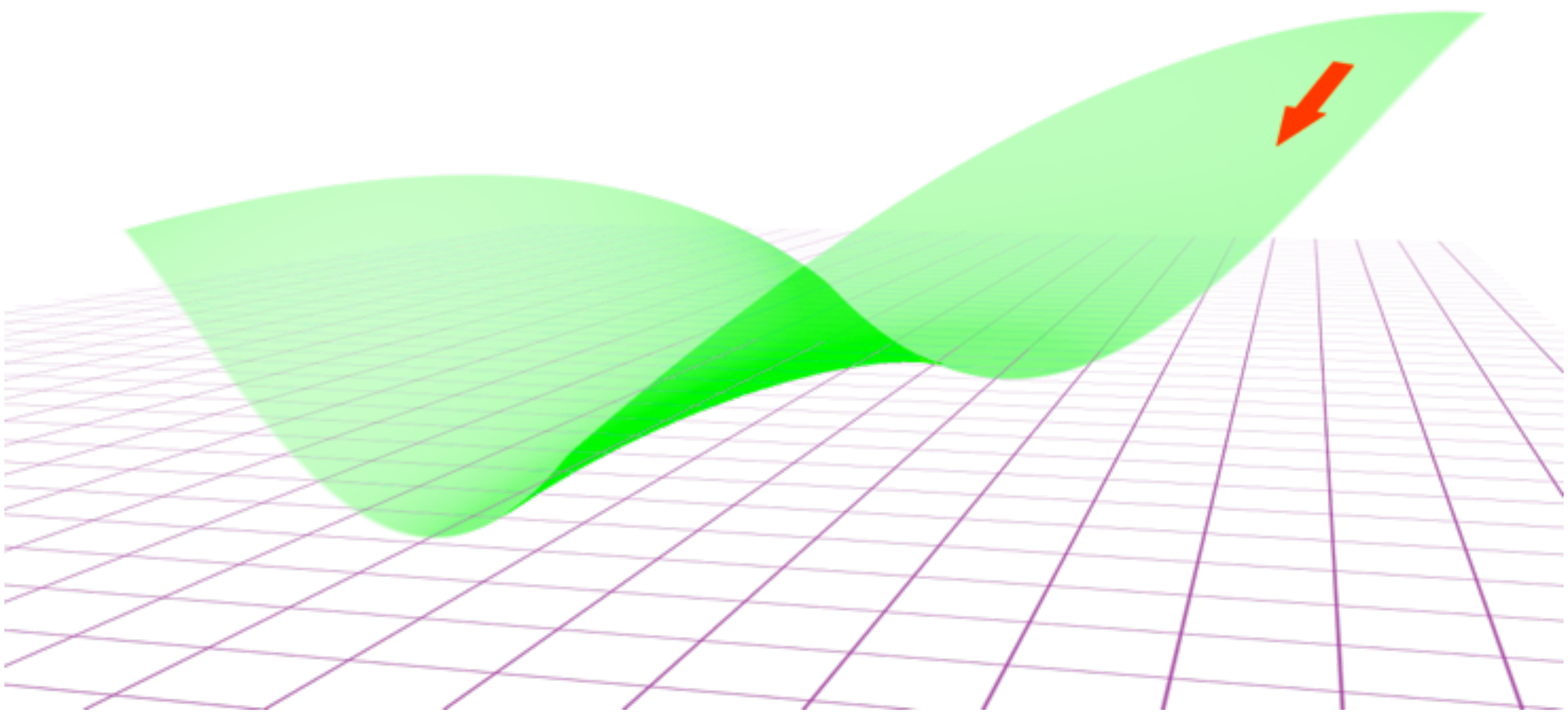
Potentials and fields

$$\Phi \quad : \quad \text{Global absolute value}$$

$$\mathbf{E} = -\nabla\Phi \quad : \quad \text{Local vector value}$$



The problem to solve

Poisson equation

$$\nabla^2 \Phi = -\frac{\rho}{\varepsilon}$$ elliptic PDE

$$\nabla \varepsilon \nabla \Phi = -\rho$$

$$\nabla \cdot \mathbf{D} = \rho$$

with $\mathbf{E} = -\nabla \Phi$ and $\mathbf{D} := \varepsilon \cdot \mathbf{E}$

Gauss‘ law of electrodynamics!

mathematician: hyperbolic!

physicist: local!

computer scientist: $\mathcal{O}(N)$!

Maxwell equations

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\left(\frac{1}{c^2}\right)\dot{\mathbf{B}} = \nabla \times \mathbf{E}$$

$$\dot{\mathbf{D}} = \nabla \times \mathbf{B} - \mathbf{j}$$

$$F_L = q \cdot \left(\frac{\mathbf{D}}{\varepsilon} + \left(\frac{1}{c^2}\right)\mathbf{v} \times \mathbf{B}\right)$$

Lorentz force

Reformulation of Electrostatics

$$\nabla \cdot \mathbf{D} = \rho \qquad \nabla \times \frac{\mathbf{D}}{\varepsilon} = 0 \qquad F_L = q \cdot \frac{\mathbf{D}}{\varepsilon}$$

$$\Updownarrow$$

$$\mathcal{H}_{\mathrm{EF}} = \frac{1}{2} \int \frac{\mathbf{D}^2}{\varepsilon} d\mathbf{r}$$

transversal component minimized away,
constraint vs. Born-Oppenheimer surface

initial solution

$$\mathbf{D}(t_0) = \rho_0$$

time evolution

$$\dot{\mathbf{D}} + \mathbf{j} - \nabla \times \dot{\mathbf{\Theta}} = 0$$

Equations of motion

set of hyperbolic PDEs:

$$m_i \ddot{\mathbf{r}}_i = -\frac{\partial U}{\partial \mathbf{r}_i} - q_i \frac{\mathbf{D}}{\varepsilon} + q_i \mathbf{v}_i \times \mathbf{B}$$

$$\dot{\mathbf{D}} = c^2 \, \nabla \times \mathbf{B} - \mathbf{j}$$

$$\dot{\mathbf{B}} = -\nabla \times \frac{\mathbf{D}}{\varepsilon}$$

with

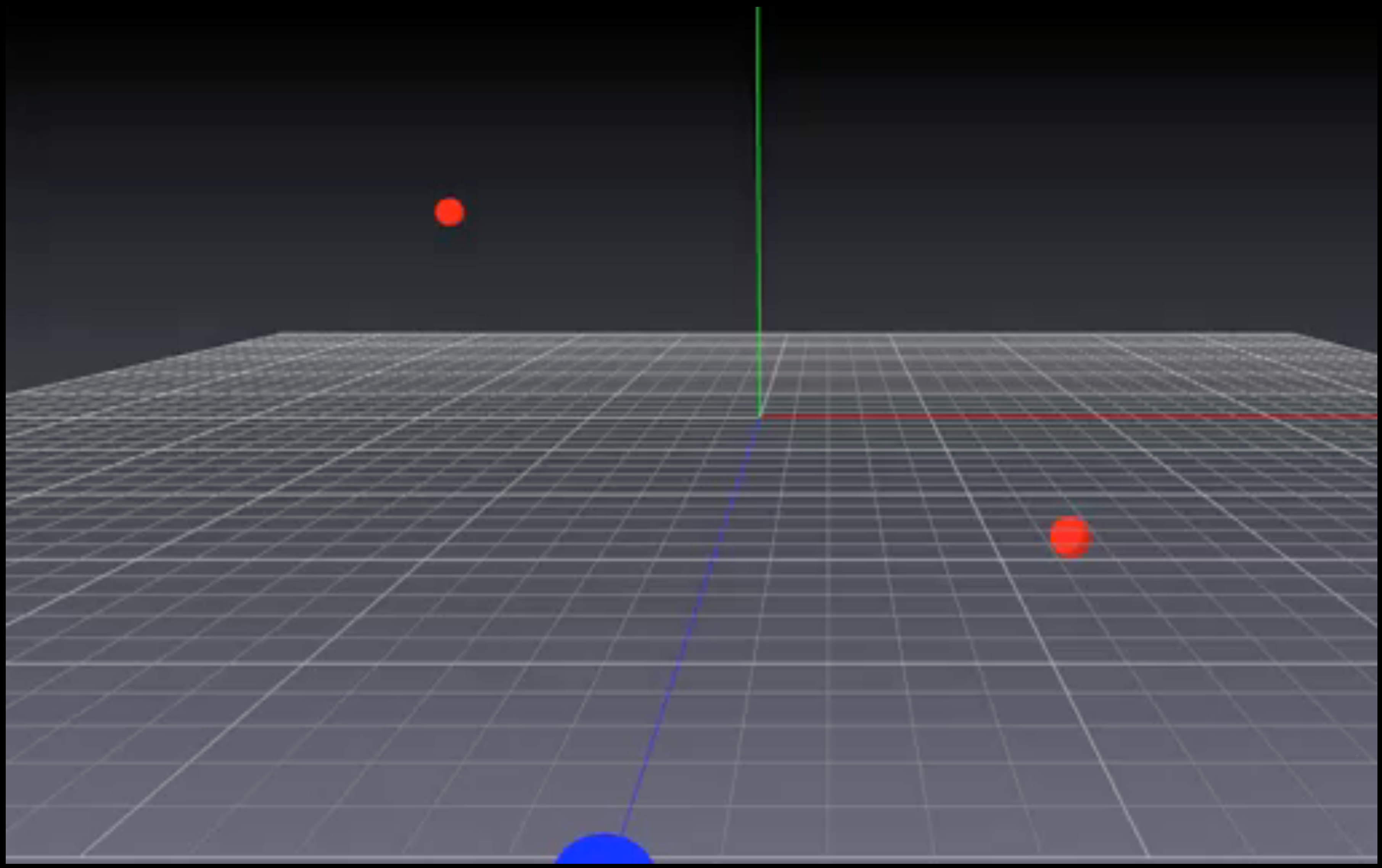
$$f_{\text{mass}} := \frac{1}{c^2}$$

$$\mathbf{B} := \nabla \times \mathbf{A}$$

- initial solution
- time propagation of particles and fields

What it does, graphically

- no instantaneous interaction
- current onto lattice
- magnetic field propagation
- act on particle



CPMD: Treat separate time scales with artificial dynamics

CPMD	MEMD
ion cores	charges
wave function	fields
artificial dynamics for ψ	artificial dynamics for **D**, **B**
electron mass	$f_{\text{mass}} = 1/c^2$

Static observables via statistical physics

Transversal and parallel component

$$\mathcal{H} = \mathcal{H}_\perp + \mathcal{H}_{||}$$

$$\Downarrow$$

Boltzmann factor factorizes:

$$\exp\left(-\frac{\mathcal{H}}{k_B T}\right) = \exp\left(-\frac{\mathcal{H}_\perp}{k_B T}\right) \cdot \exp\left(-\frac{\mathcal{H}_{||}}{k_B T}\right)$$

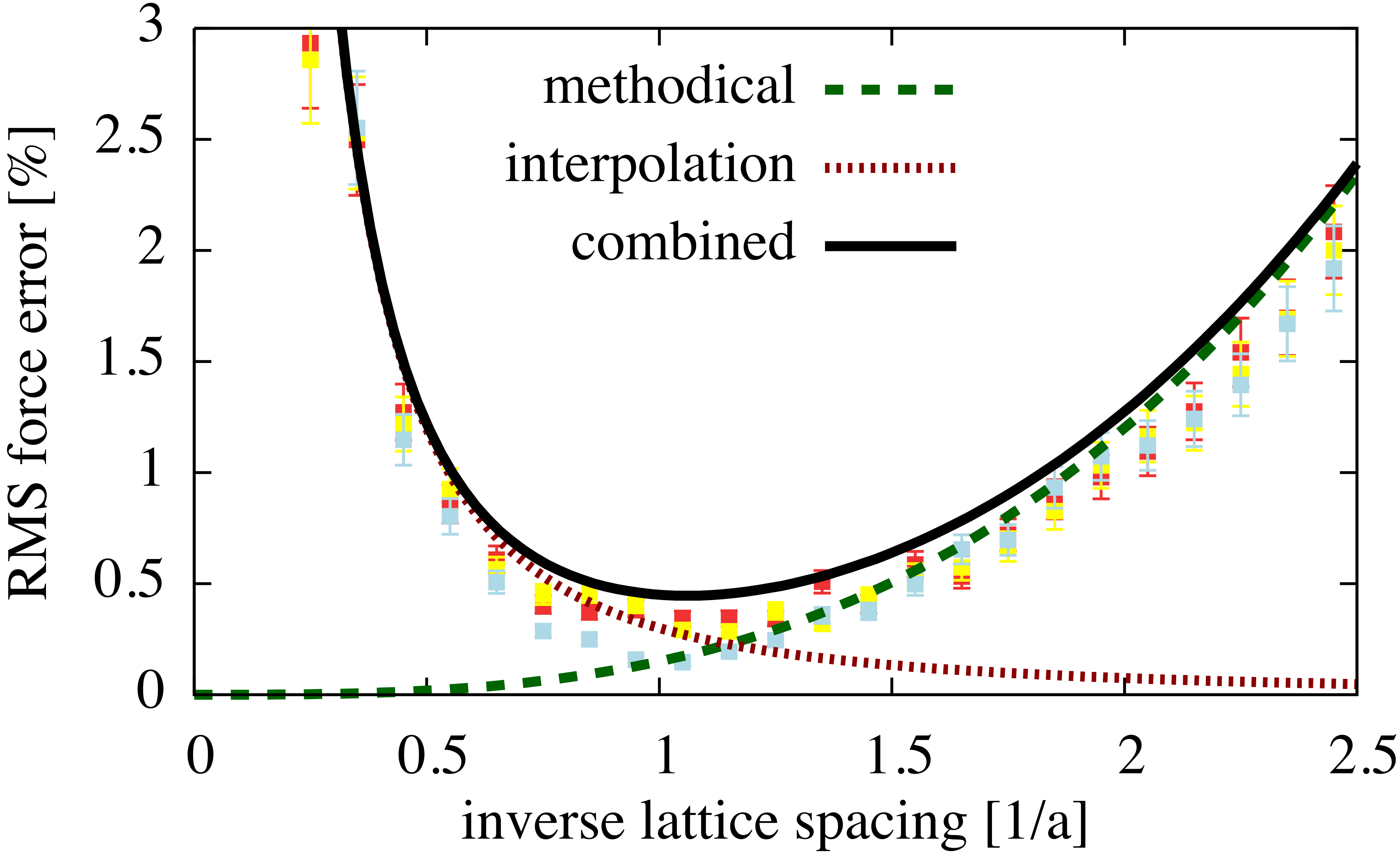
$$\Downarrow$$

The artificial transverse degree of freedom
is statistically independent!

Numerical errors

$$\dot{\mathbf{D}} = c^2 \nabla \times \mathbf{B} - \frac{\mathbf{j}}{\varepsilon}$$

Courant stability $c \ll \frac{a}{dt}$



What it does, numerically

- calculate current on the lattice $\mathbf{j} = \dot{\rho}$
- update local magnetic field $\dot{\mathbf{B}} = -\nabla \times \mathbf{D}$
- propagate magnetic field $\ddot{\mathbf{B}} = c^2 \, \nabla \times \nabla \times \mathbf{B}$
- increment electric field $\dot{\mathbf{D}} = c^2 \, \nabla \times \mathbf{B} - \frac{\mathbf{j}}{\varepsilon}$
- backinterpolate from lattice

When can I use MEMD?

- static observables in canonical ensemble
- cubic system
- slowly moving charges
- no electric current
- no high accuracy needed
- no fixed charges
- concept of „time step“

How can I use MEMD?

- Three parameters: a, c, dt
- Lattice spacing roughly the „size“ of particles
- Time step from MD simulations so that particles move „slow“ (~0.1a per dt)
- Speed of light from stability criterion $c \ll \frac{a}{dt}$

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cellsystem domain_decomposition -no_verlet_list
inter coulomb l_B memd f_mass mesh [epsilon ε∞]
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l_B: bjerrum length
f_mass: f_mass = 1/c^2
mesh: mesh size (1D)
ε∞: BCs at infinity

Thank you!

Further reading:

A. C. Maggs and V. Rosseto.
"Local Simulation Algorithms for Coulombic interactions".
Phys. Rev. Lett. 88(196402), *2002.*

I. Pasichnyk and B. Dünweg.
"Coulomb interactions via local dynamics: A molecular-dynamics algorithm".
J. Phys.: Condens. Matter 16(38)(3999-4020), 2004.

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"Computing Coulomb Interaction in Inhomogeneous Dielectric Media via a Local Electrostatics Lattice Algorithm".
http://arxiv.org/abs/1309.7859, 2013

Group picture!!!