Multiscale Simulations Using Particles

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KITP

June 5, 2012

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Troy, The movie

MULTISCALING as CAUSALITY

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adapted from Robert E. Ulanowicz

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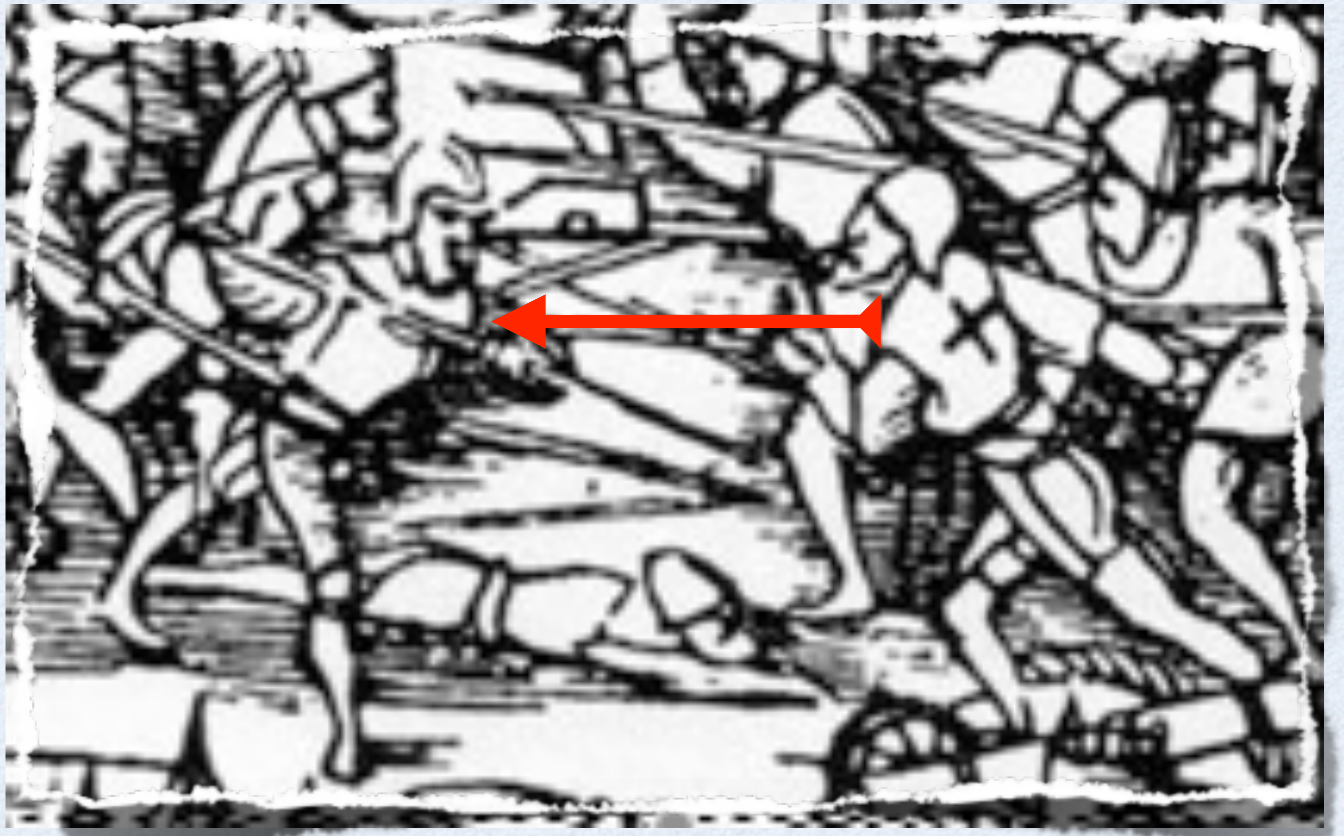

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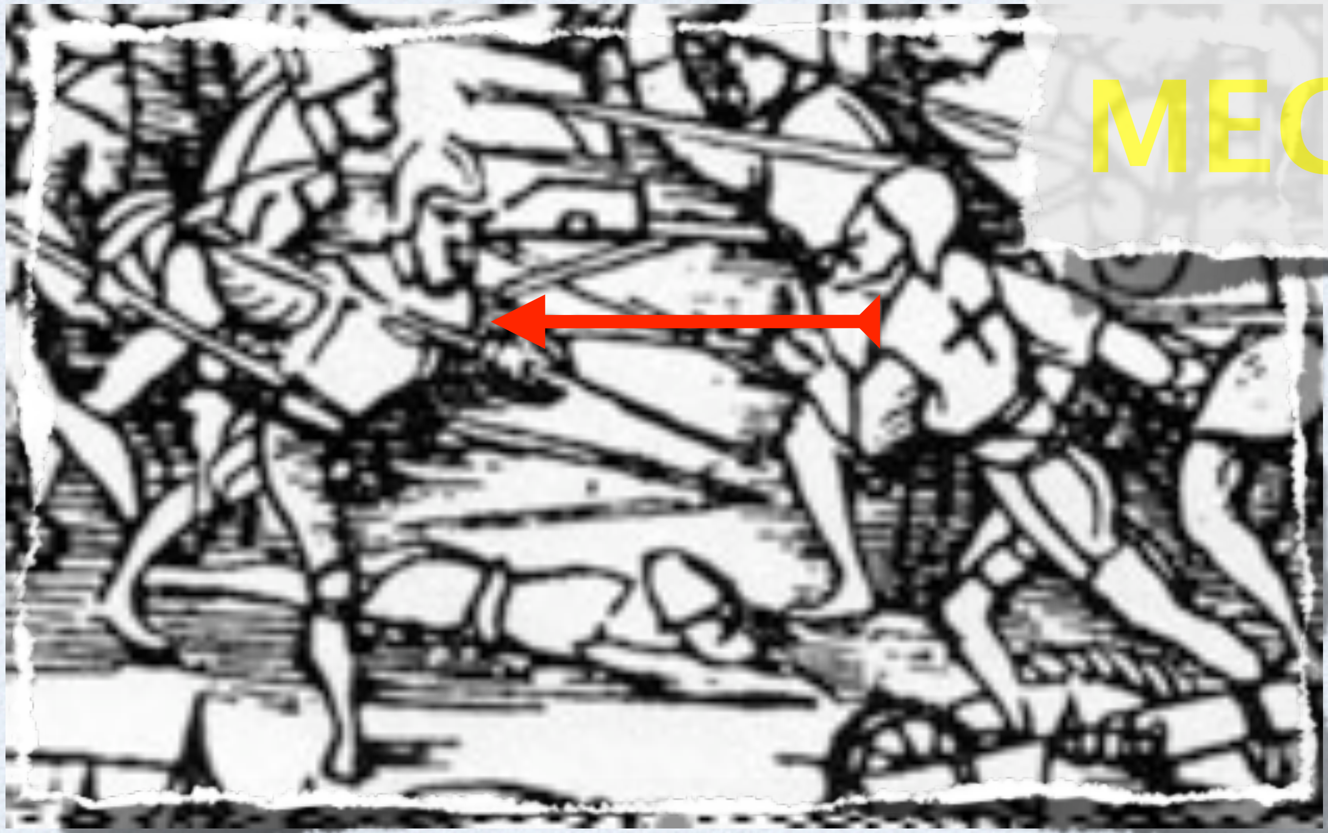

MATERIAL

MECHANICAL

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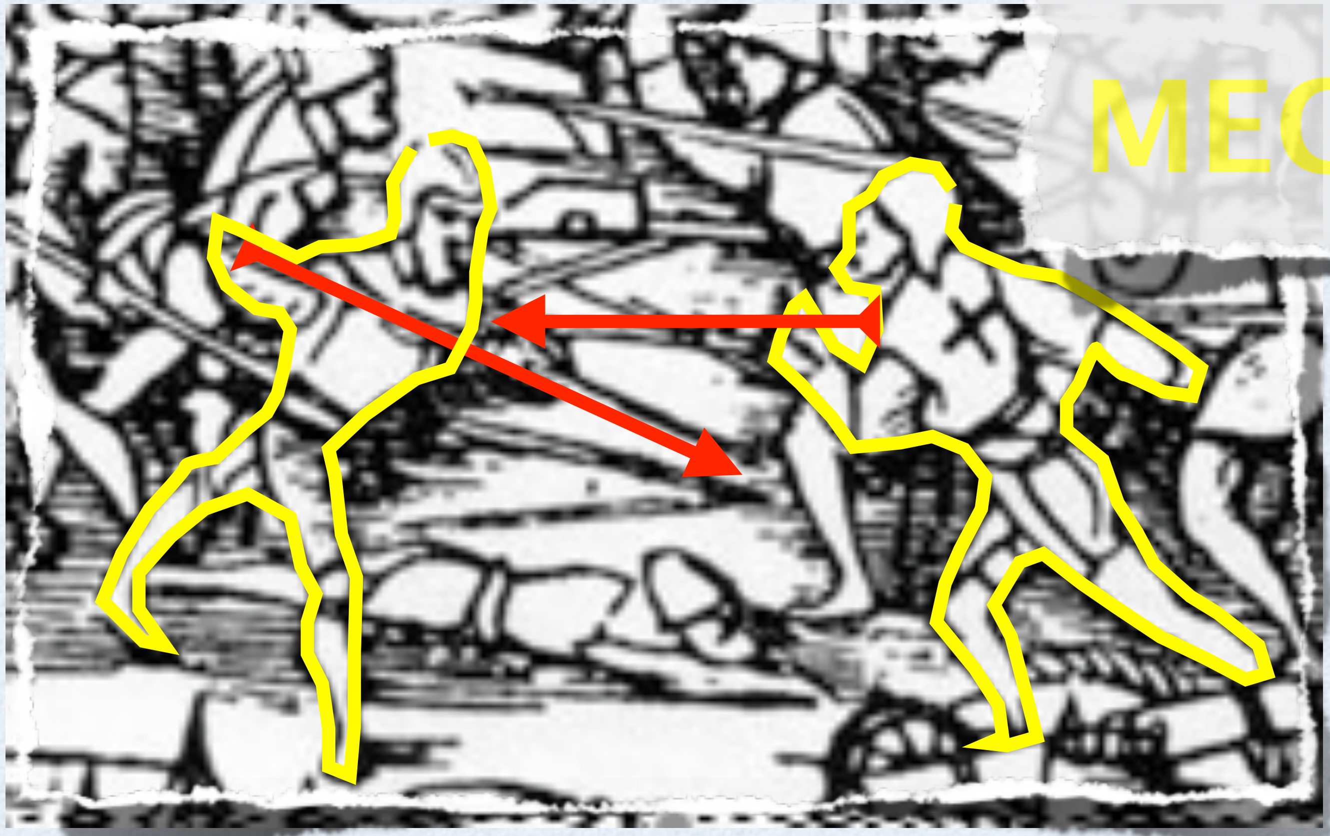

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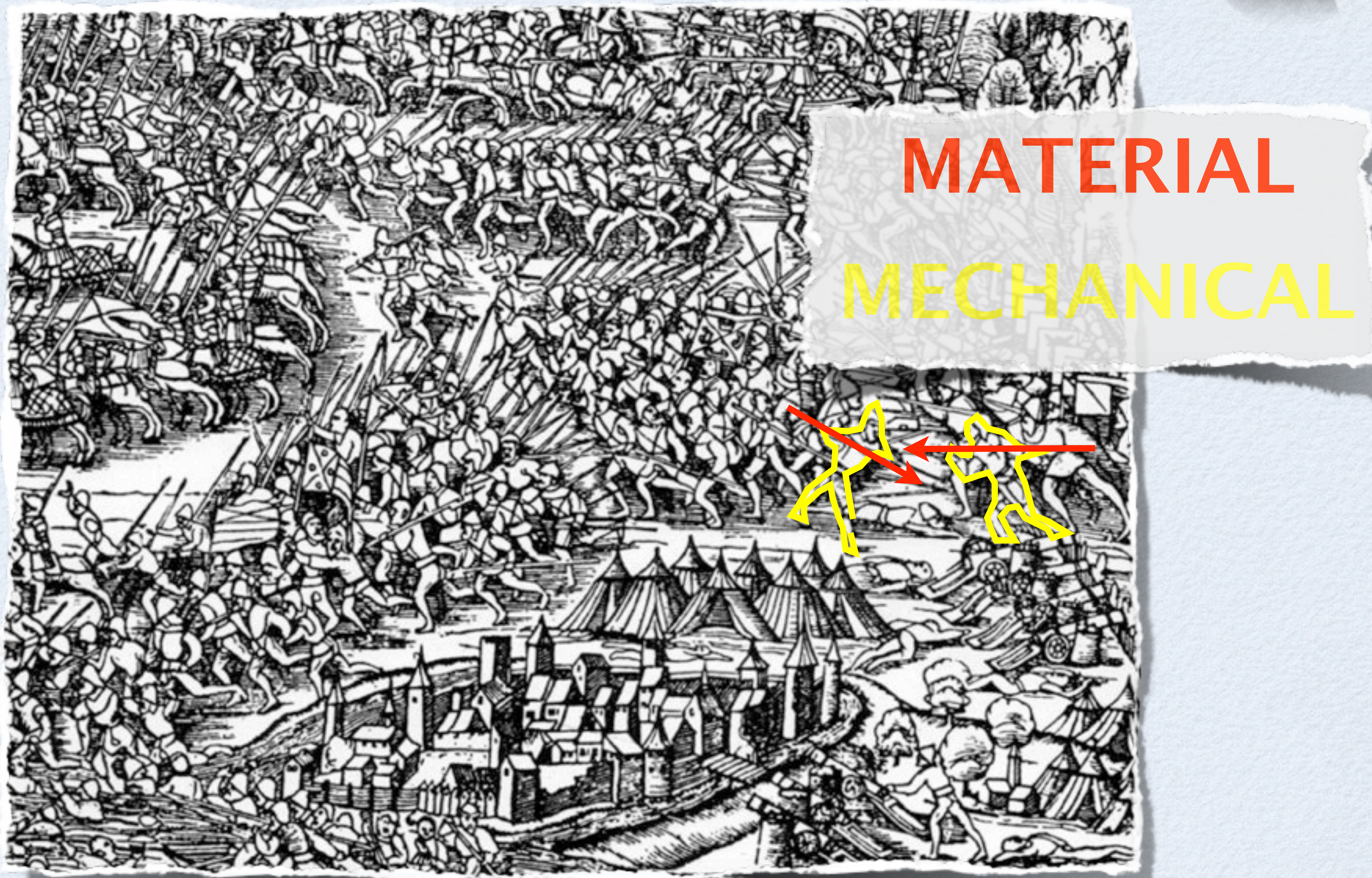

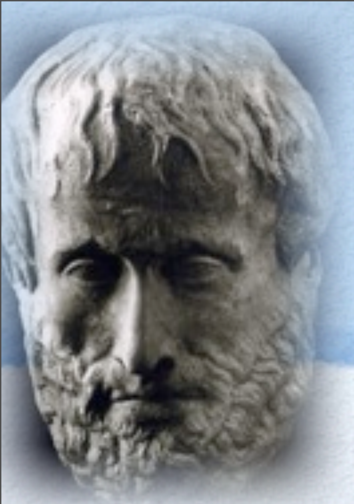

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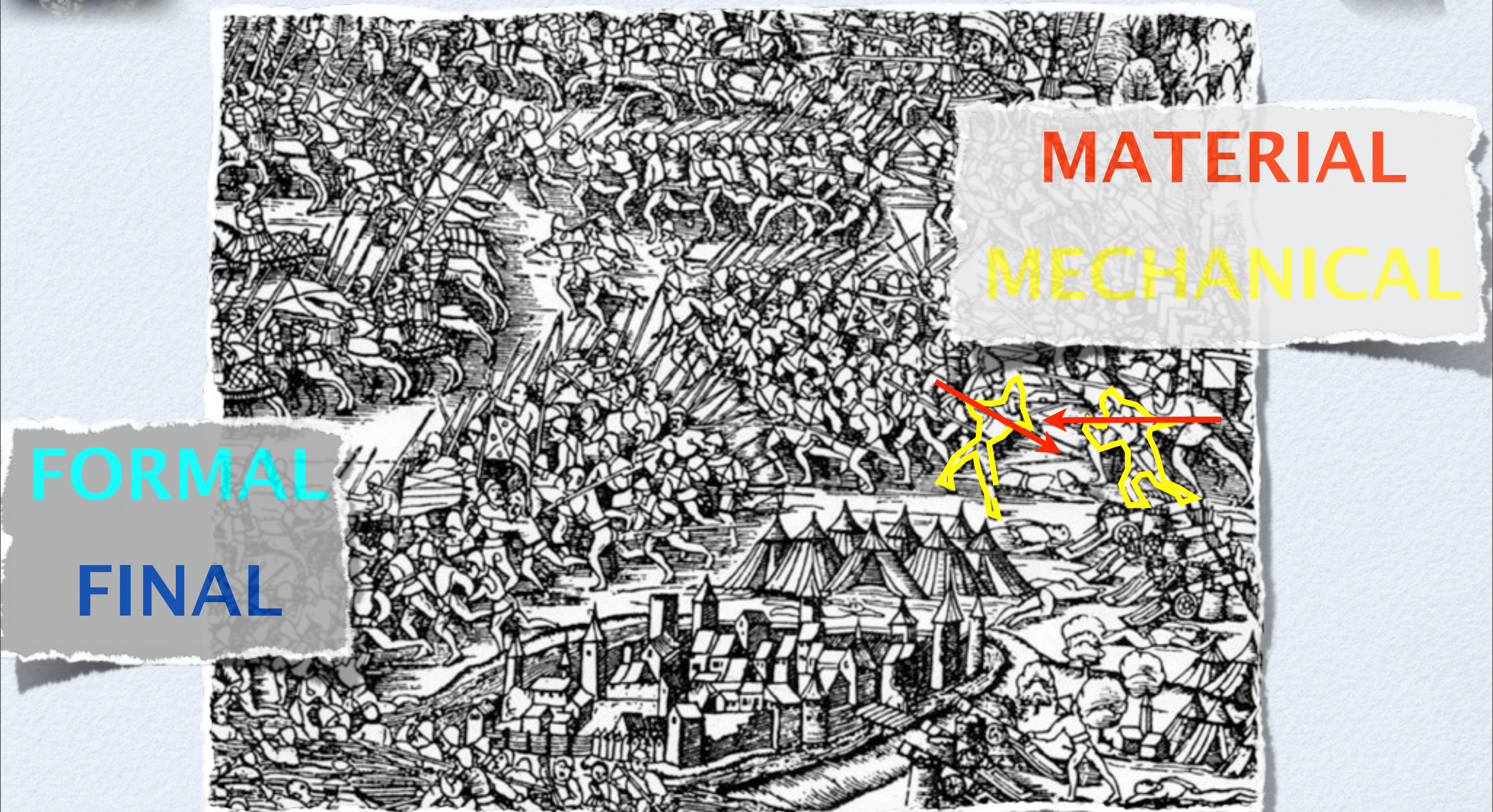

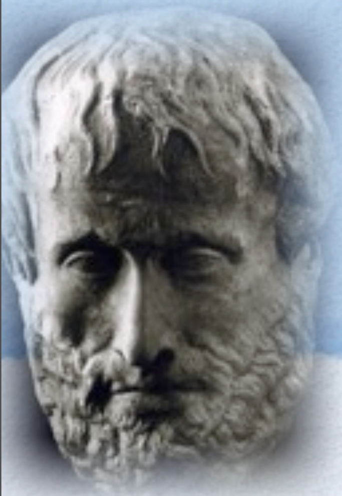

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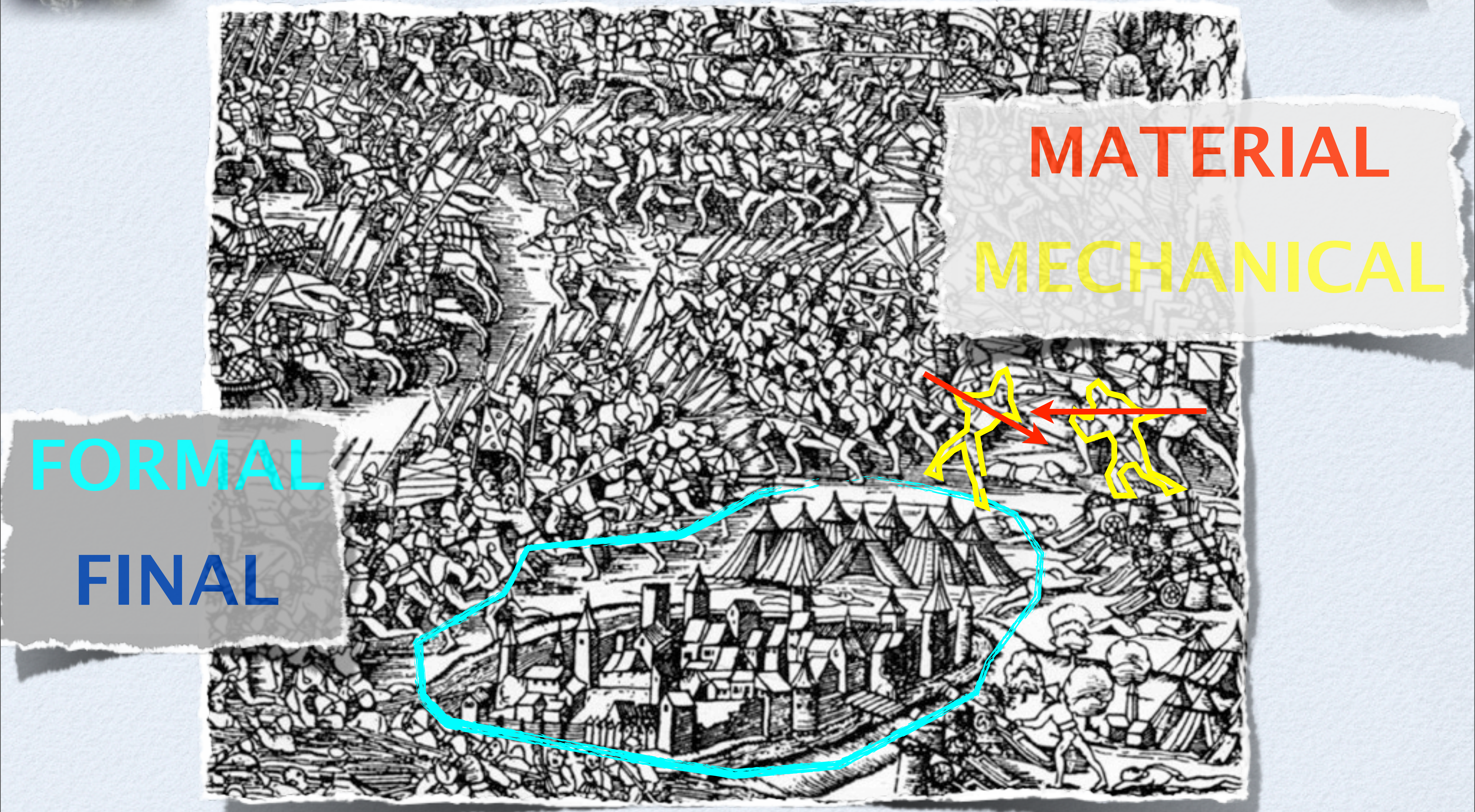

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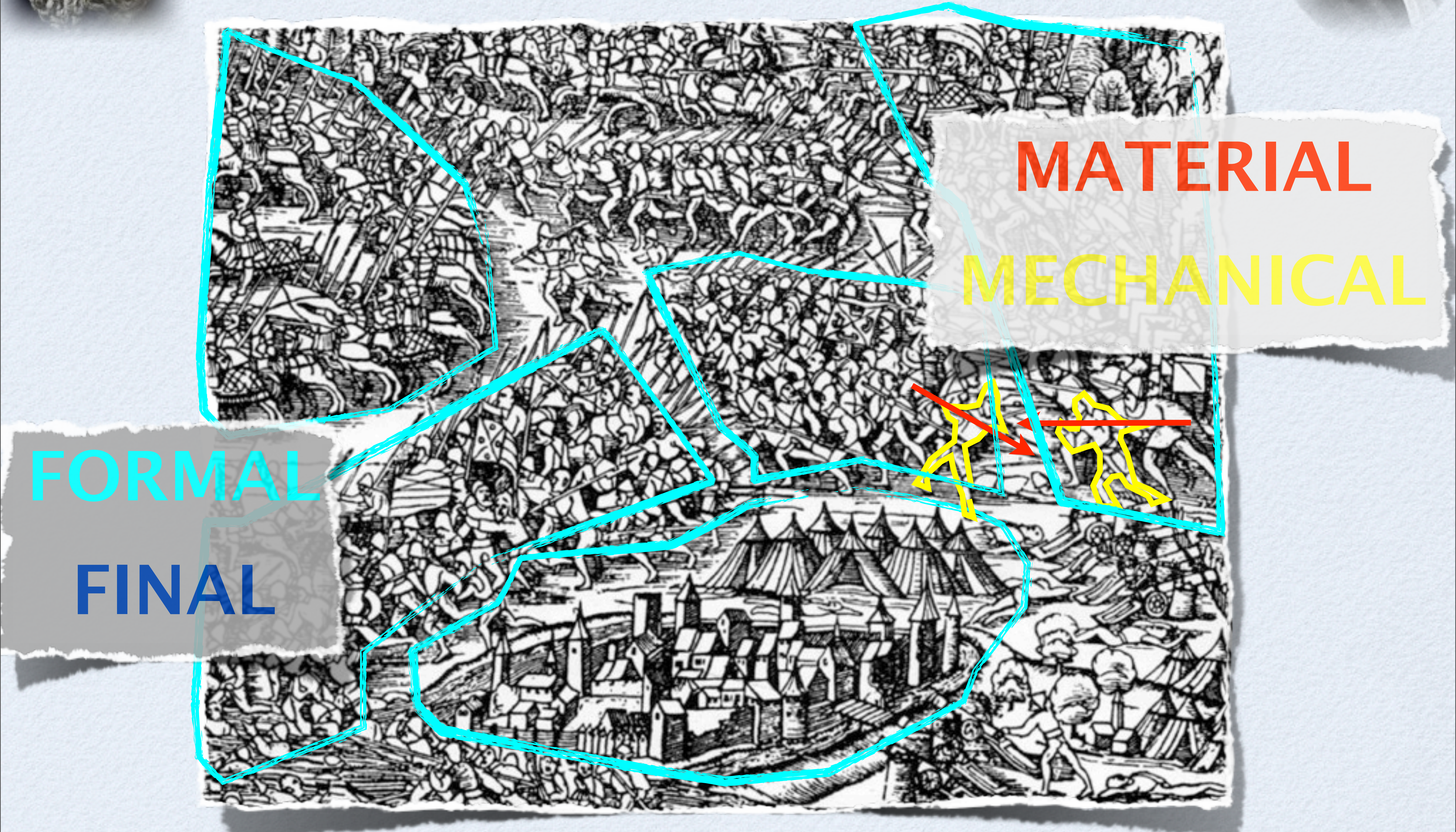

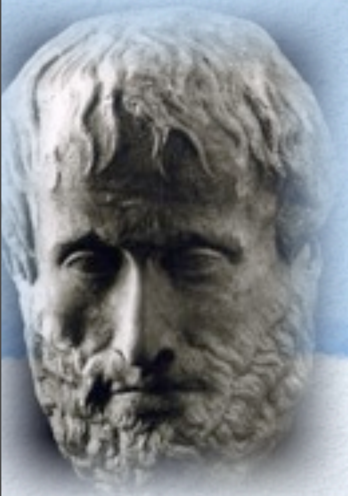

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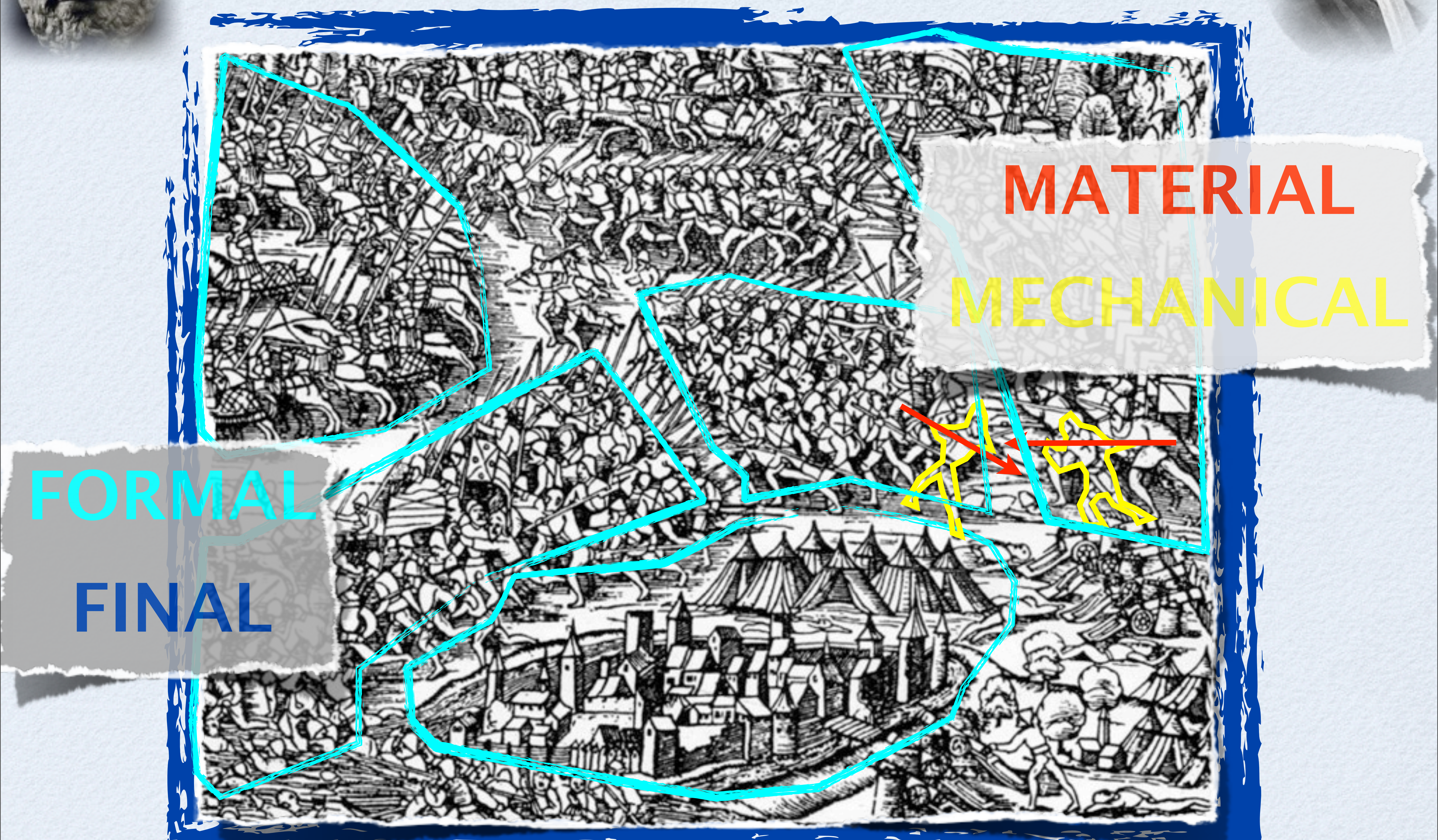

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  - Particles: a superset of Grids

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- RESULTS and OUTLOOK

PARTICLES : Lagrangian, Conservation and Other Laws

$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u}_p$$

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SPH, Vortex Methods

$$\rho_p \frac{D\mathbf{u_p}}{Dt} = (\nabla \cdot \sigma)_p$$

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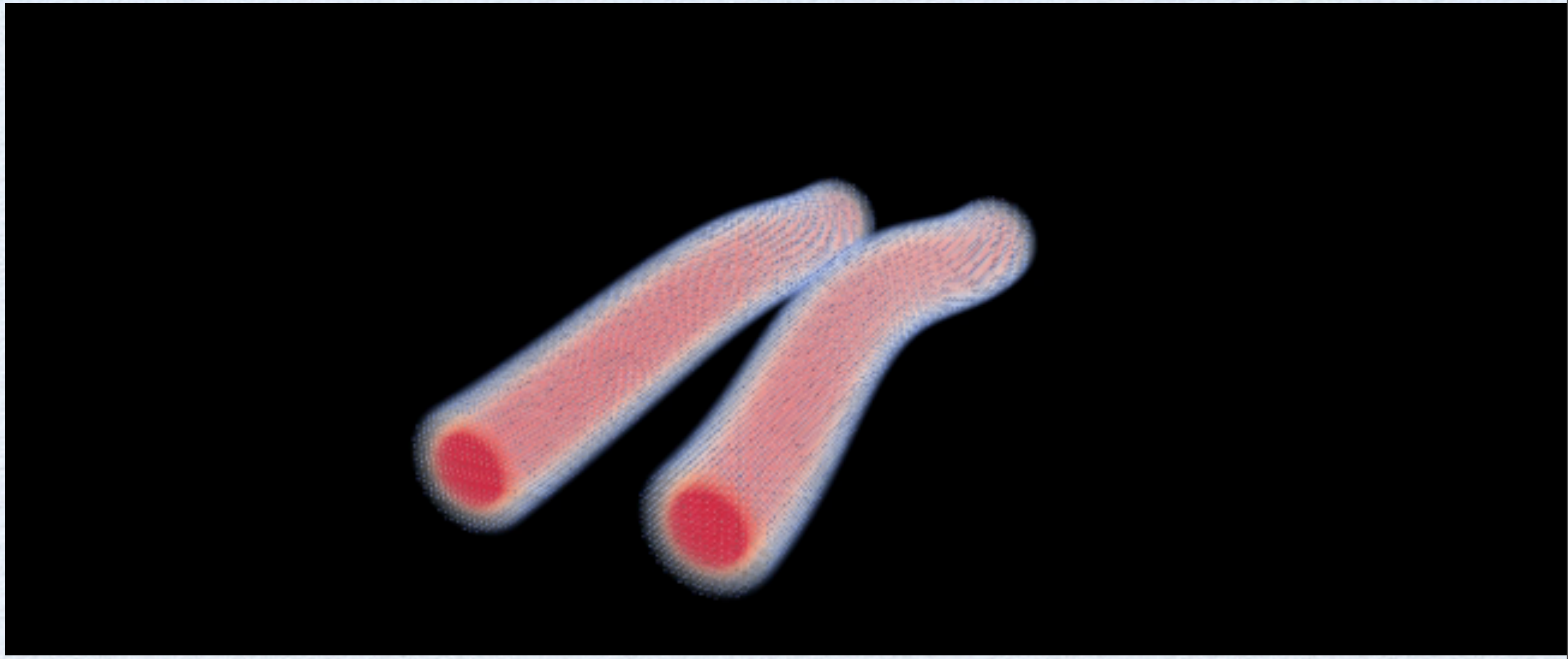

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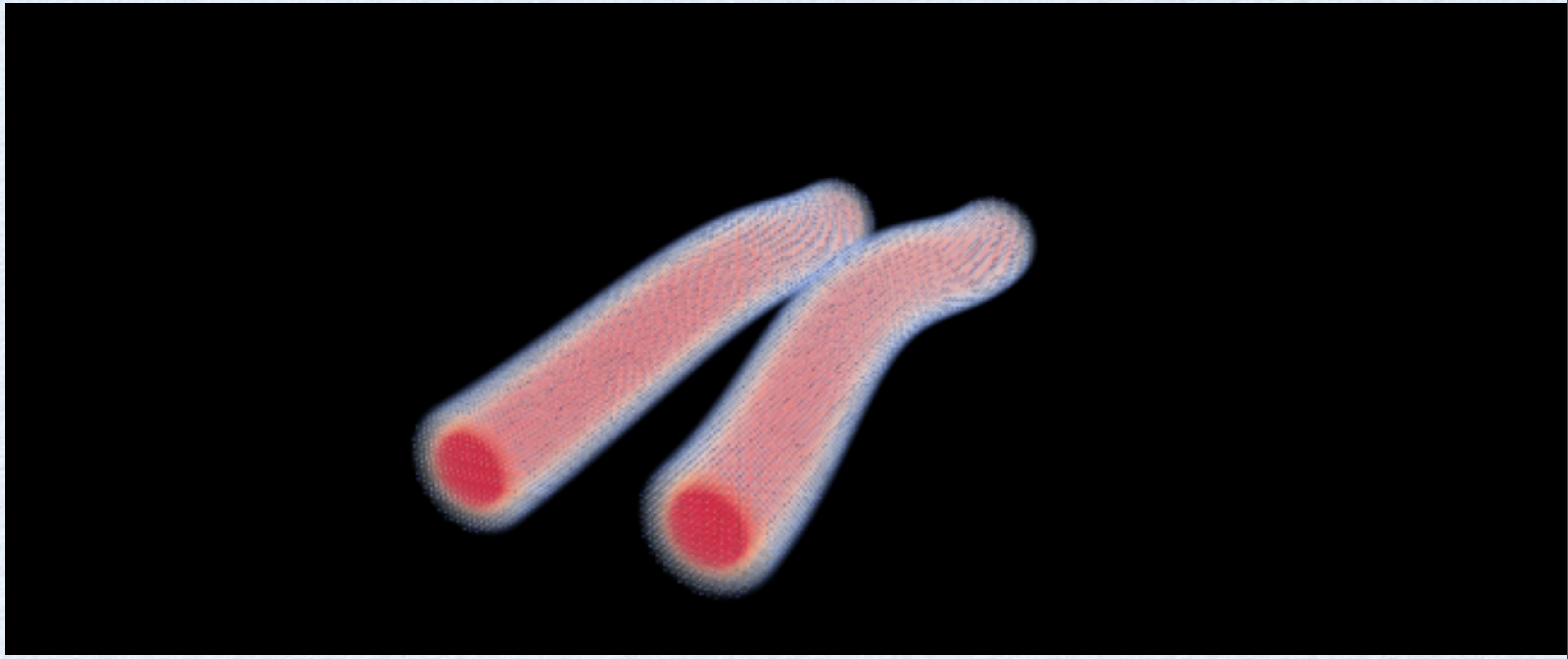

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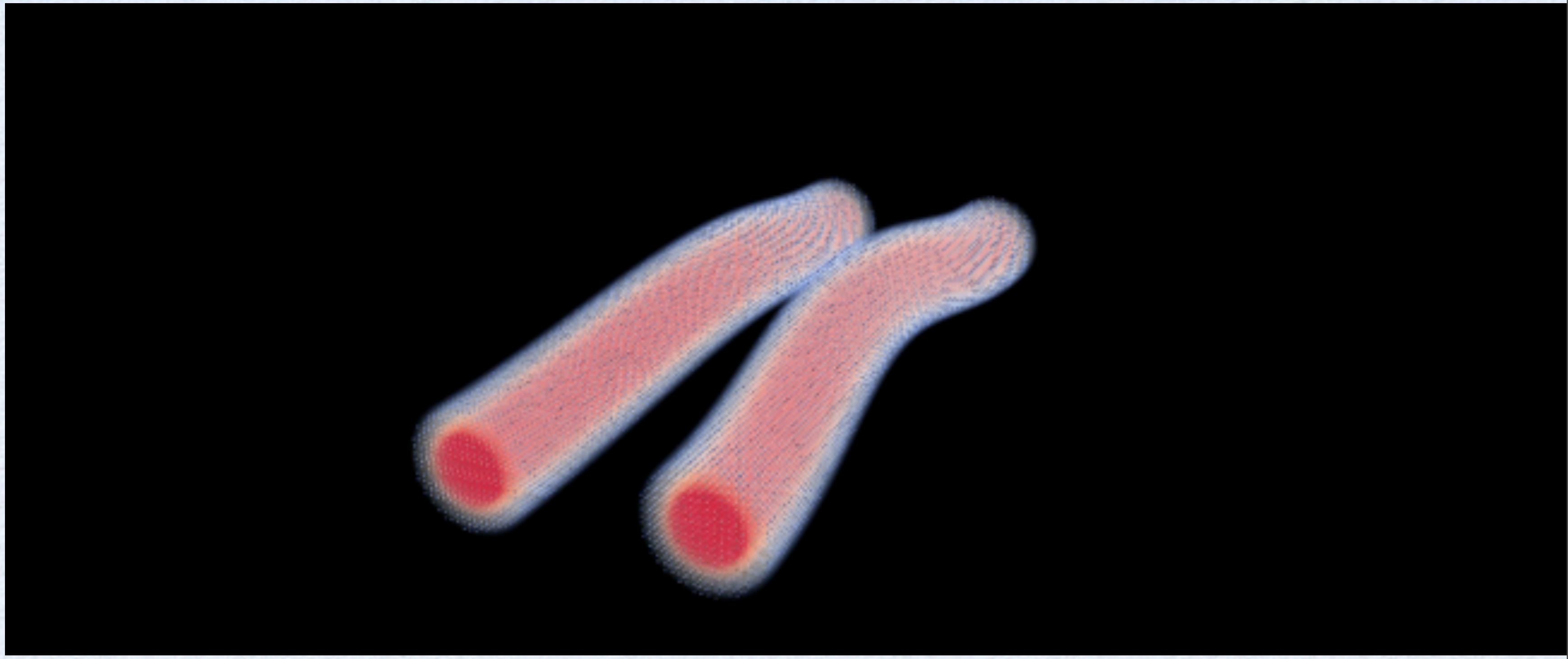

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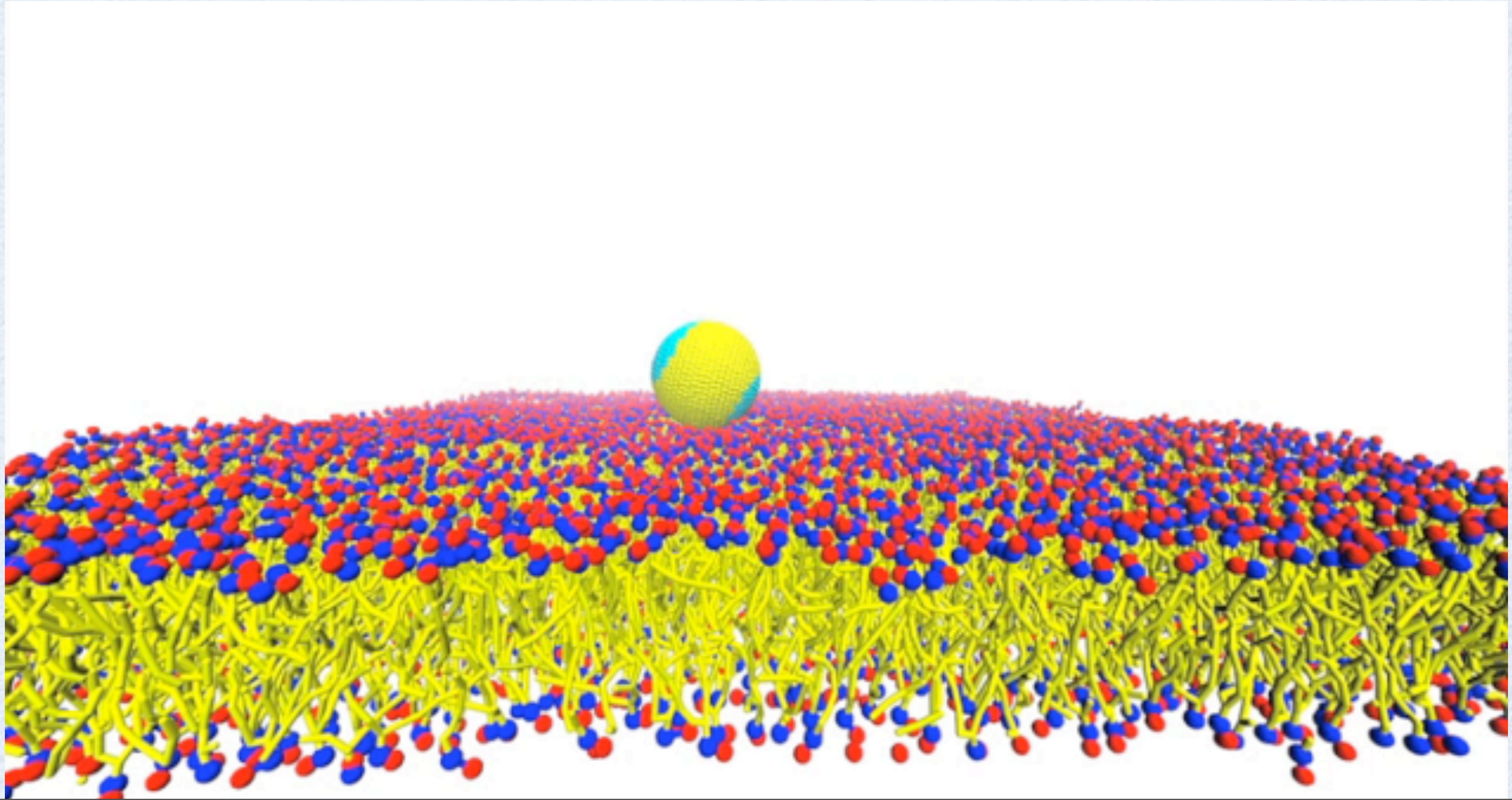

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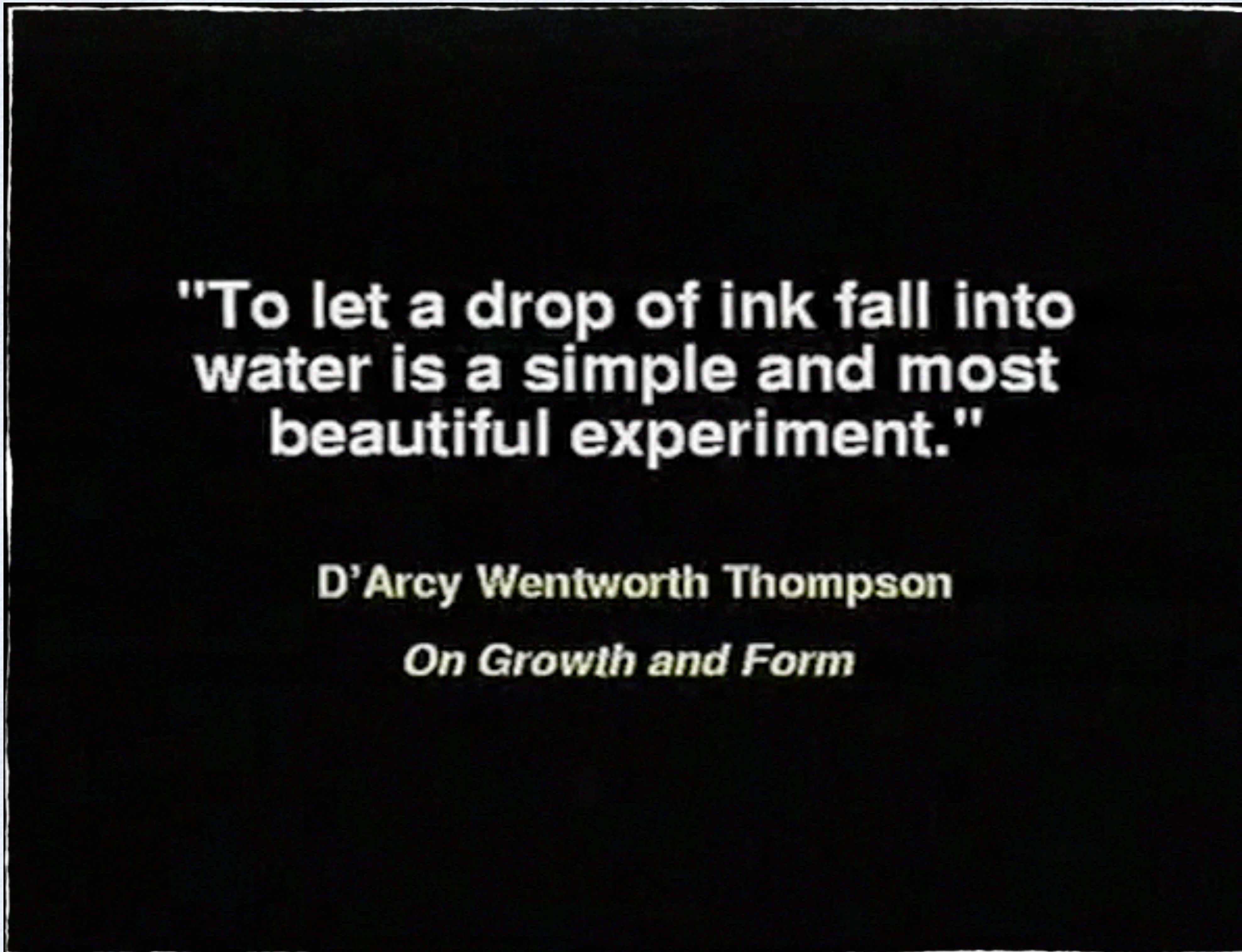
MODELING – APPROXIMATION



J. H. Walther, P. Koumoutsakos, Three-dimensional vortex methods for particle-laden flows with two-way coupling, **J. Comput. Phys.**, 167, 39-71, 2001 multi Scale **Simulations using Particles**

PK, **Ann. Rev. Fluid Mechanics**, **2005**

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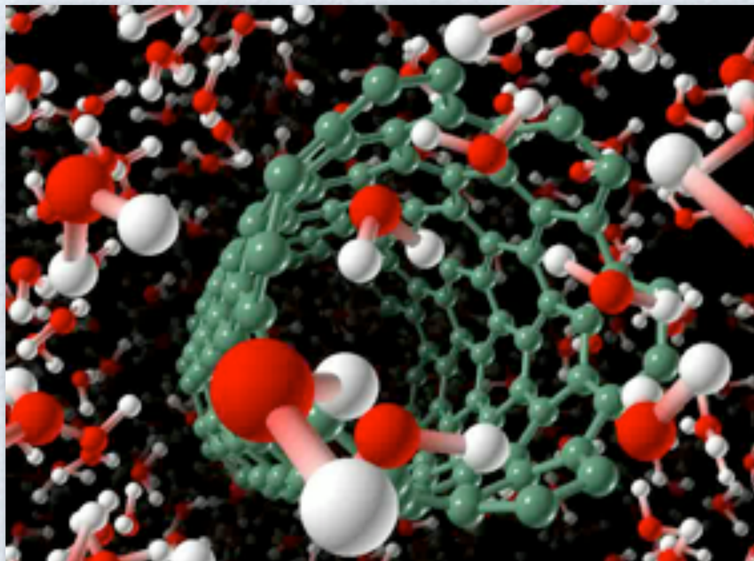

Water and CNTs

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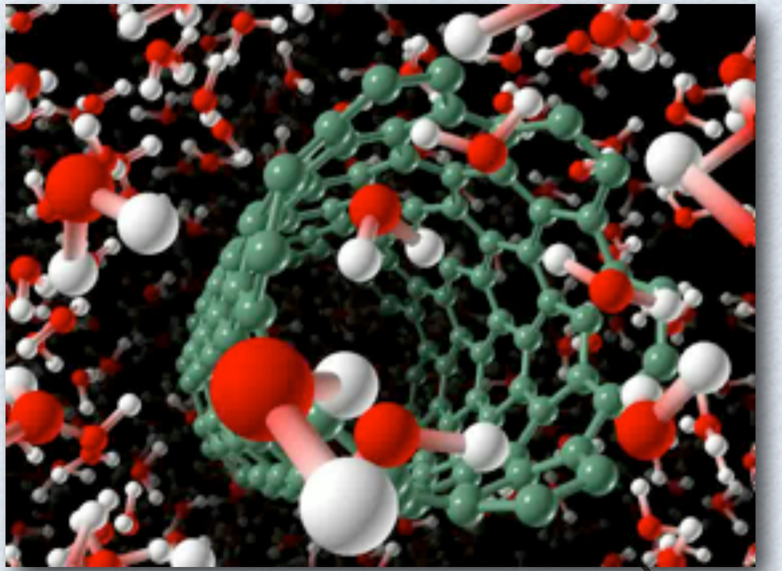

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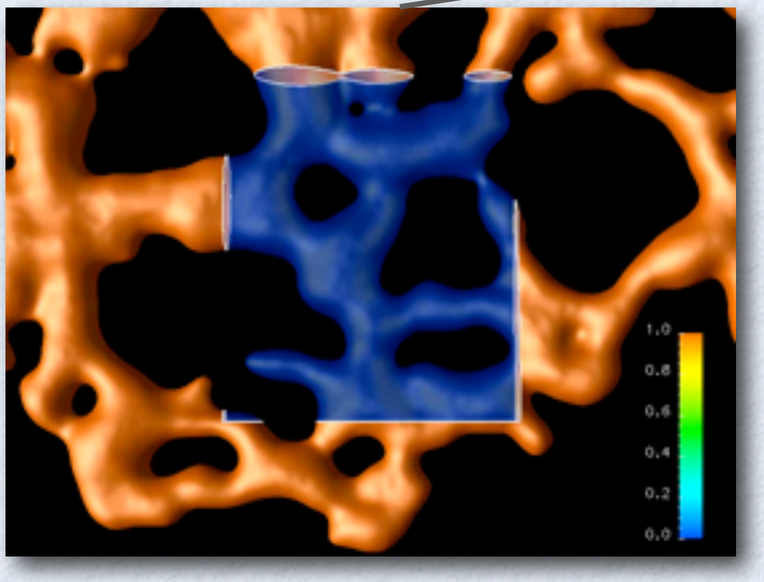

Diffusion in/on Cell Organelles

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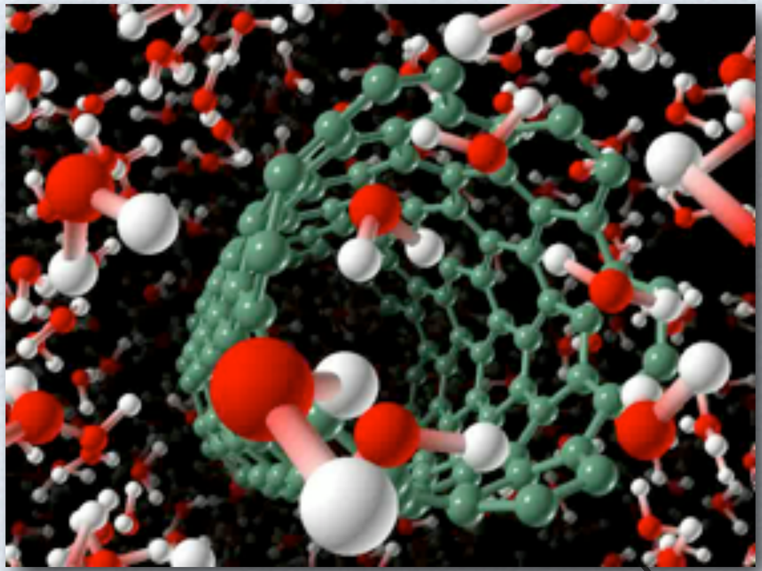

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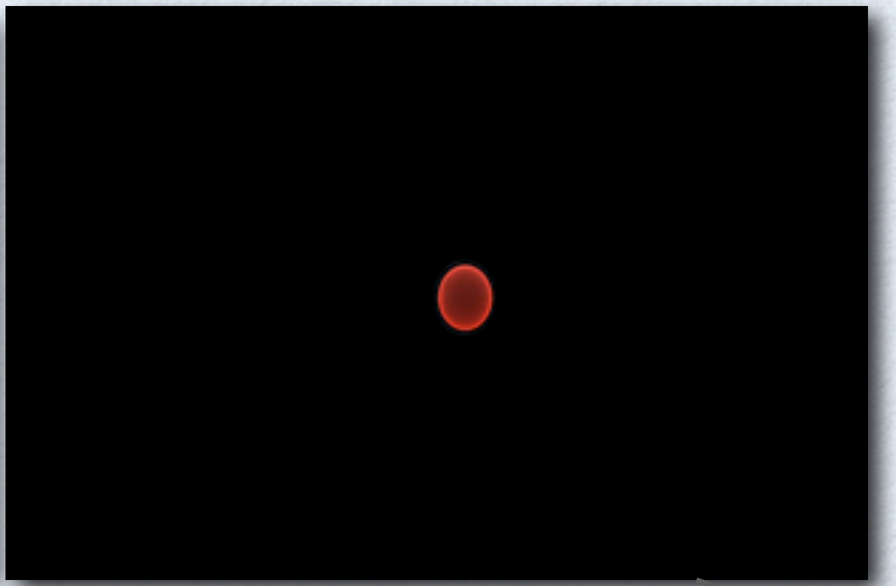
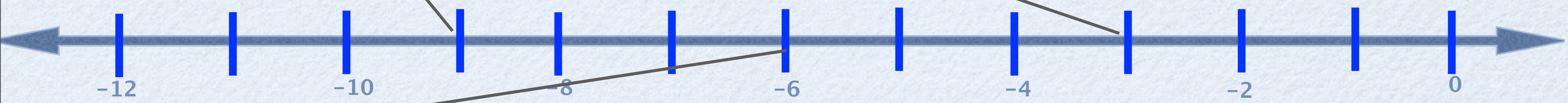
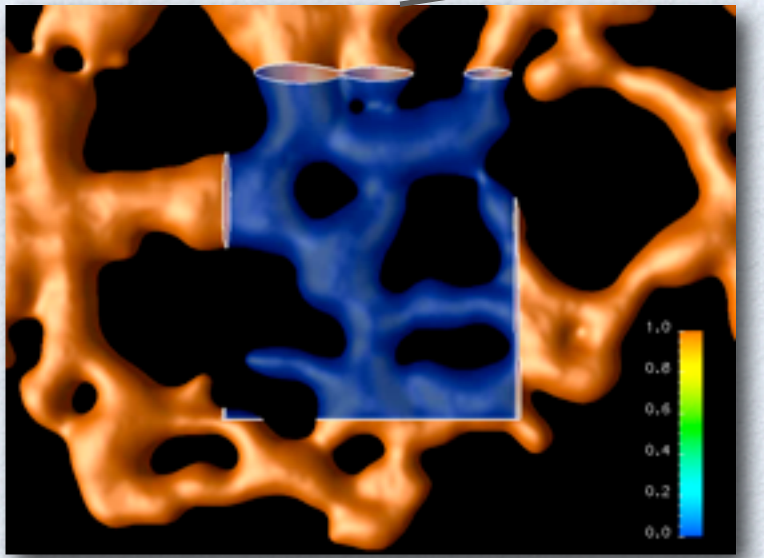


Cell Proliferation





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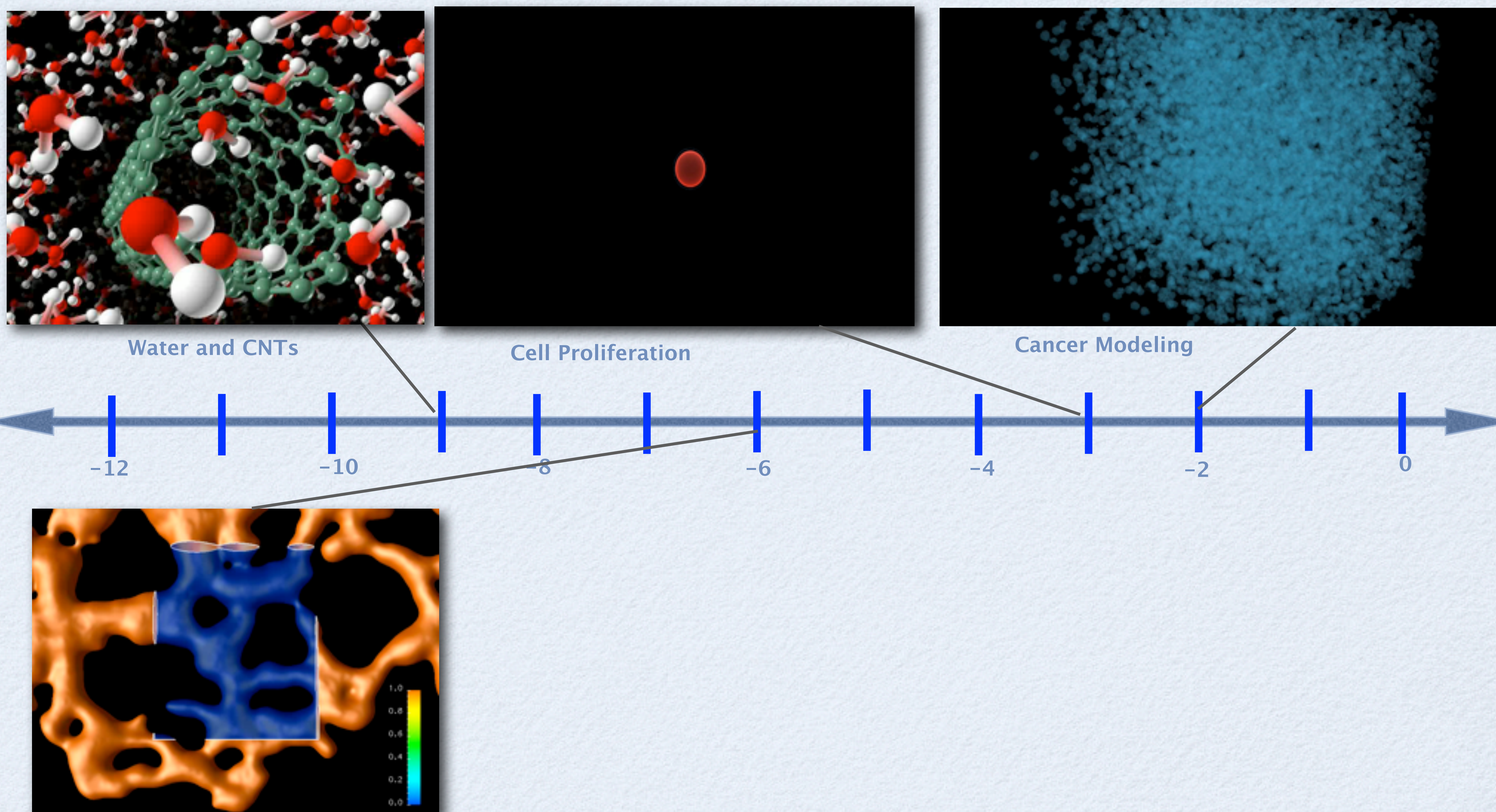

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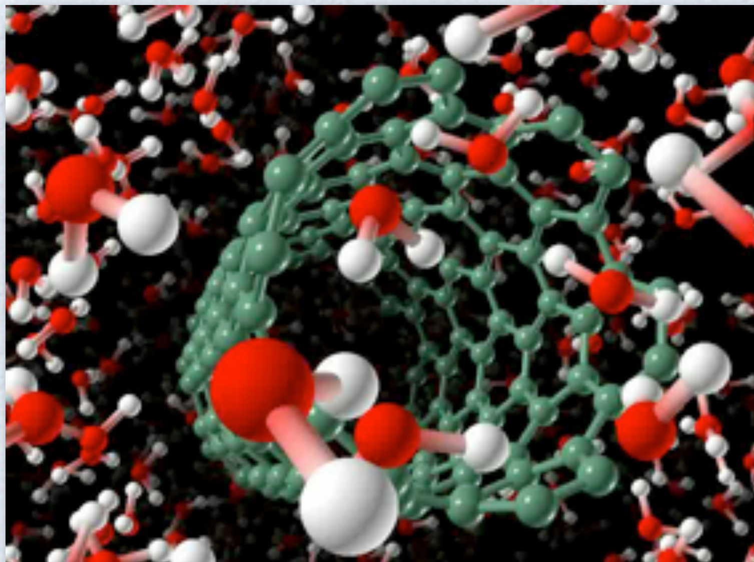

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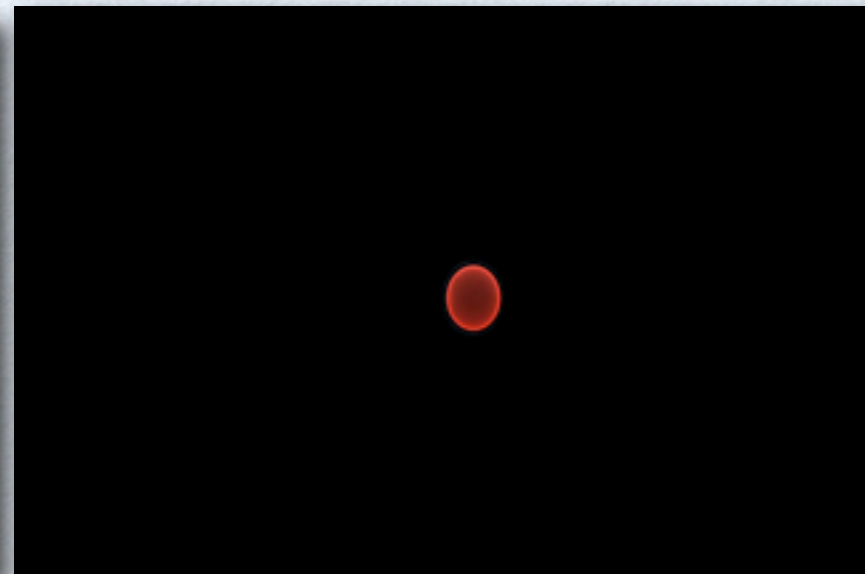

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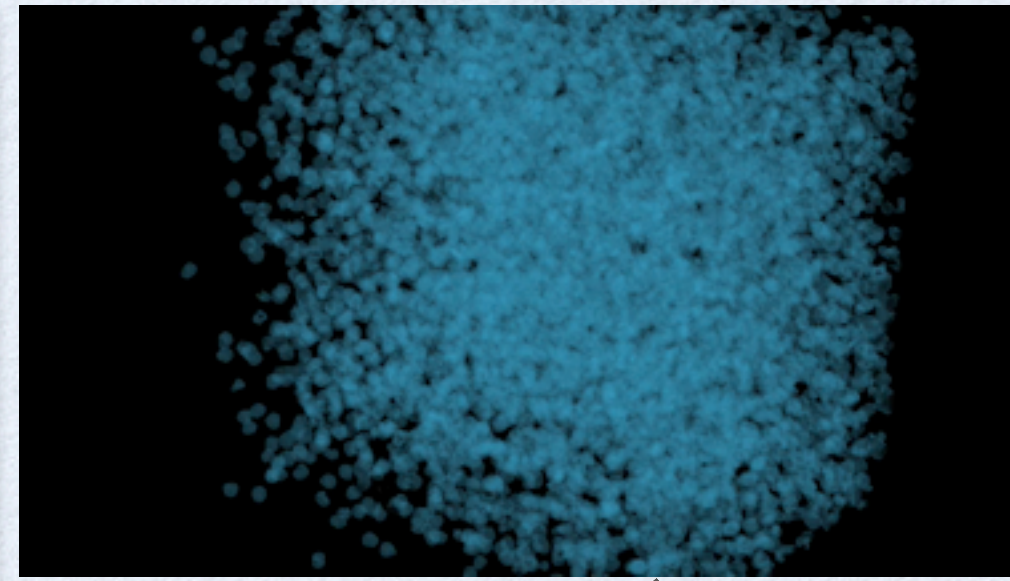
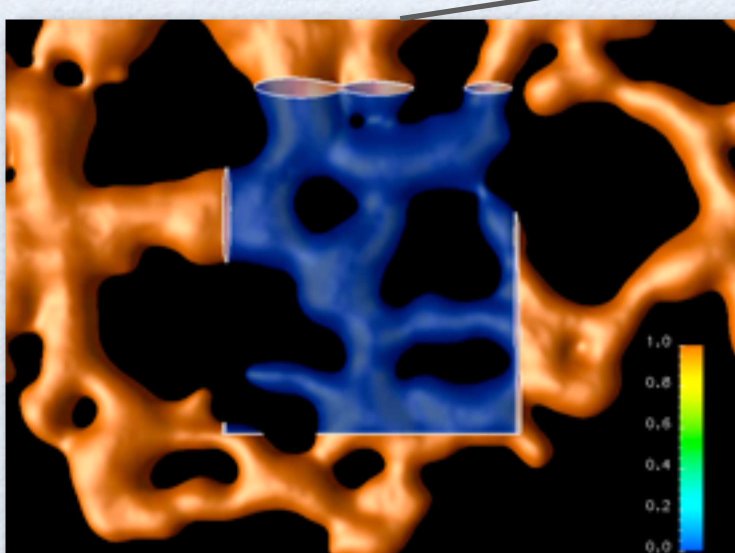


Cancer Modeling



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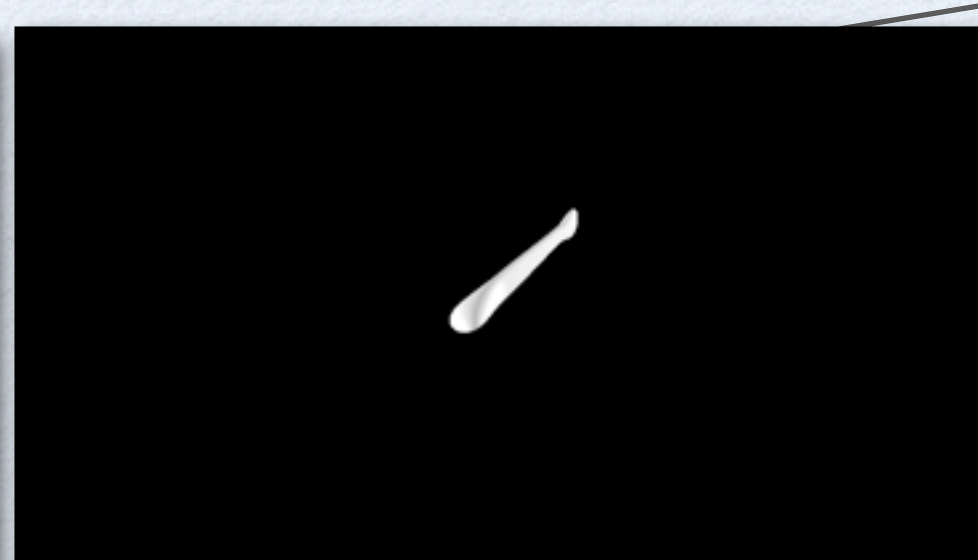

Swimming Organisms

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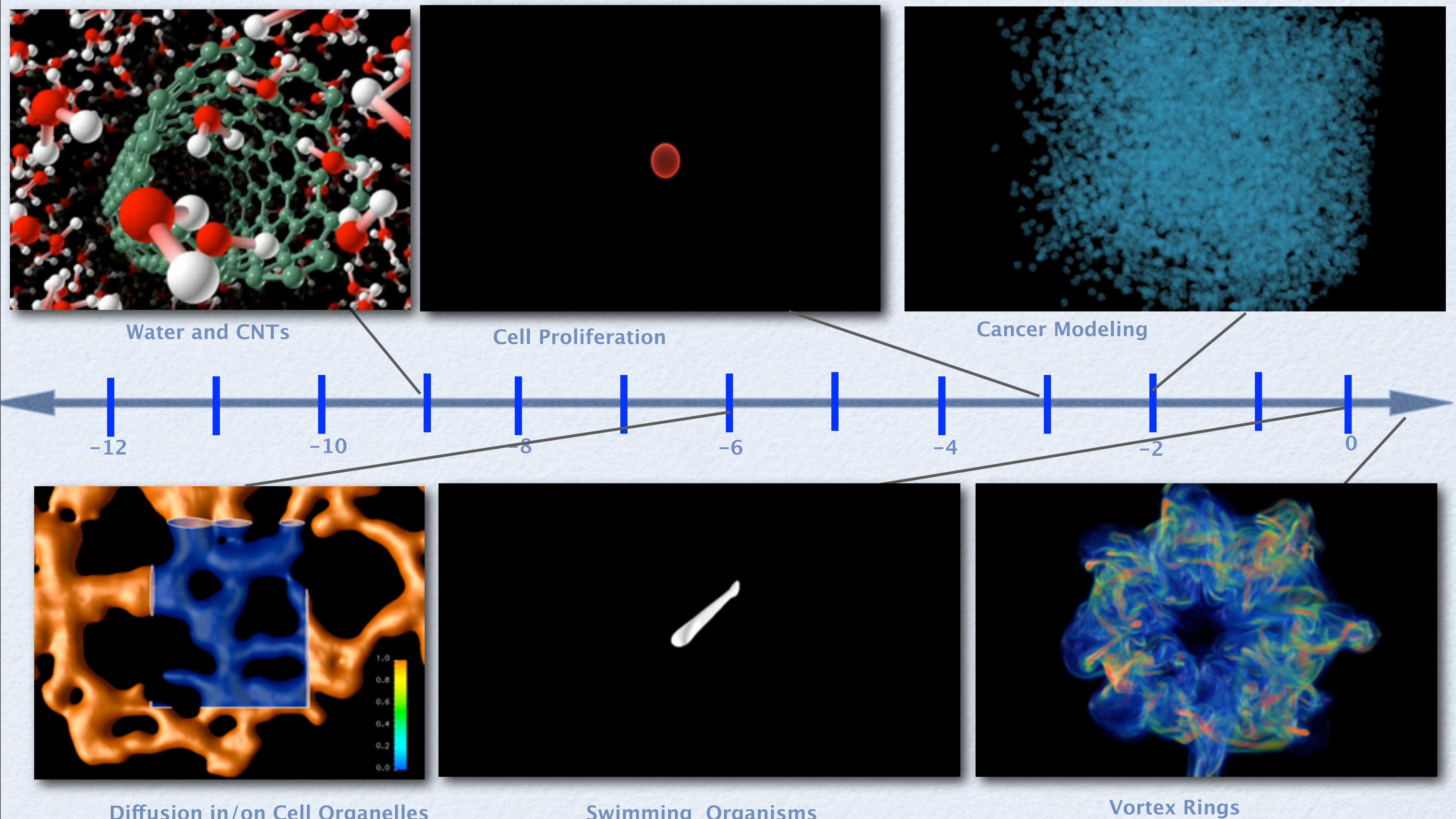

FUNCTIONS and PARTICLES

Integral Function Representation

$$\Phi(x) \;=\; \int \Phi(y)\,\delta(x-y)\,dy$$

Function Mollification

$$\Phi_\epsilon(x) \;=\; \int \Phi(y)\,\zeta_\epsilon(x-y)\,dy$$

Point Particle Quadrature

$$\Phi^h(x,t) \;=\; \sum_{p=1}^{N_p} h_p^d\,\Phi_p(t)\,\delta(x-x_p(t))$$

Smooth Particle Quadrature

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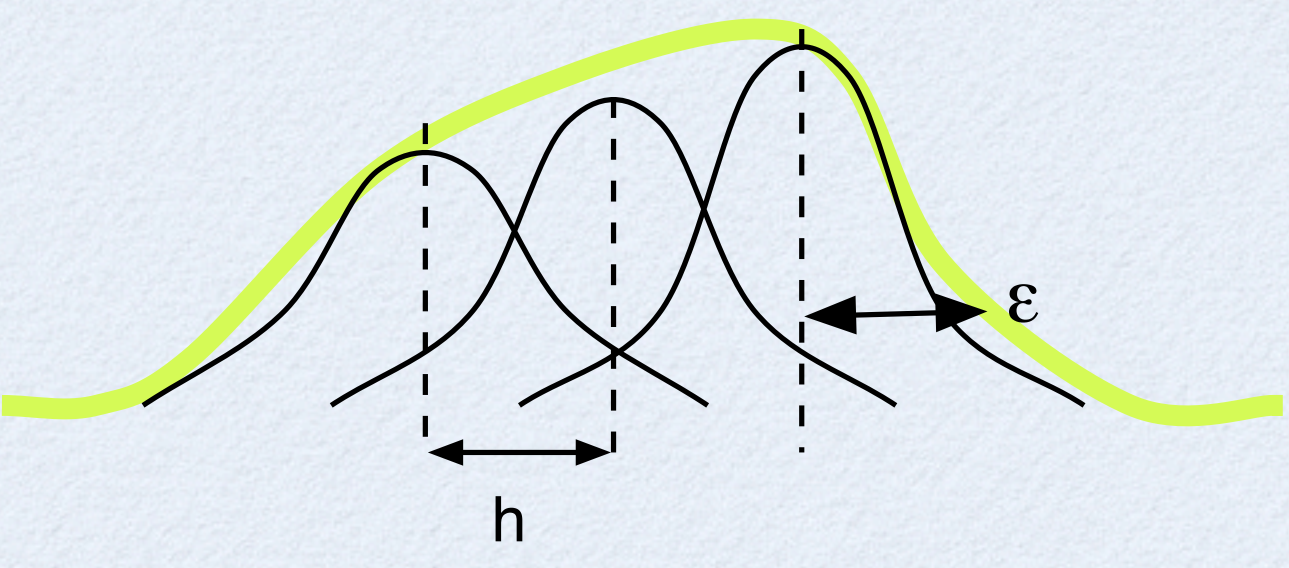

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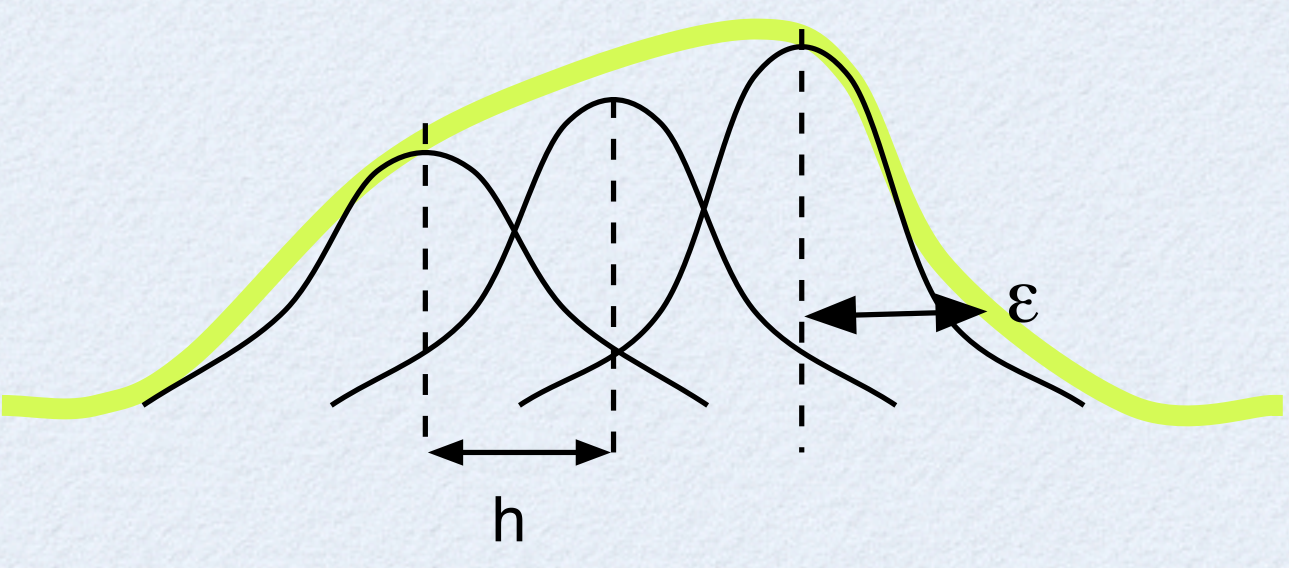

Particles are “mesh” free

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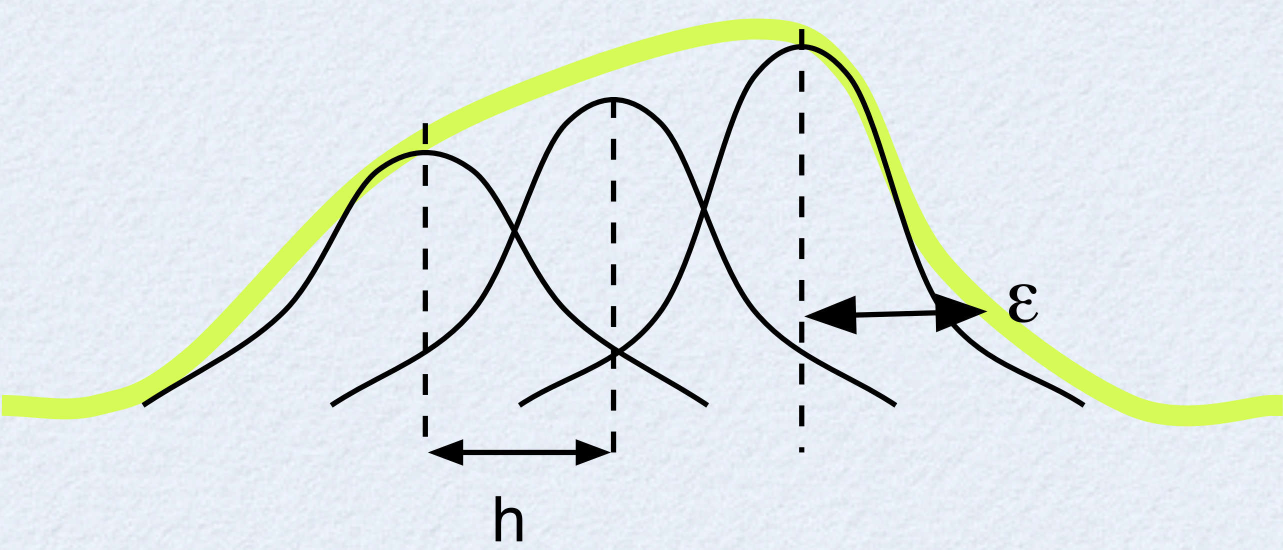

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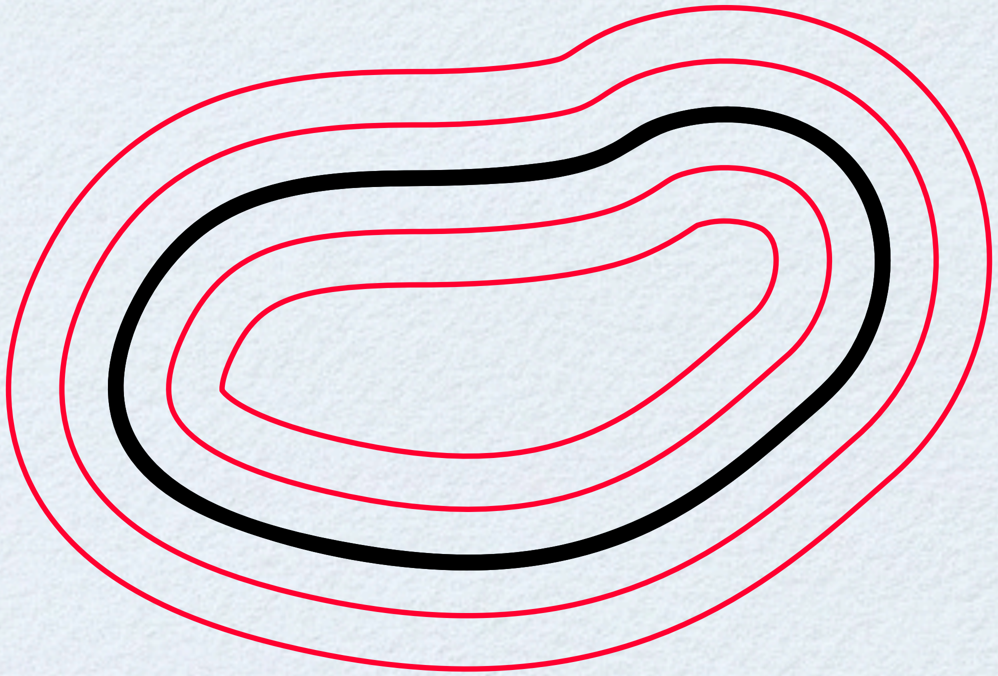
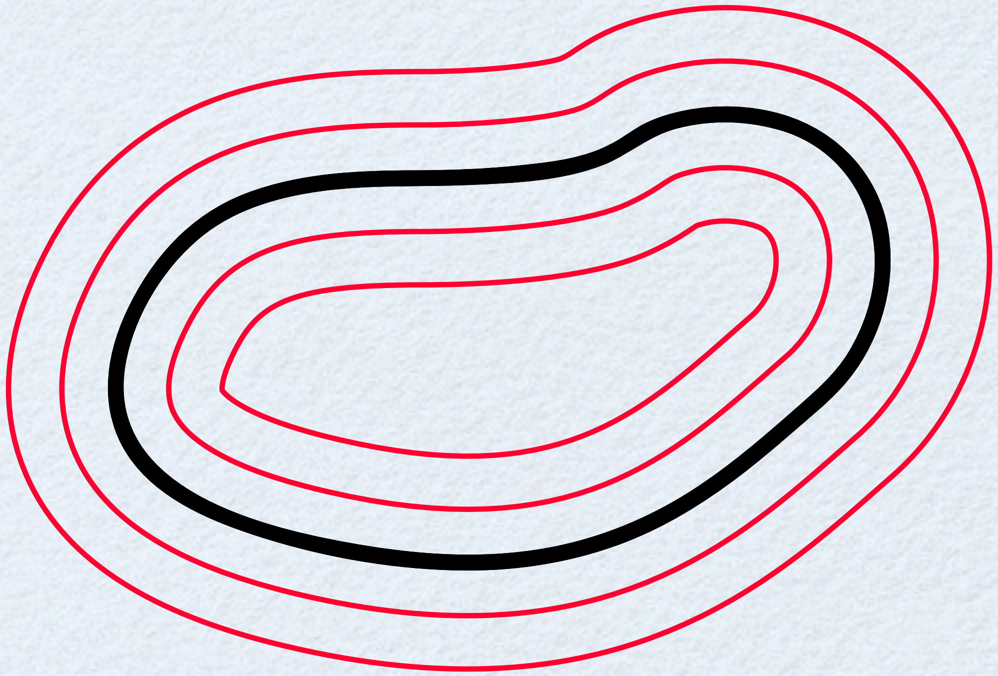


EXAMPLE : LEVEL SETS

$$\Gamma(t) = \{\mathbf{x} \in \Omega \mid \phi(\mathbf{x}, t) = 0\}$$

$$|\nabla \phi| = 1$$



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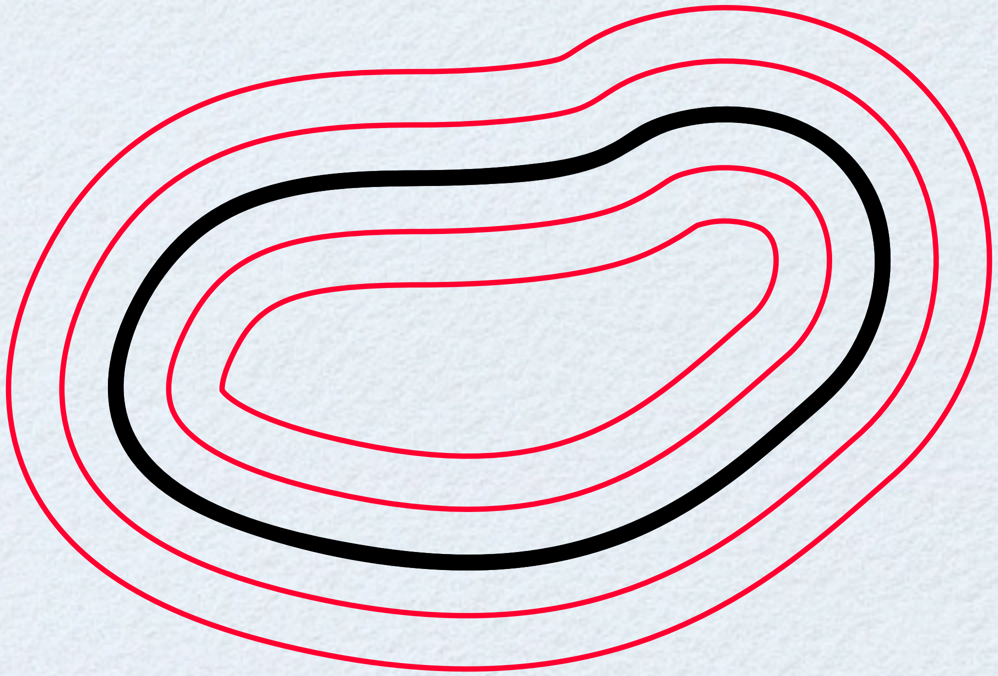

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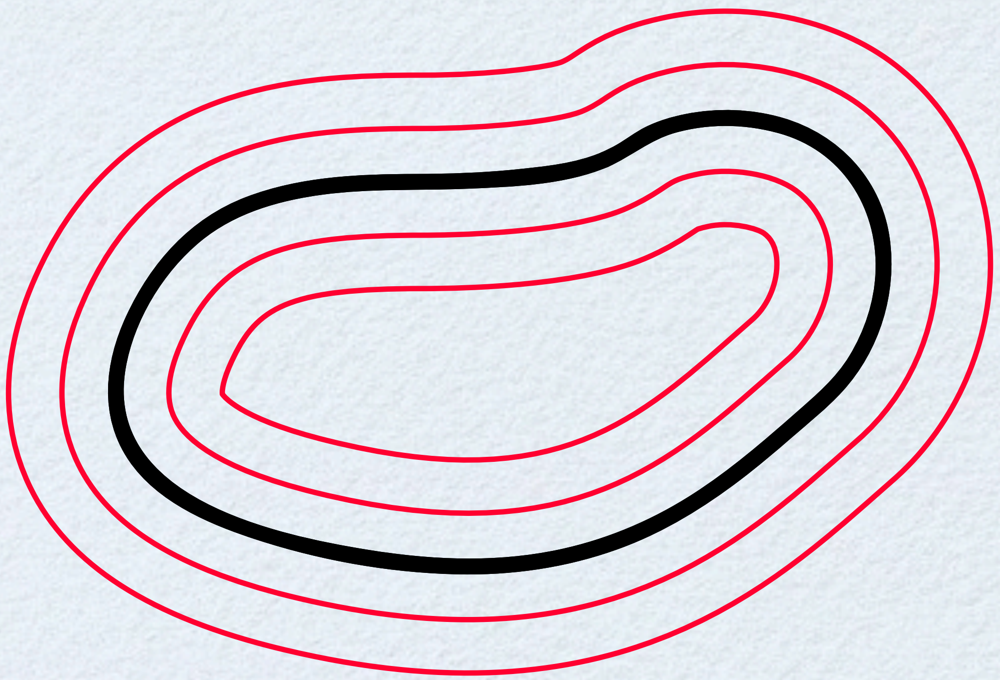

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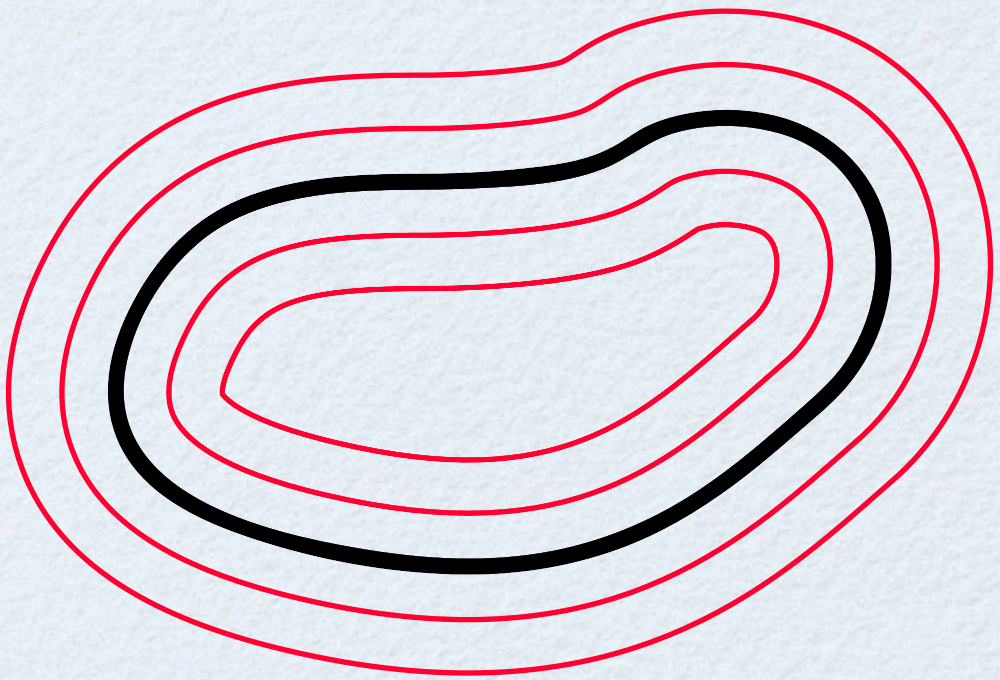

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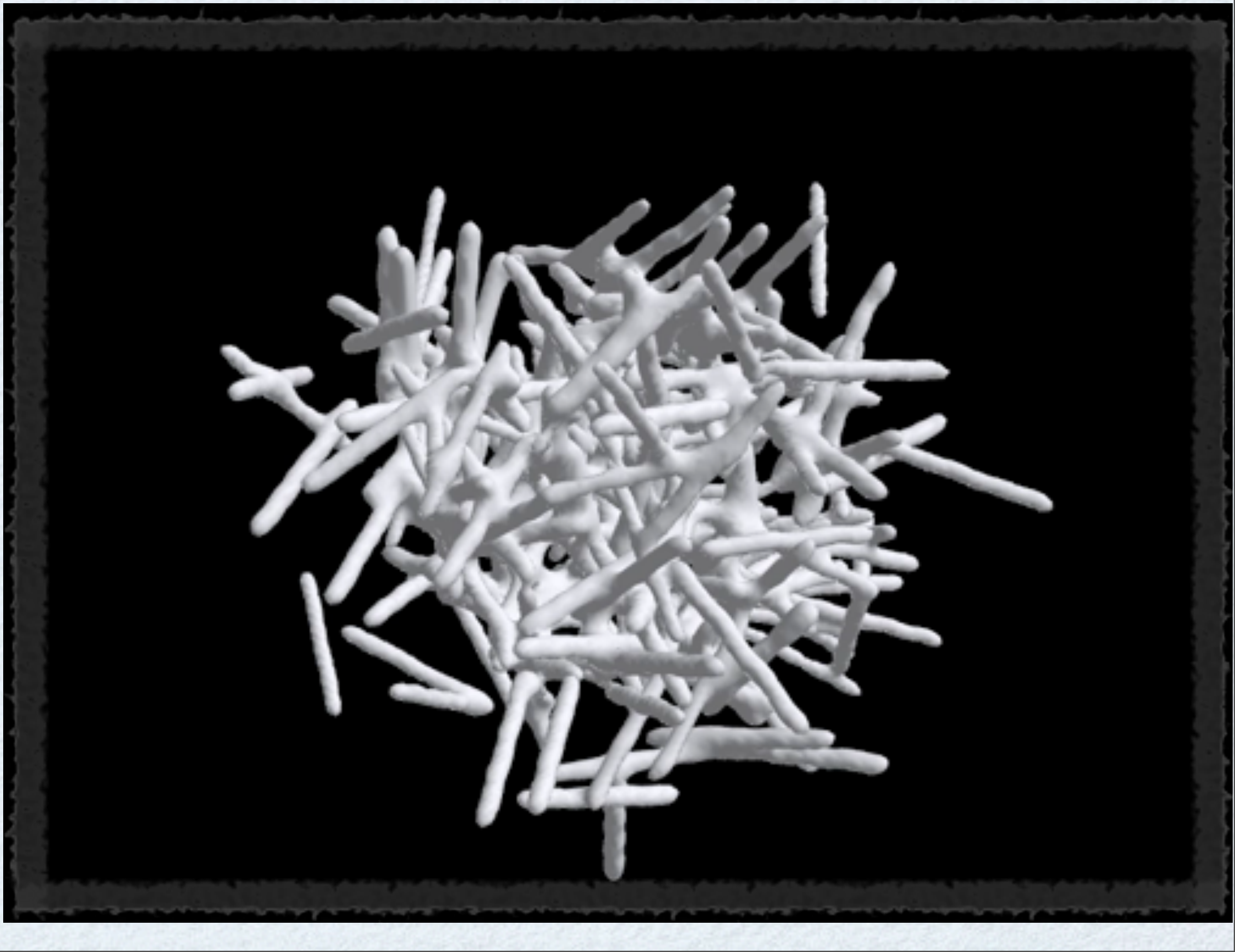

Lagrangian vs Eulerian Descriptions

S. E. Hieber and P. Koumoutsakos. A Lagrangian particle level set method. **J. Computational Physics**, 210:342-367, 2005

$$\Phi(\mathbf{x}, t) = \Phi_0(\mathbf{x} - \mathbf{u}t)$$

- **PARTICLE LEVEL SETS** exact for rigid body motion

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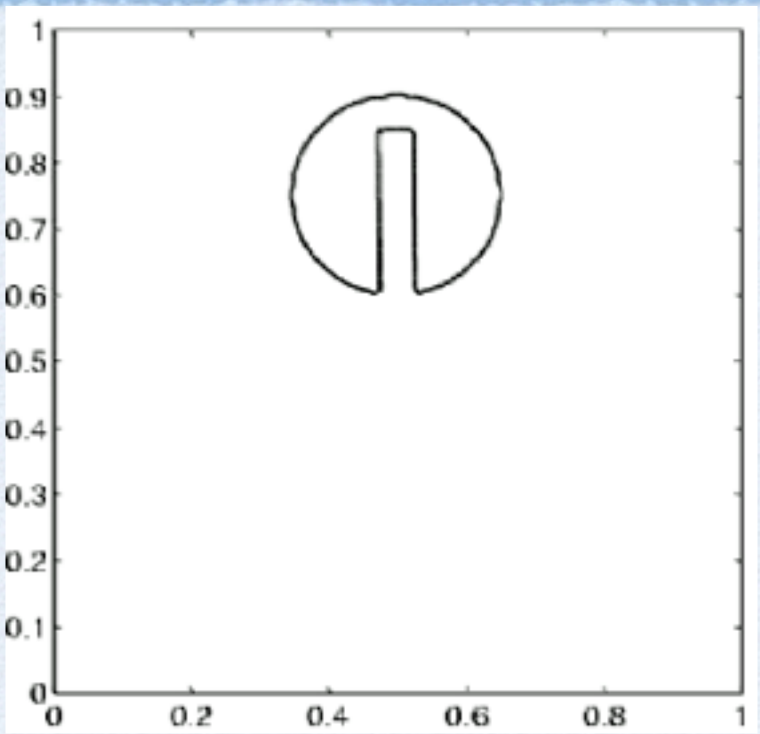

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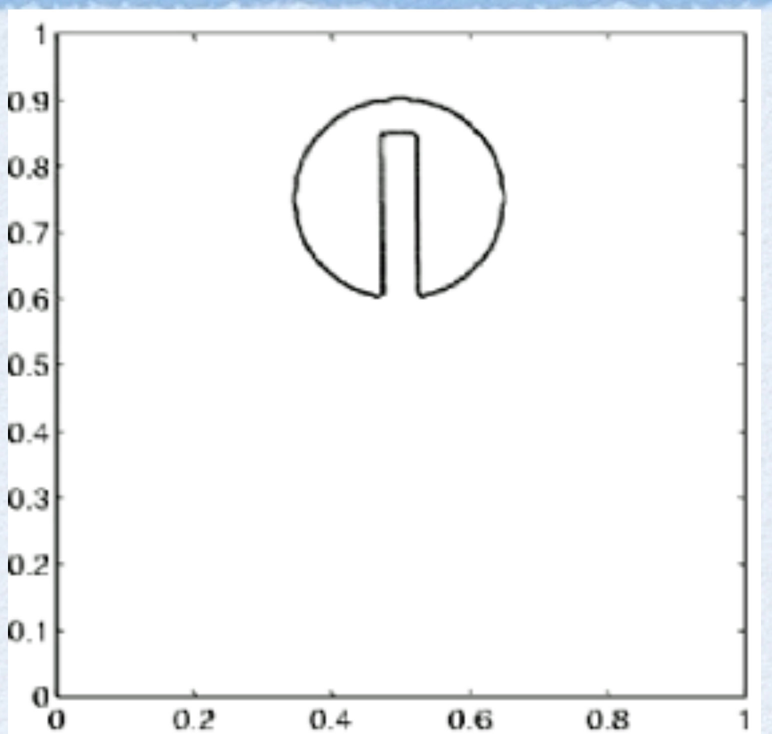

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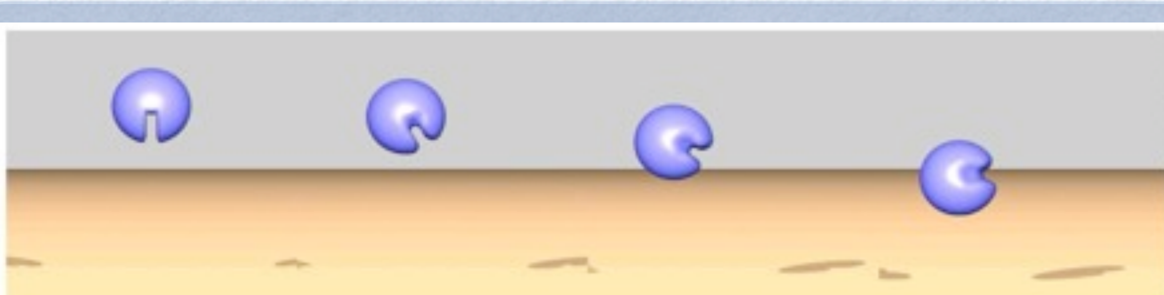
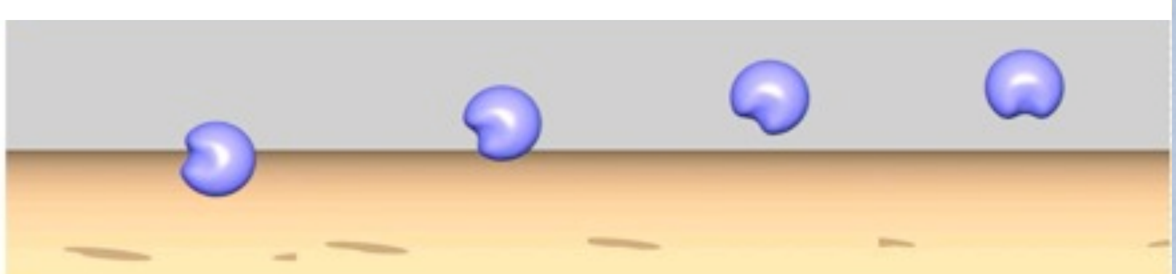
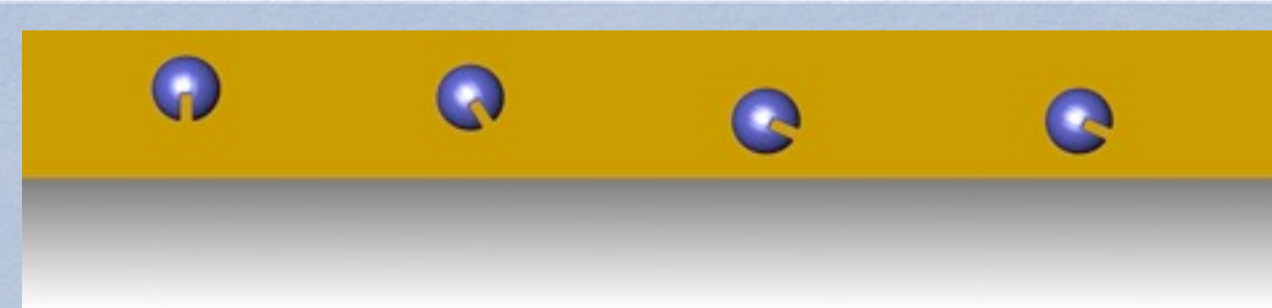


Hubrid Particle-Grid Level Sets
(Enright and Fedkiw, 2002)





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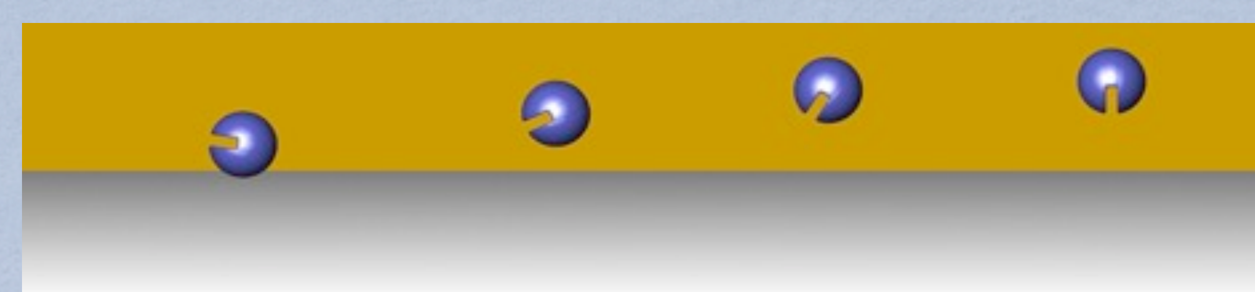
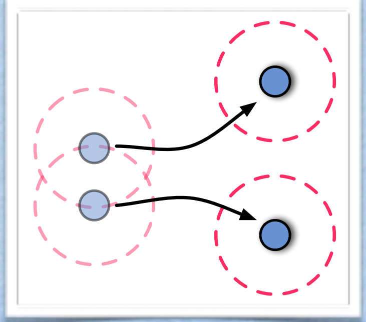


LAGRANGIAN DISTORTION

- loss of overlap -> loss of convergence



Particles follow flow trajectories - Location distortion

EXAMPLE :

Incompressible 2D Euler Equations

$$\omega = \nabla \times \mathbf{u} \quad \nabla \cdot \mathbf{u} = 0$$

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There is an exact axisymmetric solution

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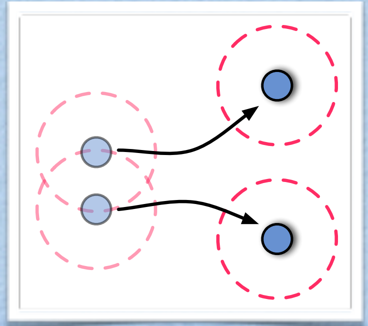

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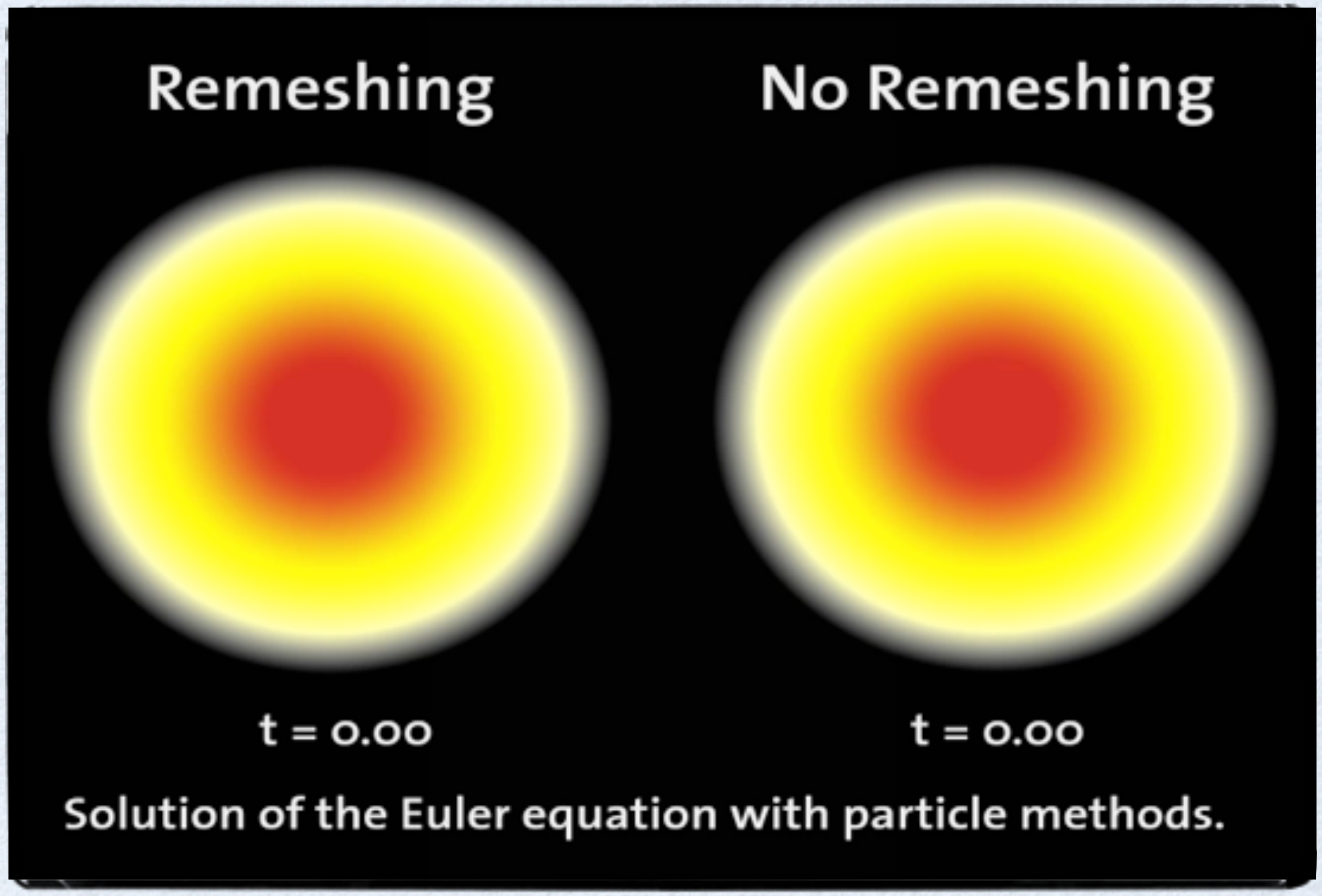
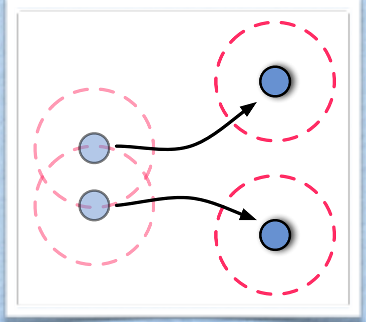


LAGRANGIAN DISTORTION

- loss of overlap -> loss of convergence



Particles follow flow trajectories - Location distortion

EXAMPLE :

Incompressible 2D Euler Equations

$$\omega = \nabla \times \mathbf{u} \quad \nabla \cdot \mathbf{u} = 0$$

$$\frac{D\omega}{Dt} = 0$$

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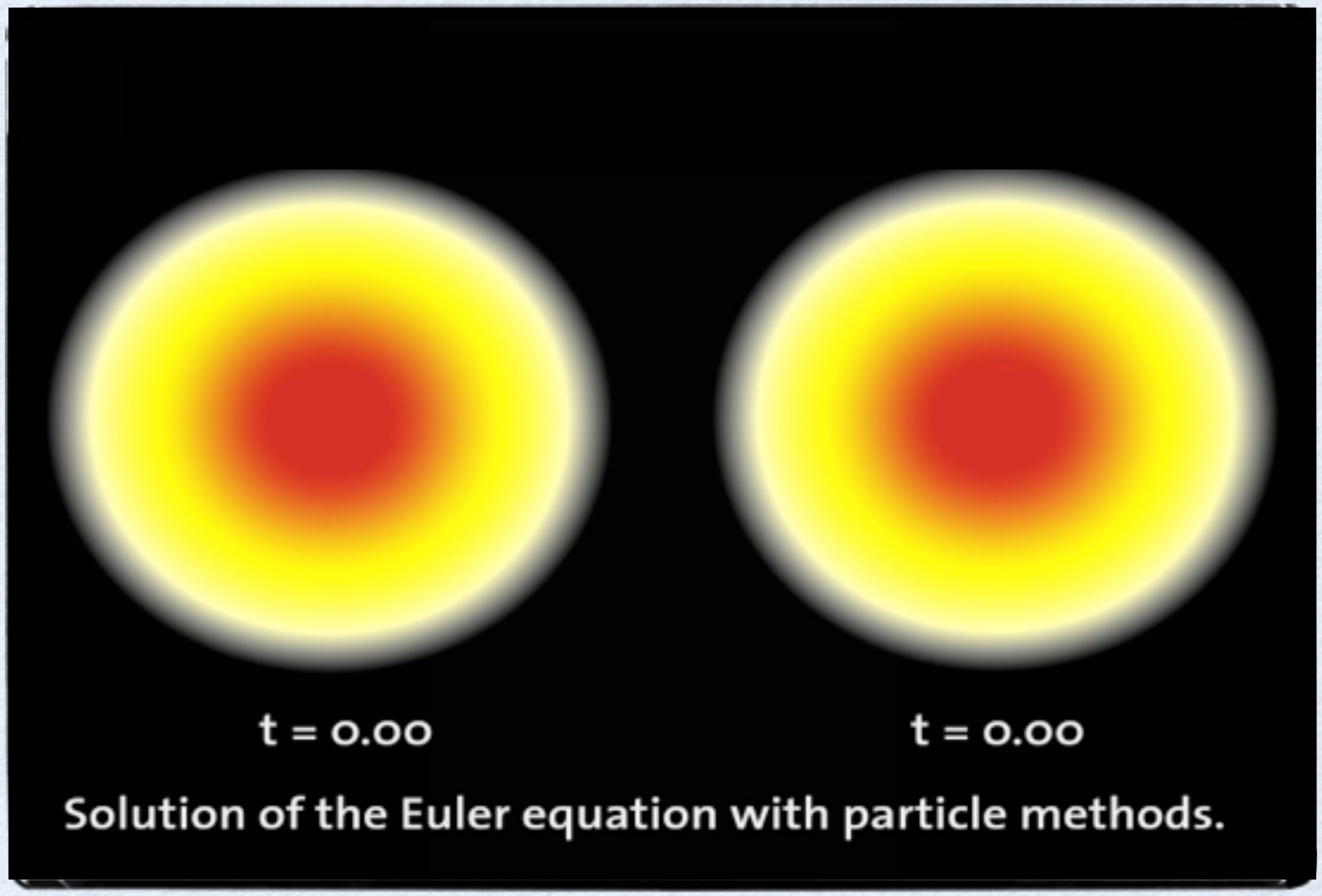

SMOOTH PARTICLES MUST OVERLAP

Integral Function Representation

$$\Phi(x) \; = \int \Phi(y)\,\delta(x-y)\,dy$$

Function Mollification

$$\Phi_\epsilon(x) \; = \int \Phi(y)\,\zeta_\epsilon(x-y)\,dy$$

$$\int \zeta\, x^\alpha\, dx = 0^\alpha \qquad 0 \le \alpha < r$$

Point Particle Quadrature

$$\Phi^h(x,t) \; = \sum_{p=1}^{N_p} h_p^d\, \Phi_p(t)\, \delta(x - x_p(t))$$

Smooth Particle Quadrature

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TOTAL ERROR

$$\begin{aligned} ||\Phi - \Phi_\epsilon^h|| &\le ||\Phi - \Phi_\epsilon|| + ||\Phi_\epsilon - \Phi_\epsilon^h|| \\ &\le (C_1\, \epsilon^r + C_2\, (\frac{h}{\epsilon})^m)\, ||\Phi||_\infty \end{aligned}$$

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Need h/ε < 1 for accuracy

PARTICLES MUST OVERLAP

Hald, Beale and Majda, (80‘s) Anderson, Cottet (90’s)

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How to fix it ?

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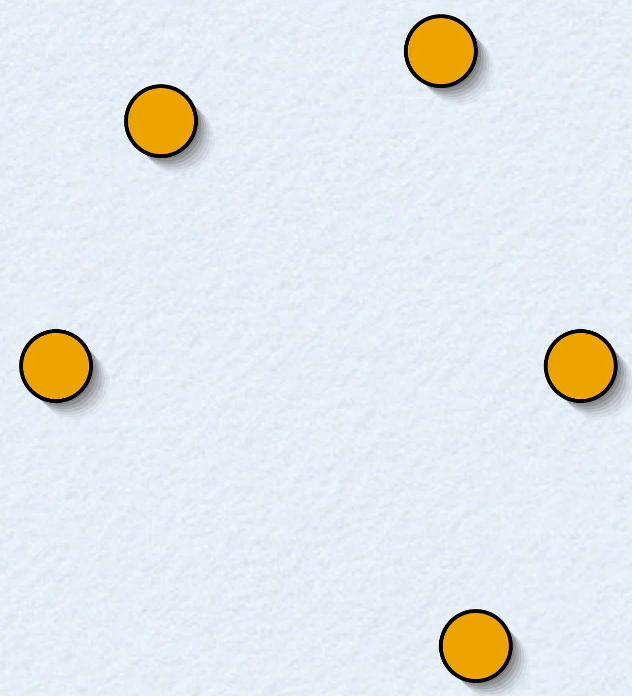

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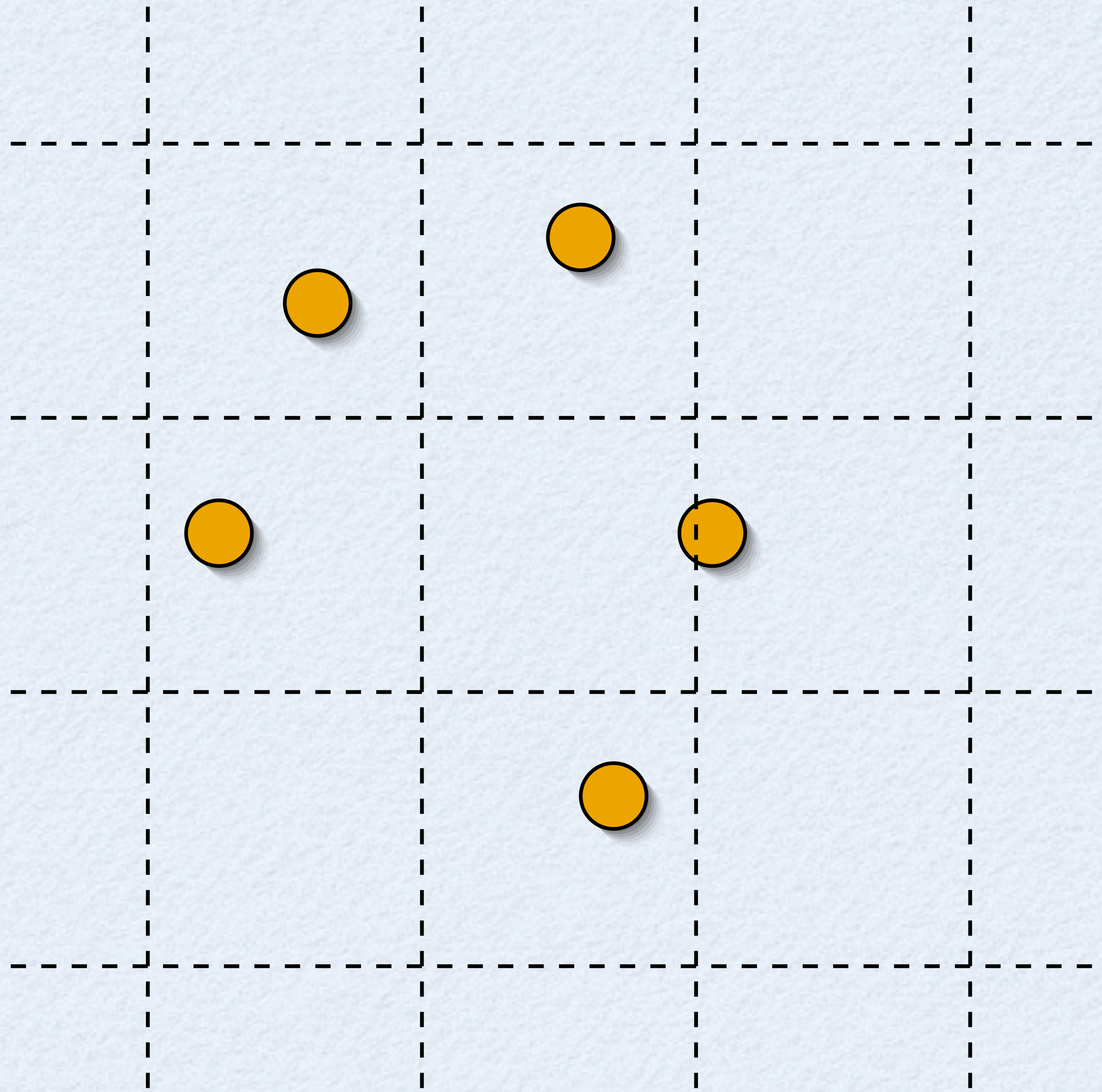

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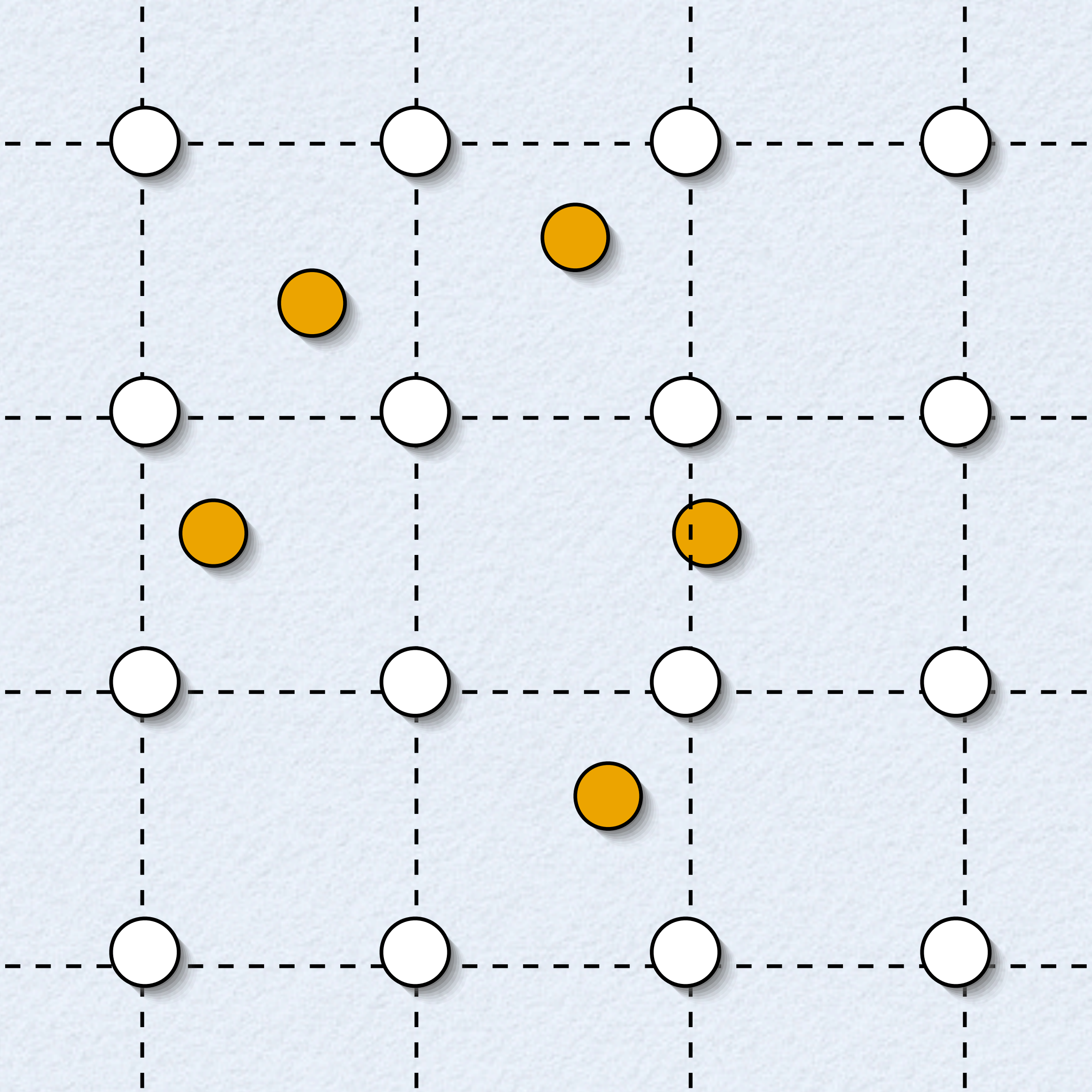

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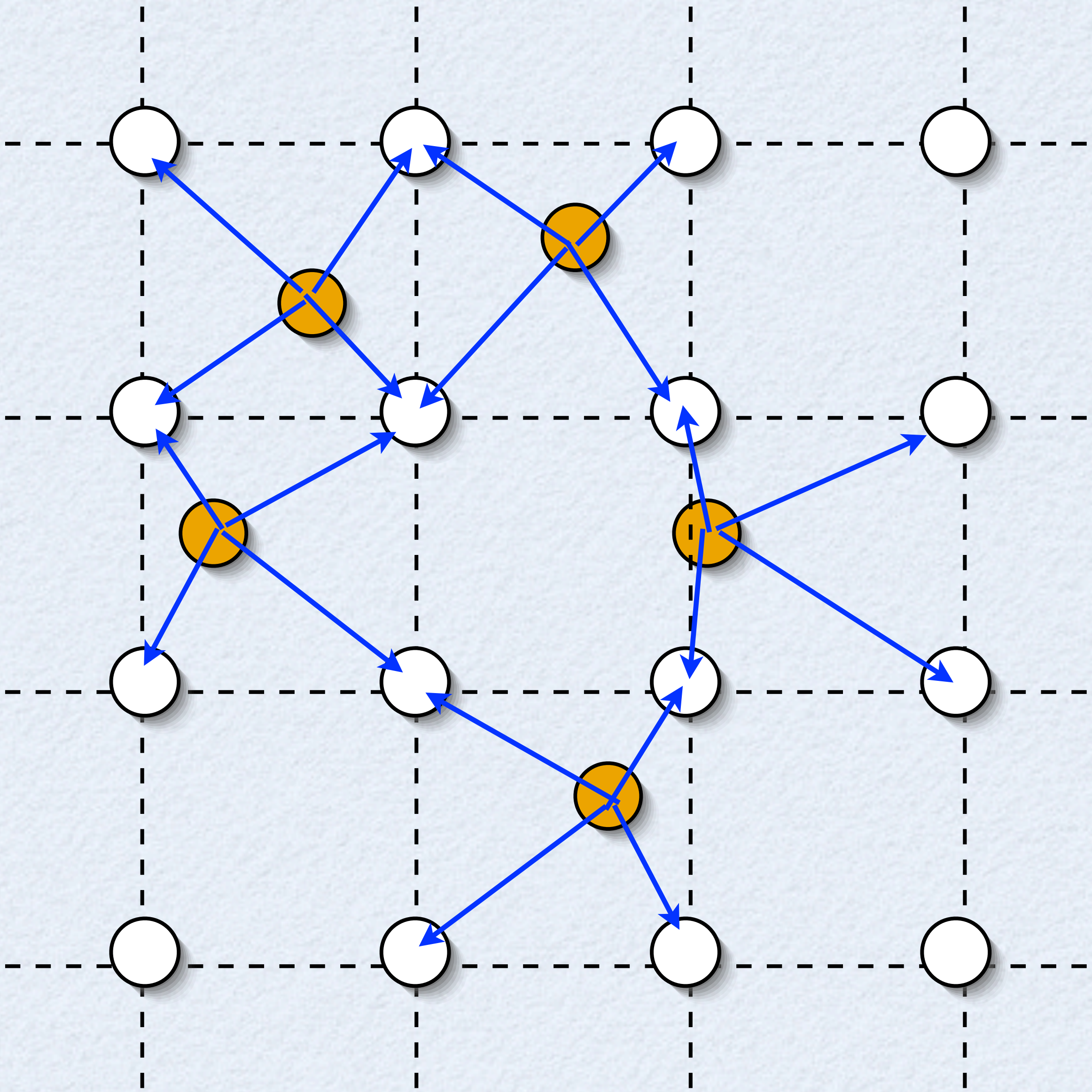

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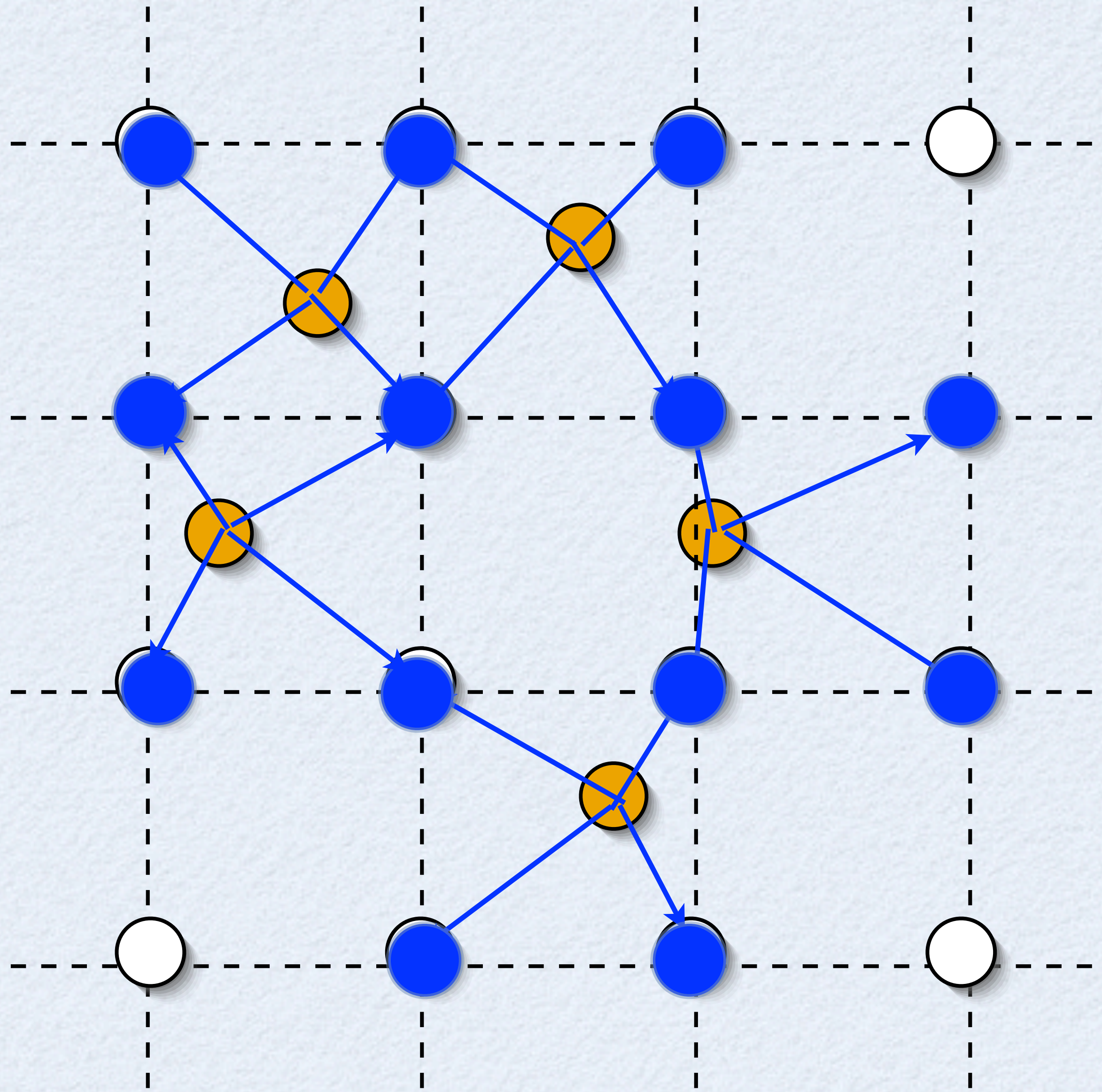

Moment Conserving Interpolation : $Q_p^{\text{new}} = \sum_{p'} Q_{p'} M(j\,h - x_{p'})$

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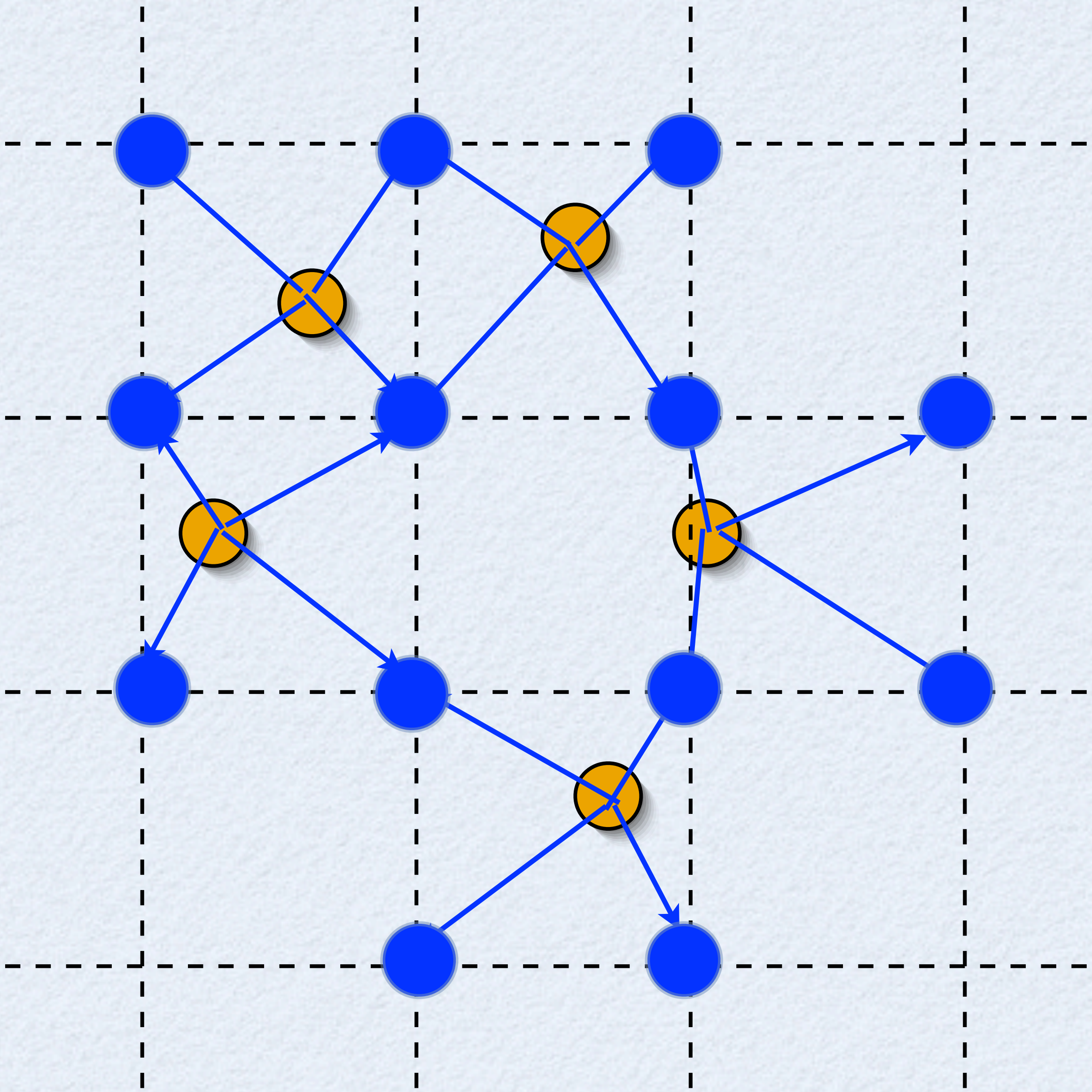

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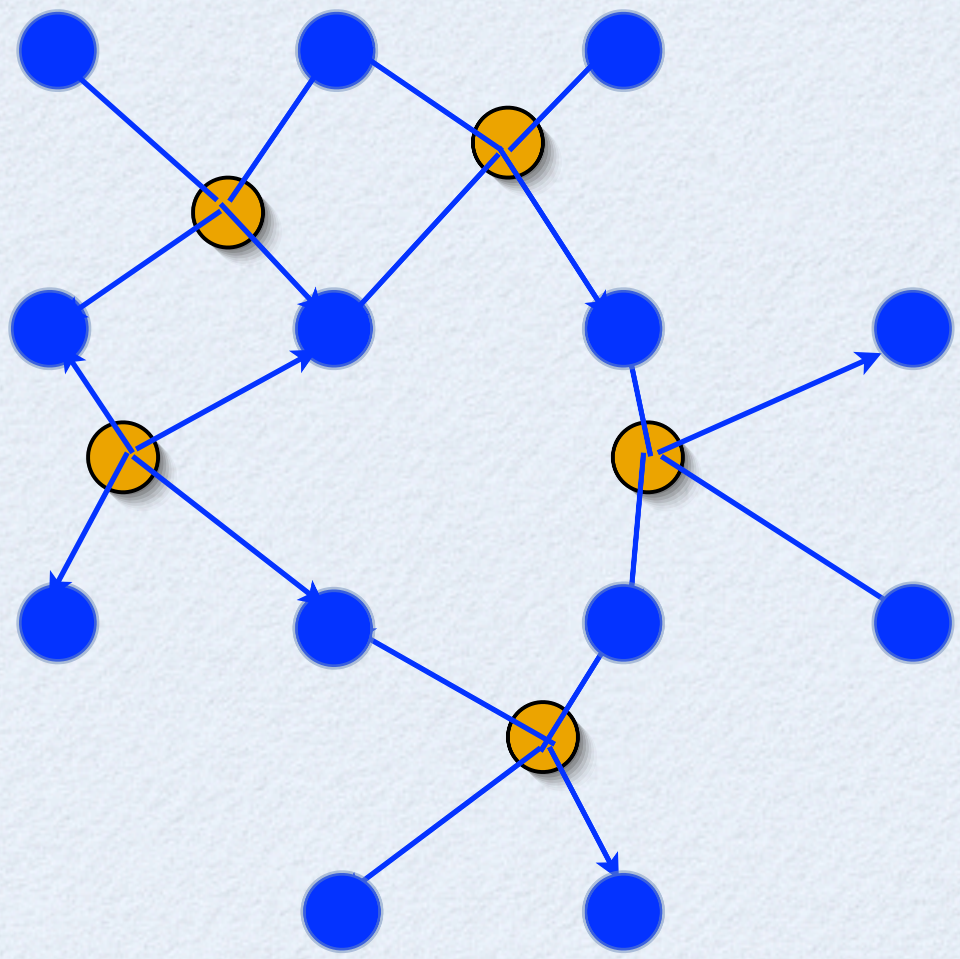

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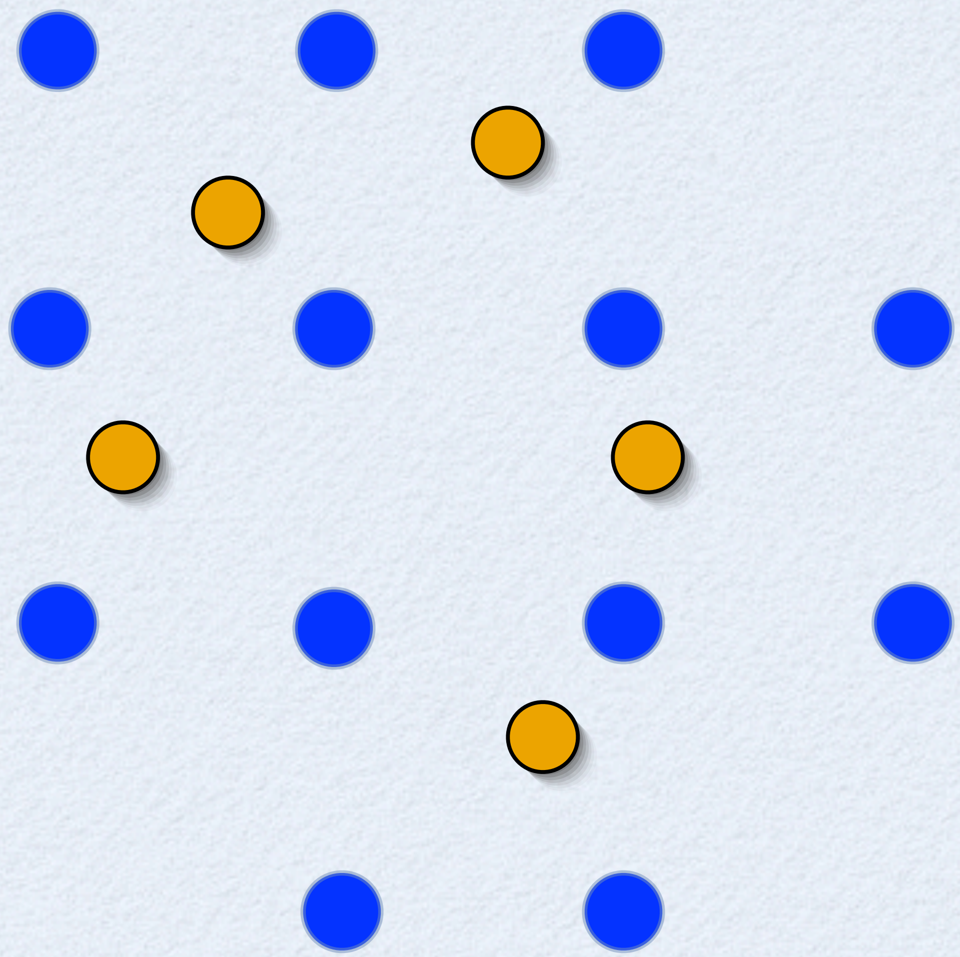

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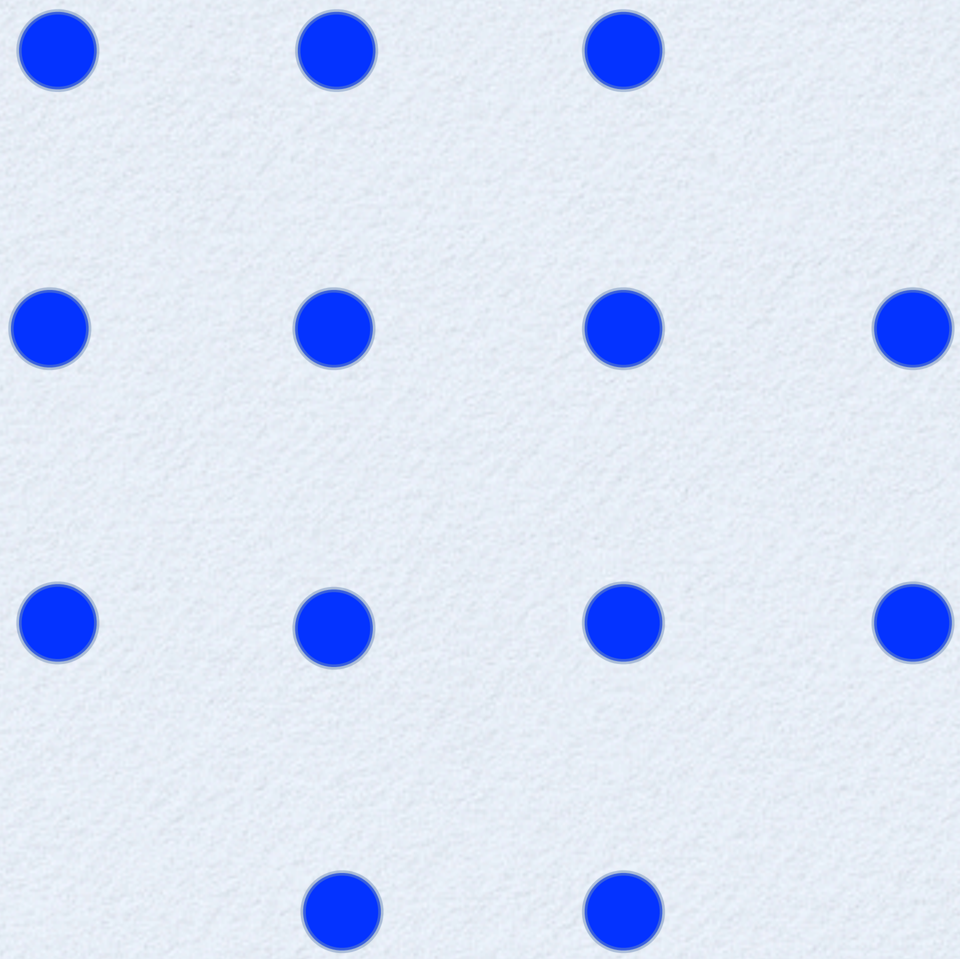

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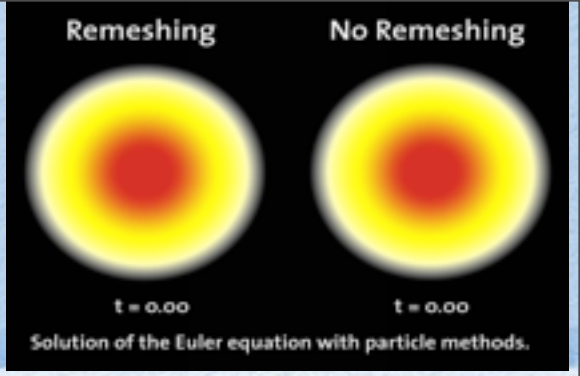

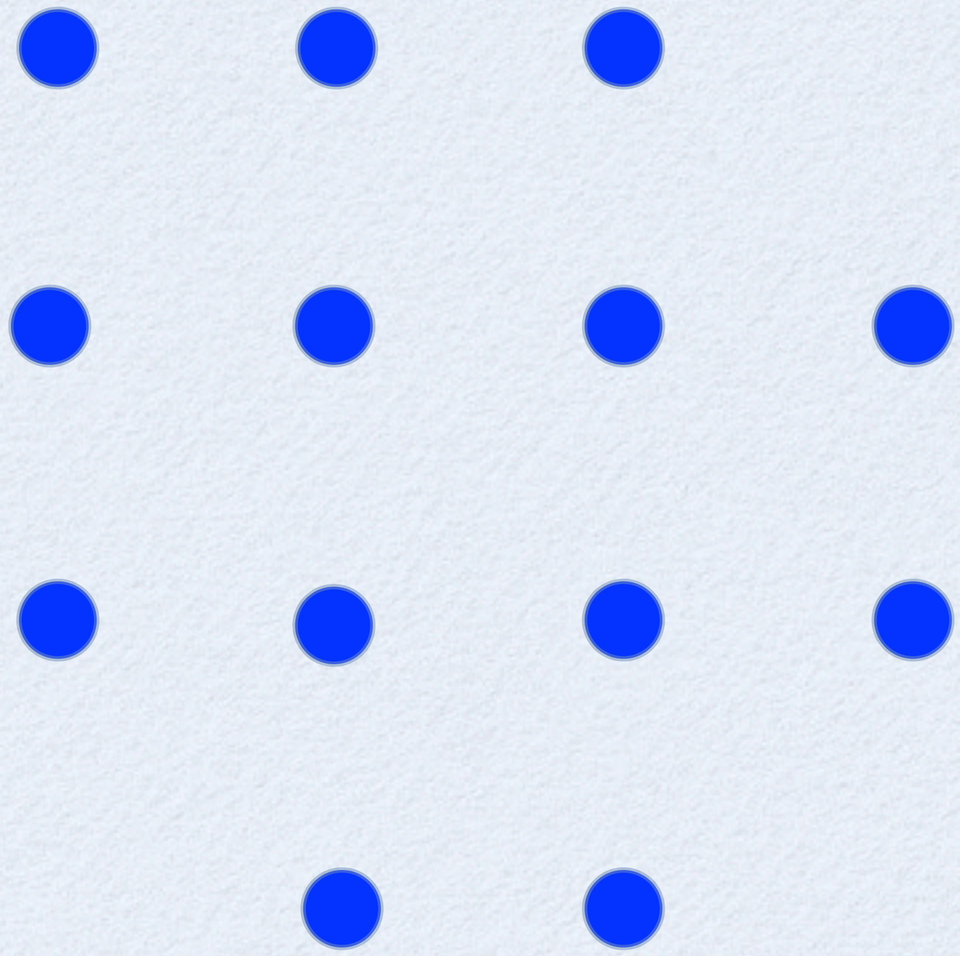

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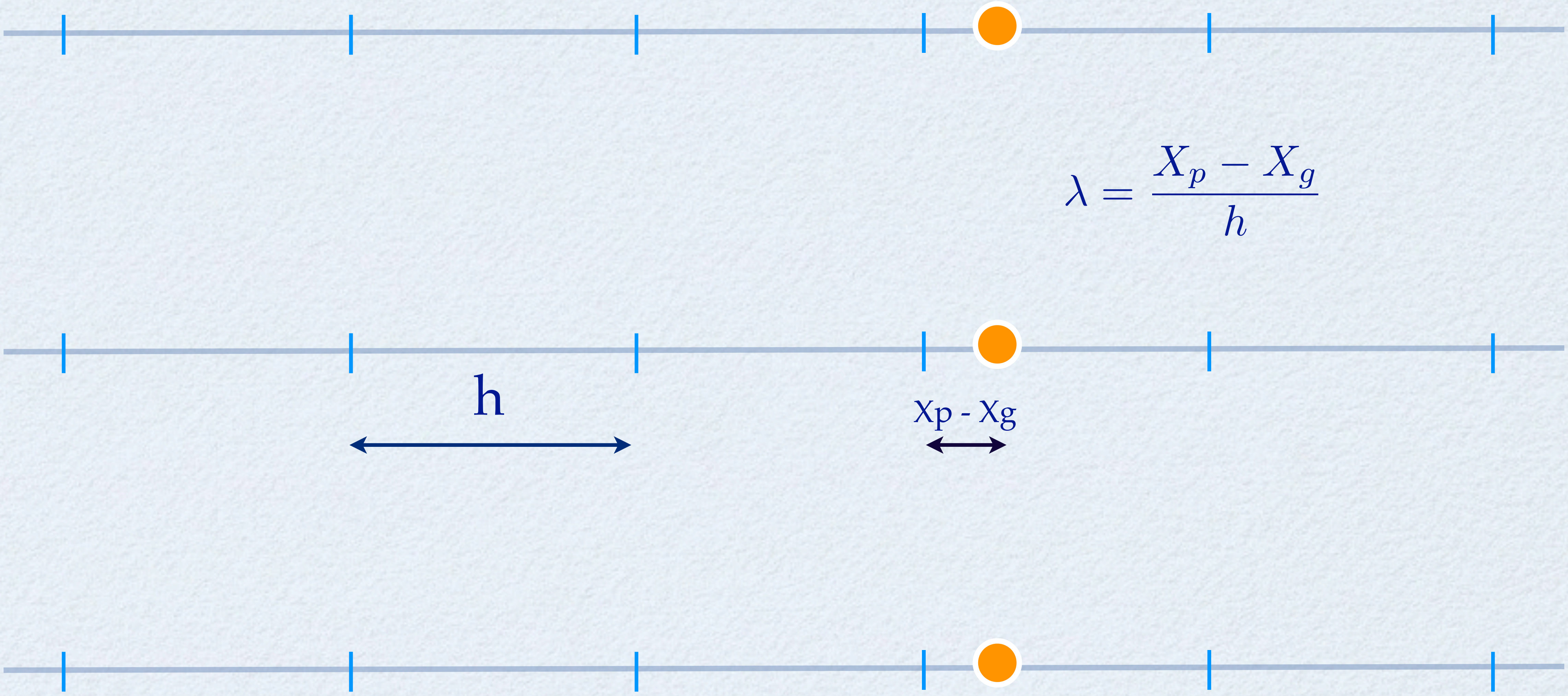
4:RESAMPLE: Mesh Nodes BECOME Particles

Size of Remeshing Stencil = # Conserved Moments



$$\lambda = \frac{X_p - X_g}{h}$$

Bergdorf et. al., MMS,2005
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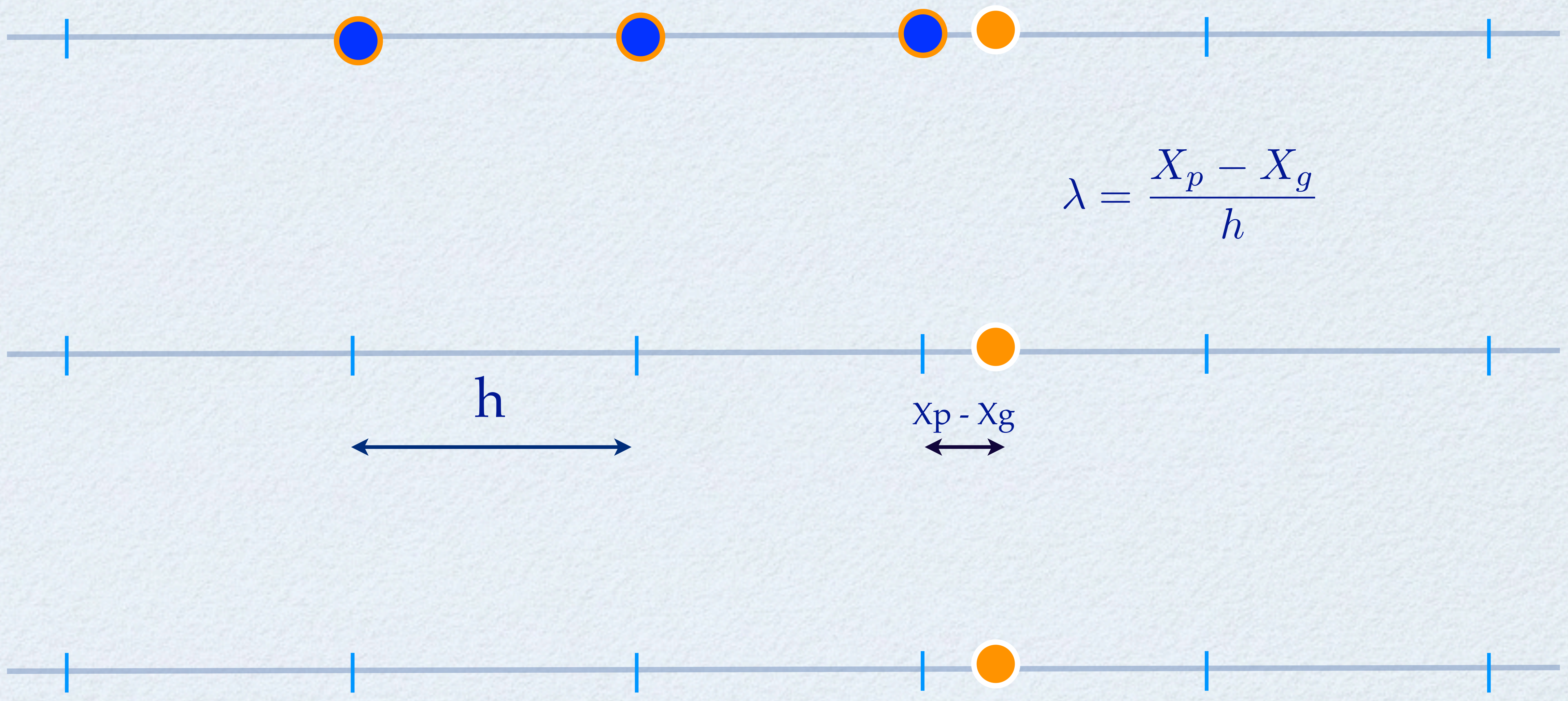

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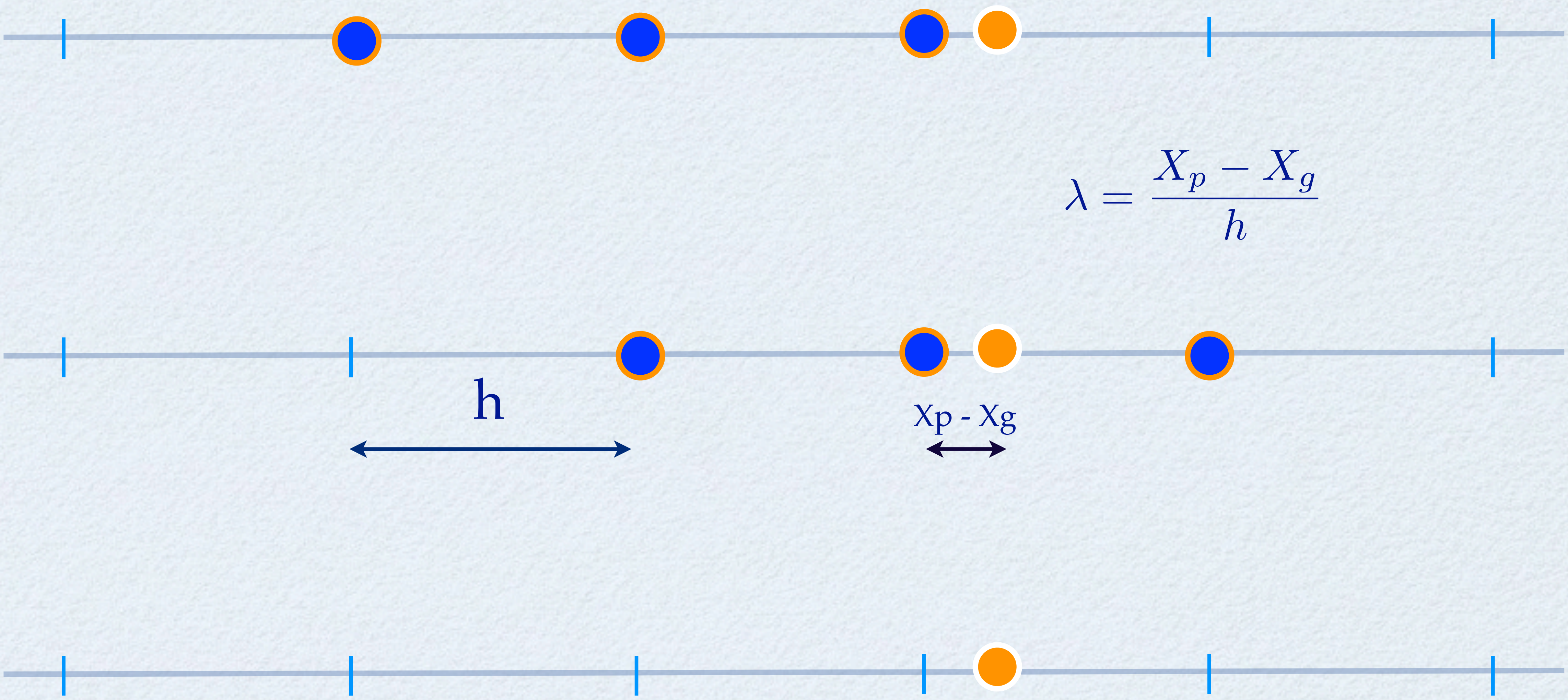

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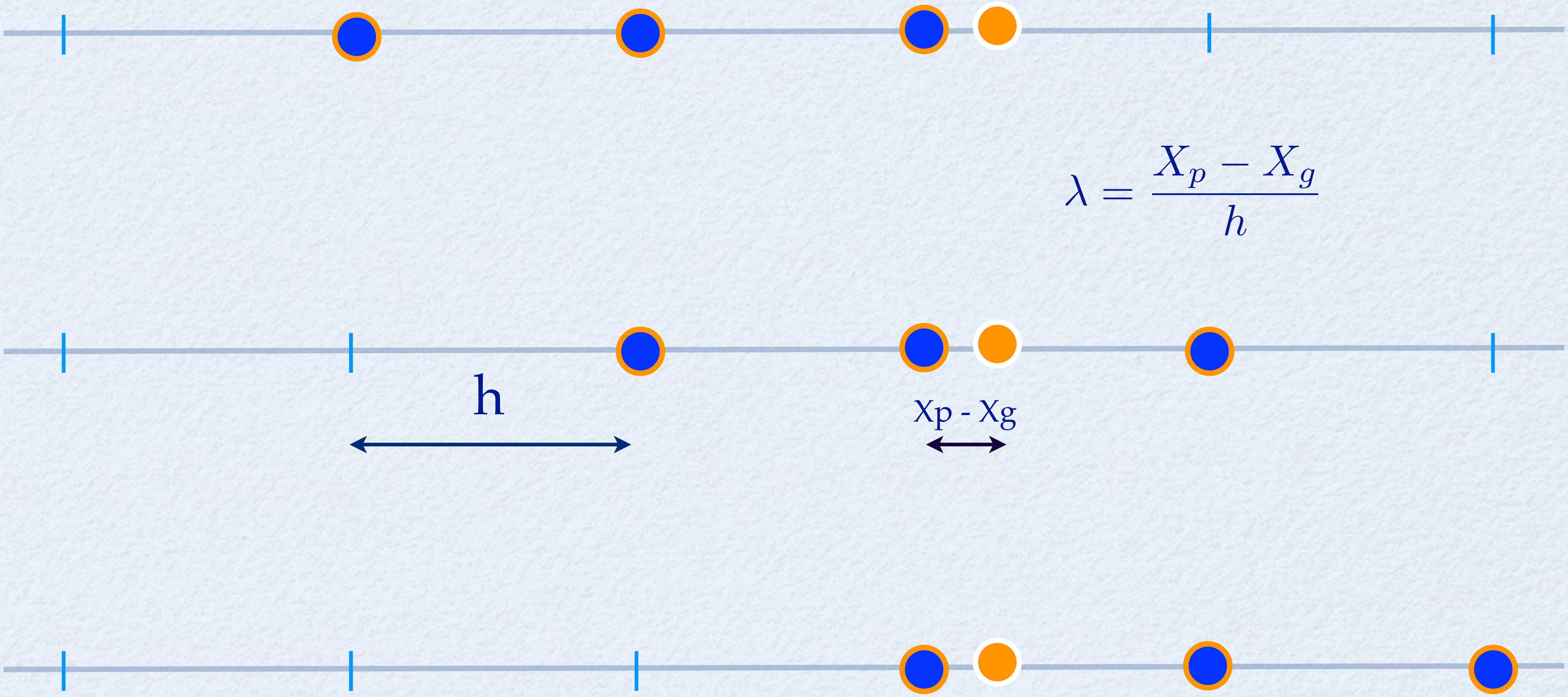

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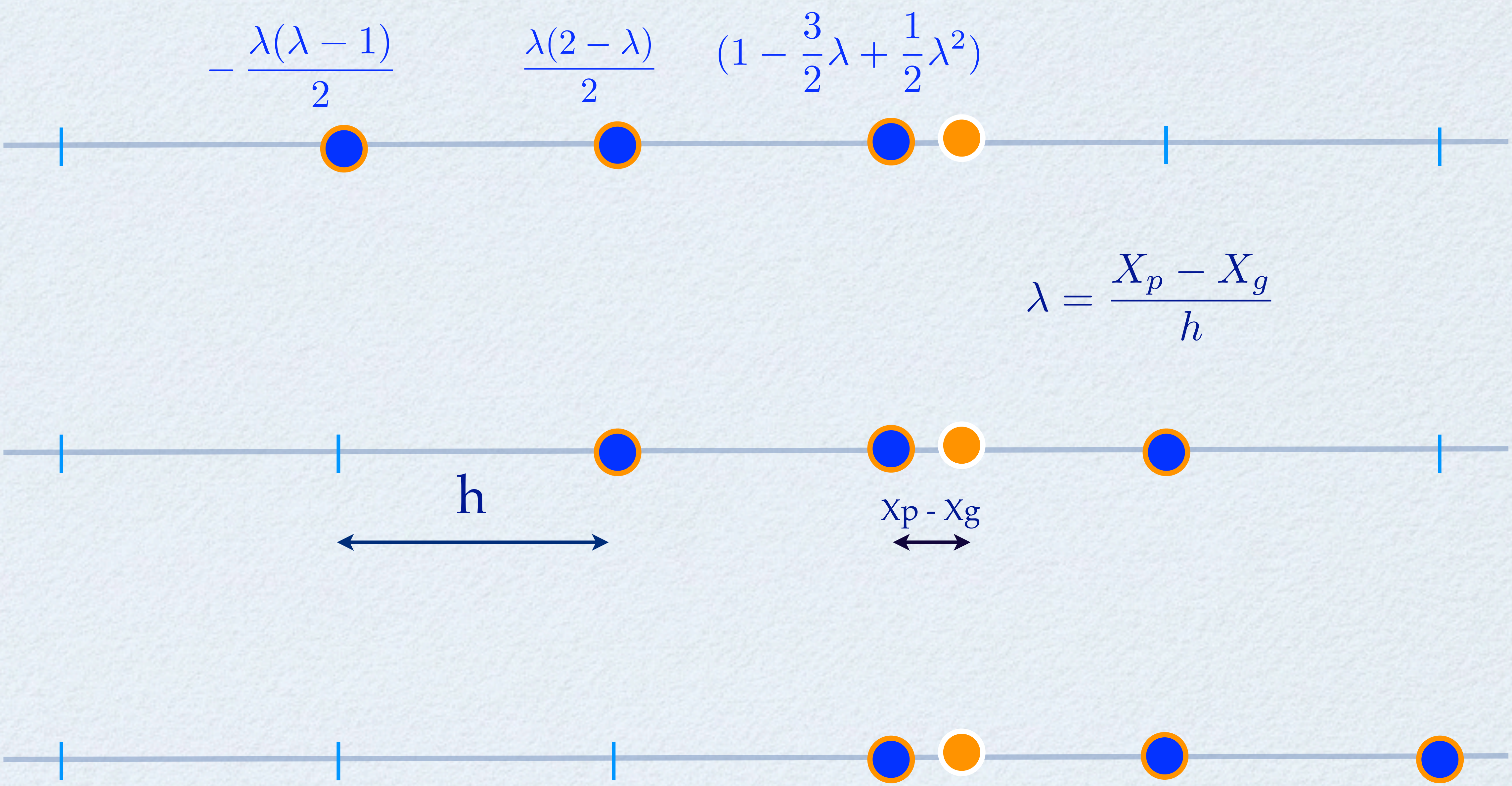

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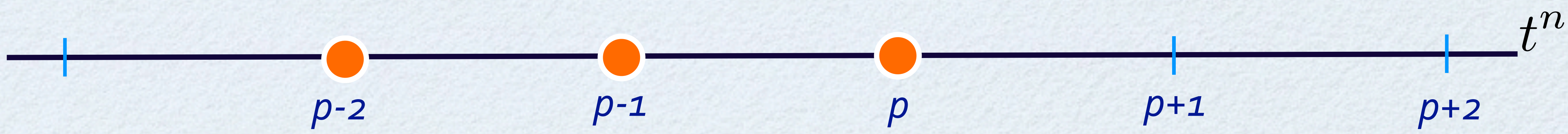
+ REMESH



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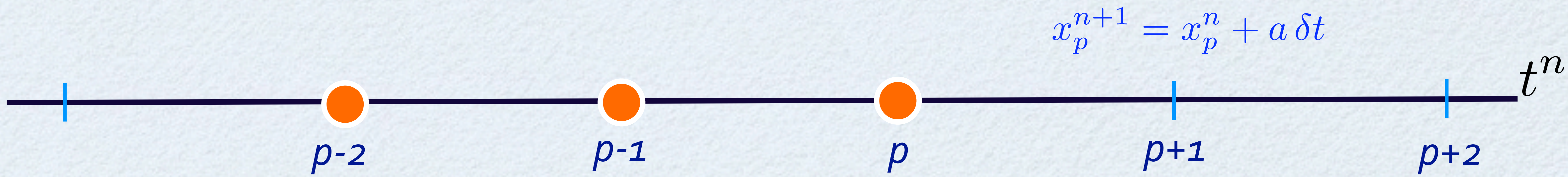

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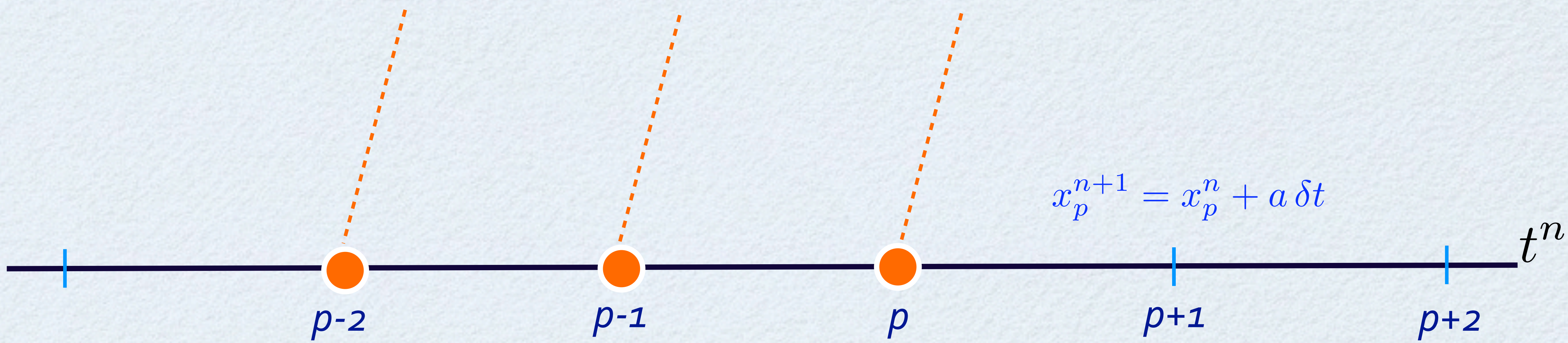

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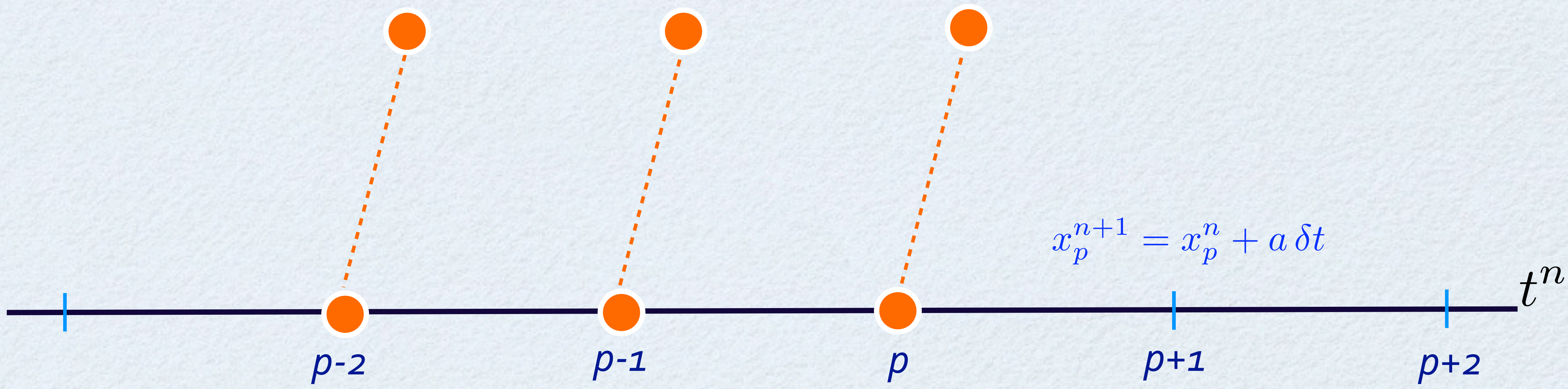

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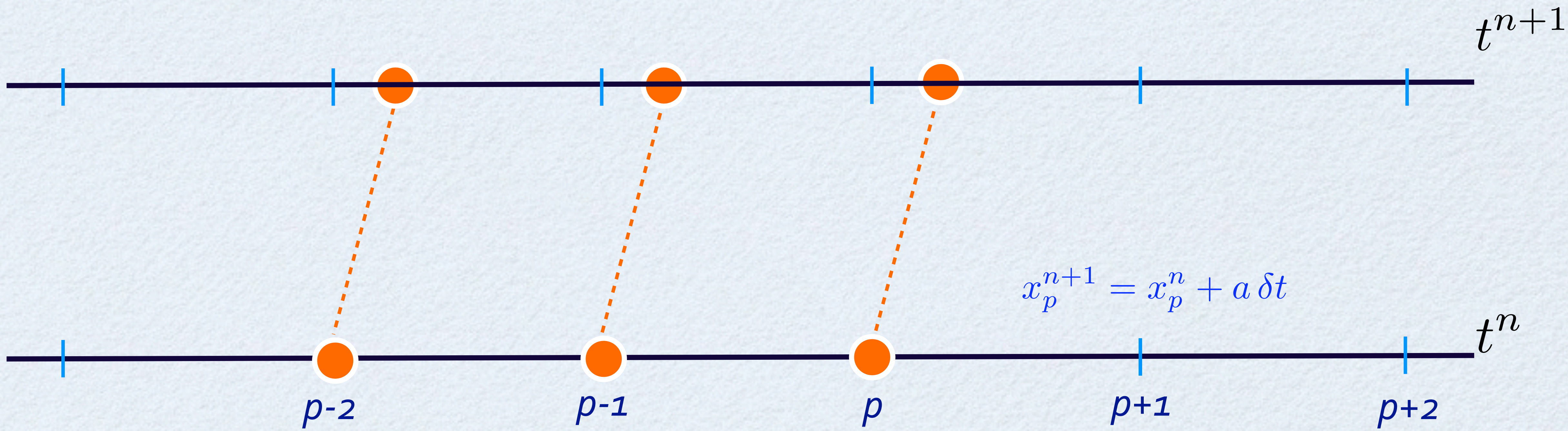

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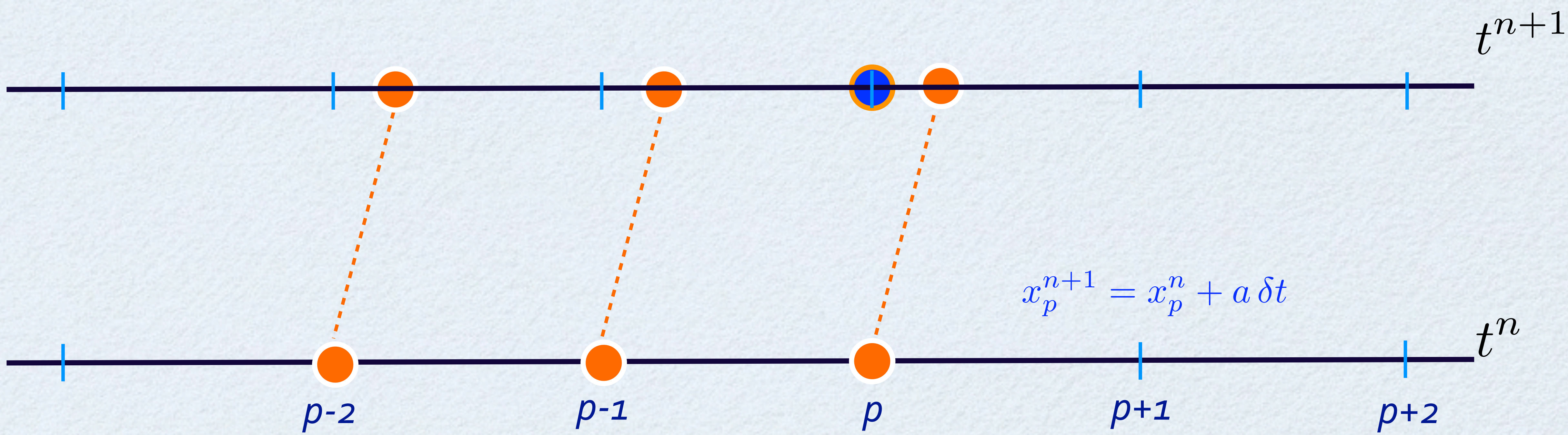

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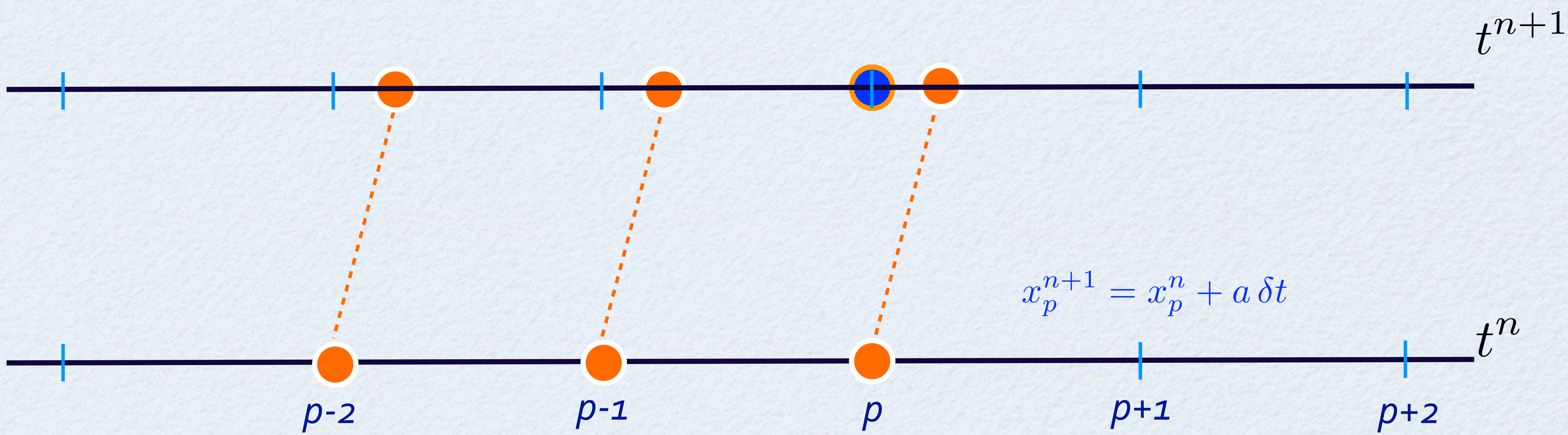

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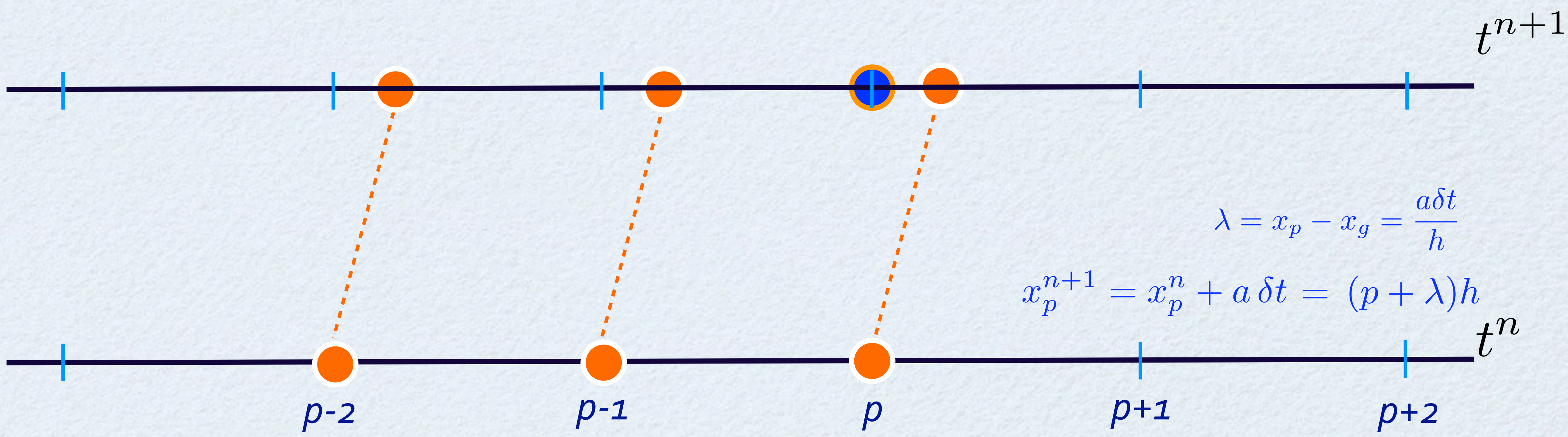

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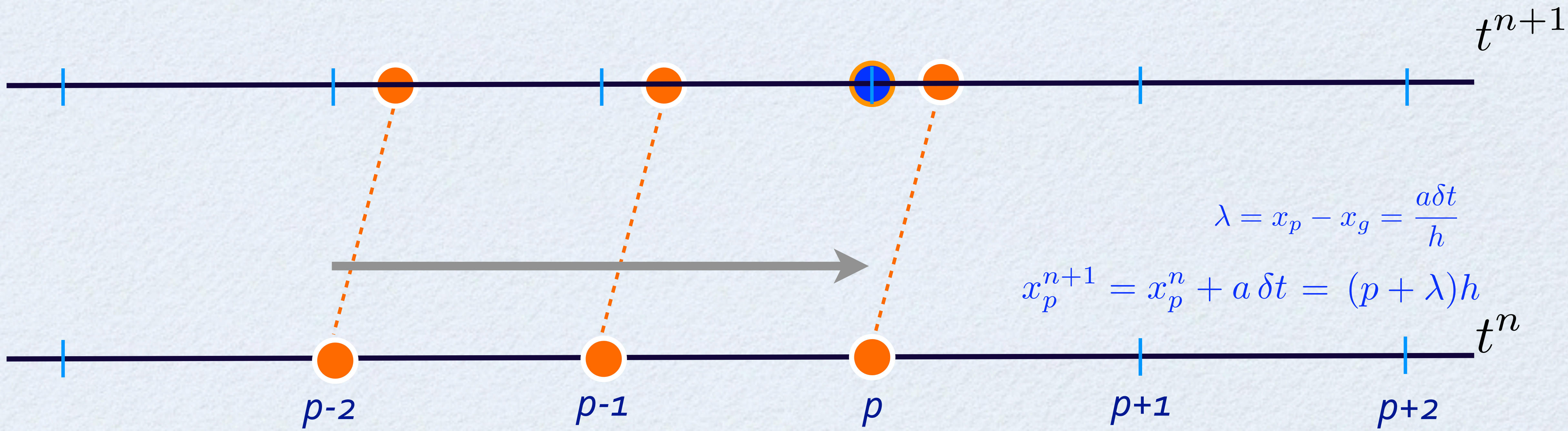

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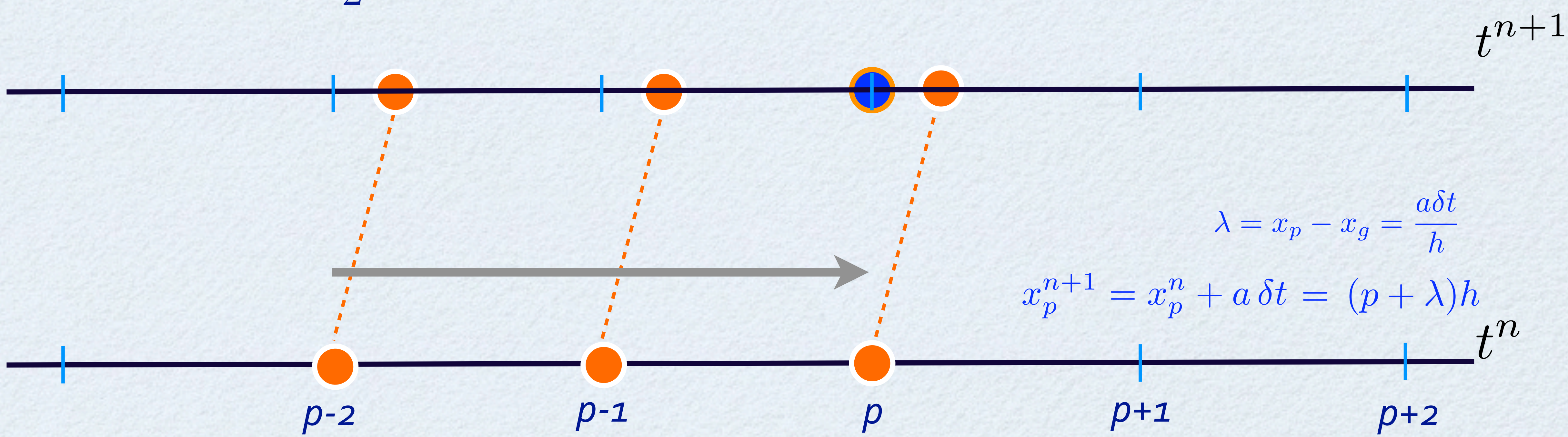
+ REMESH

$$u_p^{n+1} = -\frac{\lambda(\lambda-1)}{2} u_{p-2}^n$$



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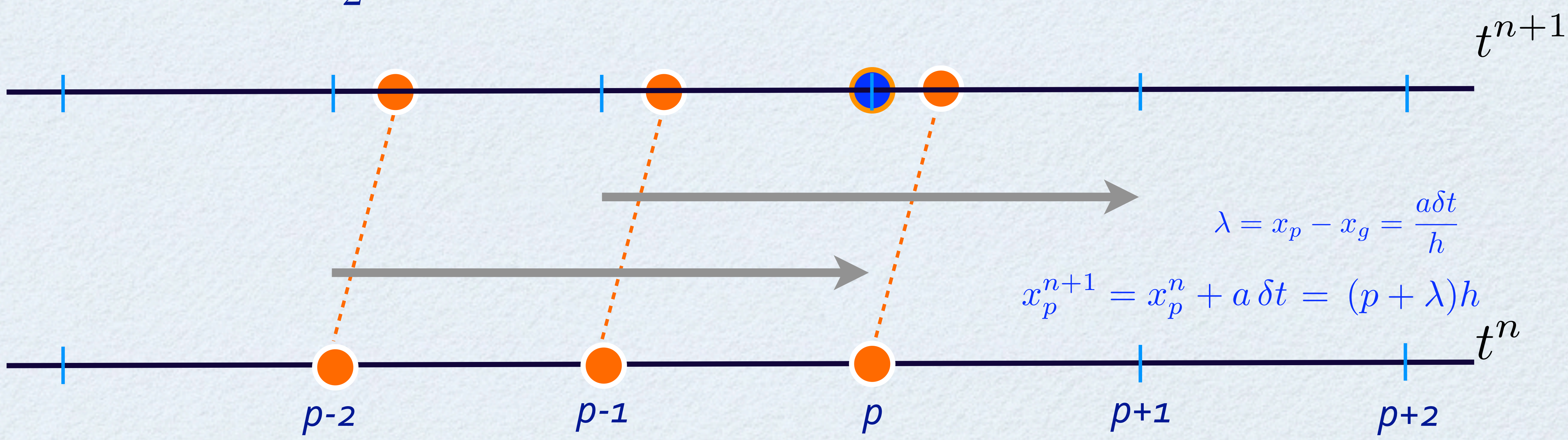
$$\frac{du_p}{dt} = 0 \qquad \frac{dx_p}{dt} = a$$

+ REMESH

$$u_p^{n+1} = -\frac{\lambda(\lambda-1)}{2} u_{p-2}^n$$



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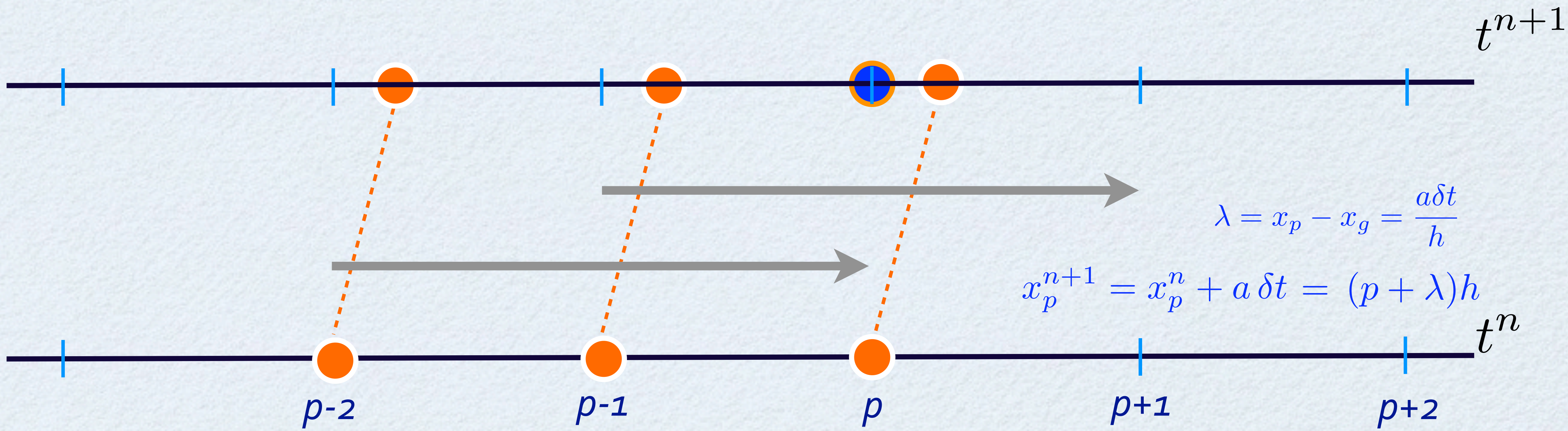

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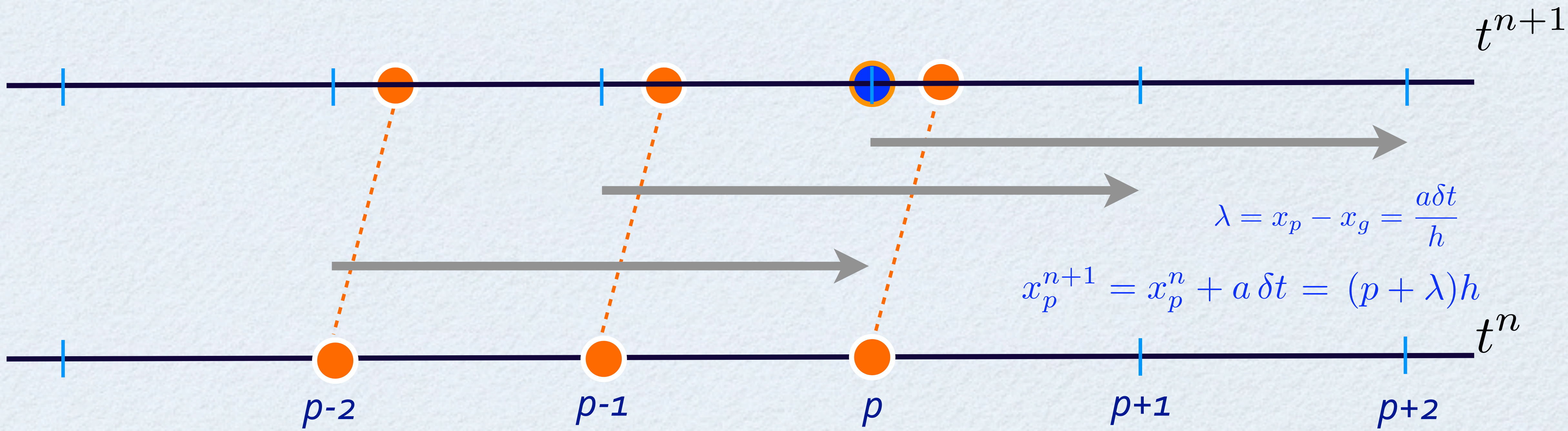

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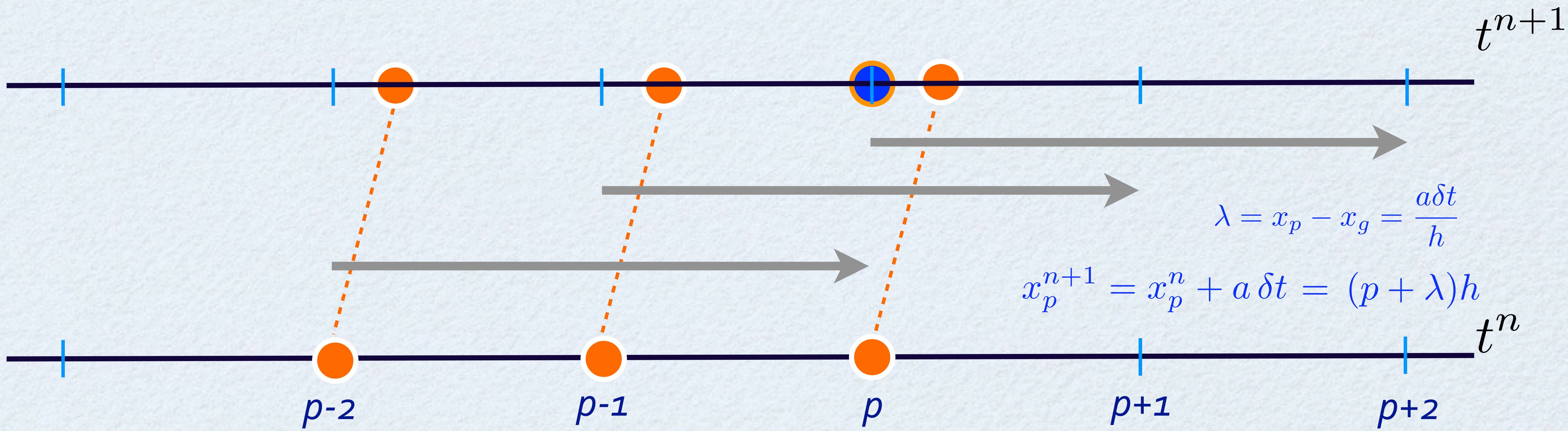

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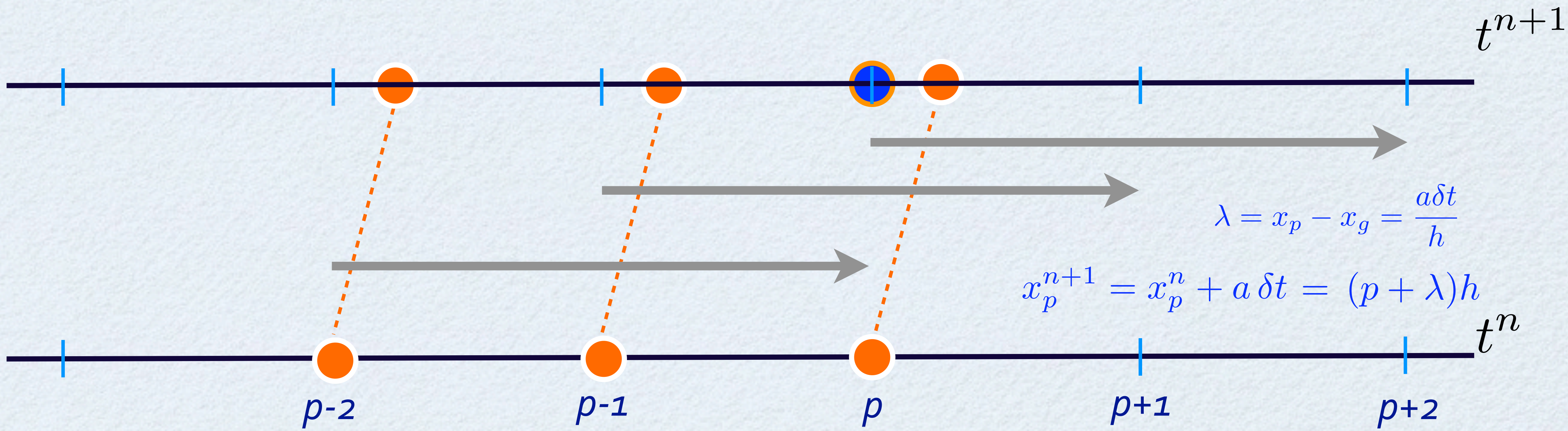

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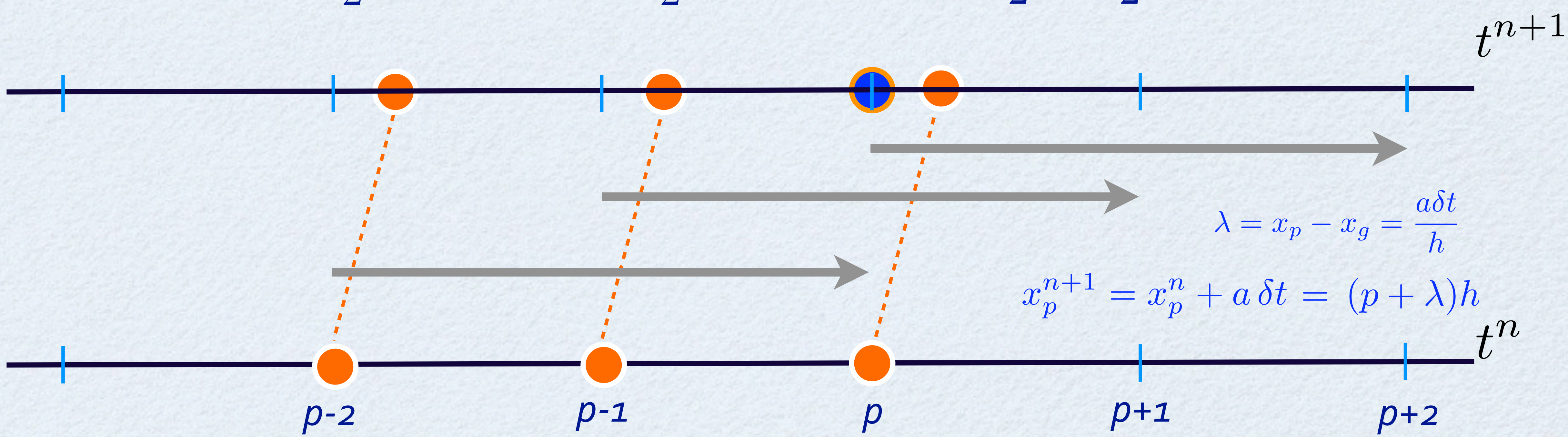

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Euler Advect + One-sided Remesh = Beam-Warming FD

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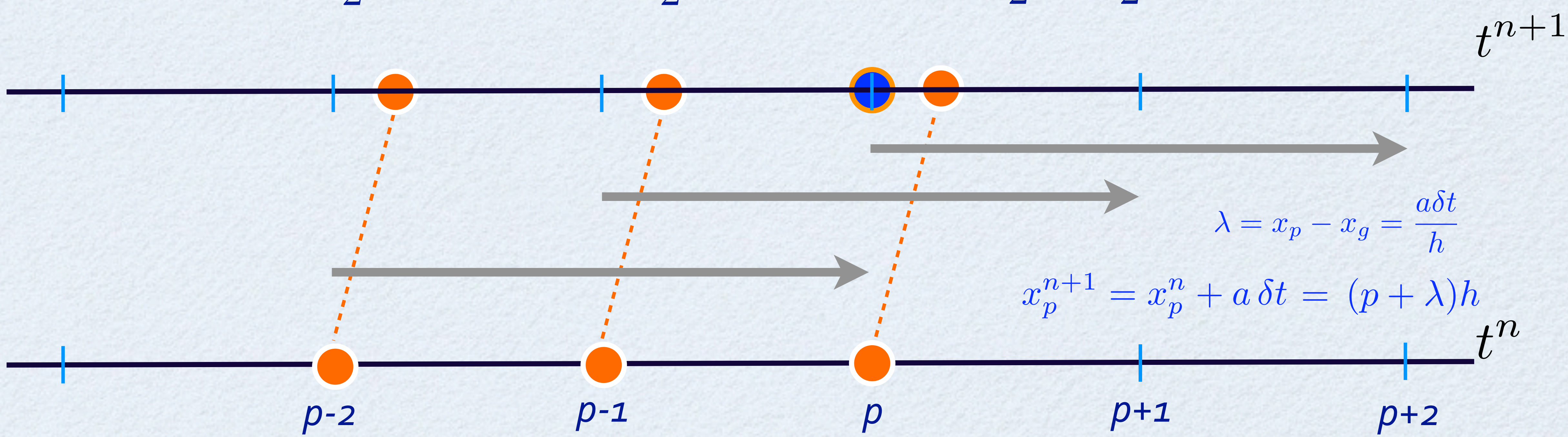

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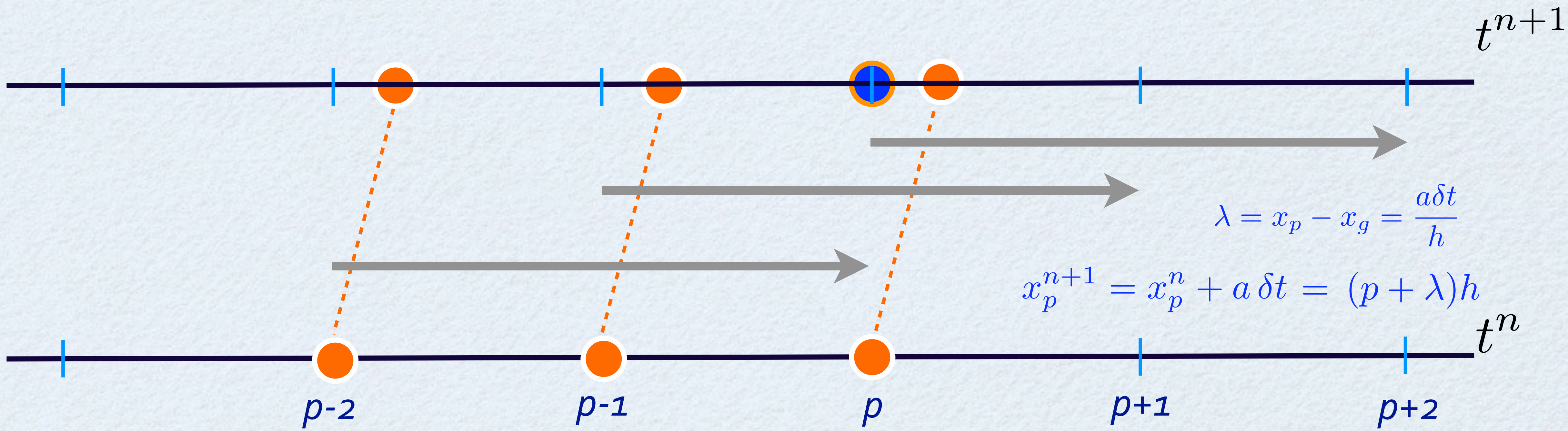

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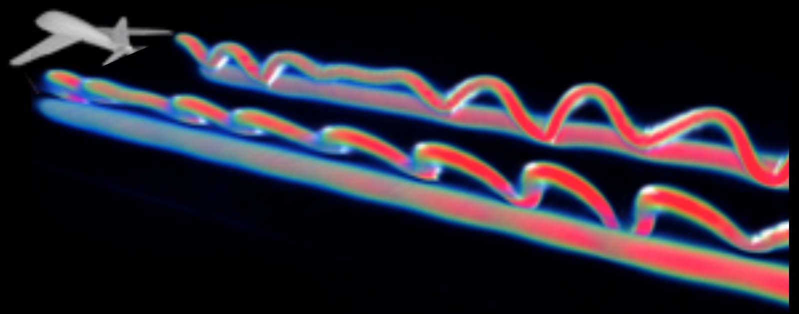
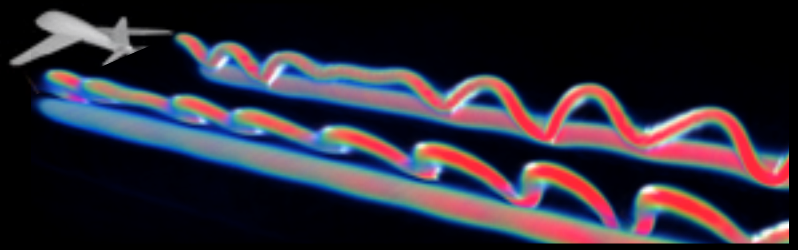
Euler Advect + One-sided Remesh = Beam-Warming FD

Euler Advect + Central Remesh = Lax - Wendroff FD ....



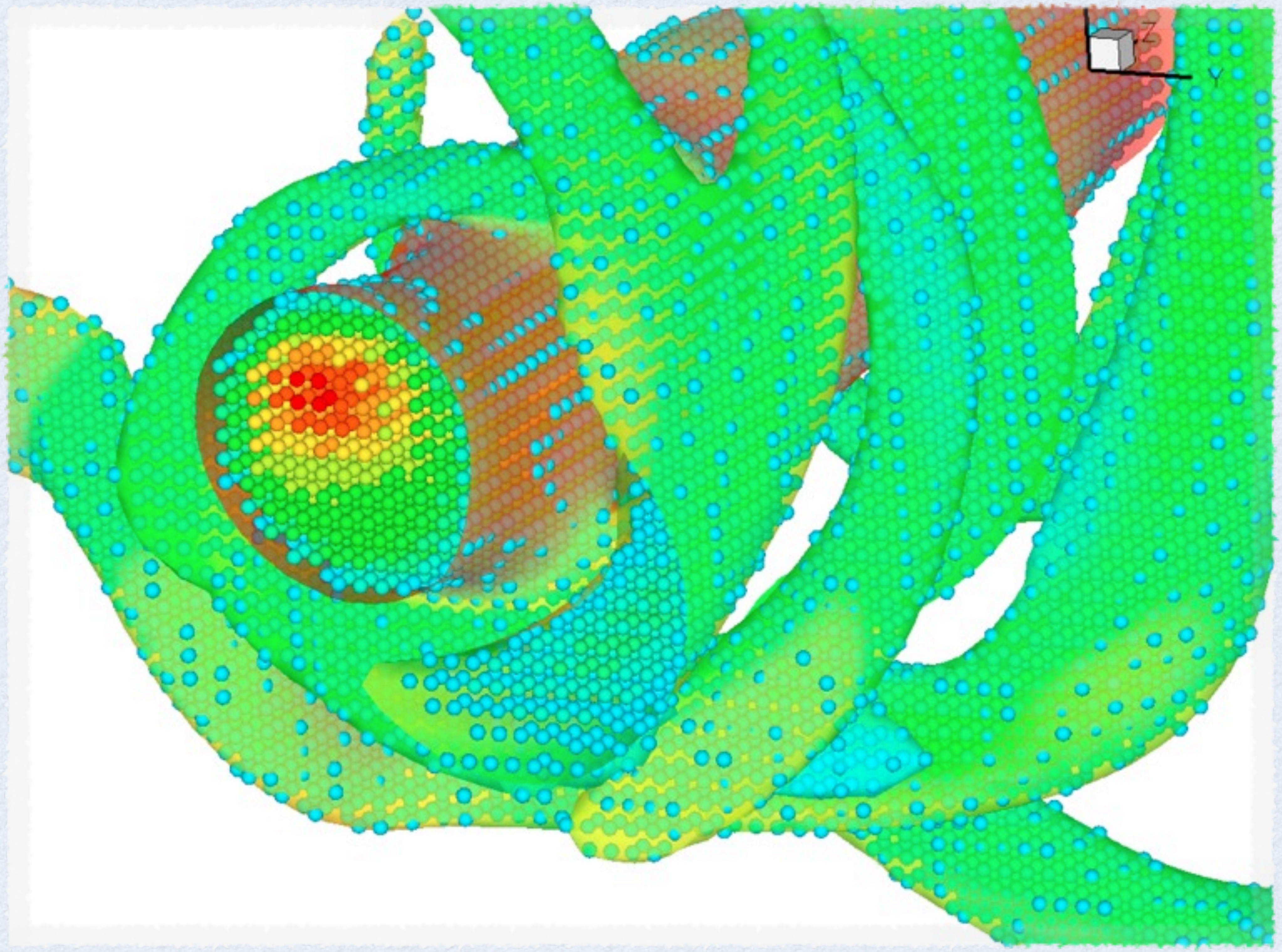
16K Cores – 10 Billion Particles – 60%

Runs at IBM Watson Center - BLue Gene/L



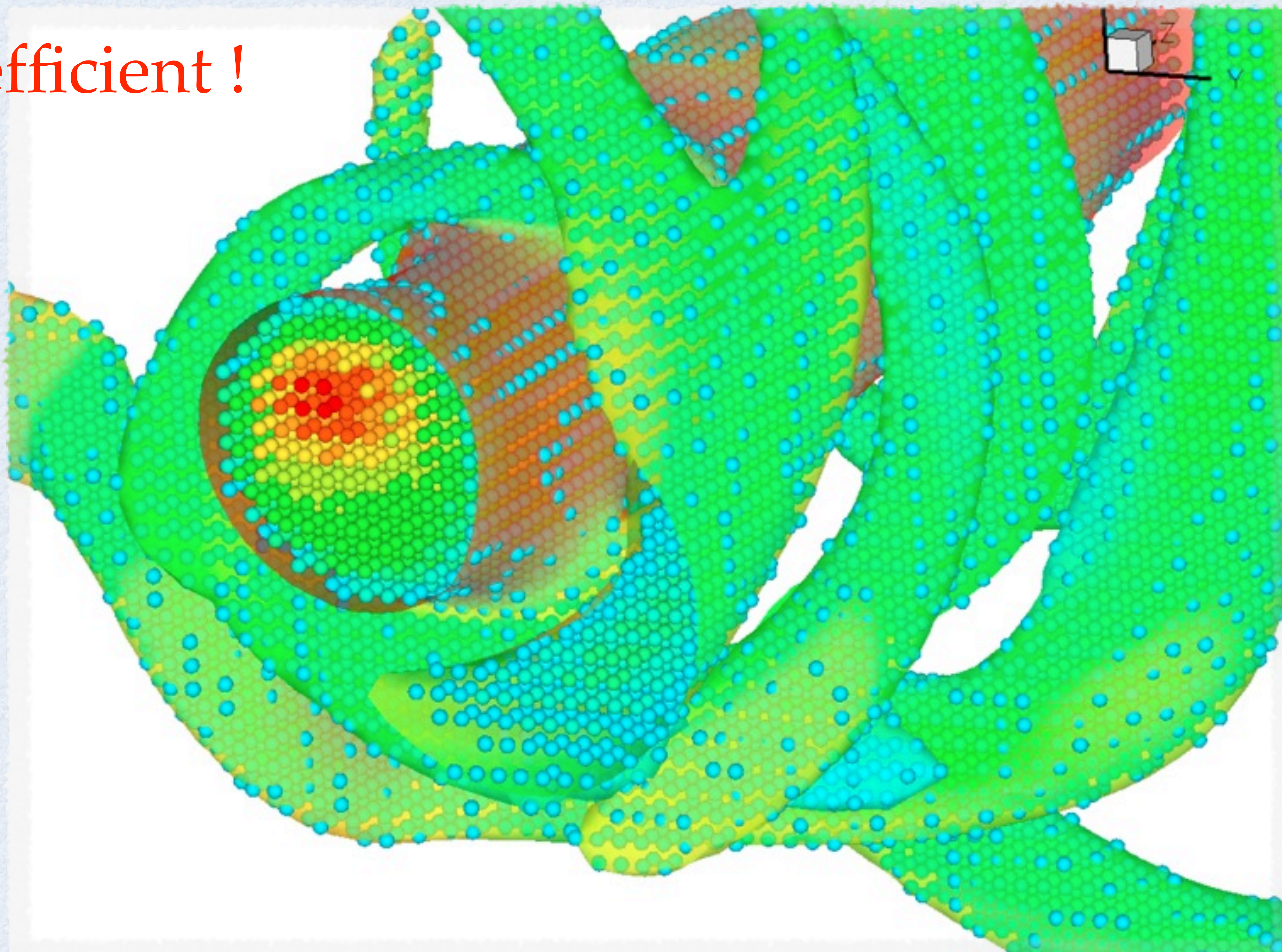
Chatelain P., Curioni A., Bergdorf M., Rossinelli D., Andreoni W., Koumoutsakos P., Billion Vortex Particle Direct Numerical Simulations of Aircraft Wakes, Computer Methods in Applied Mech. and Eng. 197/13-16, 1296-1304, 2008

PARTICLES ARE ADAPTIVE



PARTICLES ARE ADAPTIVE

yet inefficient !



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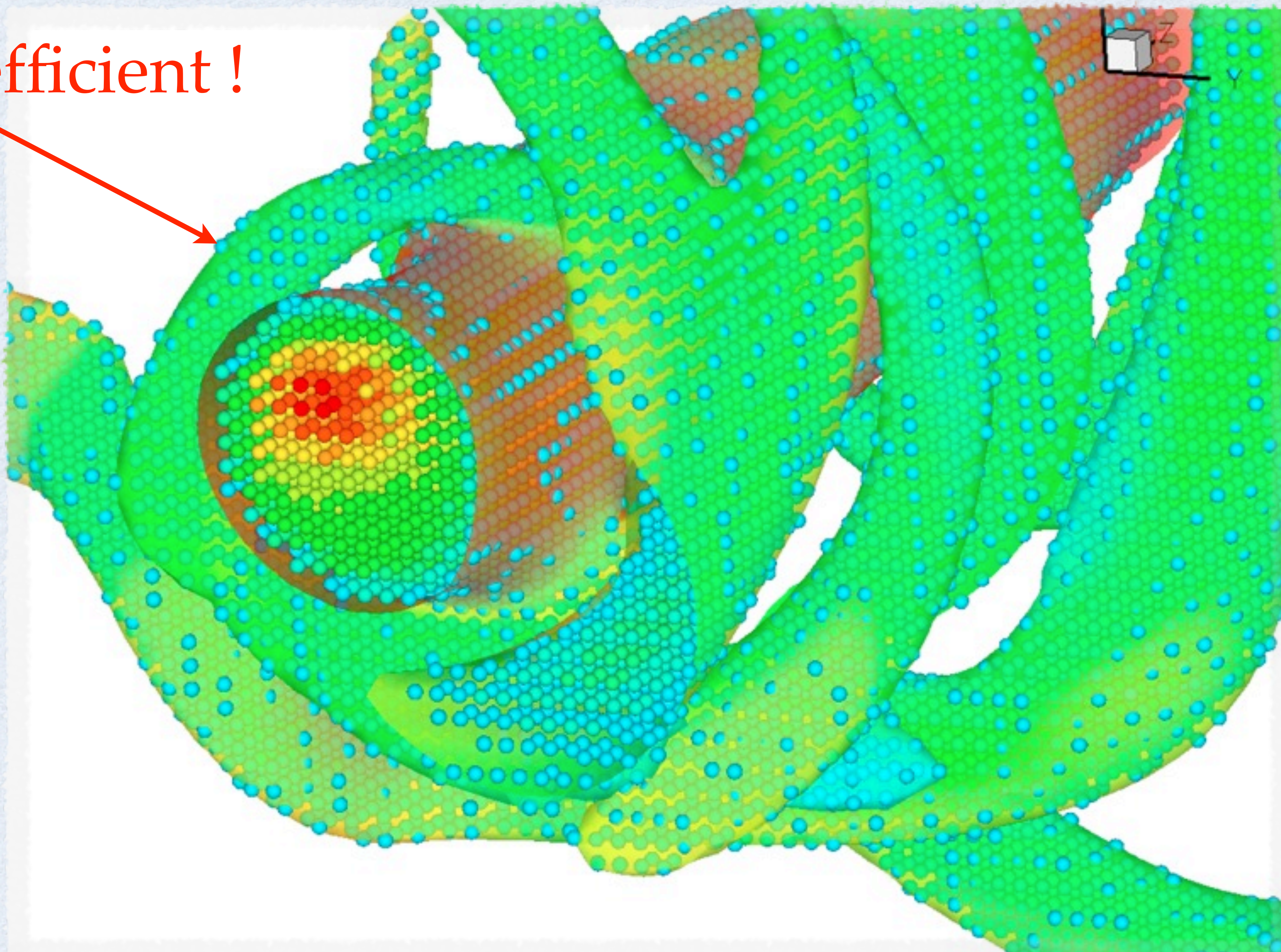
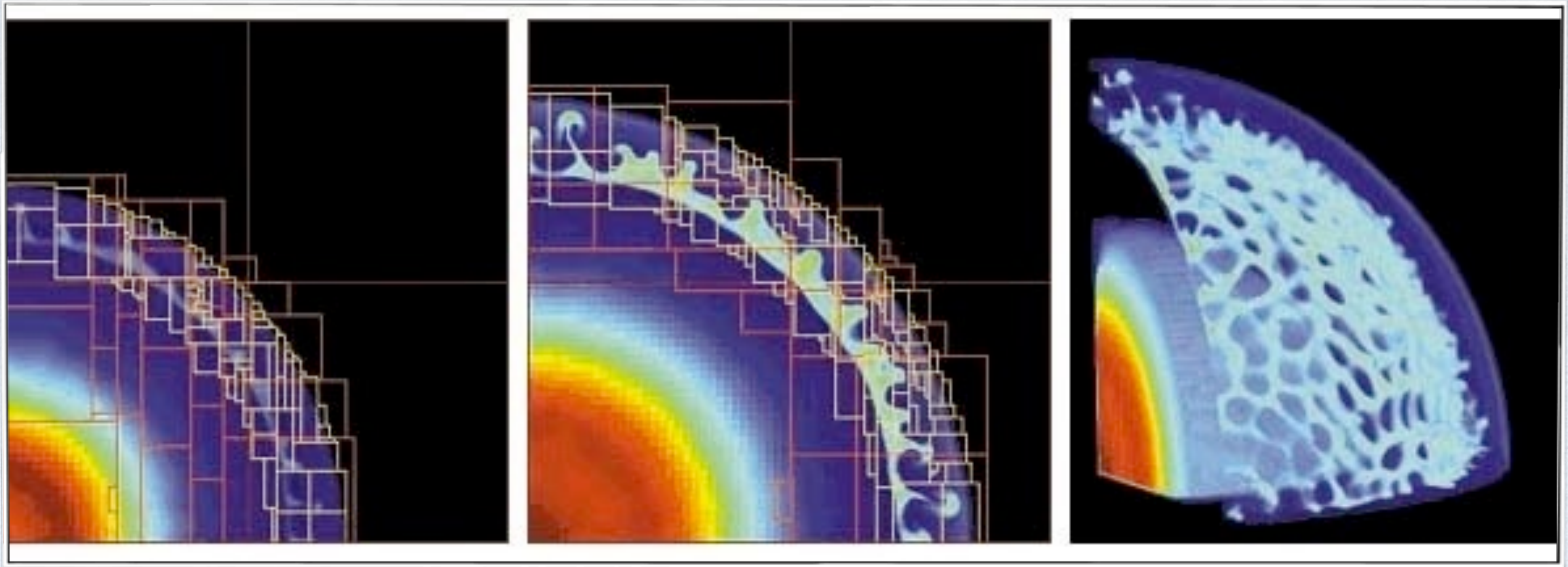


Adaptive Mesh Refinement



Berger, Colella,J. Comp. Phys., 1989

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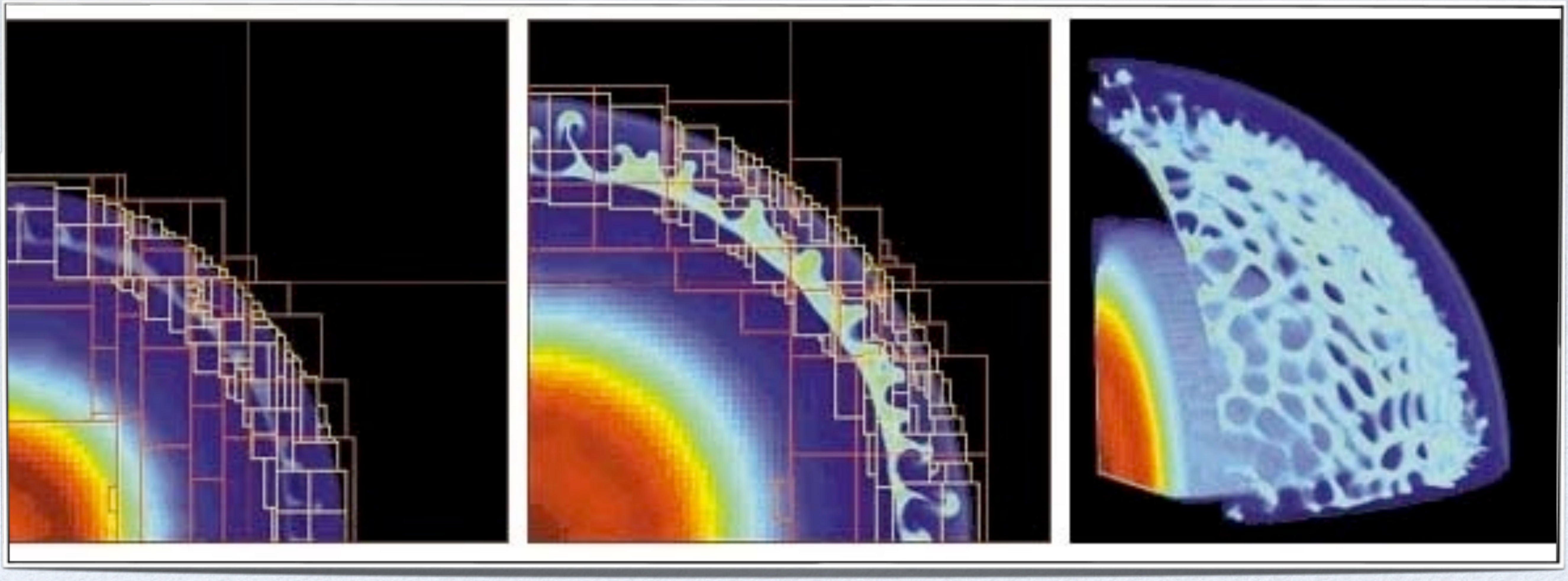
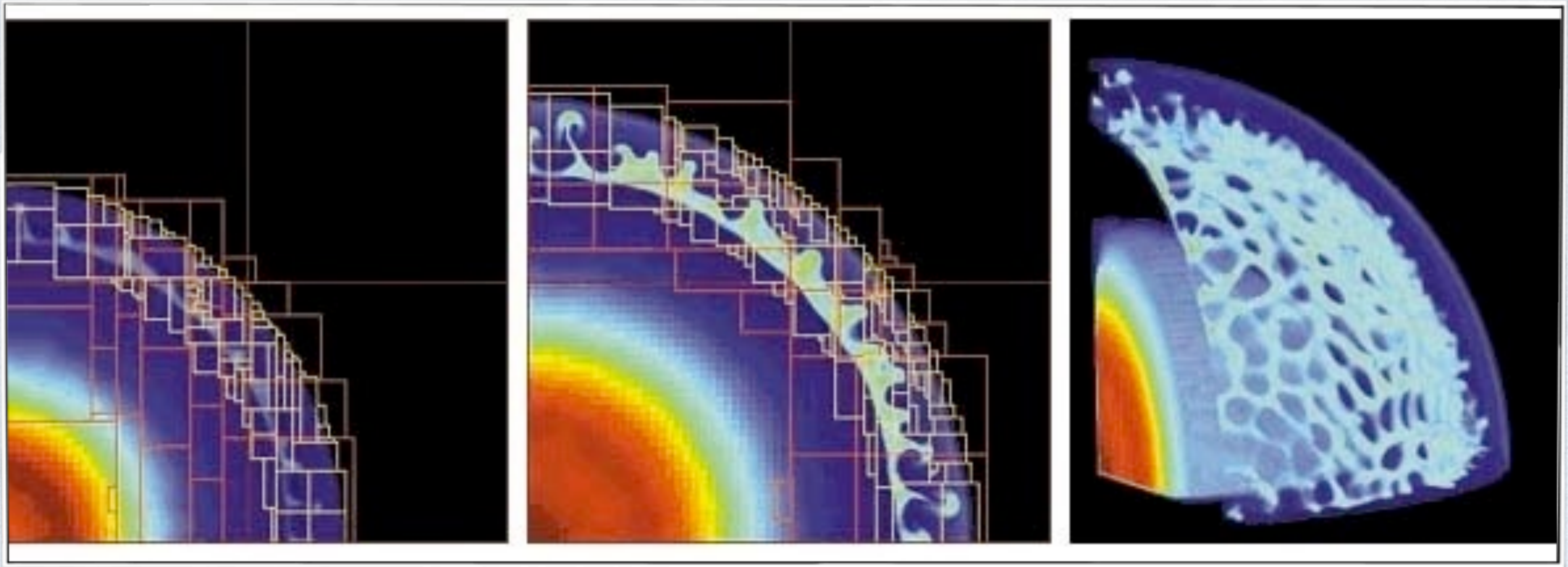


- Support of unstructured grids

Berger, Colella,J. Comp. Phys., 1989

Adaptive Mesh Refinement



- Support of unstructured grids
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Berger, Colella,J. Comp. Phys., 1989

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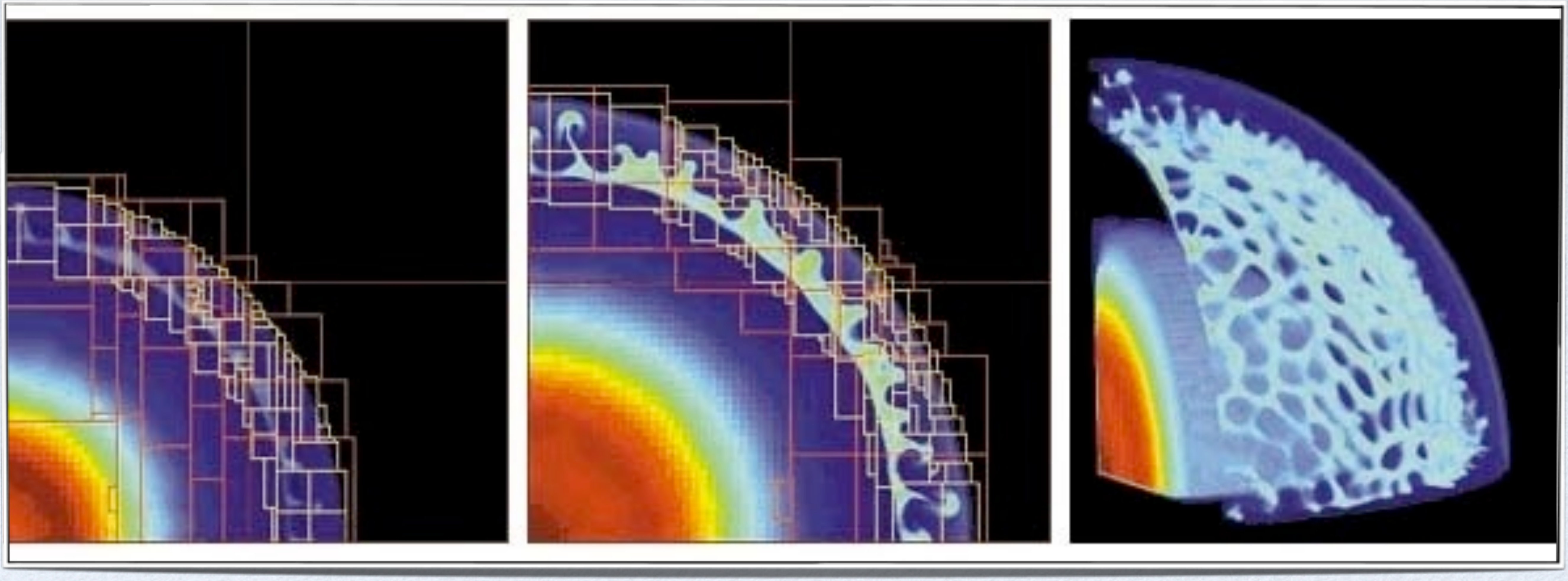

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- Low compression rate (Gradient, curvature)

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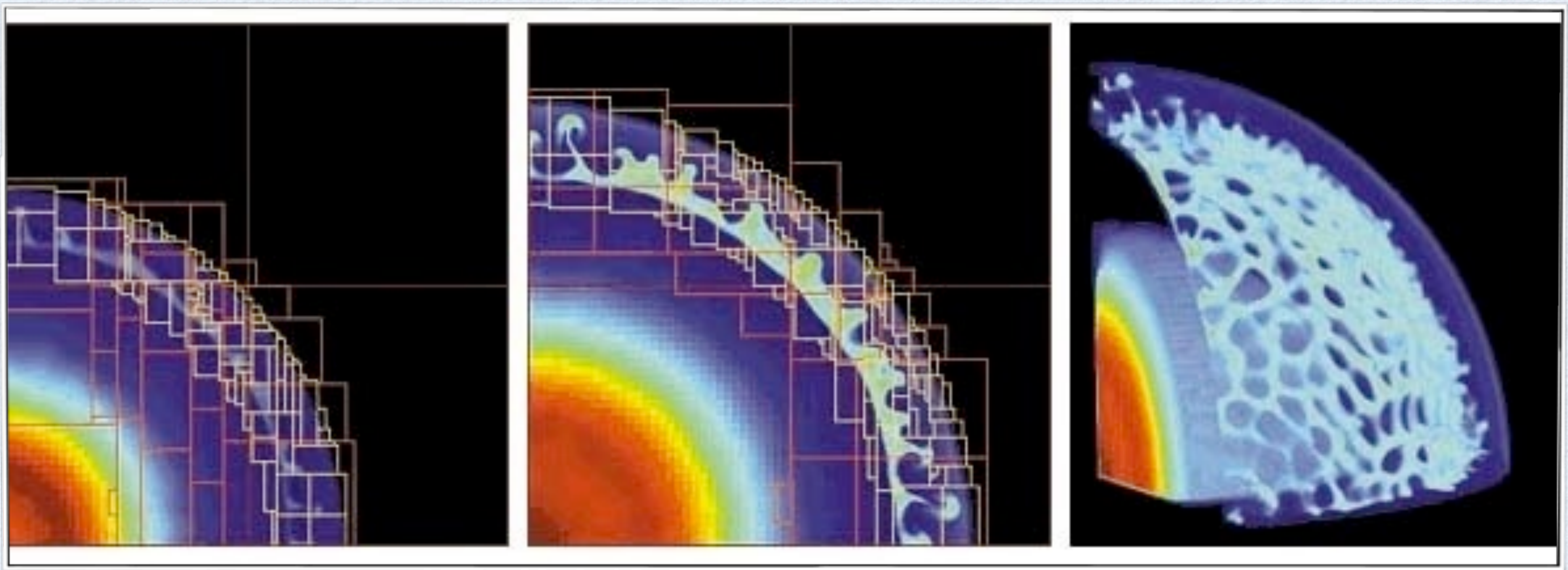


- Support of unstructured grids
- Different mesh orientations

- Low compression rate (Gradient, curvature)
- No explicit control on the compression error

Berger, Colella,J. Comp. Phys., 1989

Wavelet Compression

50:1

Multiresolution function representation:

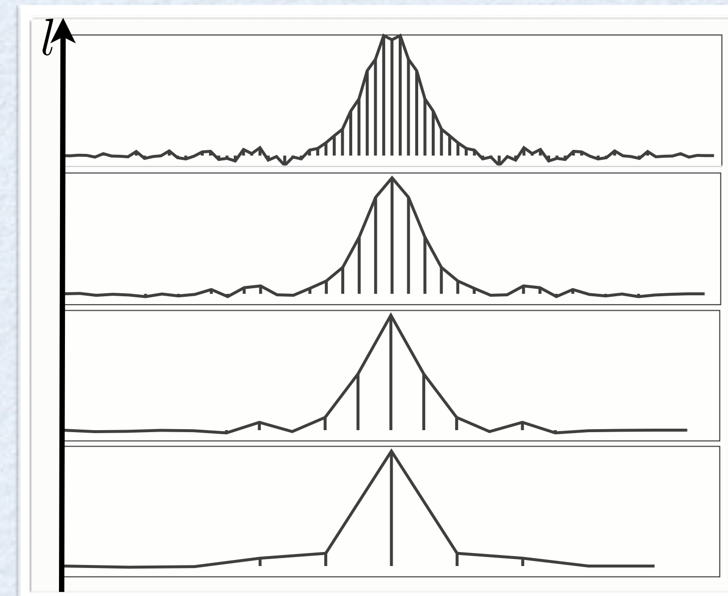
Analysis (collocation): d_k^l ~ | fine - Prediction(coarse) |

$$q^L = \sum_k c_k^0 \zeta_k^0 + \sum_{l<L} \sum_k d_k^l \psi_k^l$$

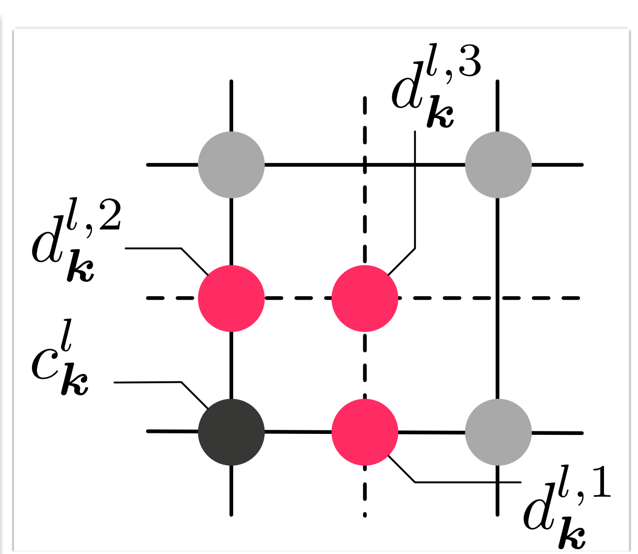
GROUND LEVEL

DETAIL COEFFICIENTS

WAVELETS



Each wavelet is associated with a specific grid point/particle (2D)



Compression / Adaptation:

Discard insignificant detail coefficients: $|d_{\boldsymbol{k}}^{l,m}| < \varepsilon$

Compressed function representation:

$\|q^L - q_{\geq}^L\| < \varepsilon$ → Adapted grid

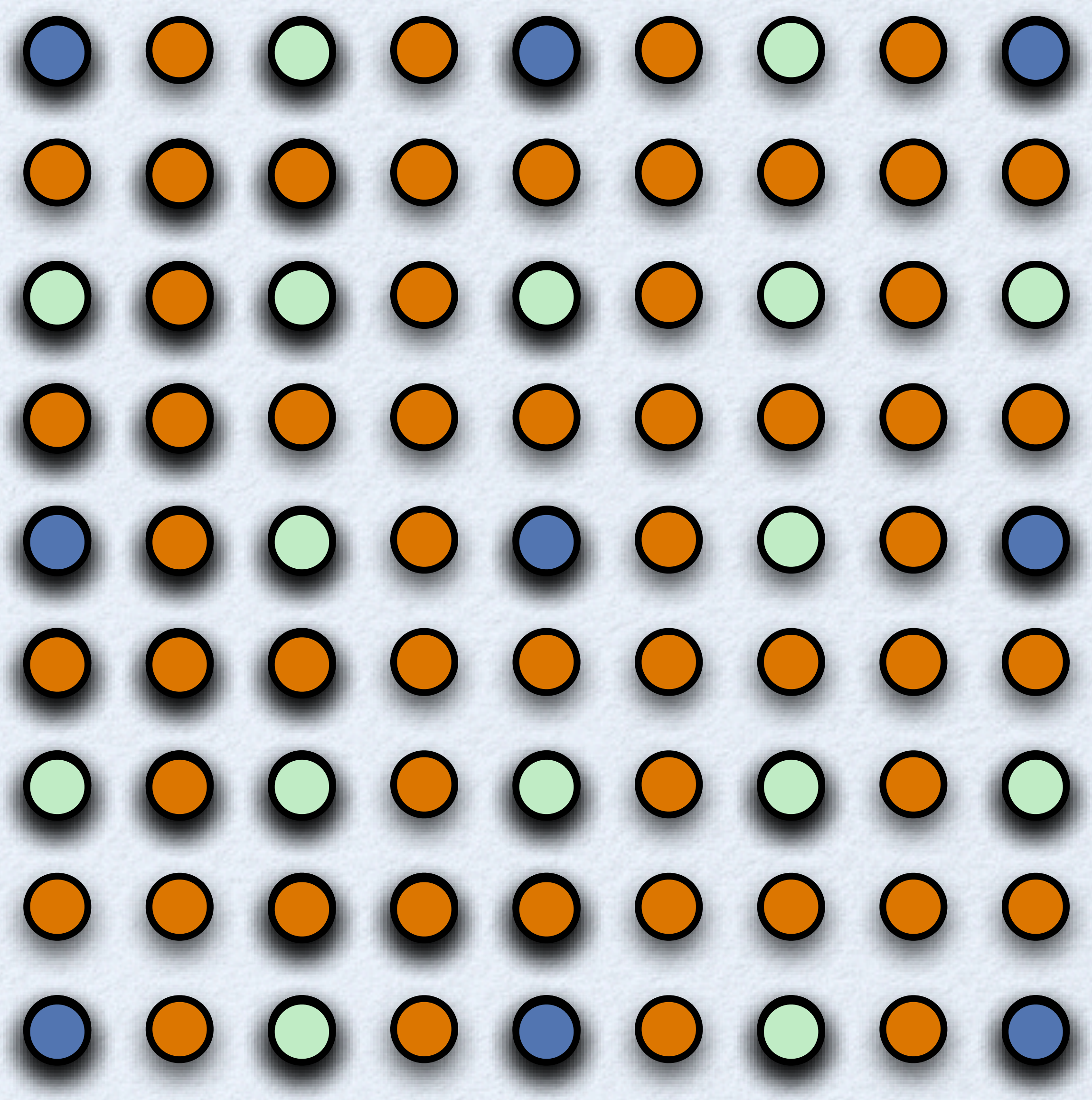
PARTICLETS : REMESHED PARTICLES + WAVELETS

$$q^L = \sum_k c_k^0 \, \zeta_k^0 + \sum_{l<L} \sum_k d_k^l \, \psi_k^l$$

"ground" level

detail coefficients

wavelets



```
1.Remesh
2.Wavelets- Compress/Adapt
3.Convect
4.Wavelets Reconstruct
5.GOTO 1
```

M. Bergdorf, P. Koumoutsakos. A Lagrangian Particle-Wavelet Method, Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, 5(3), 980-995, 2006

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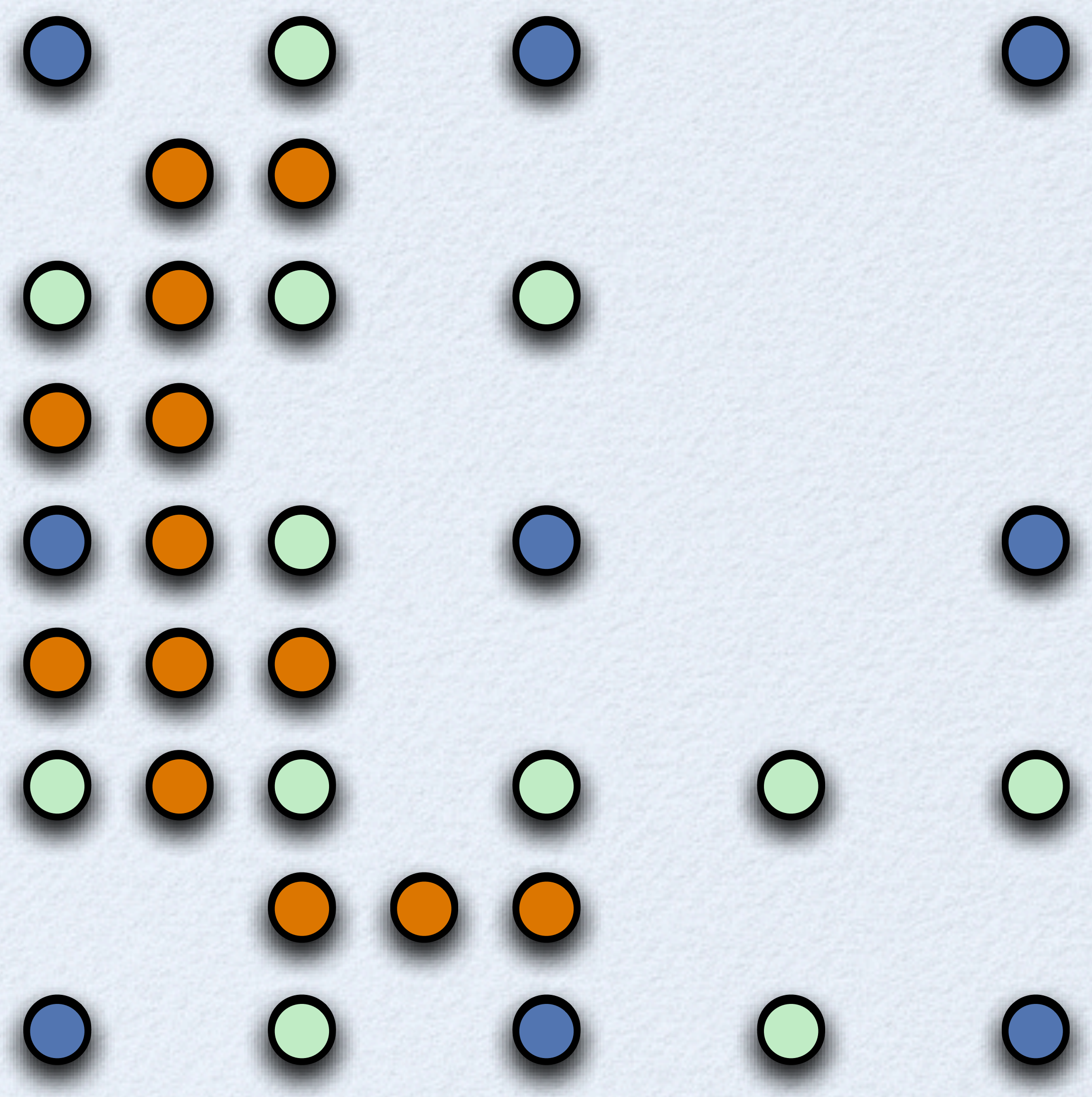

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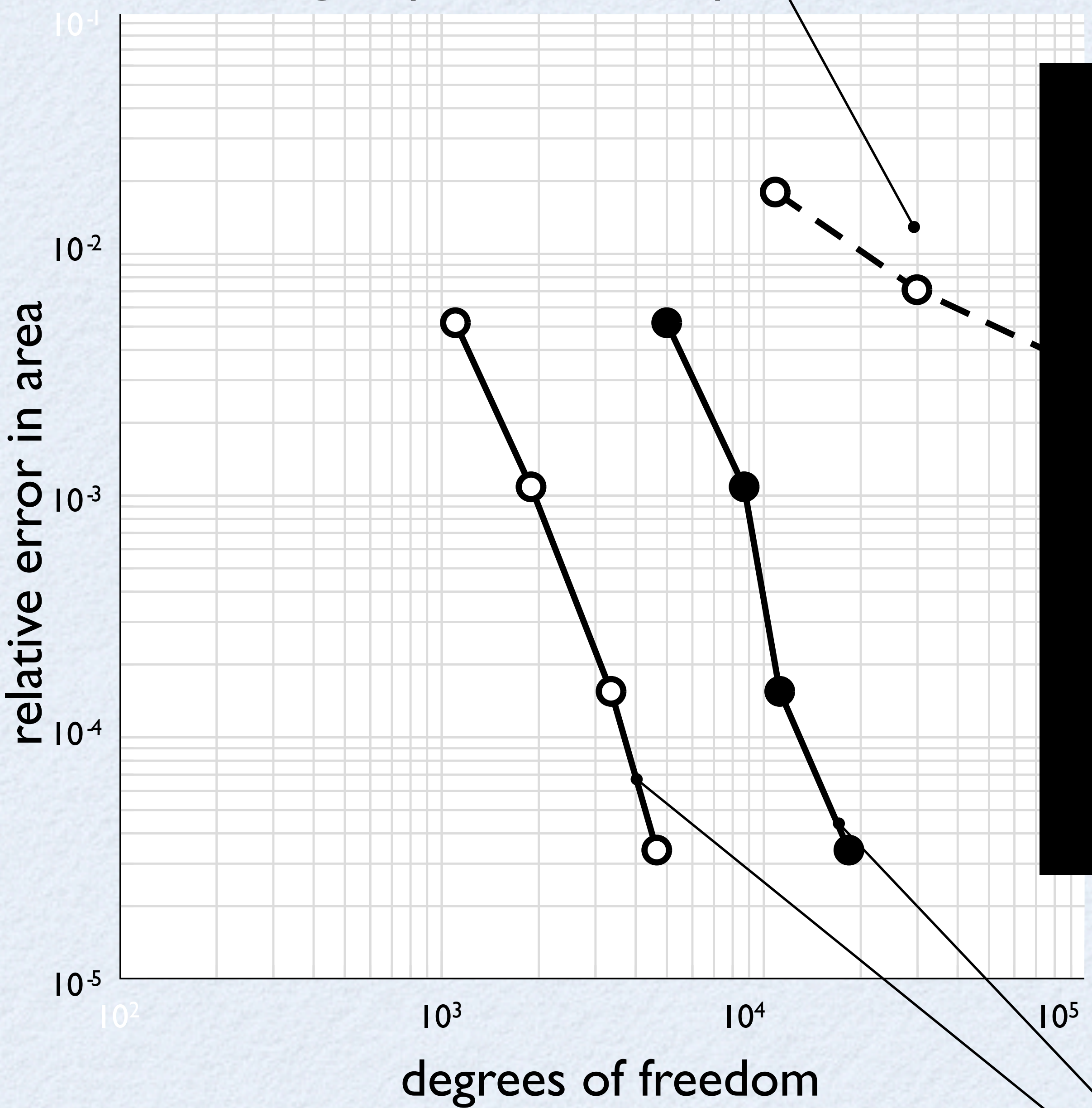
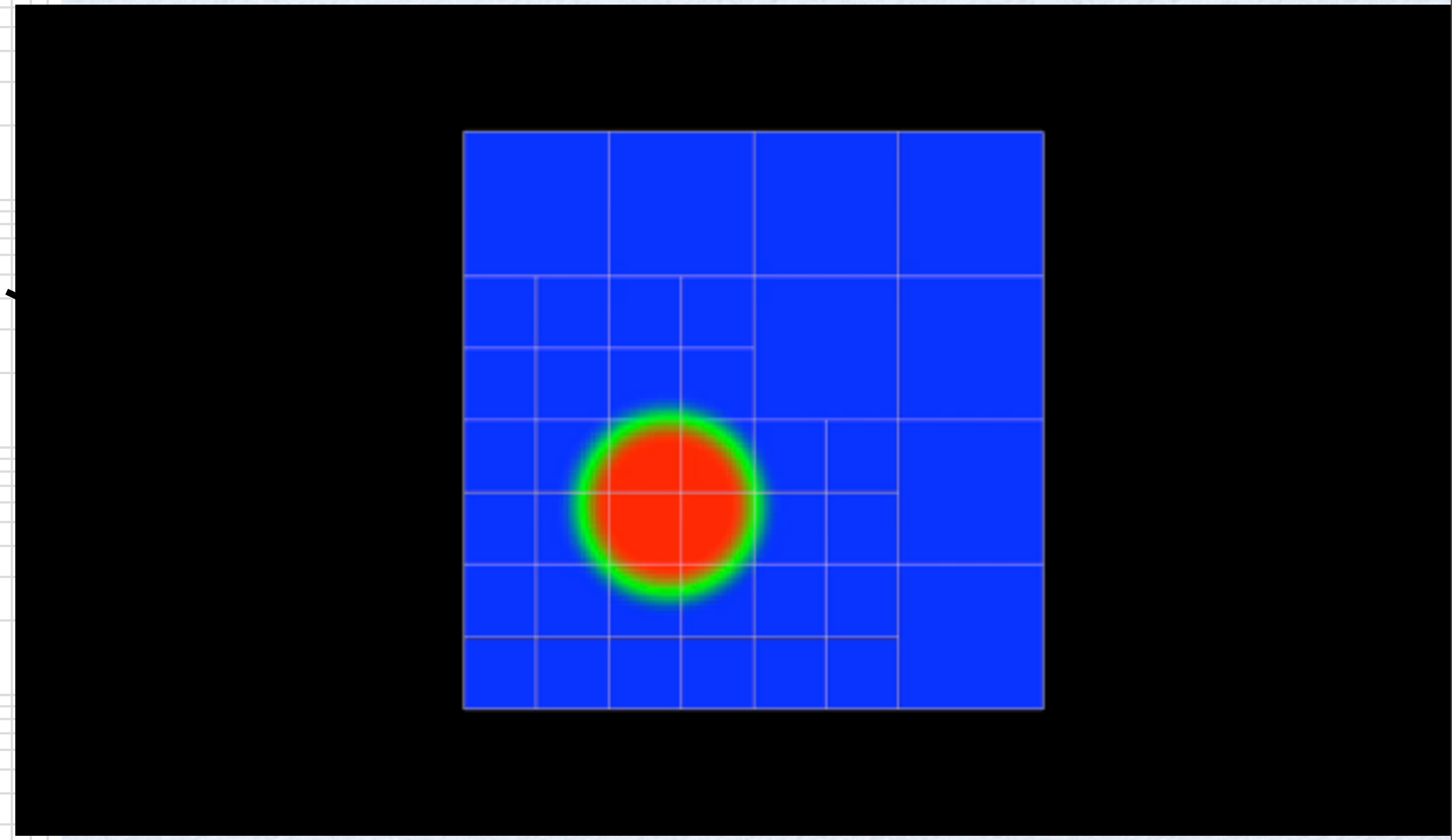
M. Bergdorf, P. Koumoutsakos. A Lagrangian Particle-Wavelet Method, Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, 5(3), 980-995, 2006

MULTIRESOLUTION LEVEL SETS

M. Bergdorf, P. Koumoutsakos. A Lagrangian Particle-Wavelet Method, Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, 5(3), 980-995, 2006

Enright, Fedkiw et al, 2002
dof = # grid points + aux. particles at t=0.0





Present Method
dof = # active gp/particles at t=0.0
dof = # active gp/particles at final time

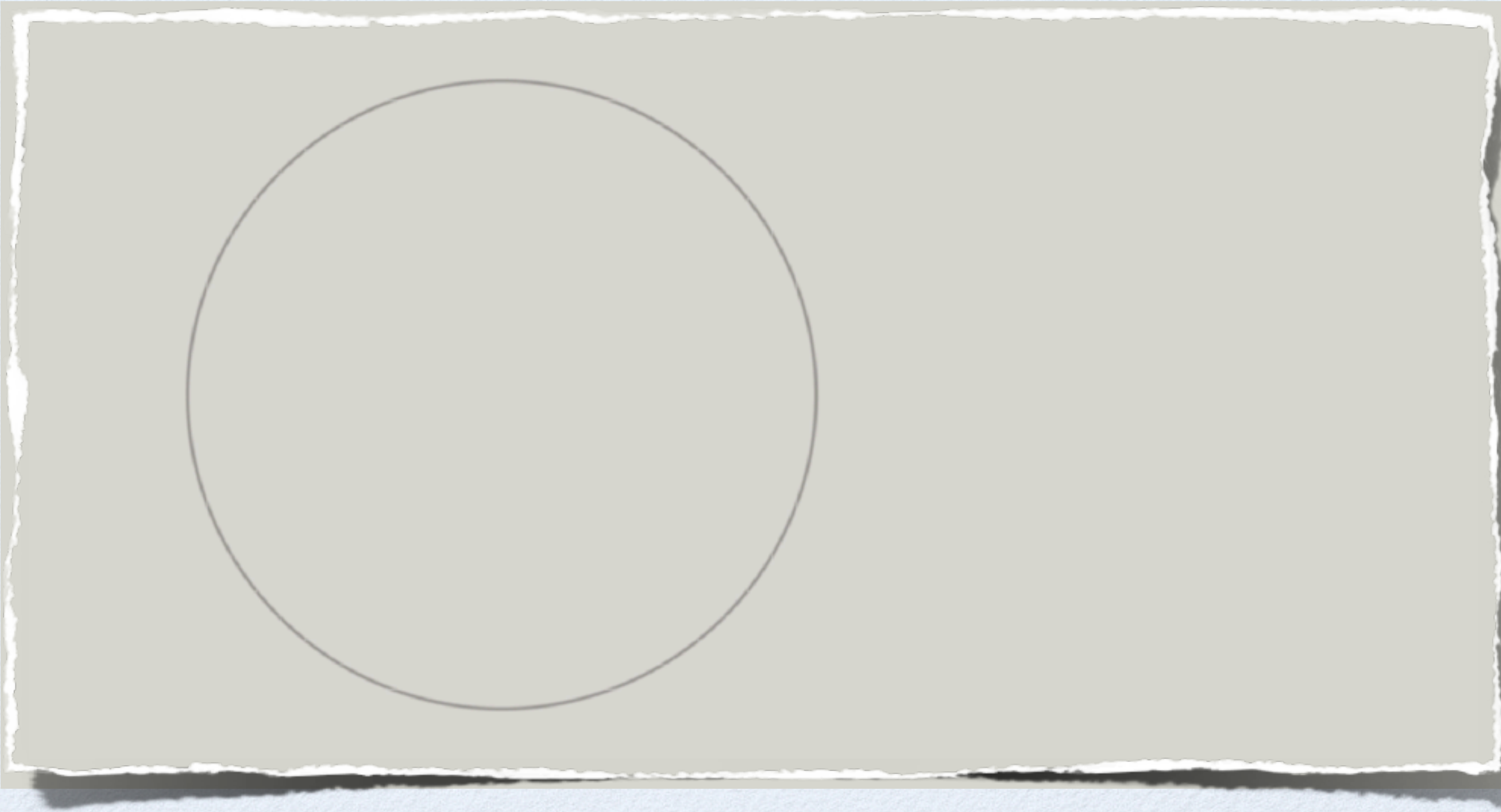
$CFL_{max} \sim 40$

Shock Bubble Interaction

(M=3, At=0.8)

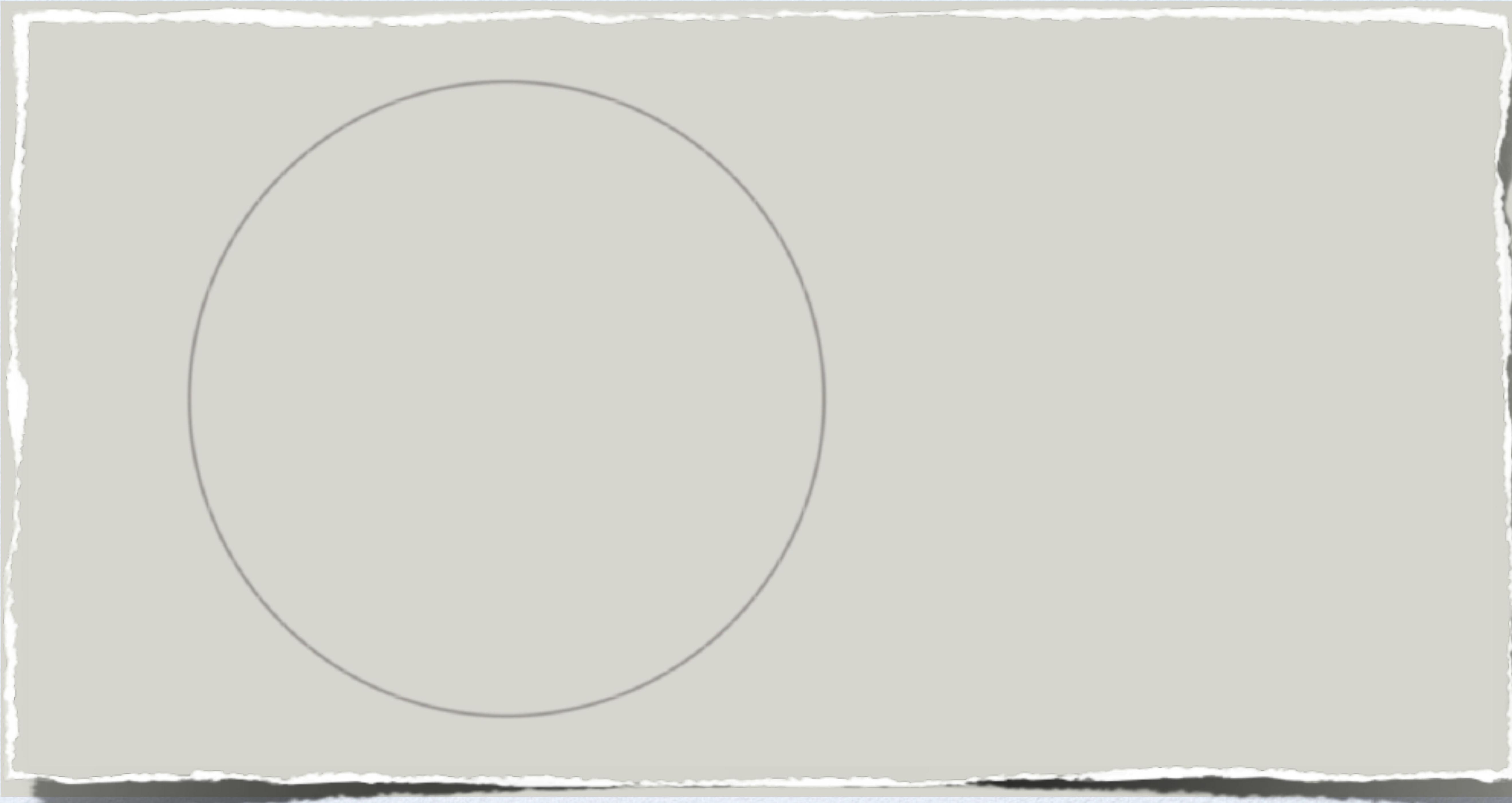
Shock Bubble Interaction

(M=3, At=0.8)



Shock Bubble Interaction

(M=3, At=0.8)



FINEST RESOLUTION EQUIVALENT : 8000 x 8000 uniform grid

~40 times smaller adaptive grid

BOUNDARIES + ALGORITHMS

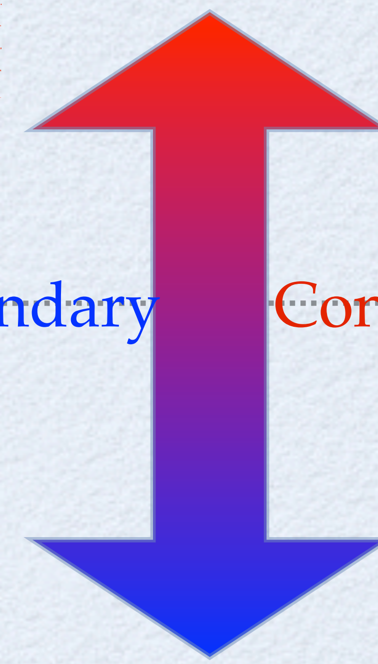
COUPLING AND BOUNDARY CONDITIONS

Atomistic:

Molecular Dynamics

$$m\frac{d^2r}{dt^2} = F$$

+ Fc



Boundary Conditions

+ Fa

m : mass **r** : position **F** : force

Continuum:

Navier- Stokes Eqs.

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho}\nabla P + \nu\nabla^2\mathbf{u}$$

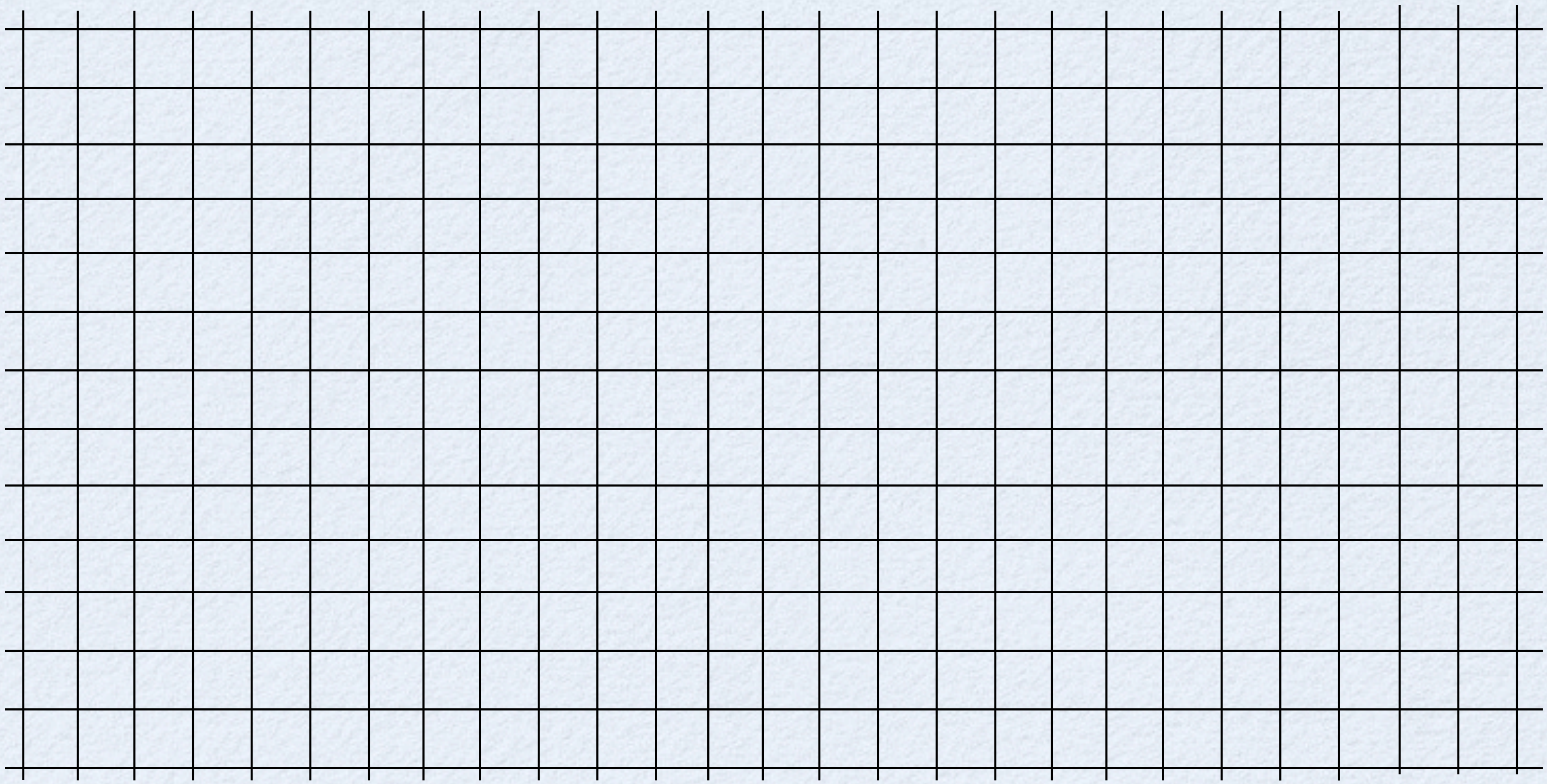
$$\frac{D\rho}{Dt} = \rho\nabla\cdot\mathbf{u}$$

u : velocity, **P** : pressure, ρ : density, ν : viscocity

Boundary Conditions = Coupling

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + f (\text{enforces b.c.})$$

Boundary Conditions = Coupling



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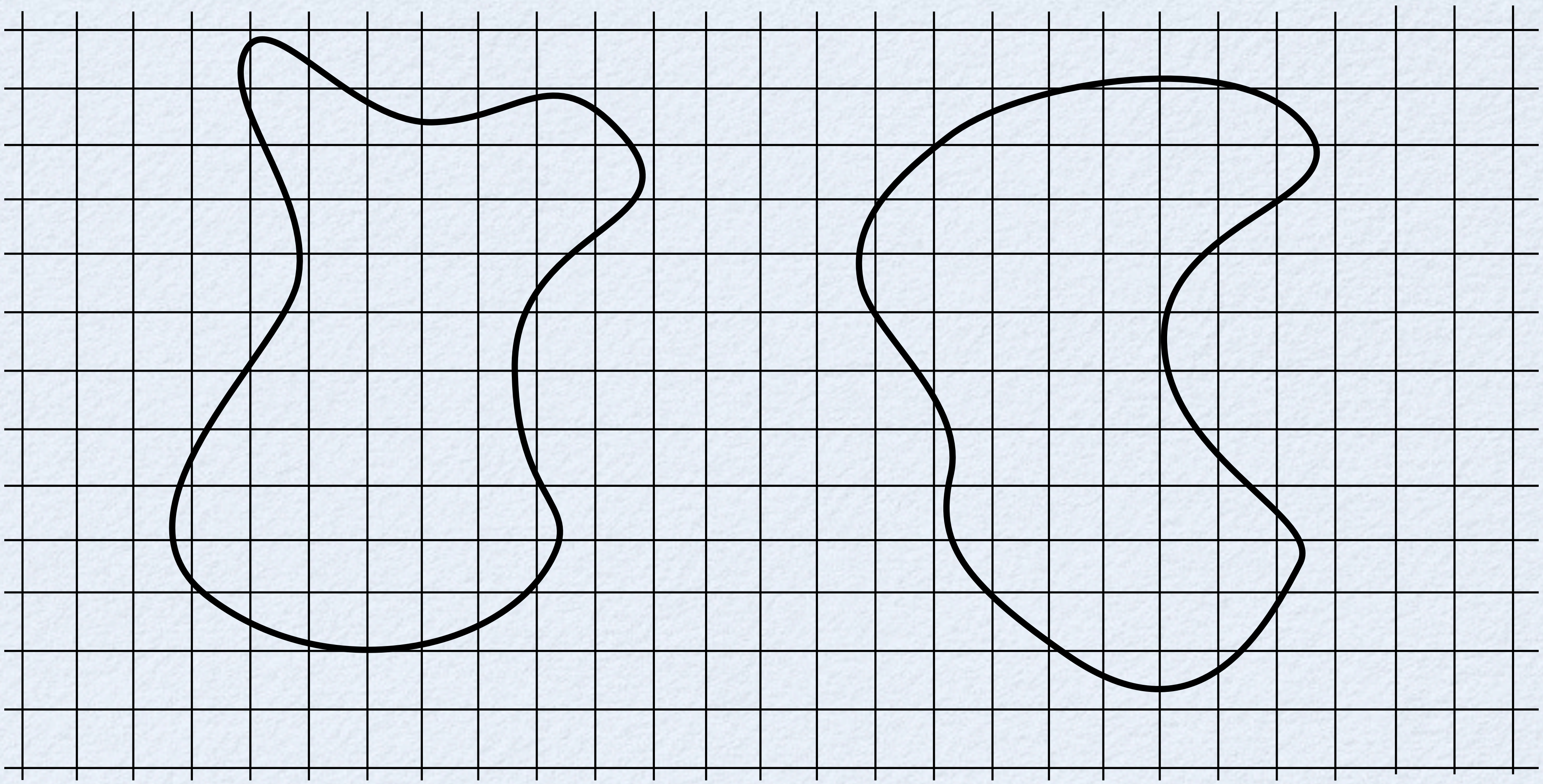

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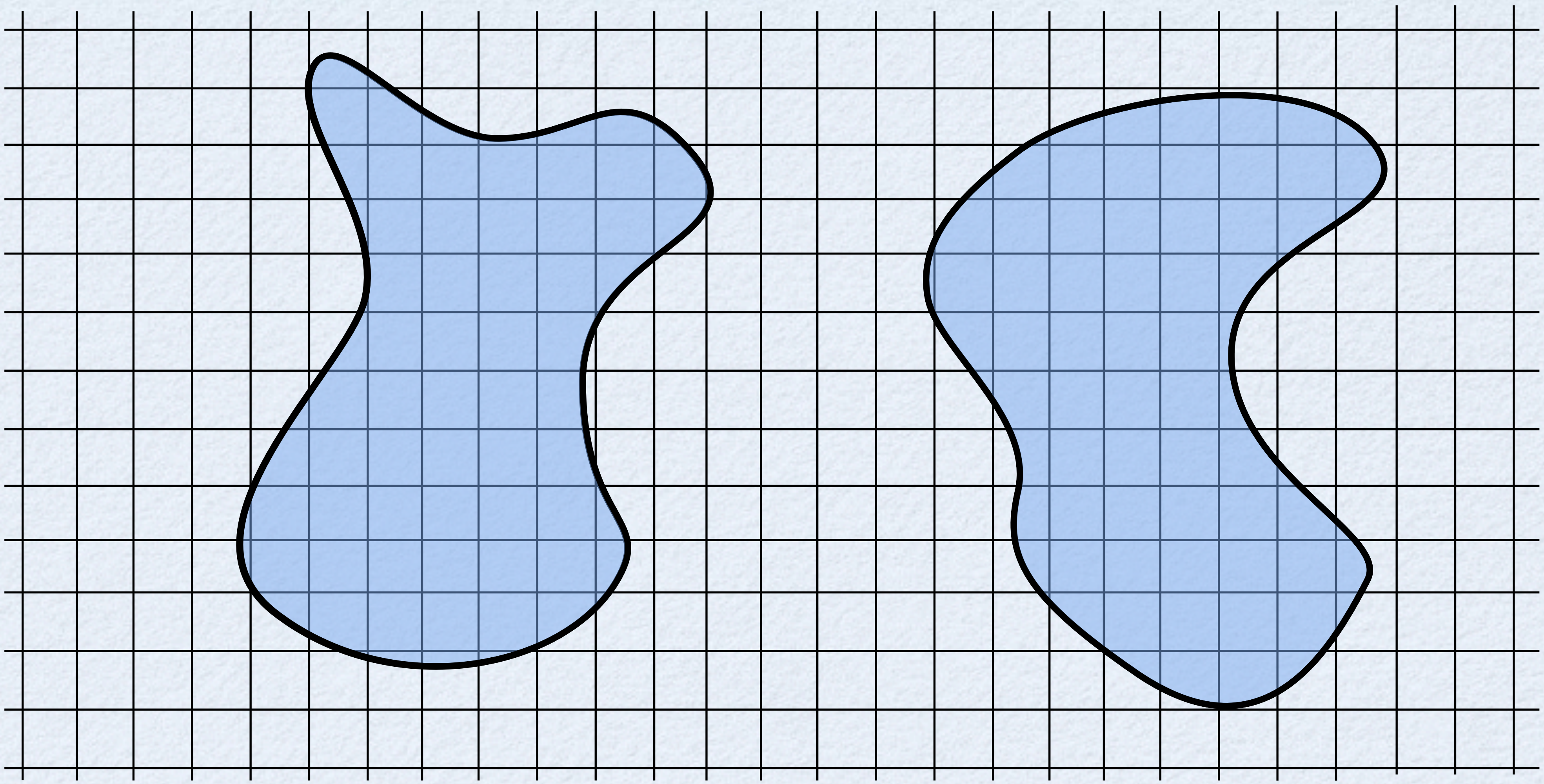
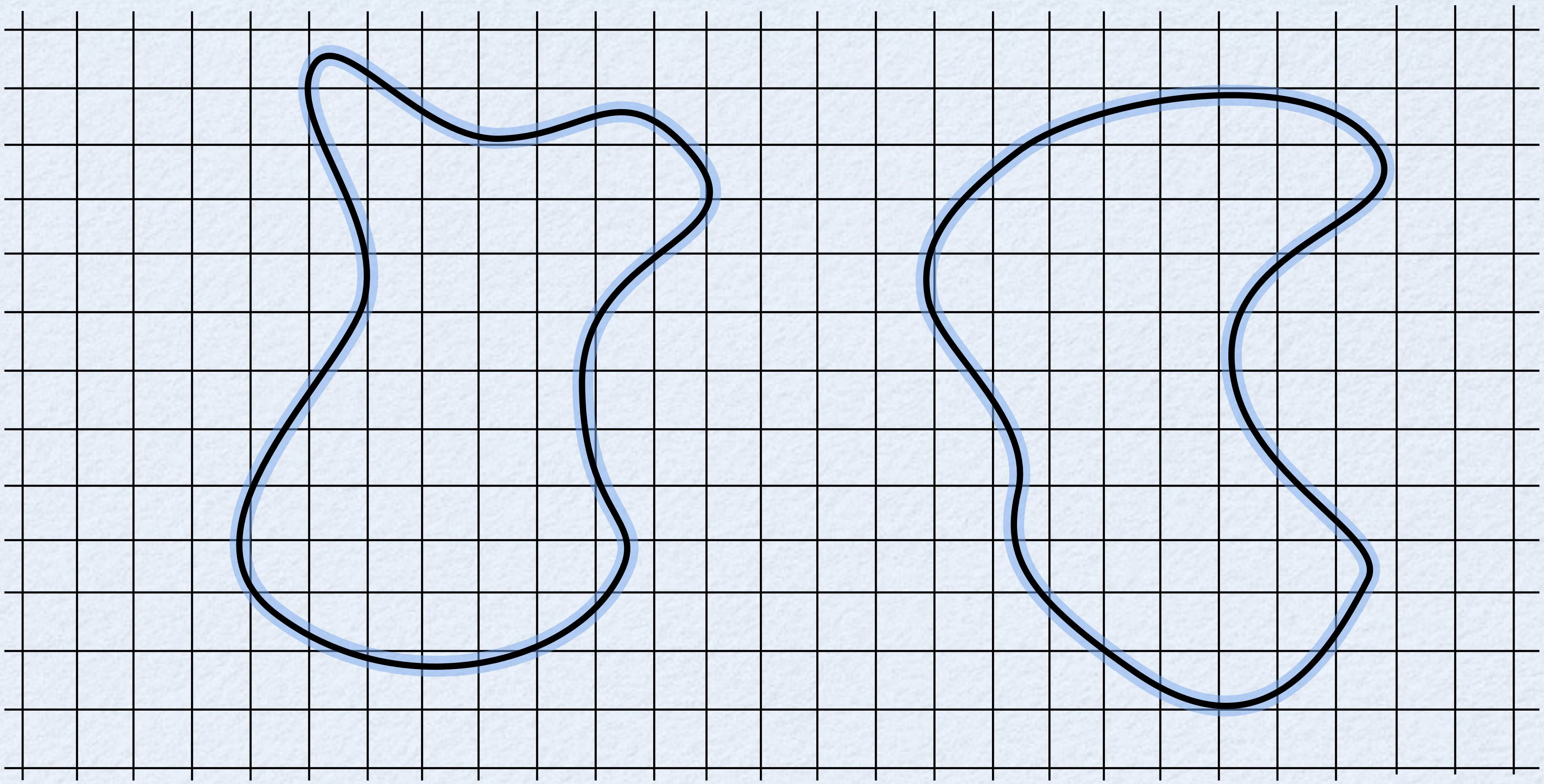


$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} \; + f(\text{enforces b.c.})$$

Penalization Method: $f(\mathbf{x}) = \lambda \chi_S (\mathbf{u}_S - \mathbf{u})$

Boundary Conditions = Coupling



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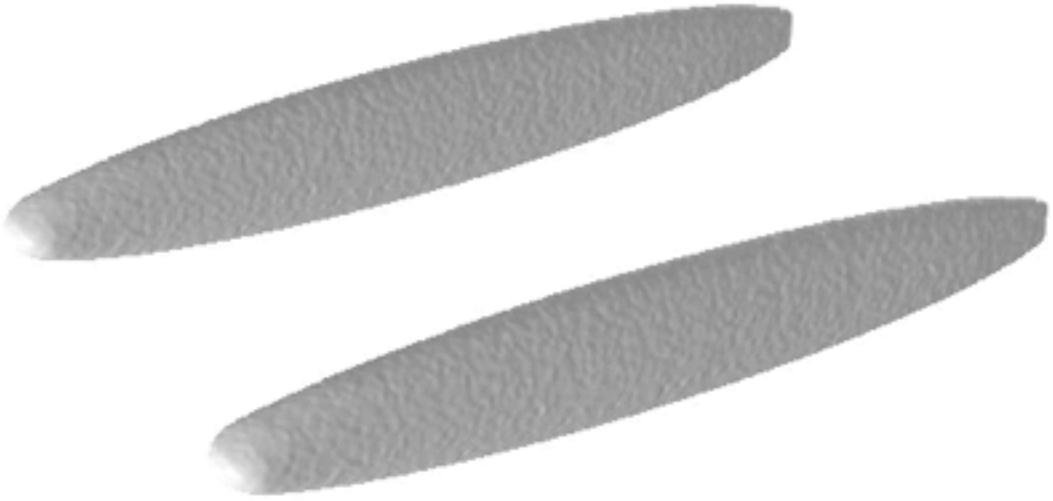
P. Angot, C. H. Bruneau, and P. Fabrie,, Numer. Math. , 1999

Immersed Boundary: $f(\mathbf{x}) = \kappa \delta_S (\mathbf{x}_S - \mathbf{x})$

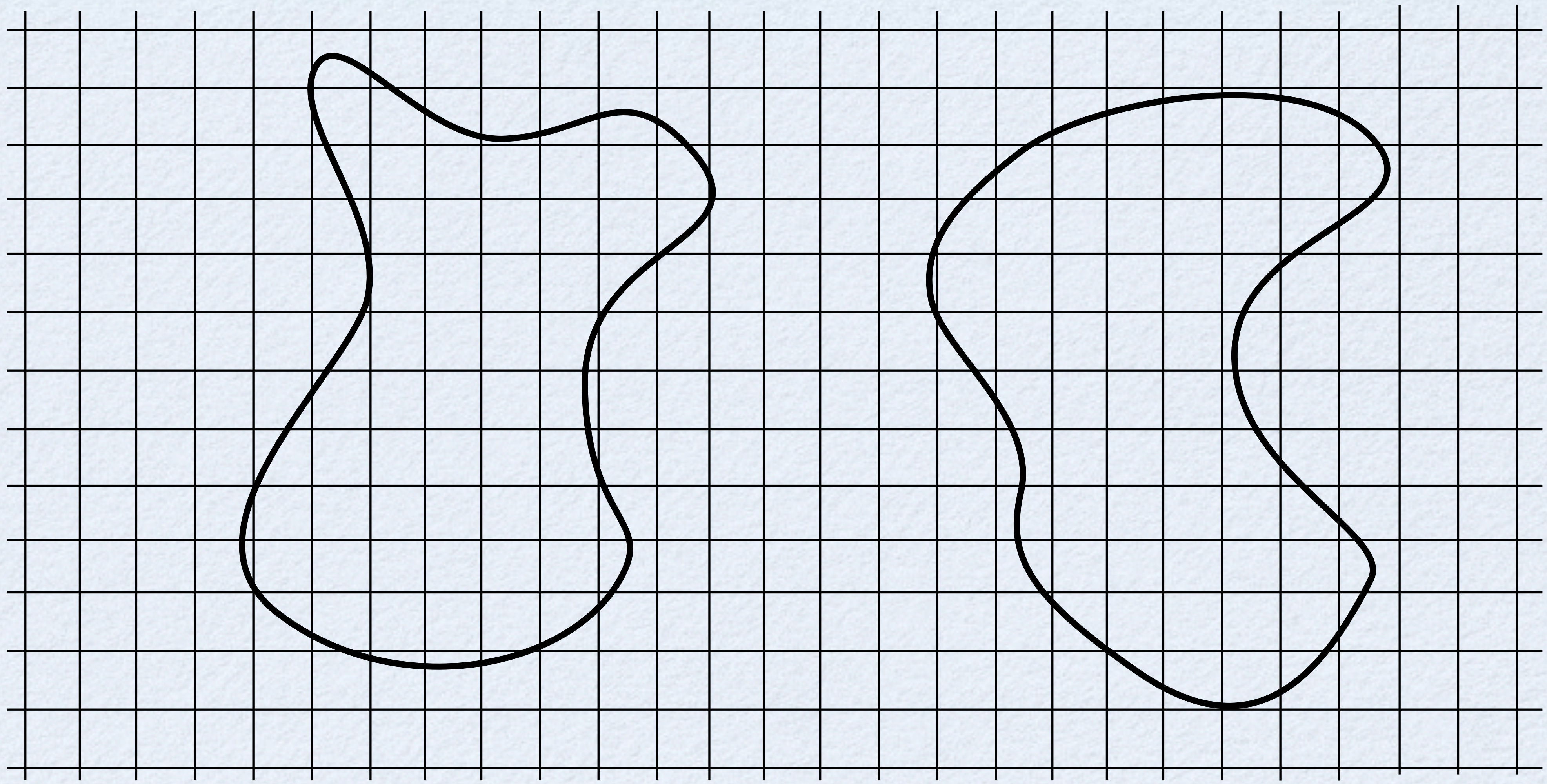
C.S. Peskin, J. Comput. Phys., (1977)

FISH SCHOOLING



2 FISH (OBVIOUSLY)

Boundary Conditions = Coupling



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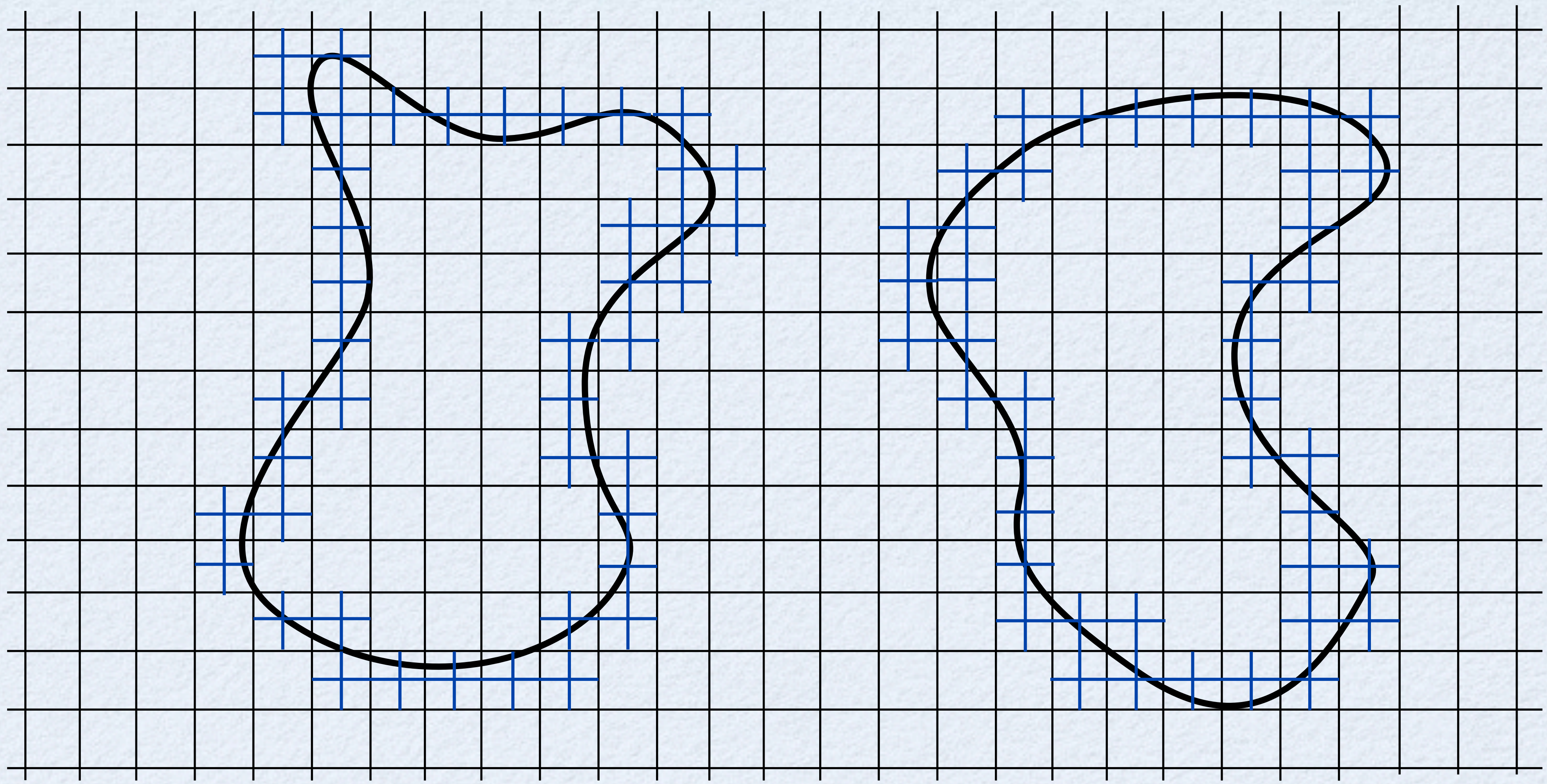

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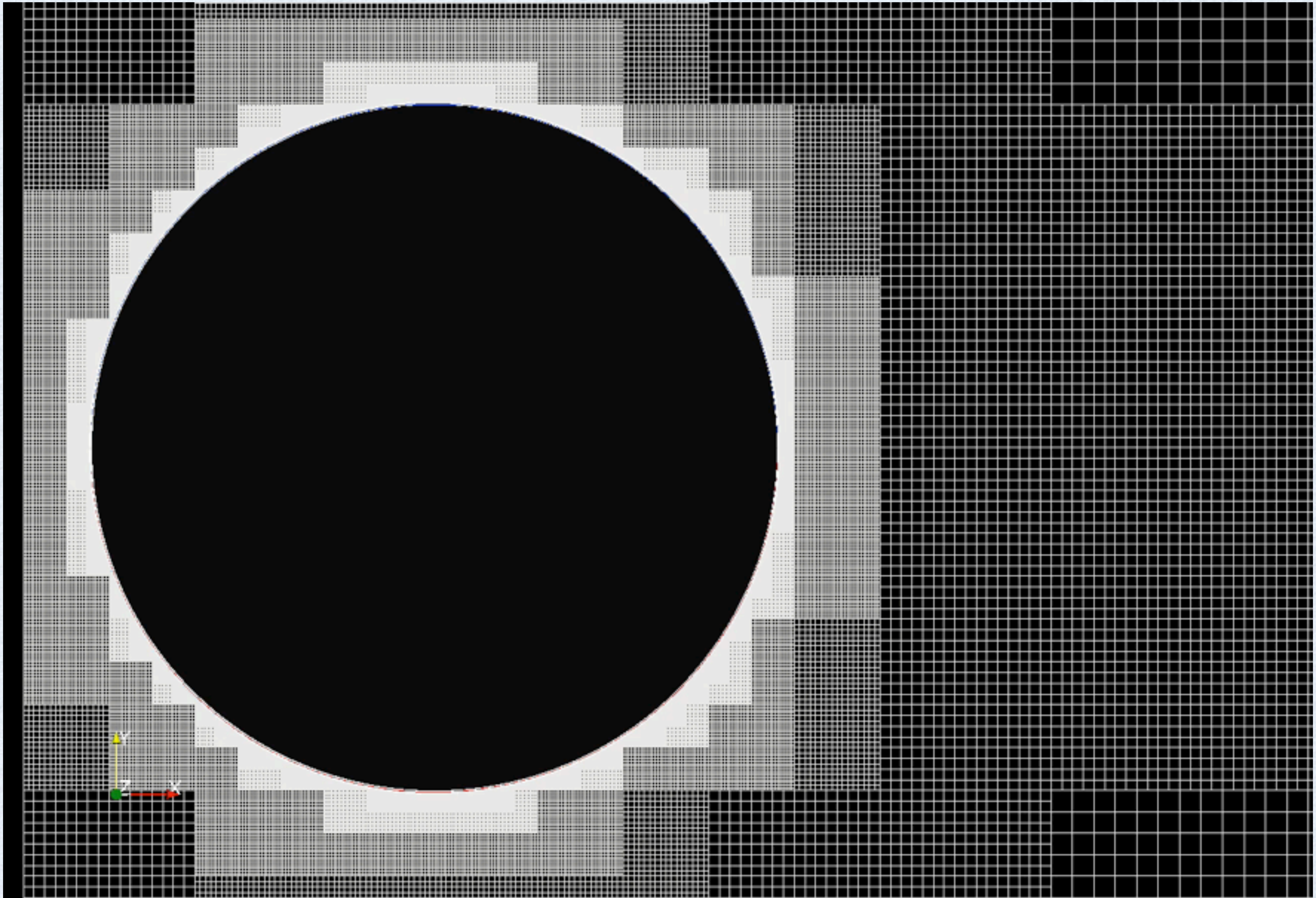
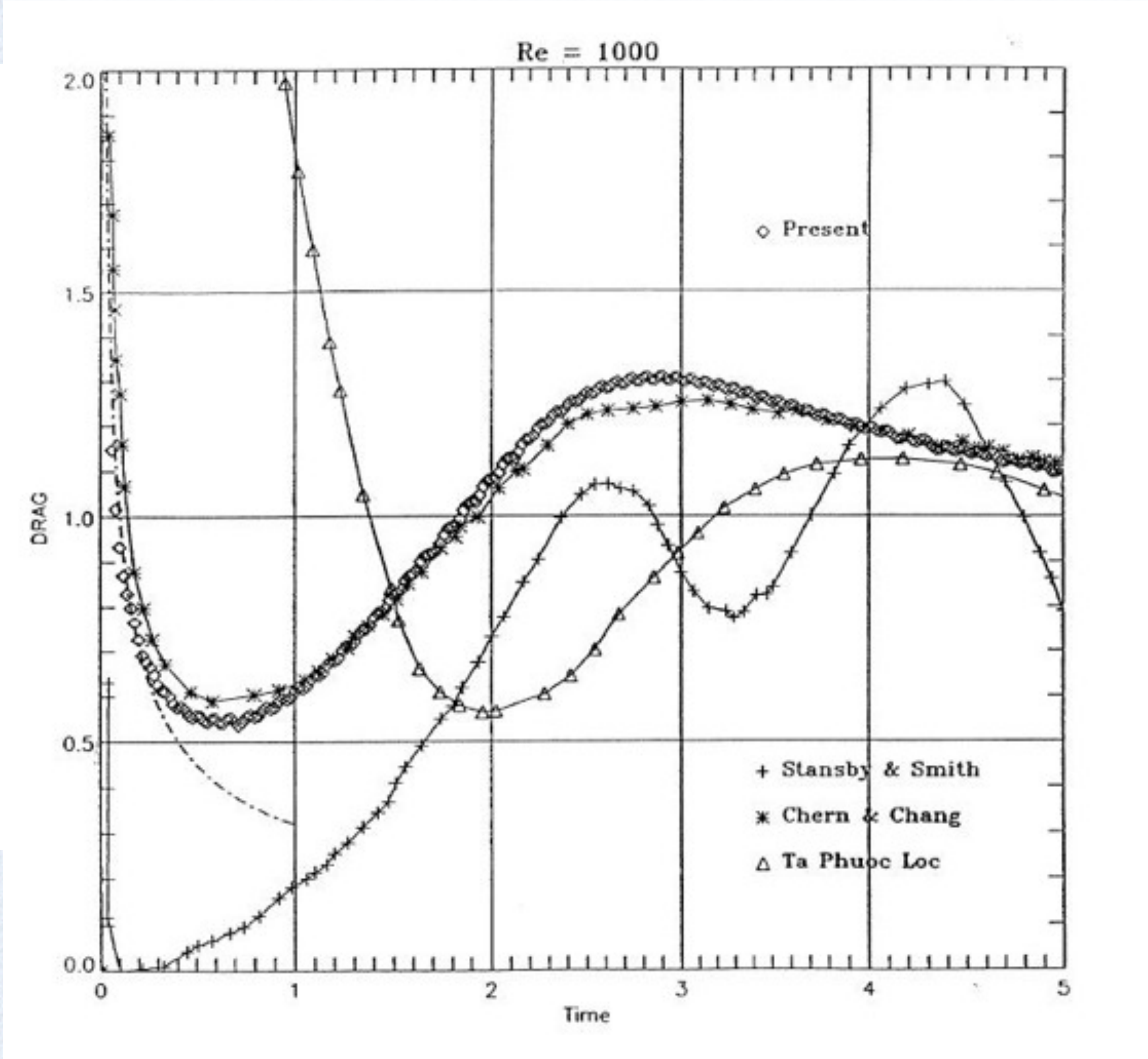
Re 9500 : Multiresolution + Multicores + (multi)GPUs



Benchmark : The Impulsively Started Cylinder



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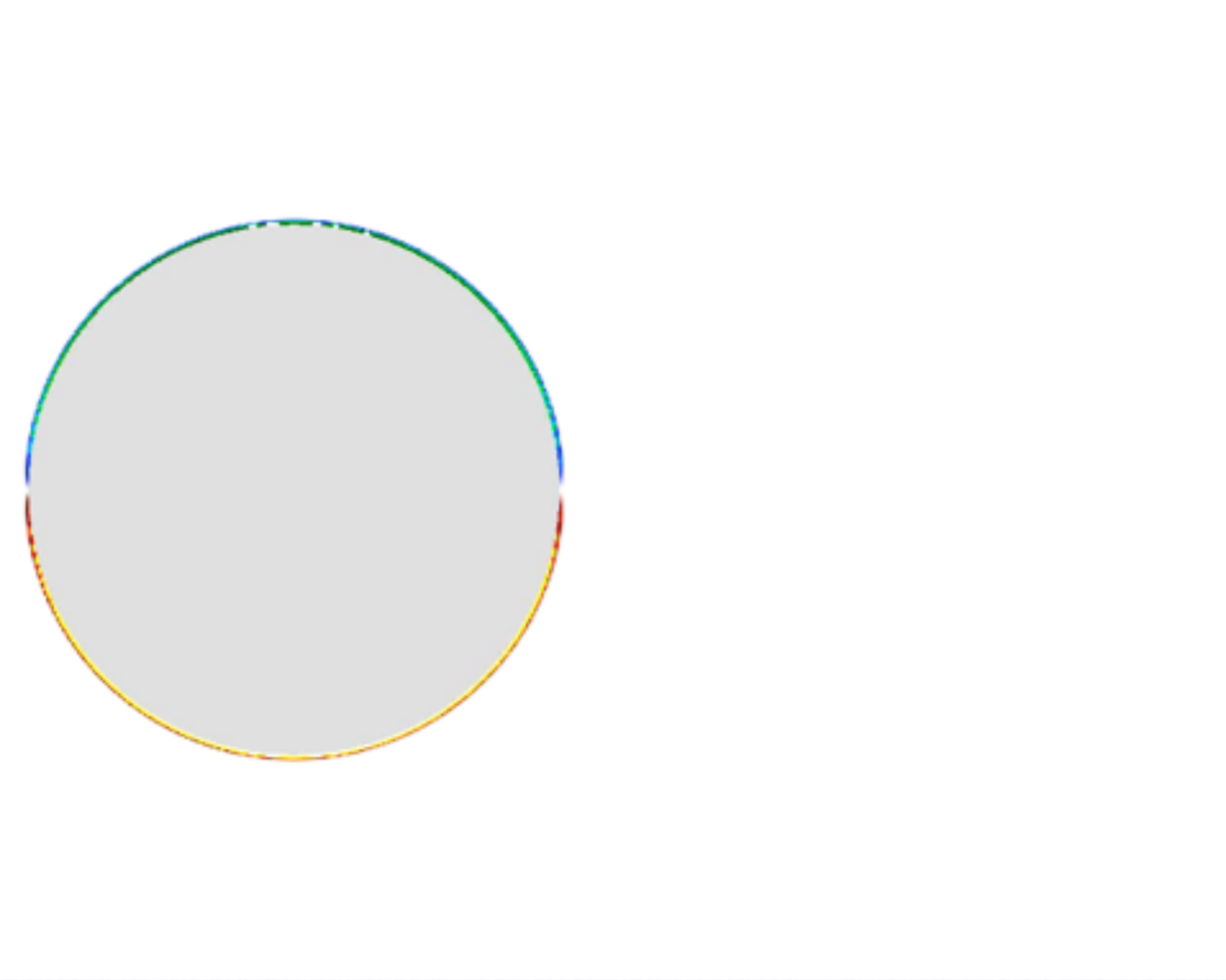
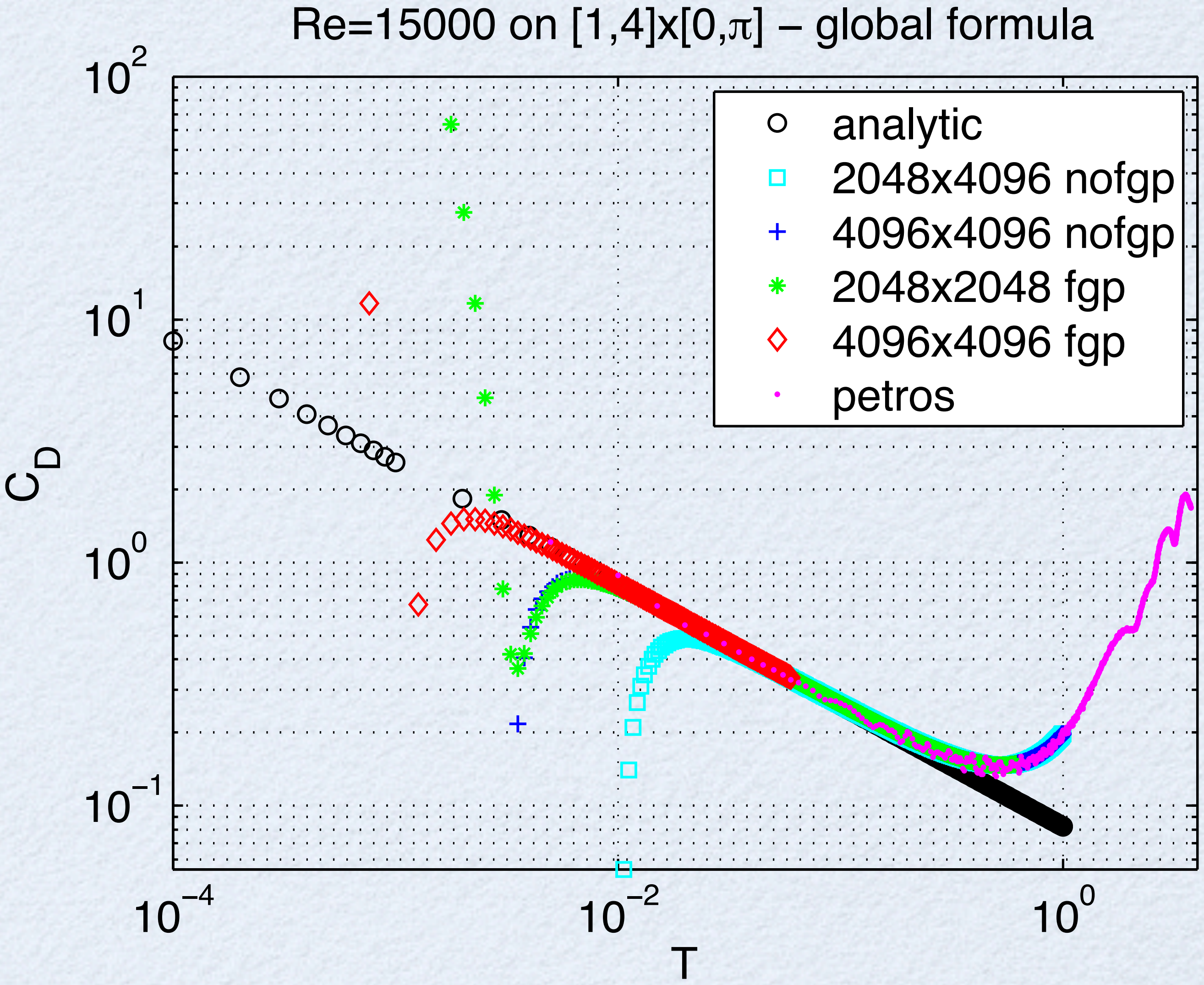
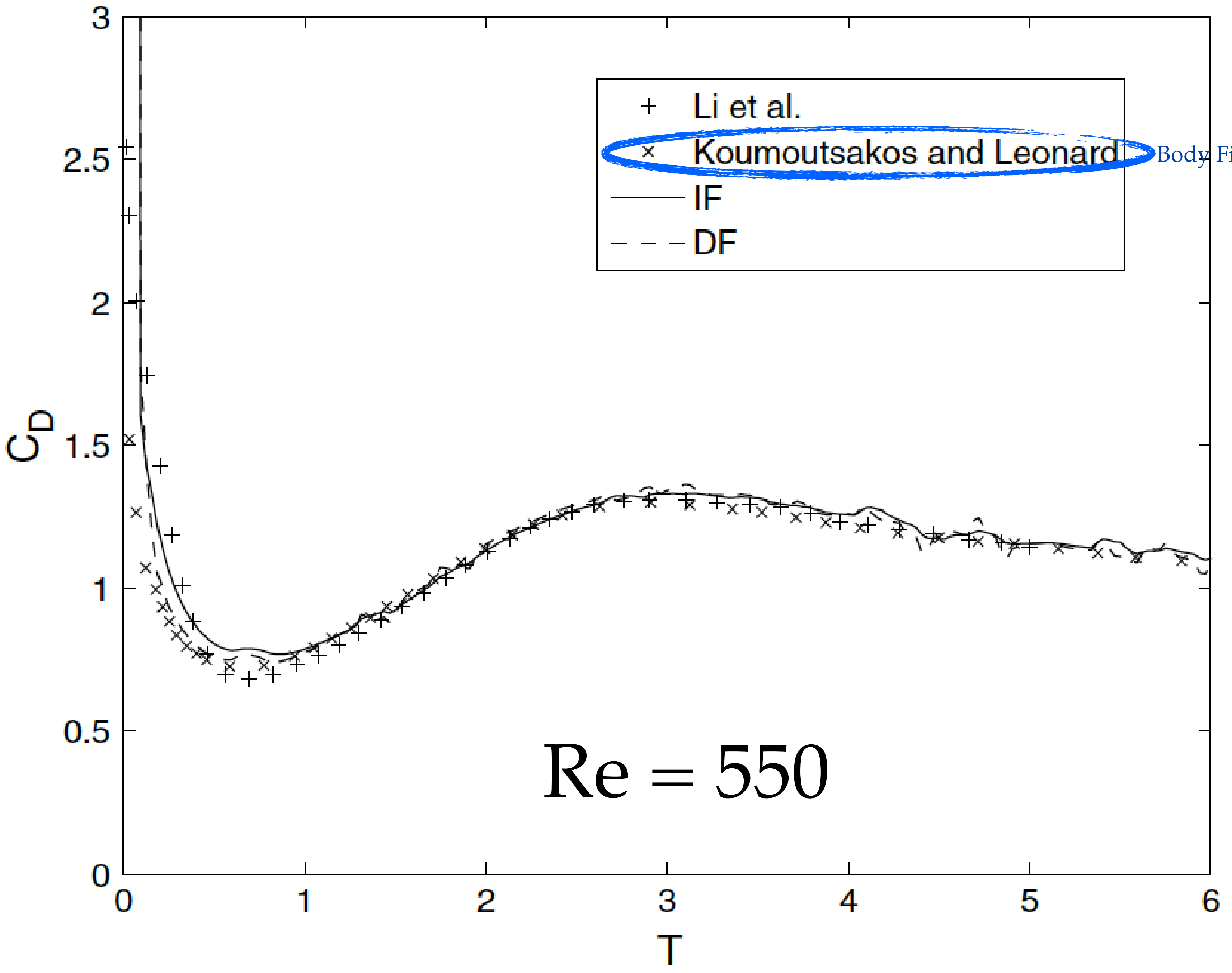
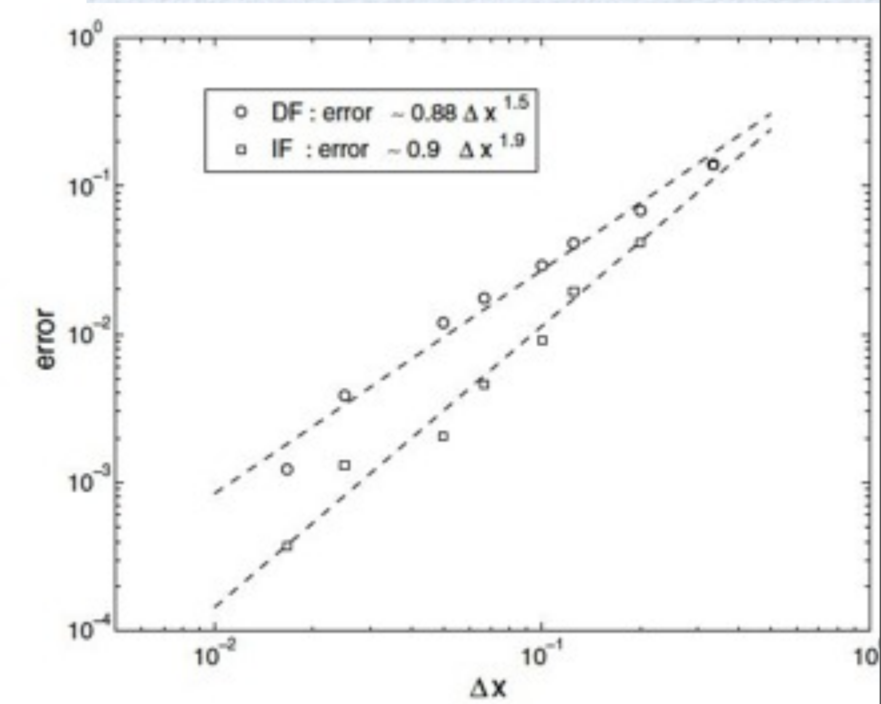




Lattice Boltzmann + Immersed Boundaries



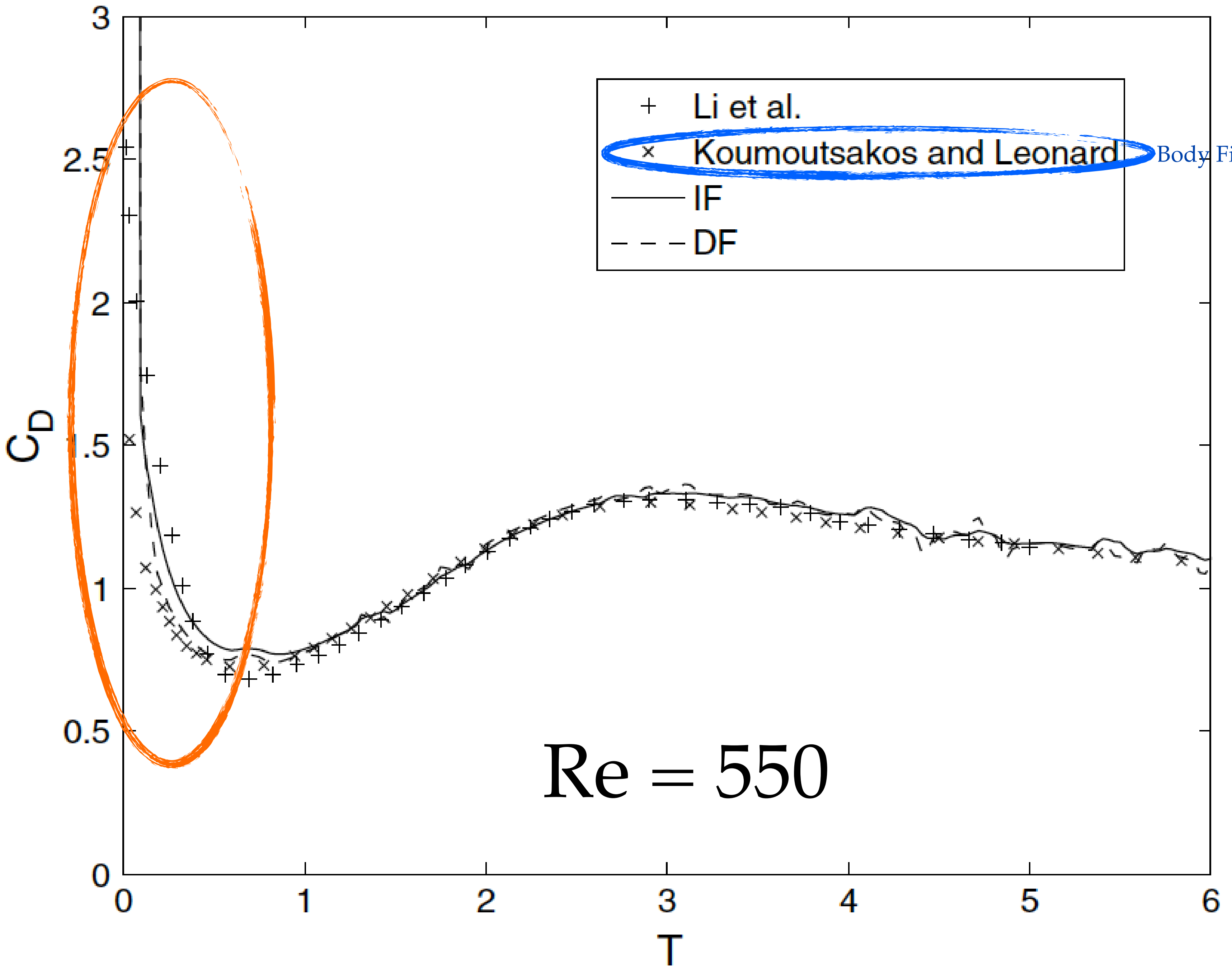
Body Fitted Grids + Vorticity Boundary Conditions

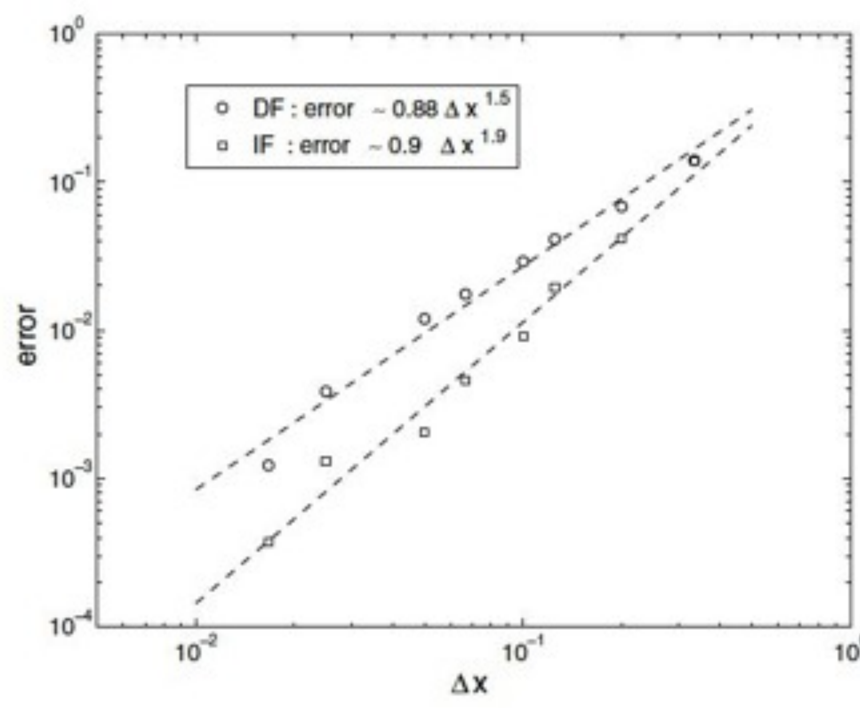


Convergence Rate

Dupuis A., Chatelain P., Koumoutsakos P., An Immersed Boundary-Lattice Boltzmann Method for the Simulation of the Flow Past an Impulsively Started Cylinder, **J. Computational Physics**, 227, 9, 4486-4498, 2008

Lattice Boltzmann + Immersed Boundaries

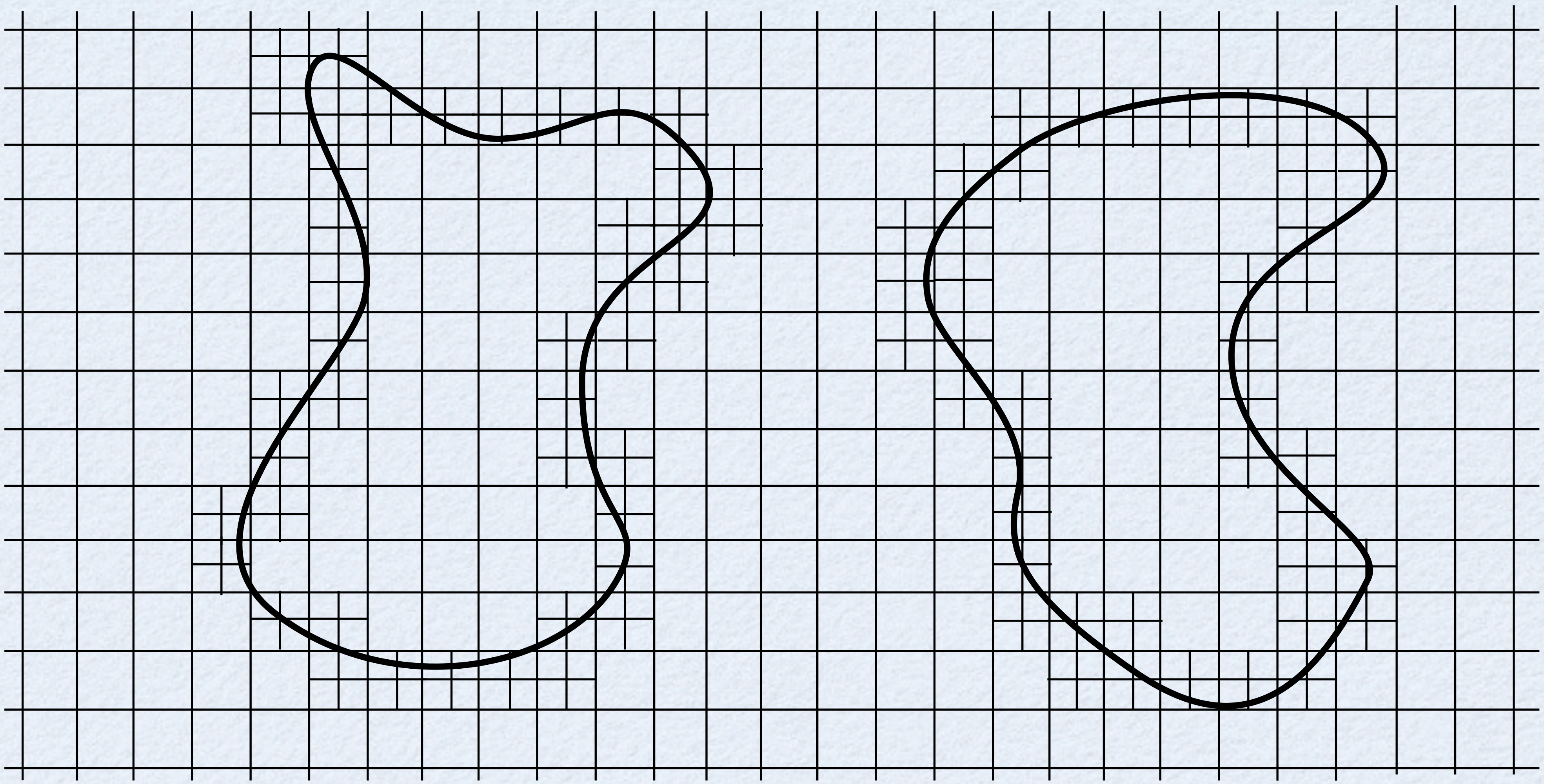




Convergence Rate

Dupuis A., Chatelain P., Koumoutsakos P., An Immersed Boundary-Lattice Boltzmann Method for the Simulation of the Flow Past an Impulsively Started Cylinder, **J. Computational Physics**, 227, 9, 4486-4498, 2008

Boundary Conditions = Coupling



$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} \; + f(\text{enforces b.c.})$$

Multiphysics/Multiscale

$$f(\mathbf{x}) \approx F(\text{Atomistic Simulations})$$

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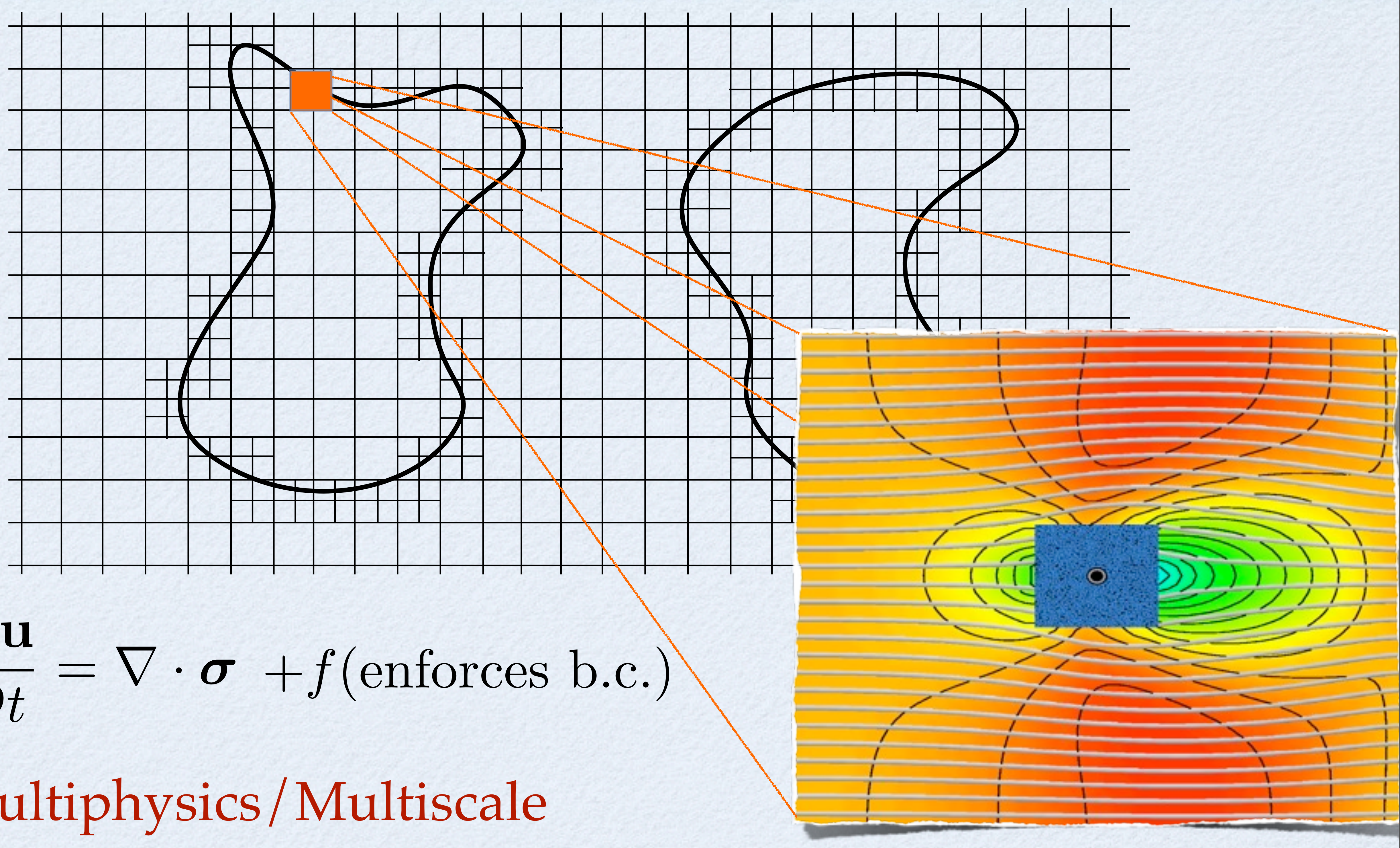

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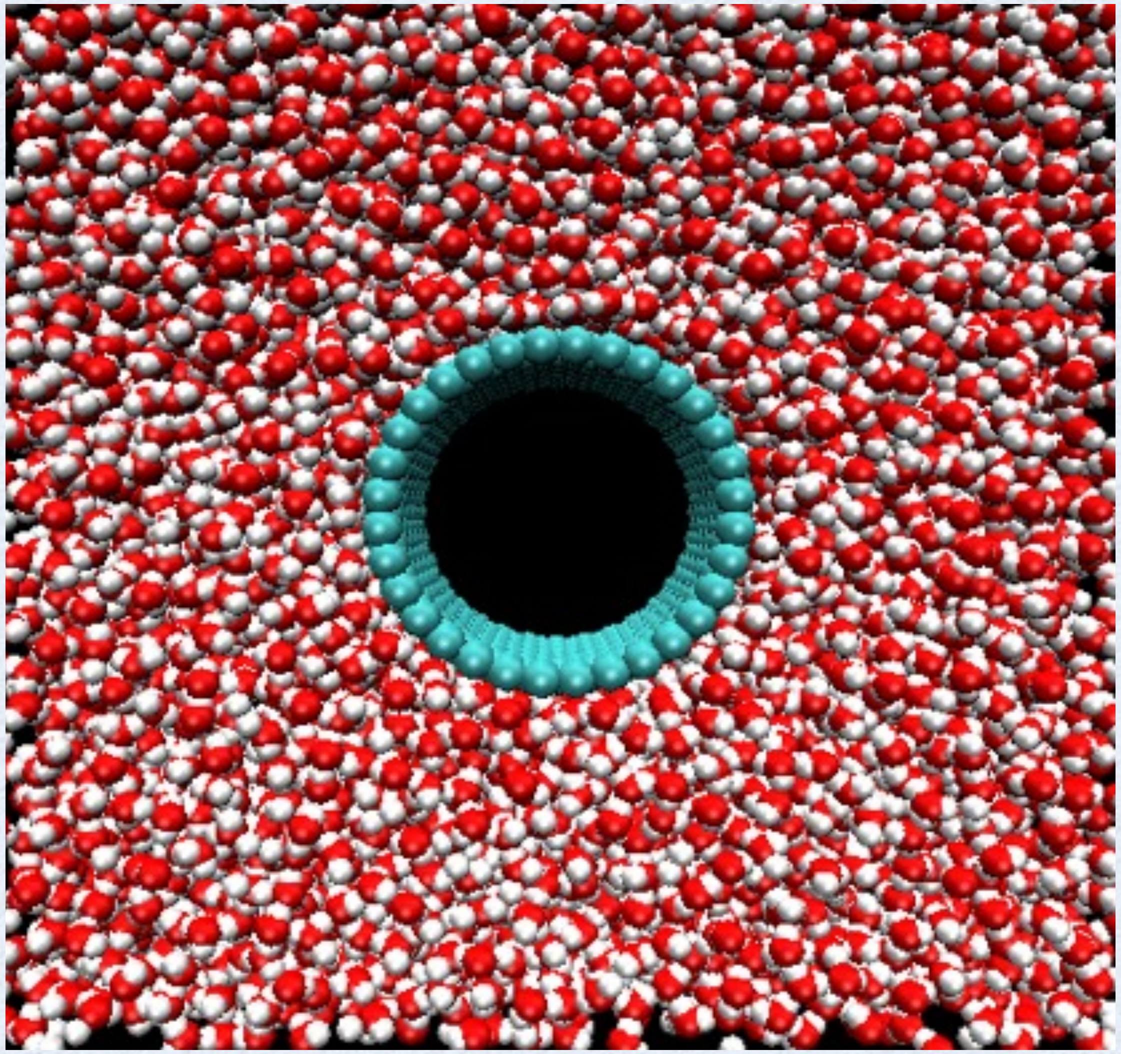
Schwarz DD for Liquids

T. Werder, J. H. Walther, P. Koumoutsakos, Hybrid atomistic-continuum method for the simulation of dense fluid flow, **J. Computational Physics**, 205, 373 - 390, 2005



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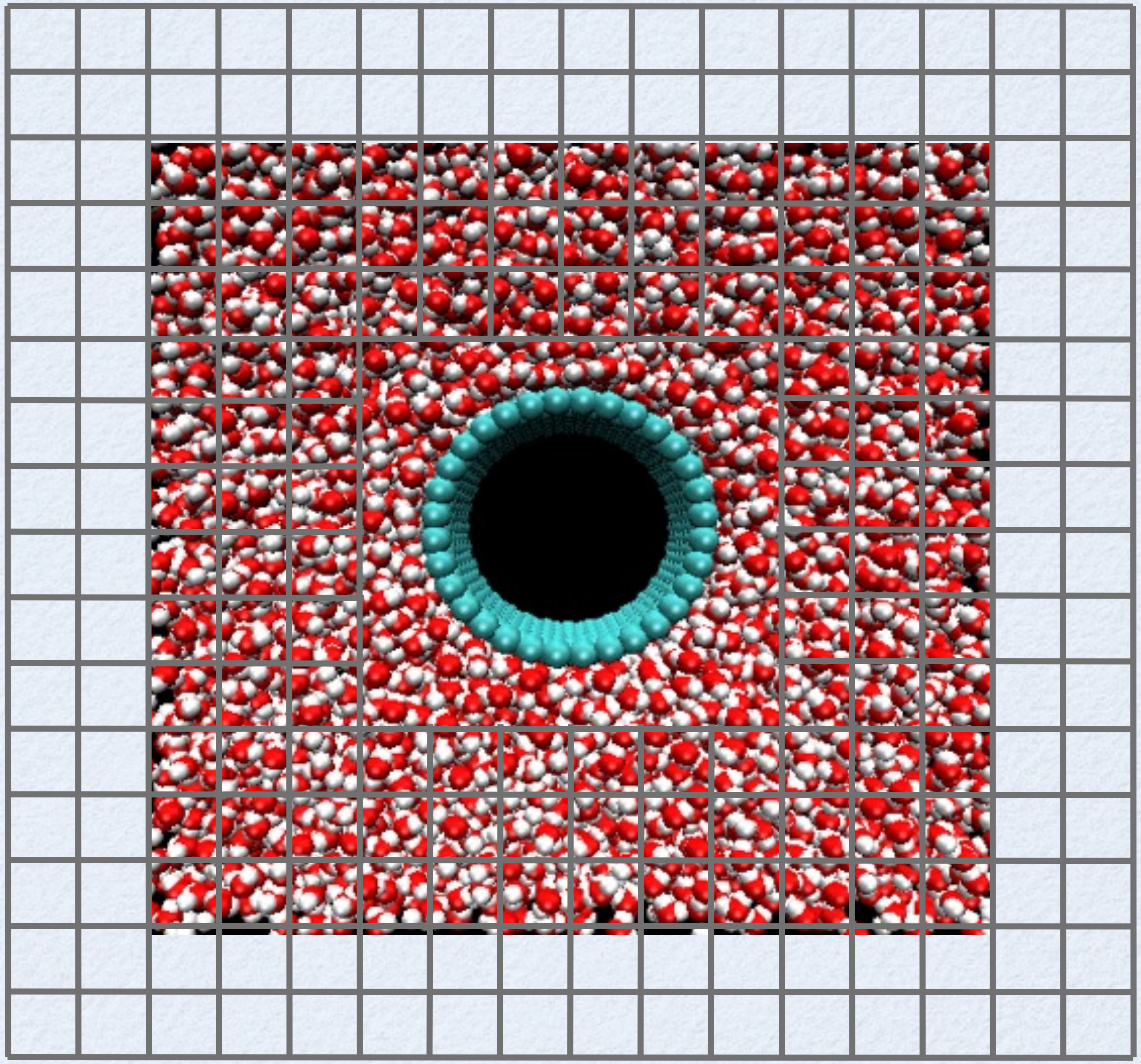

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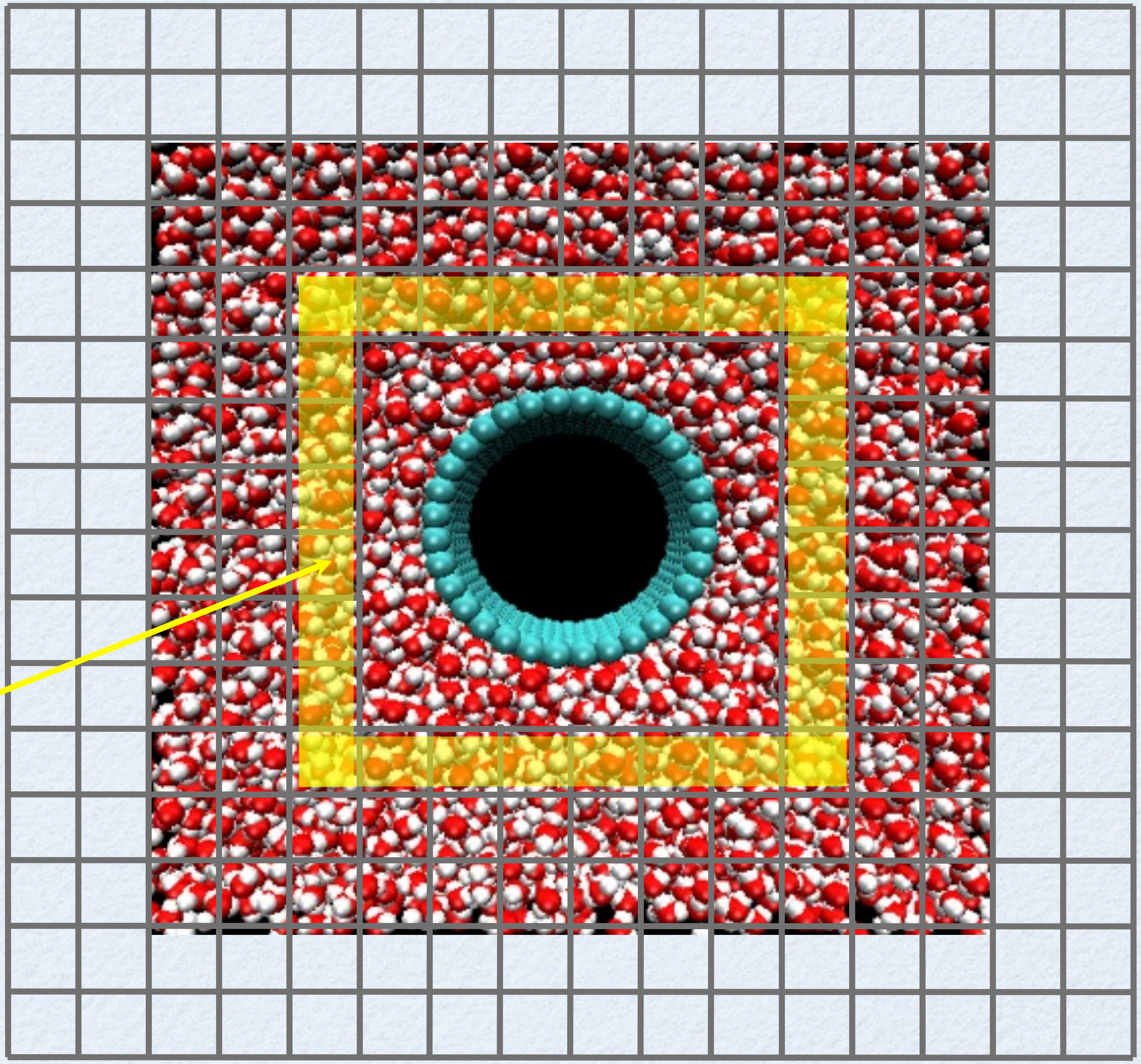

Measure
A→C

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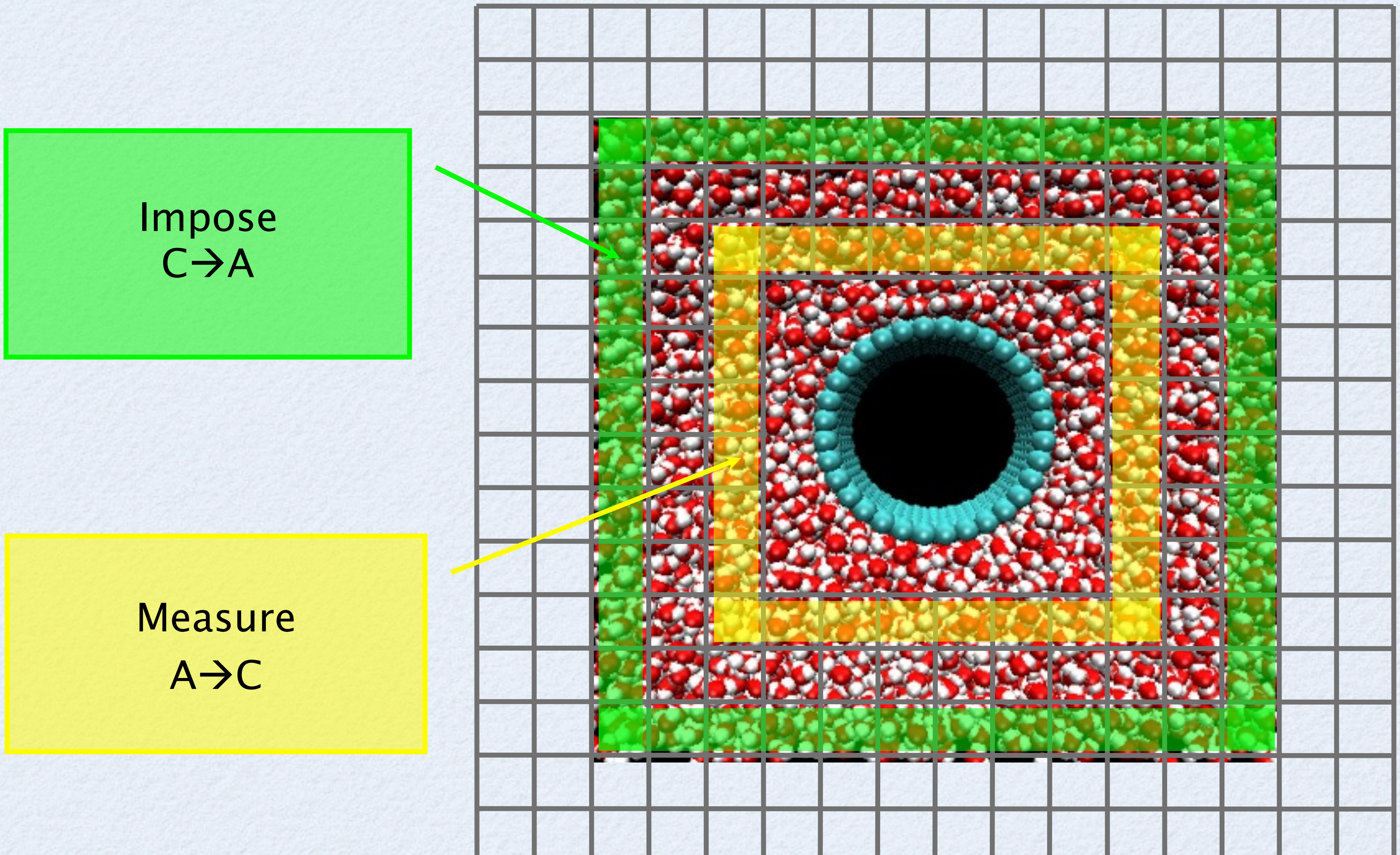

- Iterate, until the solution in the overlap region converges.
- Conservative scheme – transport coefficients in A and

Bridging FLUX & SCHWARZ DD Algorithms

Dupuis A., Kotsalis E.M, Koumoutsakos P., Coupling Lattice Boltzmann and Molecular Dynamics Models for Dense Fluids, **Physical Review E**, 75, 046704, 2007

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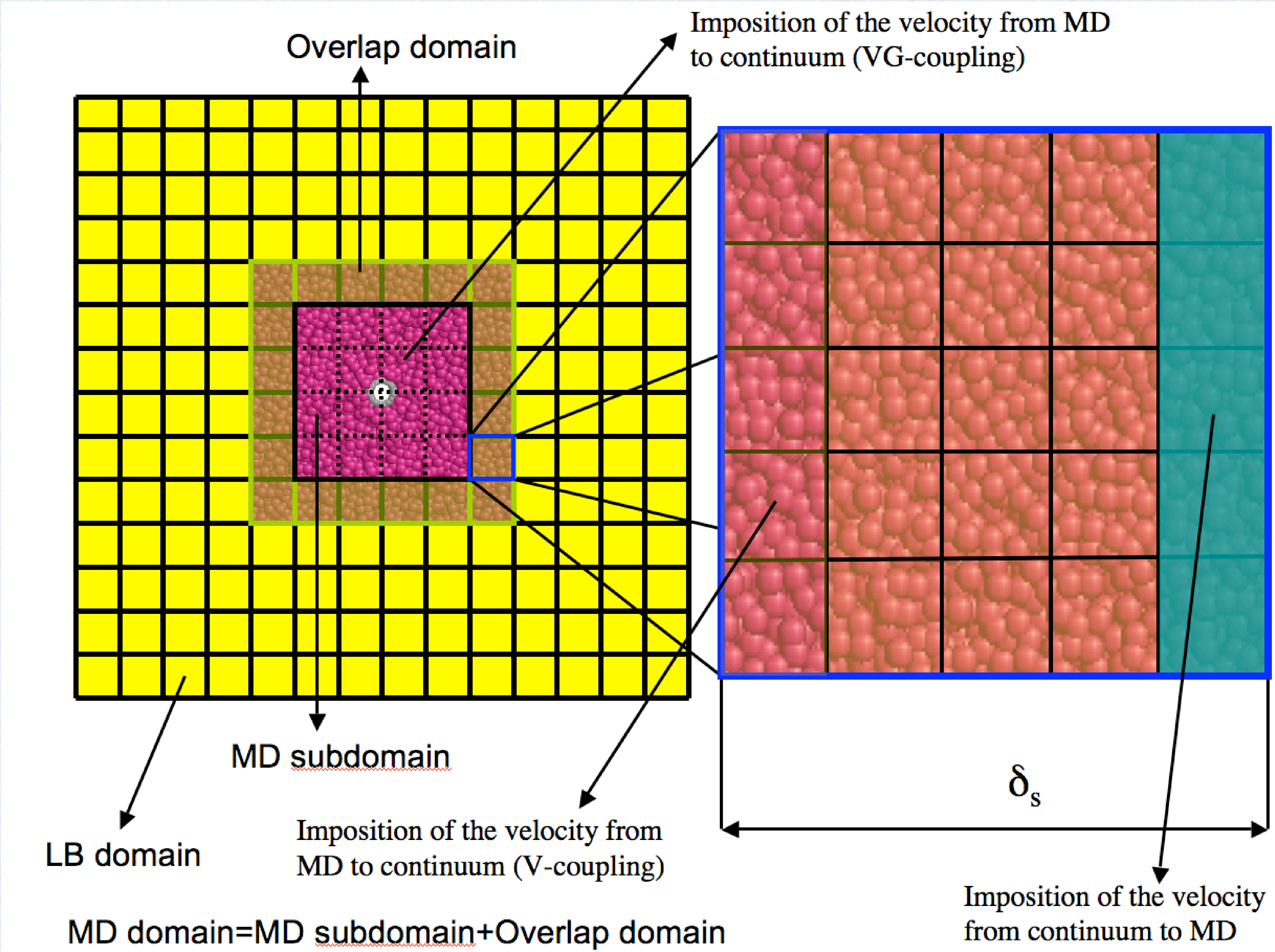

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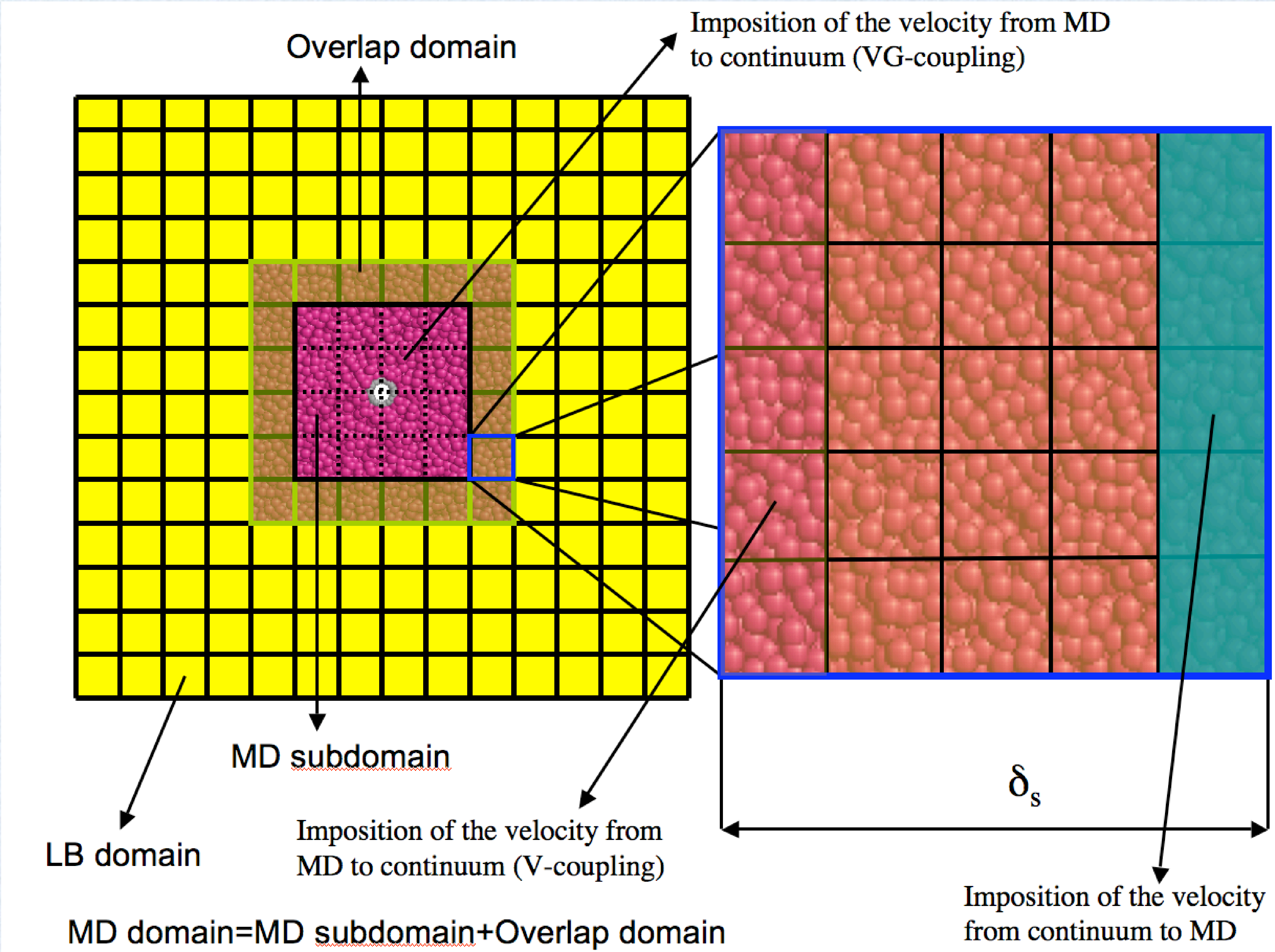

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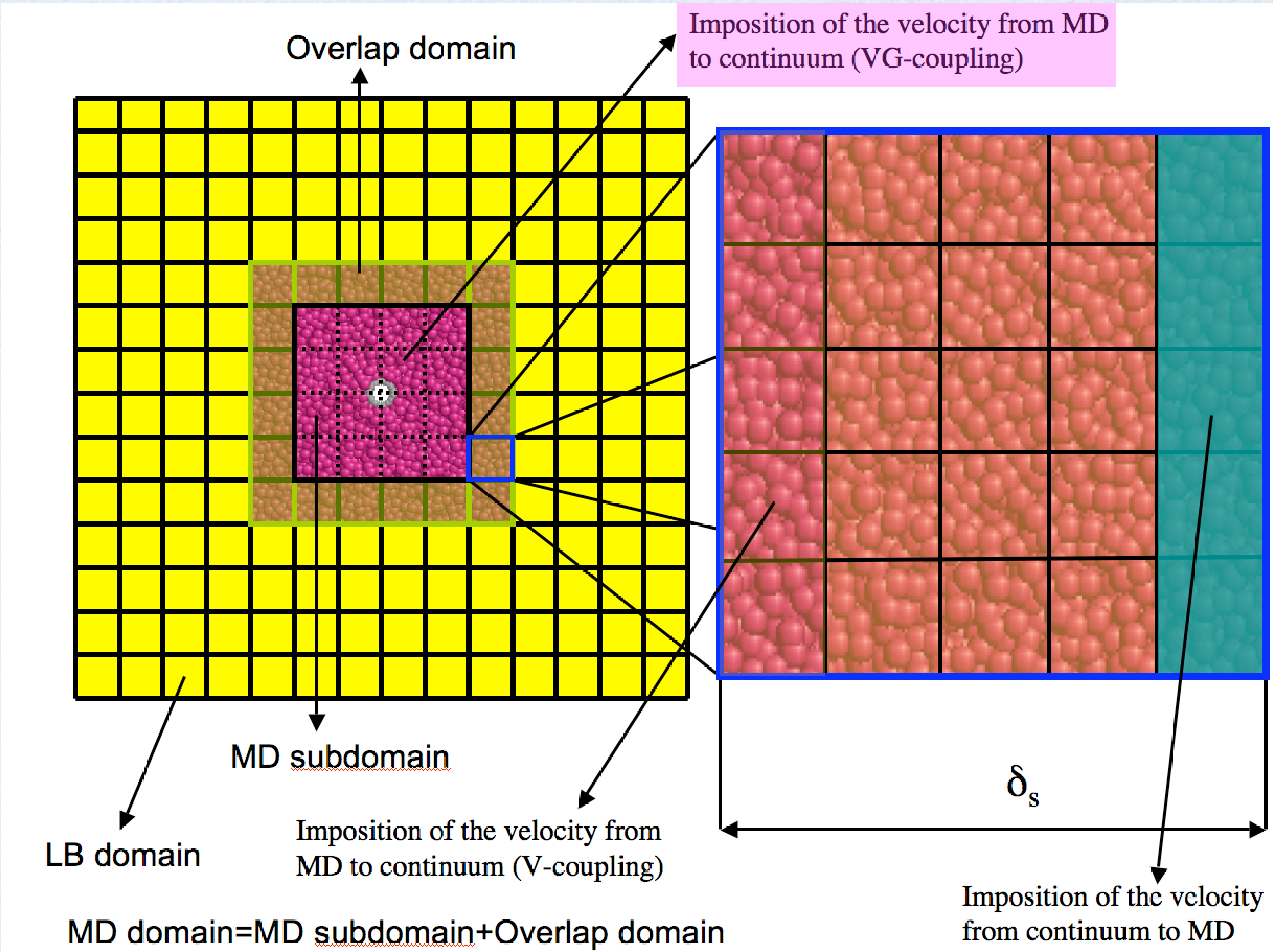

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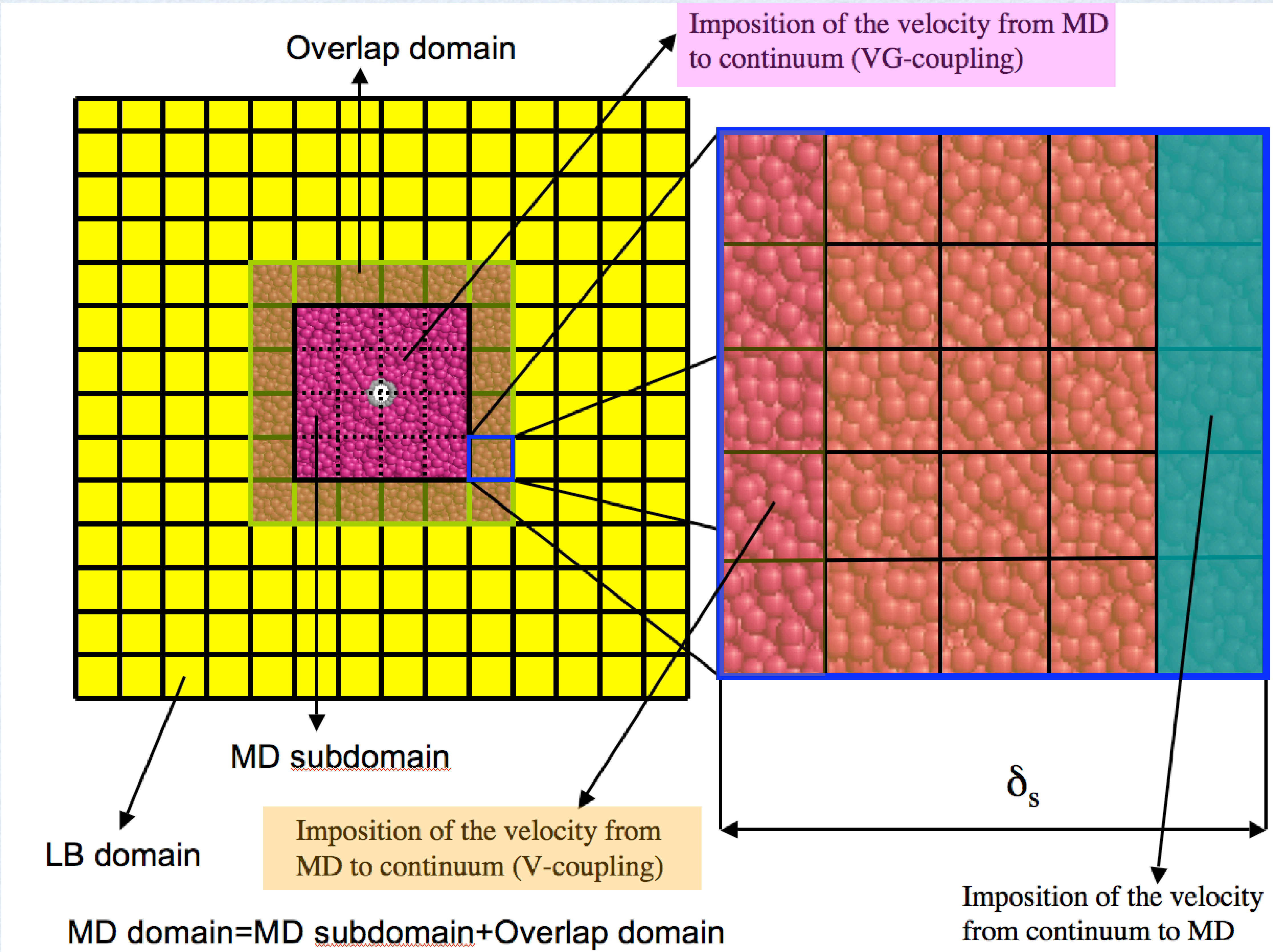
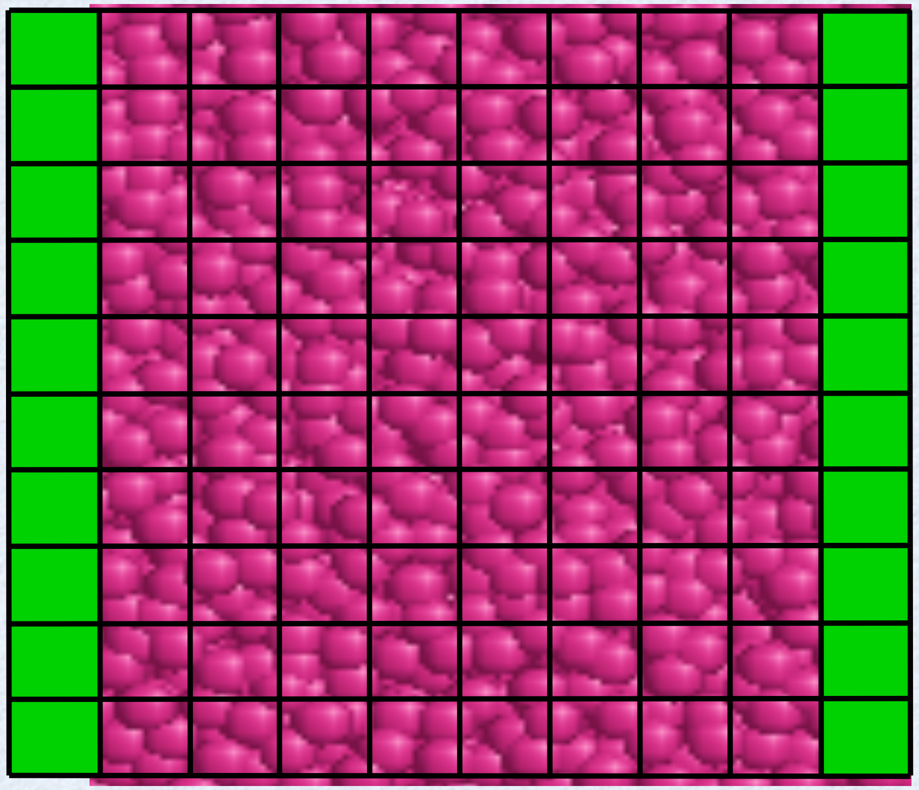
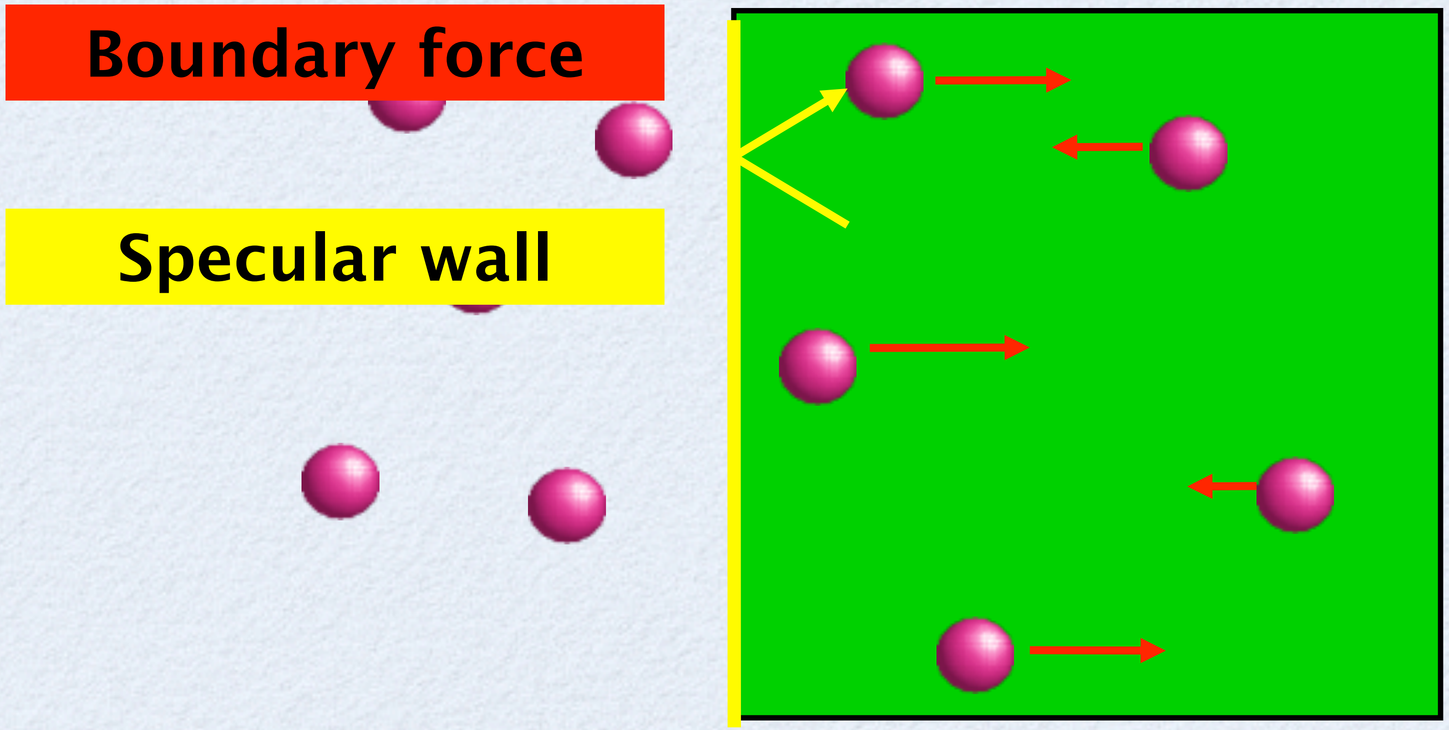


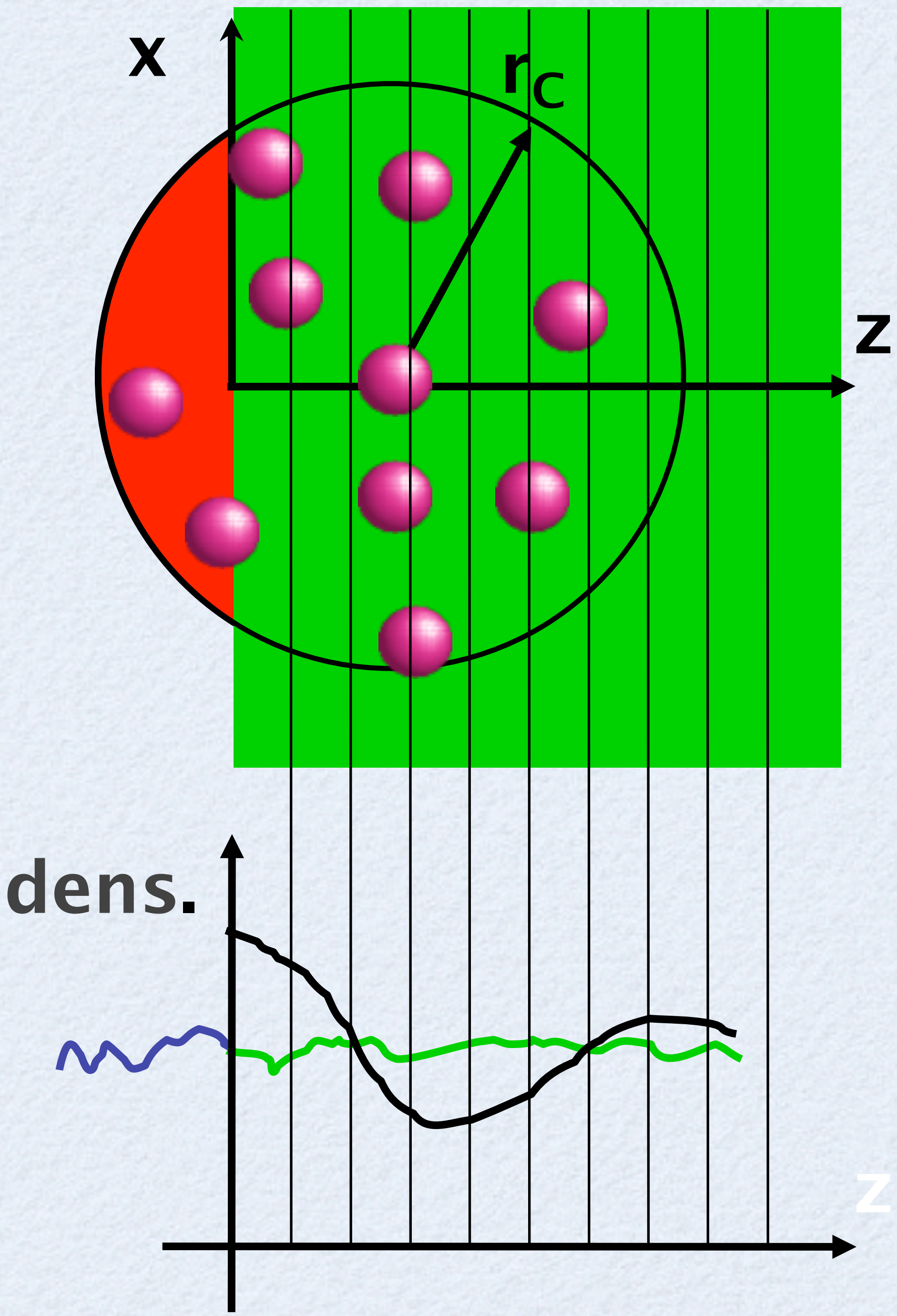
TEST 1 : EQUILIBRIUM   Non-Periodic MD





NON_PERIODICITY & BOUNDARY FORCE

How can we account for the particles in the red domain?



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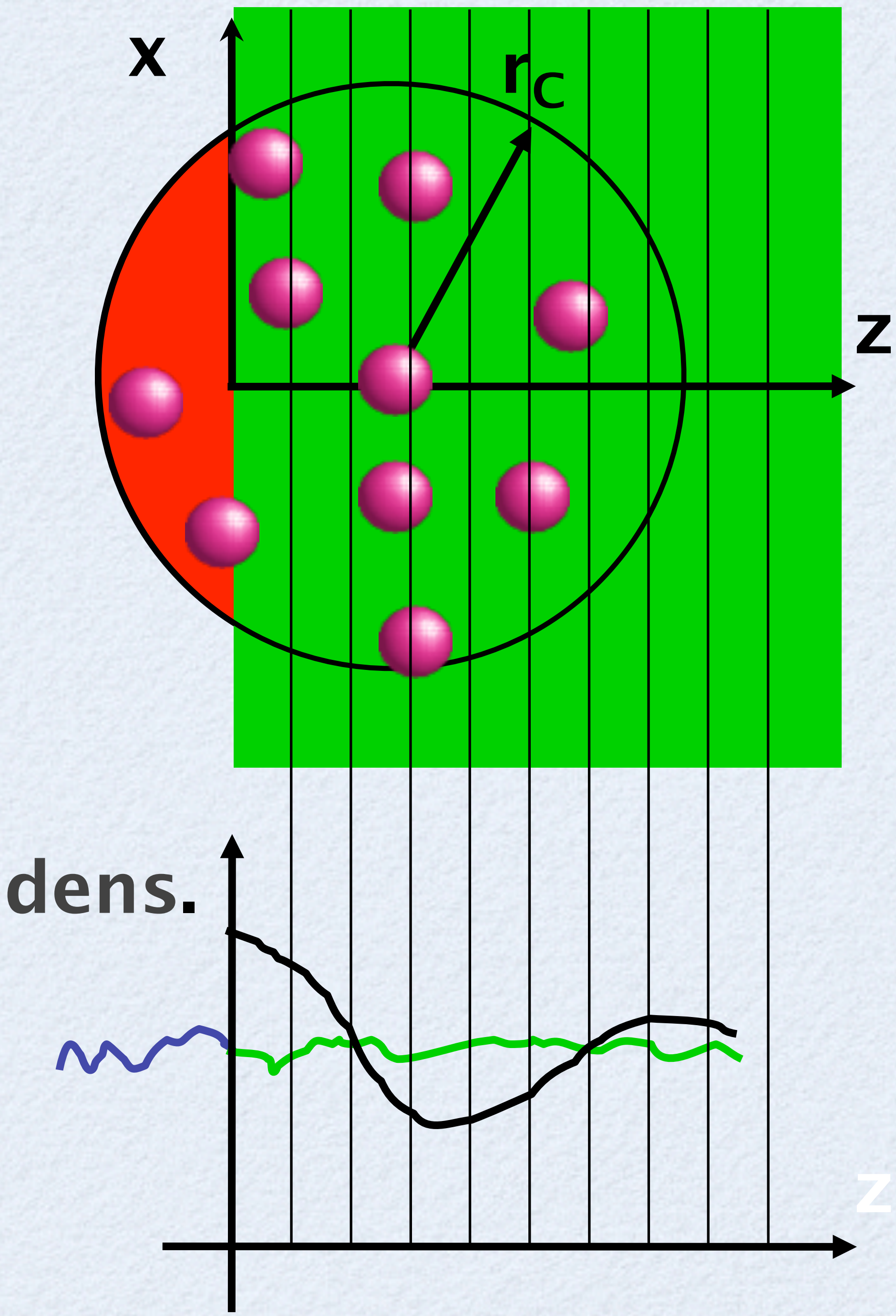
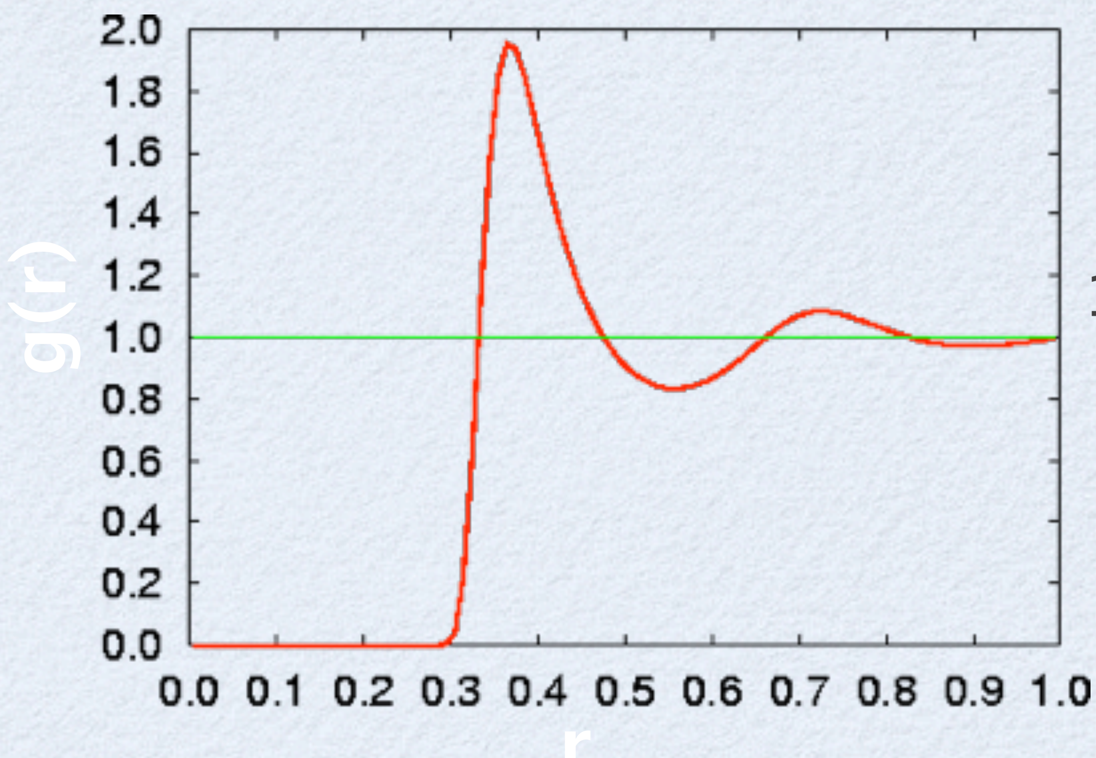


Take fluid structure into

$$\rho(r) = \int_0^r 4\pi r'^2 \rho g(r') dr'$$

$$F_m(z) = -2\pi\rho \int_{\text{red}} g(r) \frac{\partial U(r)}{\partial r} \frac{z}{r} x dx dz$$

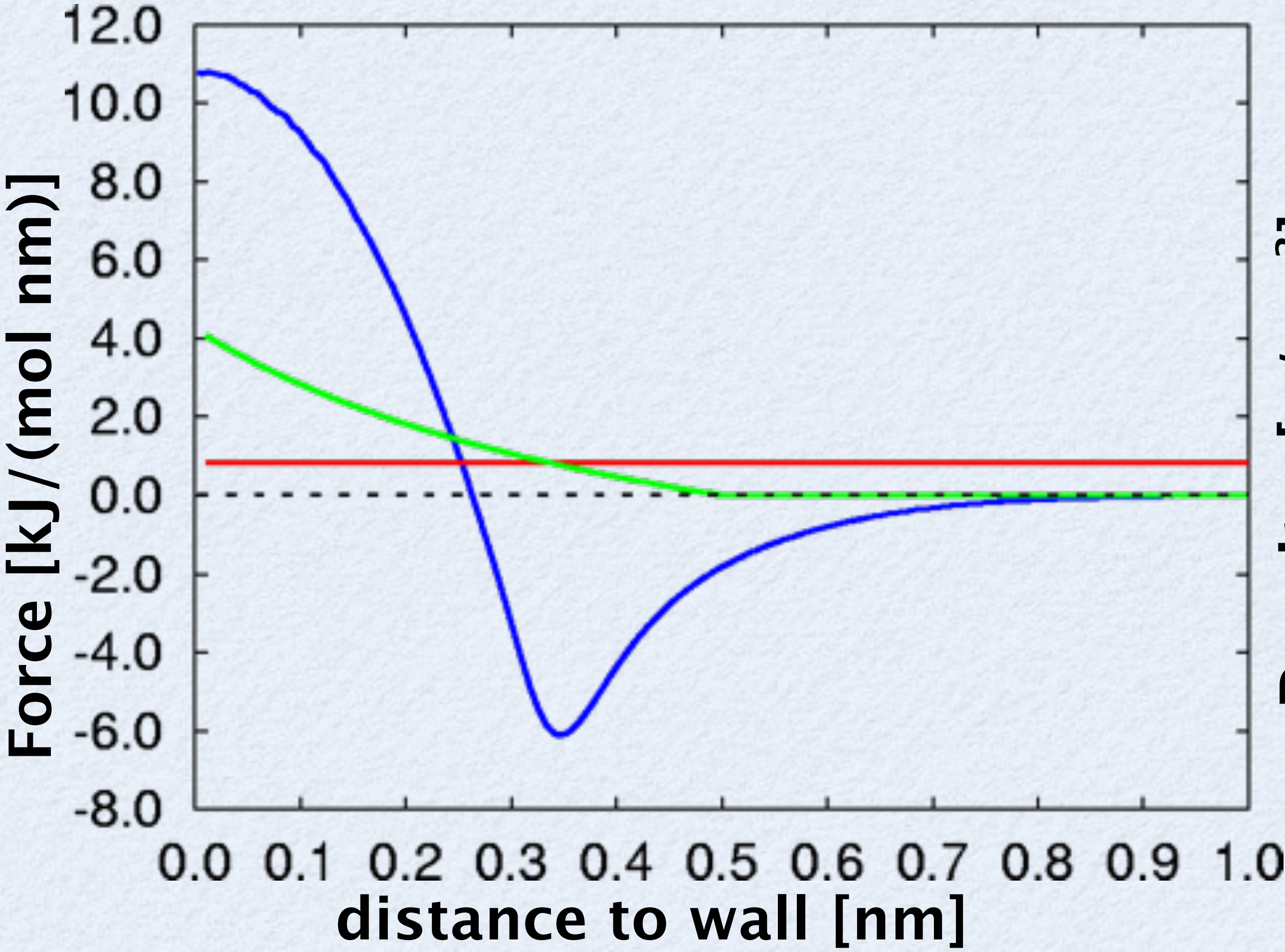


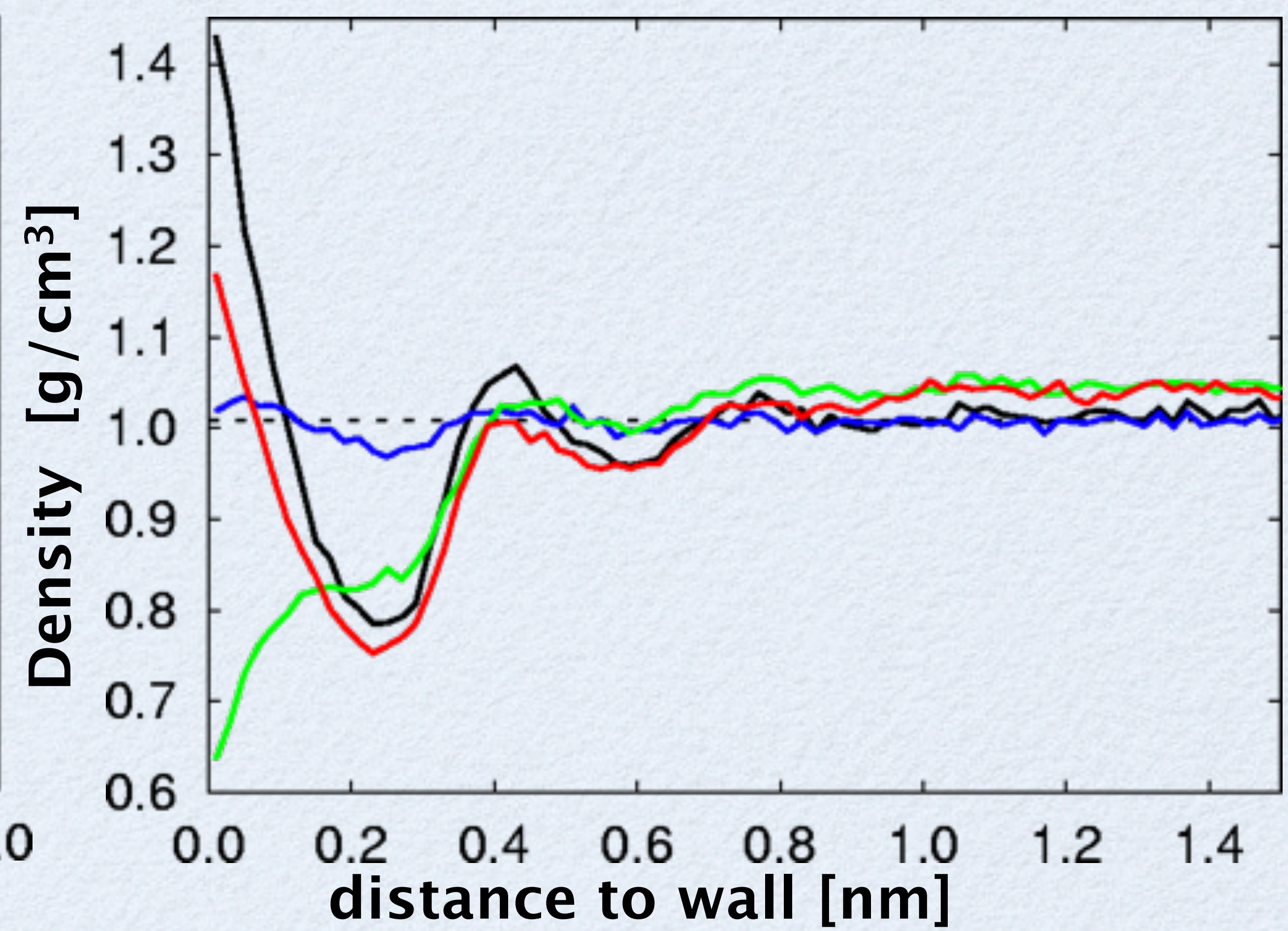
215 K
1.0 gcm^{-3}

A comparison of Forces

No force

Uniform distribution (O'Connell 1995[A])





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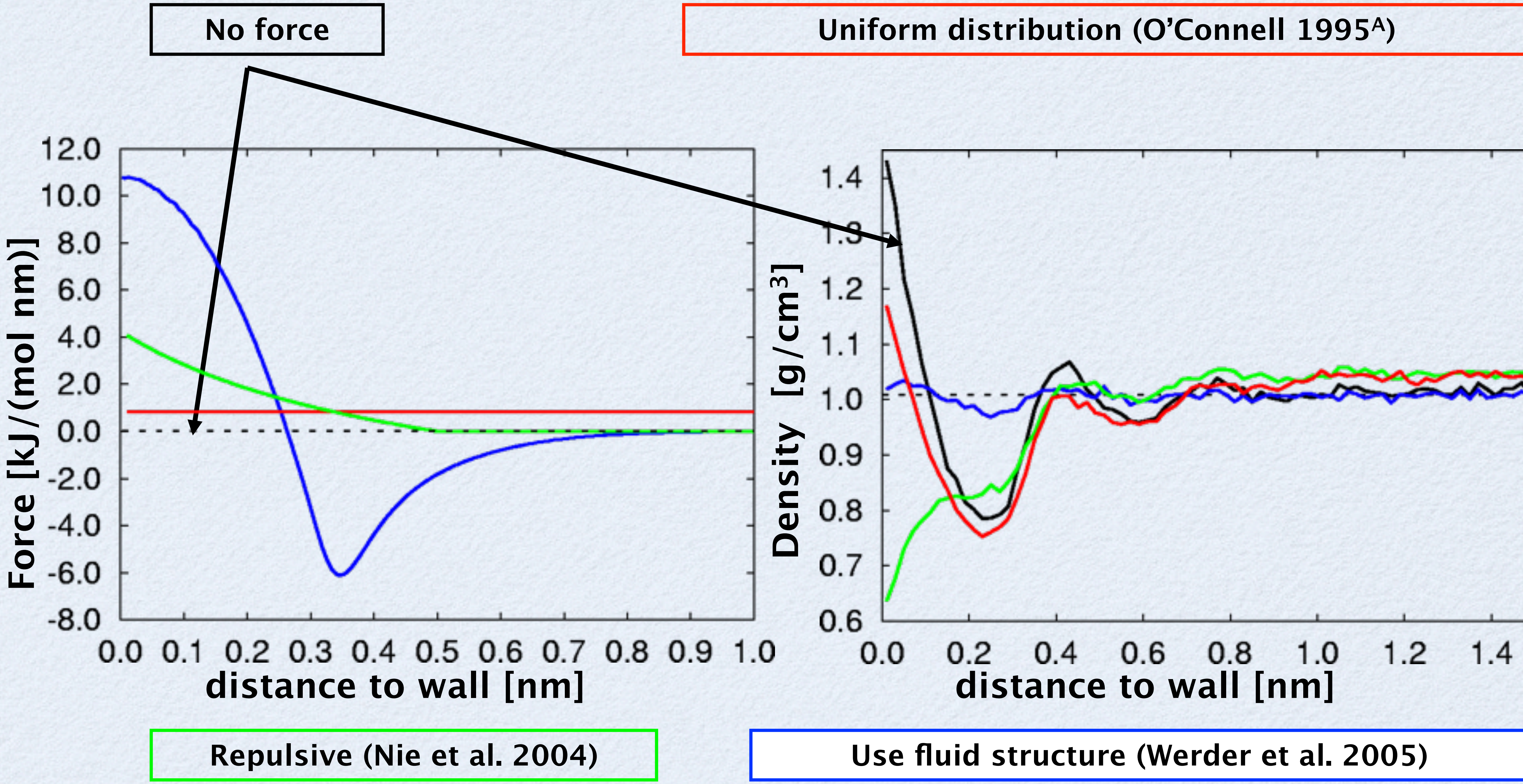

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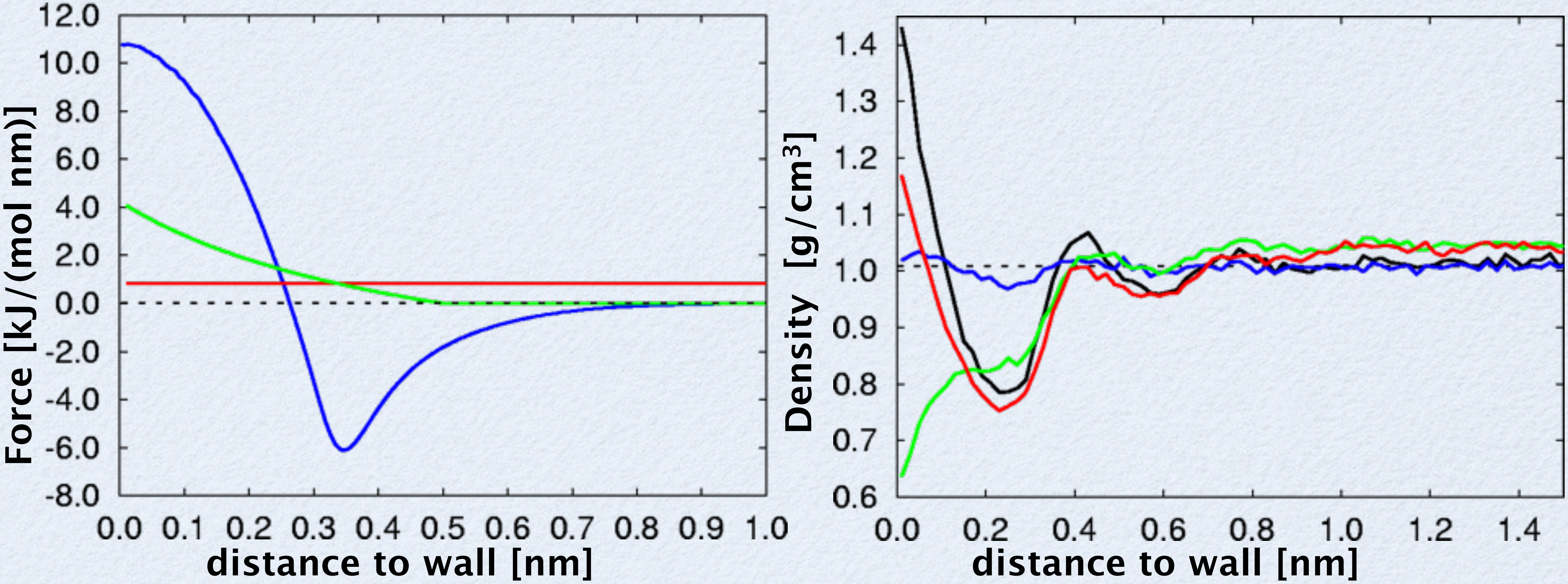

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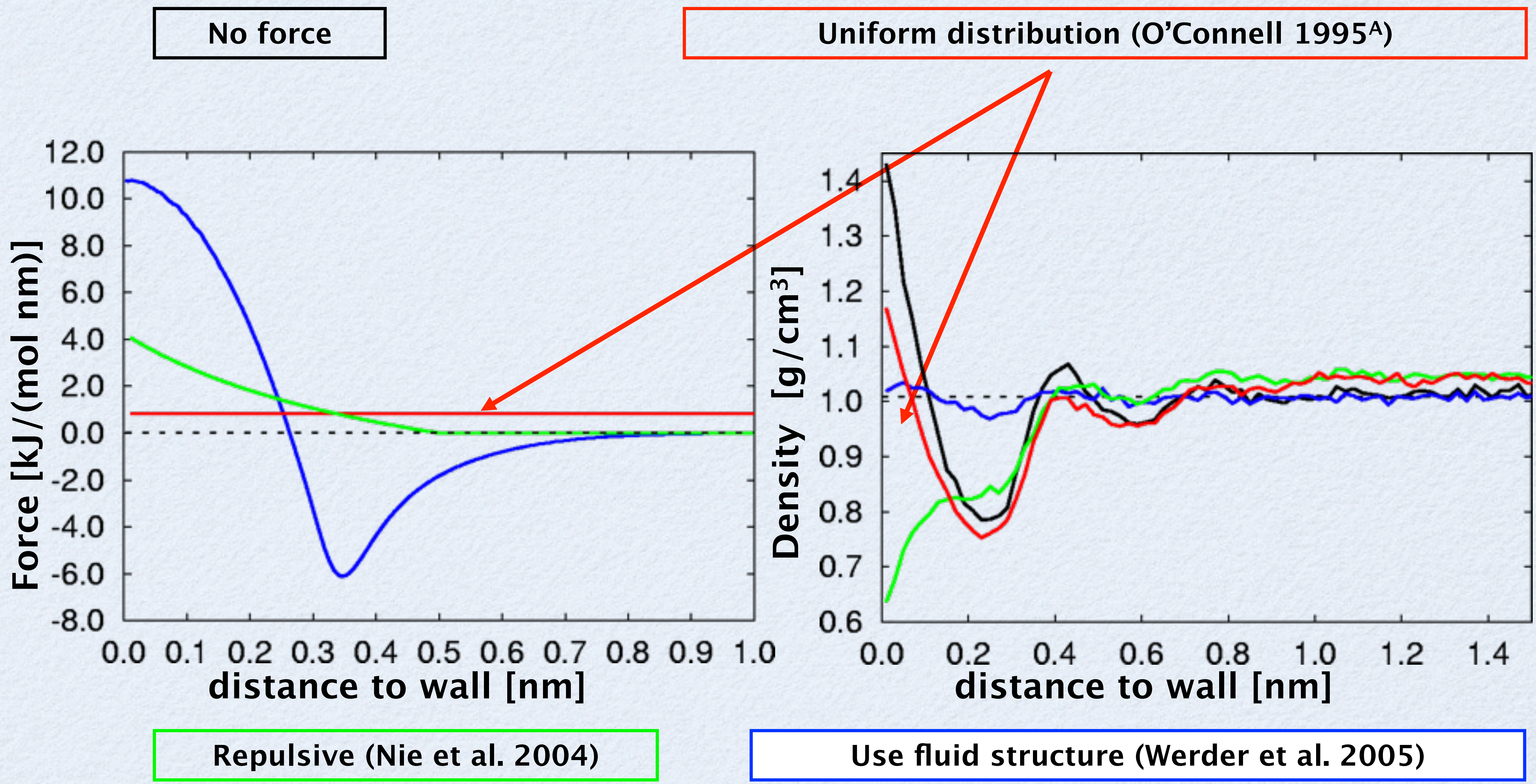

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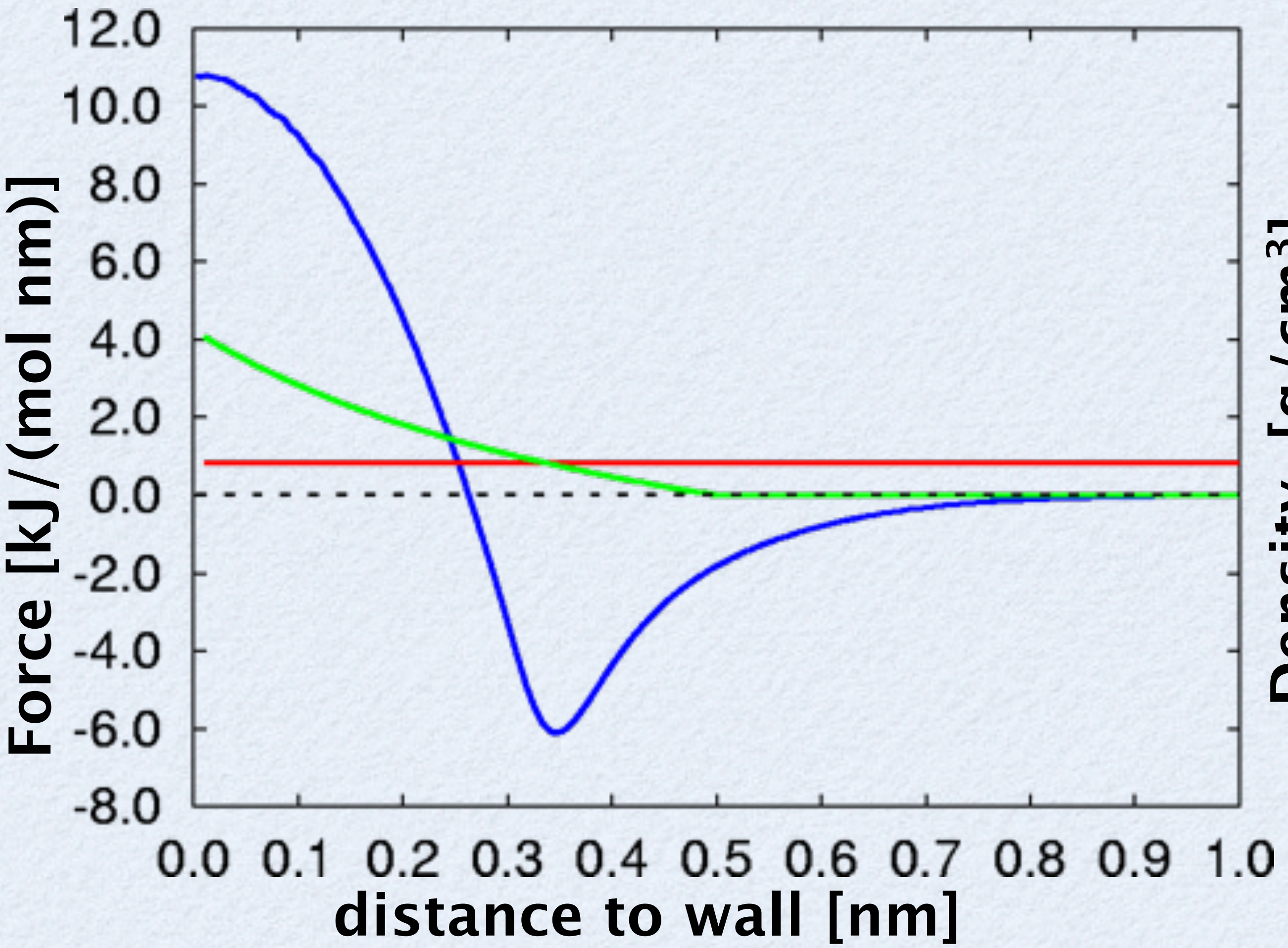

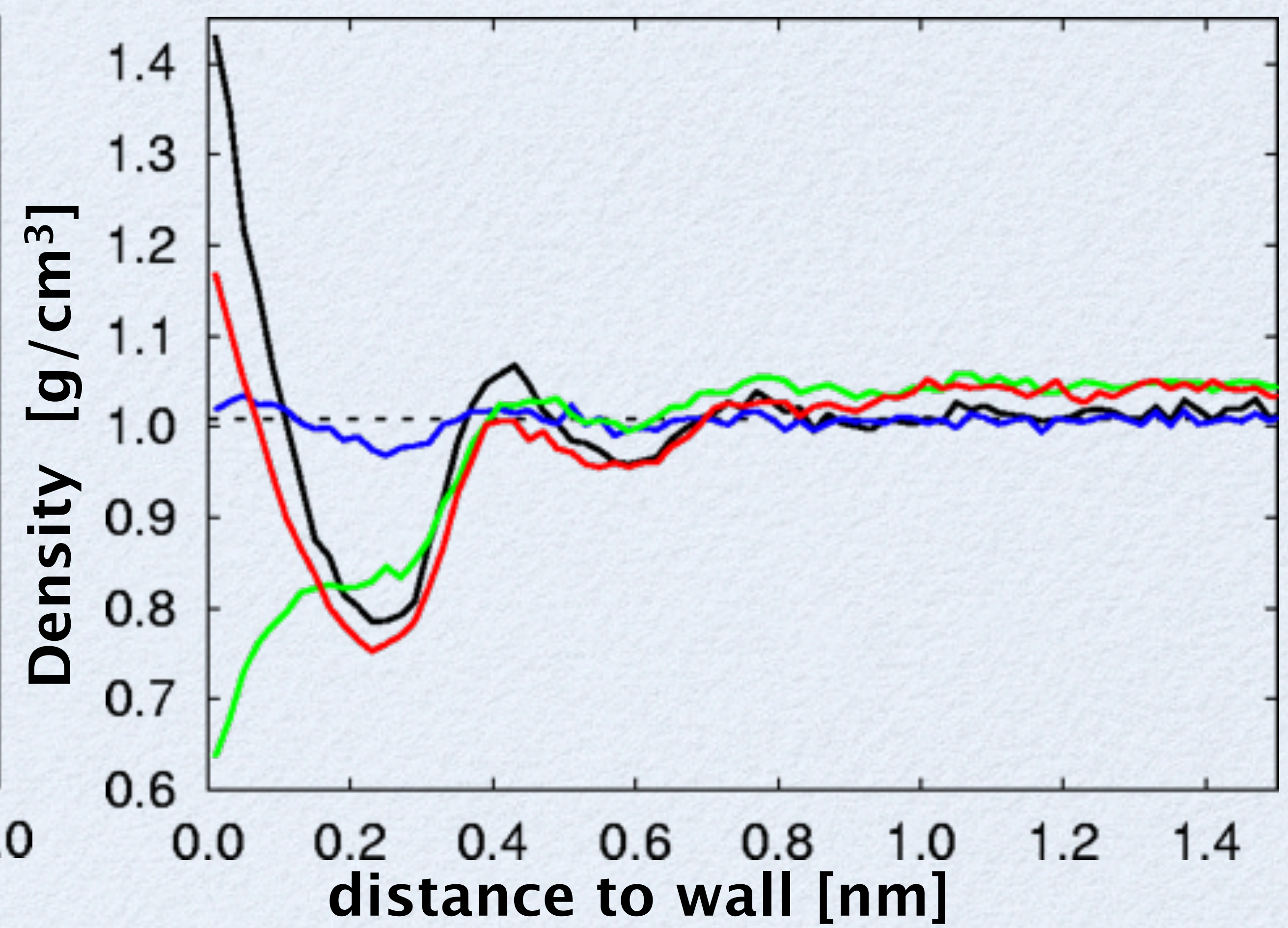

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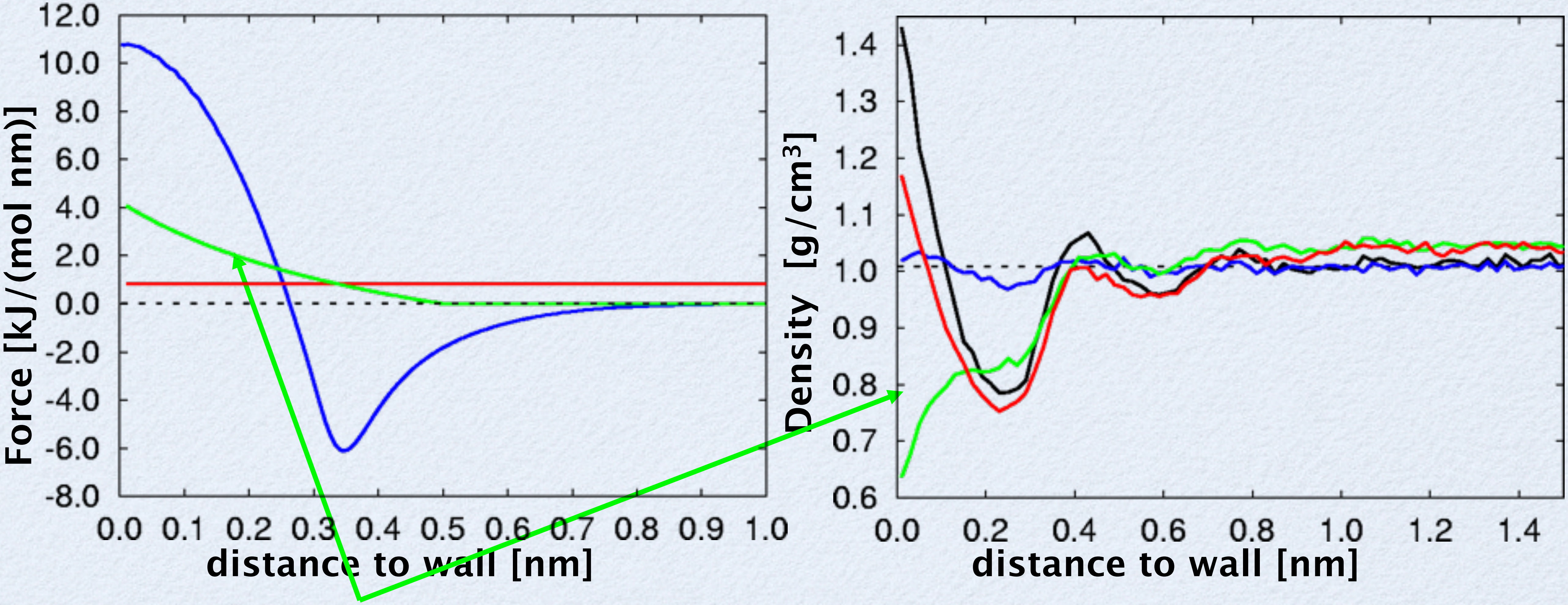

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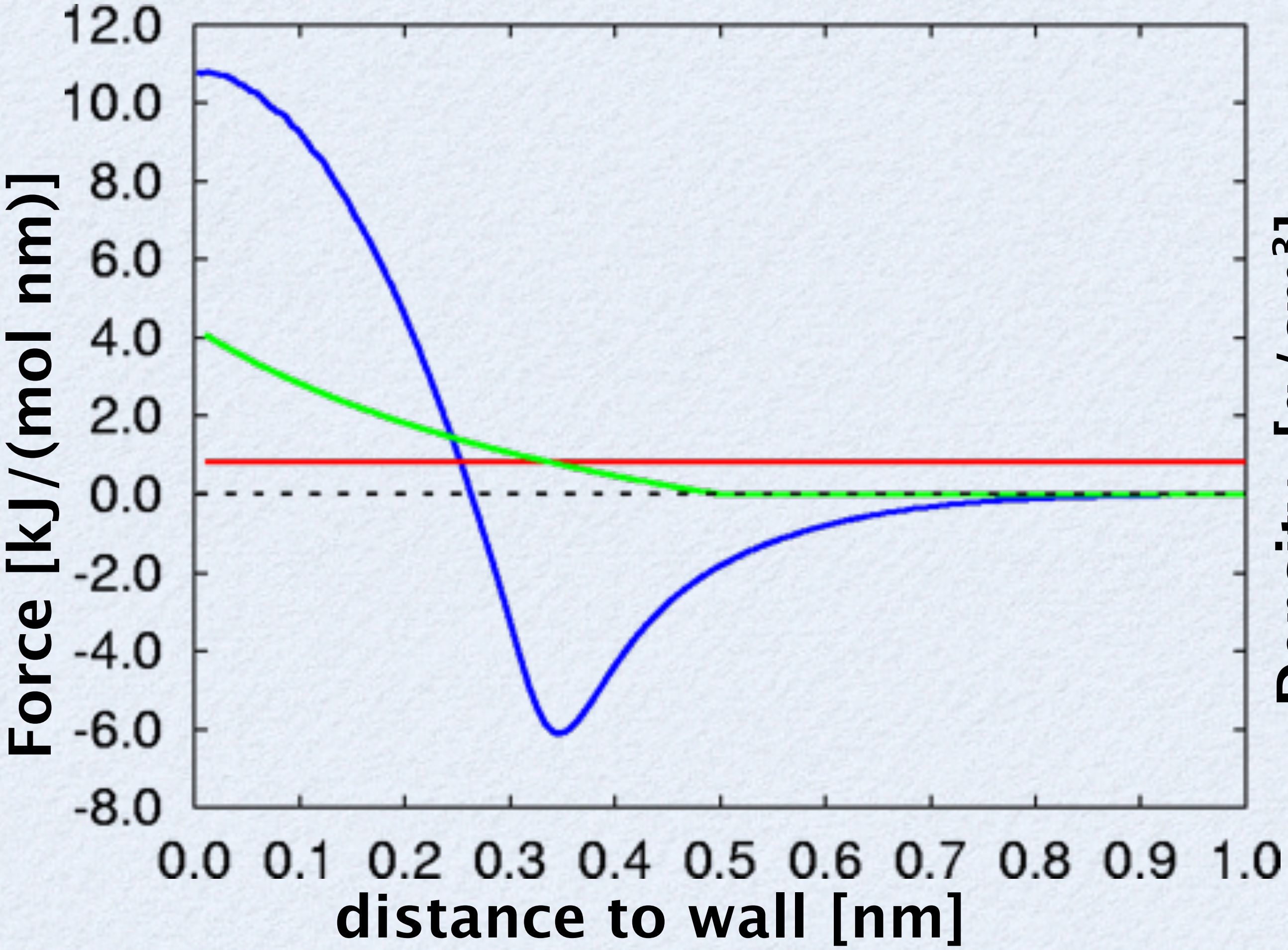

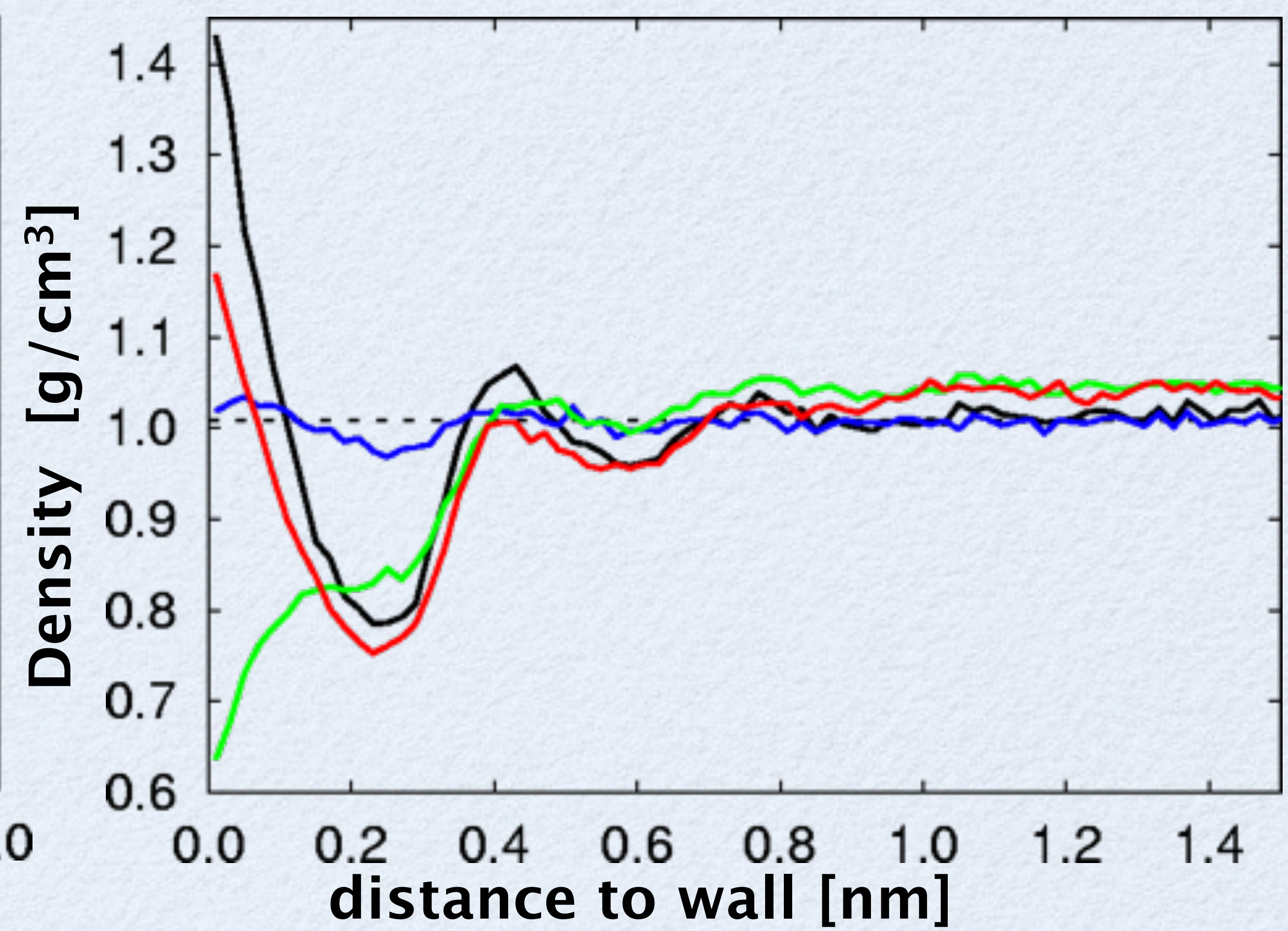

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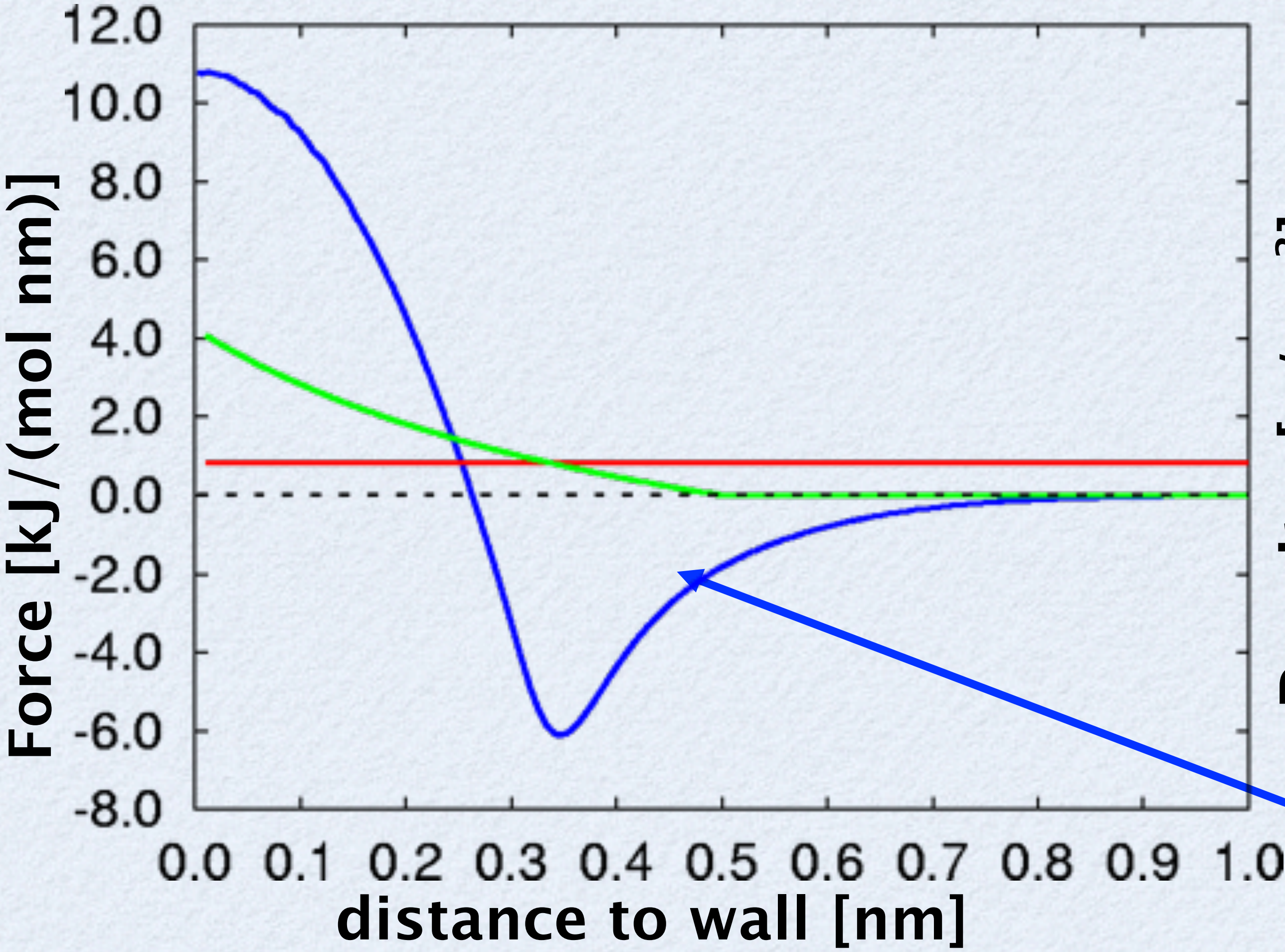

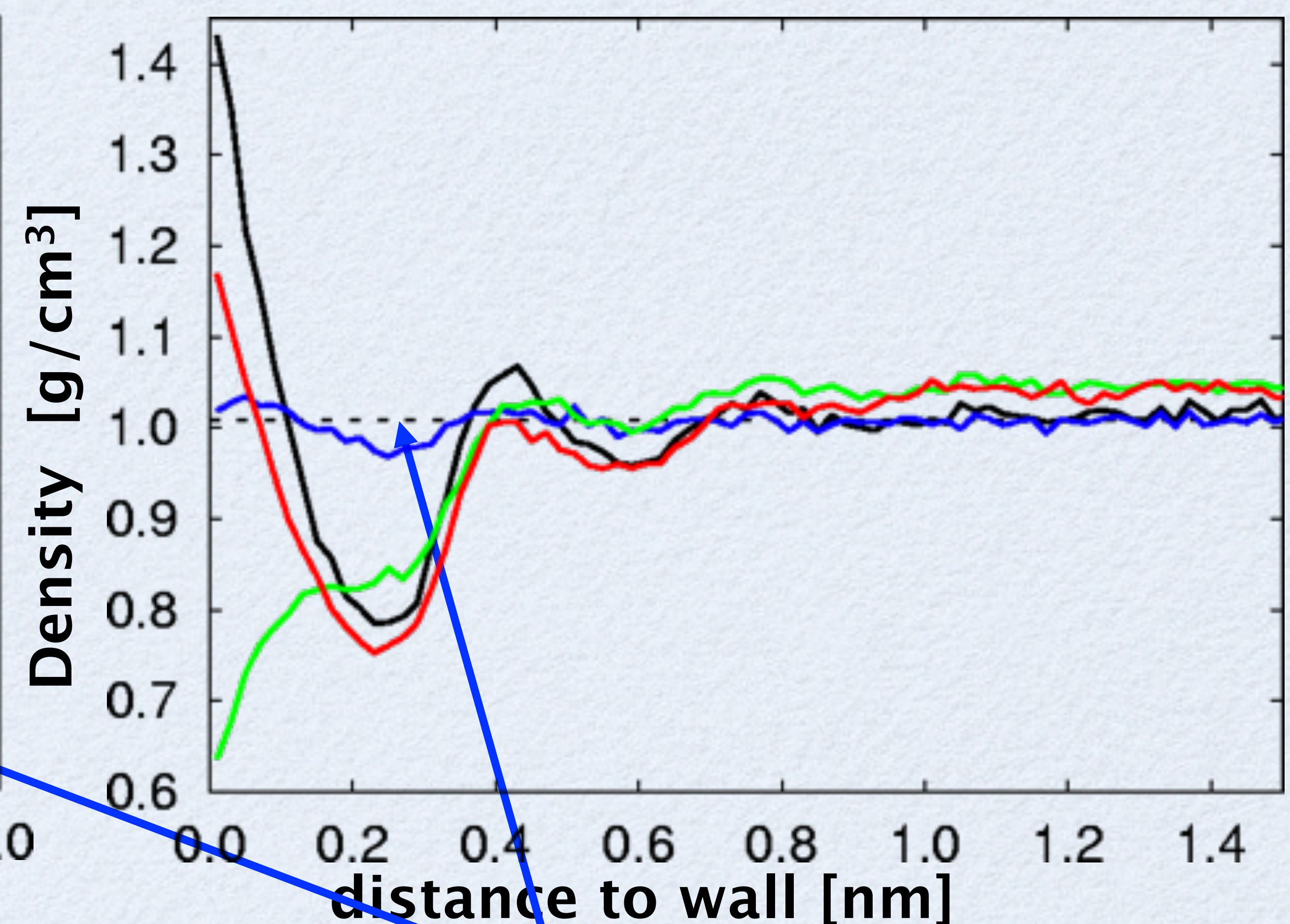

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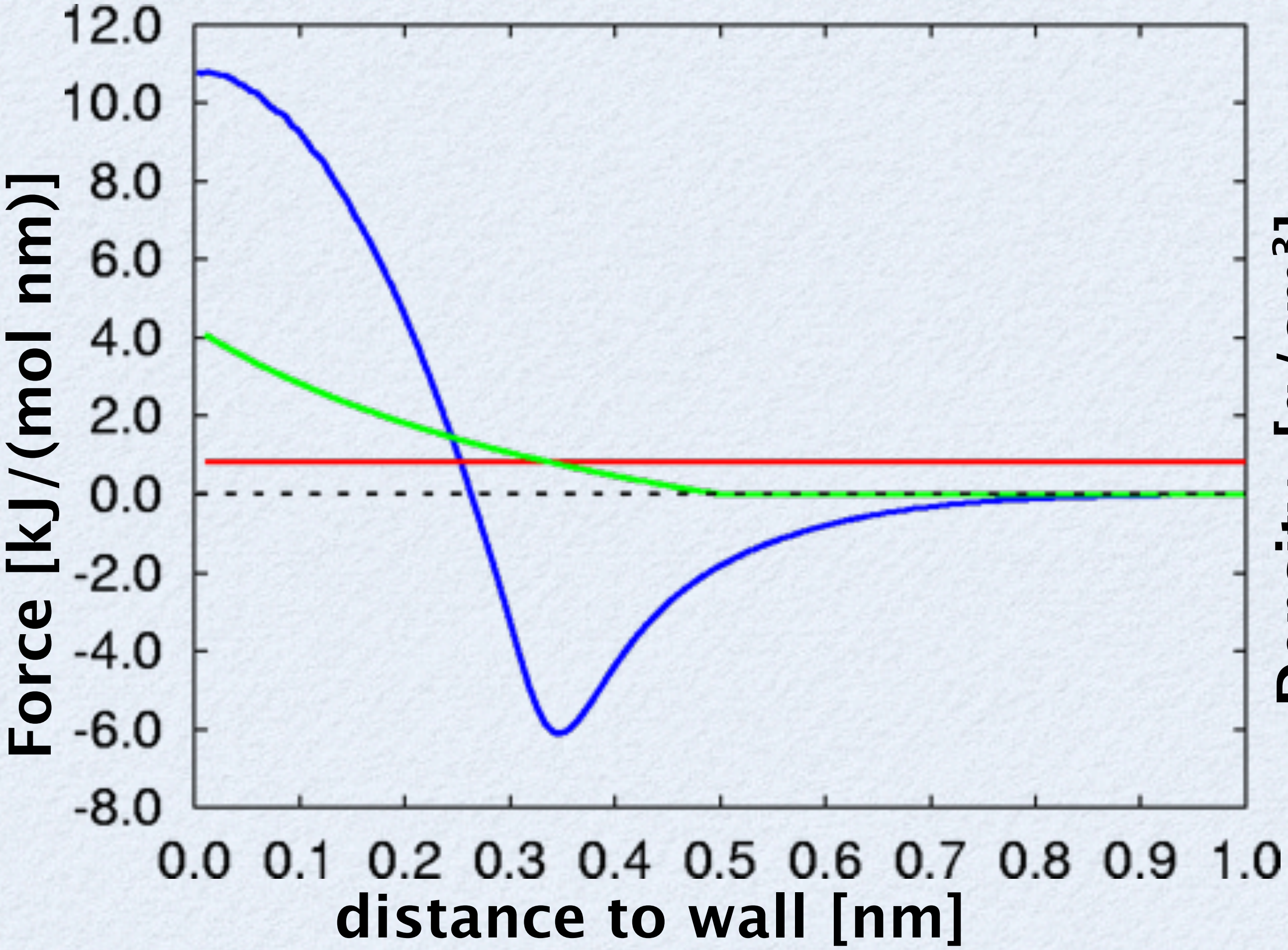

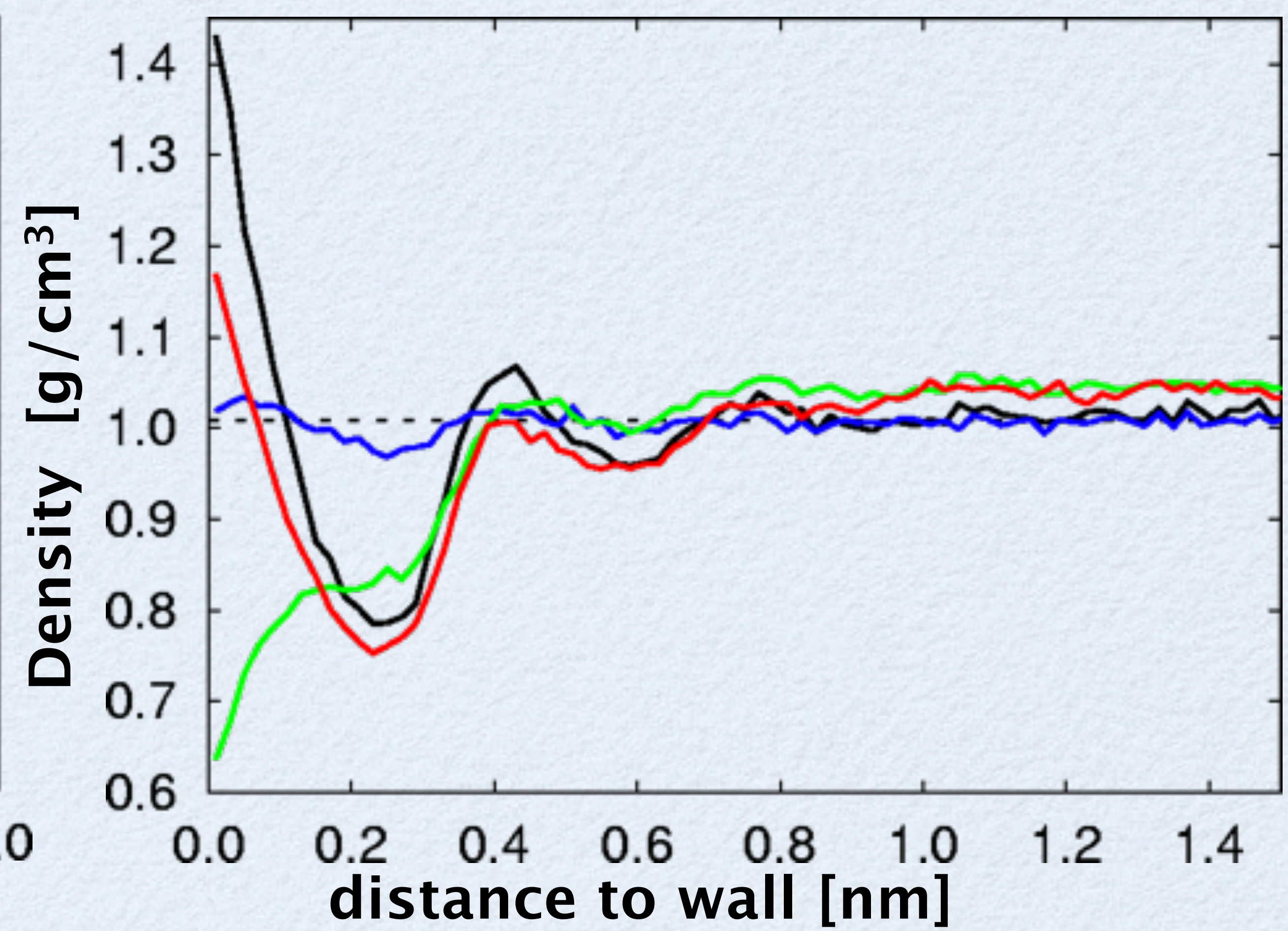

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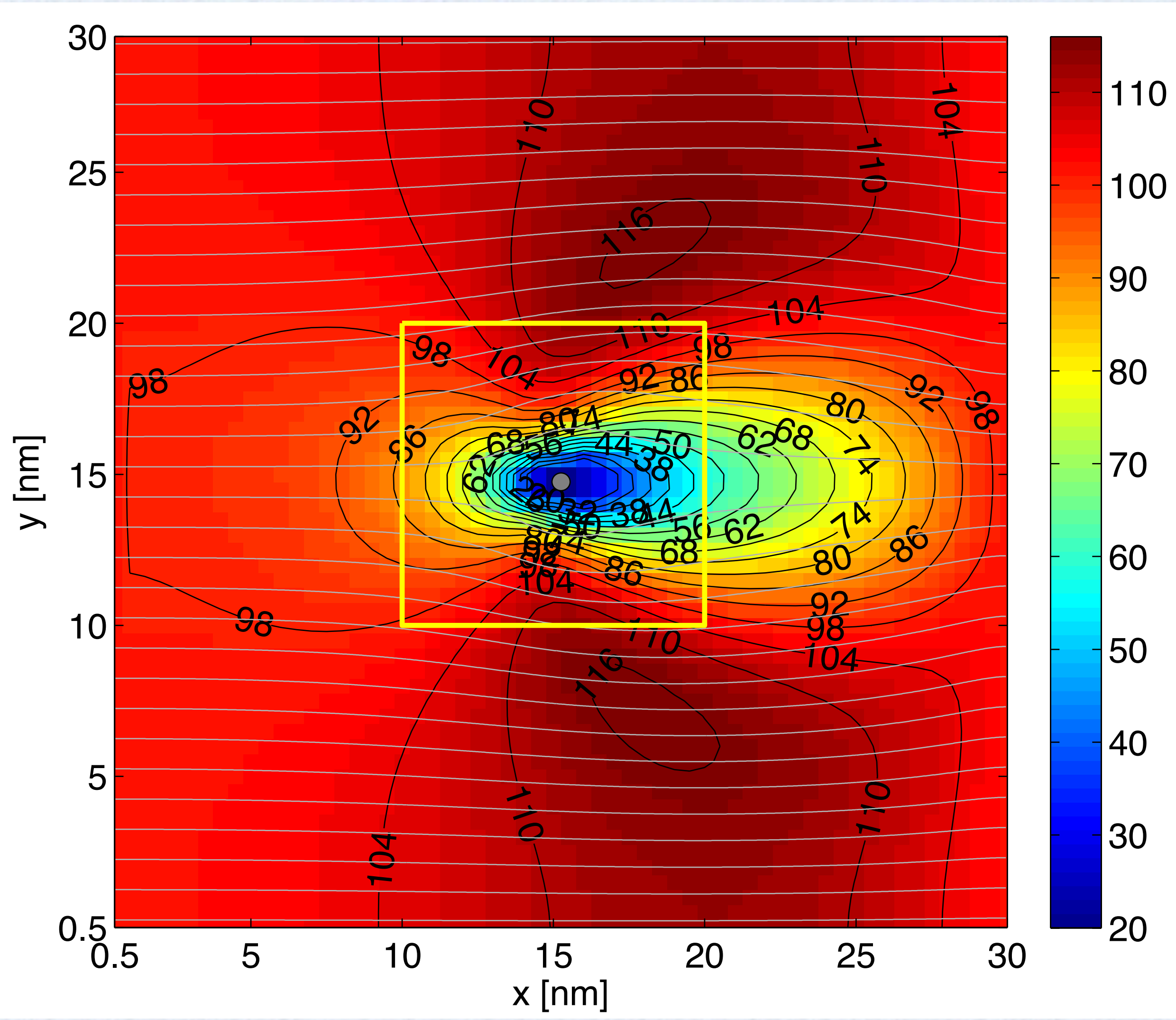
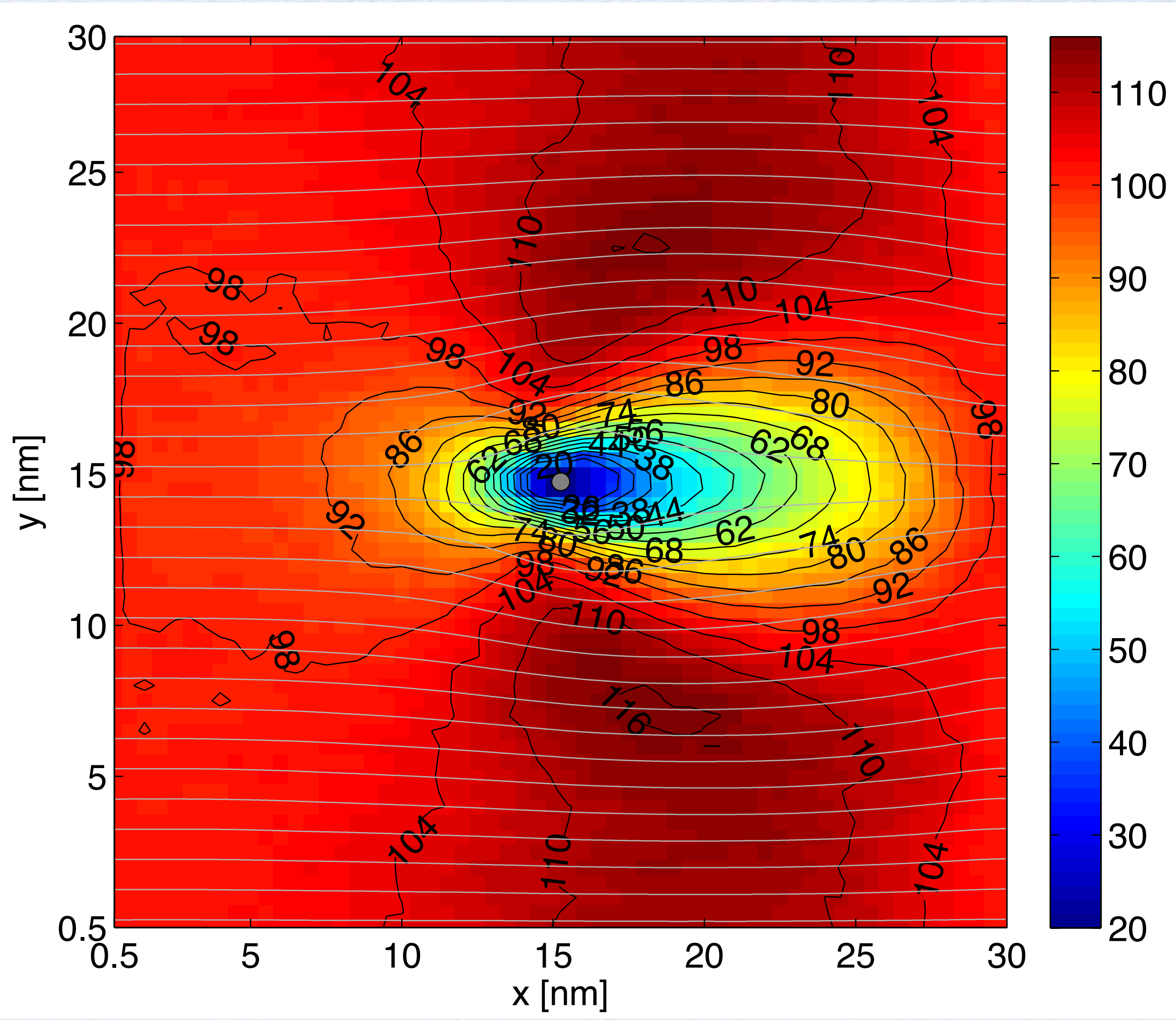
MD vs Hybrid scheme



Hybrid solution



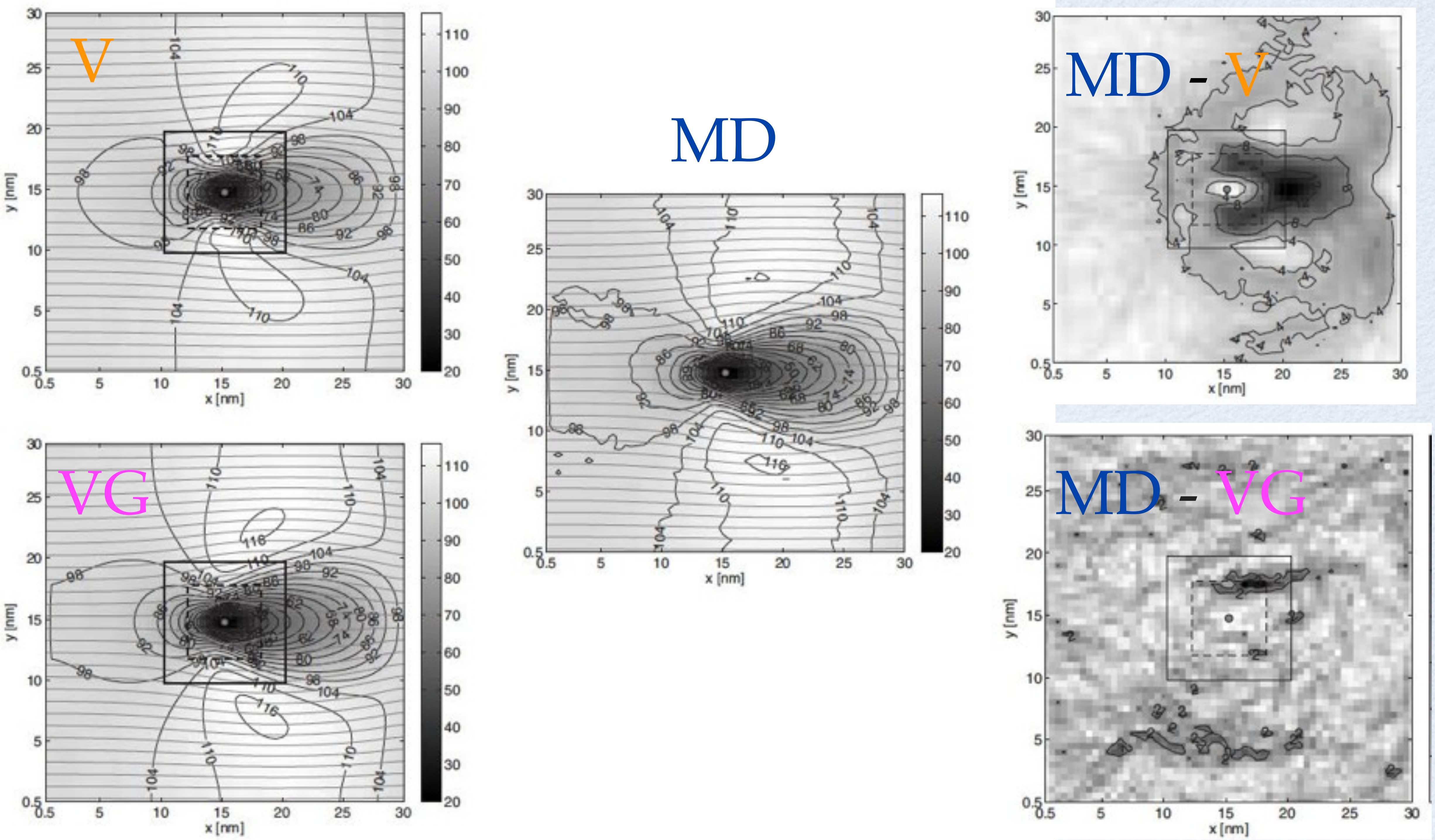
Reference MD solution

Relative Error ~ 1.3%

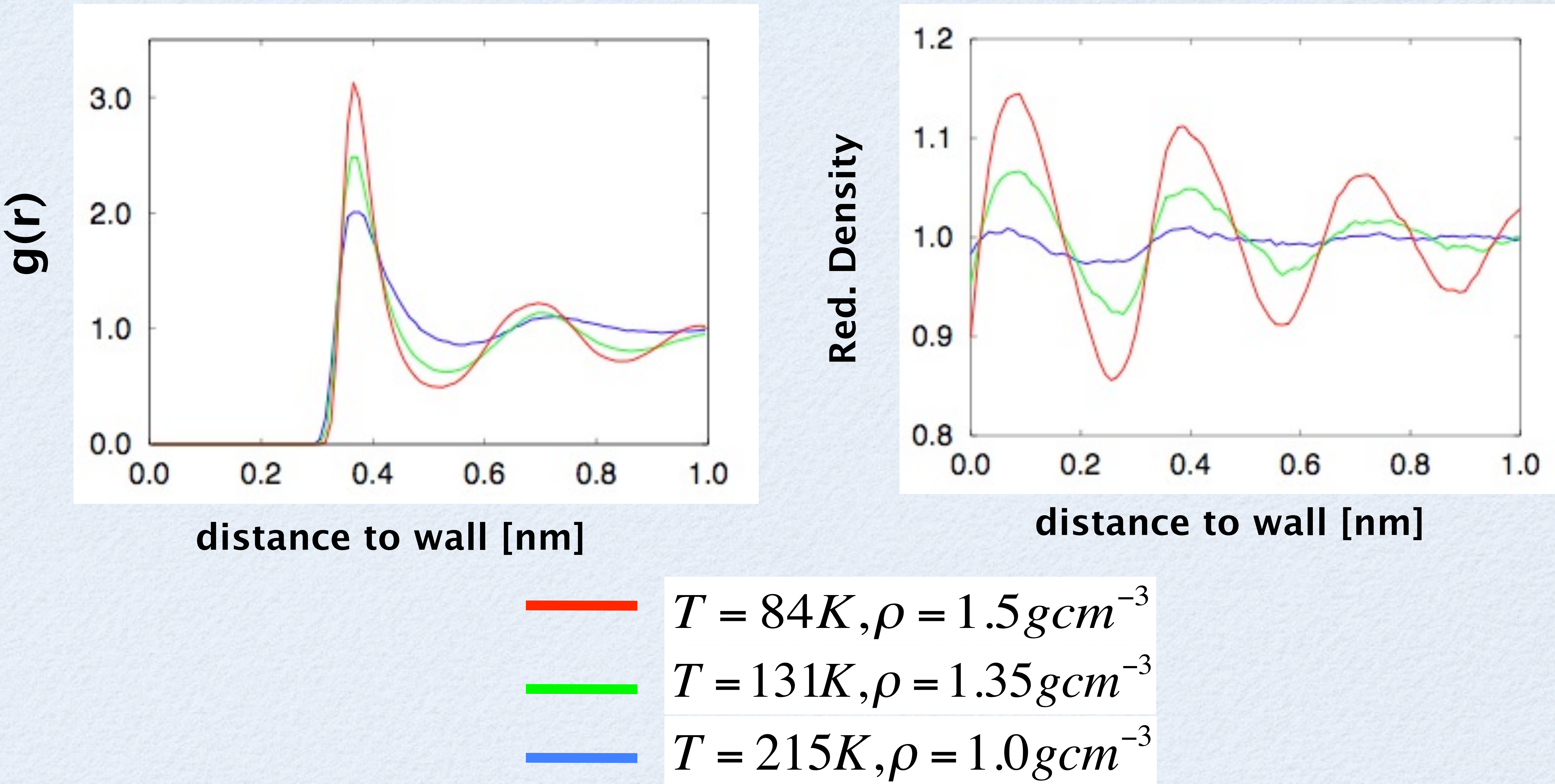
The hybrid scheme is ~ (L/R)3 times faster for a computational domain of size L and a MD subdomain of size R.**

A. Dupuis, E.M. Kotsalis, and PK., Coupling lattice Boltzmann and molecular dynamics for dense fluids. Phys. Rev. E, 75: 046704, 2007

Errors for Different Couplings



The problem with density variations

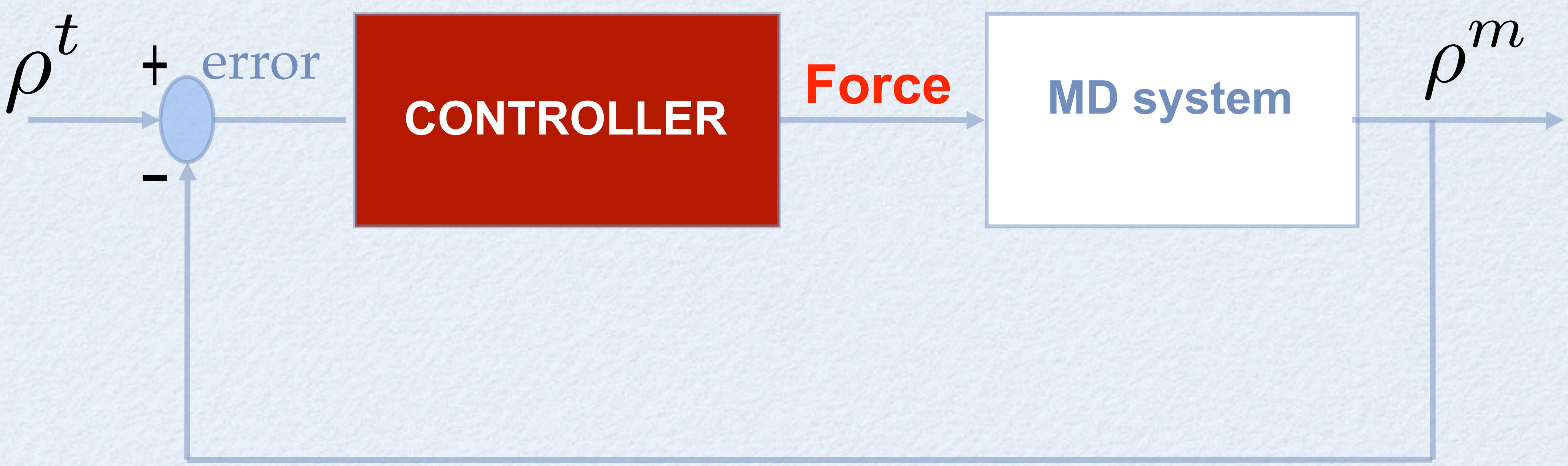


- Density variations depend on liquid state
- **Amplitude** proportional to **structural correlations** in the liquid

a simple **Control approach to Coupling**

E.M. Kotsalis, J.H. Walther, and P. Koumoutsakos., Phys. Rev. E, 2007.

- Controlling of the external boundary force
- measured density ρ^m => target density ρ^t

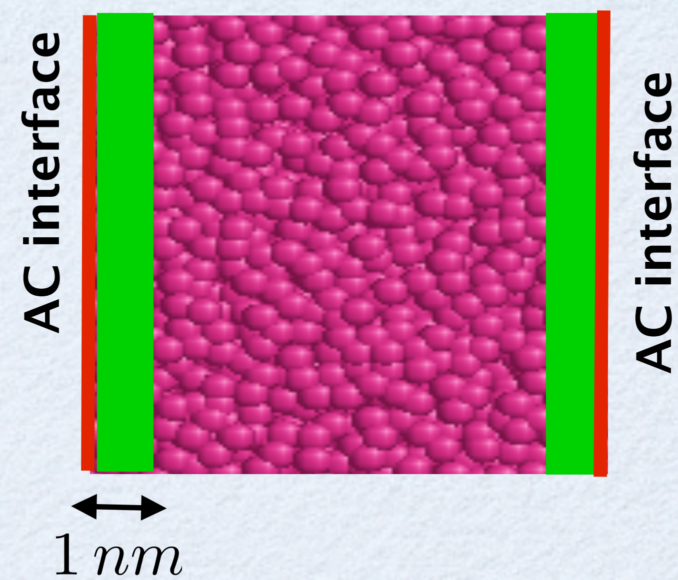


$$e(r) = \rho^t(r) - \rho^m(r)$$

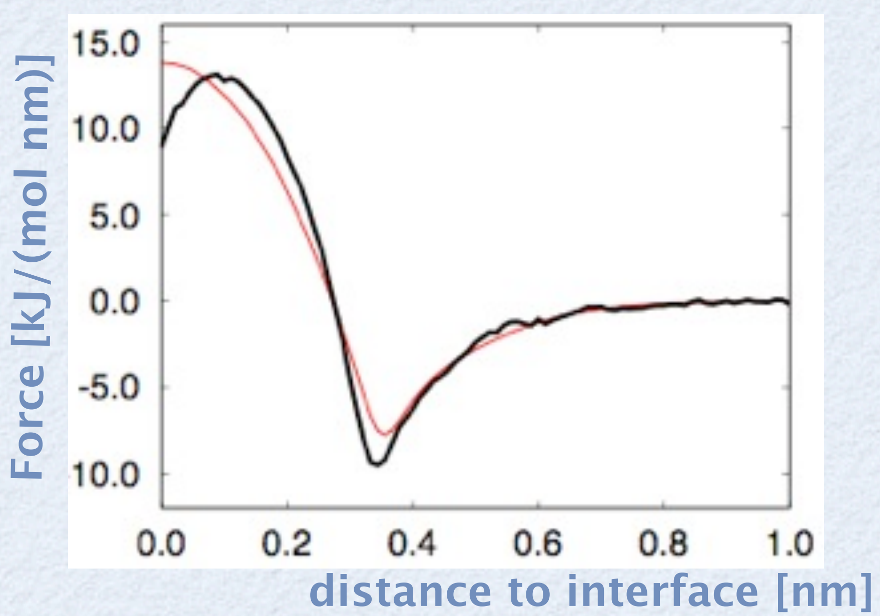
$$\textbf{Force} = k\nabla e(r)$$

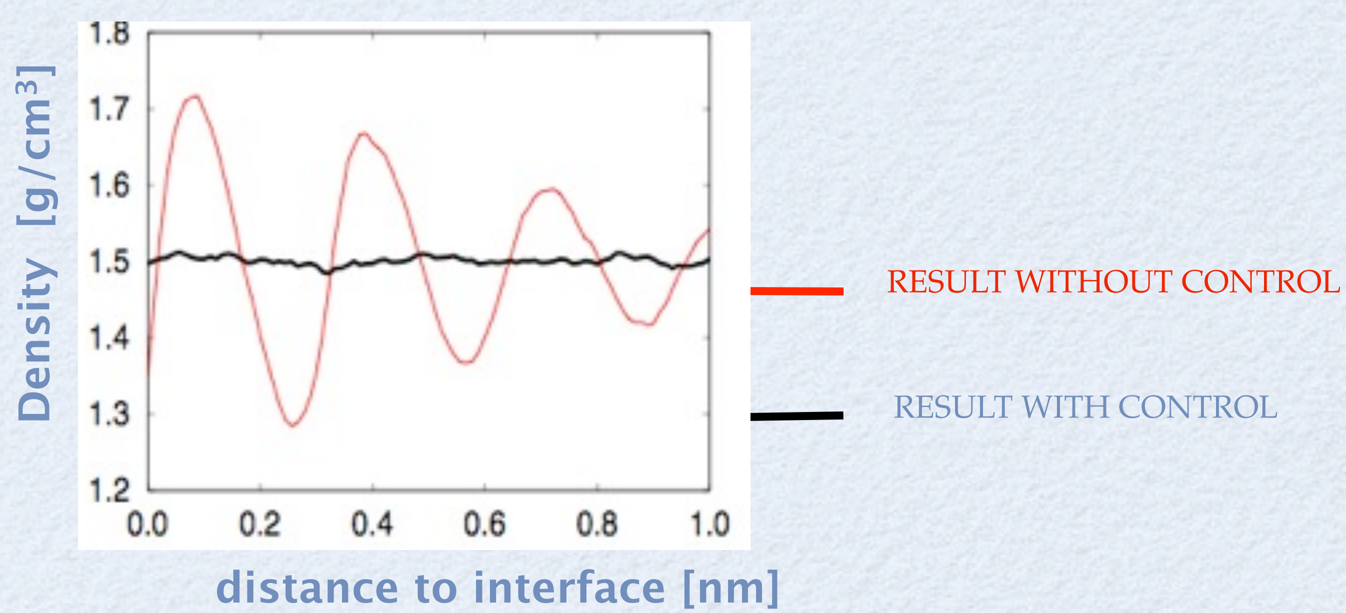
Results with Control Approach I

- at equilibrium (no flow)
- $T = 84K, \rho = 1.5gcm^{-3}$



AC interface = Elastic Boundary+External Force

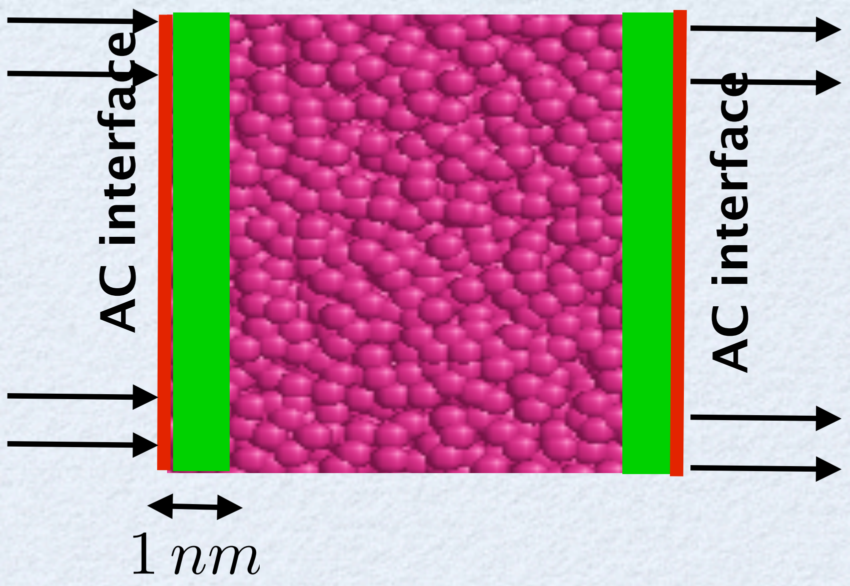




Controller deduces the boundary force

Results with Control Approach II

- uniform flow
- $T = 131K, \rho = 1.35gcm^{-3}$



Results with Control Approach II

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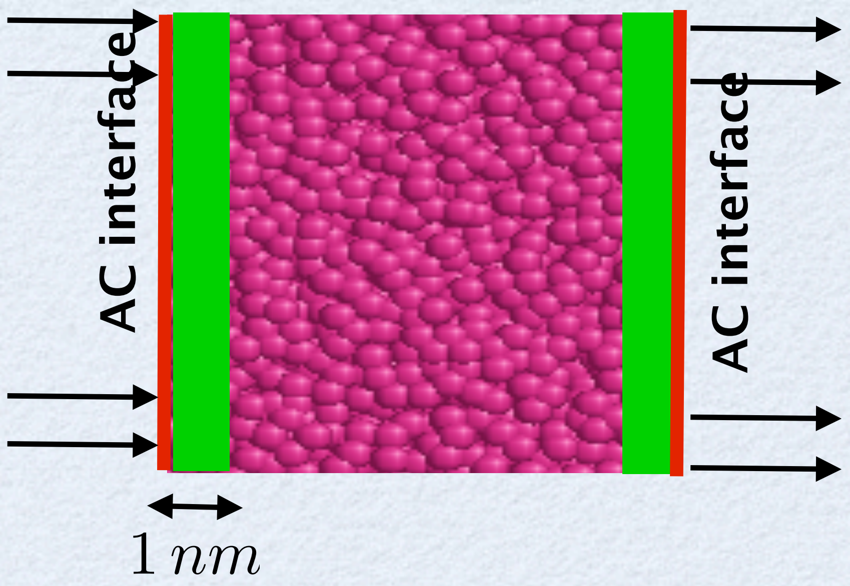
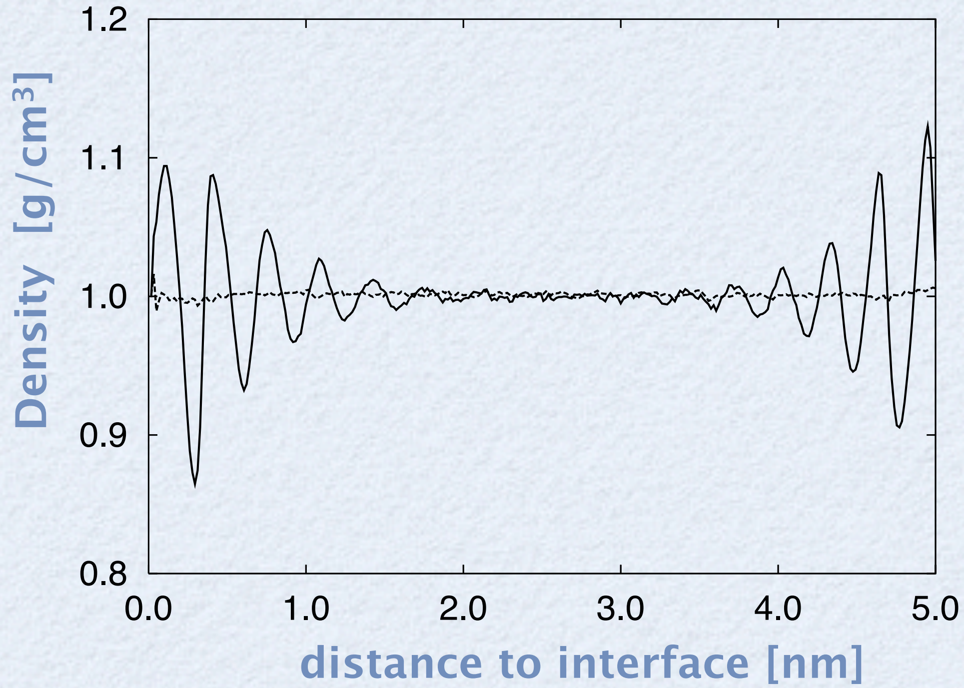
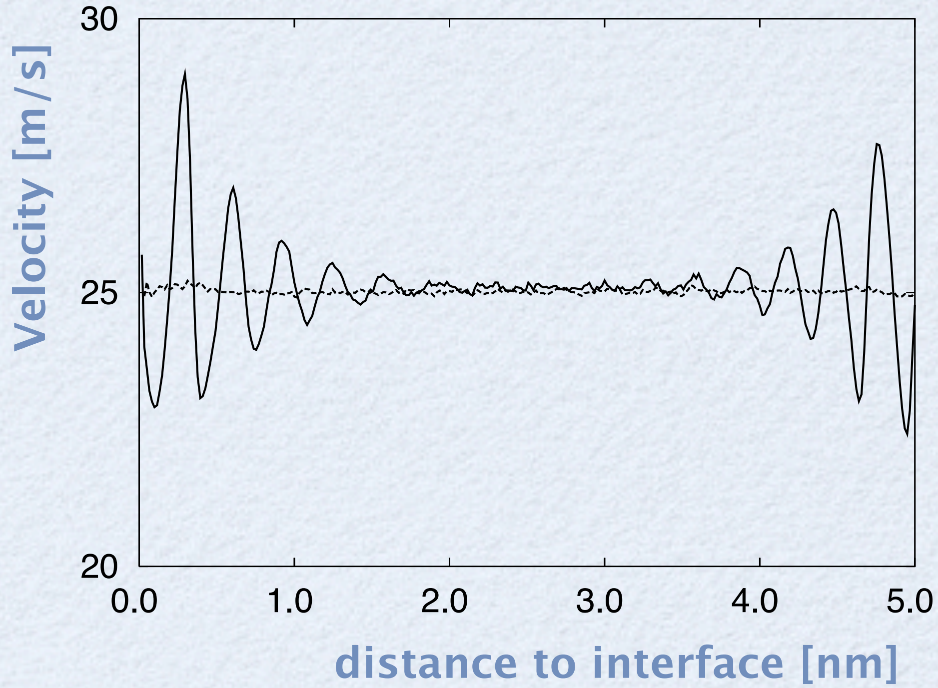


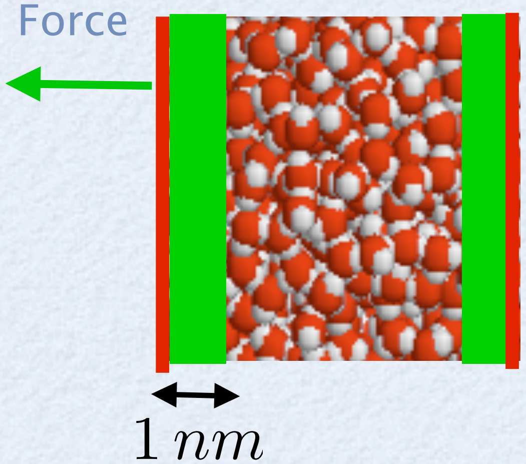




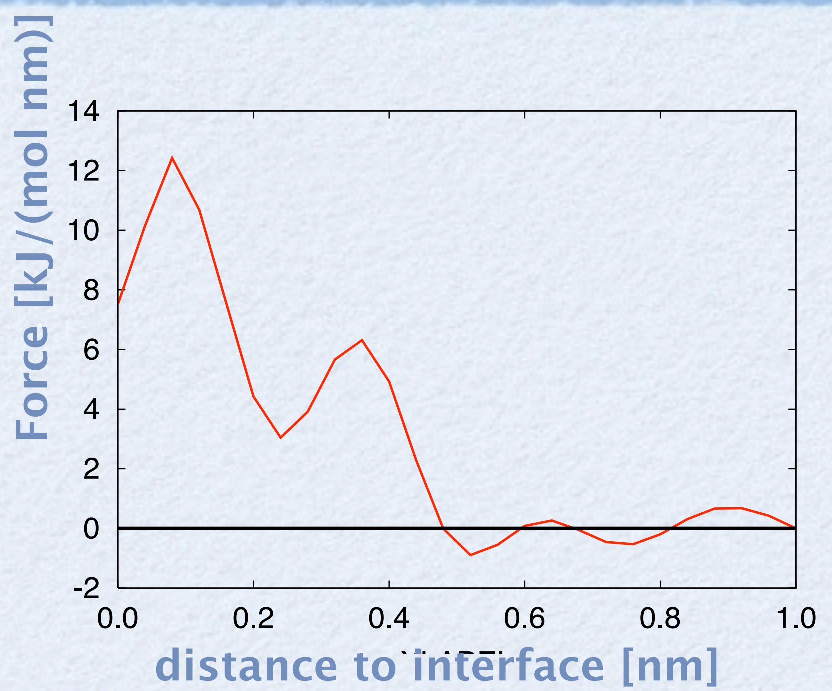
RESULT WITH CONTROL

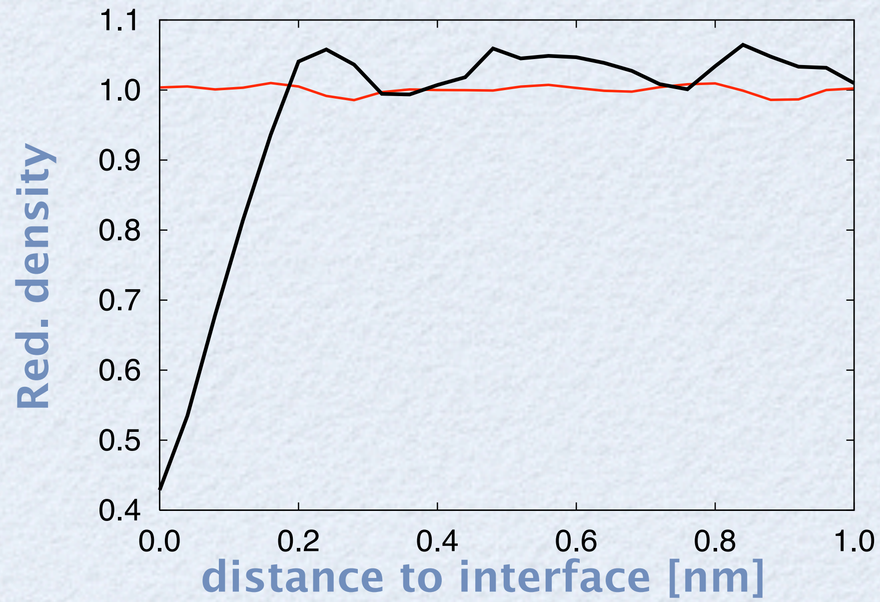
RESULT WITHOUT CONTROL

AC Interface for Water at Equilibrium



1D embedding





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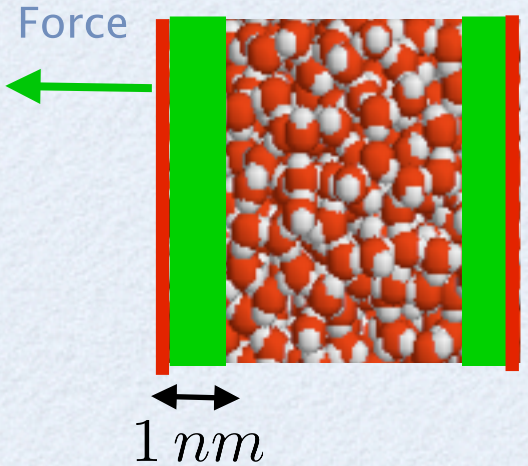
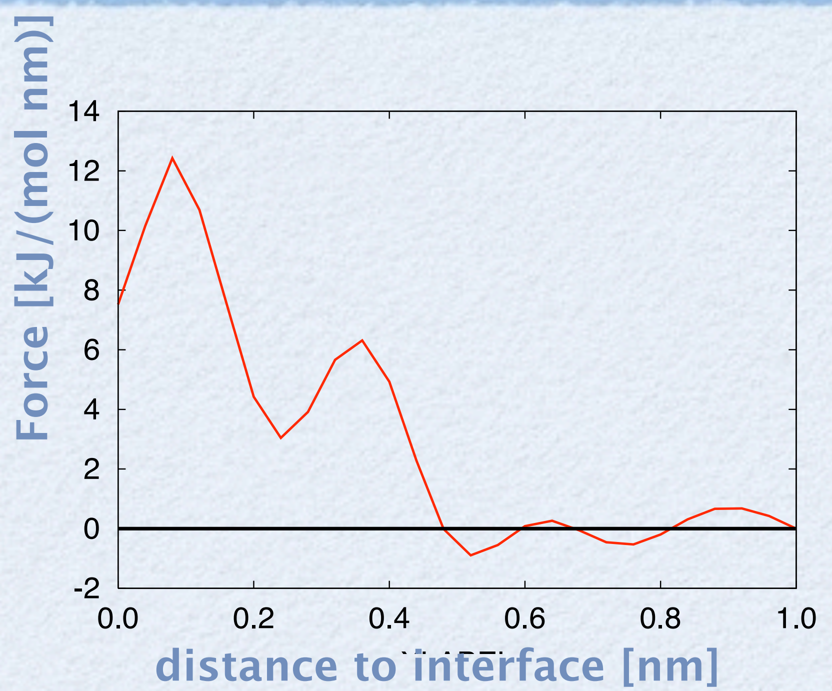
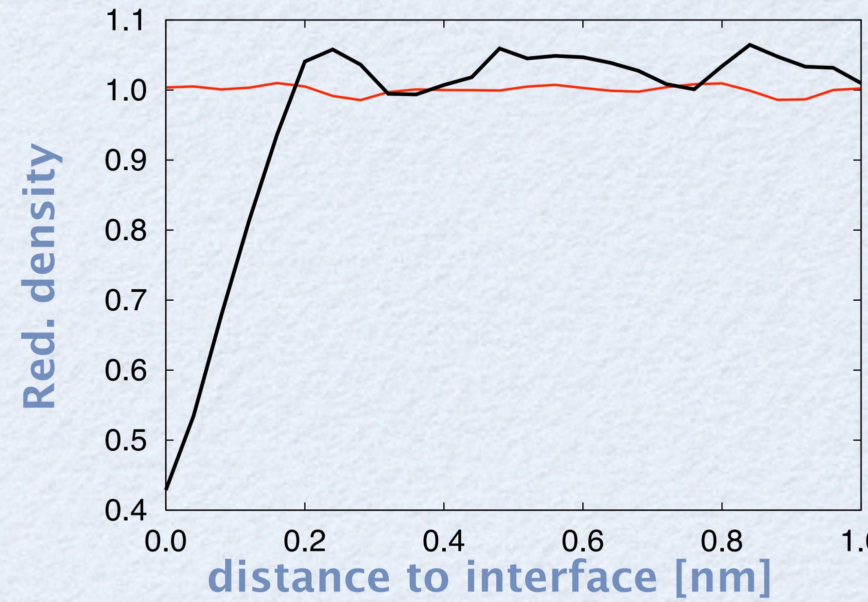


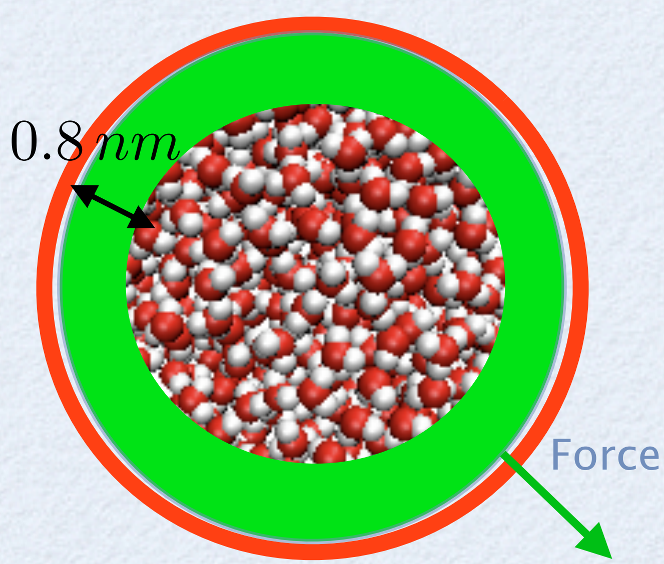
1D embedding



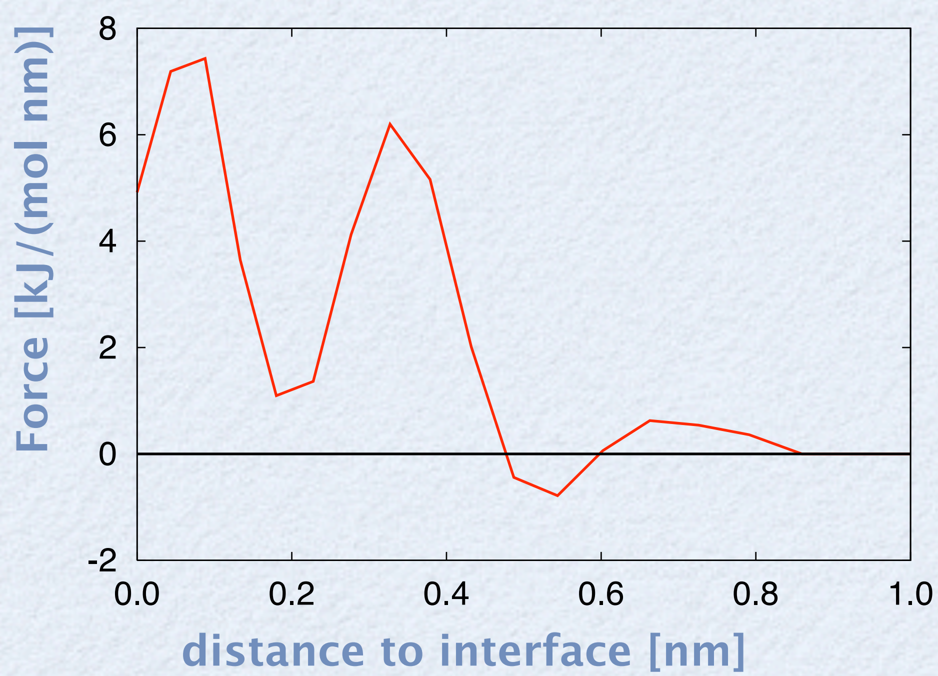


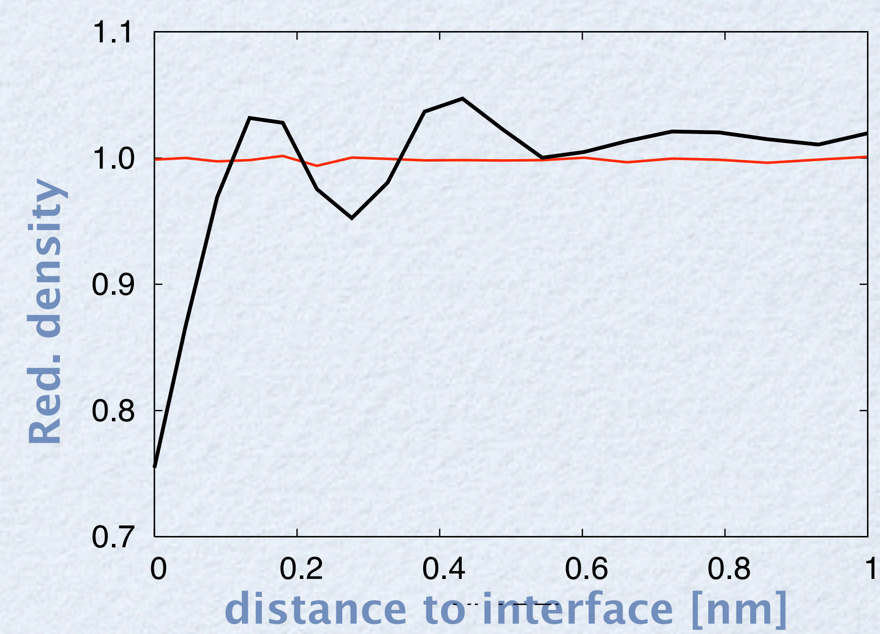
RESULT WITH CONTROL

RESULT WITHOUT CONTROL

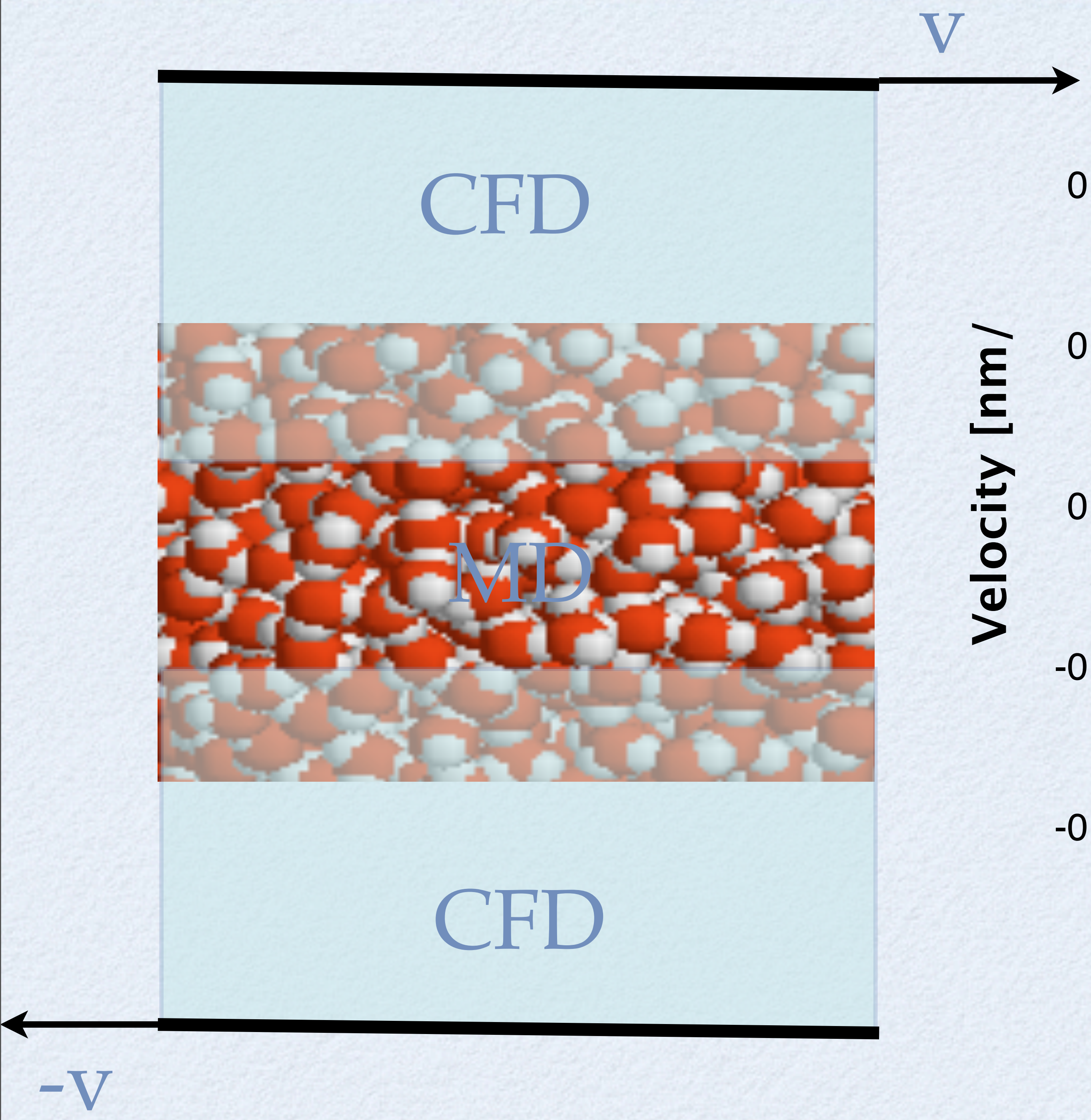


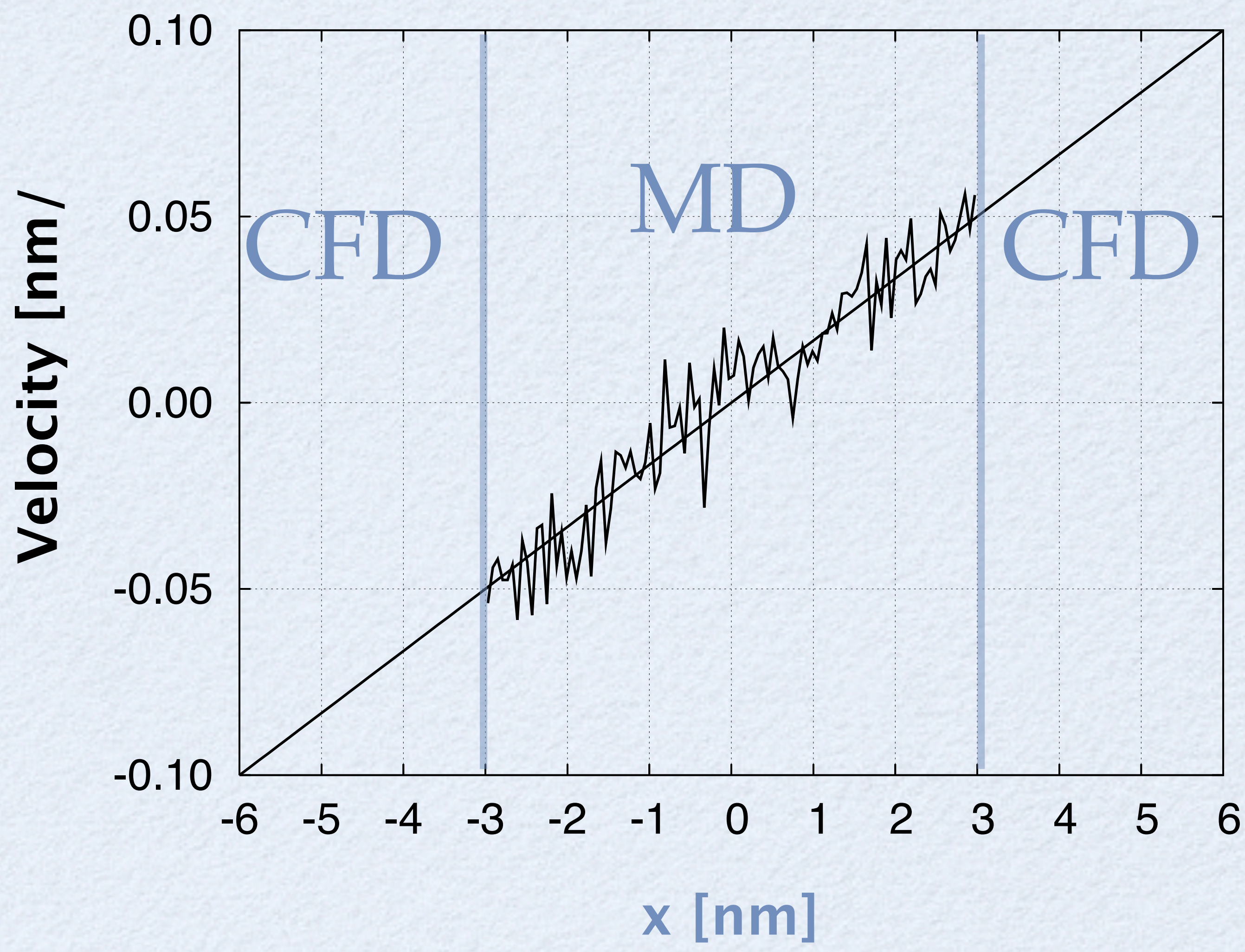
Spherical embedding



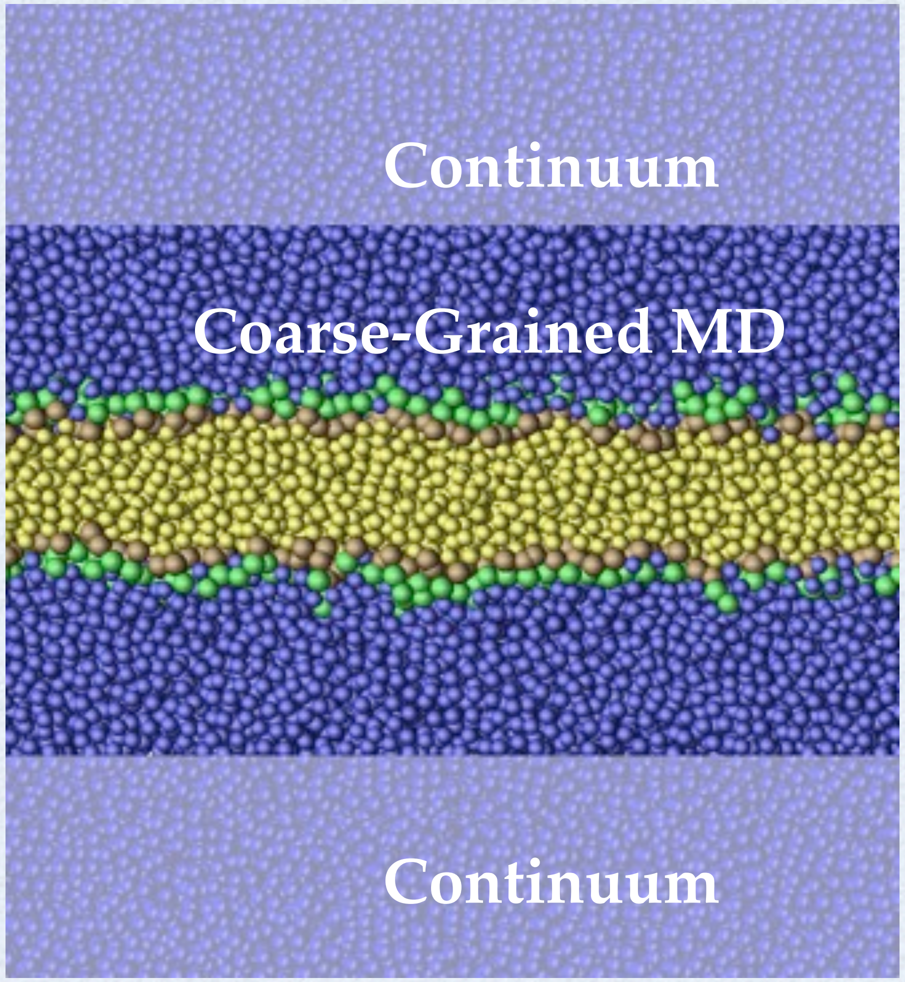


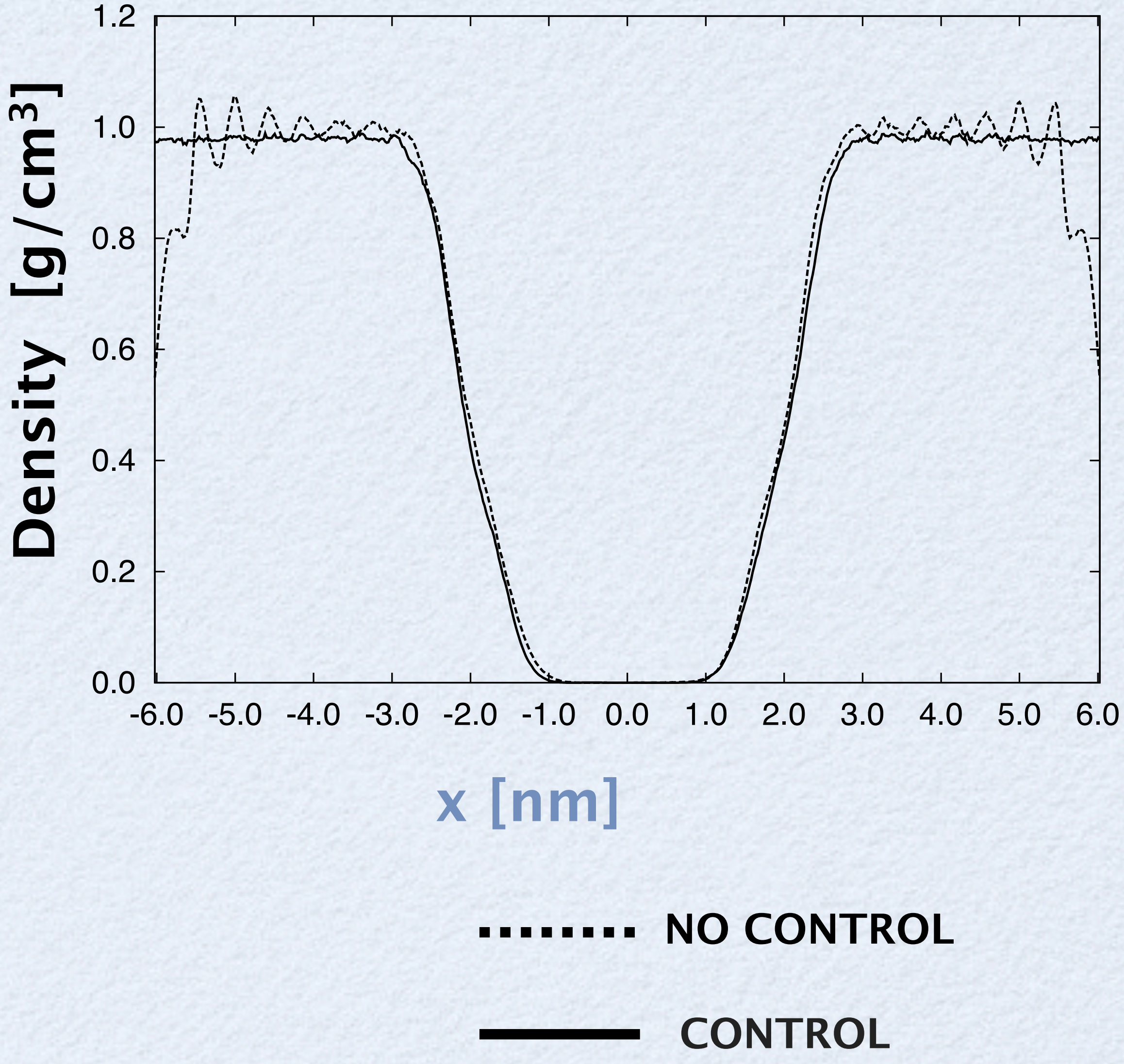
Water Couette Flow





Multiscale Membrane Simulation

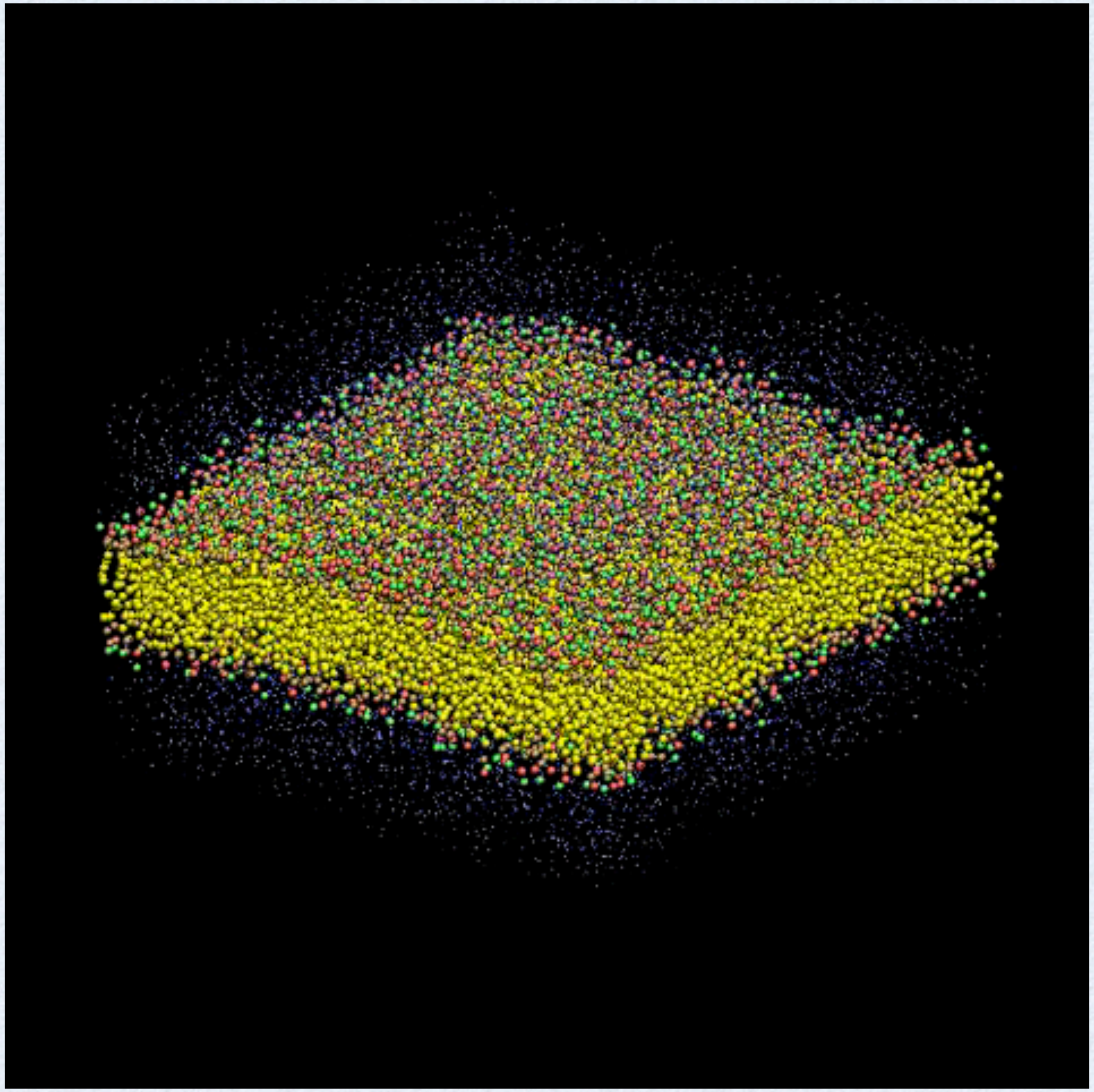


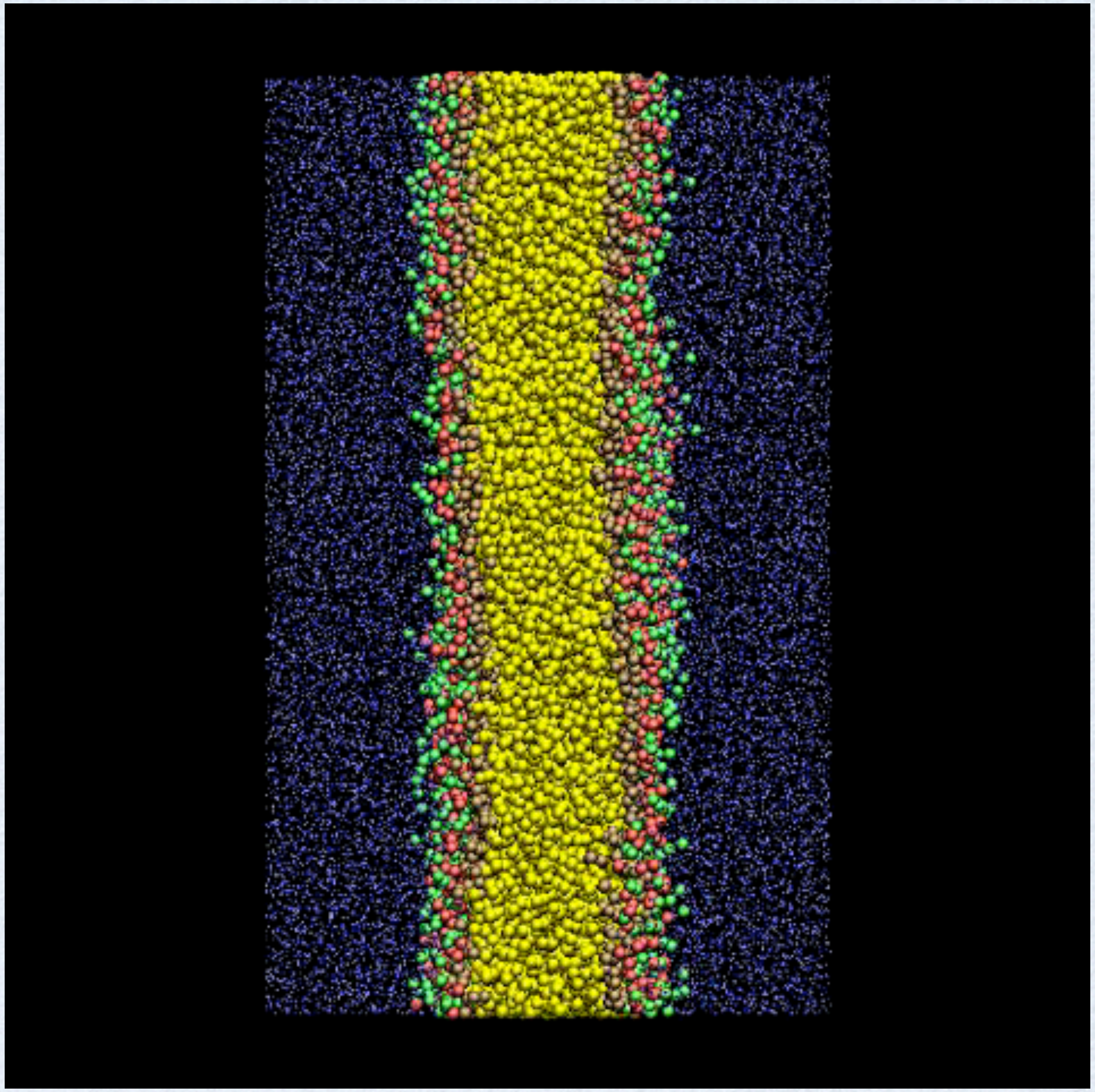


CG DPPC lipid surrounded by CG water.
Size: 12 nm x 20 nm x 20 nm

- 26250 CG water molecules
- 1250 CG lipid molecules

Multiscale Membrane Simulation





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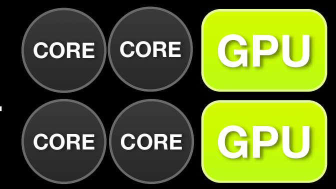
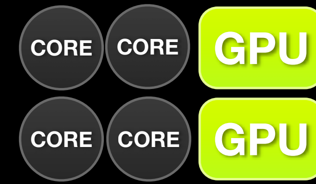
MULTISCALE METHODS

MULTISCALE METHODS +

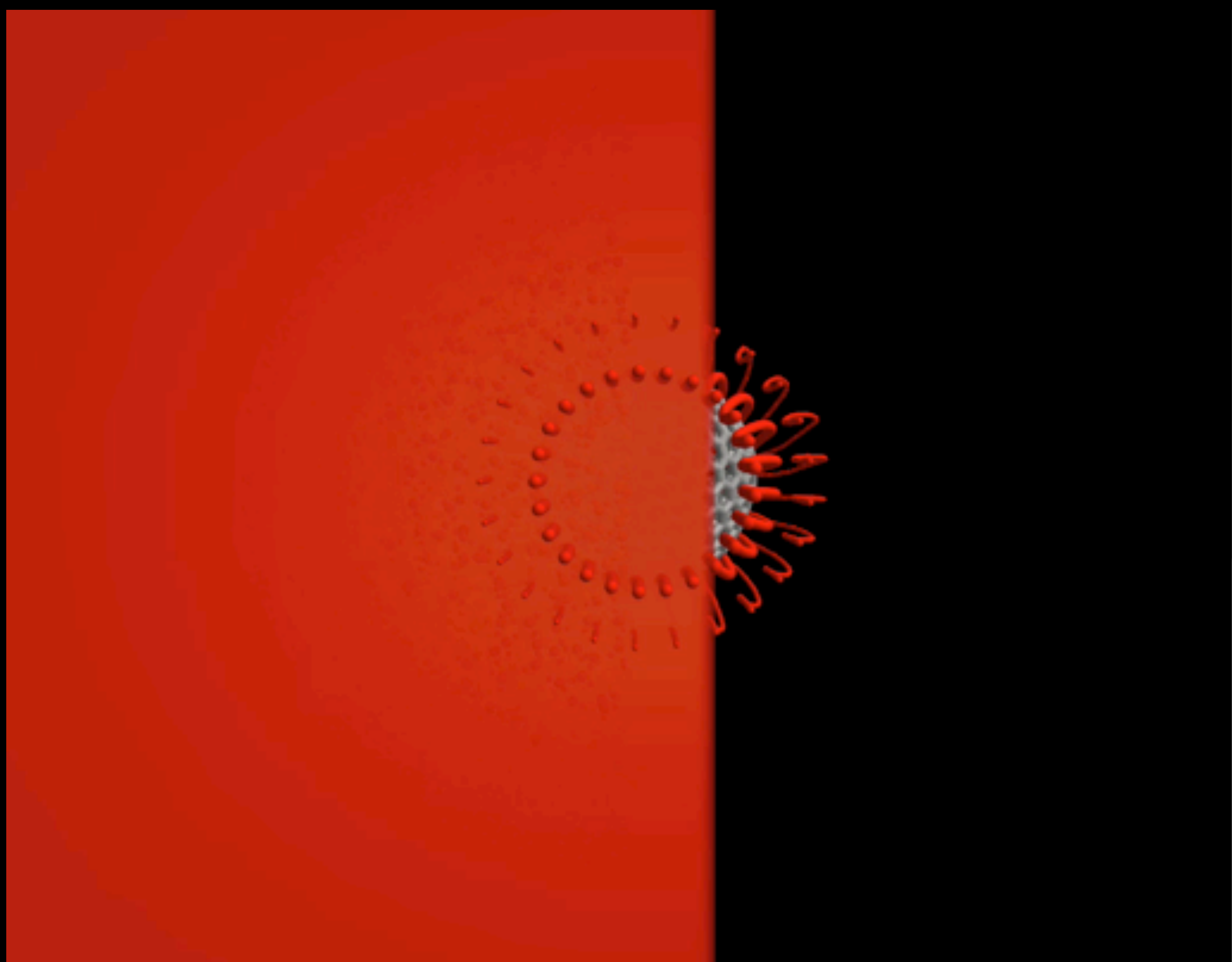


MD - Lattice-Boltzmann

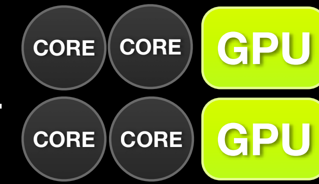
MULTISCALE METHODS +



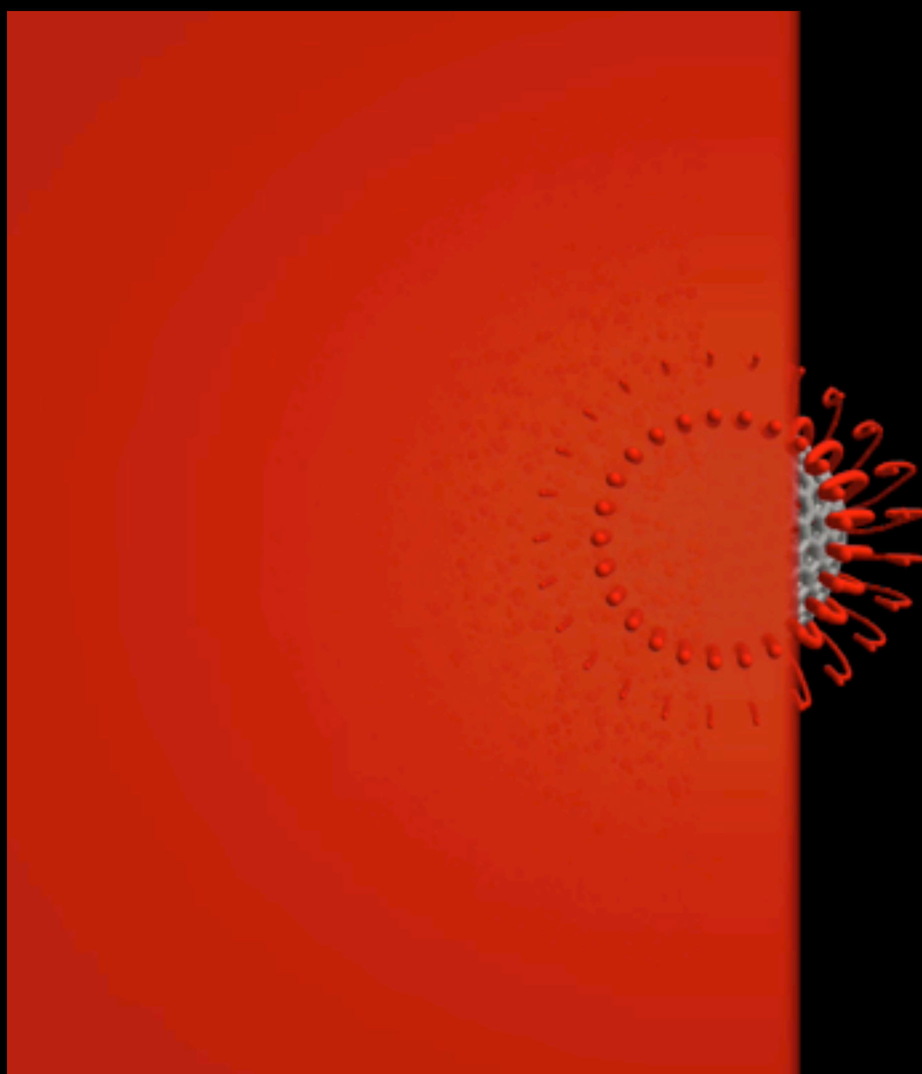
MD - Lattice-Boltzmann

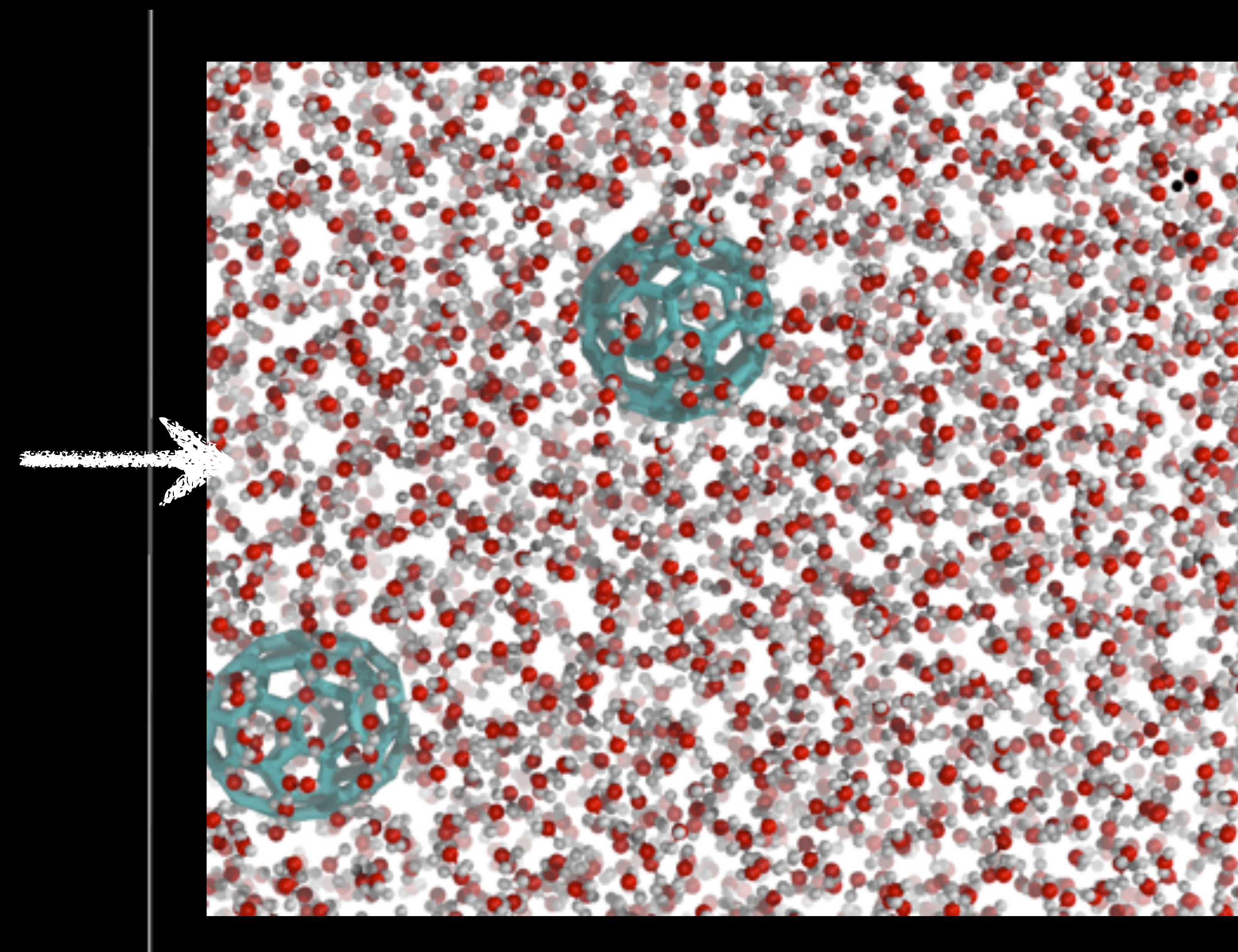


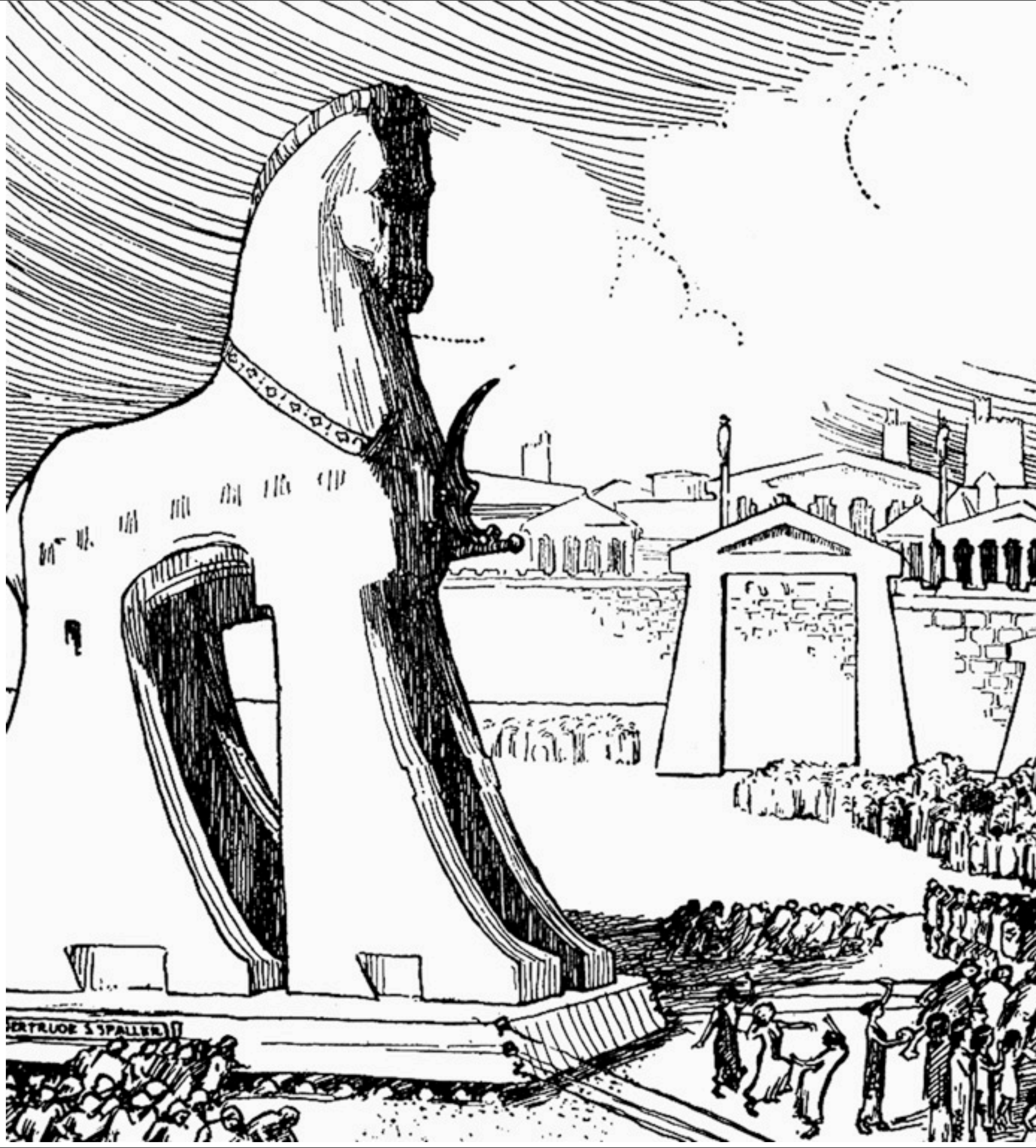
MULTISCALE METHODS +



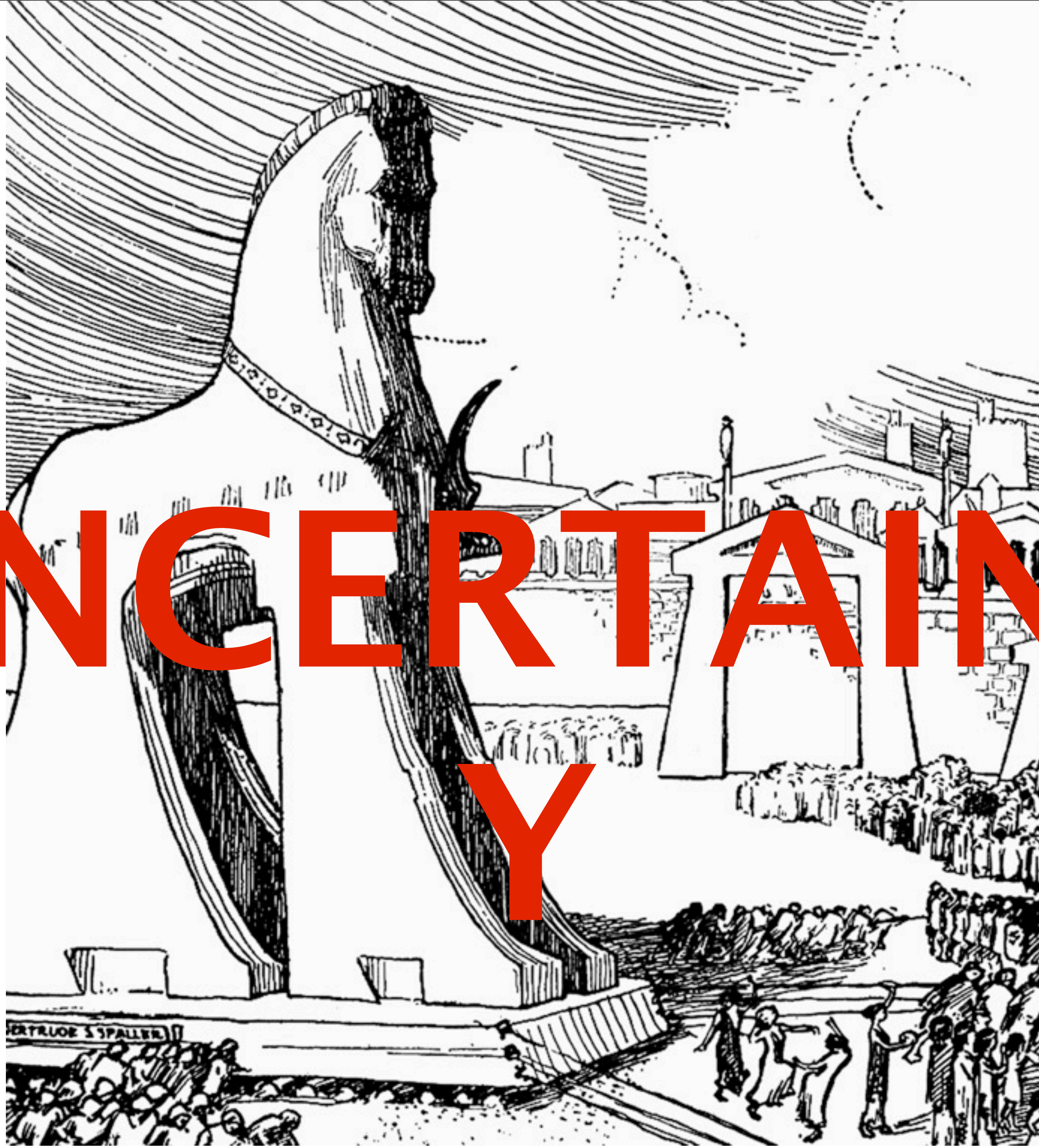
MD - Lattice-Boltzmann





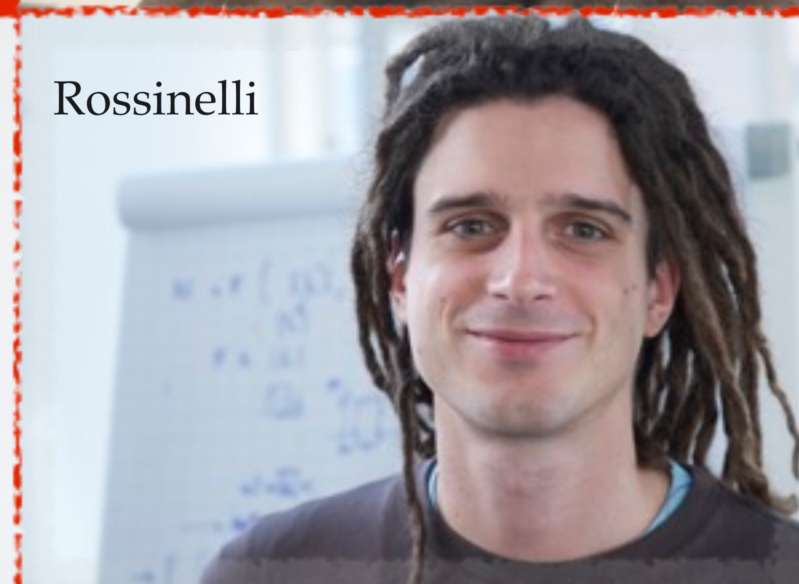

ERTRUDE S SPALLER

UNCERTAINTY




Bergdorf


Walther


Rossinelli


Chatelain


Hedjazialhosseini