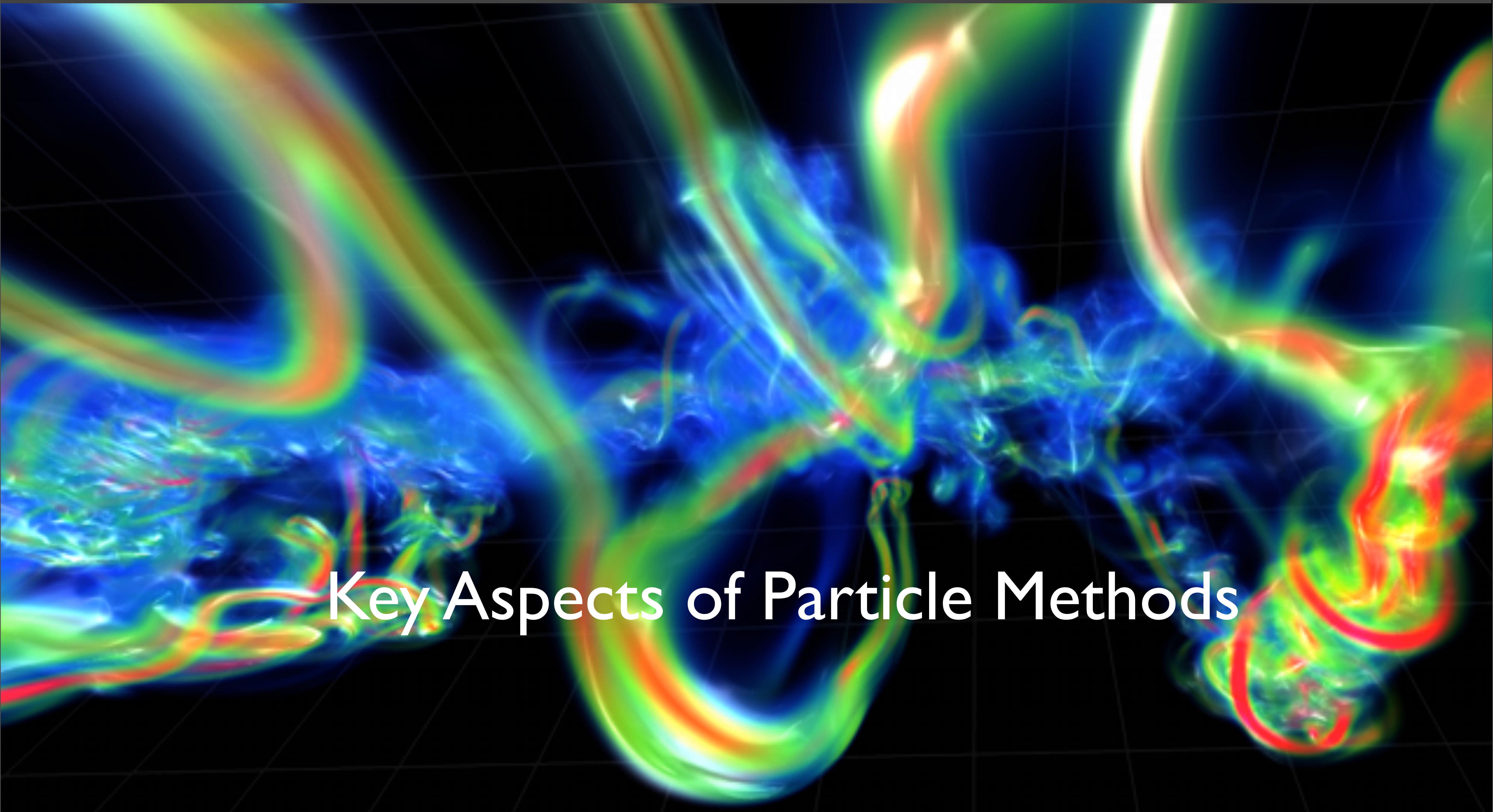


Key Aspects of Particle Methods

Simone Hieber
Biozentrum, Basel
with
Prof. Petros Koumoutsakos, CSE-Lab, ETH Zurich

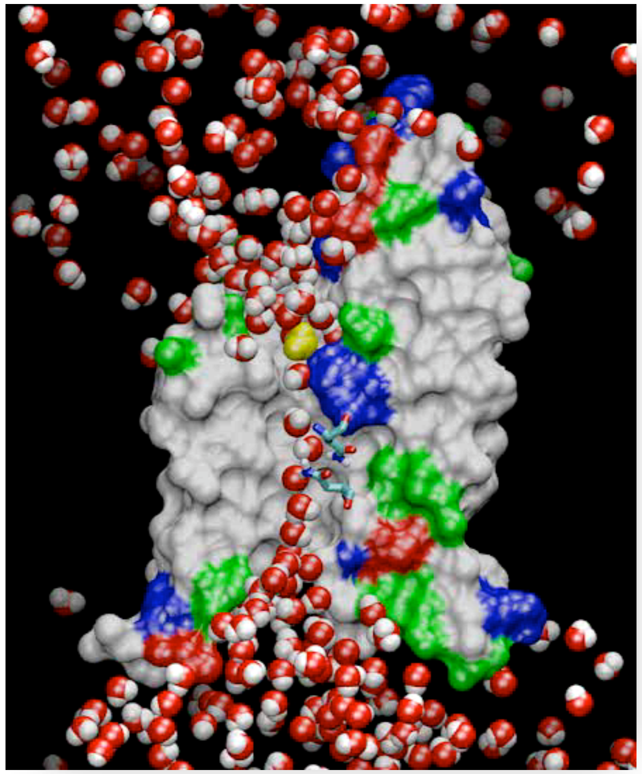
CSE Lab
ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

SIMULATIONS WITH PARTICLES

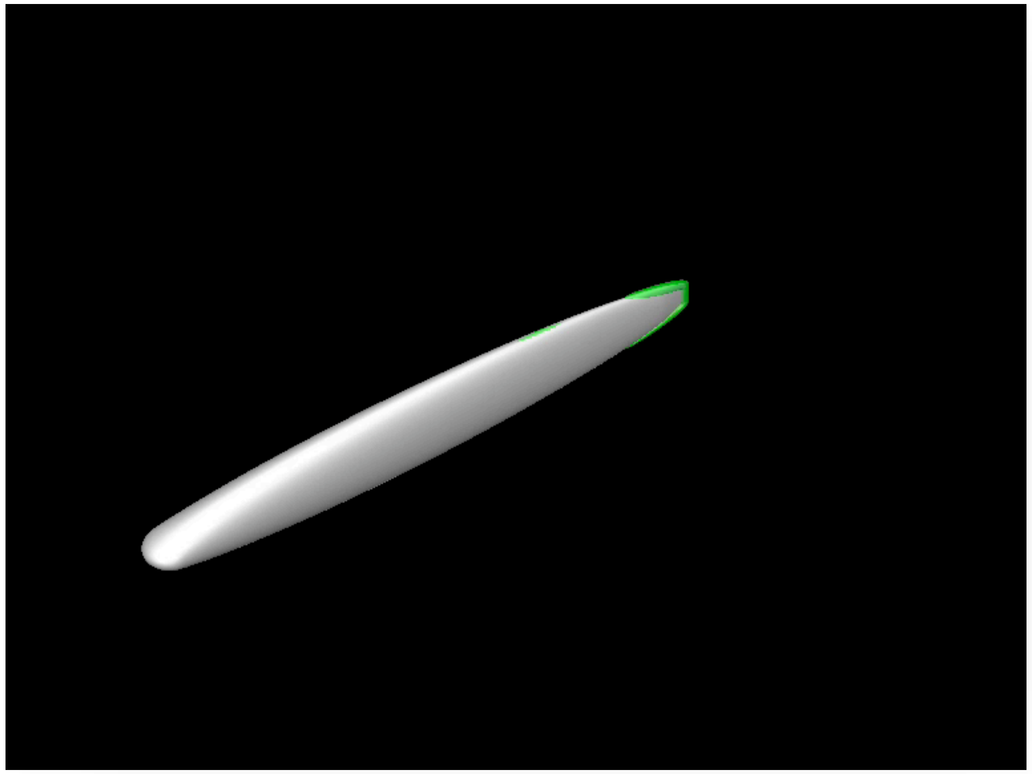
-9

0

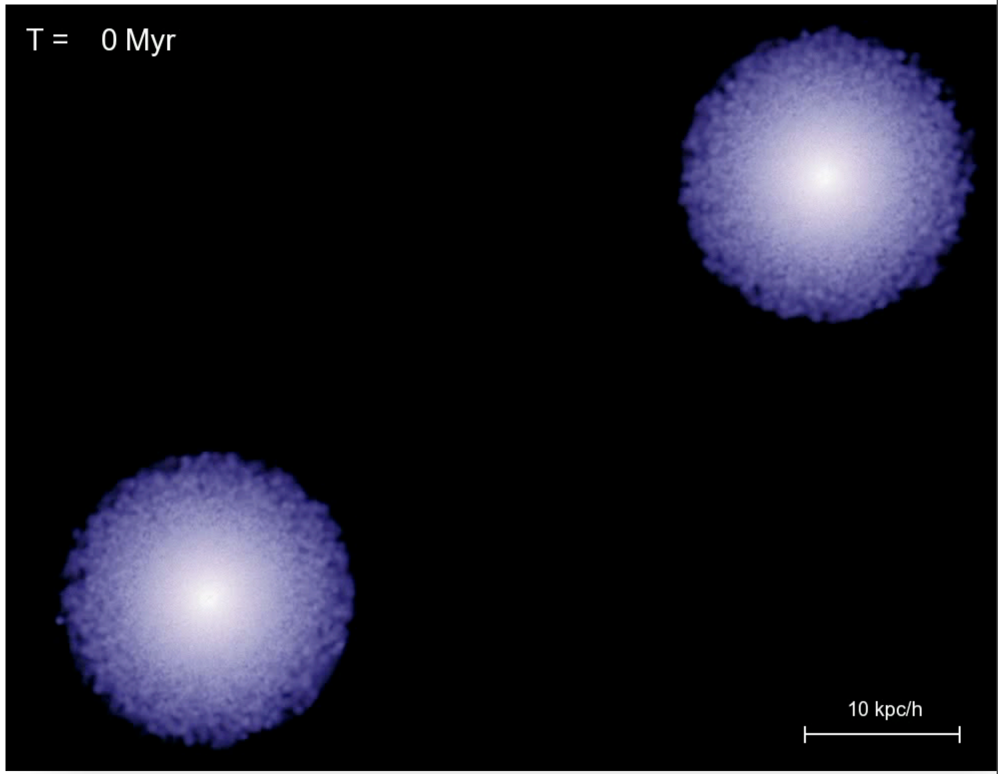
+9



Transport in aquaporins
Schulten Lab, UIUC



Anguiliform Swimmers
Koumoutsakos Lab, ETHZ

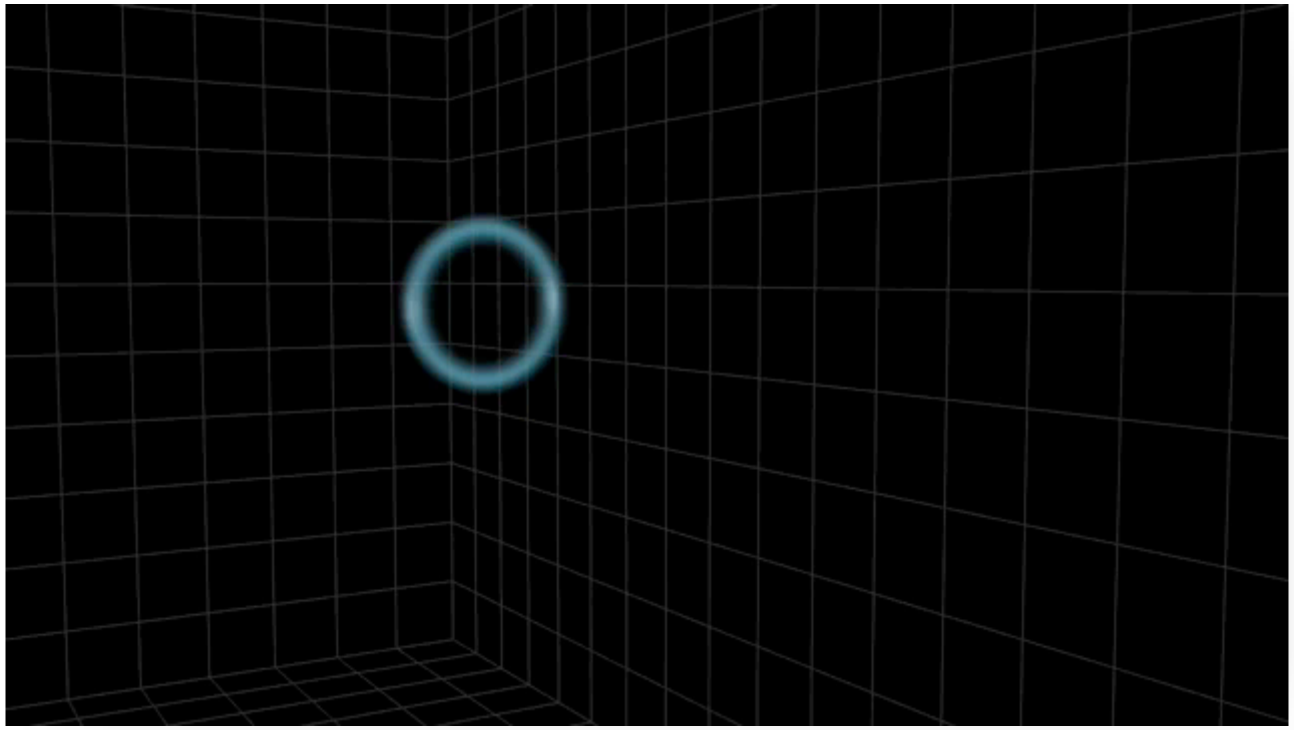


Growth of Black Holes
Springel, MPI - Hernquist, Harvard

Particles : “Smooth” - Discrete

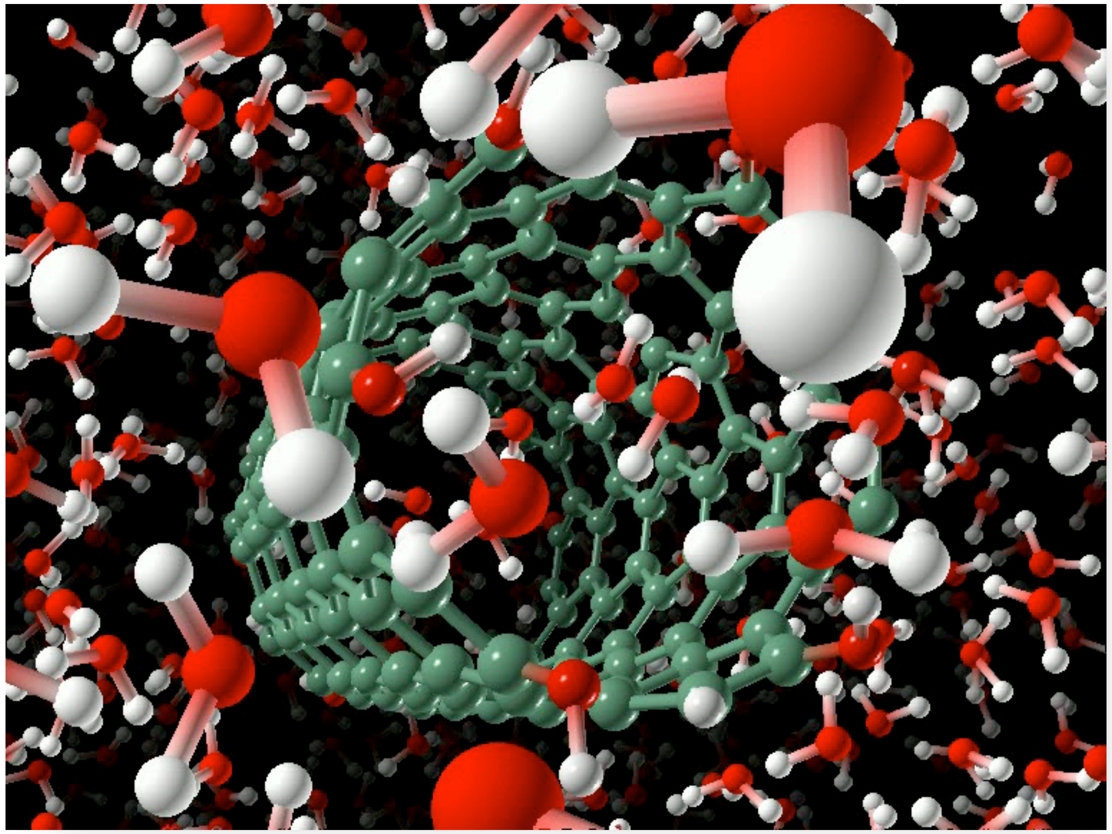
Smooth = APPROXIMATE

- Smoothed Particle Hydrodynamics
- Vortex Methods
- Lagrangian level sets



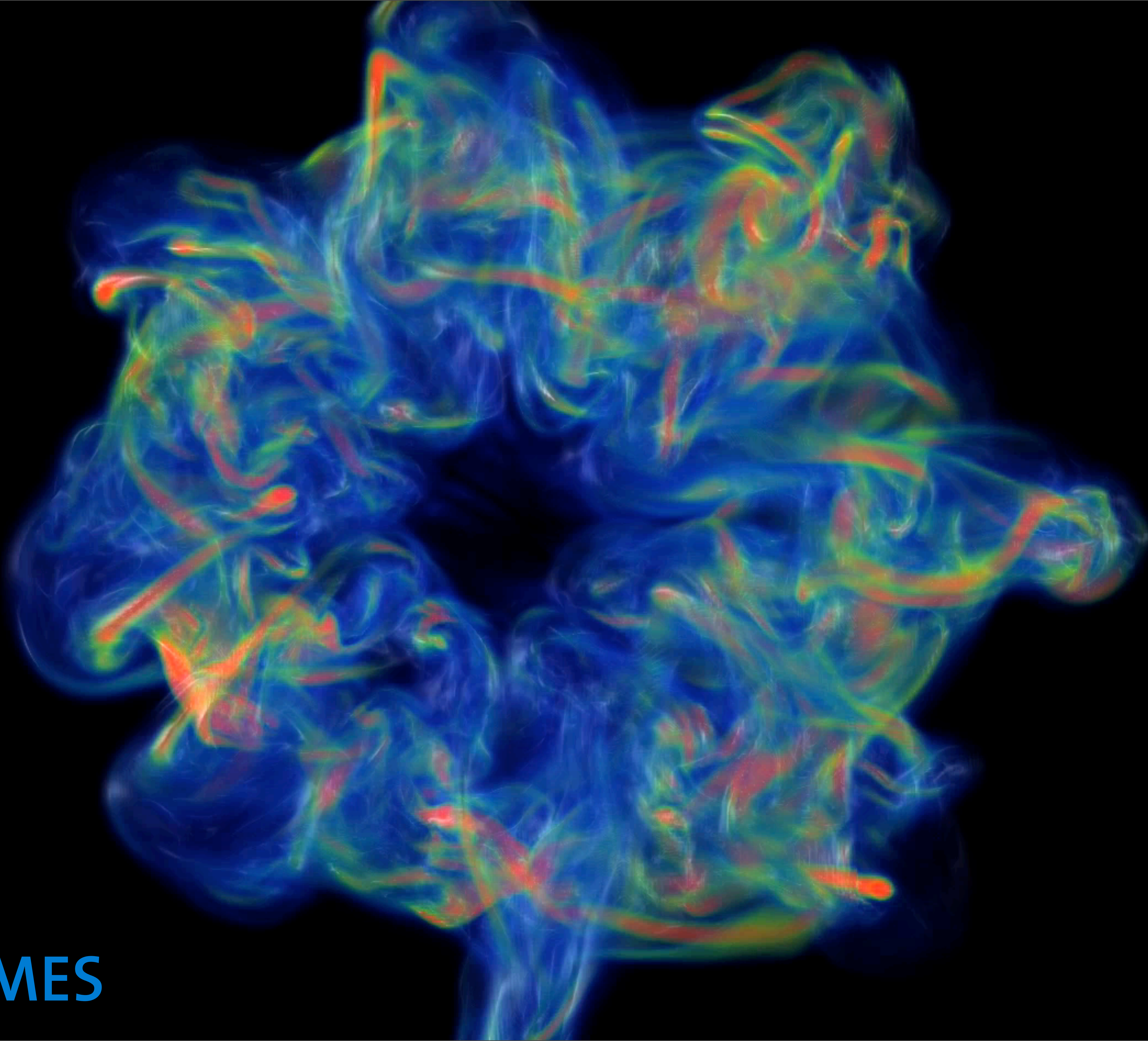
Discrete = MODEL

- Molecular Dynamics (MD)
- Dissipative Particle Dynamics
- Stochastic Simulation



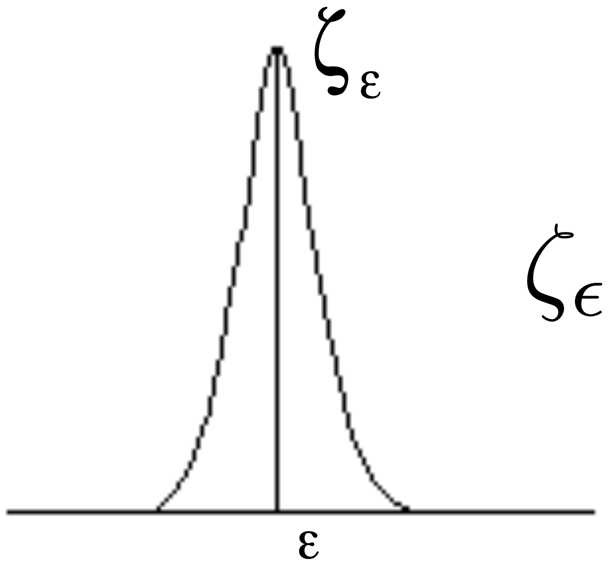
Particle Approximations

- Volumes
- Surfaces and Interfaces
- Equations

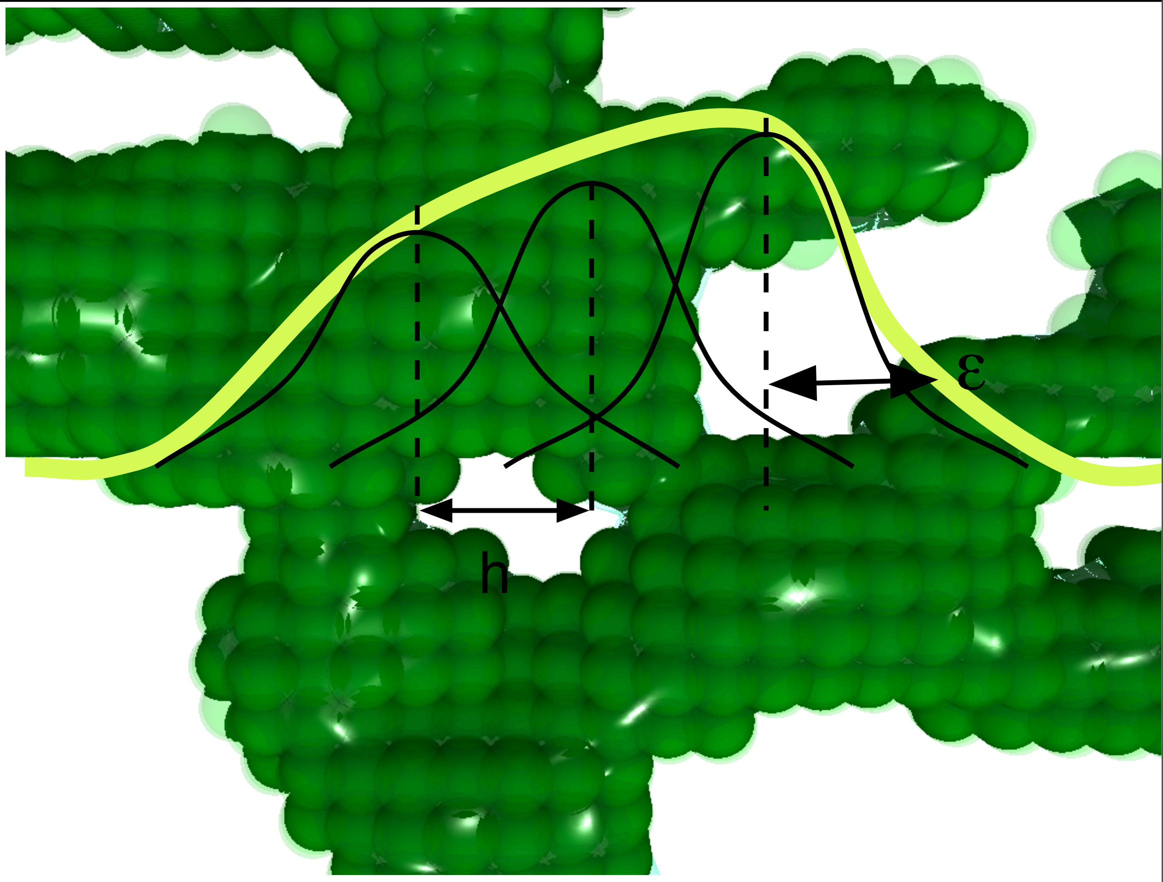


VOLUMES

Functions on Particles



$$\zeta_\epsilon = \frac{1}{\epsilon^d} \zeta(\frac{x}{\epsilon})$$



Particles $p = 1, \cdots, N$

locations x_p **volumes** $v_p = h_p^d$

properties:

$\mathbf{Q}_p(t) = q(x_p, t)$

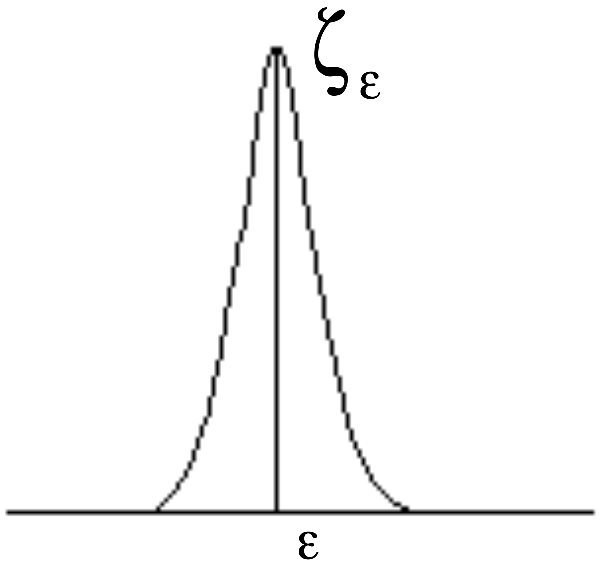
Function approximation $$q_\epsilon^h(x,t) = \sum_{p=1}^{N_p} h_p^d \, Q_p(t) \, \zeta_\epsilon(x - x_p(t))$$

Smoothing kernels approximate the Dirac-function

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

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

For $\mathbf{\Phi}$ *(with* **r** *continuous derivatives):* $\quad ||\Phi \; - \; \Phi_\epsilon|| \; \leq \; C\, \epsilon^r \; ||\Phi||_\infty$



$$\zeta_\epsilon \; = \; \frac{1}{\epsilon^d}\, \zeta(\frac{x}{\epsilon})$$

Cutoff Function : ζ must satisfy the following properties:

$$\int x^\alpha \zeta(x) dx = 0 \qquad 1 \leq |\alpha| \leq r-1$$

$$\int |x|^r |\zeta(x)| dx < \infty$$

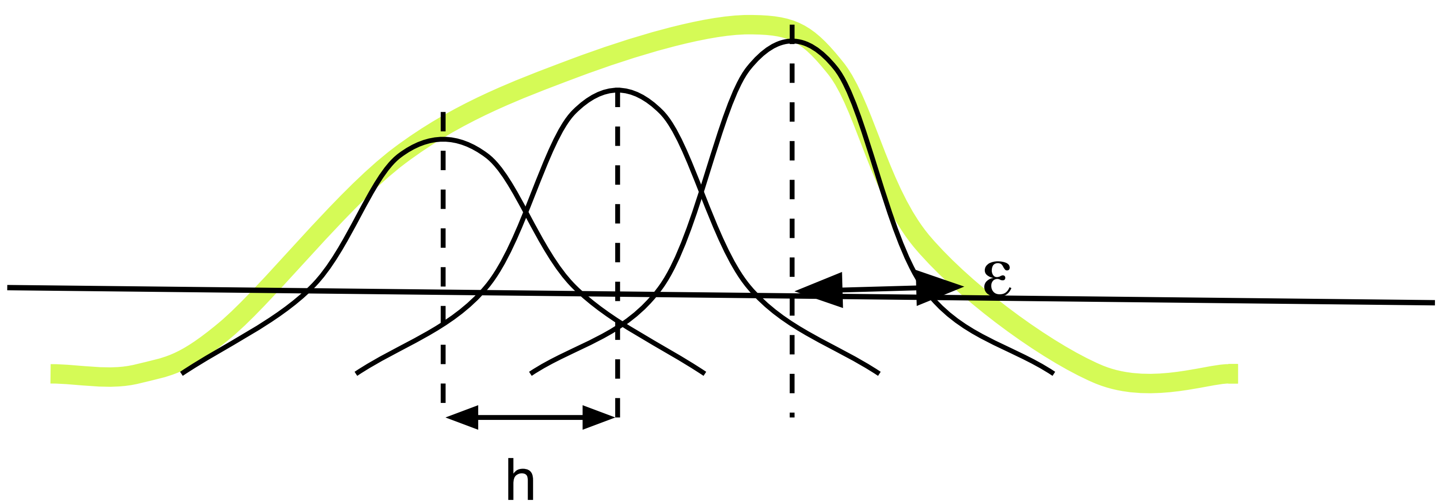
$$\int \zeta(x) dx = 1$$

Particles are quadrature points - Flexible locations

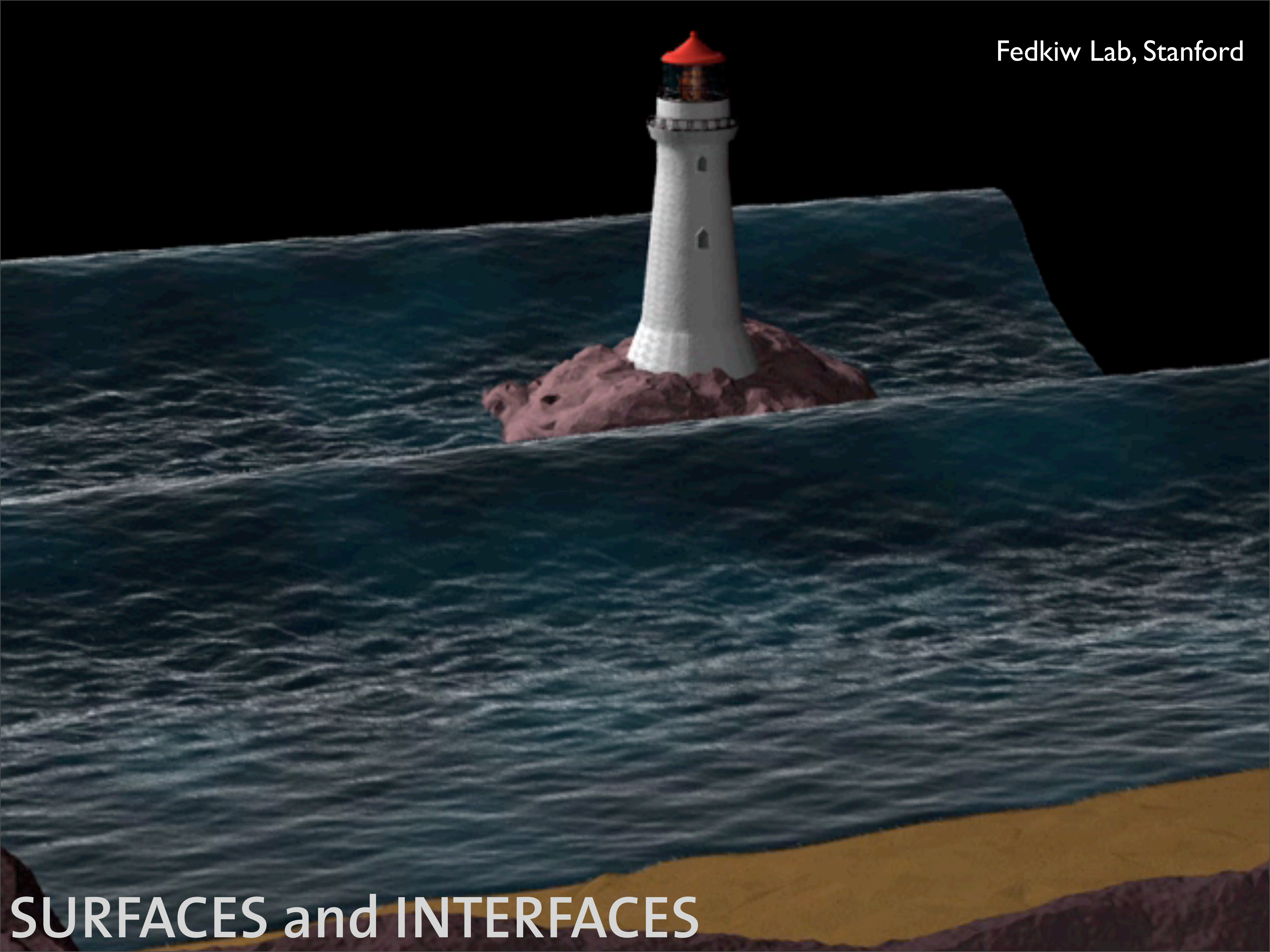
$$\Phi_\epsilon(x) = \int \Phi(y)\,\zeta_\epsilon(x-y)\,dy$$

quadrature

$$\Phi_\epsilon^h(x,t) = \sum_{p=1}^{N_p} h_p^d\,\Phi_p(t)\,\zeta_\epsilon(x - x_p(t))$$



Note : $||\Phi_\epsilon^h - \Phi_\epsilon|| \le C\left(\frac{h}{\epsilon}\right)^m ||\Phi||_\infty$


Fedkiw Lab, Stanford
SURFACES and INTERFACES

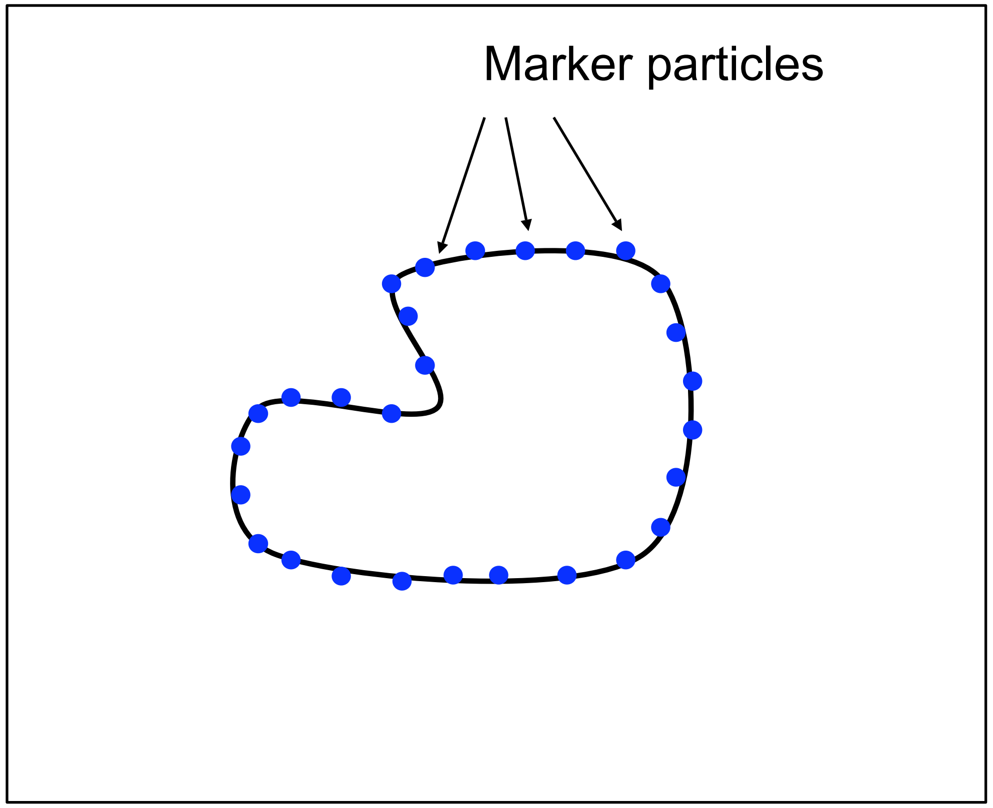
Interface Tracking versus Capturing

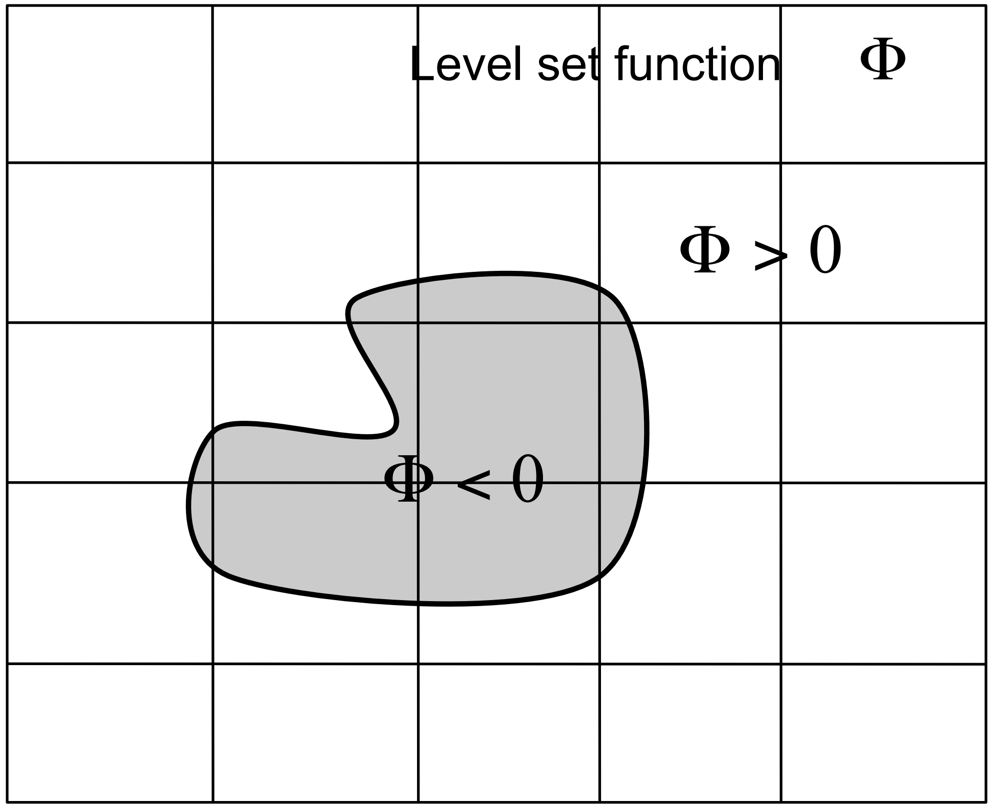
Tracking

- Explicit description
- Lagrangian framework
- Interface distortion requires reseeding

Capturing

- Implicit description
- Eulerian framework
- Evolution leads to numerical diffusion



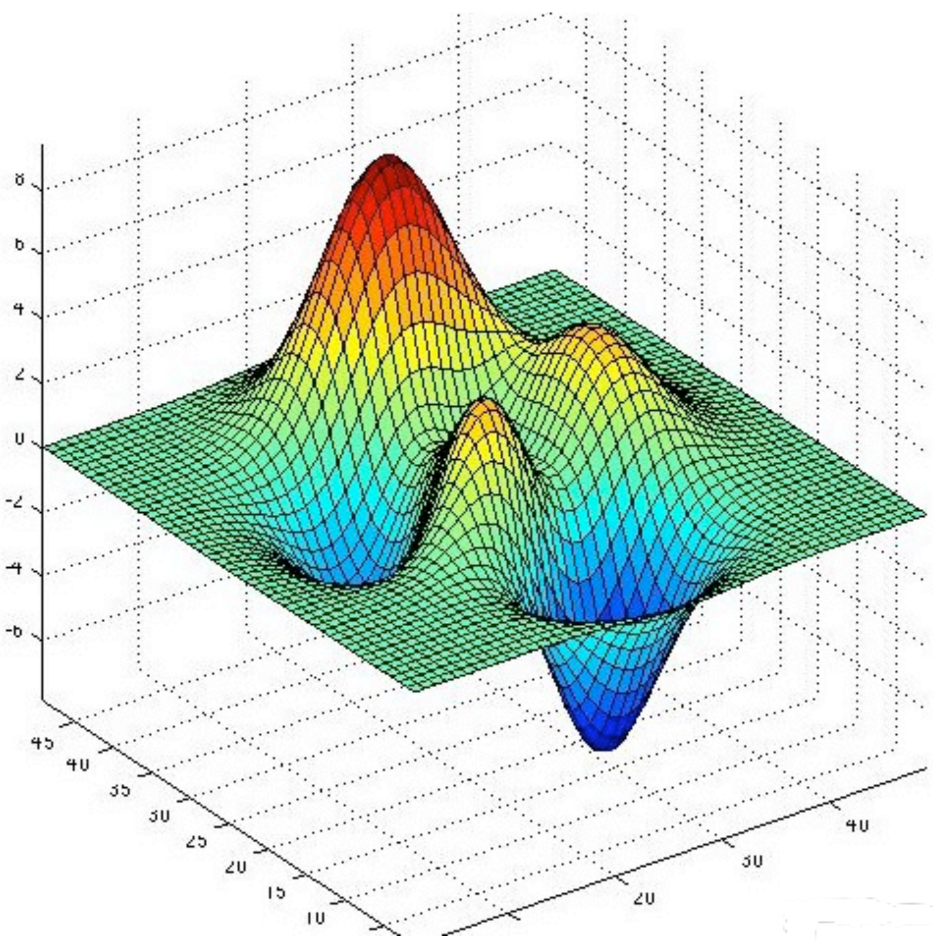


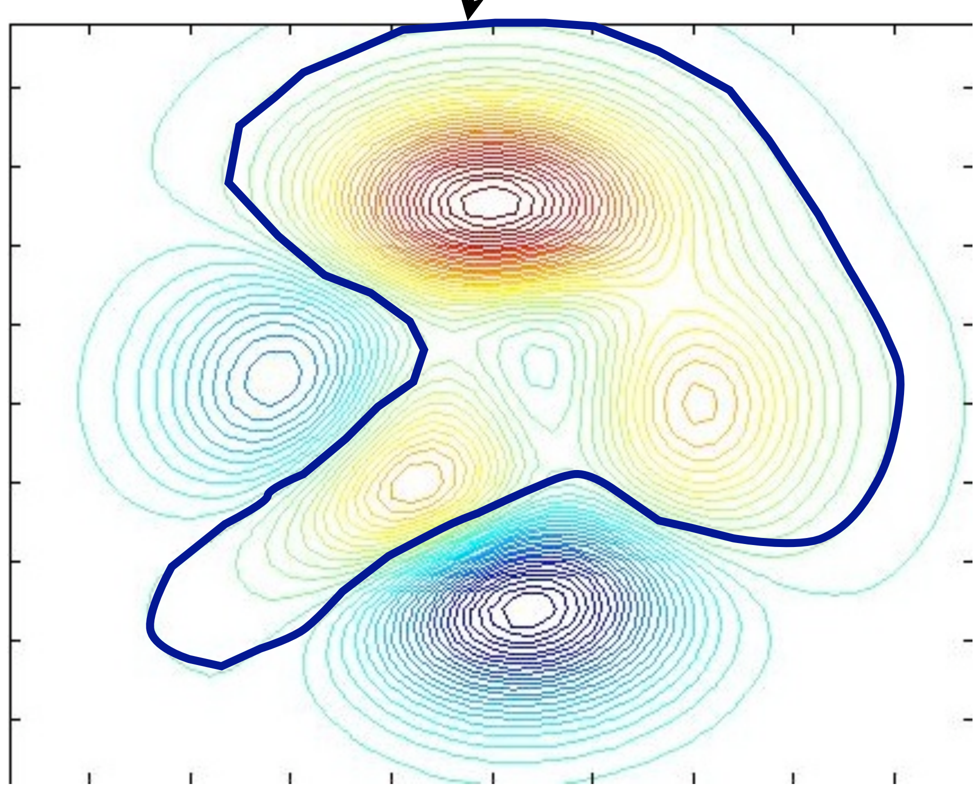
Level Sets for Surface Representation

Level Set: **implicit** surface

$$M = \{x : \Phi(x) = 0\}$$

Sethian, PNAS 93:1591. 1996.

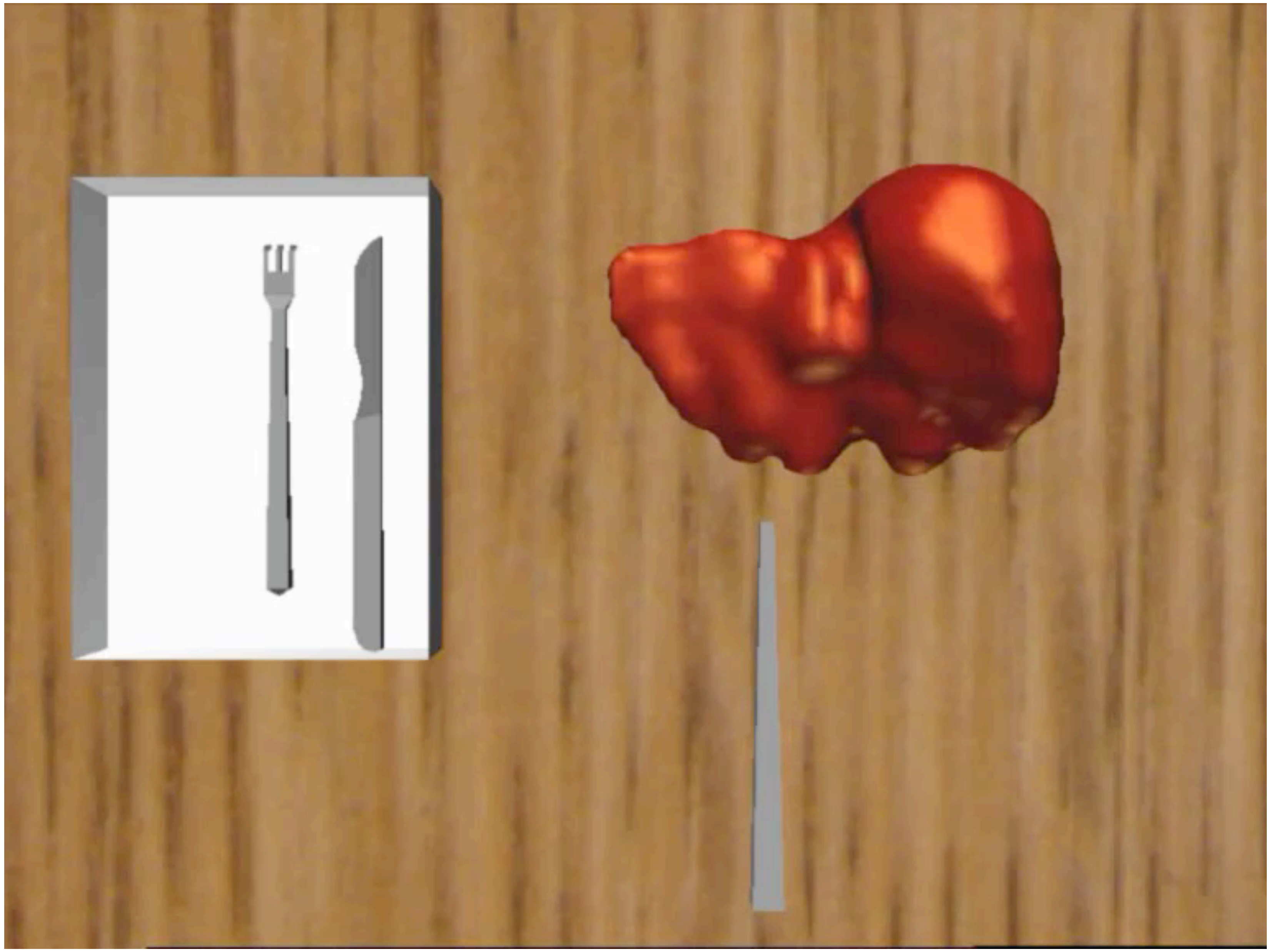




Why? → **surface** can be treated **in space**: one method

Virtual Reality Application

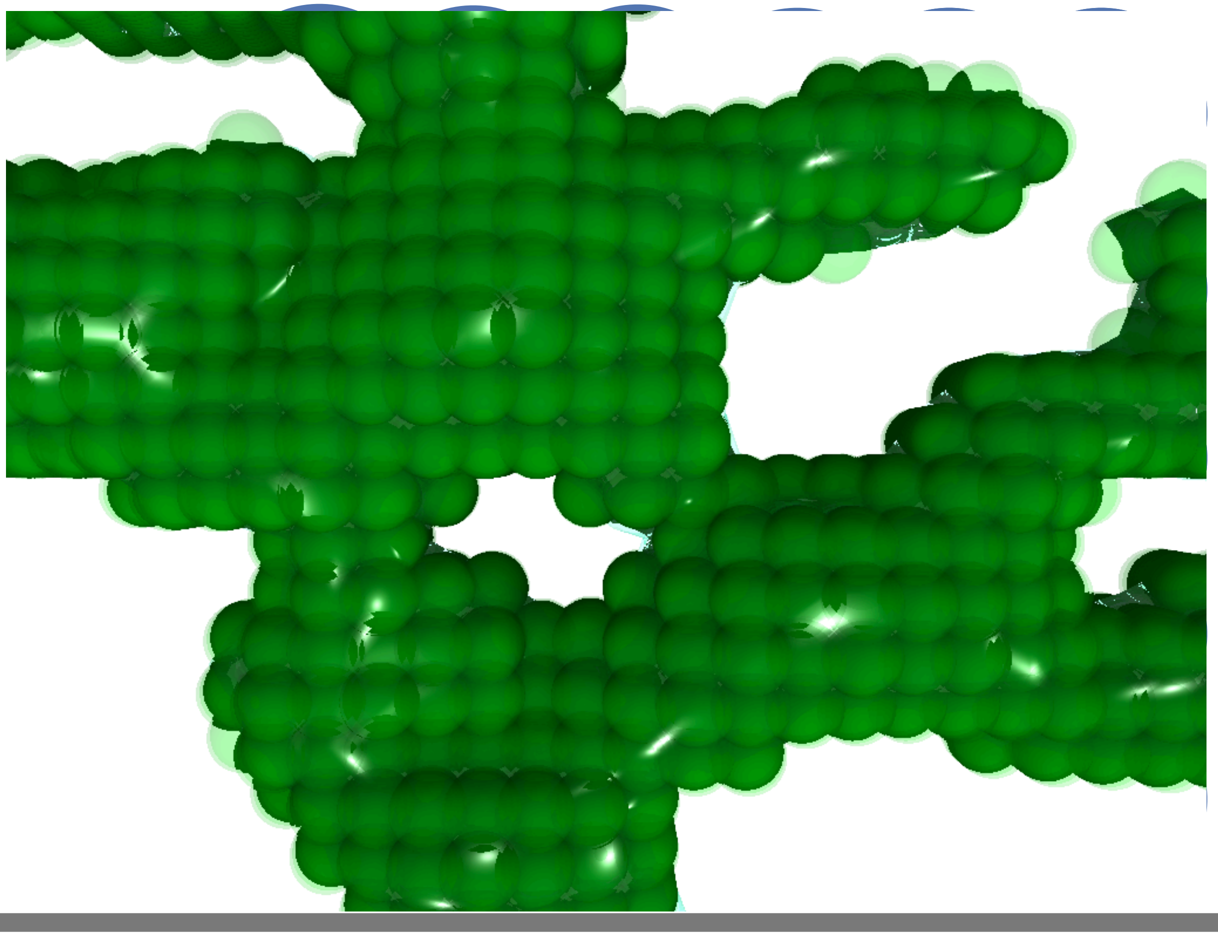
- Virtual Cutting on a Human Liver
- Shape reconstructed by Particle Level Set Method
- Collision detection library provided by Heidelberger *et al.* (2004)
- Particle affected by collision removed from level set superposition



PARTICLE METHODS : Geometry

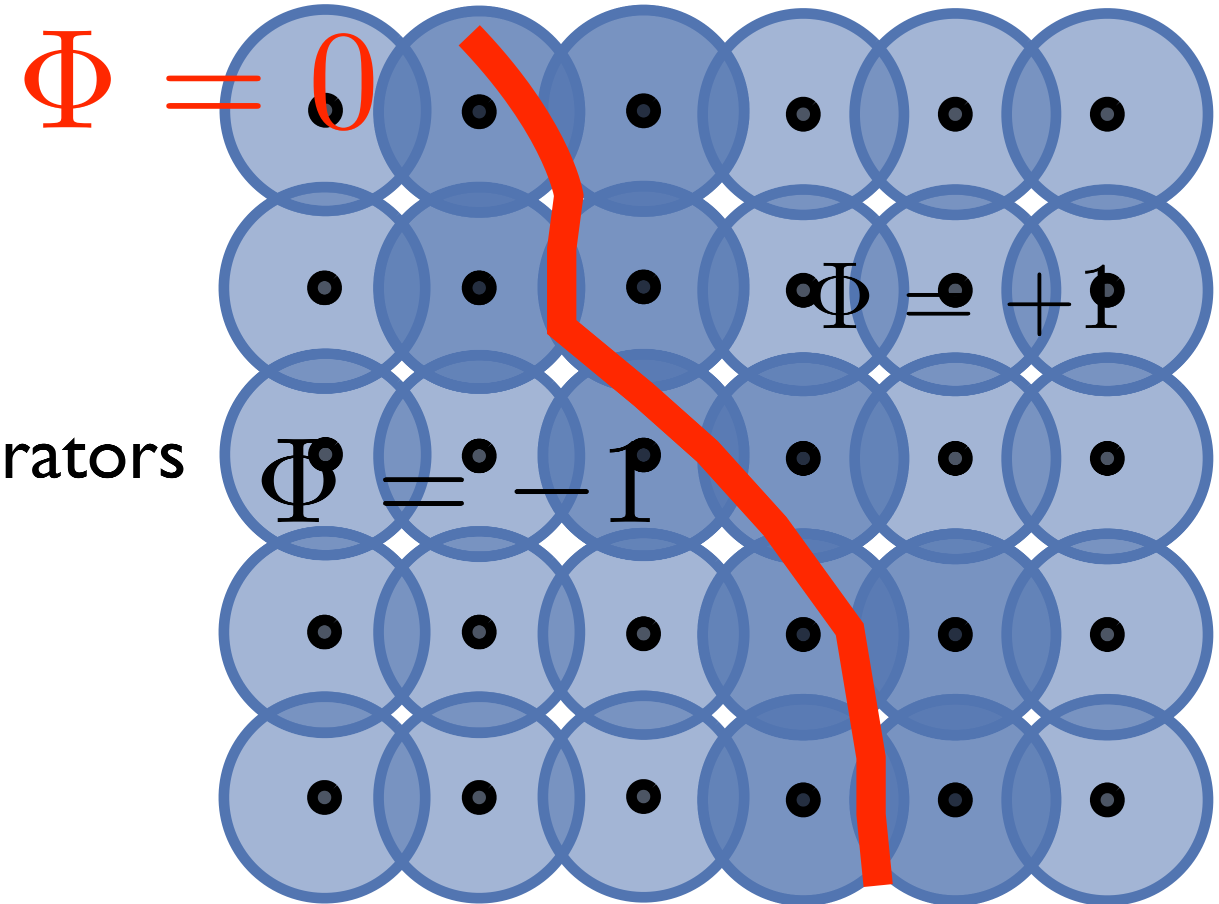
Volume particles

- Particles are quadrature points
- Easy to discretize COMPLEX GEOMETRIES



Surface particles

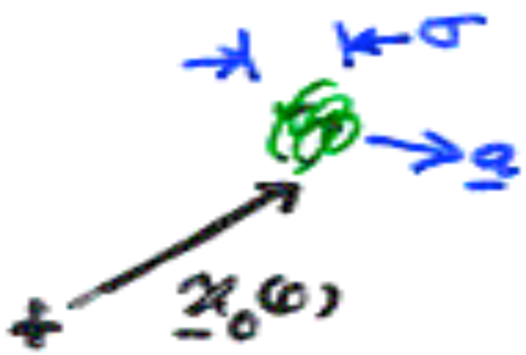
- Particle - Level Sets - COMPLEX SURFACES
- Surface Operators - Anisotropic Volume Operators



Linear Evolution Equation

$$\frac{\partial \omega_i}{\partial t} + U_{jl} x_l \frac{\partial \omega_i}{\partial x_j} = \Omega_j \frac{\partial u_i}{\partial x_j} + \omega_j U_{ij} + \nu \nabla^2 \omega_i$$

Initial Condition – "spherical" vortex ring



$$\underline{\omega}(\underline{x},0) = \nabla \times \left(\underline{a}(0)\, e^{-|\underline{x}-\underline{x}_0|^2/\sigma^2} \right)$$

$$= \nabla\left(e^{-|\underline{x}-\underline{x}_0|^2/\sigma^2}\right) \times \underline{a}(0)$$

Impulse

$$\underline{I} = \frac{1}{2}\int \underline{x} \times \underline{\omega}\, dV \sim \sigma^3 \underline{a}(0)$$

Energy (Self)

$$E(0) \sim \sigma^3 |\underline{a}|^2$$

EQUATIONS

Lagrangian Adaptivity

$$\left(\frac{\partial q}{\partial t} + \nabla \cdot (\boldsymbol{u}\, q) = \mathcal{L}(q, \boldsymbol{x}, t)\right)$$

Lagrangian form: $$\frac{Dq}{Dt} = \mathcal{L}(q, \boldsymbol{x}, t)$$

PARTICLES

→ no linear stability constraints
= no CFL (dt<dx/u) condition

initial values

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}(\mathbf{x}_p, t)\ ,$$ positions — on lattice

$$\frac{dv_p}{dt} = v_p\ (\nabla \cdot \mathbf{u})\,(\mathbf{x}_p, t)\ ,$$ volumes — $v_p = h^d$

$$\frac{dQ_p}{dt} = v_p\, \mathcal{L}^{\varepsilon, h}(q, \mathbf{x}_p, t)\ .$$ weights — $Q_p = q(\boldsymbol{x}_p, 0)\, v_p$

Extension: Level sets

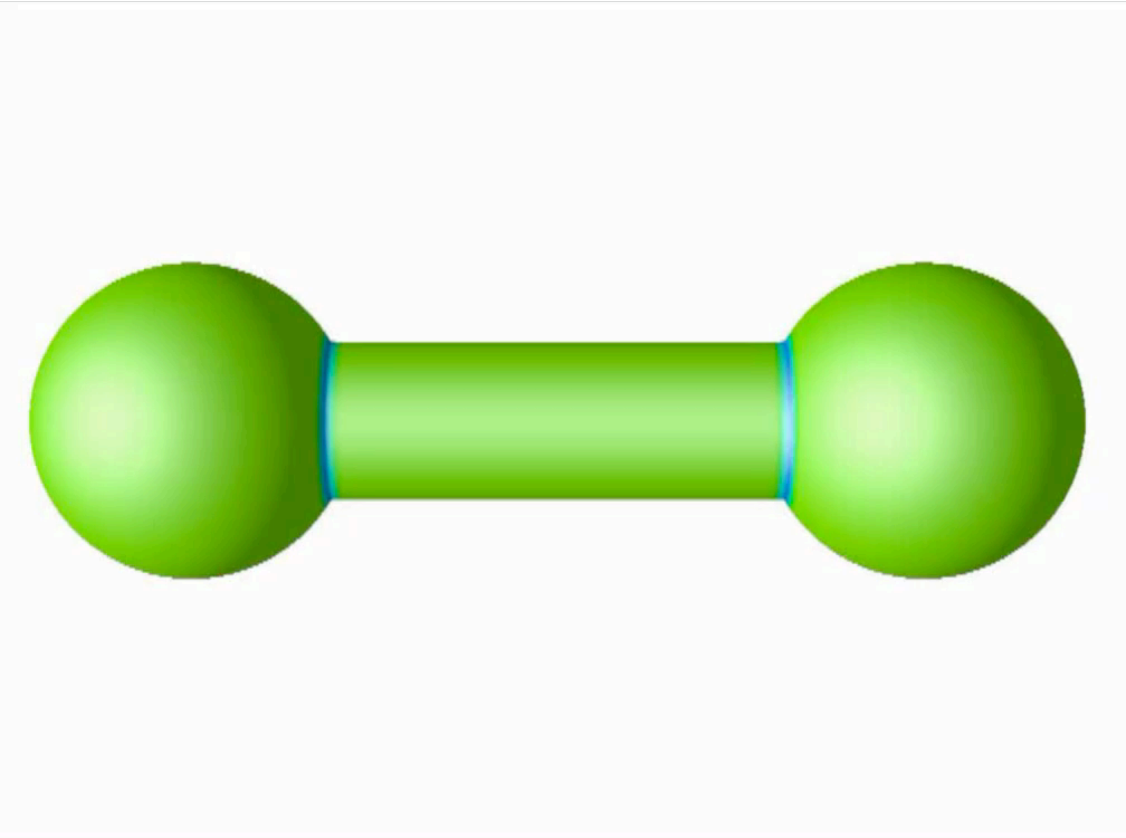
$$\frac{\partial \Phi}{\partial t} + u \cdot \nabla \Phi = 0$$

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

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

$$\frac{\partial \phi}{\partial t} + \kappa \, \boldsymbol{n} \cdot \nabla \phi = 0.$$

$$\kappa = \nabla \cdot \boldsymbol{n}$$



Solve with particles:

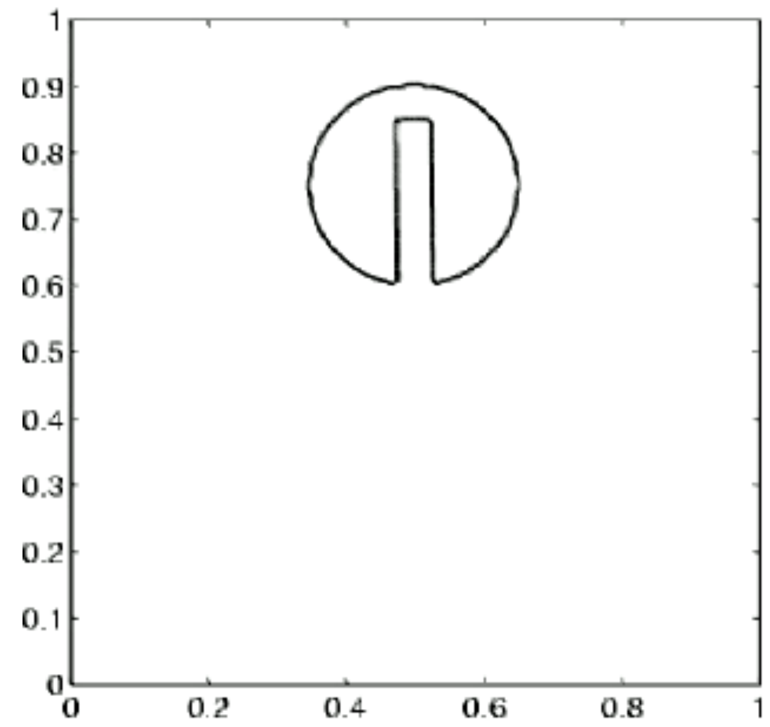
$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}(\boldsymbol{x}_p, t)$$

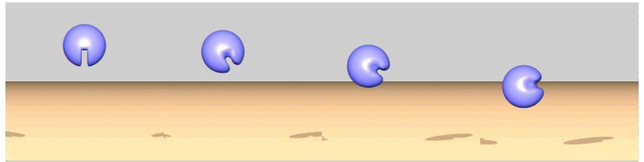
$$\frac{d\phi_p}{dt} = 0$$

Hieber and Koumoutsakos, J. Comp. Phys. 2005

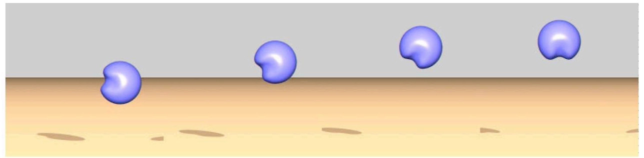
Benchmark: Rigid Body Motion

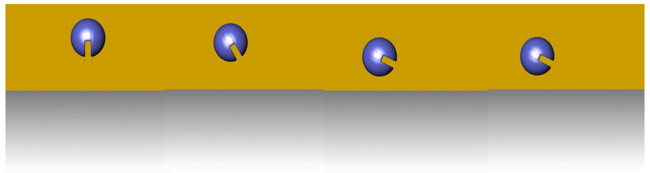
- Problem of rotating slotted disk/ sphere
- Particle level sets exact for rigid body motion
- No remeshing needed



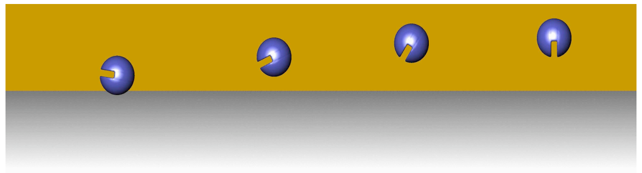


Eulerian Level Sets (Fedkiw, 2002)





Particle Level Sets (exact !)



Particle level set method

(800 particles)

How Good
(robust, efficient, stable, accurate,...) are particle methods ?

Particles go to Hollywood

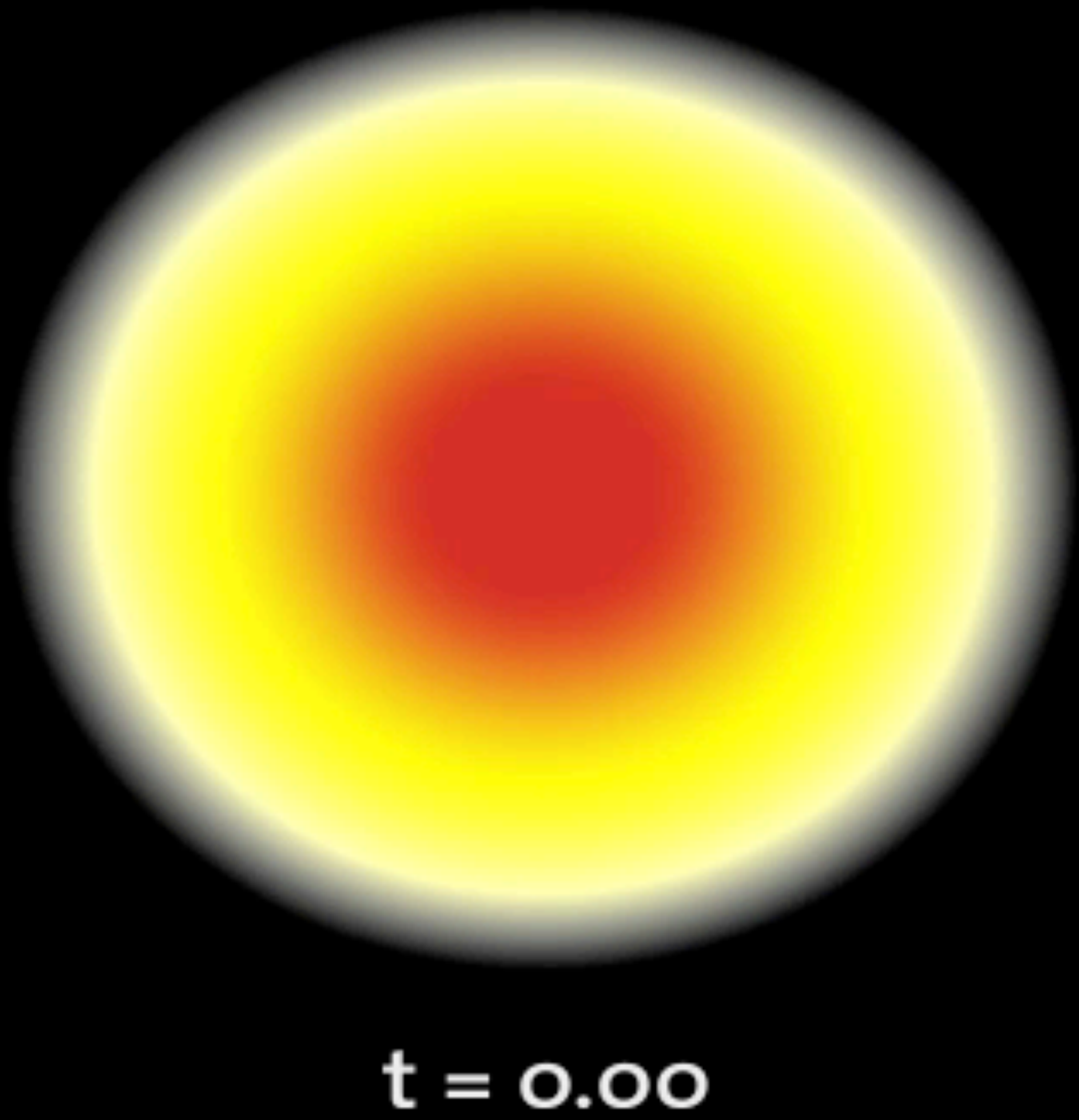
Rigid Fluid: Animating the Interplay Between Rigid Bodies and Fluid

Mark Carlson
Peter J. Mucha
Greg Turk

Georgia Institute of Technology

Sound FX by Andrew Lackey, M.P.S.E.

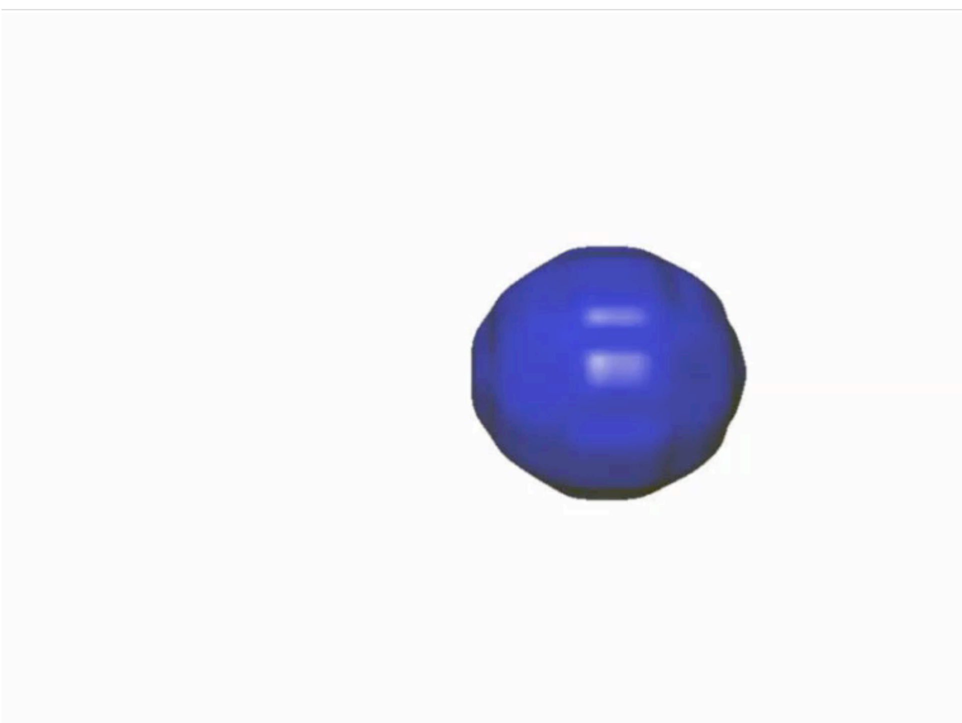
Are grid-free Particle Methods Accurate ?



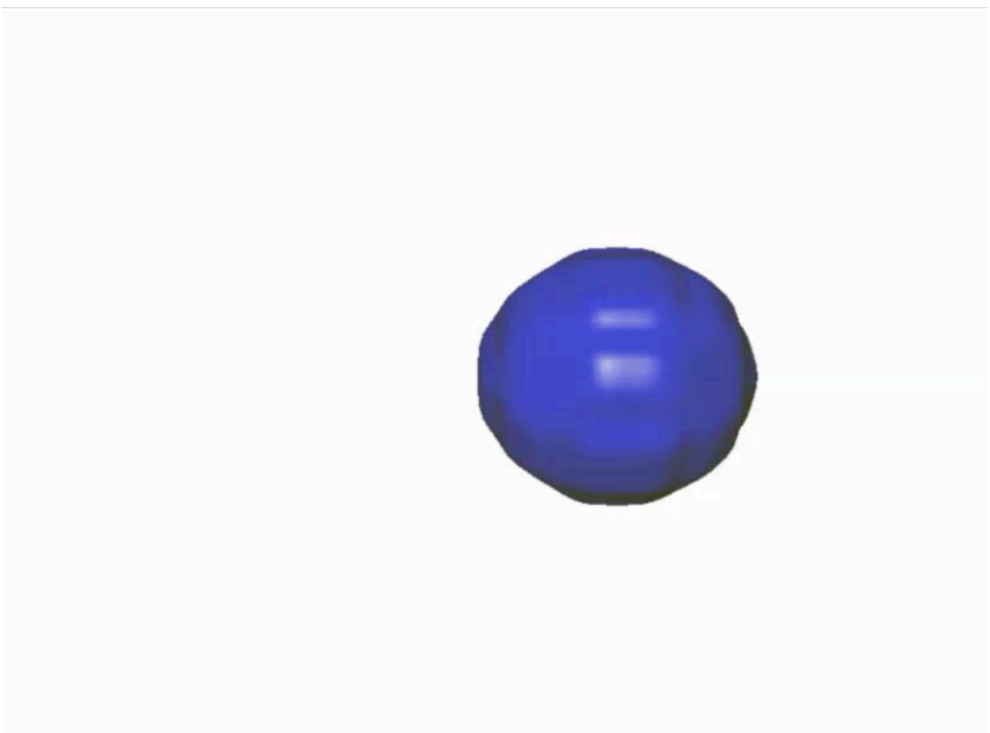
Solution of the Euler equation with particle methods.

Effect of Remeshing

- Benchmark problem with large deformations
- Velocity field prescribed in unit domain



With Remeshing



Without Remeshing

Smooth Particles must Overlap

Mollification

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

+

Quadrature

$$\Phi_\epsilon^h(x,t) = \sum_{p=1}^{N_p} h_p^d\,\Phi_p(t)\,\zeta_\epsilon(x - x_p(t))$$

$$||\Phi - \Phi_\epsilon^h|| \le ||\Phi - \Phi_\epsilon|| + ||\Phi_\epsilon - \Phi_\epsilon^h||$$

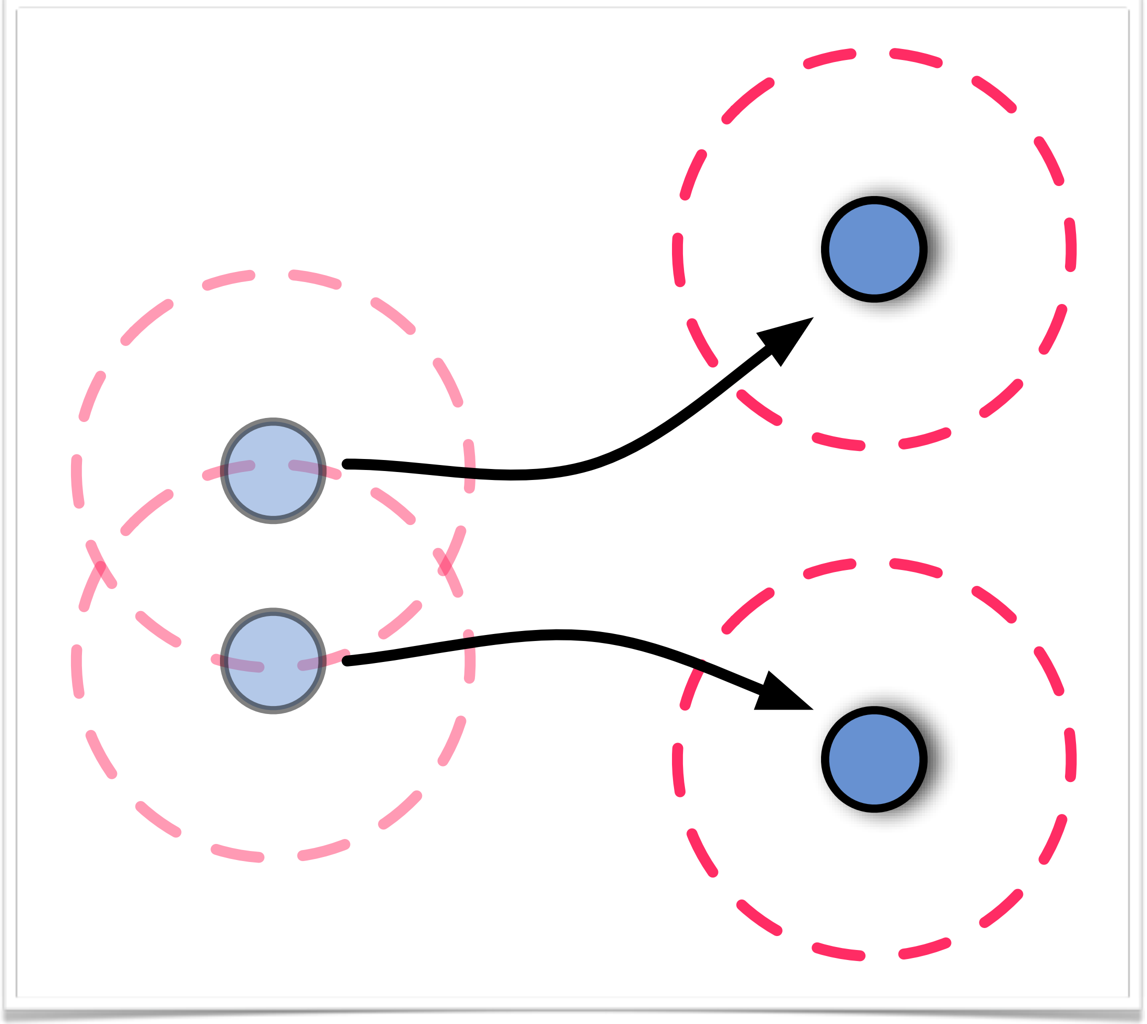
$$\le \left(C_1\,\epsilon^r + C_2\left(\frac{h}{\epsilon}\right)^m\right)||\Phi||_\infty$$

- **Must have** **$h/\varepsilon < 1$** for the quadrature to be accurate **i.e. PARTICLES MUST OVERLAP.**
- References : J. Raviart (1970's), O. Hald (1980's), T. Hou (1990's), G.H. Cottet (1990's)

Lagrangian distortion and REMESHING

Particles follow flow trajectories

- distortion of particle locations
- loss of overlap
- loss of convergence



Preventive action: remeshing

Reinitialize particles on a regular grid.

$$Q_{\boldsymbol{i}}^{\mathrm{new}} = \sum_p Q_p \, \zeta^h(\boldsymbol{i}h - \boldsymbol{x}_p)$$

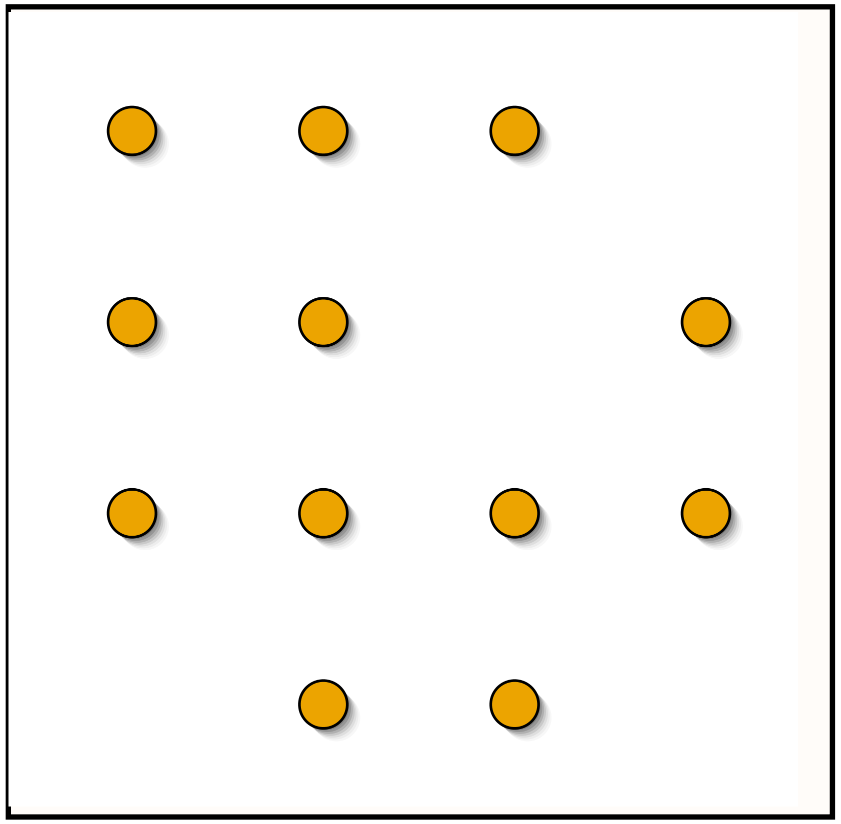
Limiting: Introduction of a grid

Enabling:

- Fast Poisson solvers
- Access versatility of finite differences
- Enabling efficient multiresolution adaptivity

Remeshing = Regularization

A new regularized particle set from the old one



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

Interpolation Kernel $M(x)$

- **Moment conserving**
- Tensorial Product of 1D kernels

REFERENCES :
Vortex Methods : PK and Leonard , JFM, 1995, and PK, JCP, 1997
SPH : Chaniotis, Poulikakos and PK, JCP, 2002

Hybrid Particle Mesh Techniques

step 1 : ADVECT Particles

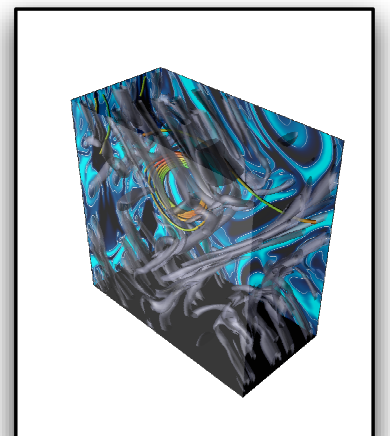
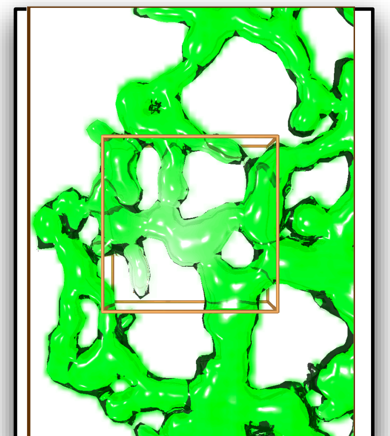
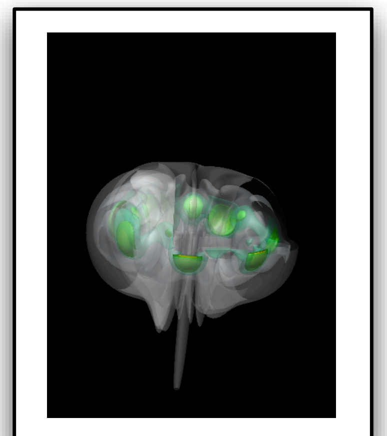
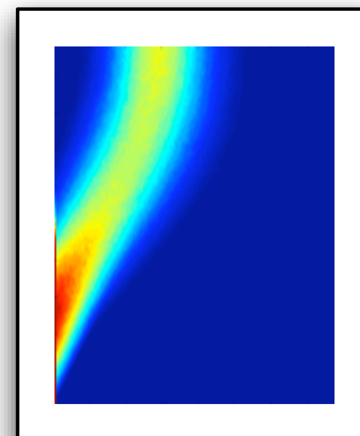
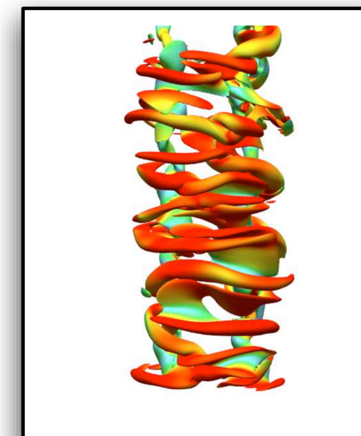
step 2 : REMESH Particles onto Grid nodes

step 3 : SOLVE field equations / DERIVATIVES on GRID

step 4 : Grid Nodes BECOME Particles

Parallel Particle Mesh library

Easy to use and efficient infrastructure for Particle-mesh simulations on parallel computers

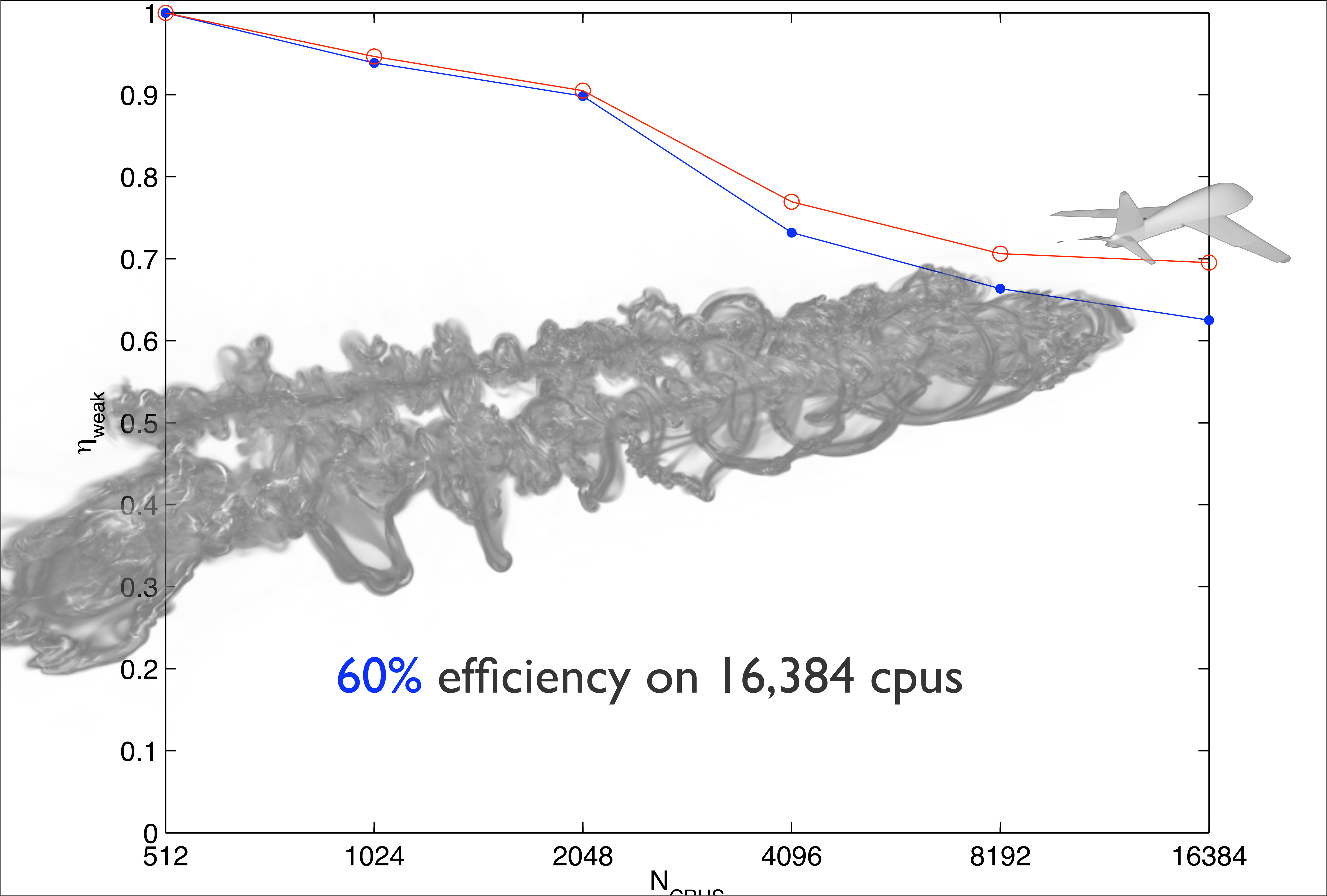






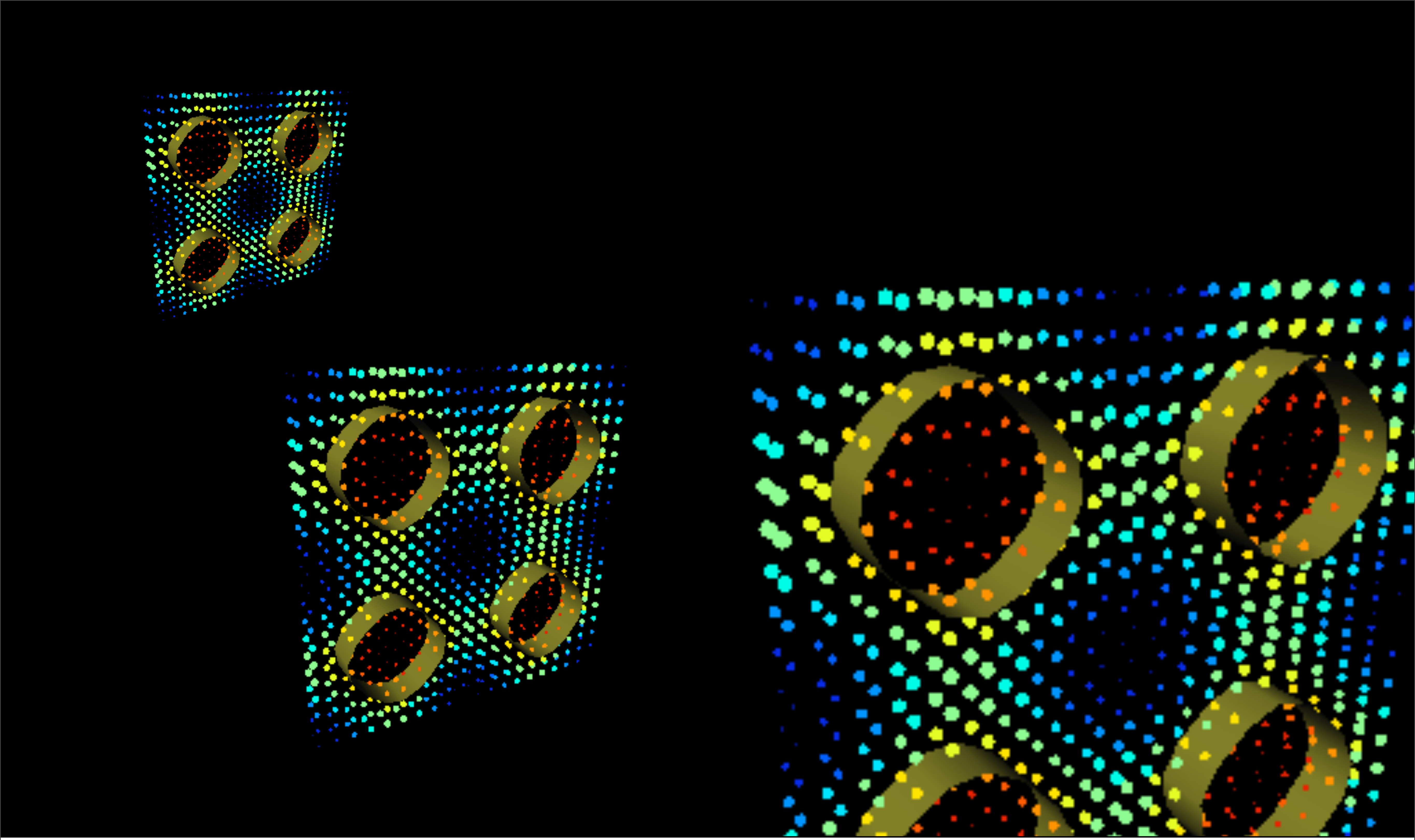
Parallel Particle Mesh Library (PPM)

Message Passing Interface (MPI) | METIS | FFTW

vector | shared memory | distributed memory | single processor

PPM + 16K processors = 10 Billion Vortex Particles





Particle Methods for Fluids and Solids

Governing Equations

Lagrangian Formulation

Isothermal Compressible Viscous Fluid

$$\frac{D\rho_l}{Dt} = -\rho_l \nabla \cdot u_l$$

$$\rho_l \frac{Du_l}{Dt} = -\nabla p_l + \nabla \tau_l$$

$$p_l = RT_0 \rho_l$$

$$\tau_{l,ij} = \mu\left(\frac{\partial u_{l,i}}{\partial x_j} - \frac{\partial u_{l,i}}{\partial x_j} - \frac{2}{3}\delta_{i,j}\frac{\partial u_{l,k}}{\partial x_k}\right)$$

Continuity equation

Momentum equation

Constitutive model

Elastic Solid

$$\frac{D\rho_s}{Dt} = -\rho_s \nabla \cdot u_s$$

$$\rho_s \frac{Du_s}{Dt} = \nabla.\sigma_s = \nabla.\left(-p_s I + S\right)$$

Linear

$$p_s = c_0^2\left(\rho_s - \rho_0\right)$$

$$\frac{DS}{Dt} = 2\mu\left(\dot{\epsilon} - \tfrac{1}{3}\delta_{ij}\dot{\epsilon}_{ij}\right)$$

$$\dot{\epsilon} = \tfrac{1}{2}\left(\nabla u + (\nabla u)^T\right)$$

Nonlinear

$$\sigma_s = f(F)$$

$$\frac{DF}{Dt} = \frac{\partial u}{\partial x} F$$

Particle Equations - Fluid

Set of ODEs

Isothermal Compressible Viscous Fluid

$$\frac{dx_p}{dt} = u_p$$

$$\frac{d\rho_p}{dt} = -\rho_p \langle \nabla \cdot u \rangle_p$$

$$\rho_p \frac{du_p}{dt} = -\langle \nabla p \rangle_p + \langle \nabla \tau \rangle_p$$

$$p_p = RT_0 \rho_p$$

$$\tau_{ij,p} = \mu \left(\left\langle \frac{\partial u_i}{\partial x_j} \right\rangle_p - \left\langle \frac{\partial u_i}{\partial x_j} \right\rangle_p - \frac{2}{3} \delta_{i,j} \left\langle \frac{\partial u_k}{\partial x_k} \right\rangle_p \right)$$

Equation of motion

Continuity equation

Momentum equation

Constitutive model

$\langle \ \rangle_p$: Approximation on particle p

Particle Equations - Solid

Set of ODEs

Elastic Solid

Equation of motion

$$\frac{dx_p}{dt} = u_p$$

Continuity equation

$$\frac{d\rho_p}{dt} = -\rho_p \langle \nabla \cdot u \rangle_p$$

Momentum equation

$$\rho_p \frac{du_p}{dt} = \langle \nabla . \sigma \rangle_p = -\langle \nabla p \rangle_p + \langle \nabla . S \rangle_p$$

Constitutive model

Linear

$$p_p = c_0^2 (\rho_p - \rho_0)$$

$$\frac{dS_p}{dt} = 2\mu \left(\dot{\epsilon}_p - \tfrac{1}{3} \delta_{ij} \dot{\epsilon}_{ij,p} \right)$$

$$\dot{\epsilon}_p = \tfrac{1}{2} \left(\langle \nabla u \rangle_p + \langle \nabla u \rangle_p^{\,T} \right)$$

Nonlinear

$$\sigma_p = f(F_p)$$

$$\frac{dF_p}{dt} = \left\langle \frac{\partial u}{\partial x} \right\rangle_p F_p$$

$\langle \; \rangle_p$: Approximation on particle p

Computational Setup

- Boundary Conditions

Fluid	Solid
Periodic boundary condition	
Fixed or no-slip boundary (prescribed velocity)	
Flow inlet (prescribe inlet velocity)	Free surface (stress-free boundary)
Flow outlet (zero-pressure condition)	

Implementation: ghost particles carrying attributes to satisfy boundary conditions

- Interfaces described by the particle level set method

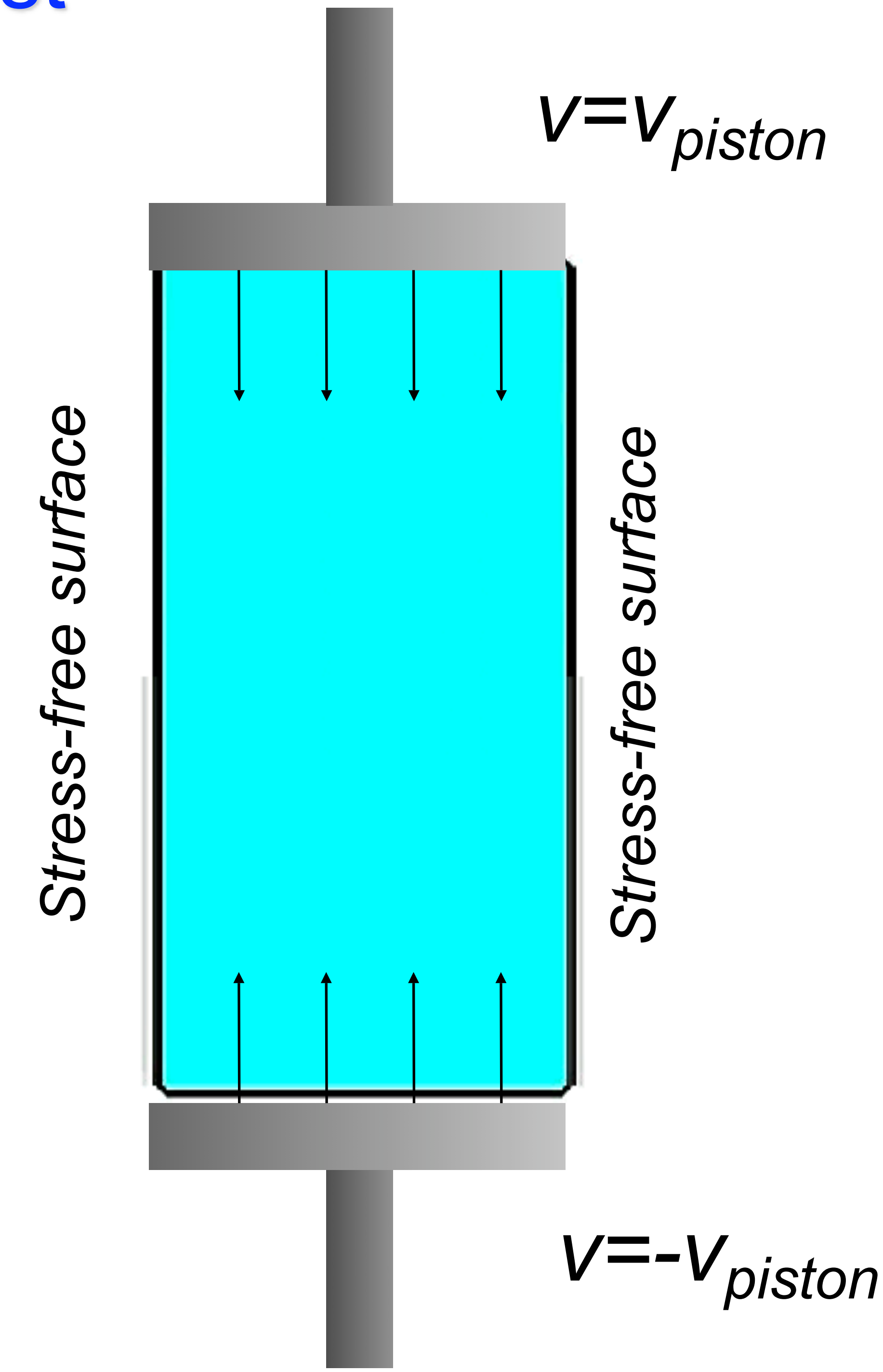
- Particle Remeshing at a constant frequency

- Reynolds number $\mathrm{Re} = \frac{\rho_0 U_0 L_0}{\mu}$ Mach number $M = \frac{U_0}{c_0}$

Particle Simulation of Elastic Solid

Plane Strain Compression Test

- Pistons move with constant velocity
- Elastic solid fixed to the pistons
- Highly dynamic deformation of large extent



Particle Simulation of Elastic Solid

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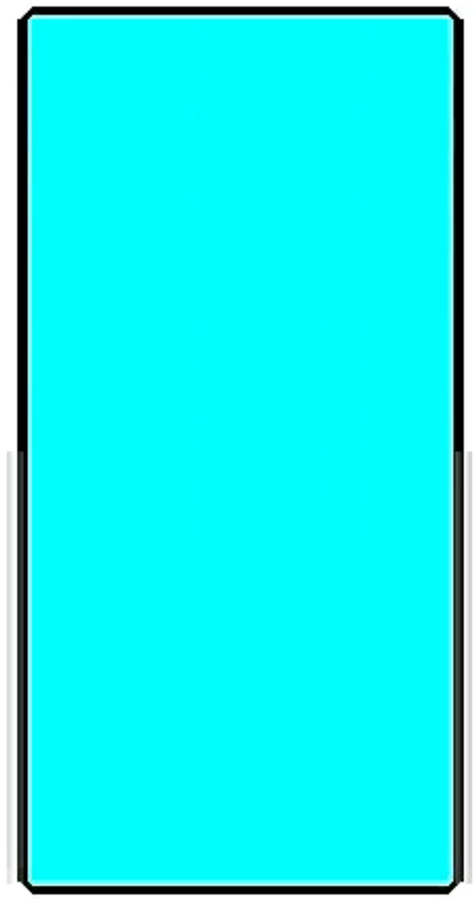


Plane Strain Compression Test

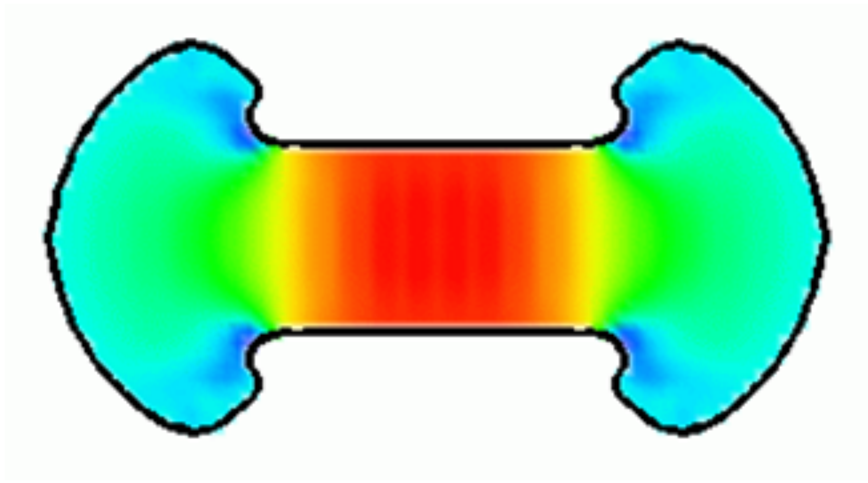
Redistributed Particle solution

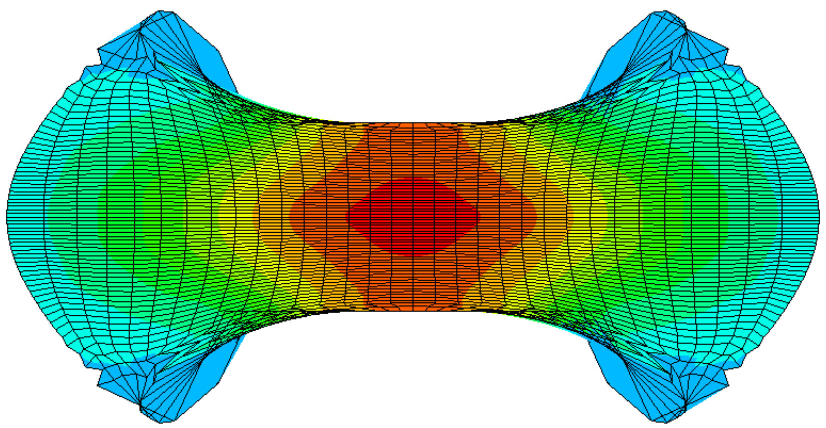
FEM solution (ABAQUS 6.4/Explicit)

Linear Elasticity

Young's Modulus =100
Poisson ratio=0.49 ~2000

particles/nodes



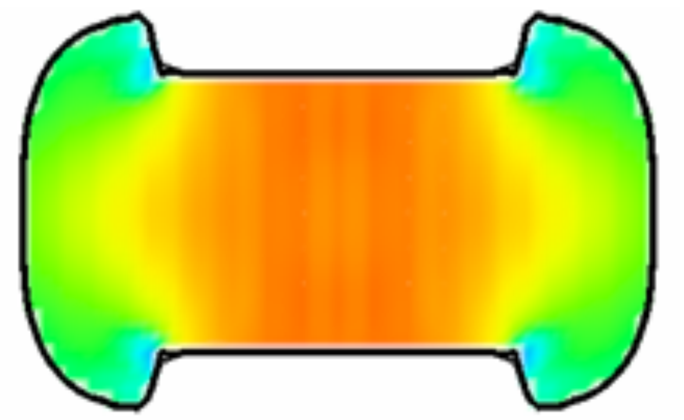


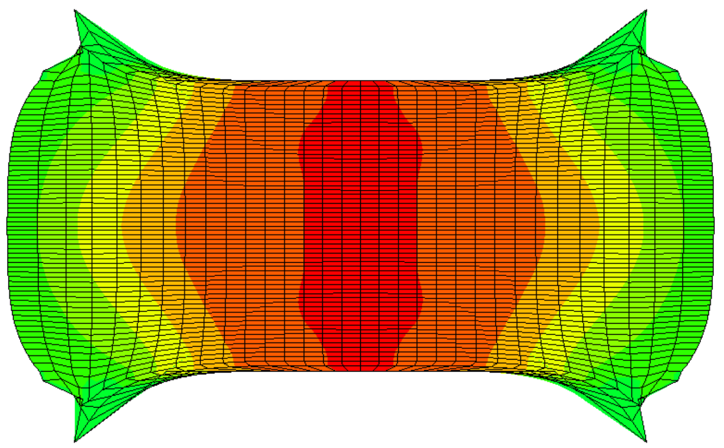
Nonlinear Elasticity

Hyperelastic Material

C_{10}=2.2, D=0.001

~2000 particles/nodes



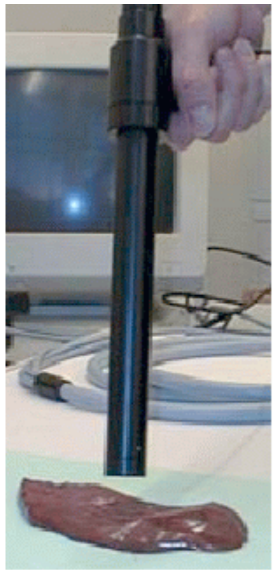


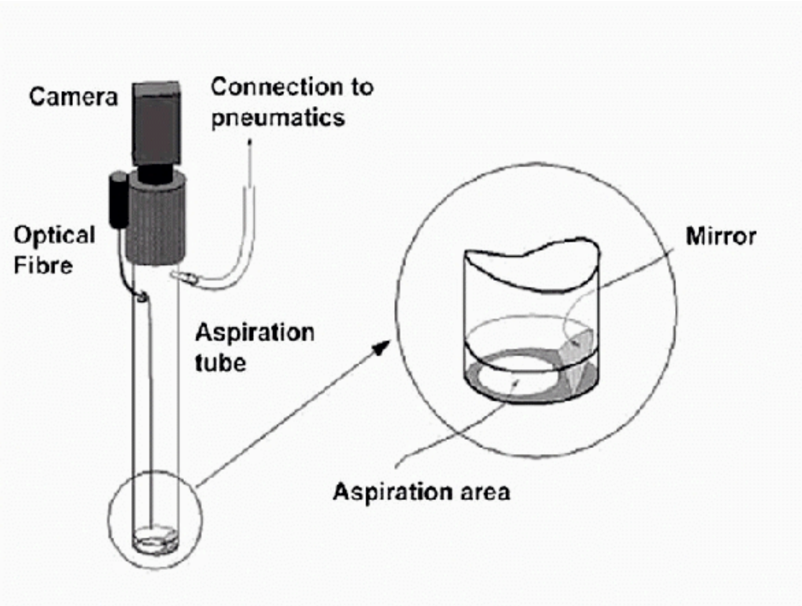
S.E. Hieber and P. Koumoutsakos A Lagrangian particle method for the simulation of linear and nonlinear elastic models of soft tissue. *al., J. Comp. Physics, accepted*

Simulation of Liver Tissue

Aspiration Test

- Experiment to determine constitutive models for biological tissue
- A vacuum created in the aspiration devices causes the tissue to form a bubble
- The height of the tissue bubble determines the parameters of the nonlinear model





Nava et al., Technology and Health Care,2004, vol.12,269-280

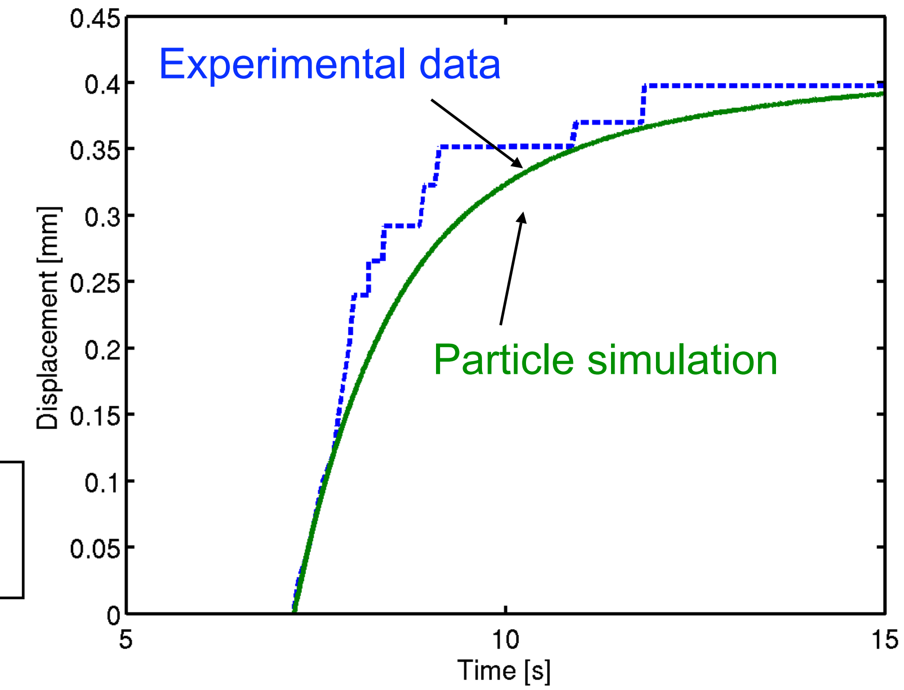
Particle Simulation of Aspiration Test

- Experiment and nonlinear model from Nava *et al.* (2004)

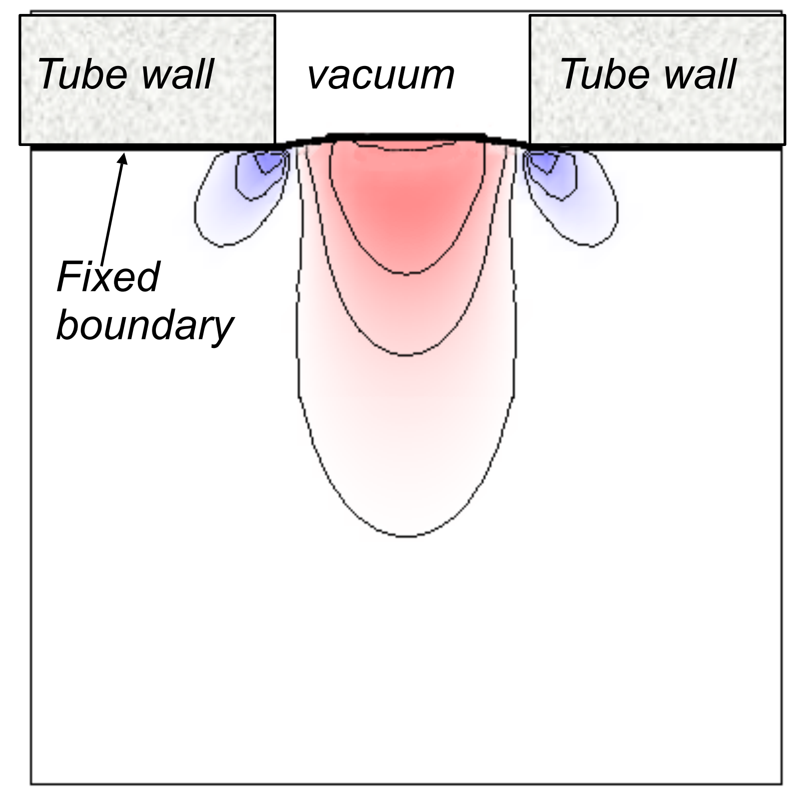
- 3D Particle simulation using $\sim 10^5$ particles

- Good agreement with experimental results in the tissue displacement

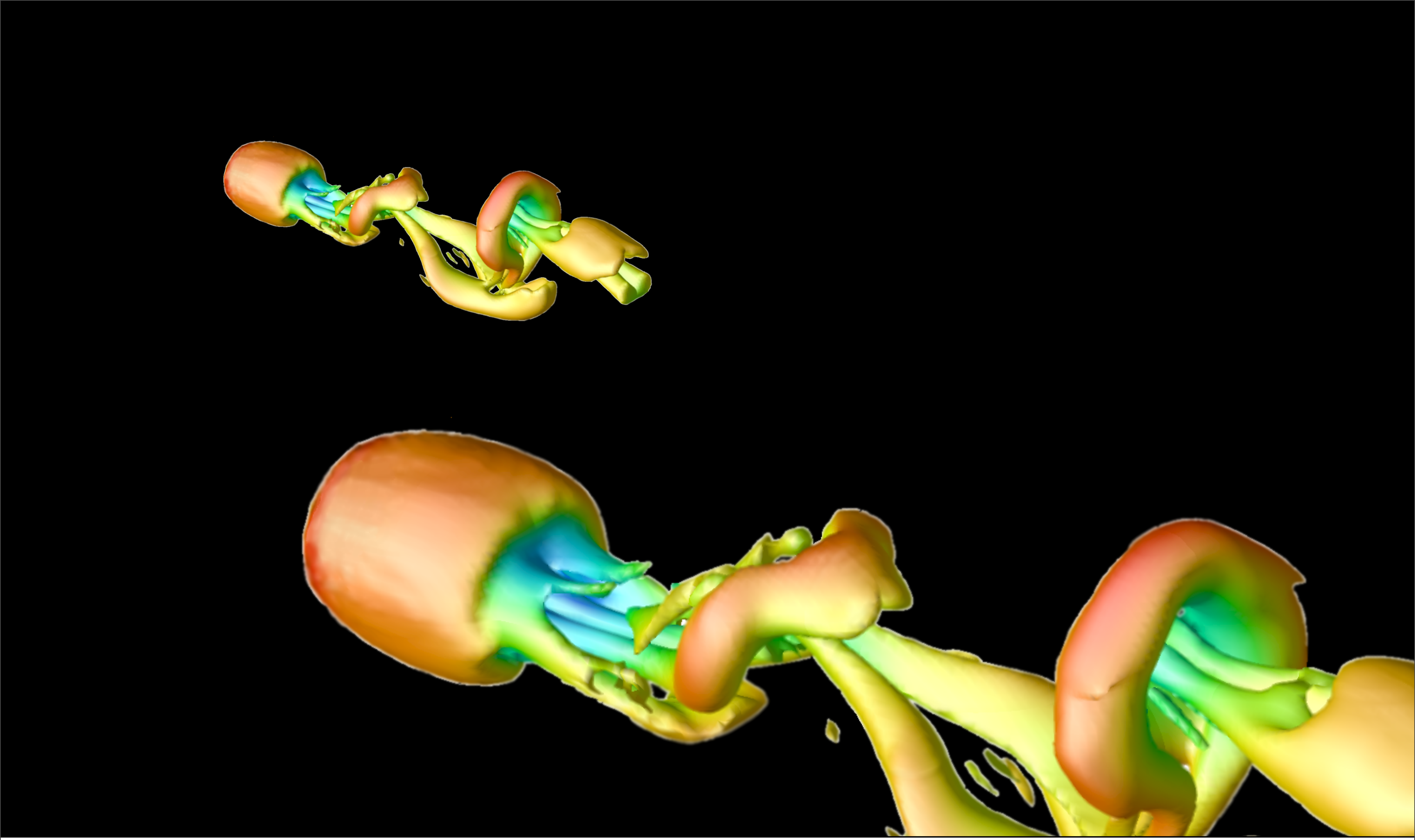
Tissue Displacement



Stretch distribution



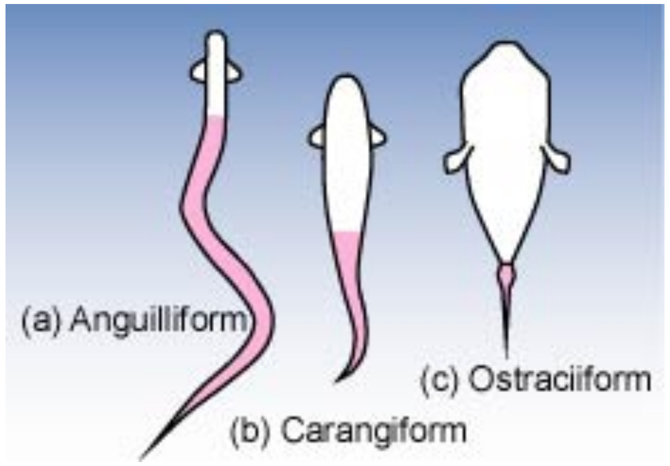
Experimental Data and Model from *Nava et al., Technology and Health Care,2004, vol. 12,269-280*



A Particle Immersed Boundary Method

Motivation

- Complex boundaries in fluid environment
- Flow-structure interactions
- Eulerian Methods: Immersed Boundary Method established



Particle Immersed Boundary approach for complex boundaries

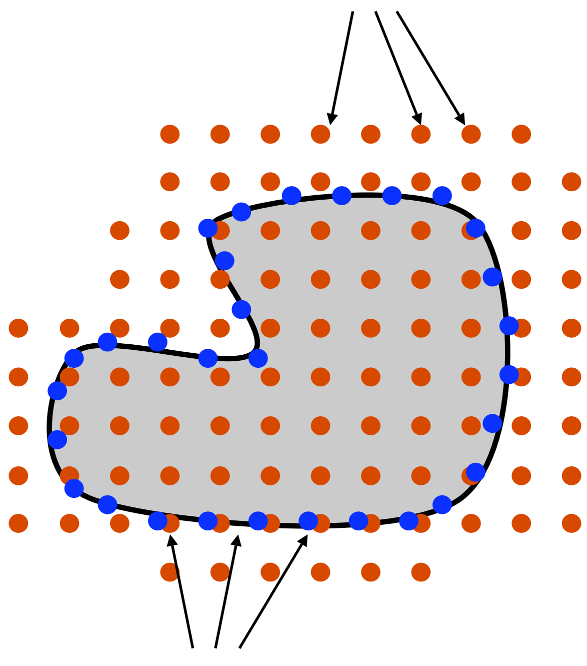
Methology

- Enforcement of no-slip condition by bodyforce field **f**

$$\rho \frac{Du}{Dt} = -\nabla p + \nabla . \tau + f$$

- Approximation of the bodyforce field **f** on the boundary

$$\frac{Du}{Dt} \approx \frac{u_{desired} - u}{\Delta t} \quad \Rightarrow f = \rho \frac{u_{desired} - u}{\Delta t} - (-\nabla p + \nabla \tau)$$



- Particle equations

$$\rho_p \frac{du_p}{dt} = -\langle \nabla p \rangle_p + \langle \nabla \tau \rangle_p + \langle f_{bp} \rangle_p$$

$$f_{bp} = \rho \frac{u_{desired}}{\Delta t} + \left\langle \rho_p \frac{-u_p}{\Delta t} - \left(-\langle \nabla p \rangle_p + \langle \nabla \tau \rangle_p \right) \right\rangle_{bp}$$

$\langle \ \rangle_p$: Approximation on particle p

$\langle \ \rangle_{bp}$: Approximation on boundary point bp

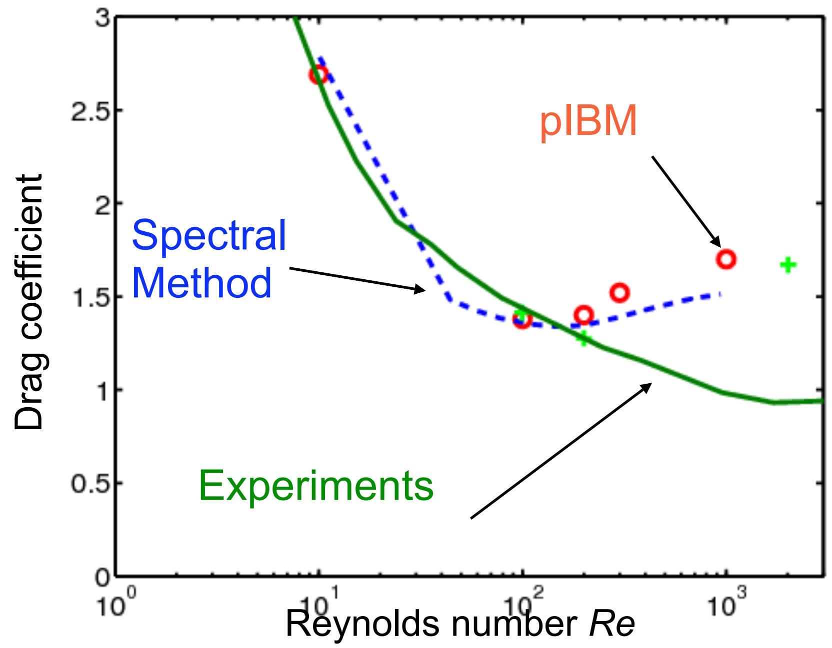
Flow past a Cylinder/Sphere

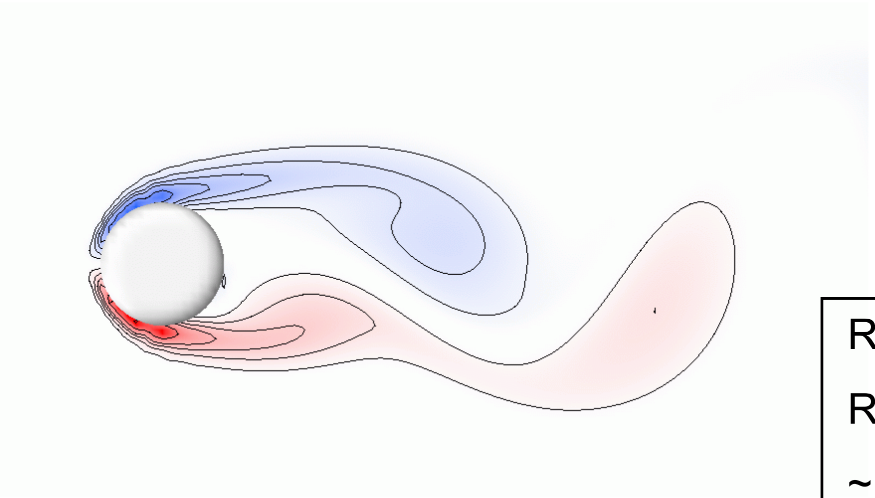
Particle Immersed Boundary Method (pIBM)

Drag coefficient

Vortex structure

Cylinder





Re = 100, Ma = 0.1

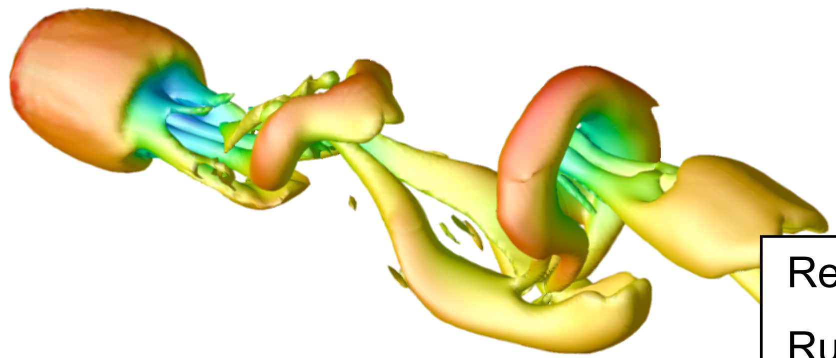
Runge Kutta 4

~10^5 particles

Sphere

Re=300

pIBM	0.71
Johnson and Patel	0.66



Vortices visualized by the Lambda-2 Method

Re = 300, Ma = 0.1

Runge Kutta 4

~10^7 particles

Flow-Structure Interactions

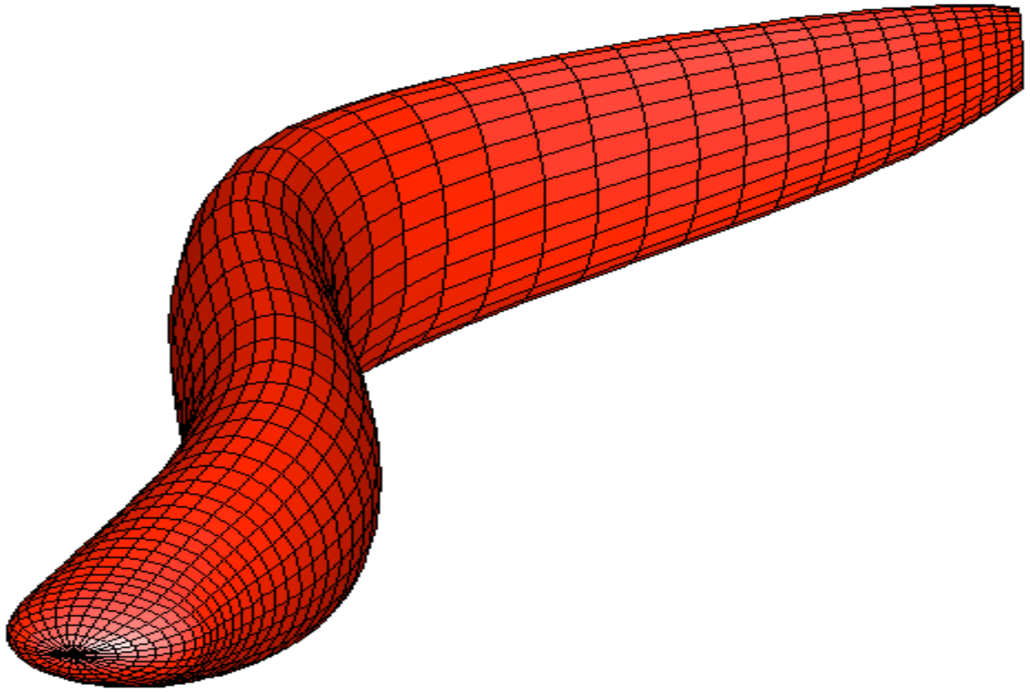
Anguilliform Swimming

- Self-propelled swimmer
  - Impact on the flow field (no-slip boundary)
  - Translation and rotation due to resulting fluid force
- Backbone Motion from Carling *et al.*(1998)

Lateral displacement of the backbone

$$\Delta y(s,t) = 0.1(s + 0.25)\sin(\omega(s - t))$$

s: normalized distance to the head
t: time



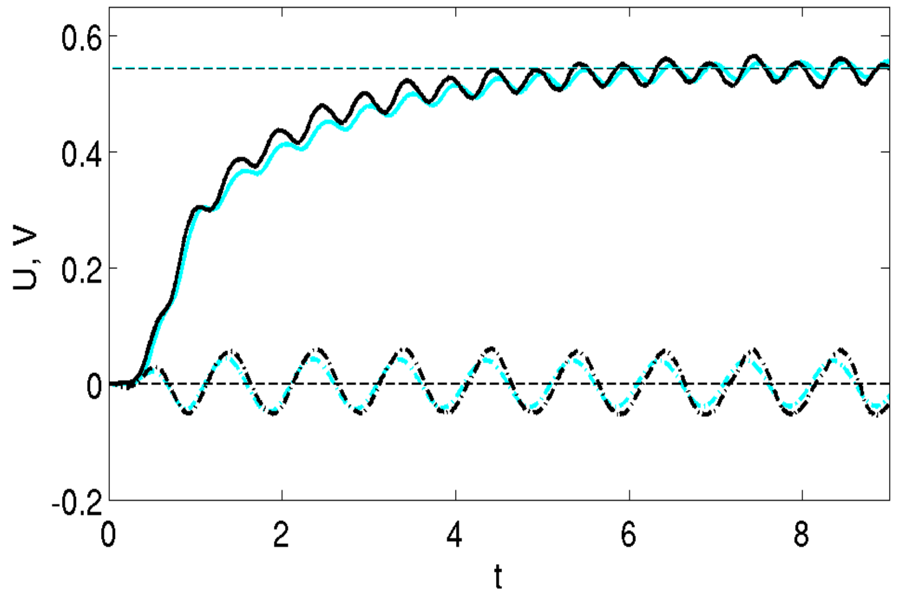
- Geometry from Kern *et al.* (2006)

Results of the 2D swimmer

Particle Immersed Boundary Method – Finite Volume Method

(Kern and Koumoutsakos 2006)

velocity 0.00



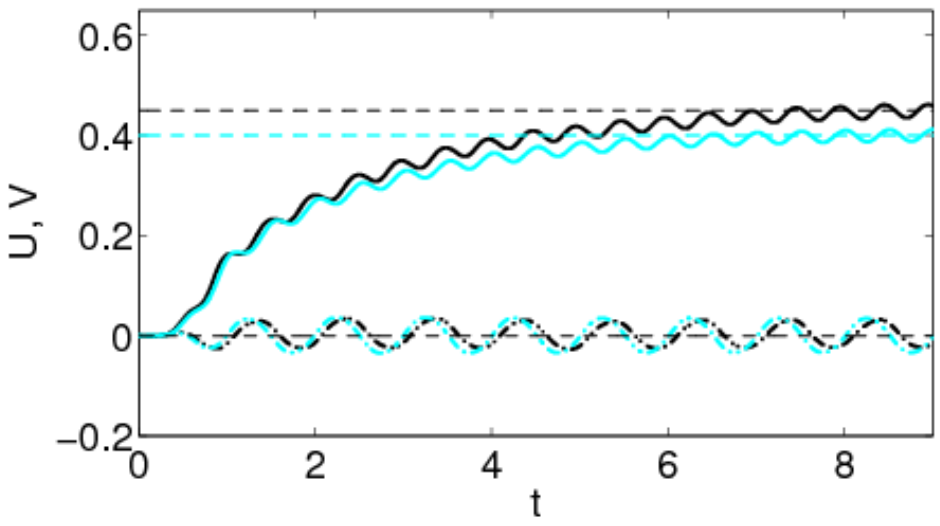
Longitudinal and lateral velocity

Ma = 0.12	RK 4th order
Re = 3800	~10^5 Particles

Results of the 3D swimmer

Particle Immersed Boundary Method – Finite Volume Method

(Kern and Koumoutsakos 2006)



Longitudinal and lateral velocity

Vortices visualized by the Lambda-2 Method

Ma = 0.05	RK 4th order
Re = 3800	~3 x10^7 Particles

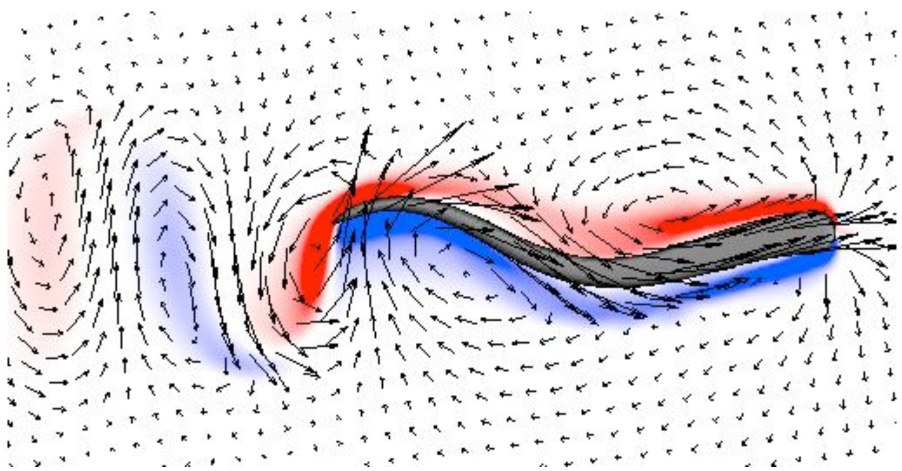
Flow Field Comparison

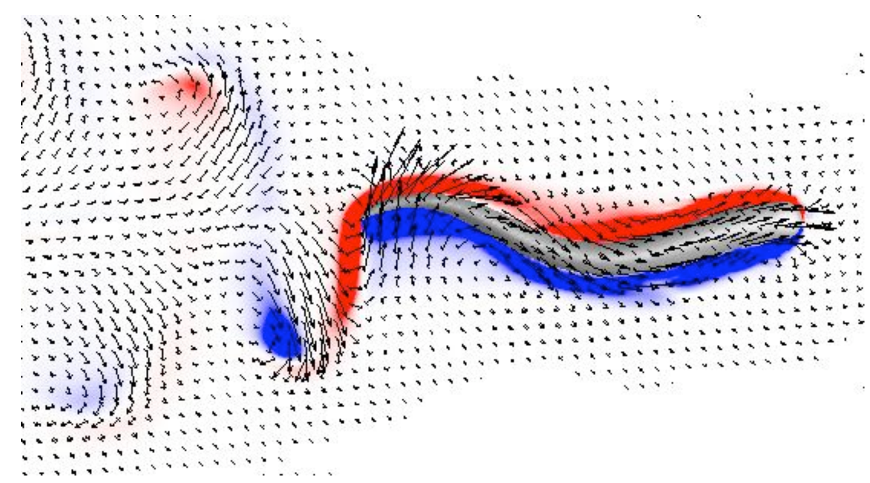
2D Swimmer

3D Swimmer

Particle Method

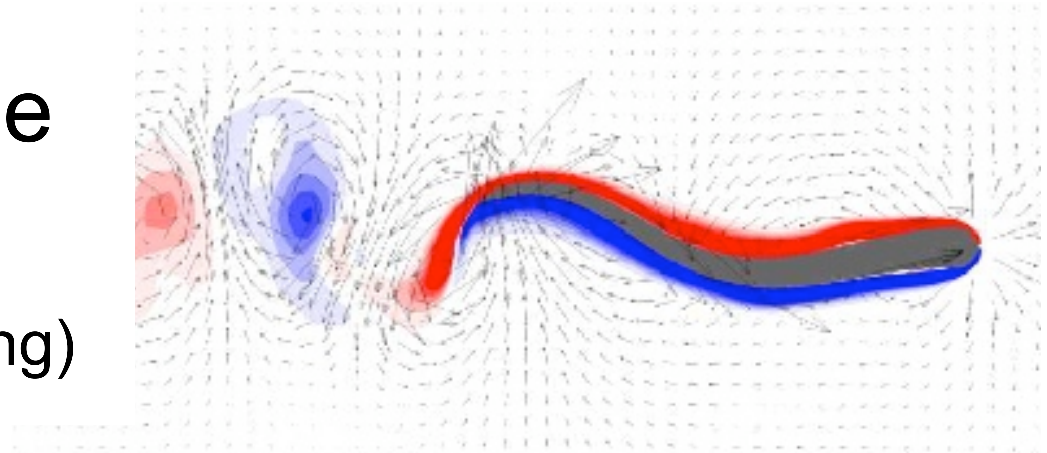
(Uniform resolution)

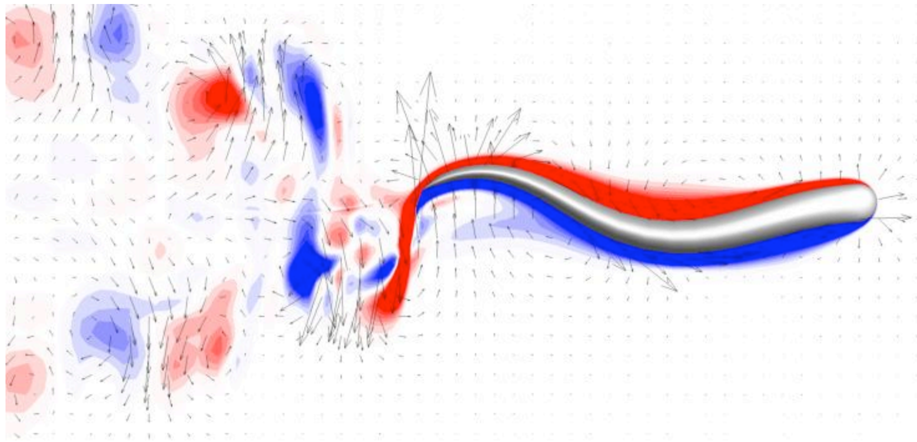




Finite Volume Method

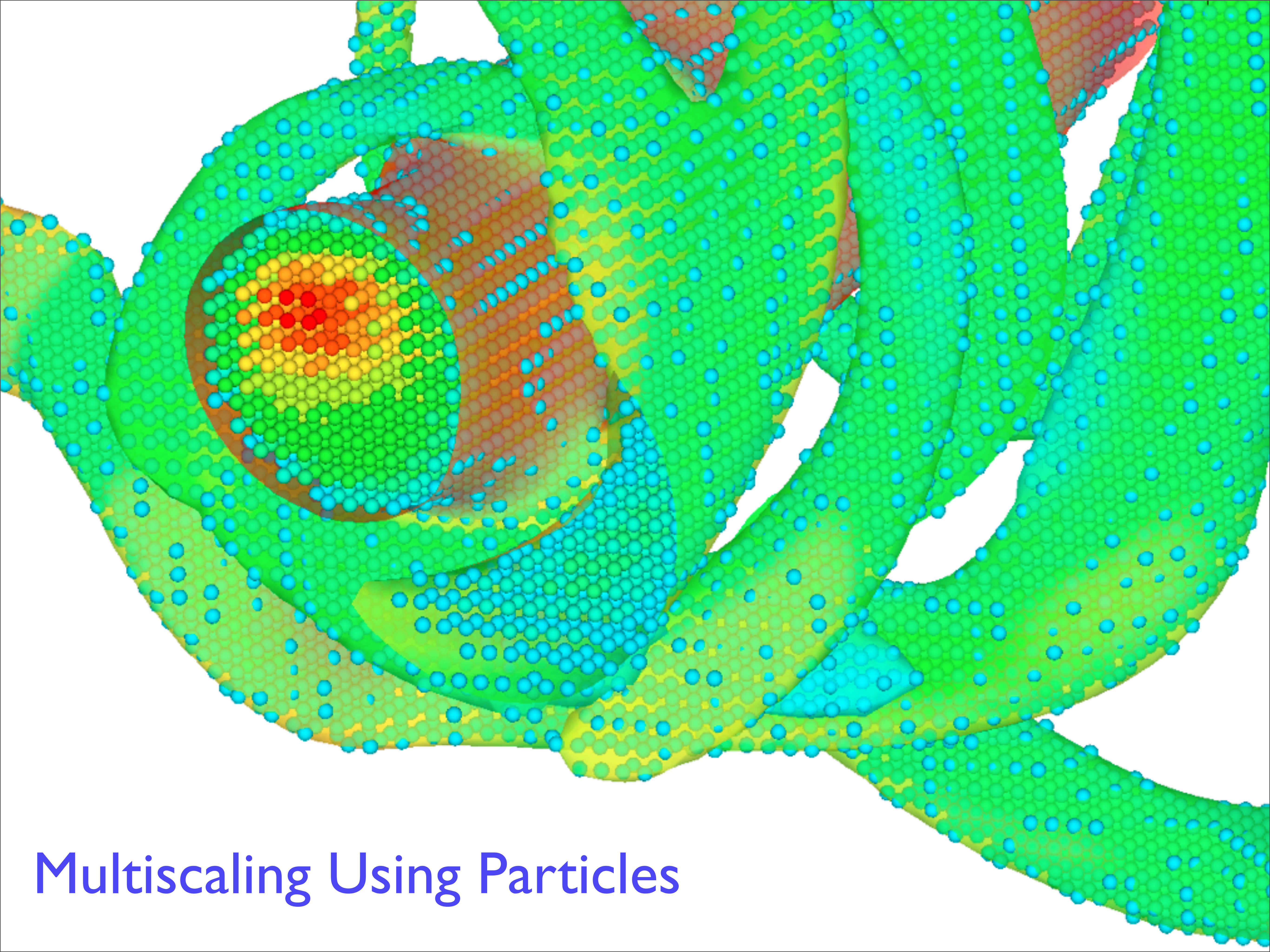
(Dynamic regridding)





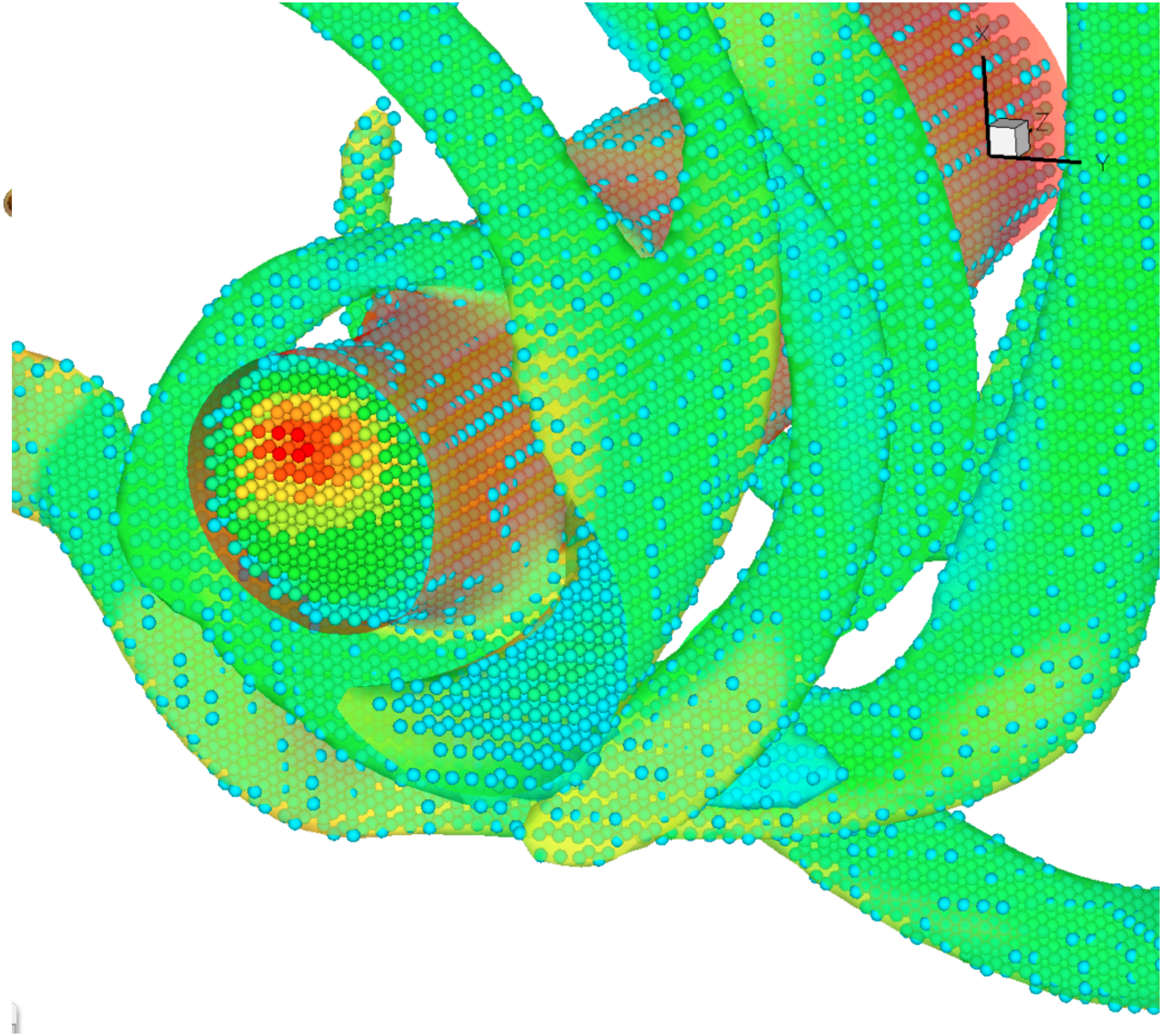
S.E. Hieber and P. Koumoutsakos. An Immersed Boundary Method for Smoothed Particle Hydrodynamics of Self-Propelled Swimmers. , *J. Comp. Physics, accepted.*

(open source) Particle Library + 16K processors = 10 Billion Vortex Particles



Multiscaling Using Particles

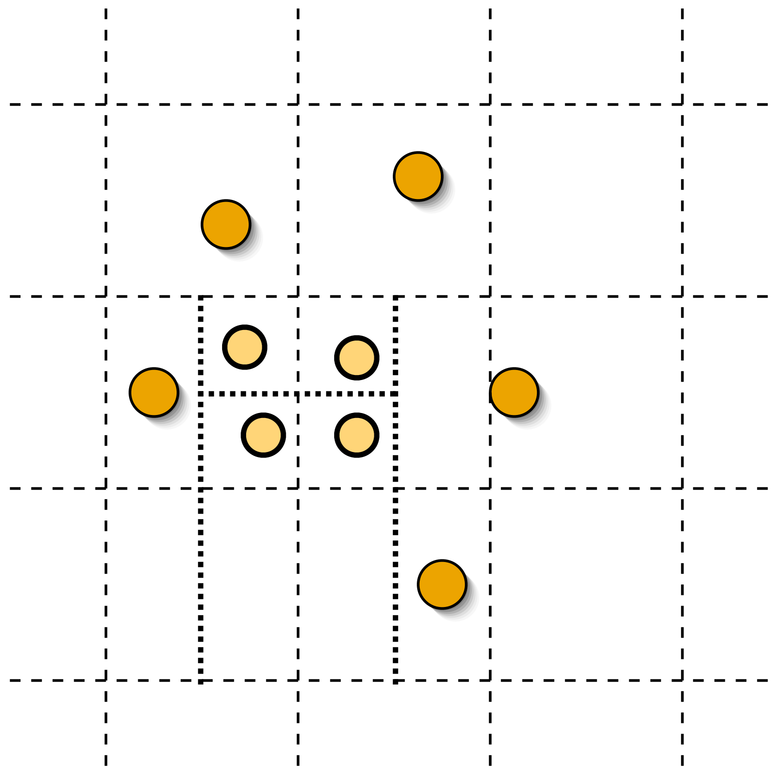
Particle Methods are Adaptive yet Inefficient



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 Mechanics and Engineering, 197/13-16, 1296-1304, 2008

Multiresolution via Remeshing

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



Grid can have variable/adaptive size

- Moment conserving
- Tensorial Product of 1D kernels
- **Programming is challenging**

Key Issue : Introduction of a **grid - The old "magic" is gone**

Enabling : • **MULTIRESOLUTION - New Magic**

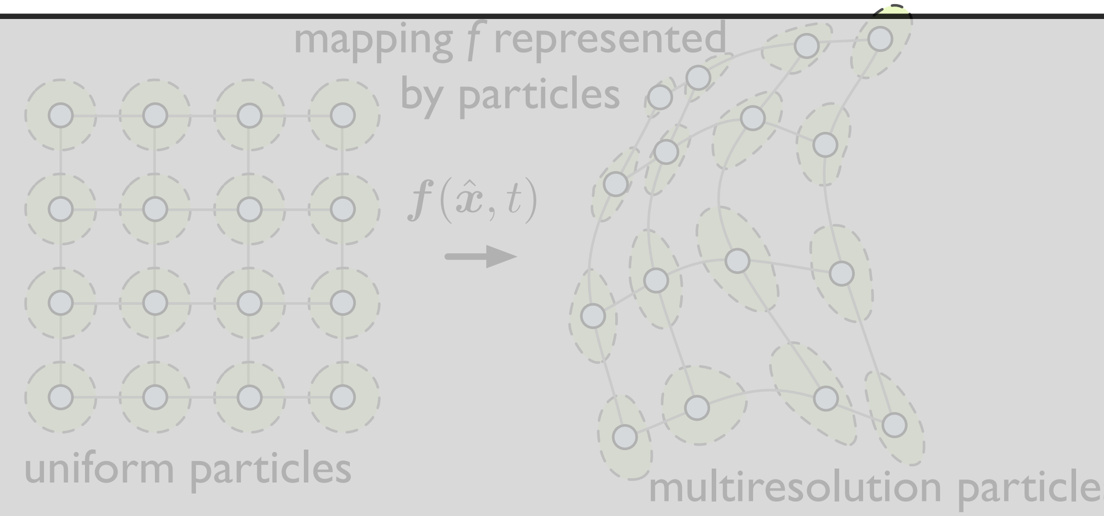
• Fast Poisson solvers - Efficient Differential operators

• Avoiding accumulation of energy in the small scales

Multiresolution Techniques for Particles

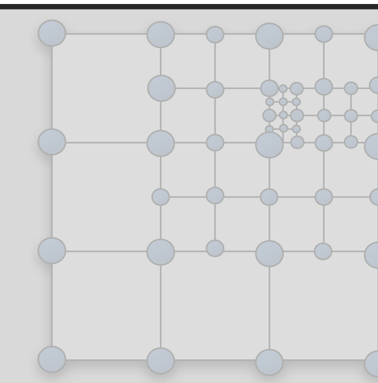
Adaptive Global Mappings

Keypoints: Adaptive mapping represented by particles



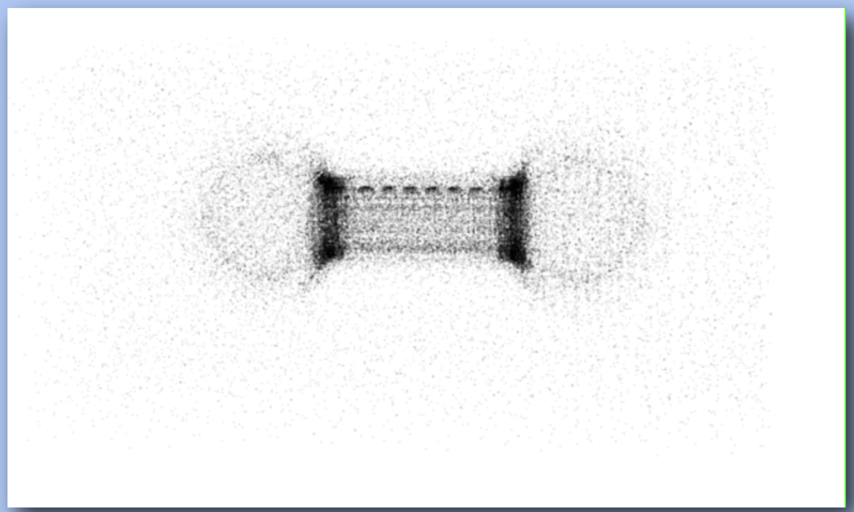
AMR-based

Keypoints: High-resolution particles are created on patches of refinement + Multilevel remeshing

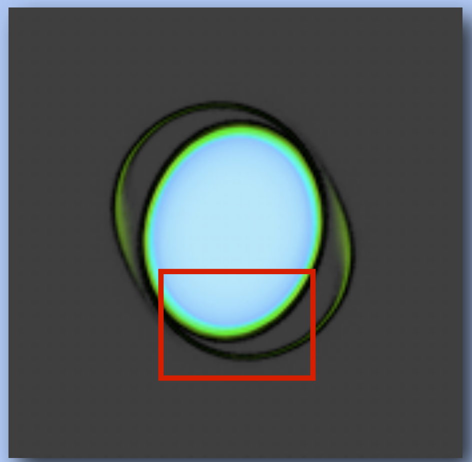


Particle-Wavelet Method

Keypoints: Wavelets guide particle refinement. Lagrangian accounting for convection of small scales



3D curvature driven collapse of a level set dumbbell



Axisymmetrization of an elliptical vortex (2D Euler)

Wavelet-particle method

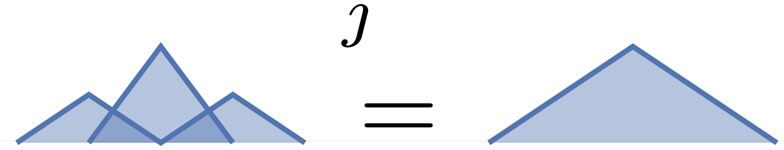
While particles are on grid locations

mollification kernel ⟷ basis/scaling function

Multiresolution analysis (MRA) $\{\mathcal{V}^l\}_{l=0}^{L}$ of particle quantities

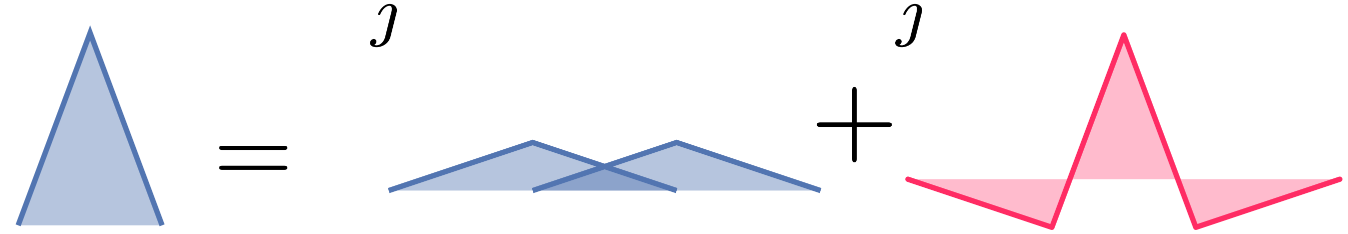
Refineable kernels as basis functions of $\mathcal{V}^l$

$$\zeta_k^l = \sum_j h_{j,k}^l \, \zeta_j^{l+1}$$



Wavelets as basis functions of the complements $\mathcal{W}^l$

$$\zeta_k^{l+1} = \sum_j \tilde{h}_{j,k}^l \zeta_j^l + \sum_j \tilde{g}_{j,k}^l \psi_j^l$$



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

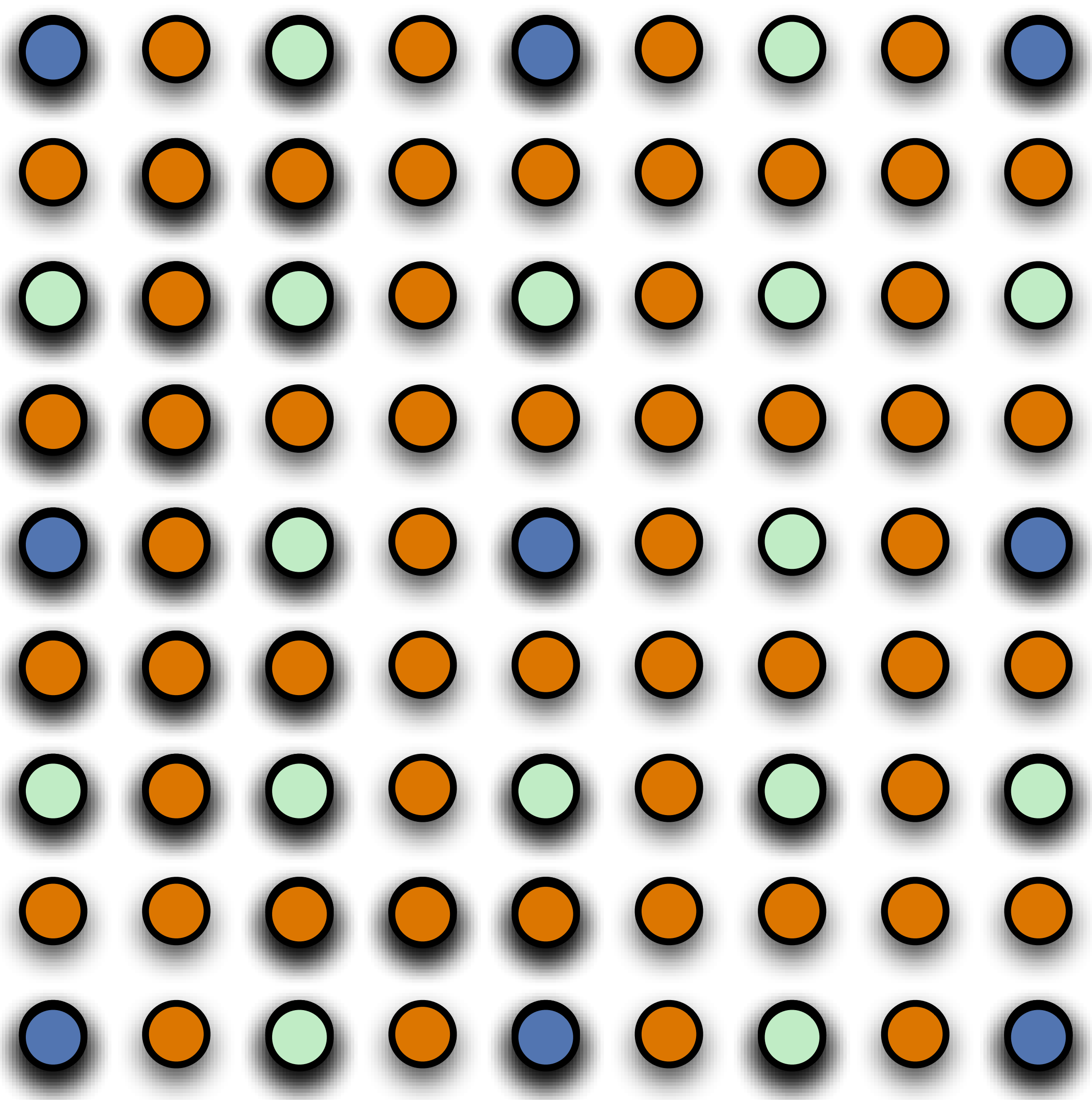
Remeshing + MultiResolution Analysis

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

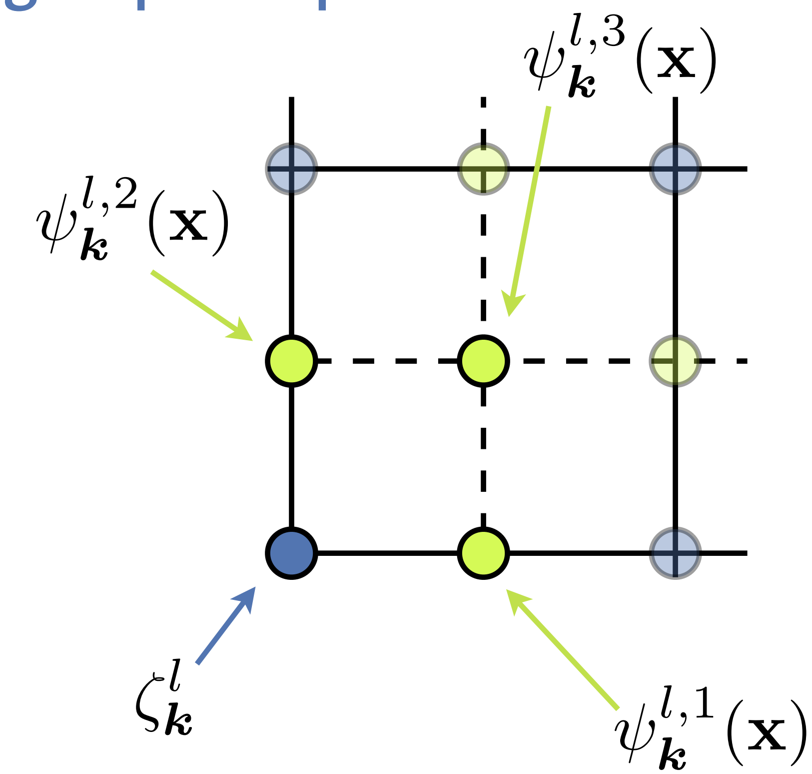
"ground" level

detail coefficients

wavelets



Each wavelet is **associated** with a **specific grid point/particle**



Discard insignificant detail coefficients:

$$\left| d_k^l \right| < \varepsilon$$

Compressed function representation: $q_{\geq}^L$

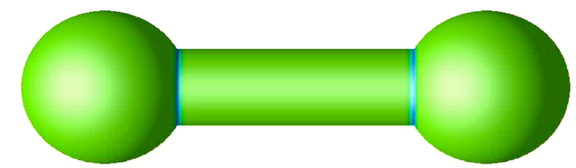
Adapted grid

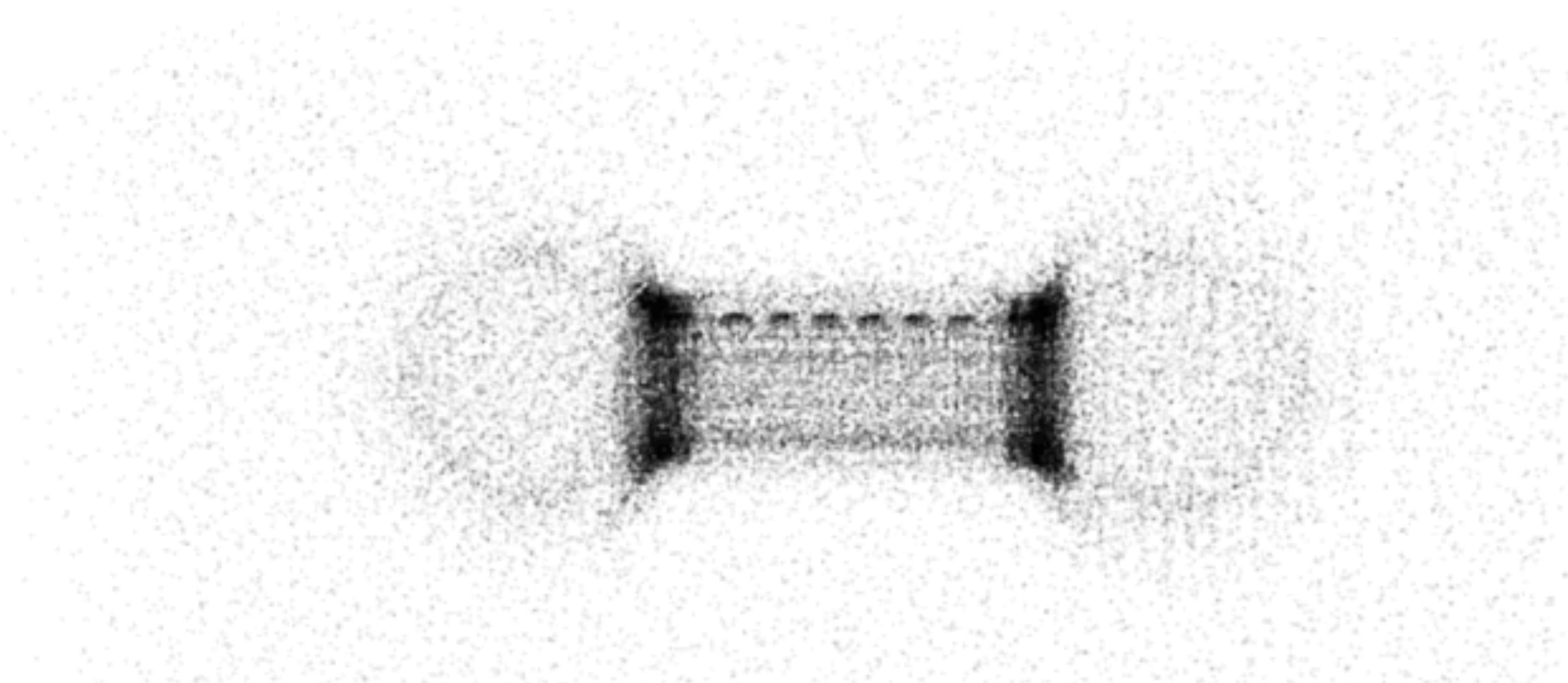
Wavelet Particle Level sets

Simulation of 3D curvature-driven flow: **Collapsing Dumbbell**

$$\frac{\partial \phi}{\partial t} + \kappa\, \boldsymbol{n} \cdot \nabla \phi = 0.$$

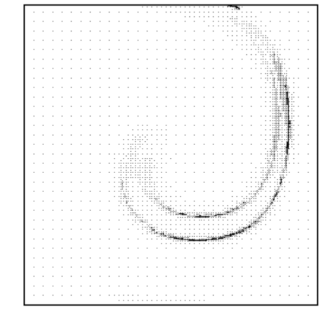
$$\kappa = \nabla \cdot \boldsymbol{n}$$

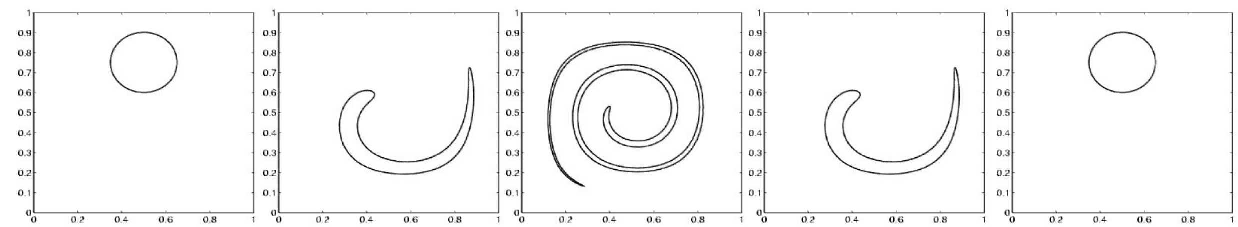


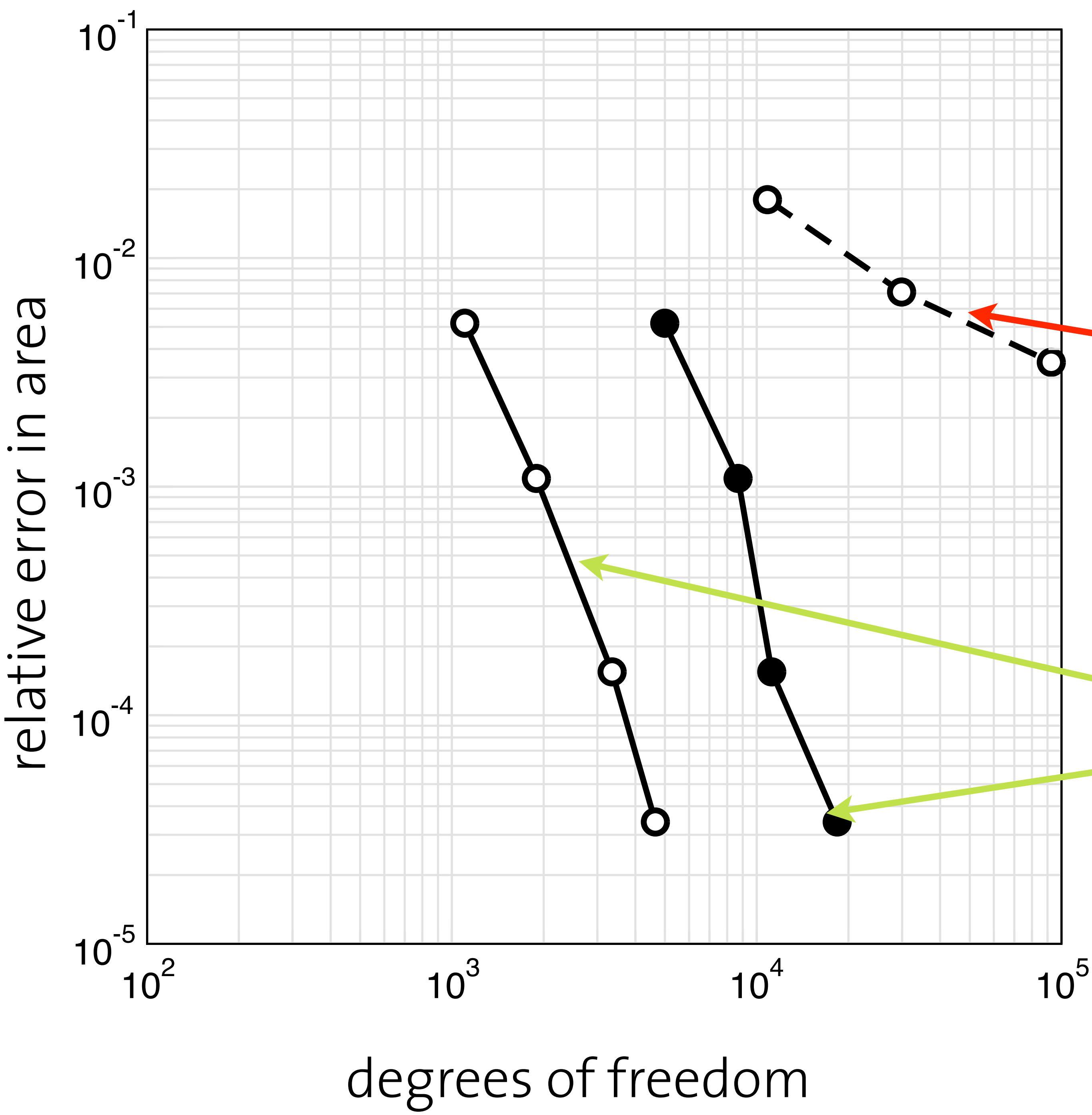


distribution of active particles

Level set volume conservation for deformation benchmark







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

$$\mathrm{CFL}_{\max} \approx 40$$

M. Bergdorf, P. Koumoutsakos, SIAM J. Multiscale Modeling and Simulation, 5(3), 980-995, 2006.

FURTHER EXAMPLES

René Magritte, *Clairvoyance* (1936)

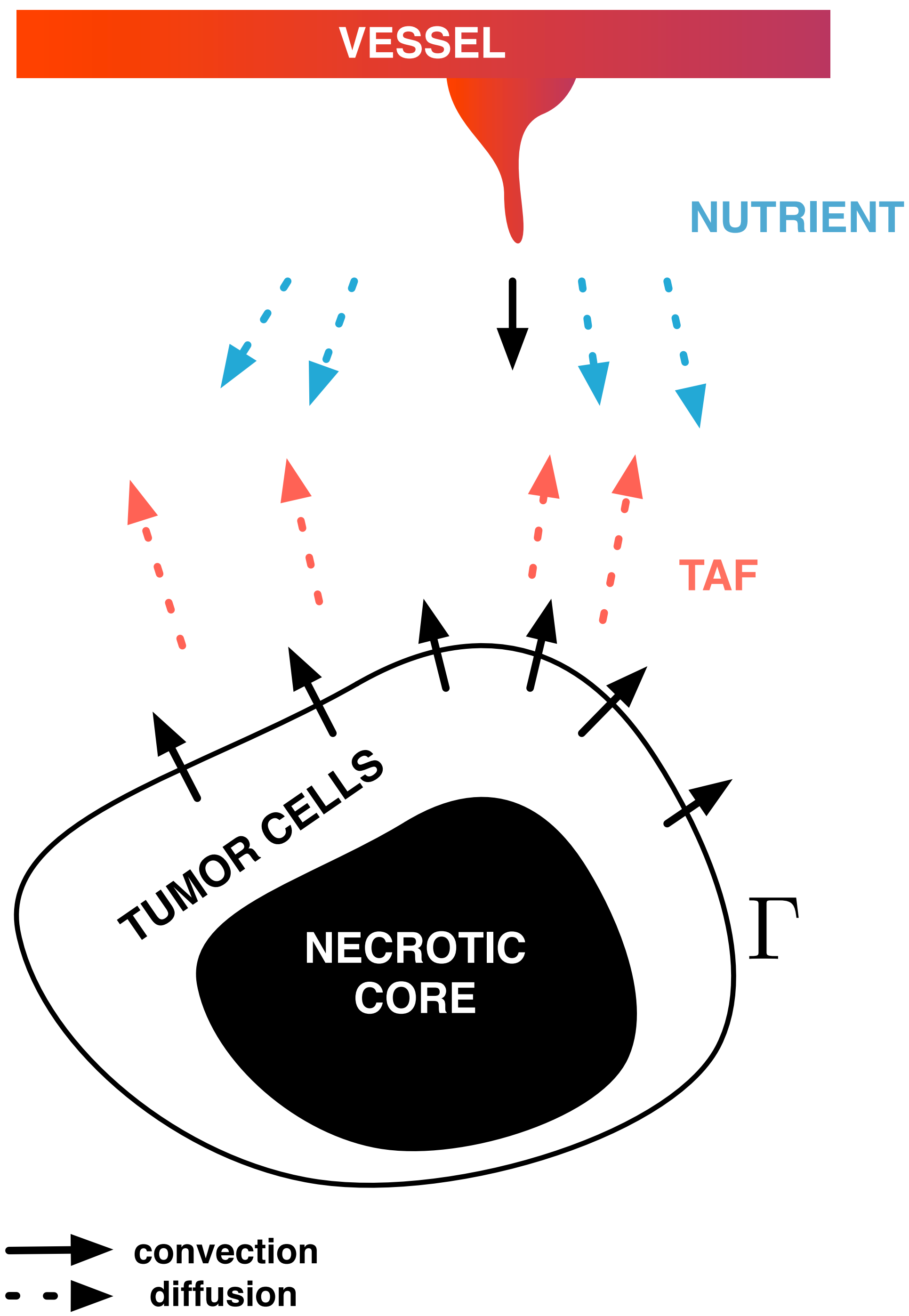
a particle - sharp interface model of Vascular Tumor growth

Reaction/diffusion/convection equation for densities carried by particles

$$\frac{Du}{Dt} = \nabla \cdot (Q \nabla u) + \Gamma(u) - L(u)$$

diffusion — proliferation/generation — death/decay

$u = u_T$	living tumor cell density
u_D	dead tumor cell density
u_C	endothelial cell density
u_N	nutrient density
u_A	TAF density



e.g. tumor cell density (only inside Γ):

$$\frac{Du_T}{Dt} = \gamma_T \, u_N \, u_T \, H(u_N - \tilde{u}_N \, u_T) - \mu_T \, H(\bar{u}_N \, u_T - u_N) \, u_T$$

proliferation — necrosis

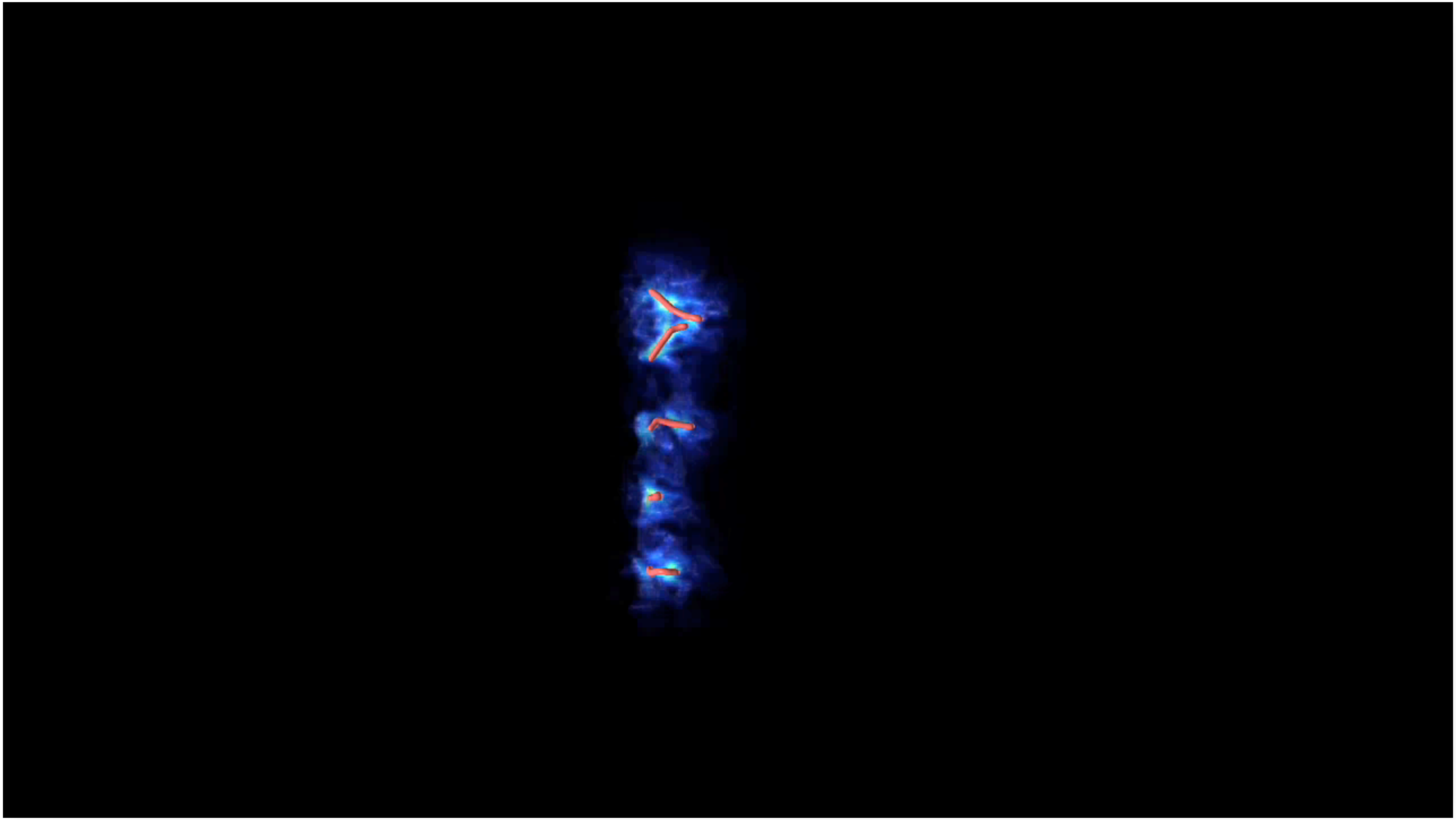
$$\boldsymbol{v} = -\nabla \left(u_T + u_D + u_C\right)$$

convection velocity

cells can proliferate if nutrient is above $\tilde{u}_N$

cells become necrotic if nutrient is below $\bar{u}_N$

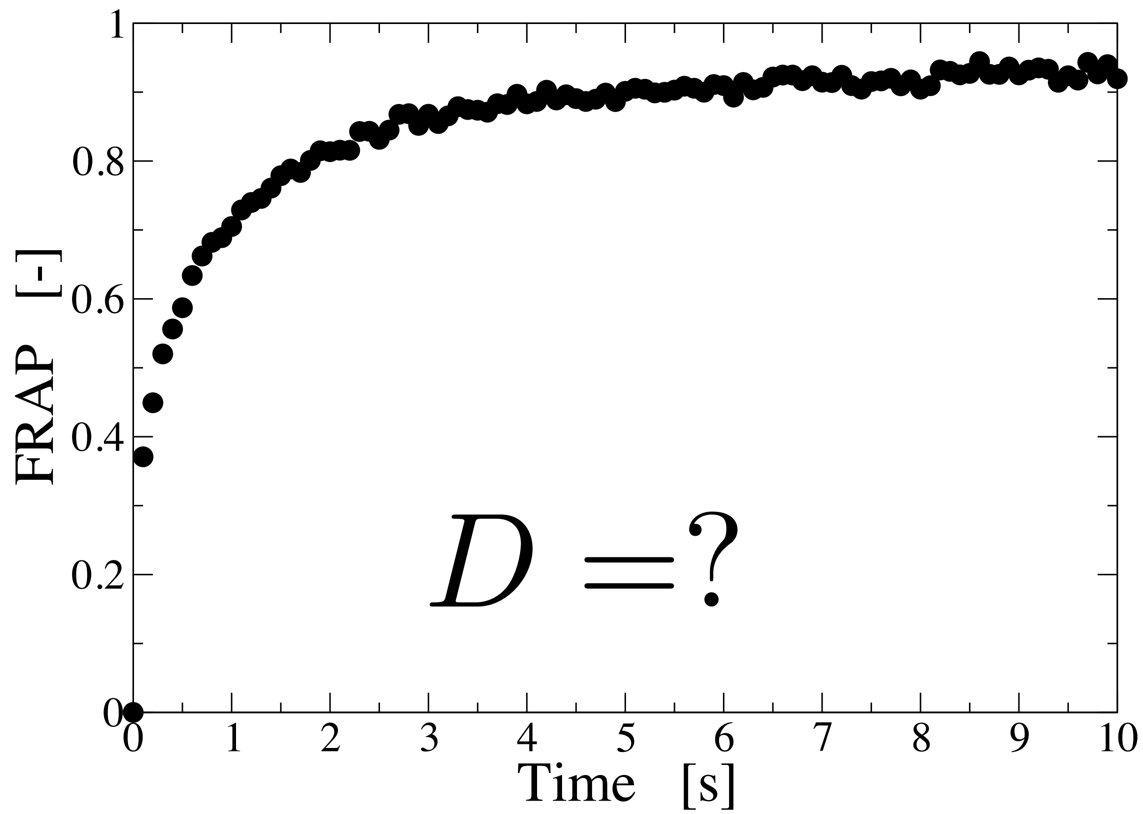
Tumor Induced Angiogenesis

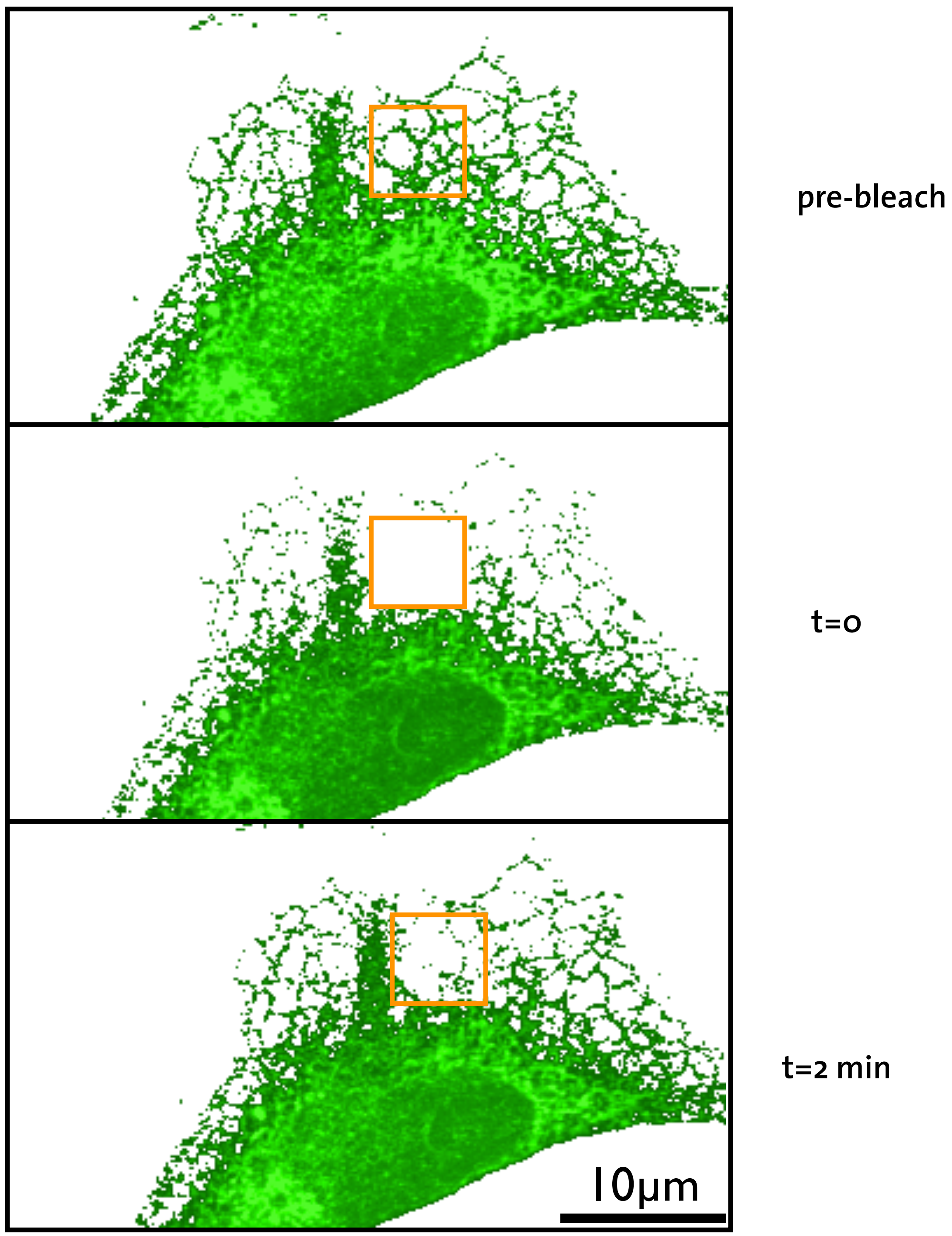


Milde F., Bergdorf M. and PK, A hybrid model of sprouting angiogenesis, Biophysical J., 2008

Diffusion in the Endoplasmatic Reticulum

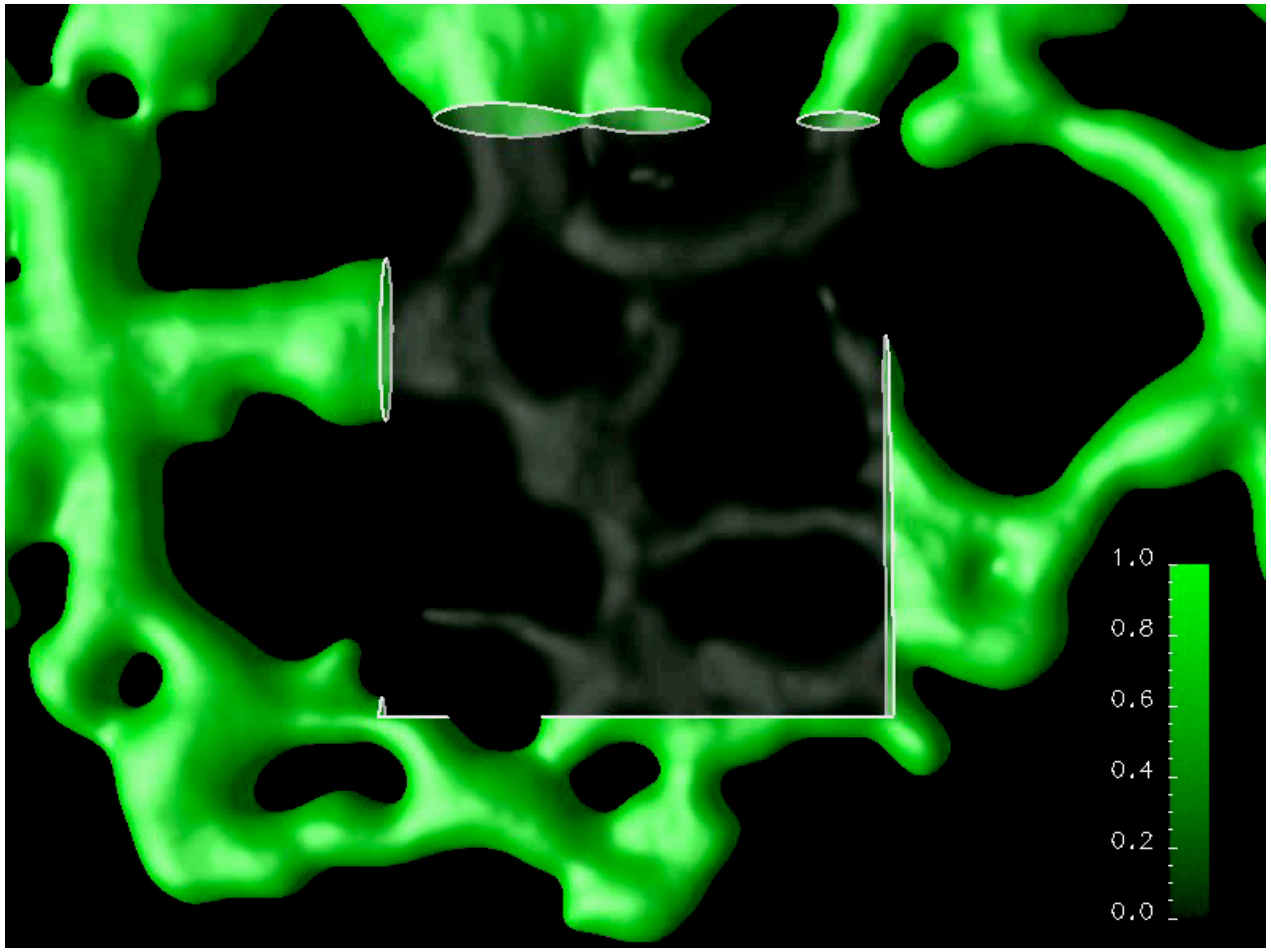
- Tag protein fluorescently
- Laser Bleach **region of interest**
- Monitor influx of unbleached protein

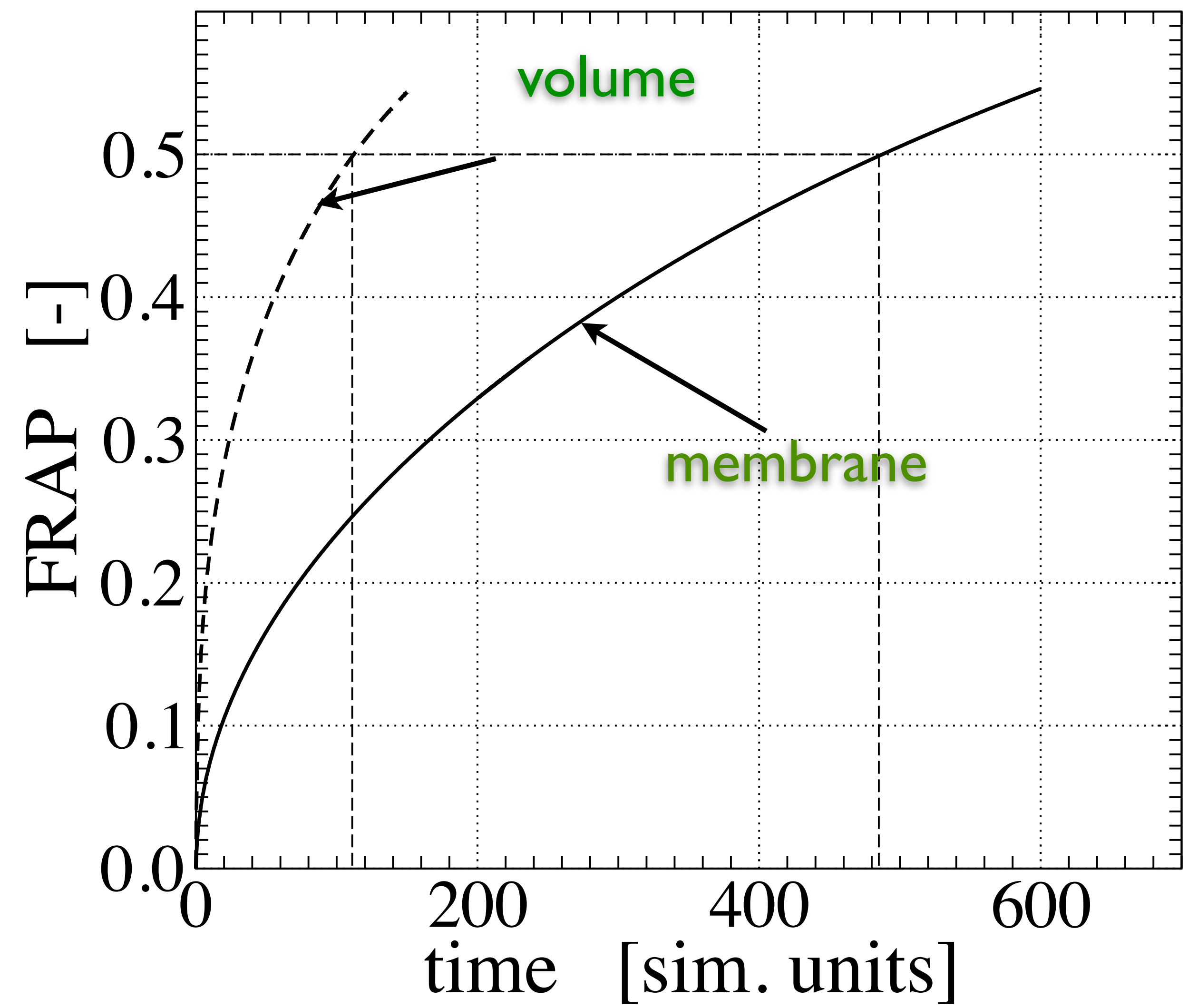




Helenius group (ETHZ)

Diffusion on reconstructed ER of VERO cells





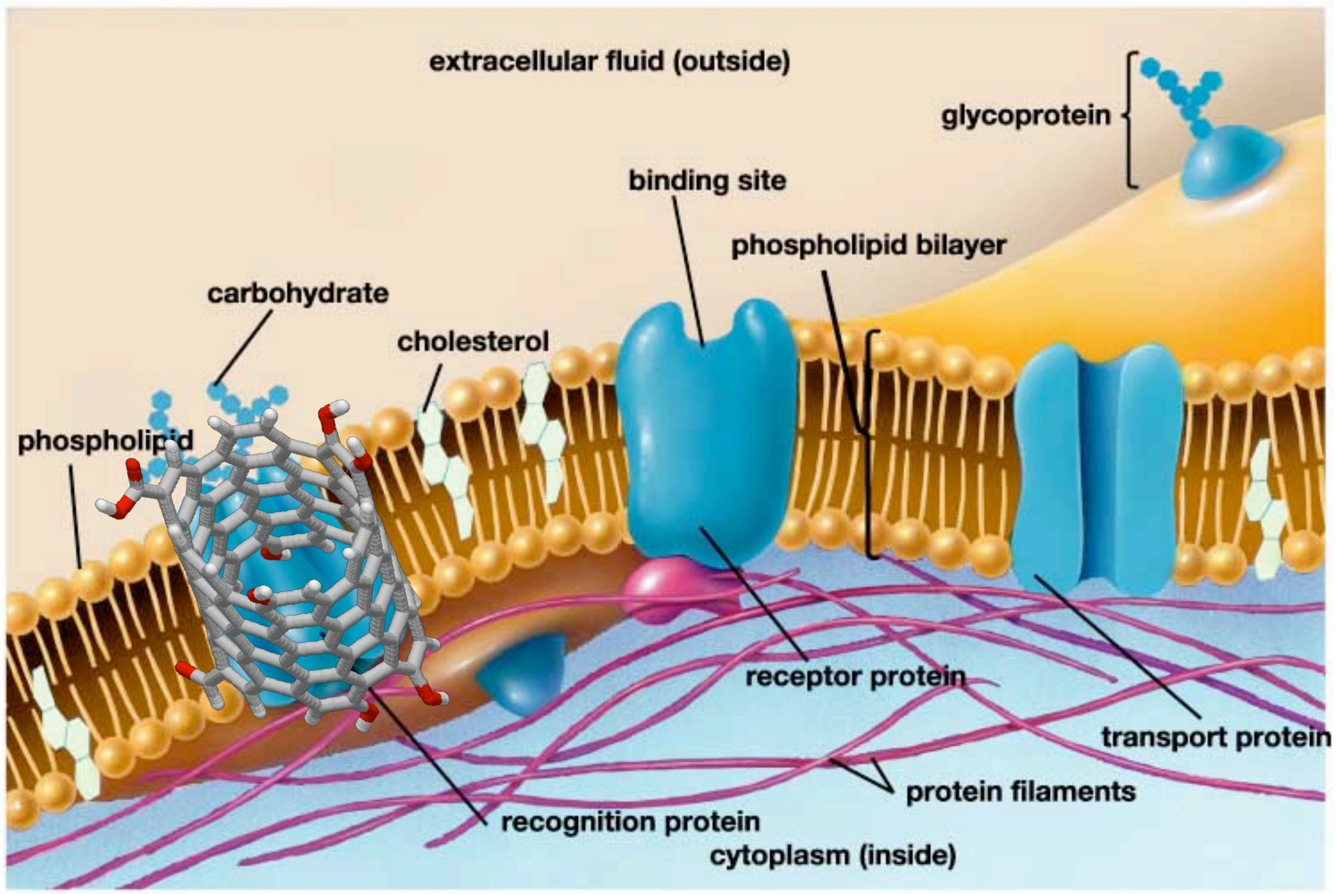
ssGFP-KDEL in the ER lumen of $\nu = 34 \pm 0.95\,\mu\mathrm{m}^2/\mathrm{s}$

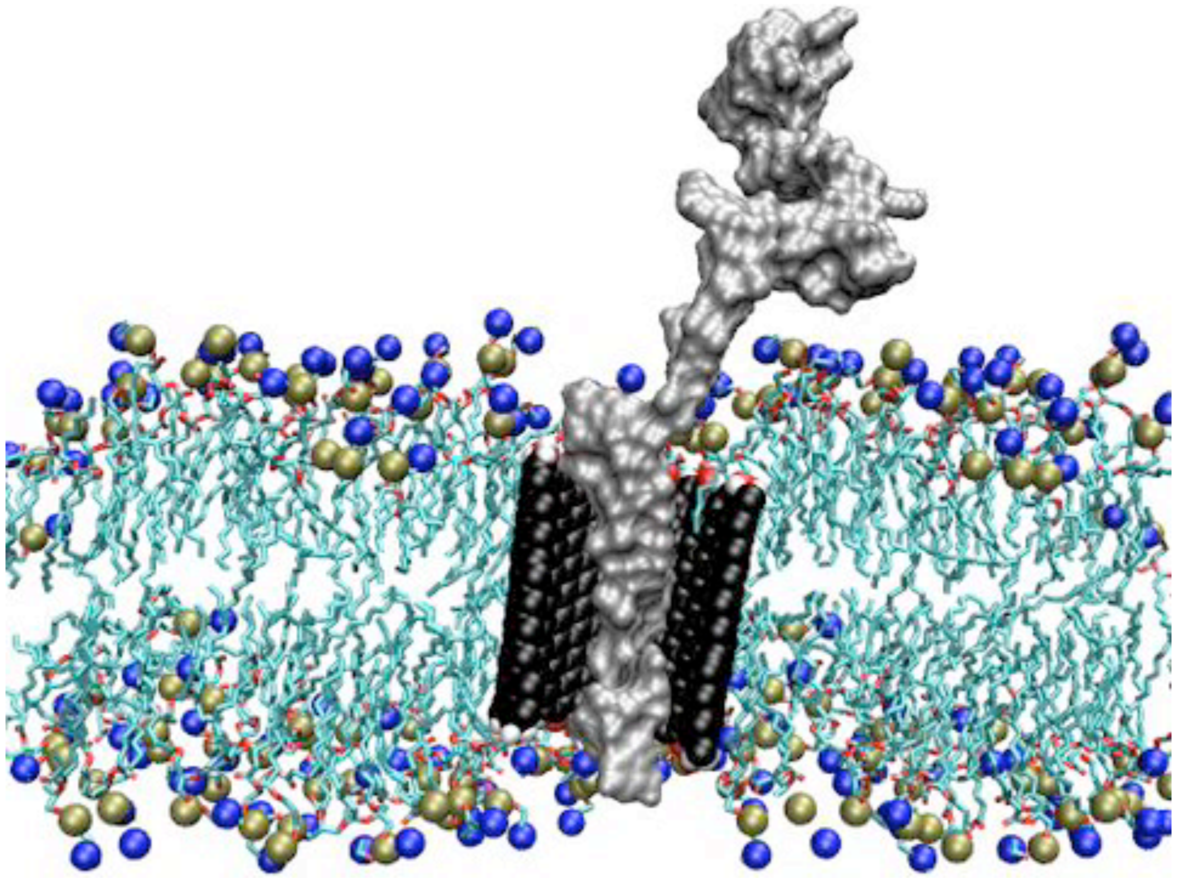
tsO45-VSVG-GFP in the ER membrane $\nu = 0.16 \pm 0.07\,\mu\mathrm{m}^2/\mathrm{s}$

Using the *same diffusion constant* recovery speed varies by ***>400%***.

I. F. Sbalzarini, A. Hayer, A. Helenius, and P. Koumoutsakos. *Biophys. J.*, 2006.

Simulations of Artificial Channels





Picture from: Teresa and Gerald Audesirik. Biology, Life on Earth. Prentice Hall, New Jersey, 1999

U. Zimmerli and P. Koumoutsakos, , Biophysical J., 2008

Conclusions

Particle Methods are well suited for

- Complex Geometries
- Efficient Remeshing
- Parallel High Performance Computing

but require special attention for

- Convergence
- Boundary Conditions
- Multiscale Approaches