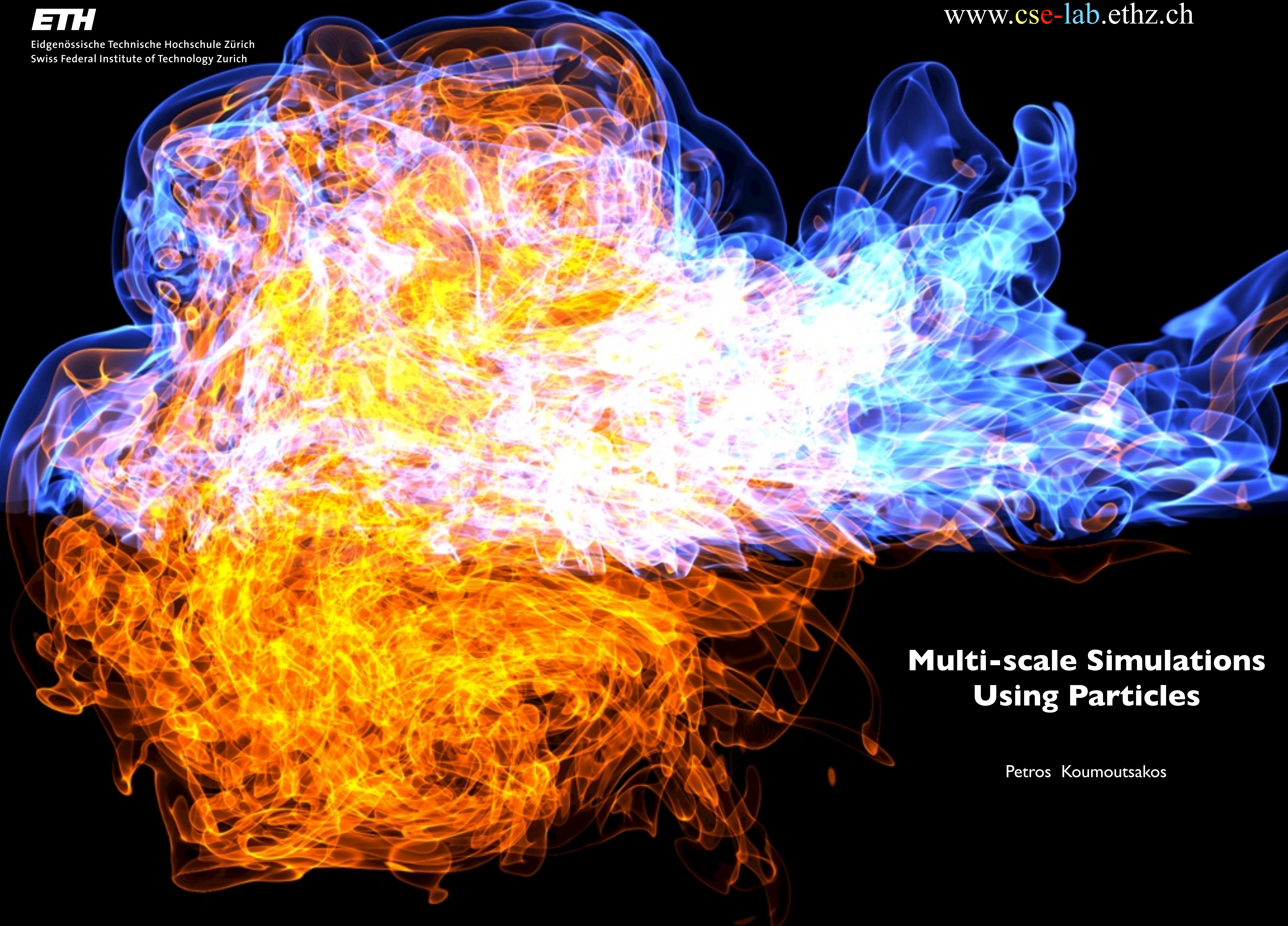
ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

www.cse-lab.ethz.ch



Multi-scale Simulations Using Particles

Petros Koumoutsakos

OUTLINE

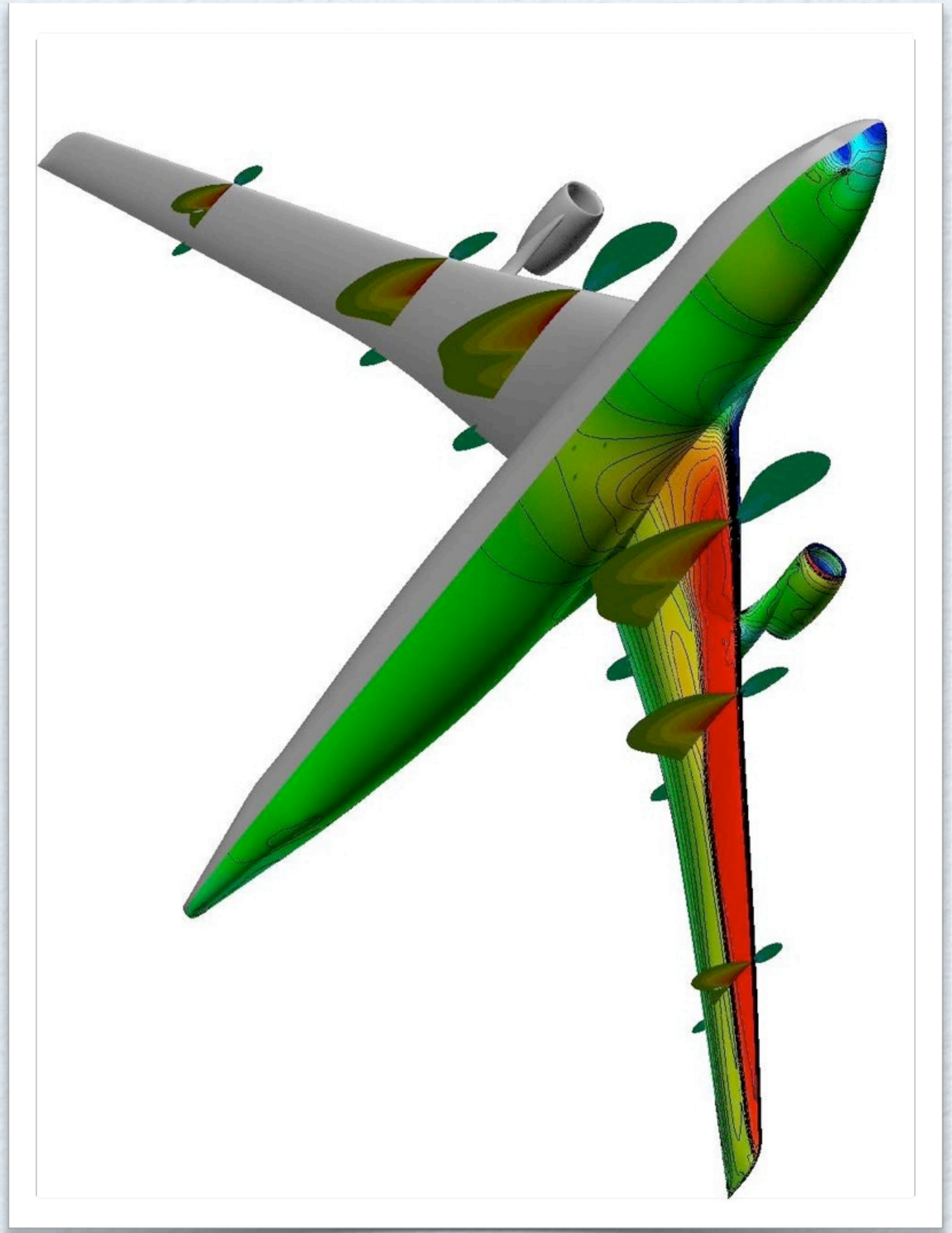
- PARTICLE METHODS
  - A computational framework
- MULTIRESOLUTION – UNBOUNDED DOMAINS
  - Particles + Wavelets
- MULTISCALING – BOUNDARIES AND INTERFACES
  - Atomistic–Mesoscale–Macroscale Particle Methods

CLASS NOTES, Links, Movies, Papers

http://www.cse-lab.ethz.ch/teaching/classes/mulsup.html

Modeling and Technology

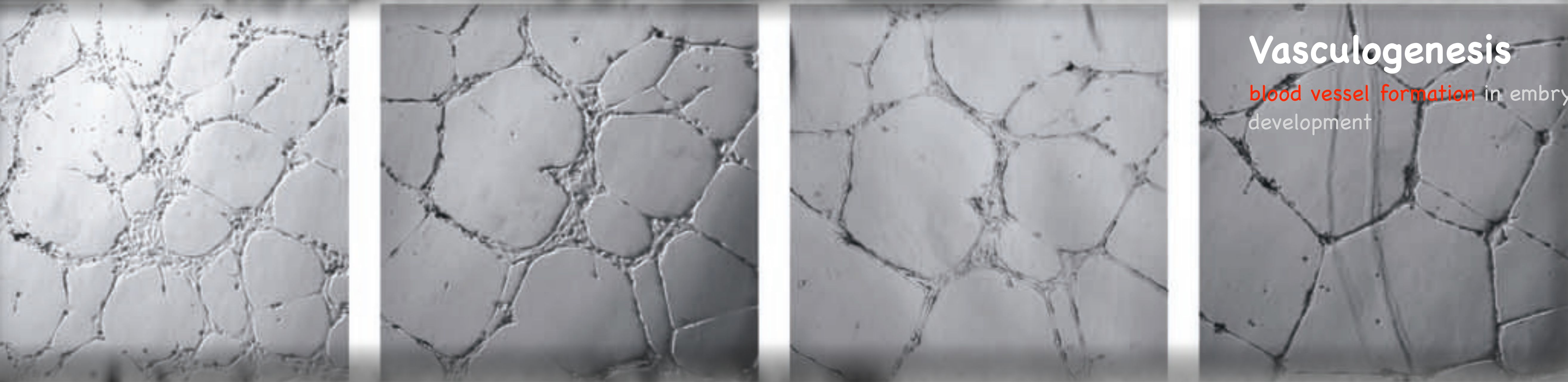
- No aircraft is flown without having been designed with complex, mechanistic simulations



Modeling and Medicine

- Heuristics and Data
- Models ?

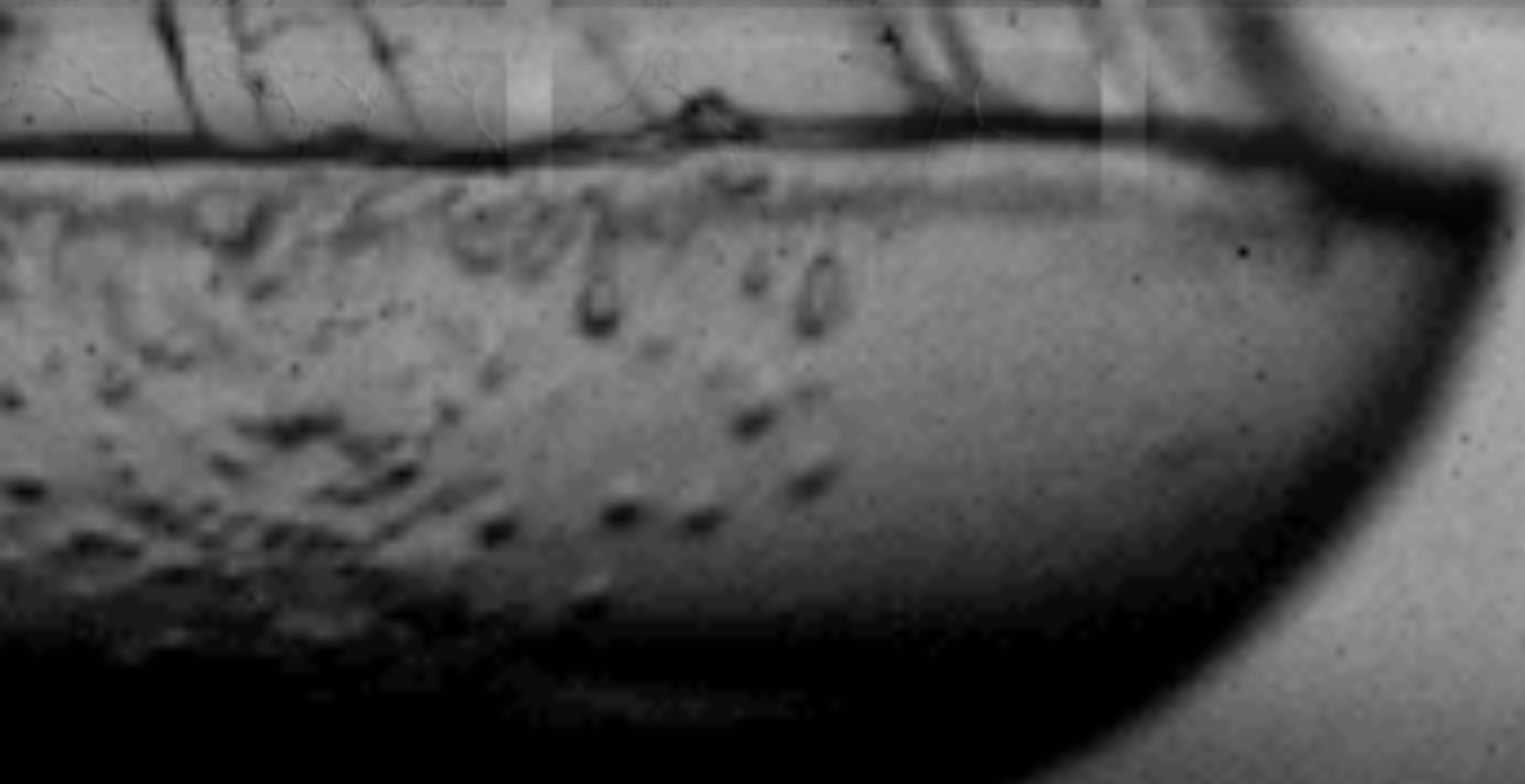
Dreamstime.com



Vasculogenesis

blood vessel formation in embryonic development

R. M. H. MERKS, S. V. BRODSKY, M. S. GOLIGORKSY, S. A.NEWMAN, AND J. A. GLAZIER. CELL ELONGATION IS KEY TO IN SILICO REPLICATION OF IN VITRO VASCULOGENESIS AND SUBSEQUENT REMODELING. DEVELOPMENTAL BIOLOGY, 289(1): 44-54, 2006.



Crown Breakup - maragoni instability

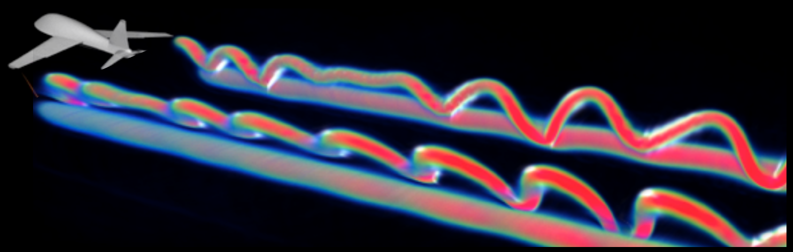
drop impact onto an ethanol sheet

[2] S. T. THORODDSEN, T. G. ETOH, AND K. TAKEHARA. CROWN BREAKUP BY MARANGONI INSTABILITY. J. FLUID MECH., 557(-1):63-72, 2006.

Τα παντα ρει

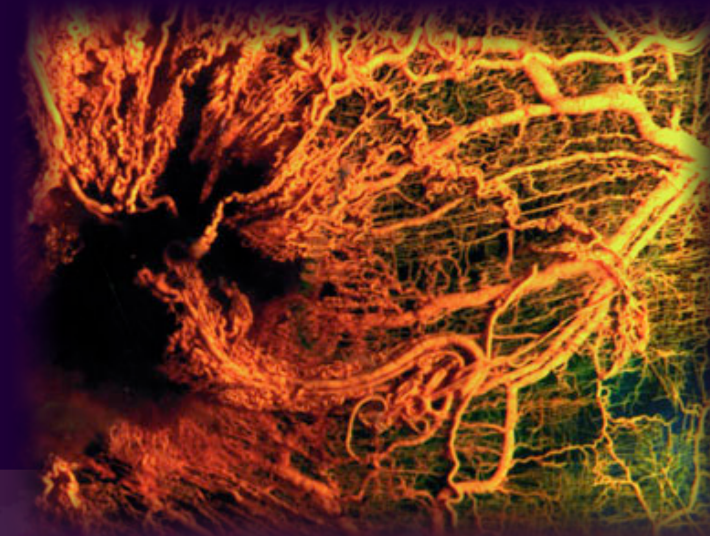
16384 Cores - 10 Billion Particles - 60% efficiency

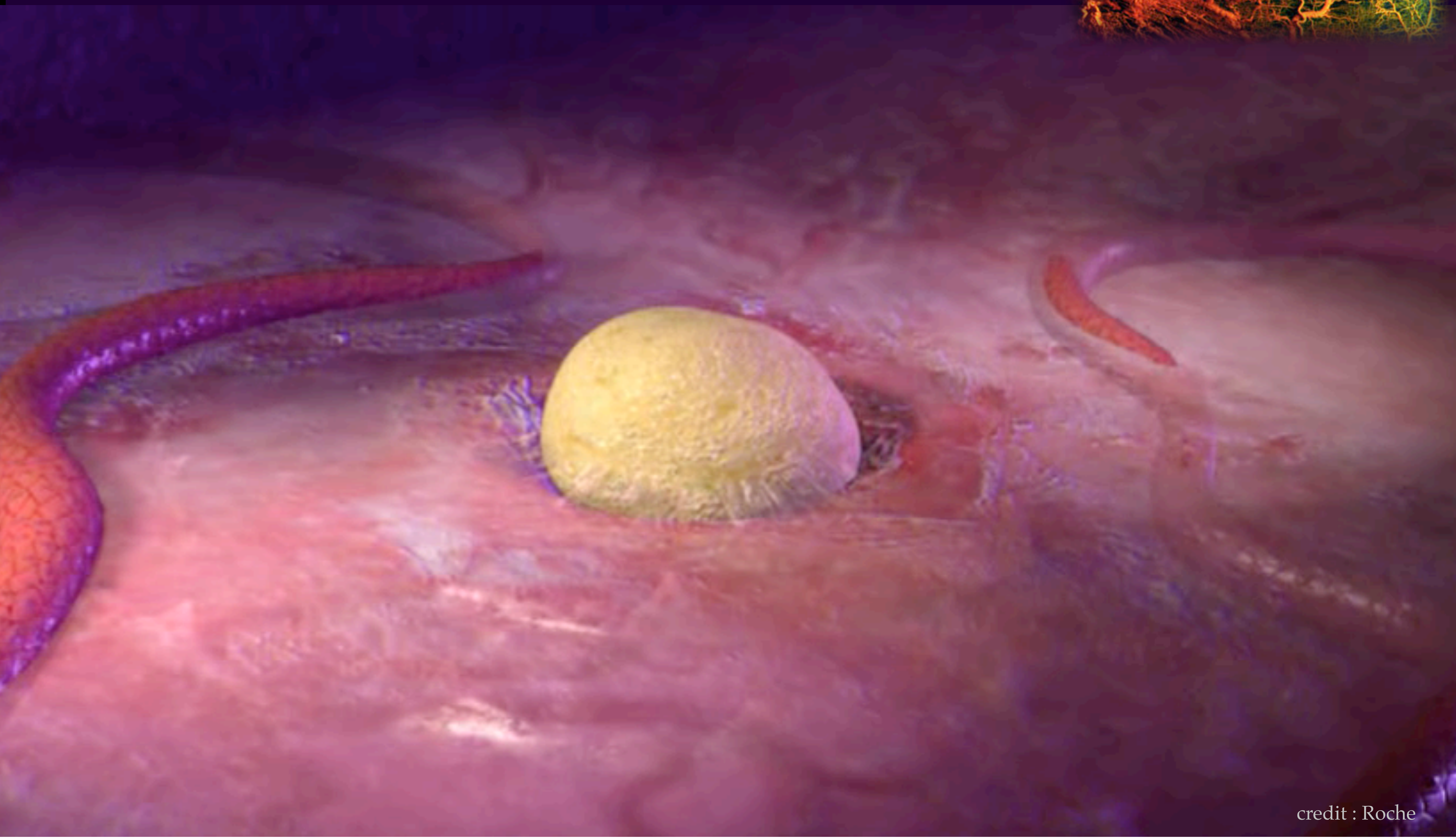
Runs at IBM Watson Center - BLue Gene/L

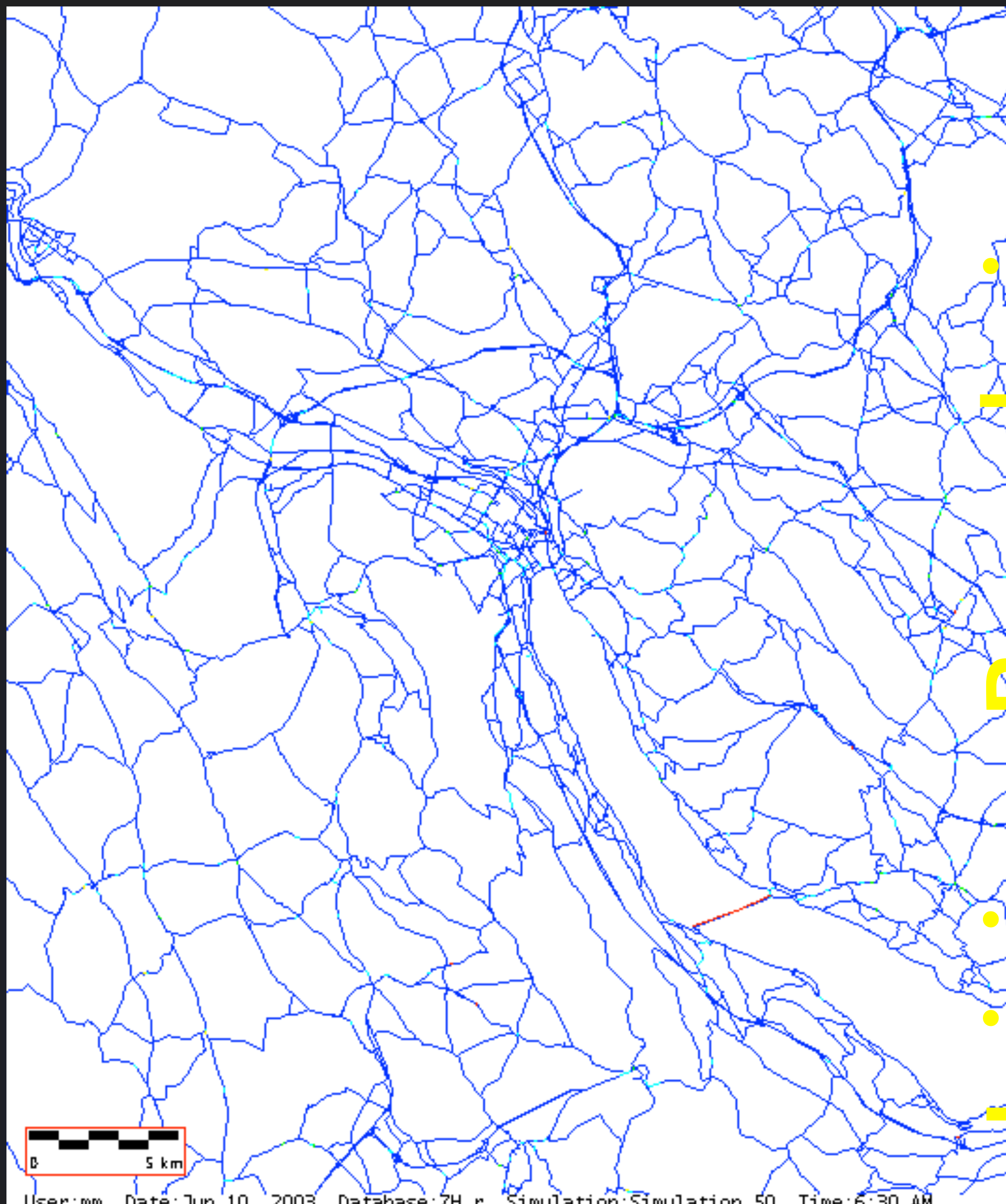


Chatelain P., Curioni A., Bergdorf M., Rossinelli D., Andreoni W., Koumoutsakos P., Billion Vortex Particle Direct Numerical Simulations of Aircraft Wakes, Computer Methods in Applied Mech. and Eng. 197/13-16, 1296-1304, 2008

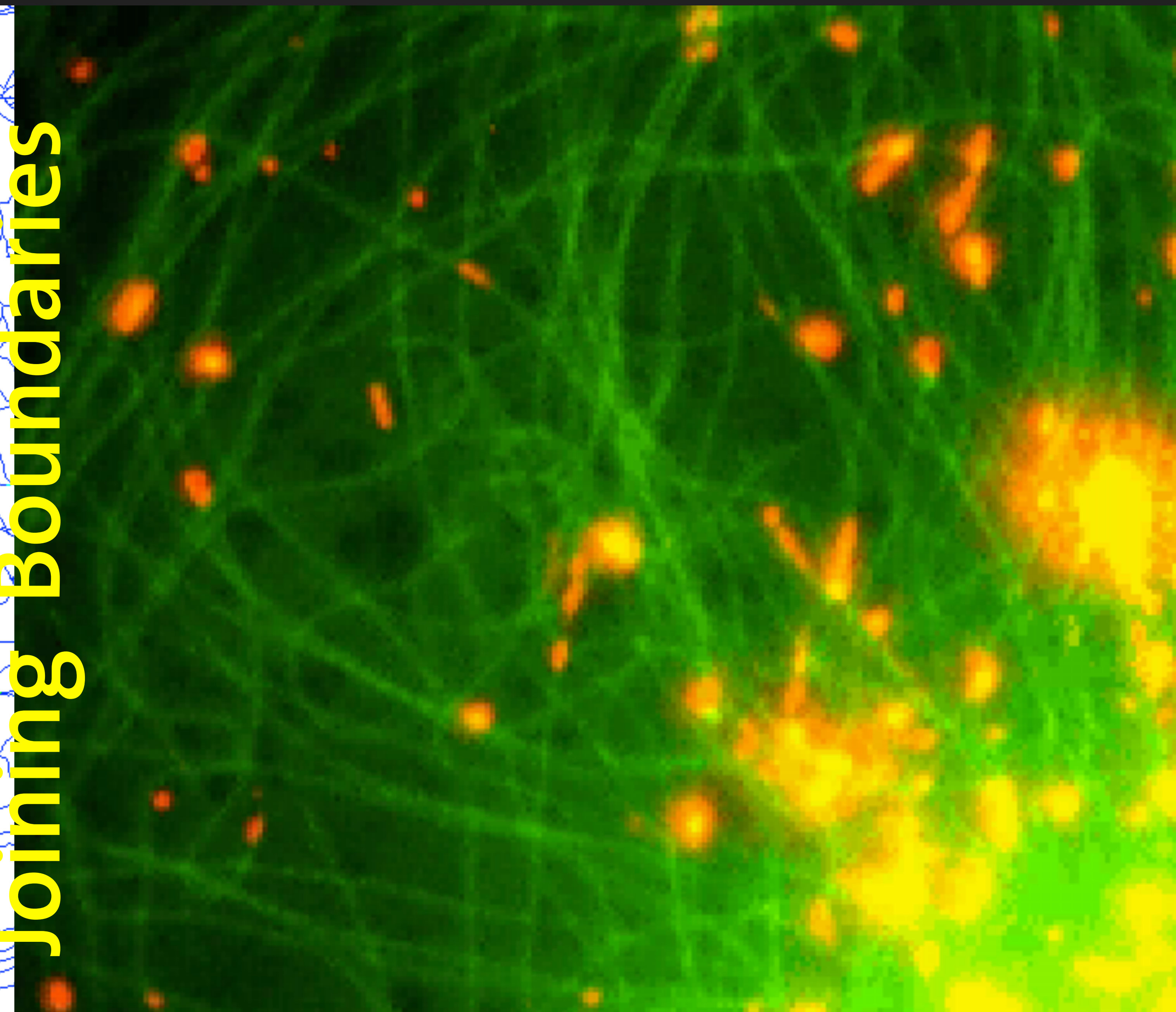
Tumor Induced Angiogenesis







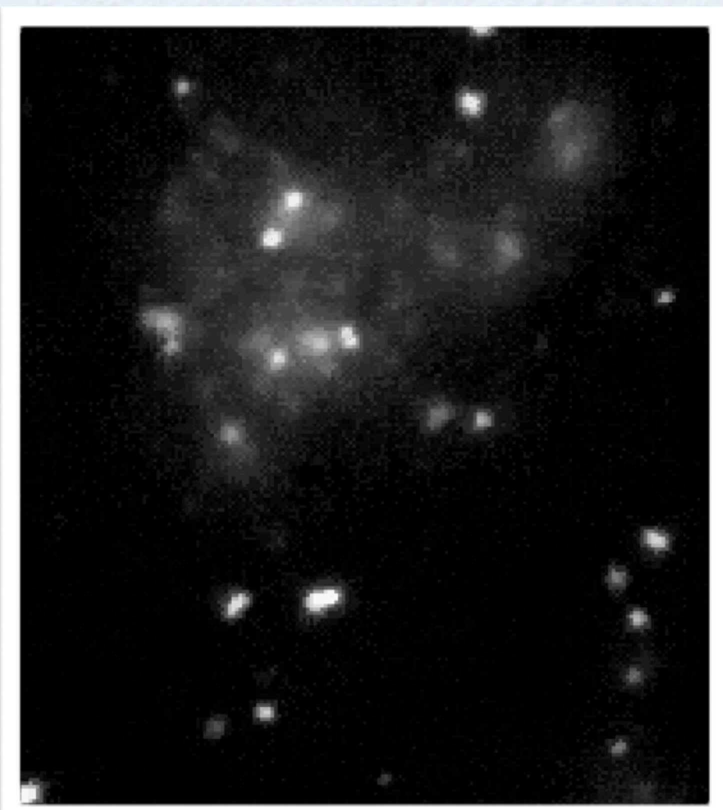
Joining Boundaries



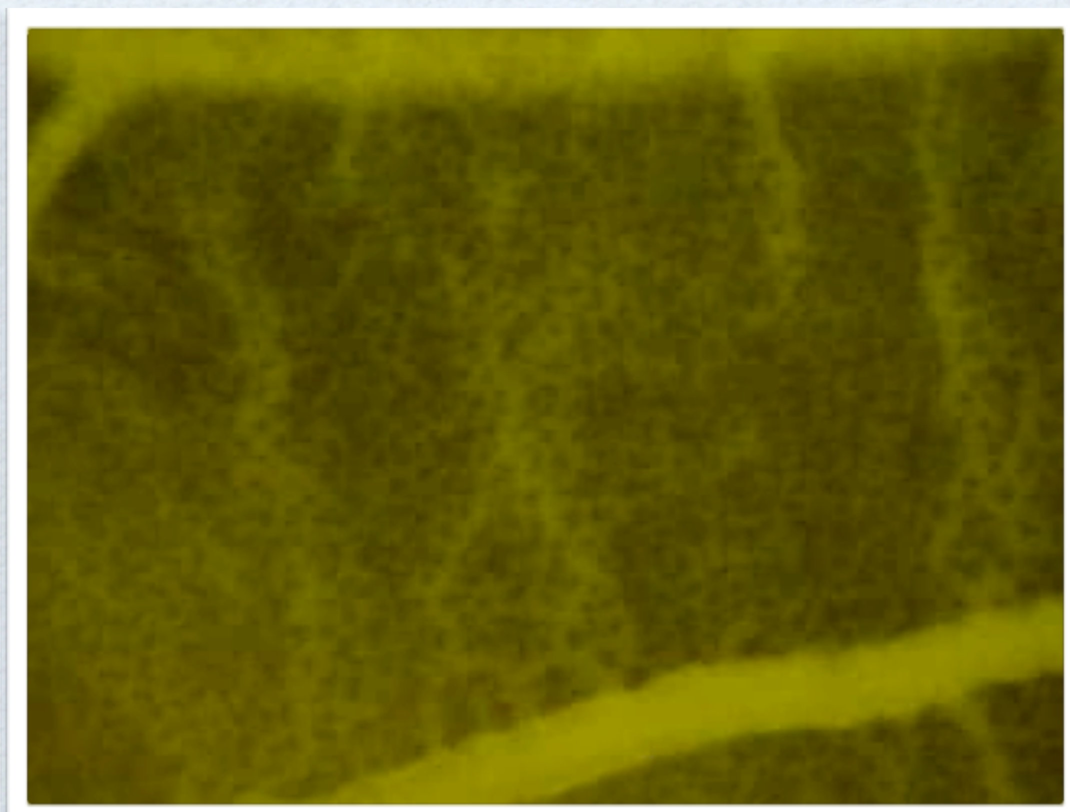
Cars
(Axhausen Lab - ETHZ)

Virus
(Helenius Lab - ETHZ)

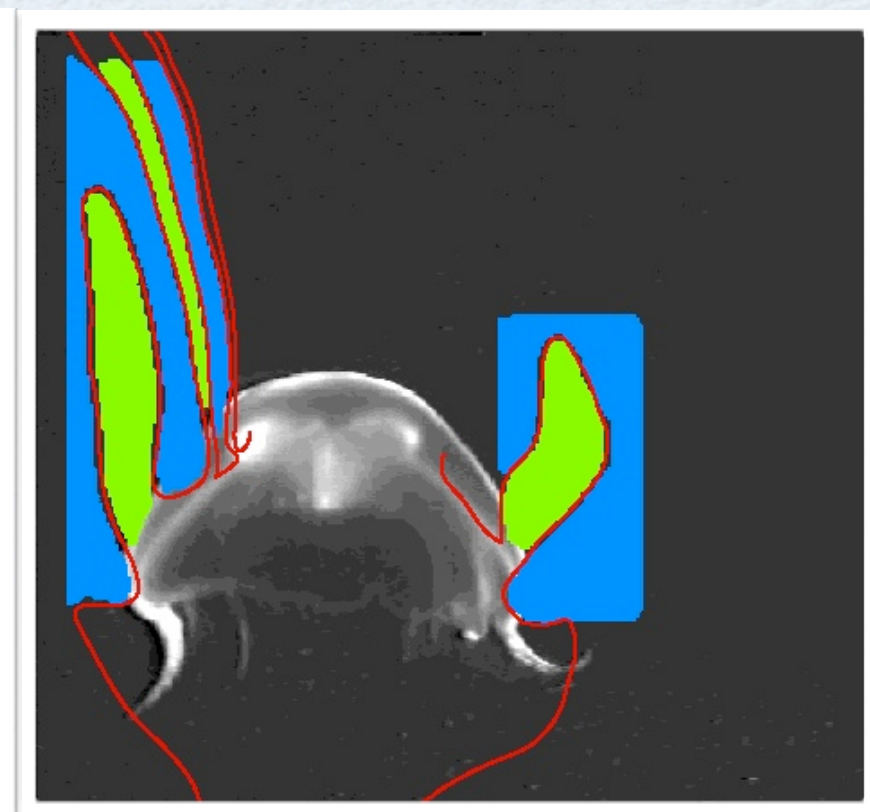
Advances
in
Hardware – Theory – Data Processing



Tracking of Adeno Virus
Greber&Koumoutsakos Lab, ETHZ



Intussuceptive Angiogenesis in the growing Chick CAM
Djonov&Burri Lab, Uni Bern



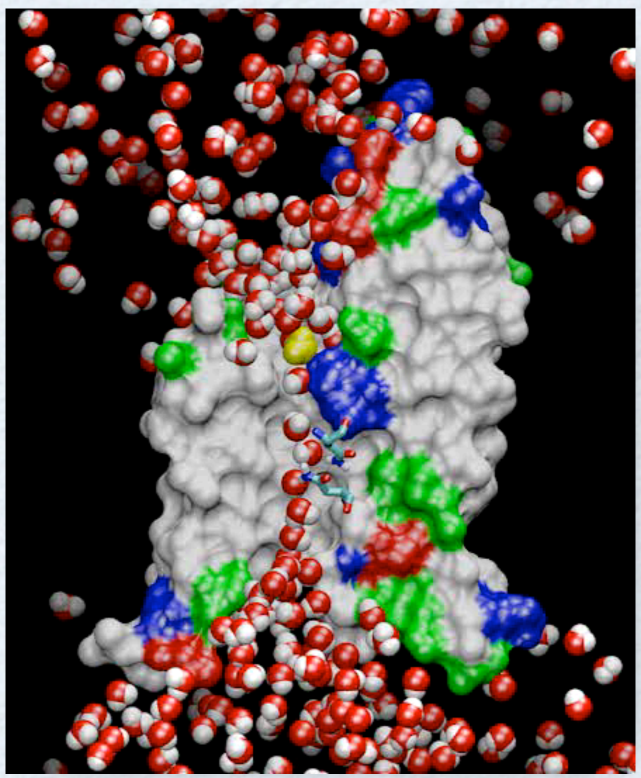
Swimming Medusa,
Dabiri Lab, Caltech

Advances
in
Hardware – Theory – Data Processing

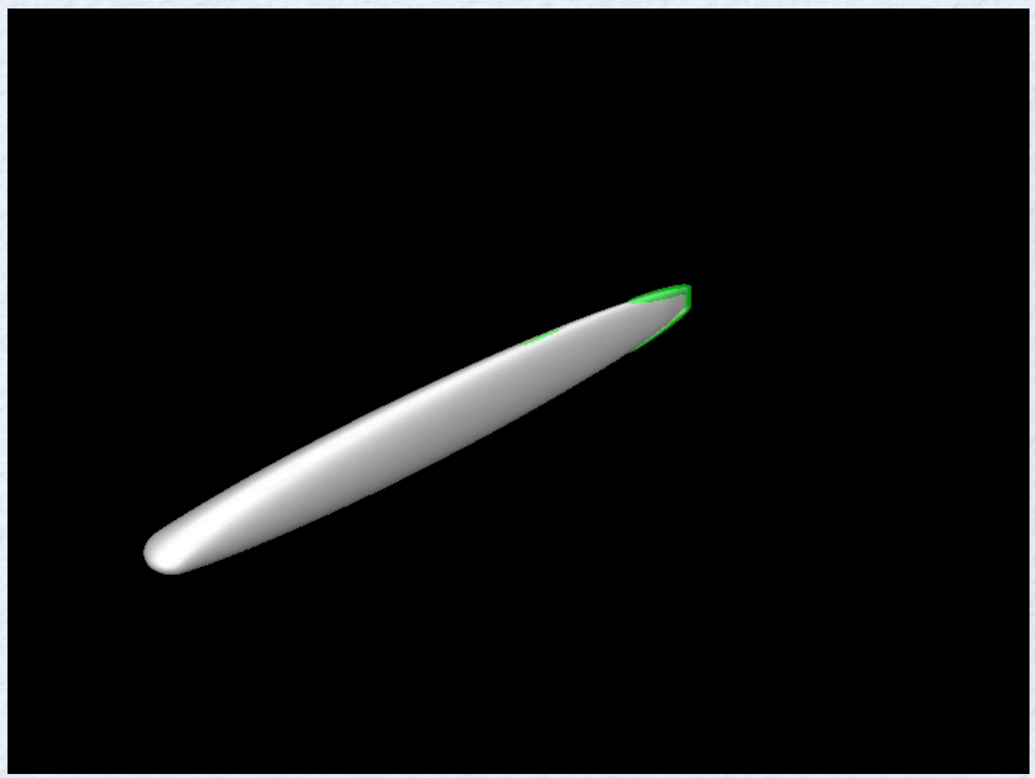
-9

0

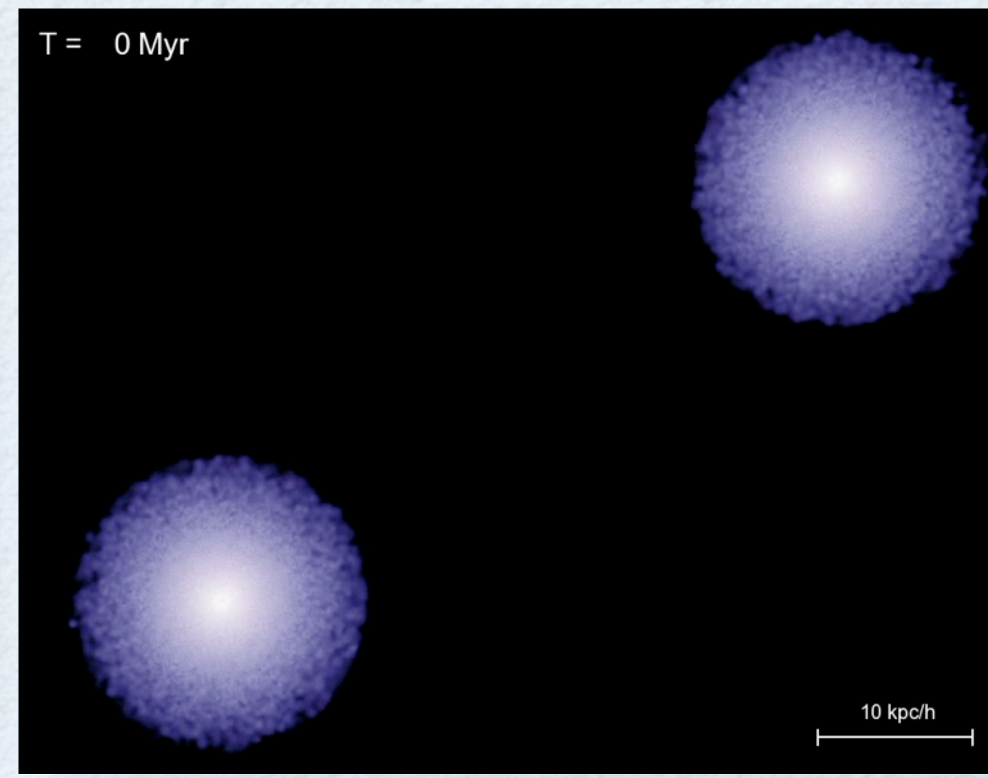
+9



Transport in aquaporins
Schulten Lab, UIUC



Anguiliform Swimmers
Koumoutsakos Lab, ETHZ



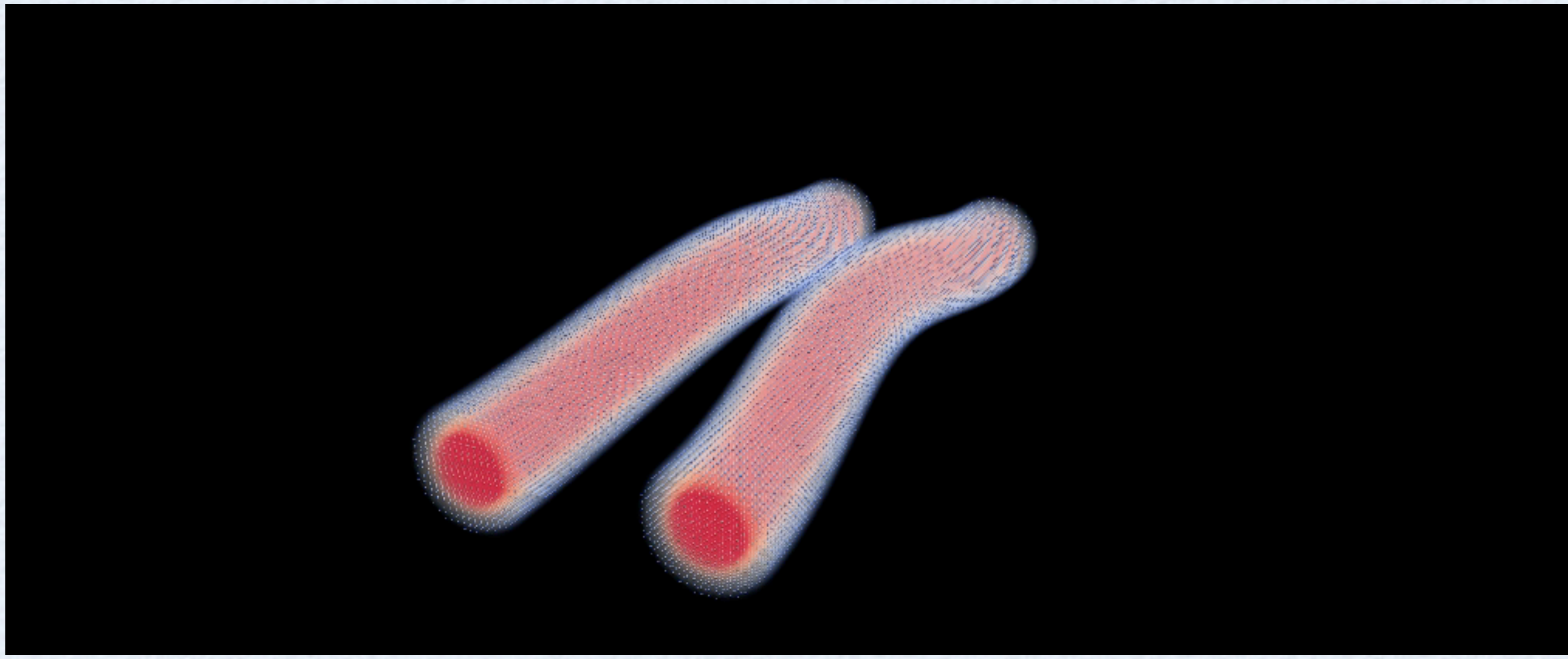
Growth of Black Holes
Springel, MPI - Hernquist, Harvard

PARTICLES : Lagrangian Form of Conservation Laws

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

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

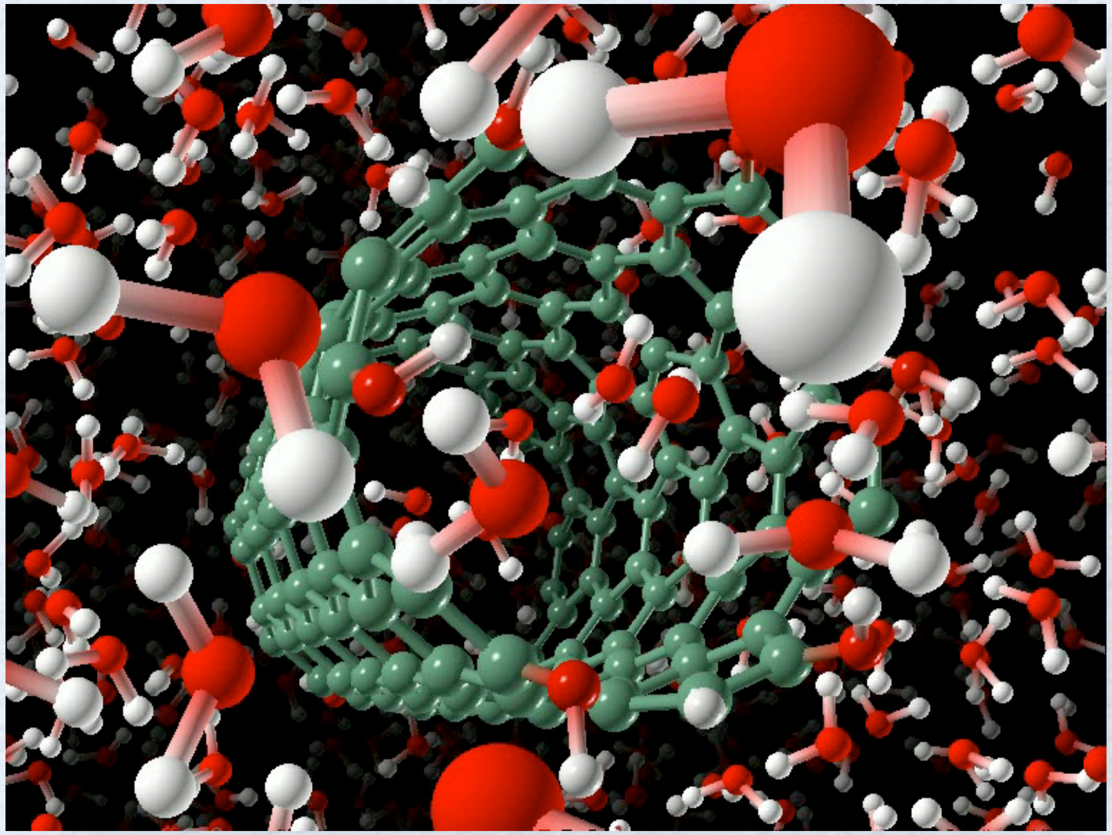
SPH, Vortex Methods



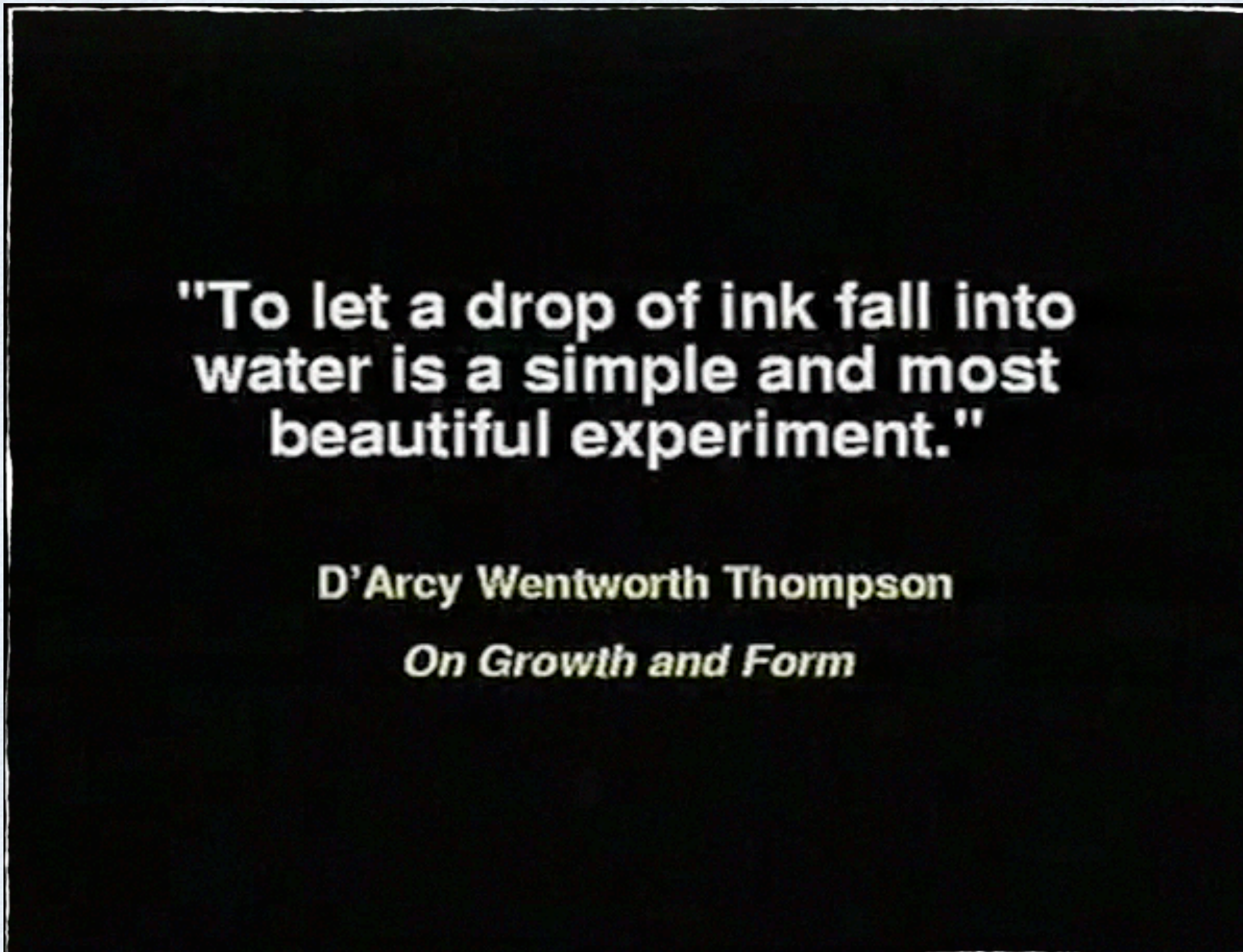
$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u}_p$$

$$m \frac{d\mathbf{u_p}}{dt} = F_p$$

Molecular Dynamics, DPD



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

Particle Methods: an N-BODY problem

Particle (position, value)

$i, j = 1, \cdots, N$

$$\frac{dx_i}{dt} = U_i(q_j, q_i, x_i, x_j, \cdots)$$

$$\frac{dq_i}{dt} = G_i(q_j, q_i, x_i, x_j, \cdots)$$

SMOOTH

Particles are quadrature points for continuum properties

RHS of ODEs: quadratures of integral equations

DISCRETE:

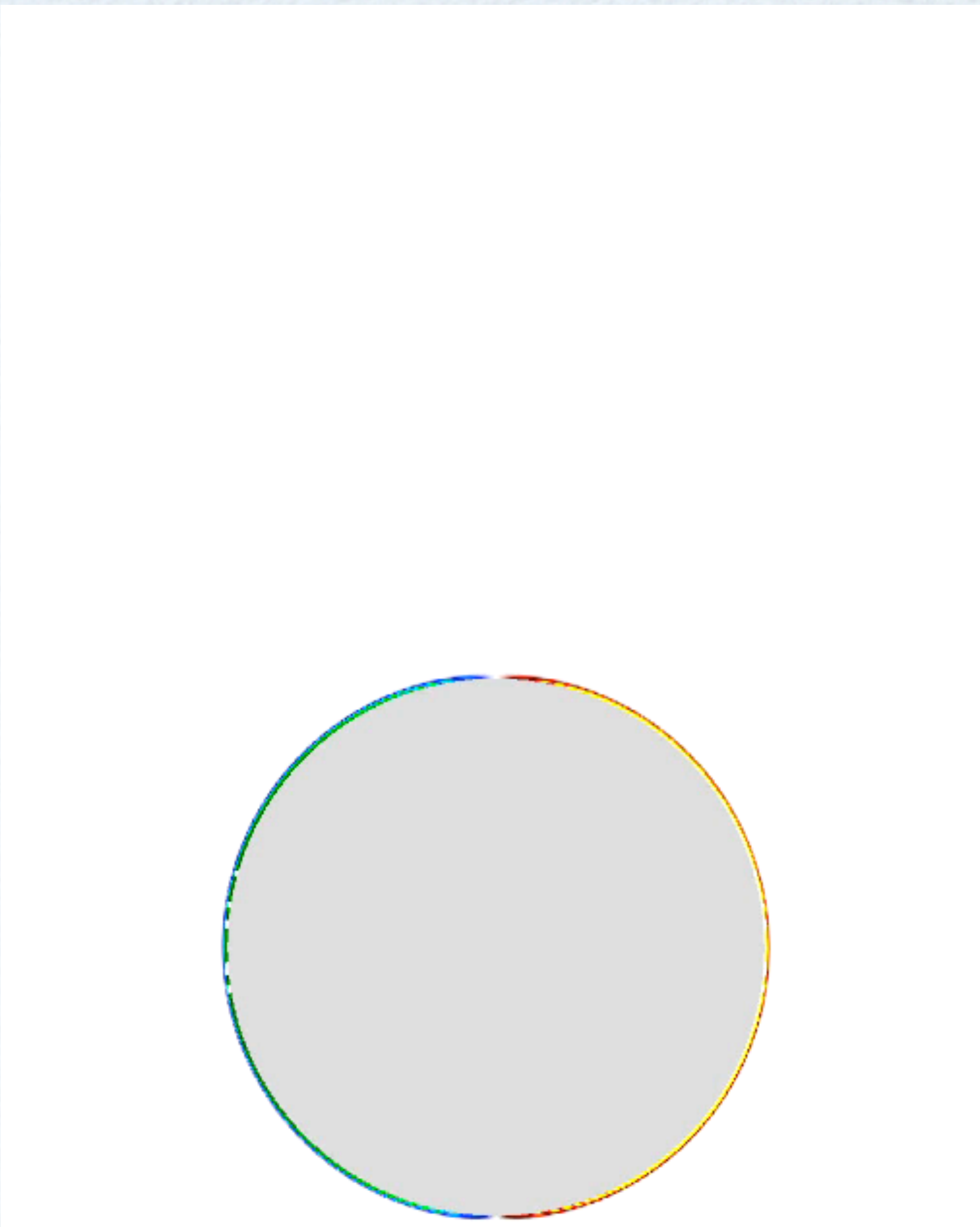
Particles are carriers of physical properties - Models

RHS of ODEs : Physical models (MD,...) - Other

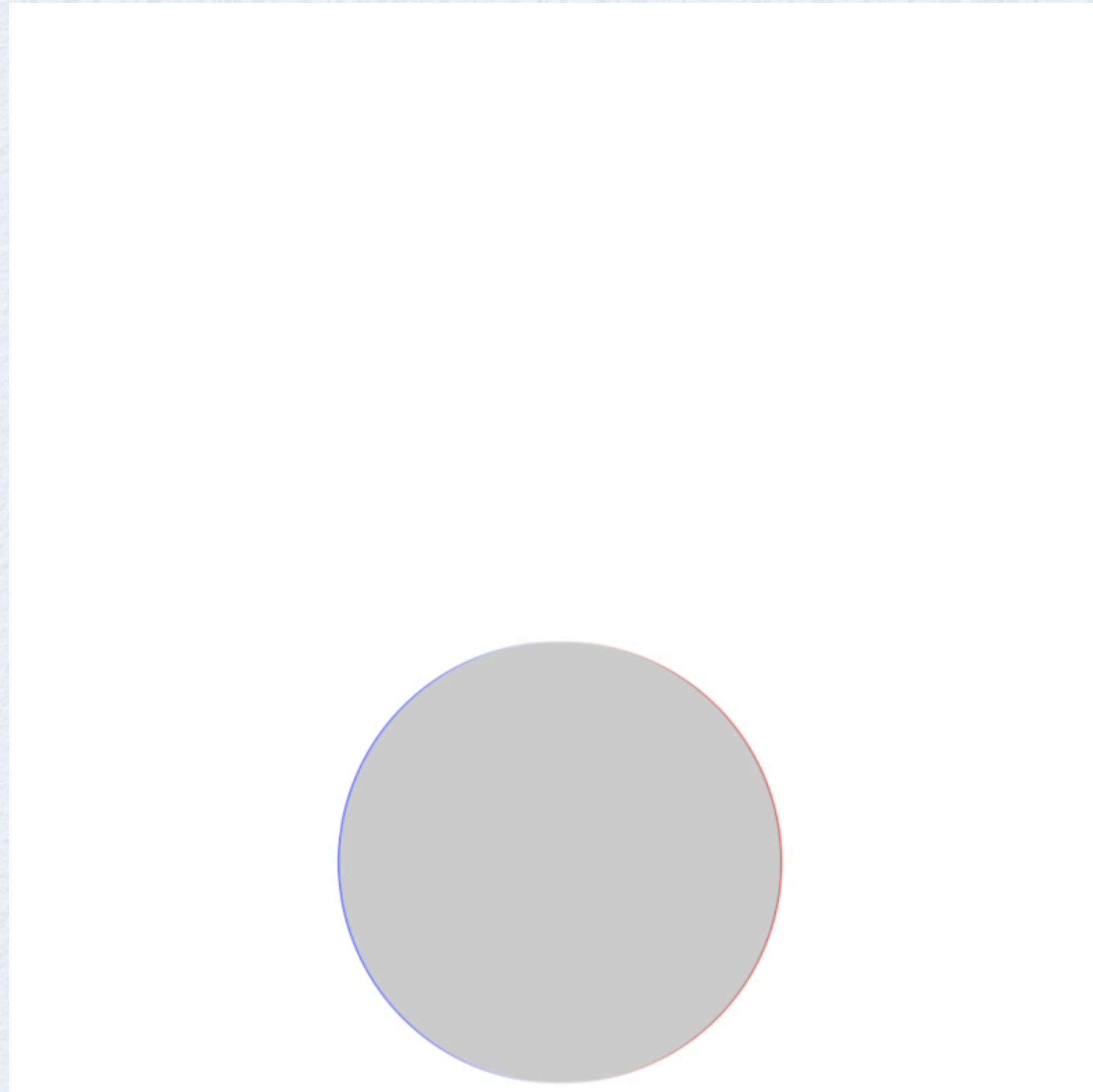
+ • Multipole Algorithms, Fast Poisson solvers , Adaptivity, multiresolution, multiphysics

CFD: Then and Now

Re = 9500 ~ 10^6 particles



1995 **20 Days** on CRAY YMP

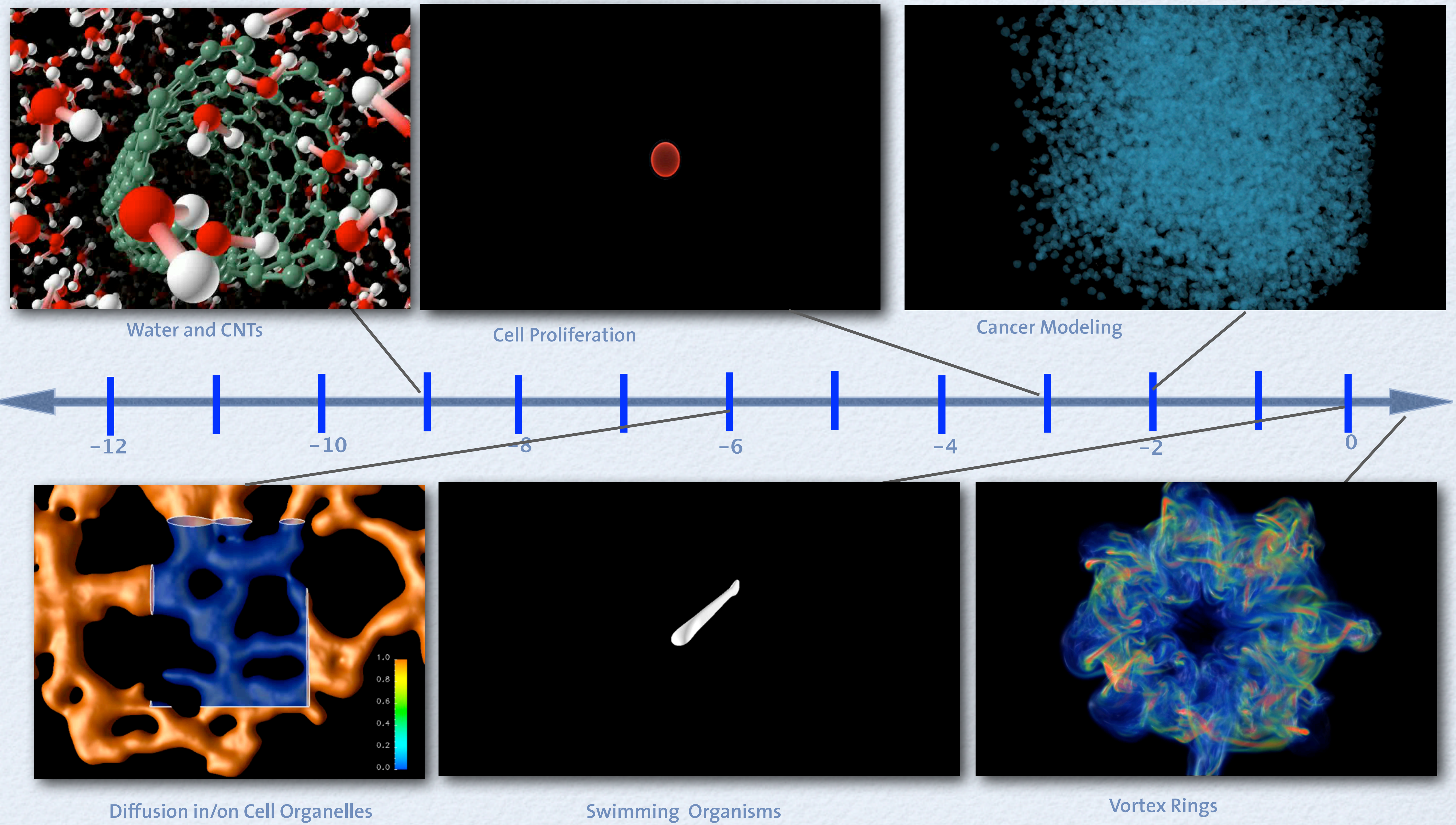


2009 **150sec** on GPU

Rossinelli D., et.al., GPU accelerated simulations of bluff body flows using vortex particle methods, **Journal of Computational Physics**, 229, 9, 3316-3333, **2010**

multi Scale Simulations using Particles

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



A BRIEF HISTORY of PARTICLE METHODS

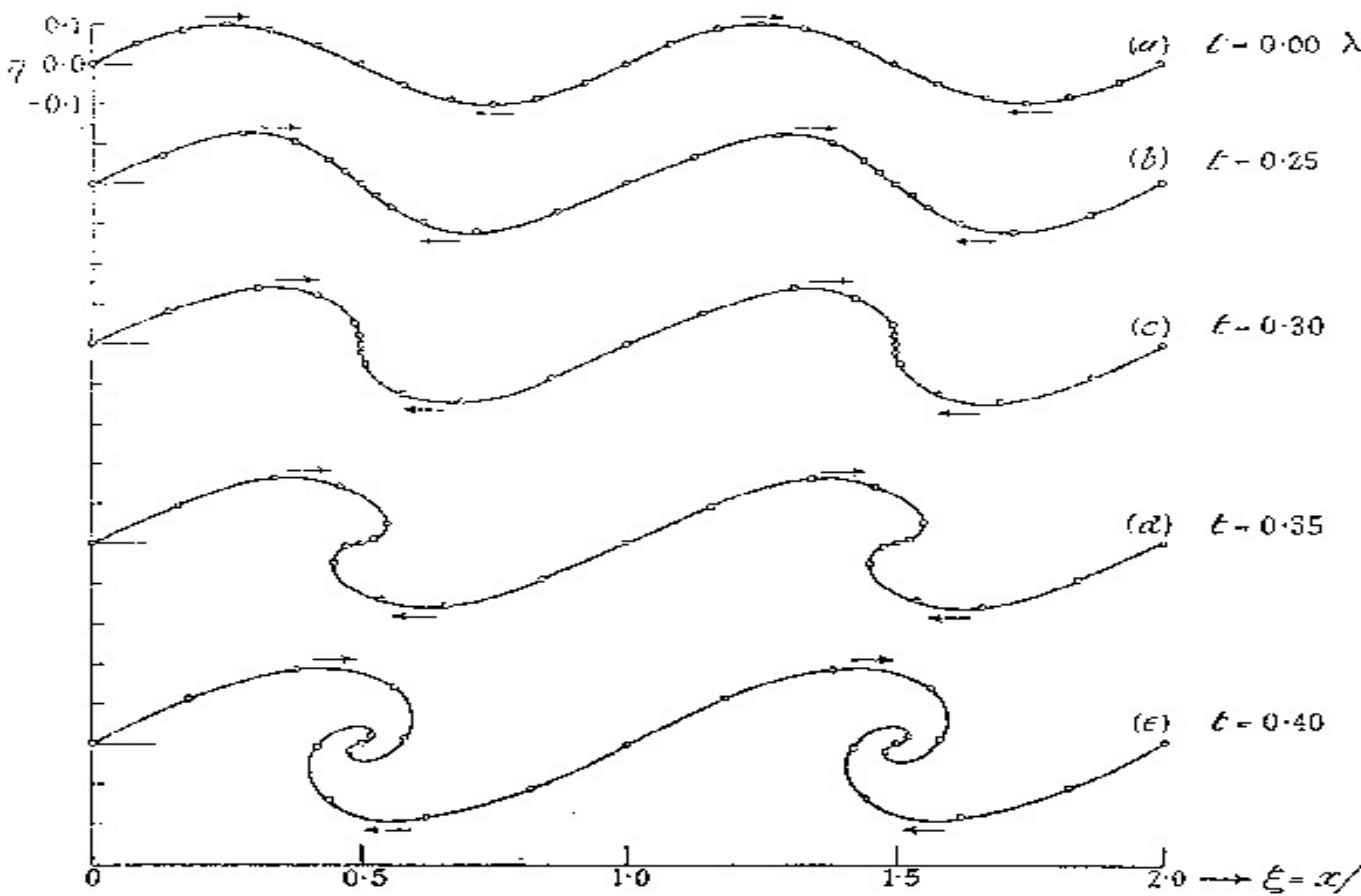


FIG. 4.

A BRIEF HISTORY of PARTICLE METHODS

CFD genesis : Vortex Particle Methods

$$\nabla \times \left(\frac{\partial u}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} \right)$$

$$\omega = \nabla \times \mathbf{u} \qquad \nabla^2 \mathbf{u} = -\nabla \times \omega$$

$$\frac{D\omega}{Dt} = \omega \cdot \nabla \mathbf{u} + \nu \nabla^2 \omega \qquad \frac{dx_p}{dt} = \mathbf{u}$$

- No pressure - Incompressibility enforced
- Poisson equation for getting the velocity
- Langragian formulation

Vortex Particle Methods : From the 20’s to the 50’s

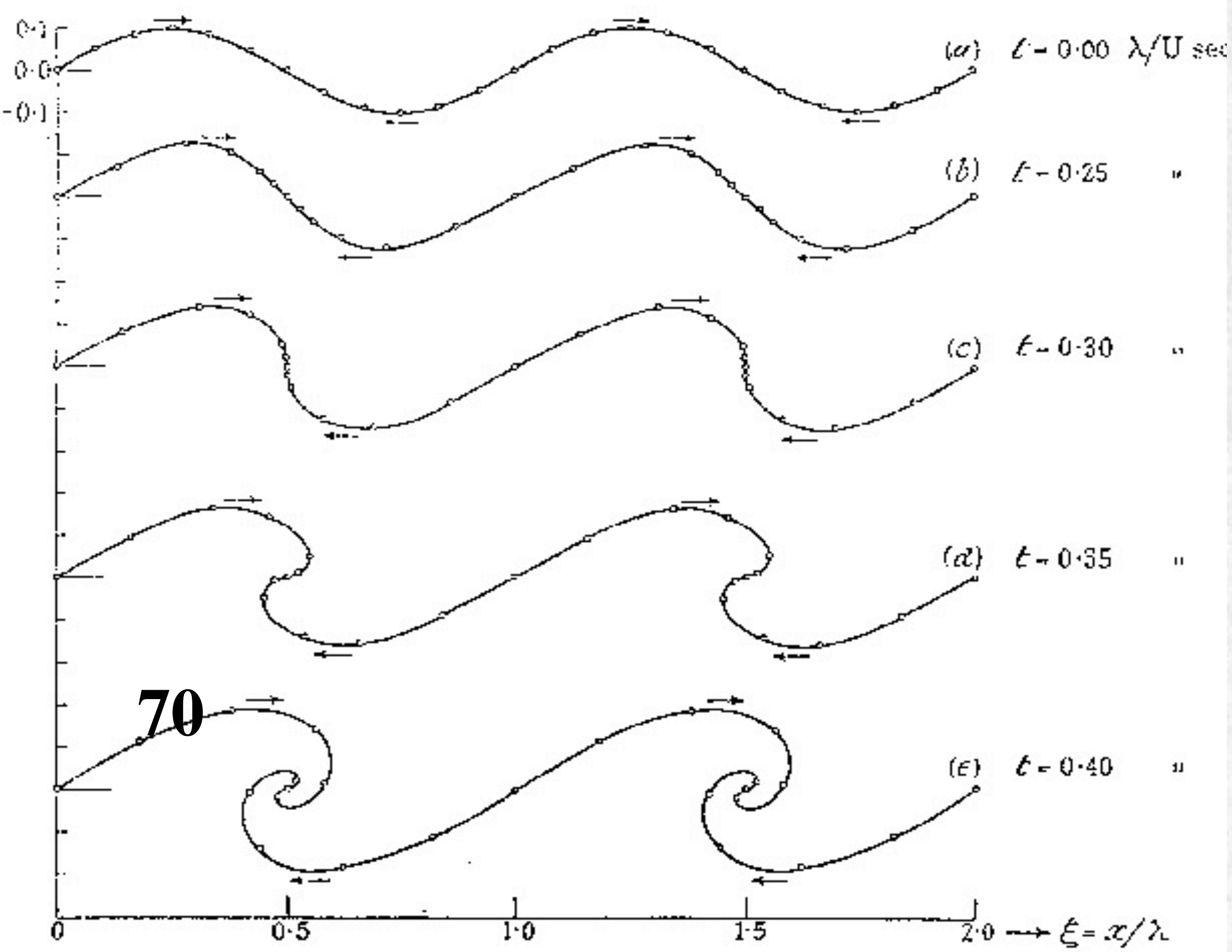
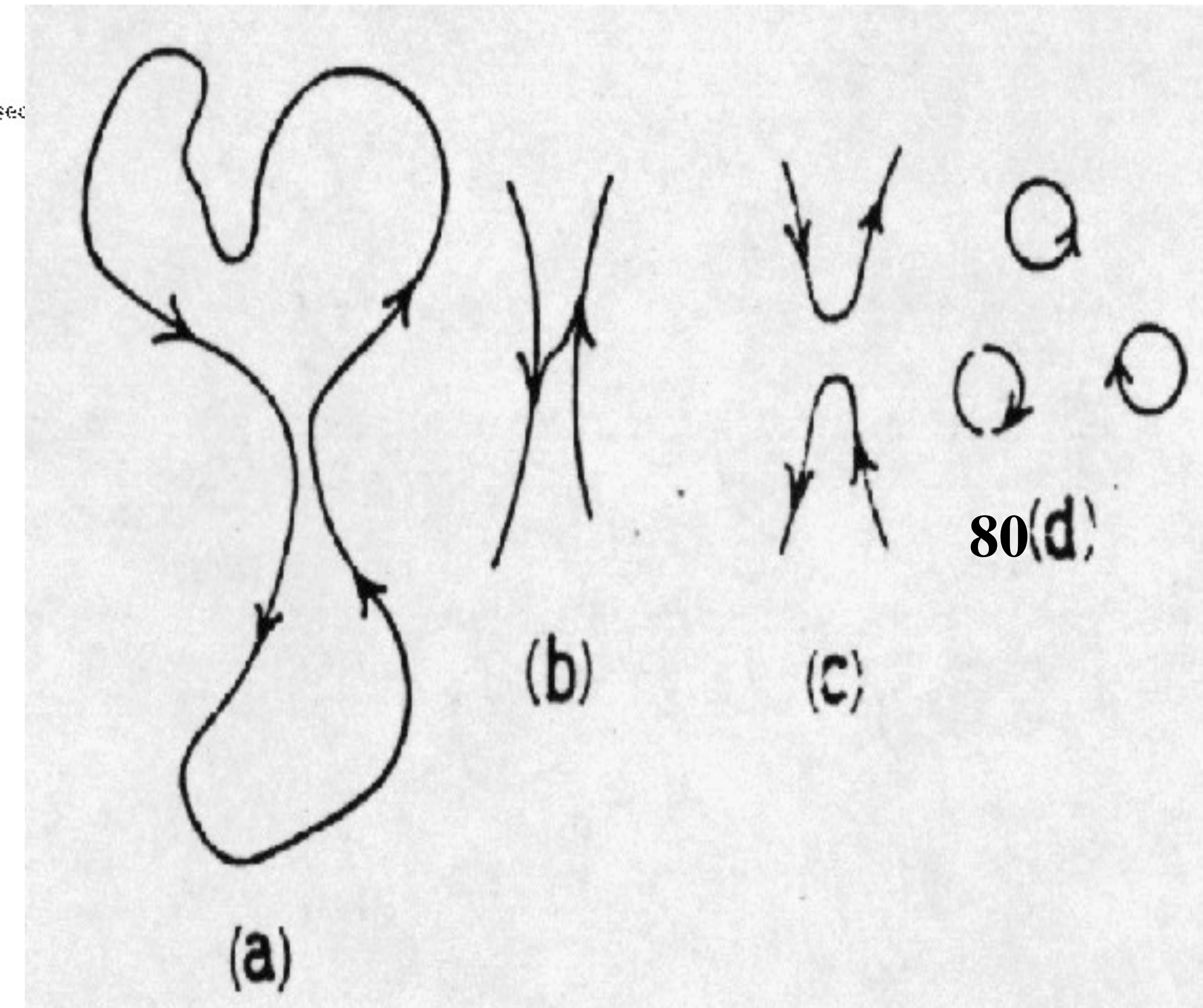


FIG. 4.

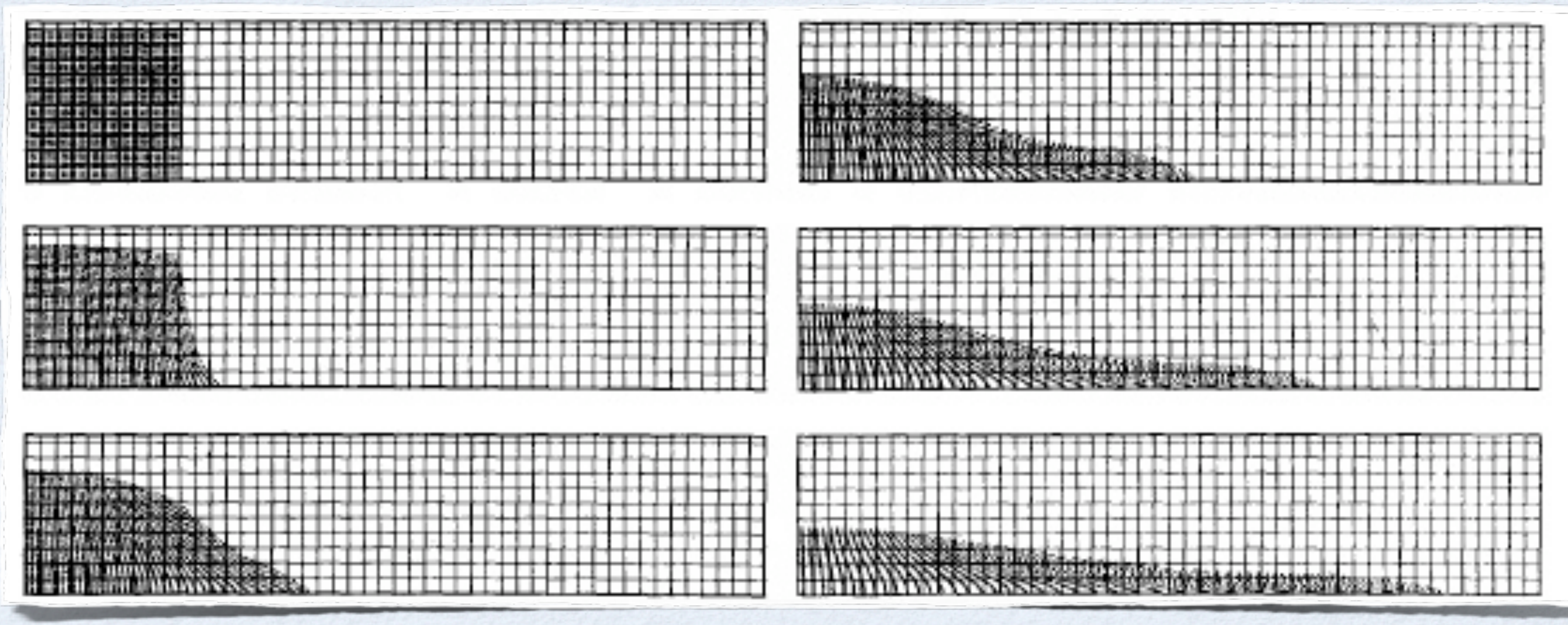


1920’s : Rosenhead

1950’s Feynman

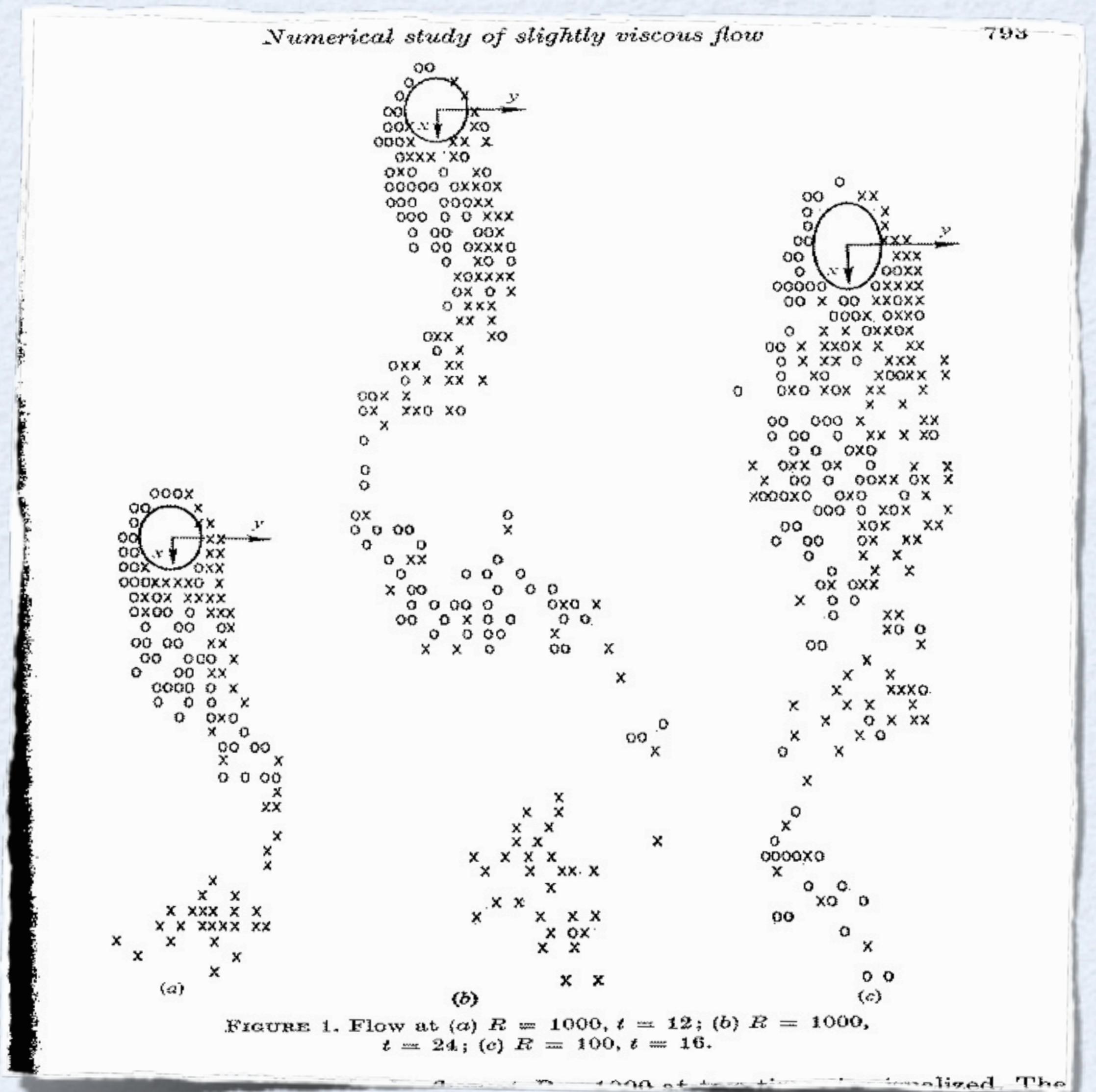
The 60's : Marker And Cell (MAC) -(velocity – pressure)

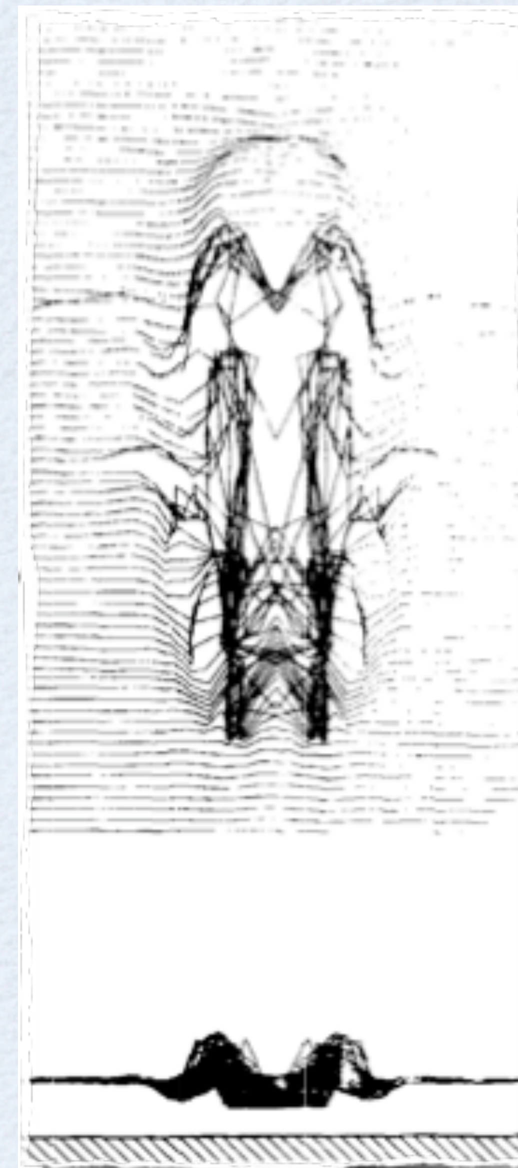
F.H. Harlow and E.J. Welch



Numerical Calculation of Time-Dependent Viscous Incompressible Flow of Fluid with Free Surface,, Harlow, Francis H. and Welch, J. Eddie, Physics of Fluids, 1965

Vortex Methods the 70–80’s



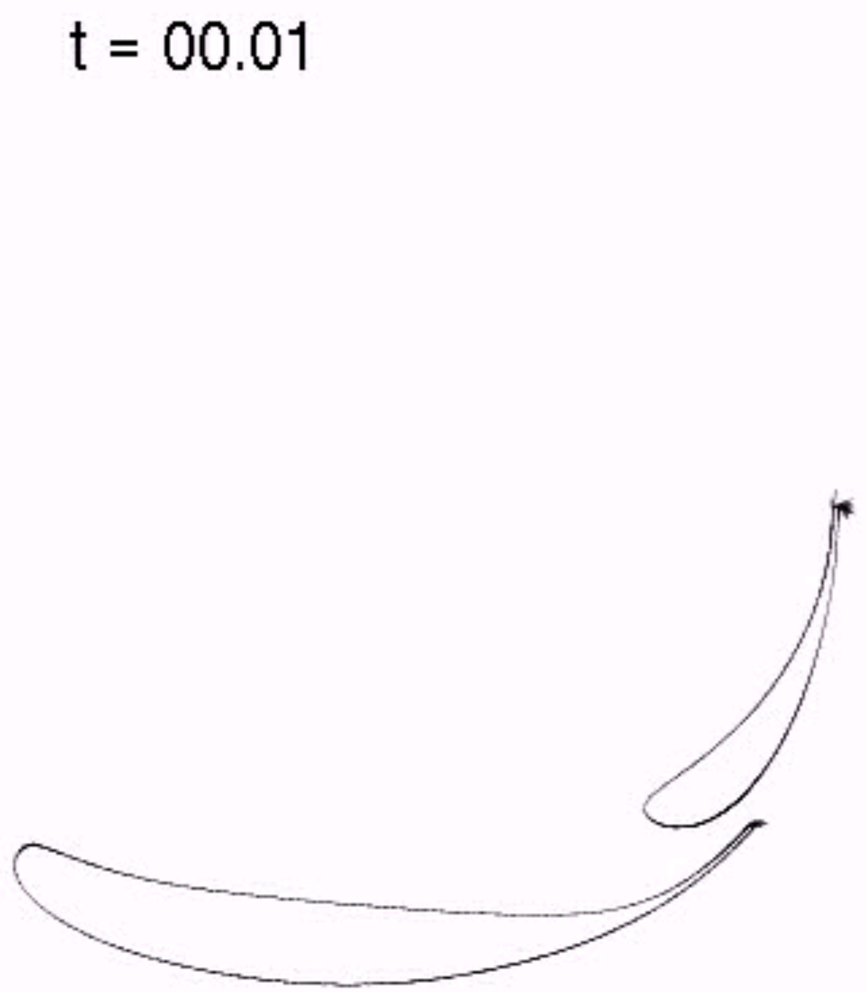


Belotserkovsky

Chorin

Leonard

vortex Particle Methods : From the 60's to the 80's



3D - Boundaries

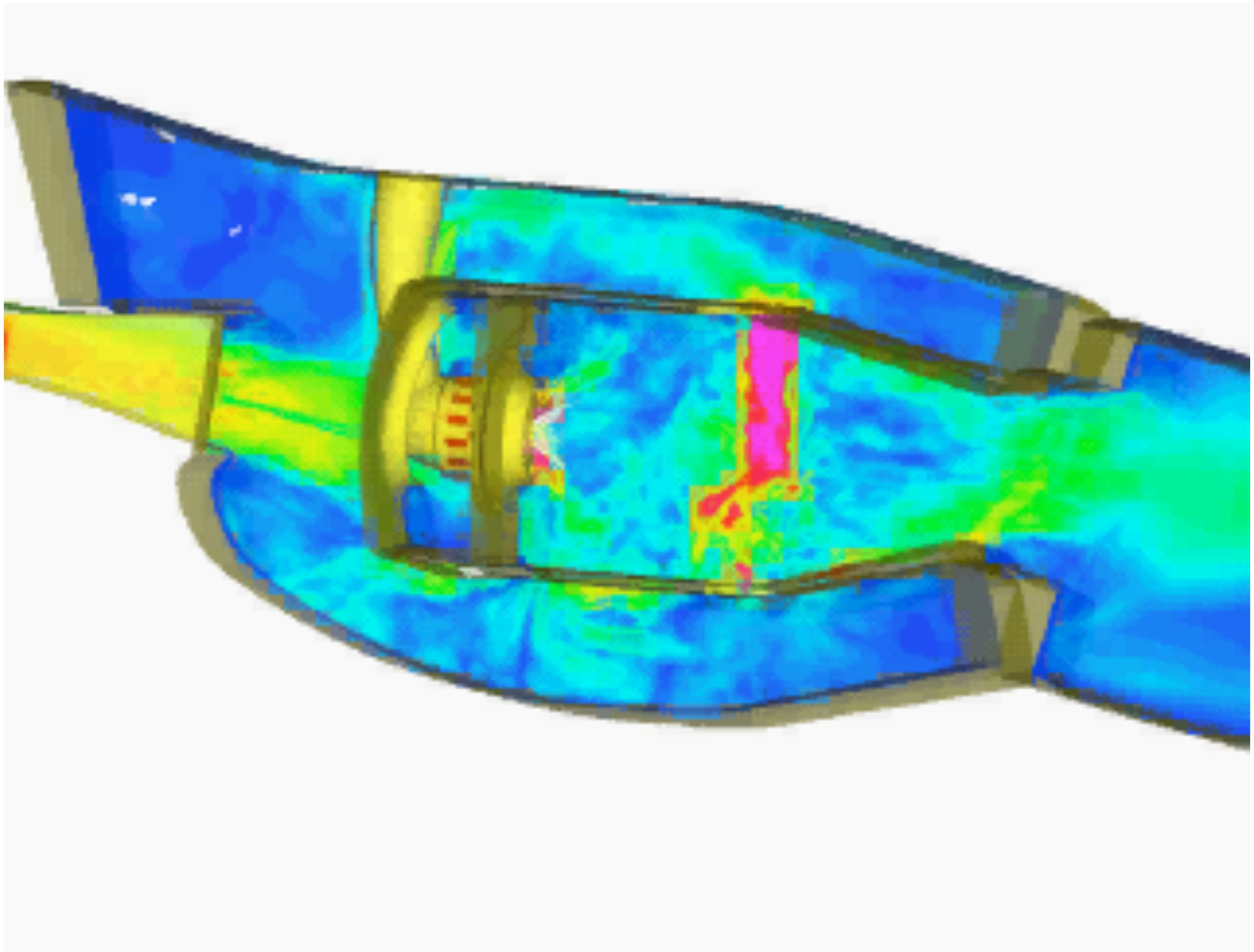
Cost

No theory of convergence

....

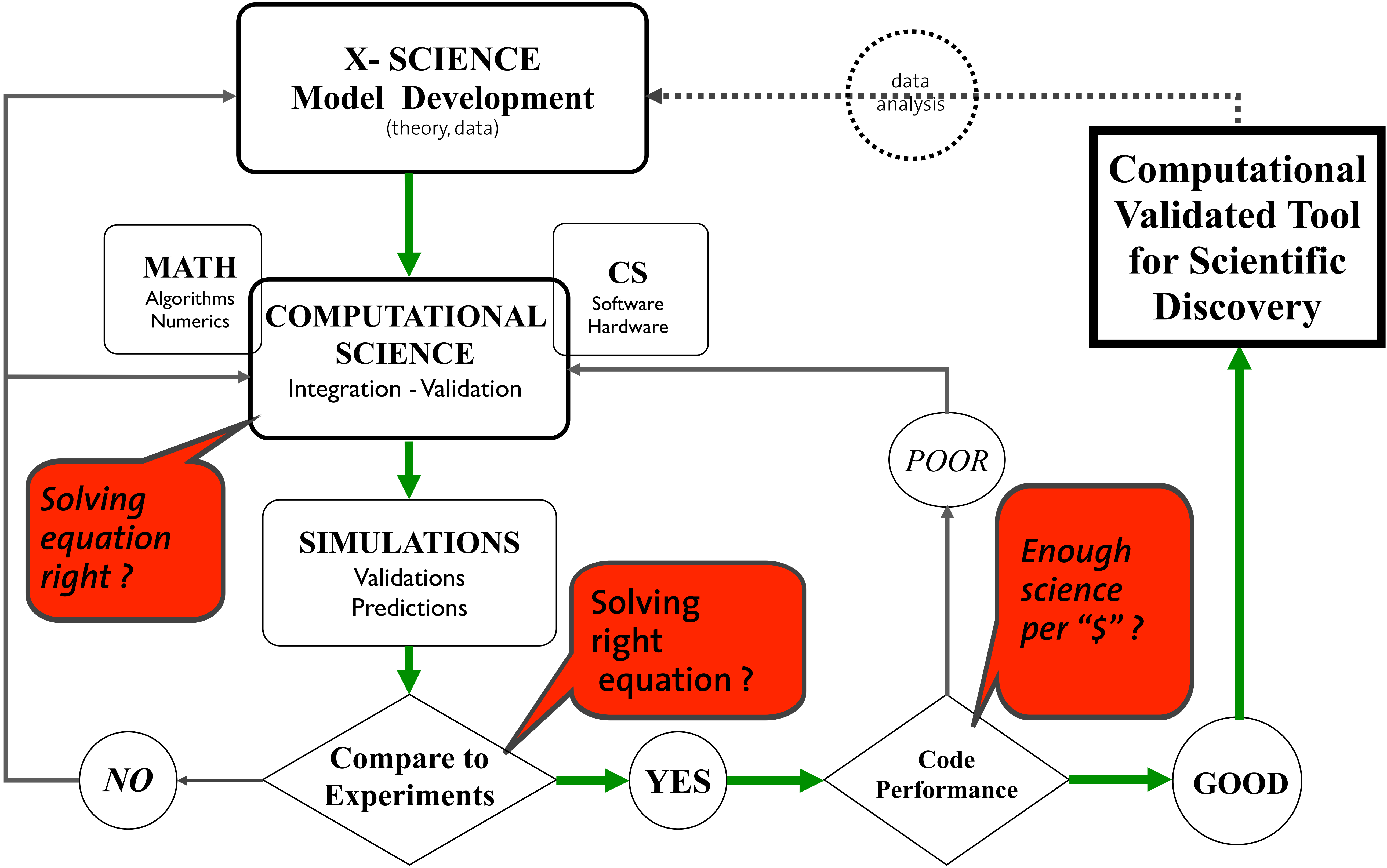
What PAUSED Vortex Methods ?

Mesh Methods for complex problems



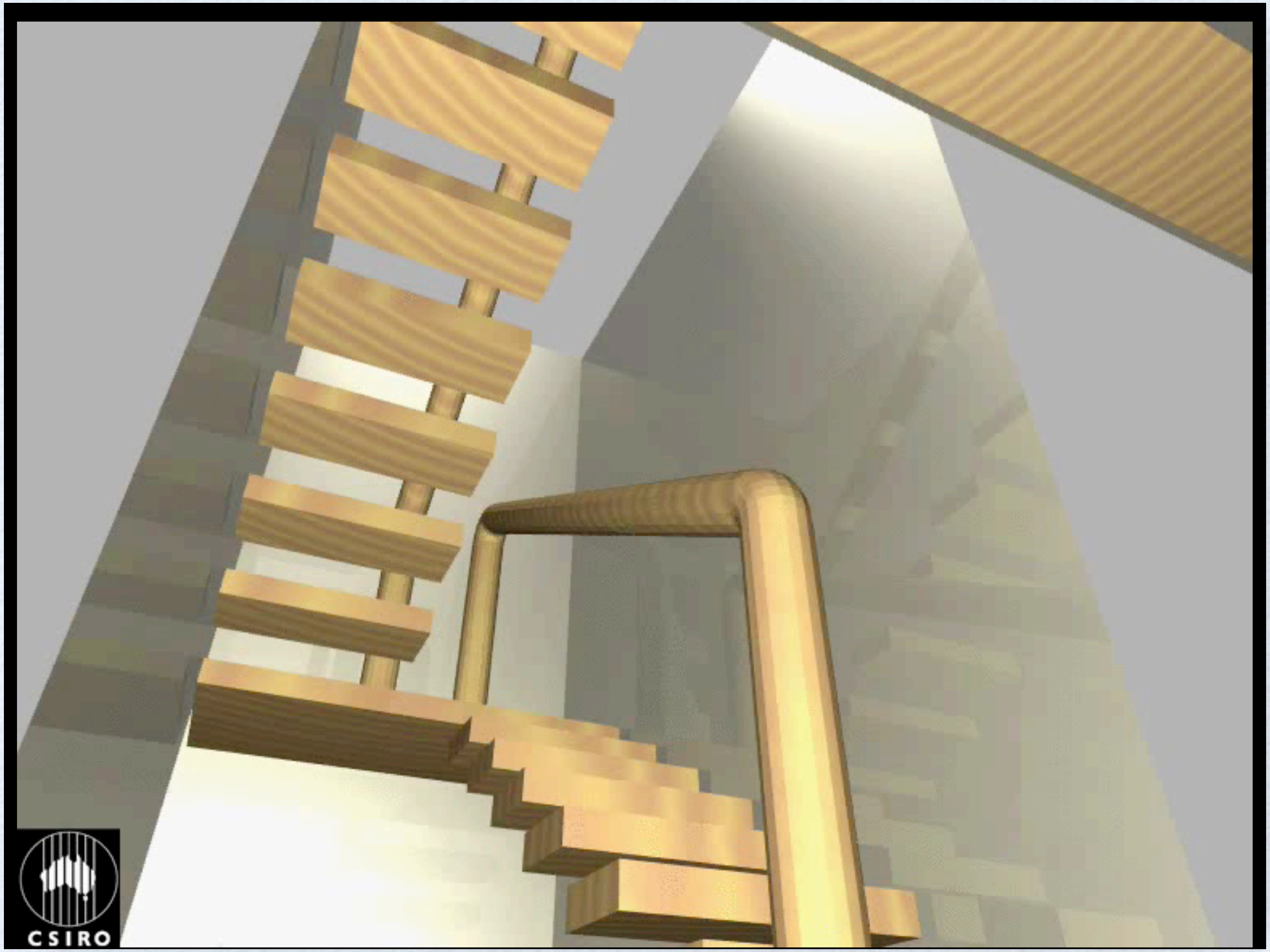
Unstructured Mesh - Center for Turbulence Research, 2005

COMPUTING : The 3 Gaps



Adapted from : US-DOE

Particles strike back : SPH (Monaghan, Lucy, 1970's)



Growth of Black Holes
Springel, MPI -
Hernquist, Harvard

GRID FREE + LAGRANGIAN / ADAPTIVE + NO POISSON EQUATION

Fluids, Particles and Graphics

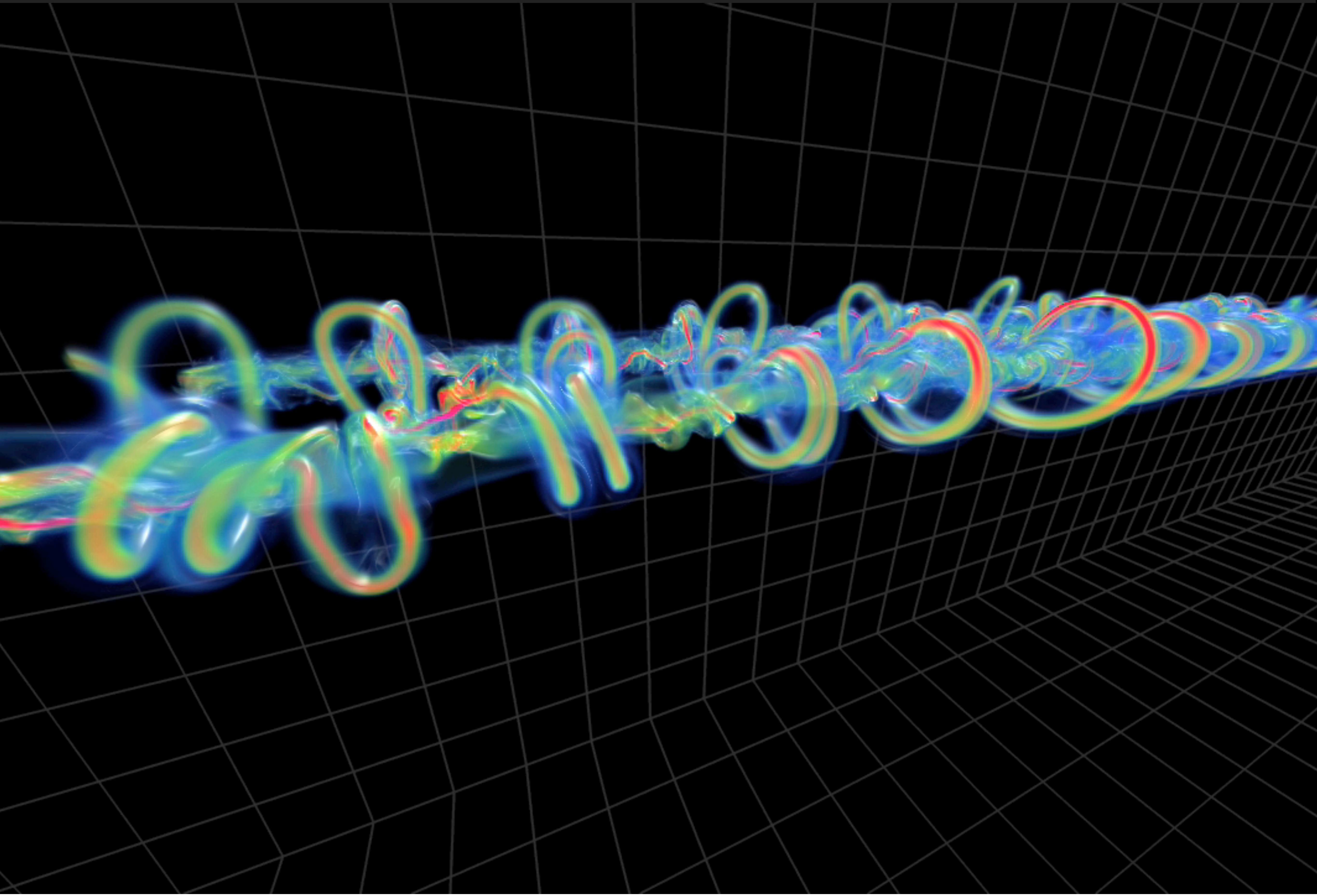
Rigid Fluid: Animating the Interplay Between Rigid Bodies and Fluid

Mark Carlson
Peter J. Mucha
Greg Turk

Georgia Institute of Technology

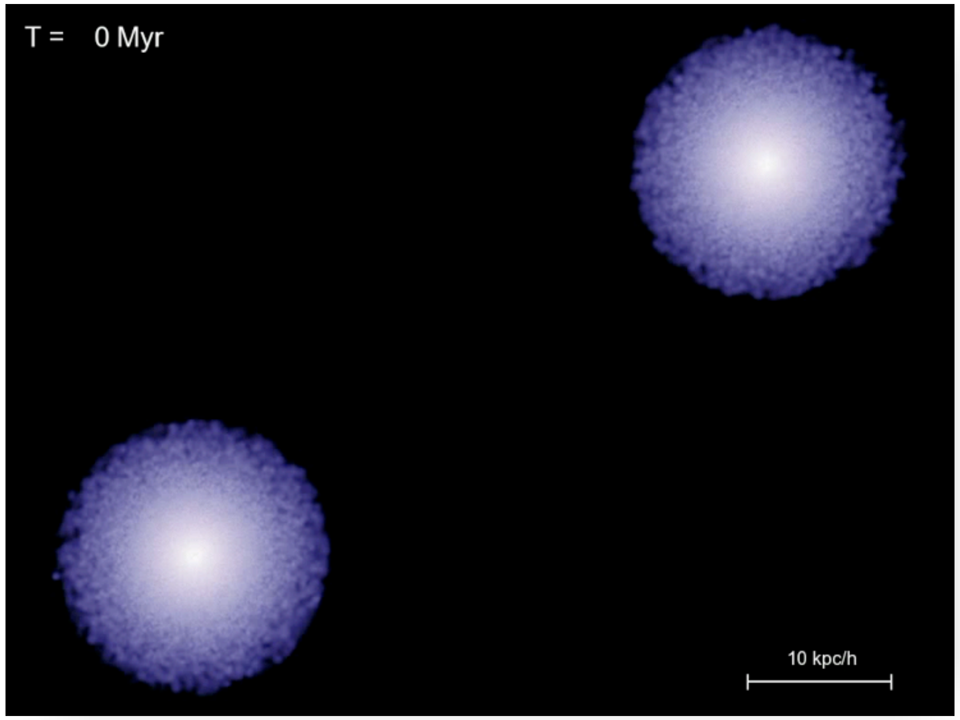
Sound FX by Andrew Lackey, M.P.S.E.

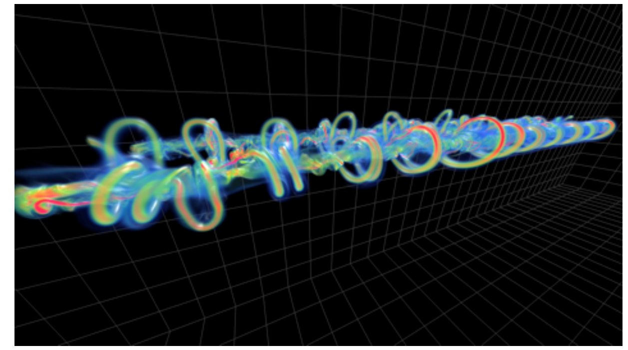
Fluids, Particles and Graphics and CFD

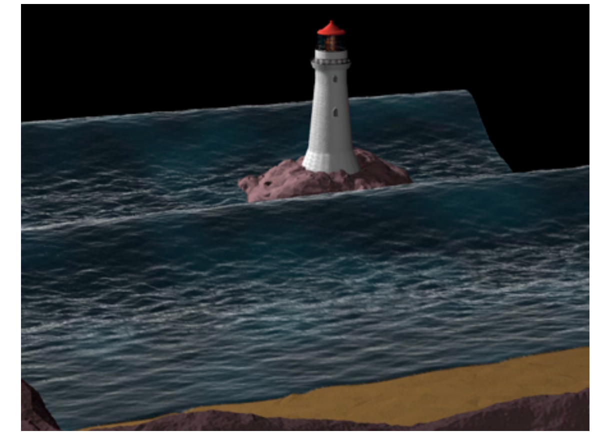


FLUIDS and PARTICLES : CFD and GRAPHICS

2000

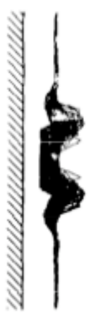


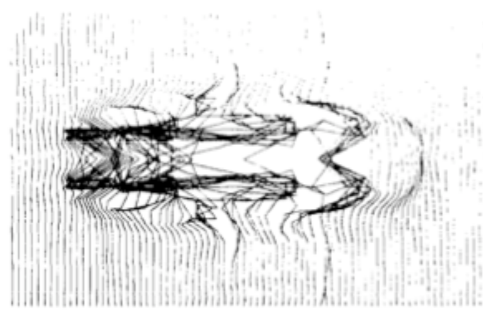


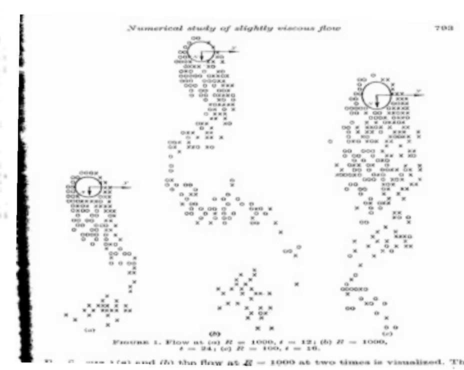


1990

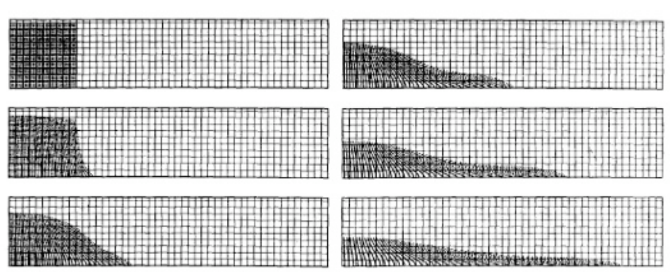
1980



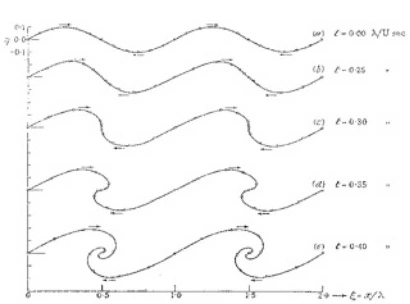




1970

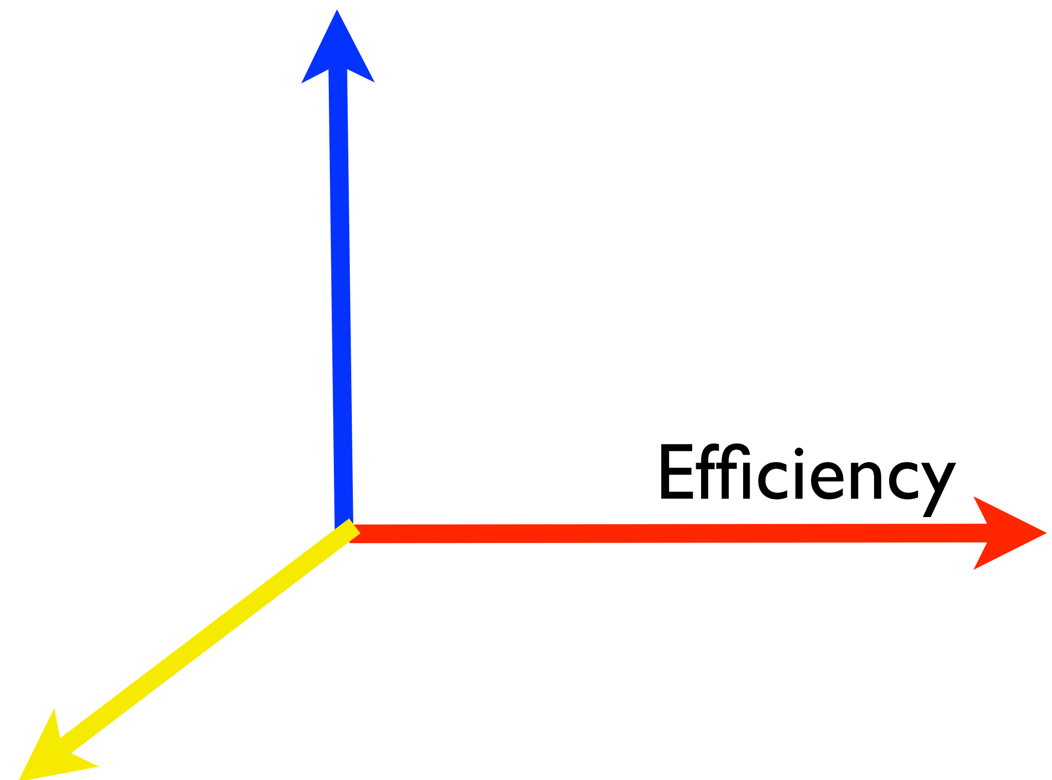


1960



1930

3 Factors for Particle Simulations



Can we precise the (V,E,P) of each simulation ?

PARTICLE METHODS

$$\frac{dx_i}{dt} = U_i(q_j, q_i, x_i, x_j, \cdots)$$
$$\frac{dq_i}{dt} = G_i(q_j, q_i, x_i, x_j, \cdots)$$

- CONTINUUM **APPROXIMATIONS**
  - Particles as quadrature points of integral approximations
- DISCRETE **MODELS**
  - Particles represent discrete elements
- COMMON ALGORITHMIC STRUCTURES
  - Algorithms, Data structures - HPC implementation

- PROS
  - Adaptivity, Robustness
  - Multiphysics

- CONS
  - Low Accuracy, Inconsistent
  - Expensive

Flow Simulations Using Particles

- Volumes
- Surfaces and Interfaces
- Equations

See : Multiscale flow simulations using particles, Koumoutsakos P, Ann. Rev. Fluid Mech., 37, 457-487, 2005

FUNCTIONS and PARTICLES

Integral Function Representation

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

Point Particle Quadrature

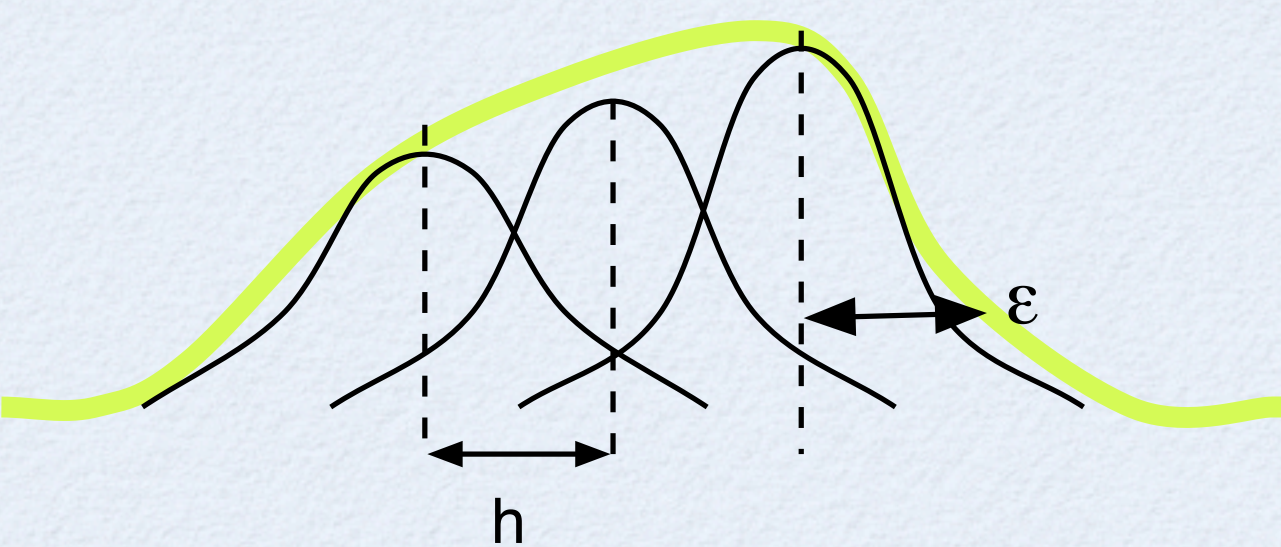
$$\Phi^h(x,t) \;=\; \sum_{p=1}^{N_p} h_p^d\,\Phi_p(t)\,\delta(x-x_p(t))$$

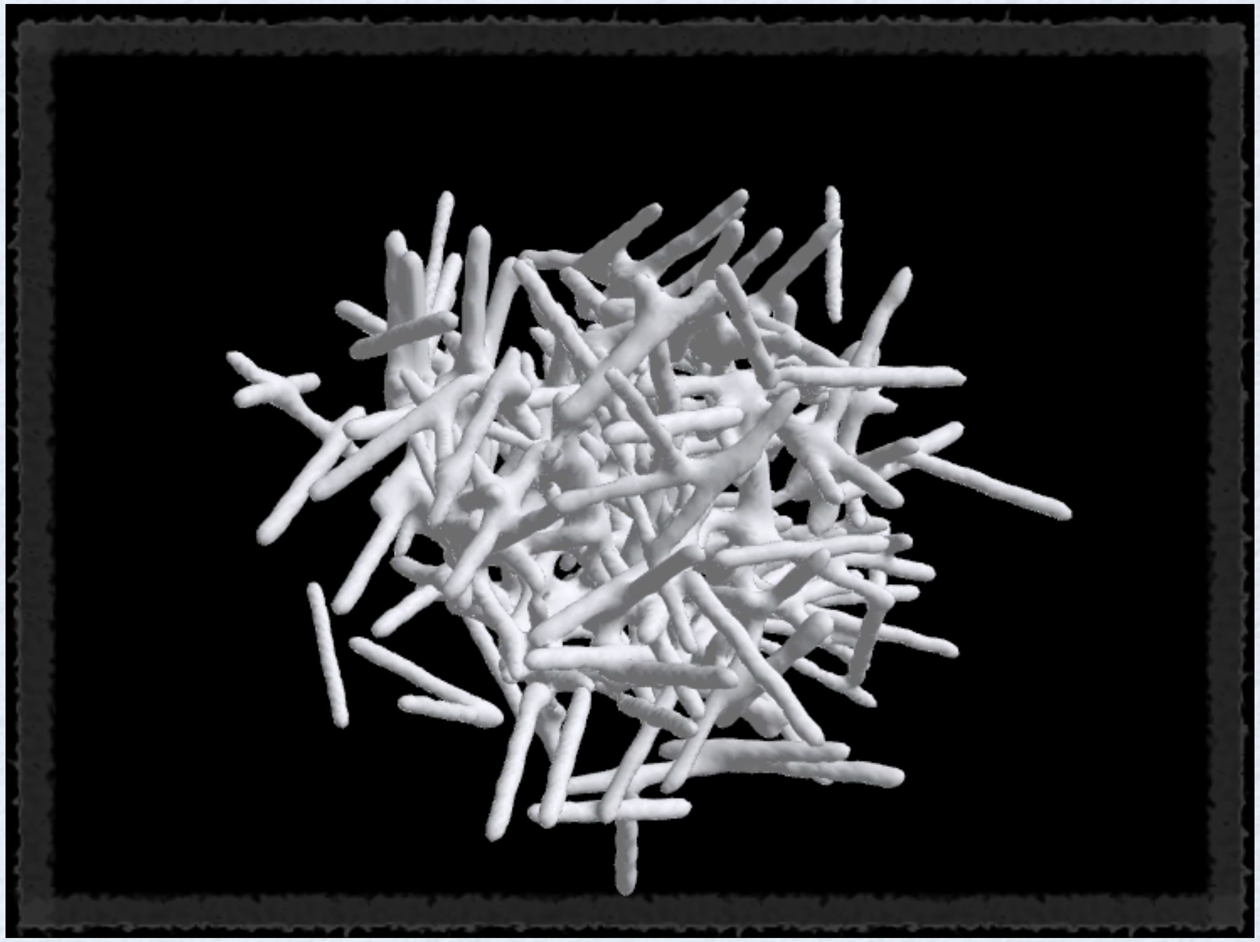
Function Mollification

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

Smooth Particle Quadrature

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



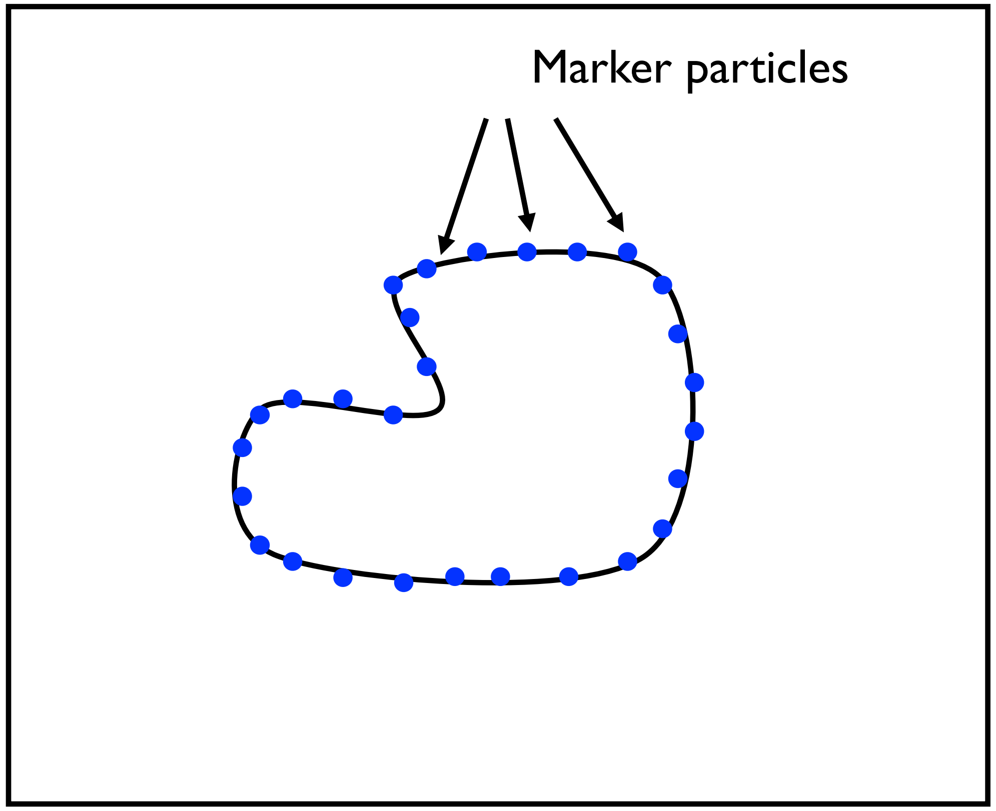


Particles are “mesh” free

Interface Tracking versus Capturing

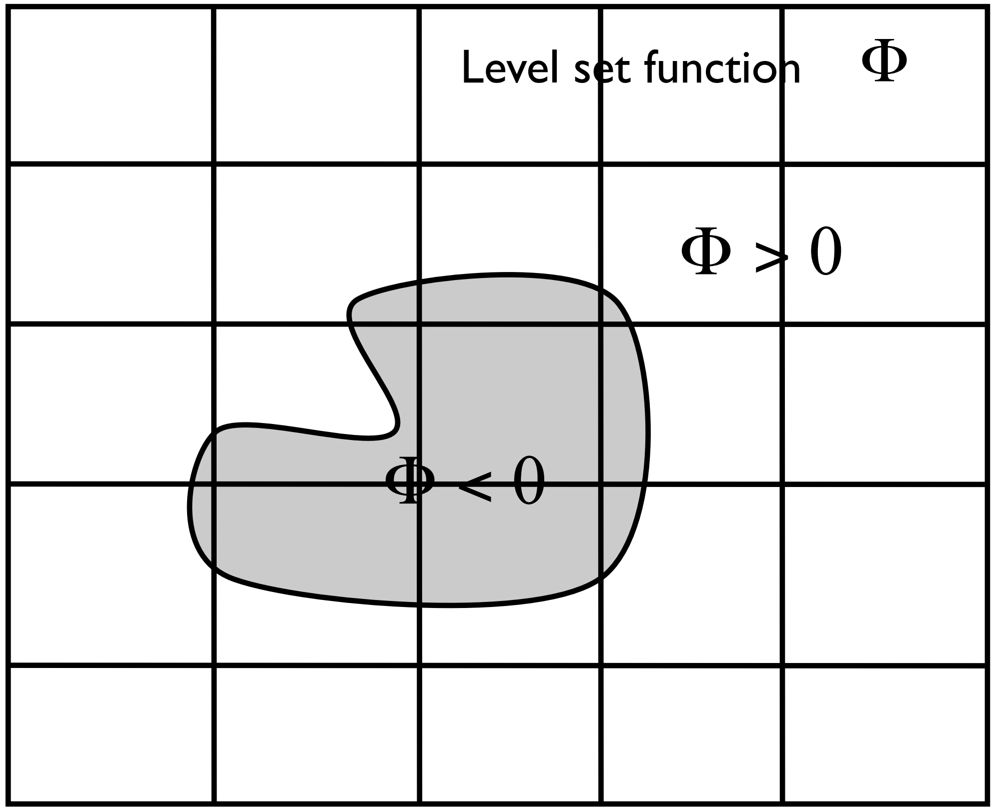
Tracking

- Explicit description
- Lagrangian framework
- Interface distortion requires reseeding



Capturing

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

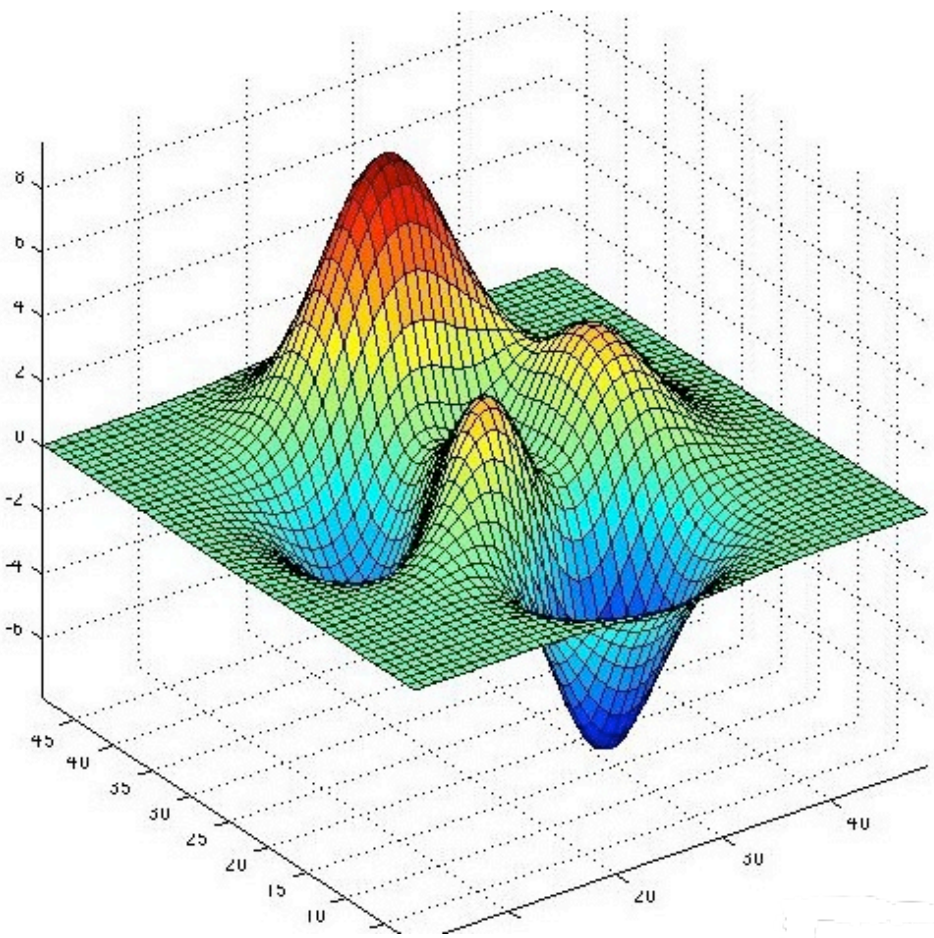


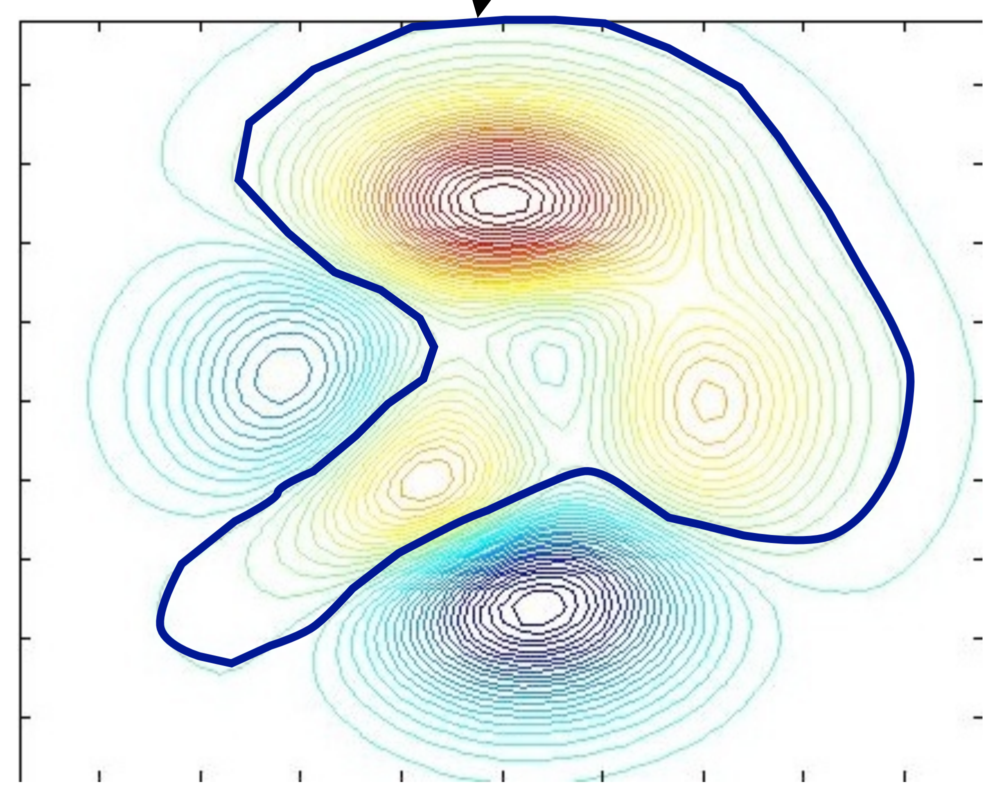
Level Sets for Surface Representation

Level Set: **implicit** surface

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

Sethian, PNAS 93:1591. 1996.

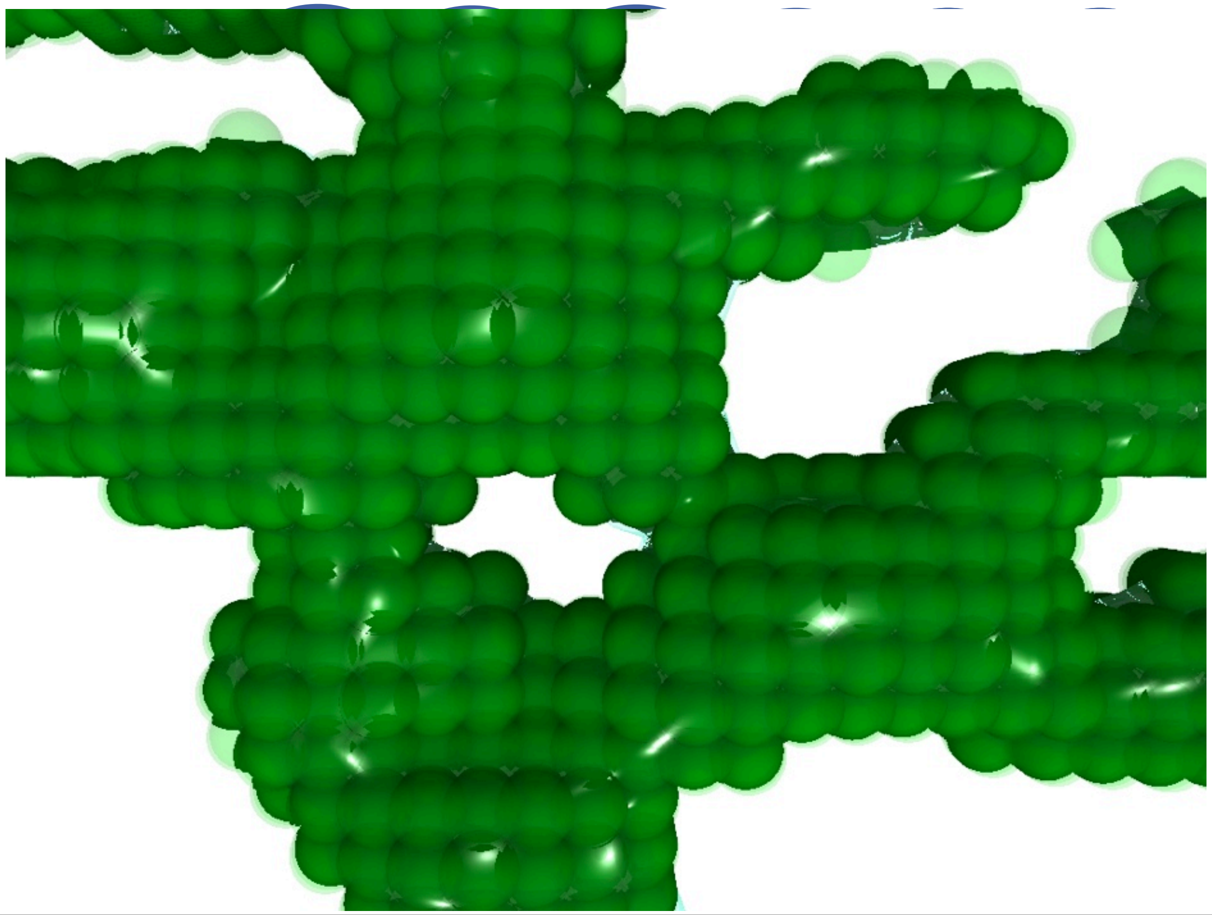




Why? → **surface** can be treated **in space**: one method

PARTICLE METHODS : Geometry

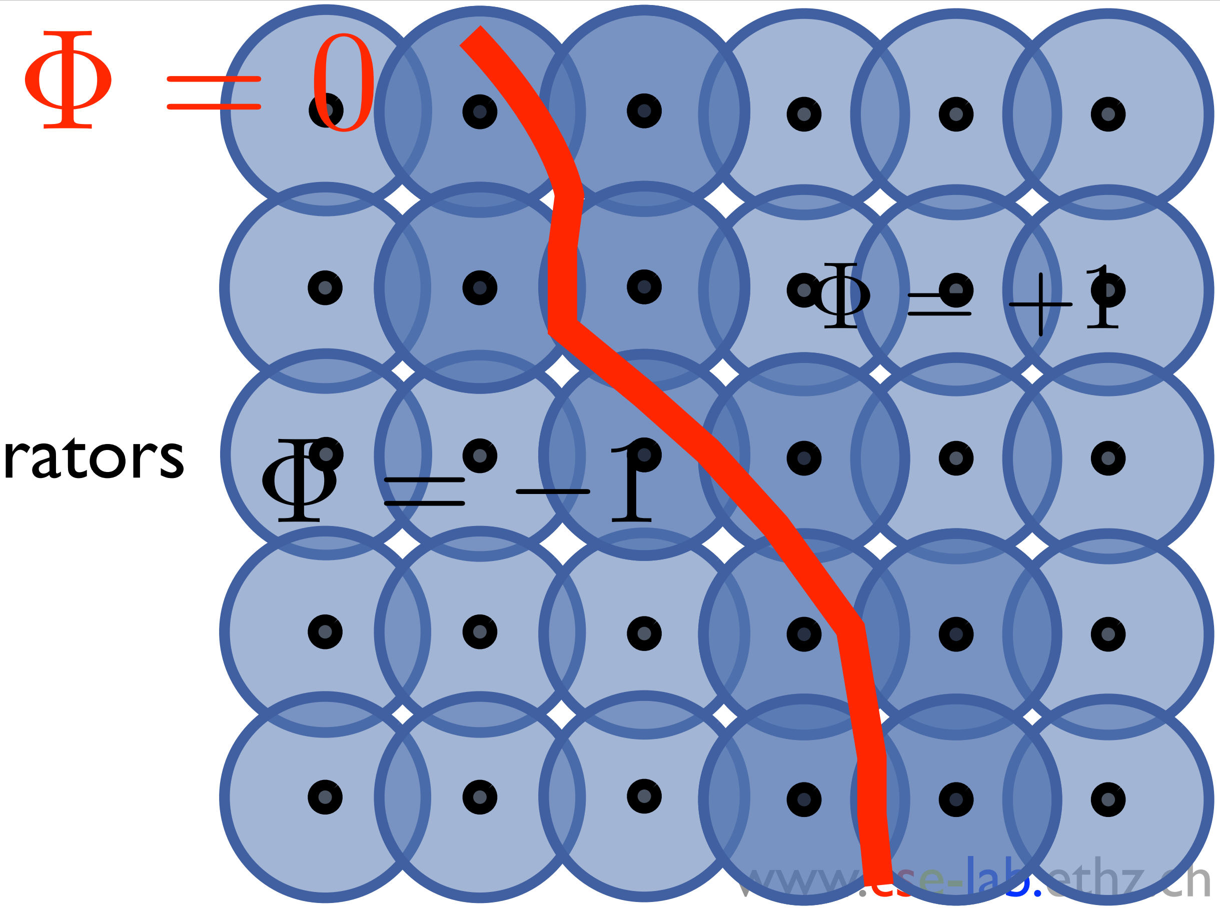
Volume particles



•Particles are quadrature points

• Easy to discretize COMPLEX GEOMETRIES

Surface particles



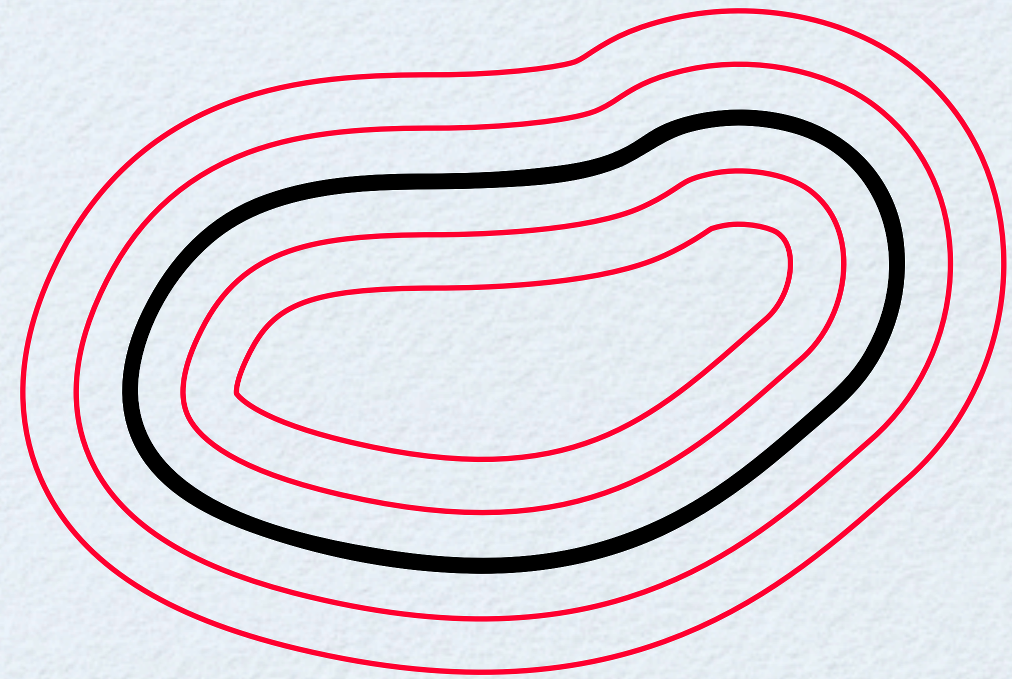
• Particle - Level Sets - COMPLEX SURFACES

• Surface Operators - Anisotropic Volume Operators

SURFACES AS LEVEL SETS

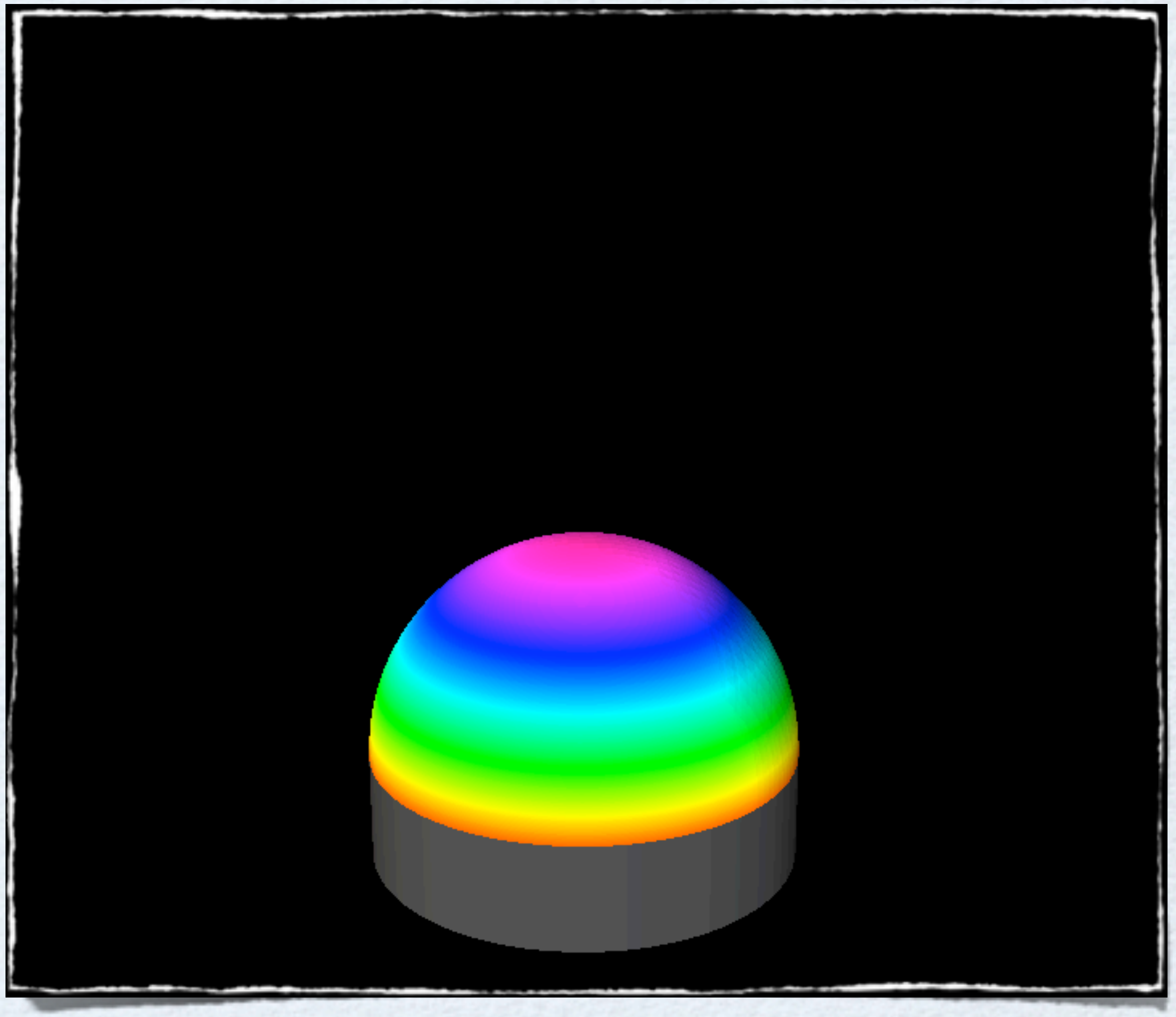
$$\Gamma(t) = \{\mathbf{x} \in \Omega \mid \phi(\mathbf{x}, t) = 0\}$$

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



EVOLVING THE LEVEL SETS

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



PARTICLE APPROXIMATION

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

Lagrangian Surface Transport

$$\frac{dx_p}{dt} = \mathbf{u_p} \qquad \frac{D\Phi_p}{Dt} = 0$$

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

Particle Level sets : 3D curvature-driven flow: Collapsing Dumbbell

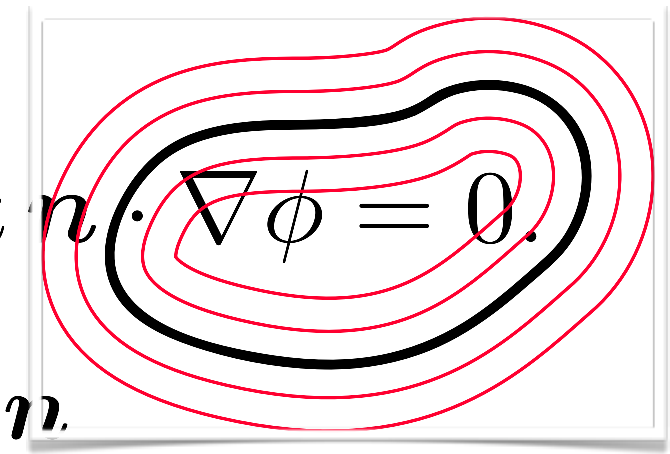
$$\frac{\partial \Phi}{\partial t} + u \cdot \nabla \Phi = 0$$

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

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

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

$$\kappa = \nabla \cdot n$$

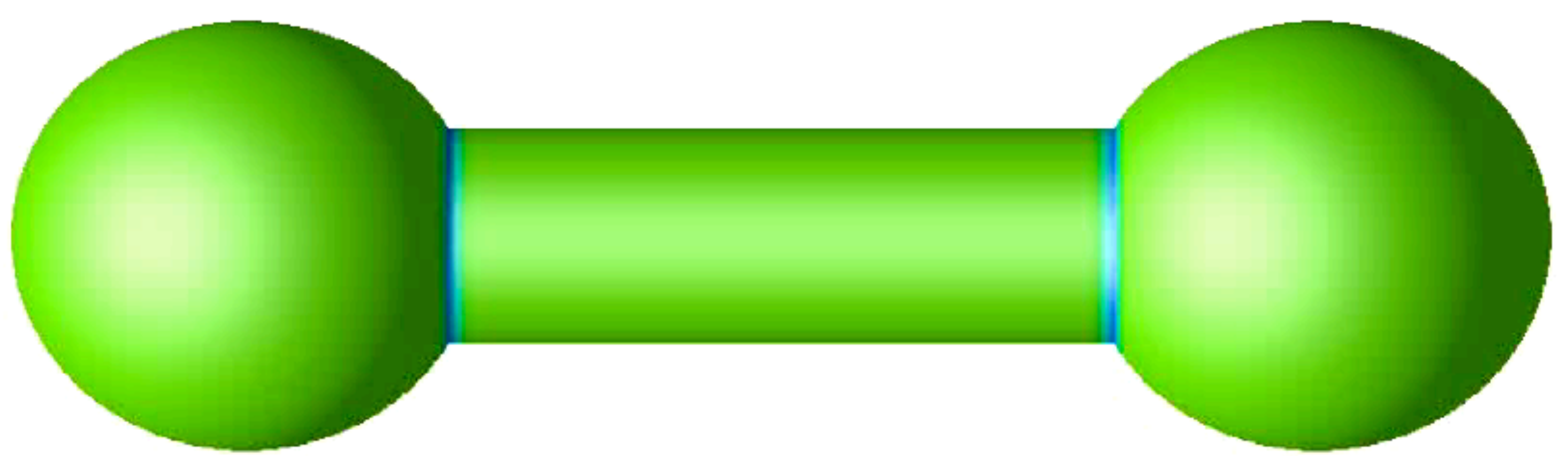


$$\Phi_\epsilon^h(x,t) = \sum_{p=1}^{N_p} h_p^d\, \Phi_p(t)\, \zeta_\epsilon(x - x_p(t))$$

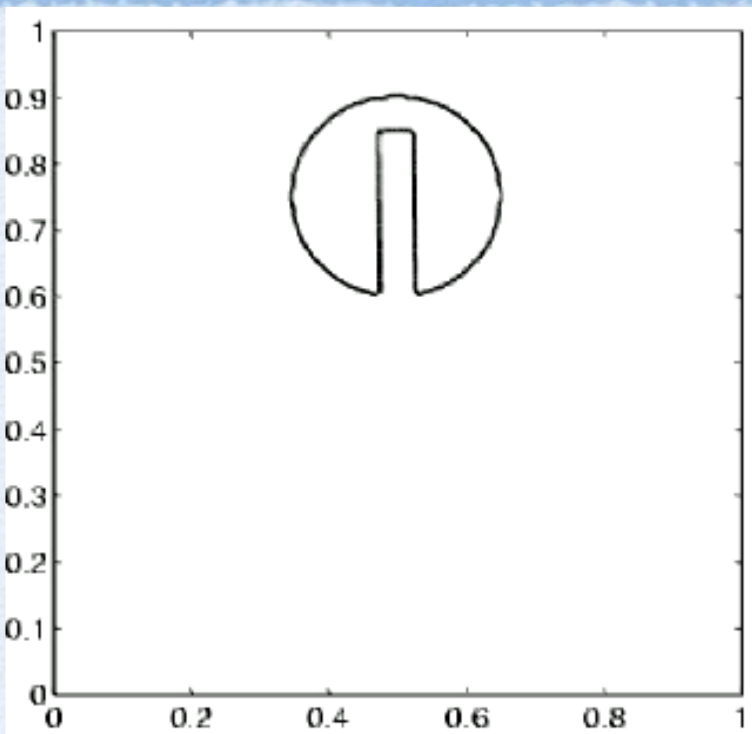
$$\frac{D\Phi_p}{Dt} = 0 \qquad \frac{dx_p}{dt} = \mathbf{u}$$

Particle Approximation

A Lagrangian Particle Level Set, Hieber and Koumoutsakos, J. Comp. Phys. 2005



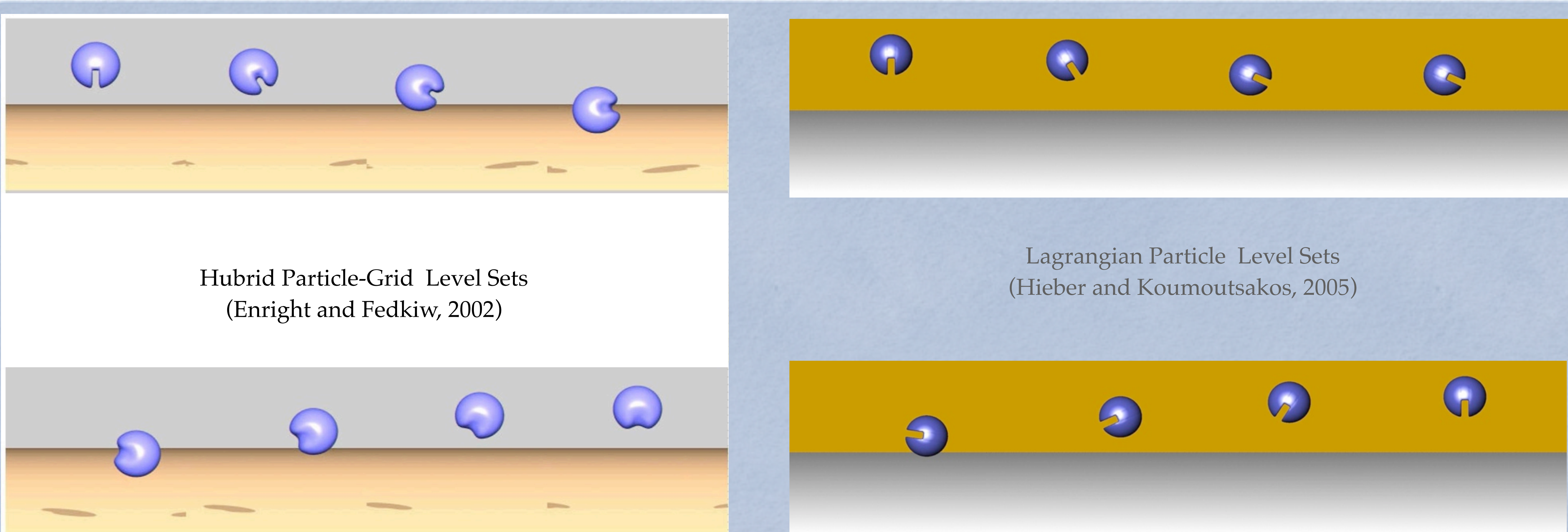
Lagrangian vs Eulerian Descriptions



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

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

Lagrangian Particle methods good for **linear** advection

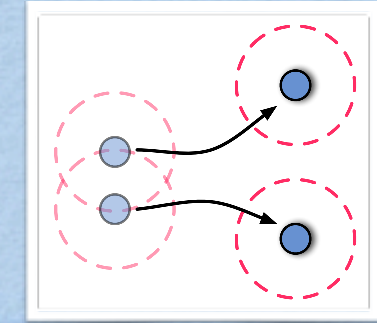


Hubrid Particle-Grid Level Sets
(Enright and Fedkiw, 2002)

Lagrangian Particle Level Sets
(Hieber and Koumoutsakos, 2005)

LAGRANGIAN DISTORTION

- loss of overlap -> loss of convergence



Particles follow flow trajectories - Location distortion

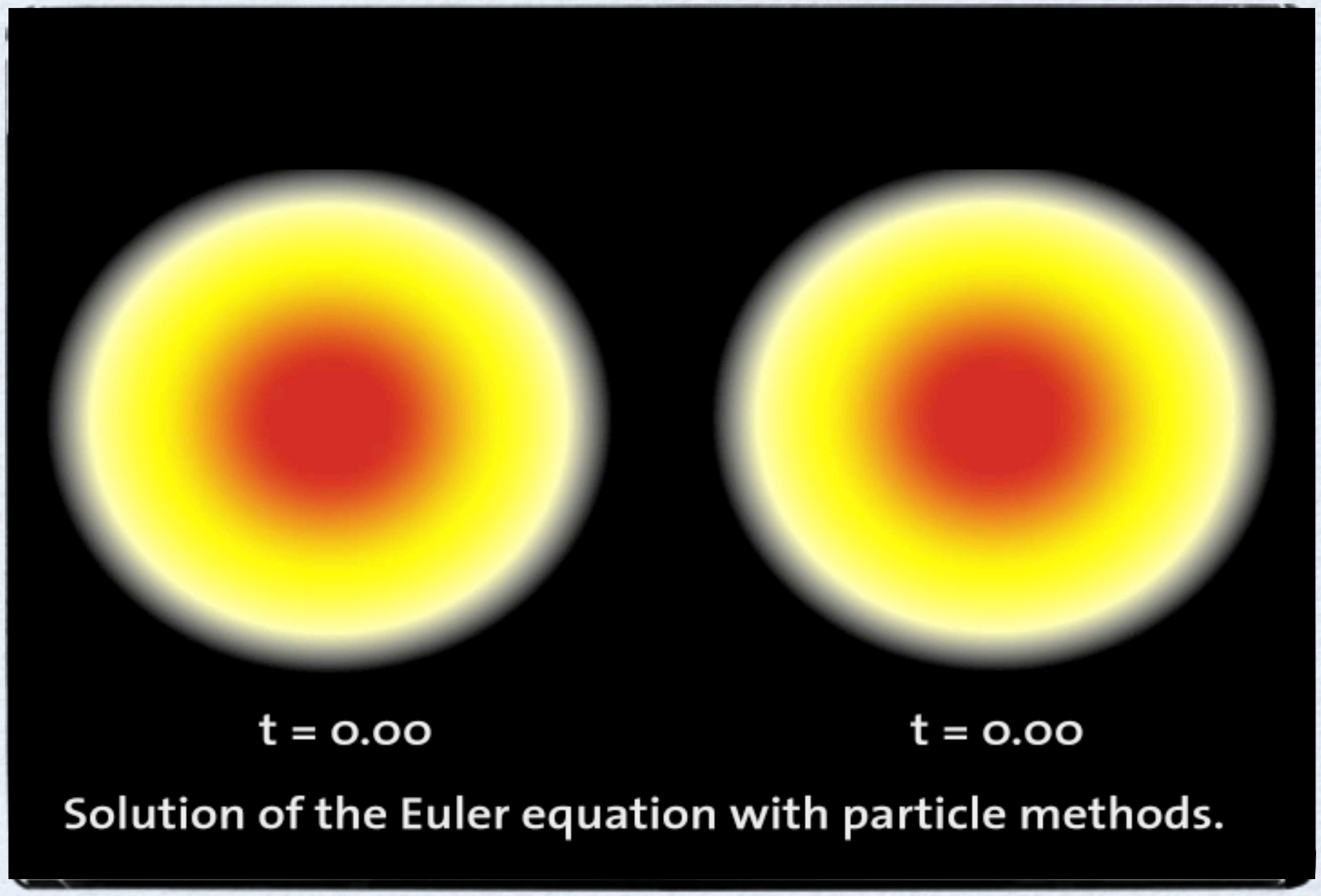
EXAMPLE :

Incompressible 2D Euler Equations

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

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

There is an exact axisymmetric solution



SMOOTH PARTICLES MUST OVERLAP

Integral Function Representation

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

Point Particle Quadrature

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

Function Mollification

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

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

Smooth Particle Quadrature

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

TOTAL ERROR

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

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

Need h/ε < 1 for accuracy

PARTICLES MUST ALWAYS OVERLAP

J. Raviart (1970's), O. Hald (1980's), Anderson, G.H. Cottet (1990's)

Are Particle Methods Grid Free ?

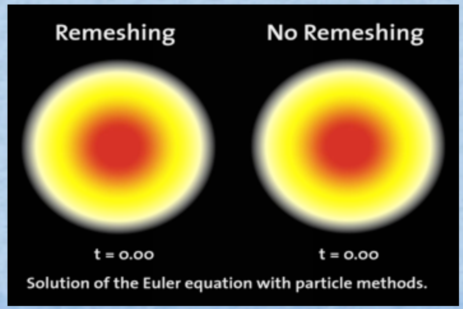
How to fix it ?

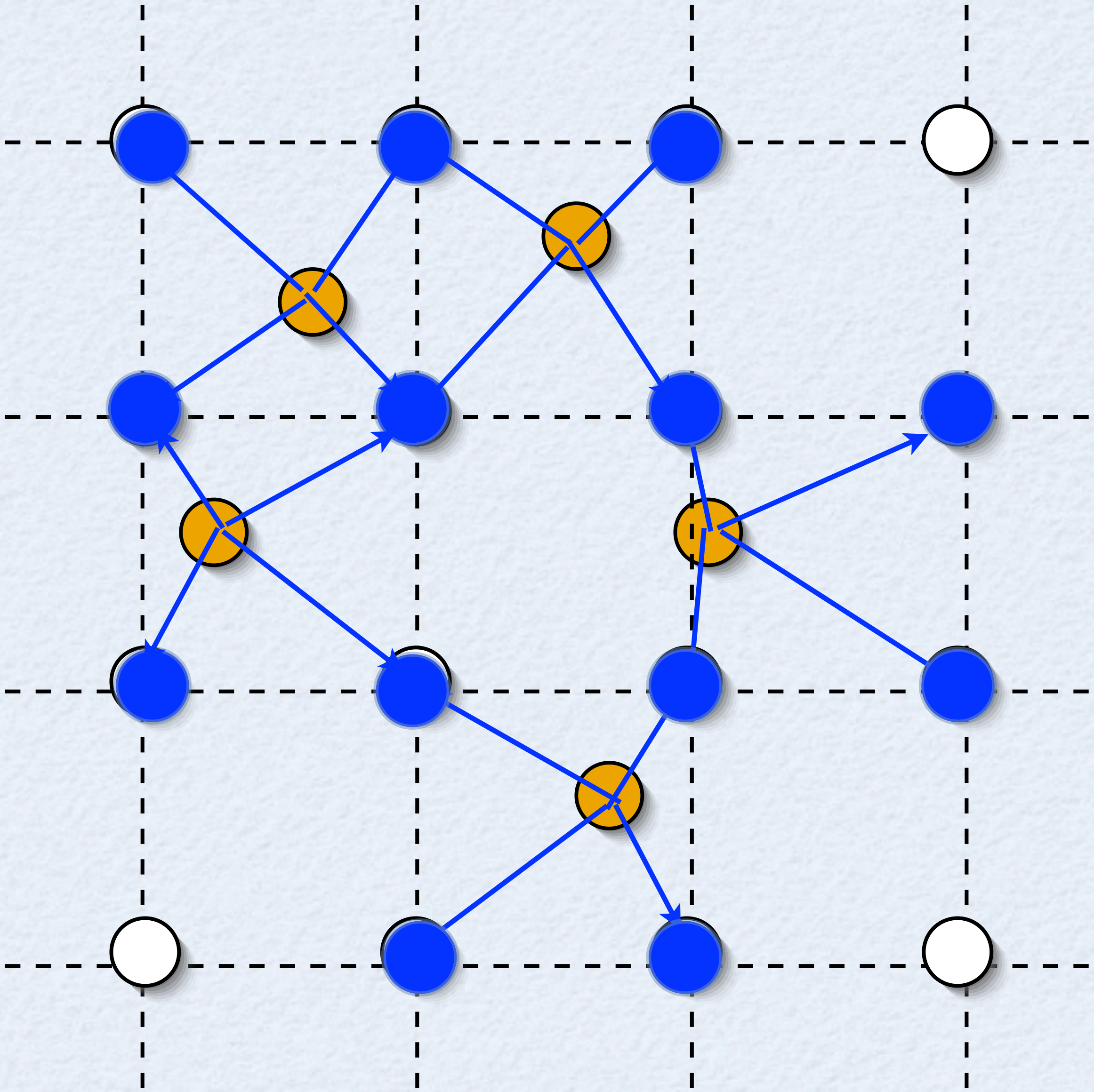
- Modify the smoothing kernels (SPH - Monaghan) — DOES NOT WORK
- Re-distribute particles with Voronoi Meshes (ALE - Russo) — EXPENSIVE - UNSTABLE
- Re-initialise particle strengths (WRKPM - Liu, Belytchko) — EXPENSIVE

REMESHING : Re-project particles on a mesh

- NO MESH-FREE particle methods
- Can use all the “tricks” of mesh based methods
- High CFL
- Multiresolution & Multiscaling
- ....

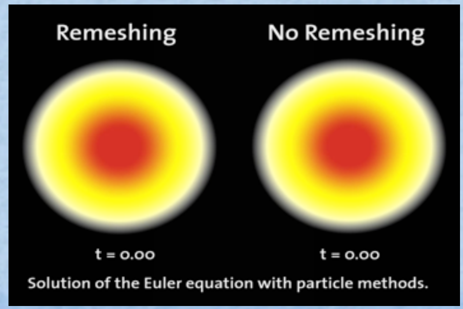
Particle Remeshing = Resampling





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

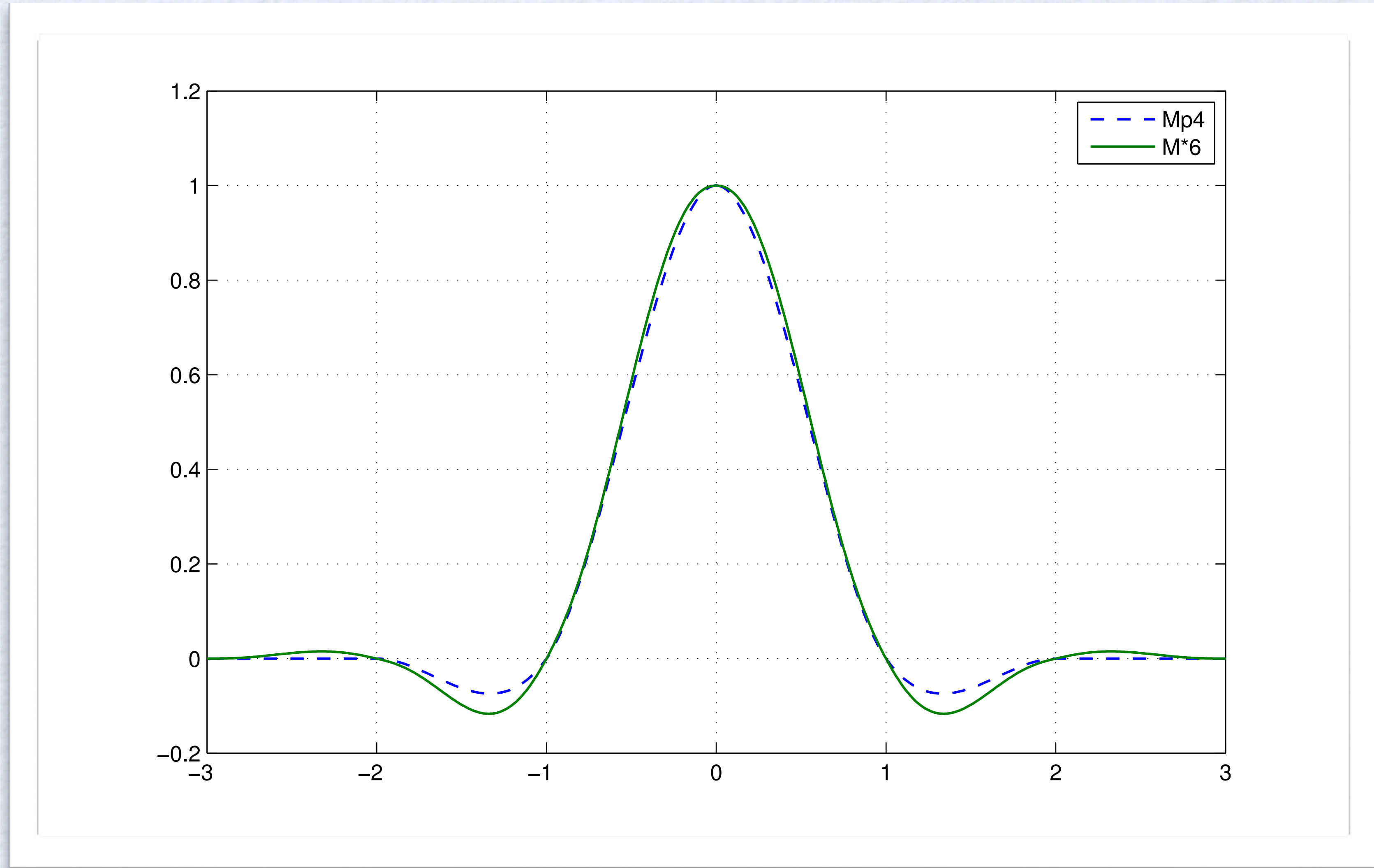
Particle Remeshing = Resampling



Moment conserving Interpolation

$$\sum_i M(x-i)\, i^\alpha = x^\alpha$$

Remesh on i = 1...L grid points
Conserving L moments a = 1....L implies
L (well posed) equations for L unknowns



Solve to derive M

$$M_6^*(x) = \begin{cases} -\frac{1}{12}(|x|-1)(24\,|x|^4 + 38\,|x|^3 - 3\,|x|^2 + 12\,|x| + 12) & |x| < 1 \\ \frac{1}{24}(|x|-1)(|x|-2)(25\,|x|^3 - 114\,|x|^2 + 153\,|x| - 48) & 1 \le |x| < 2 \\ -\frac{1}{24}(|x|-2)(|x|-3)^3(5\,|x|-8) & 2 \le |x| < 3 \\ 0 & 3 \le |x| \end{cases}$$

REMESHED PARTICLE METHODS

1. ADVECT : Particles ->Large CFL

2. REMESH : Particles to Mesh -> Vectorized

3. SOLVE: Poisson/Derivatives on Mesh ->FFTw/Ghosts

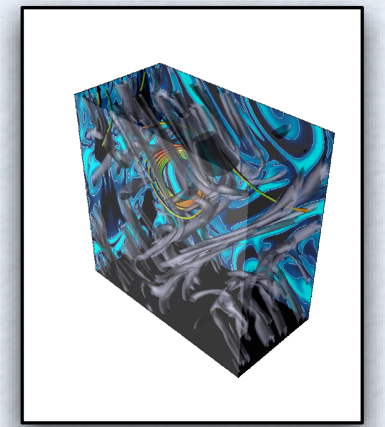
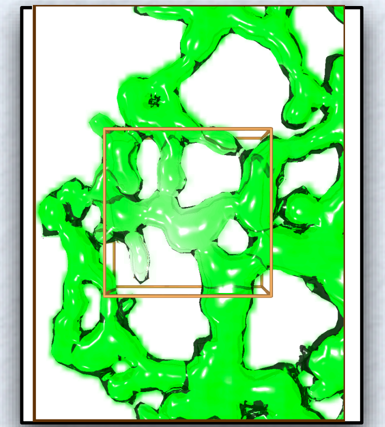
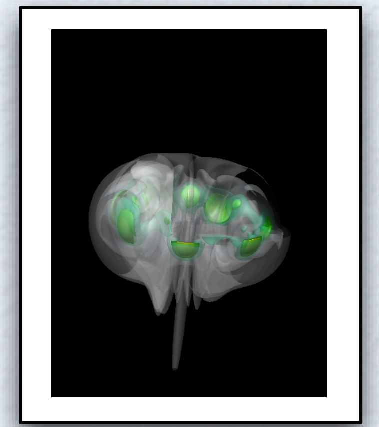
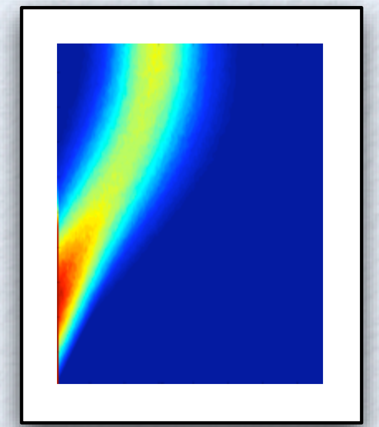
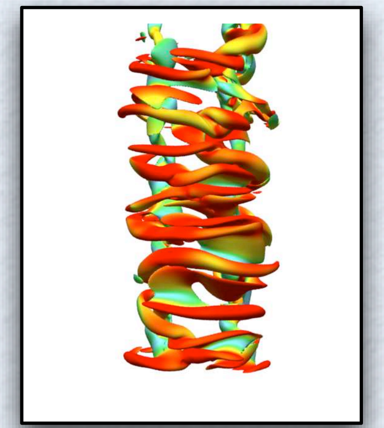
4: RESAMPLE: Mesh Nodes BECOME Particles

PPM : Parallel Particle Mesh library

www.ppm-library.org

OPEN SOURCE www.cse-lab.ethz.ch/software.html

Library for MPI parallel Particle-Mesh simulations

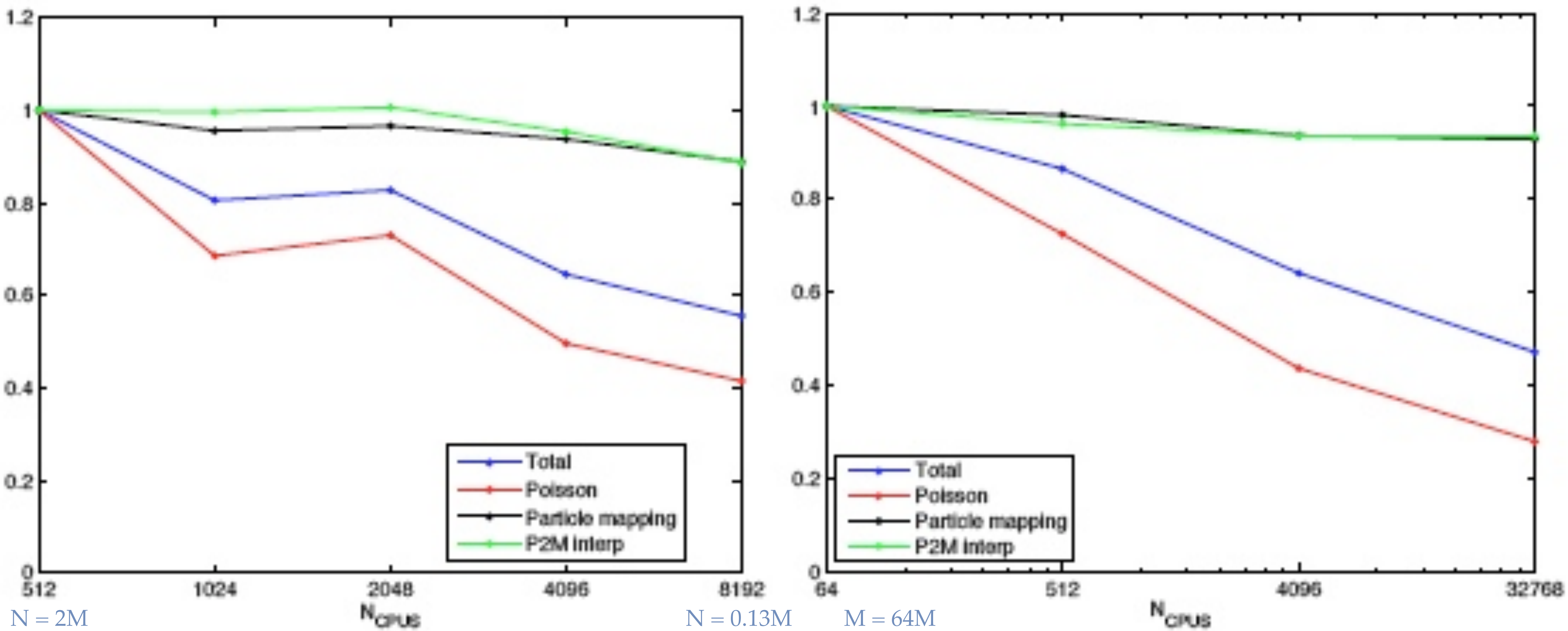
Parallel Particle Mesh Library (PPM)

Message Passing Interface (MPI) | METIS | FFTW

vector | shared memory | distributed memory | single processor

I.F. Sbalzarini, et. al.. **J. Computational Physics**,, 2006

Scalability – CRAY XT5



Strong

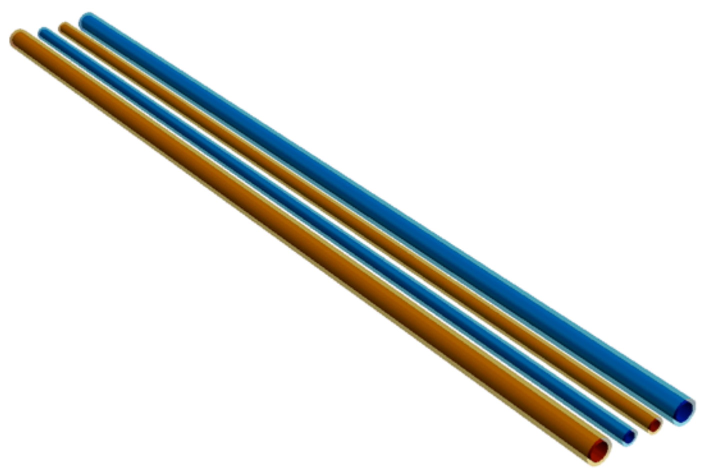
Size : 1280x1280x640

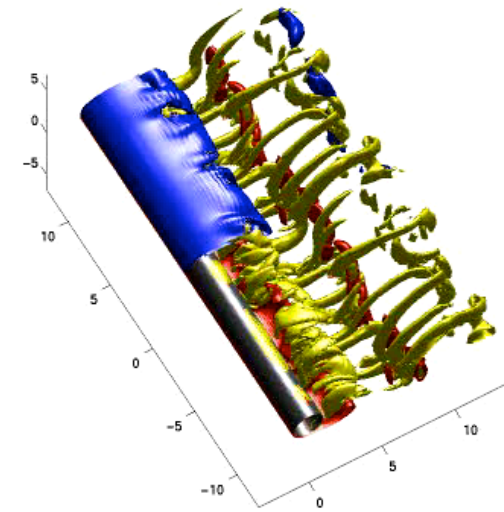
time : 512 / 90s - 8192 / 10s

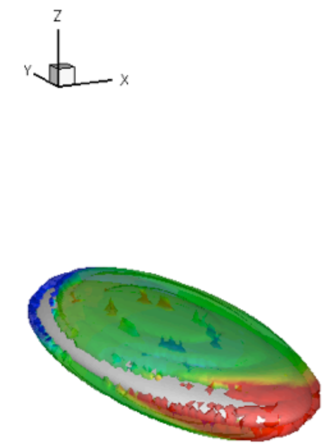
Weak

time : 64 / 40s - 32768 / 85s

Particles for Fluid Mechanics @ 2000+



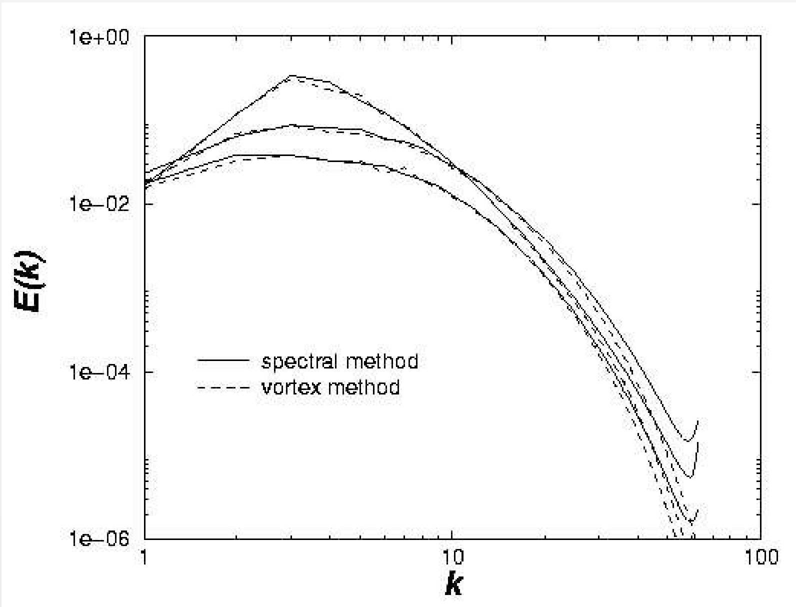


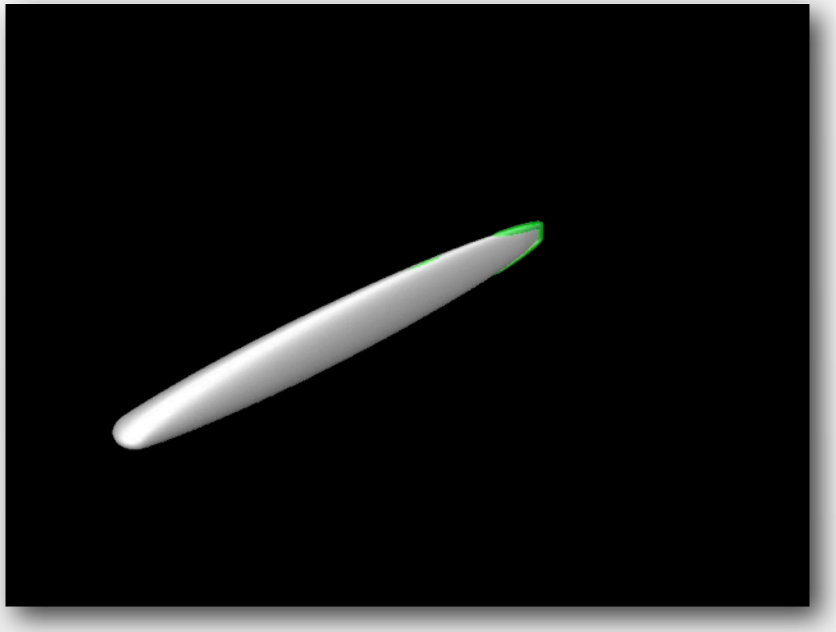


Vortex Rings and Vortex Wakes

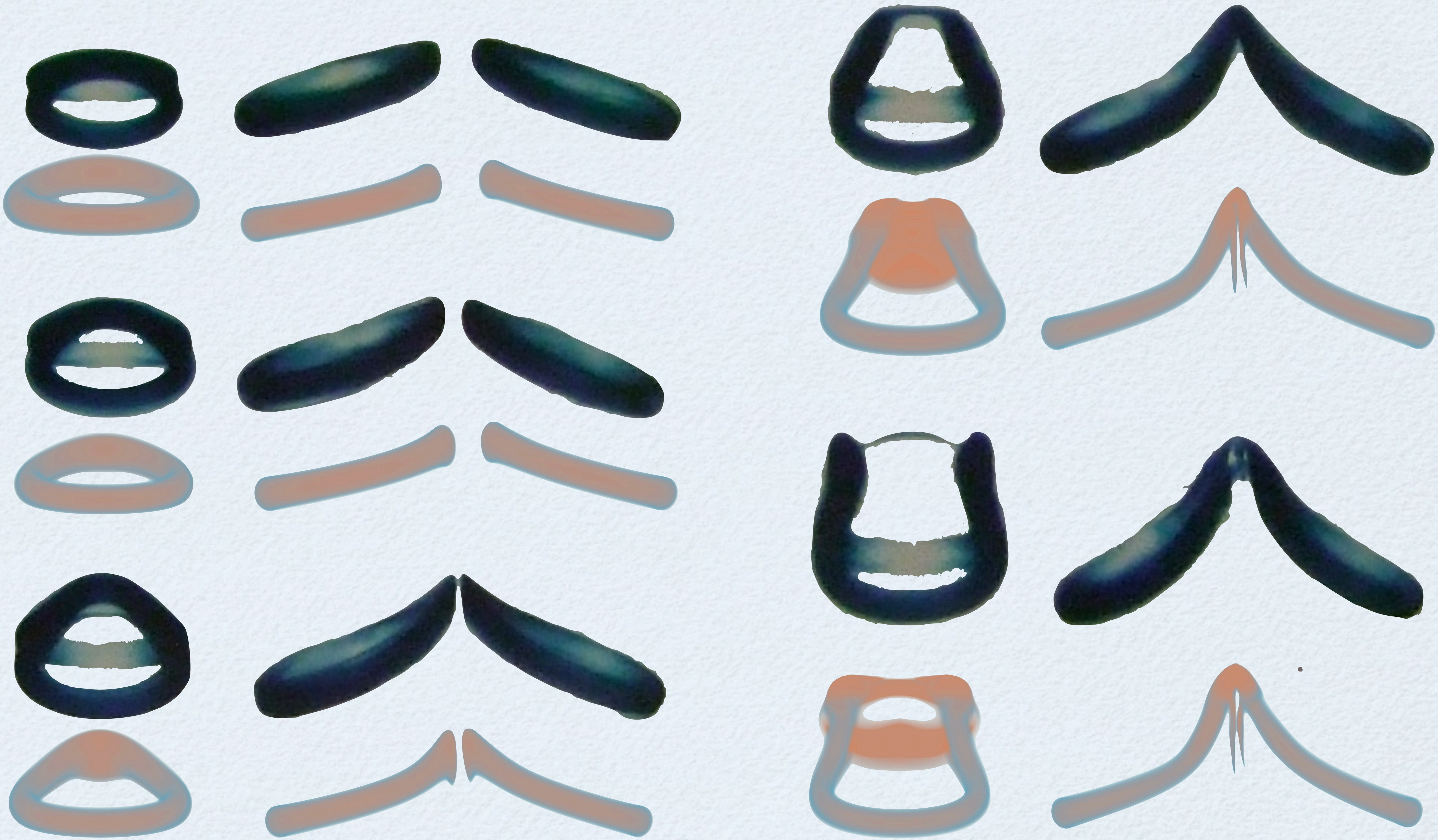
Bluff Body and Turbulent Flows

Swimming and Flying



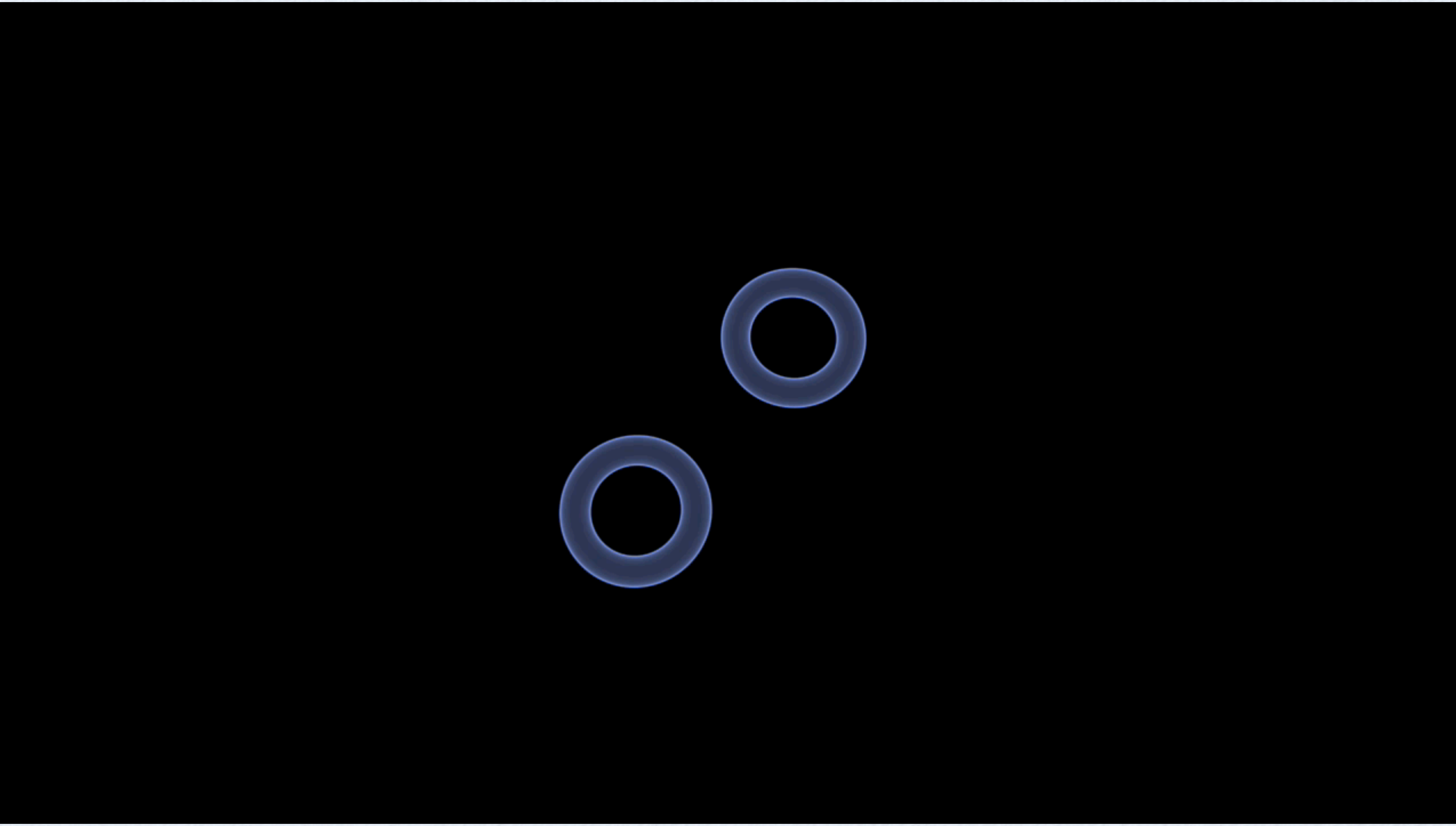


VORTEX RING COLLISION, Re = 1800

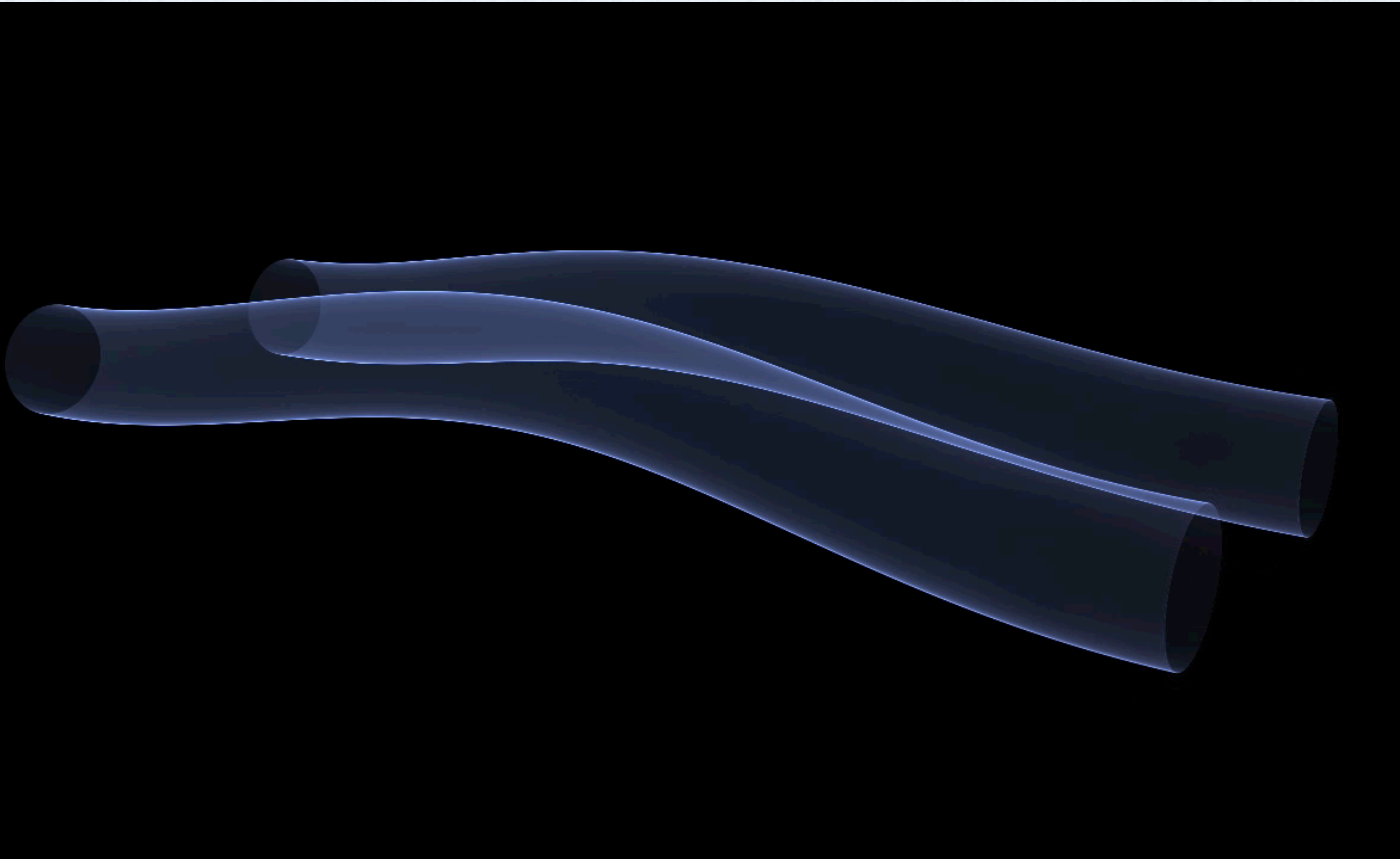


Experiments : P. Schatzle & D. Coles (1986)

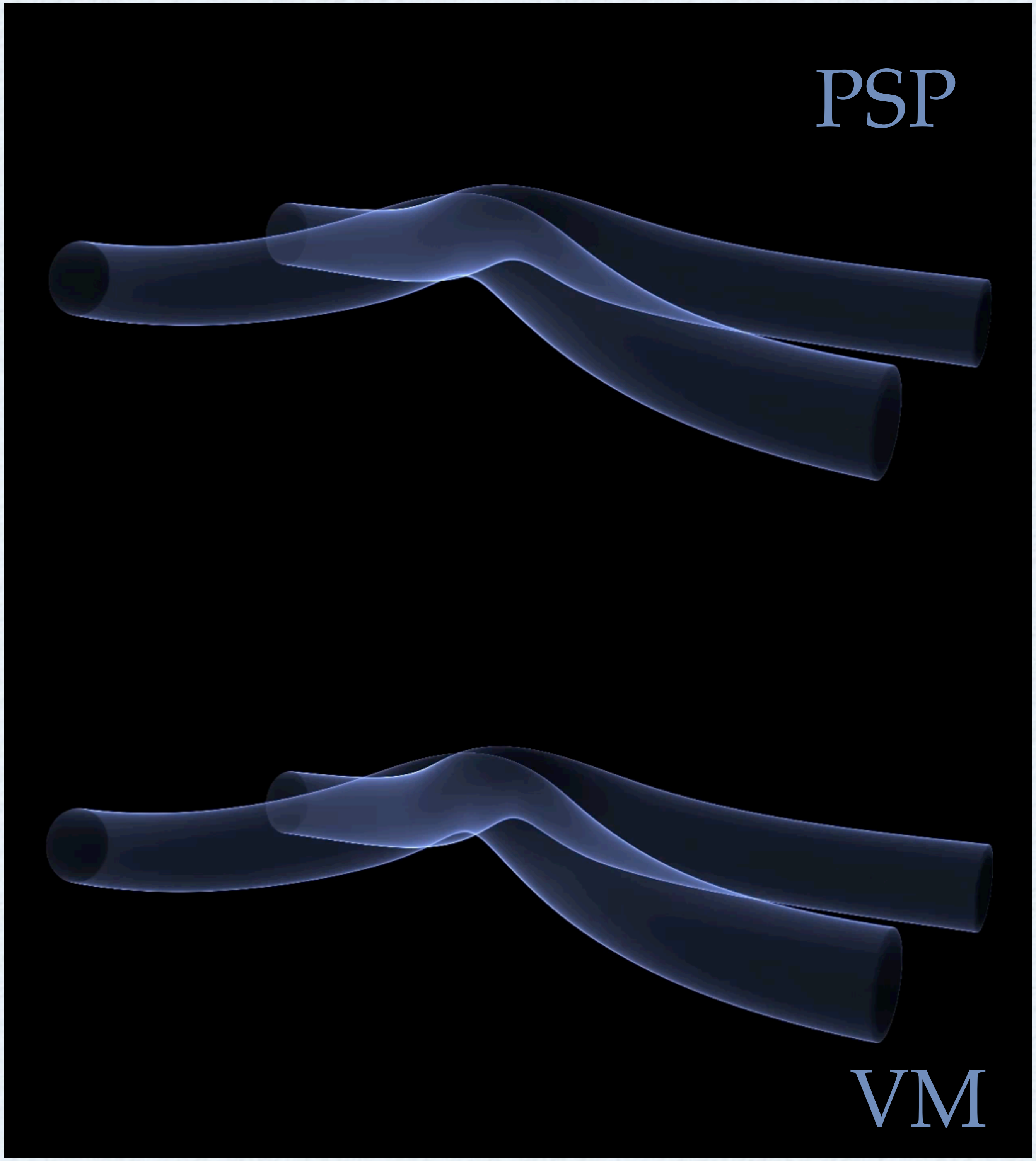
Vortex Ring Collision - Re = 10,000

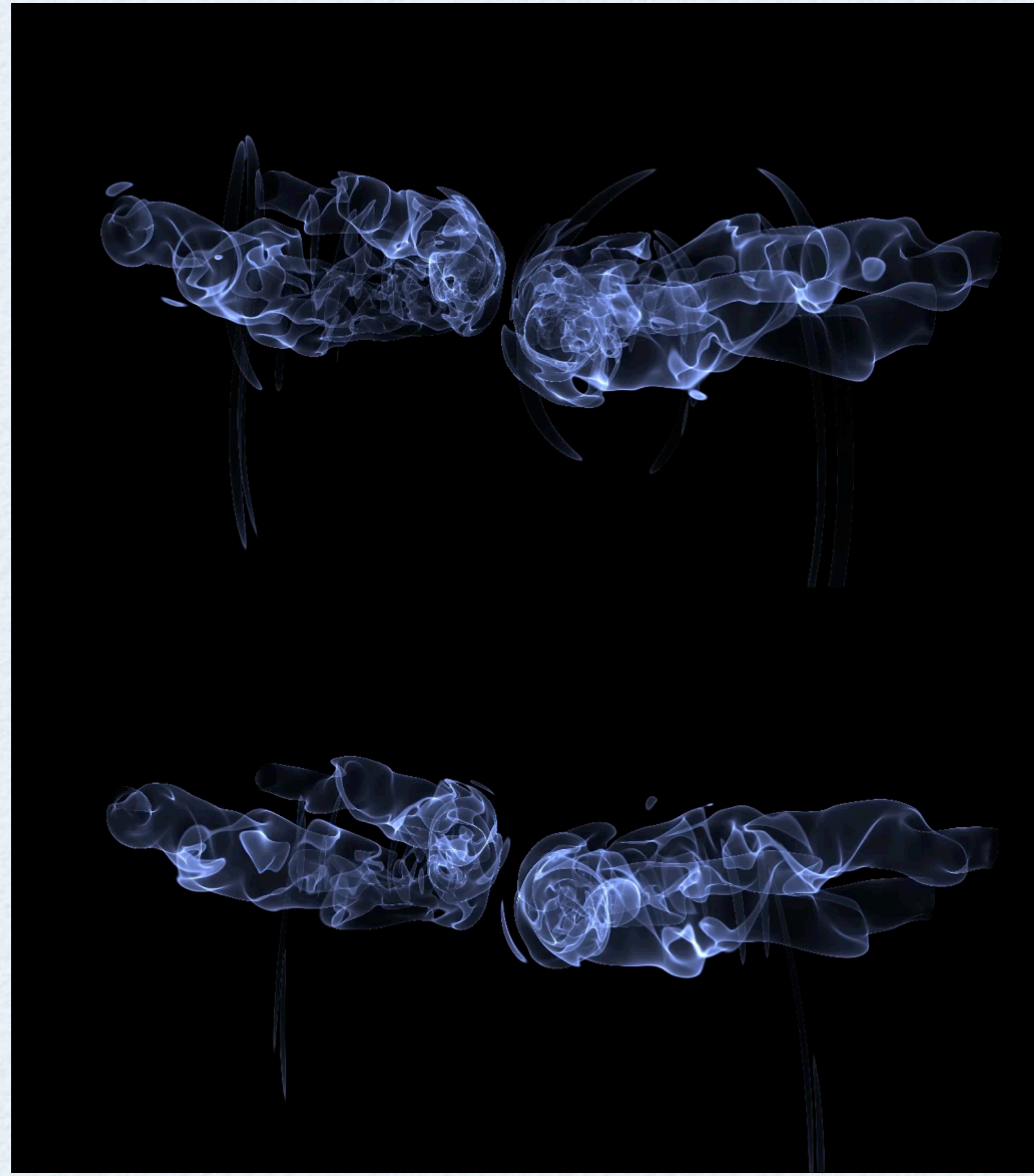


VORTEX DYNAMICS at High Re



VORTEX DYNAMICS OF TUBES @ Re = 10,000



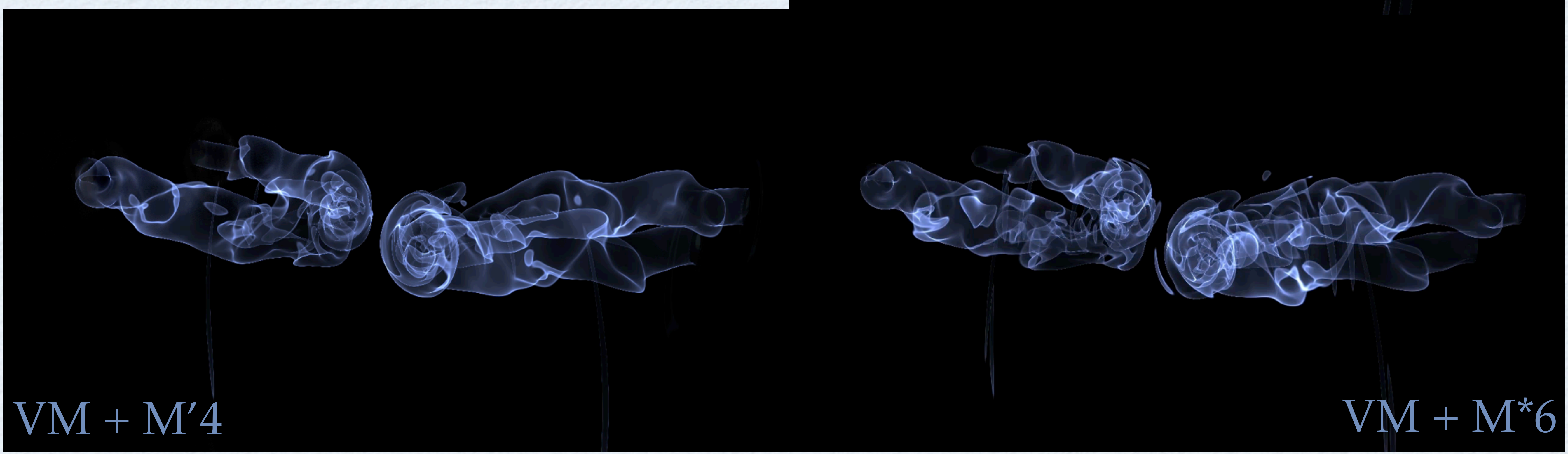


RESOLUTION : 1280 X 960 x 640 = 0.8 Billion elements

Timings : 23sec (PSP) & 12.5 sec (VM) per step (on 4096 cores) : to T = 11.5 : Nsteps (PSP - RK4) = 8400, Nsteps (VM)- RK3 = 17,000

VORTEX DYNAMICS OF TUBES @ Re = 10,000

What is the effect of Remeshing ?



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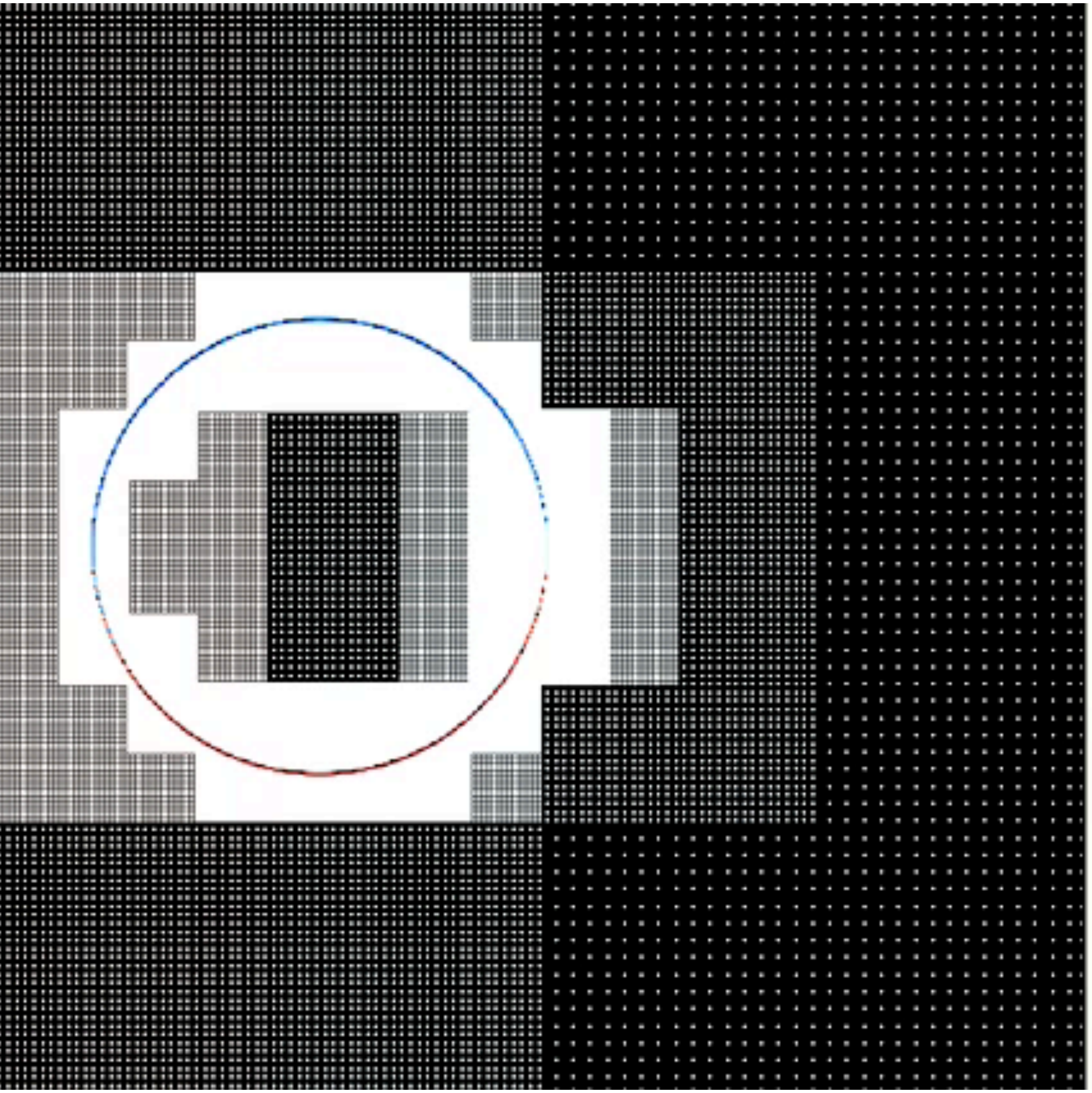
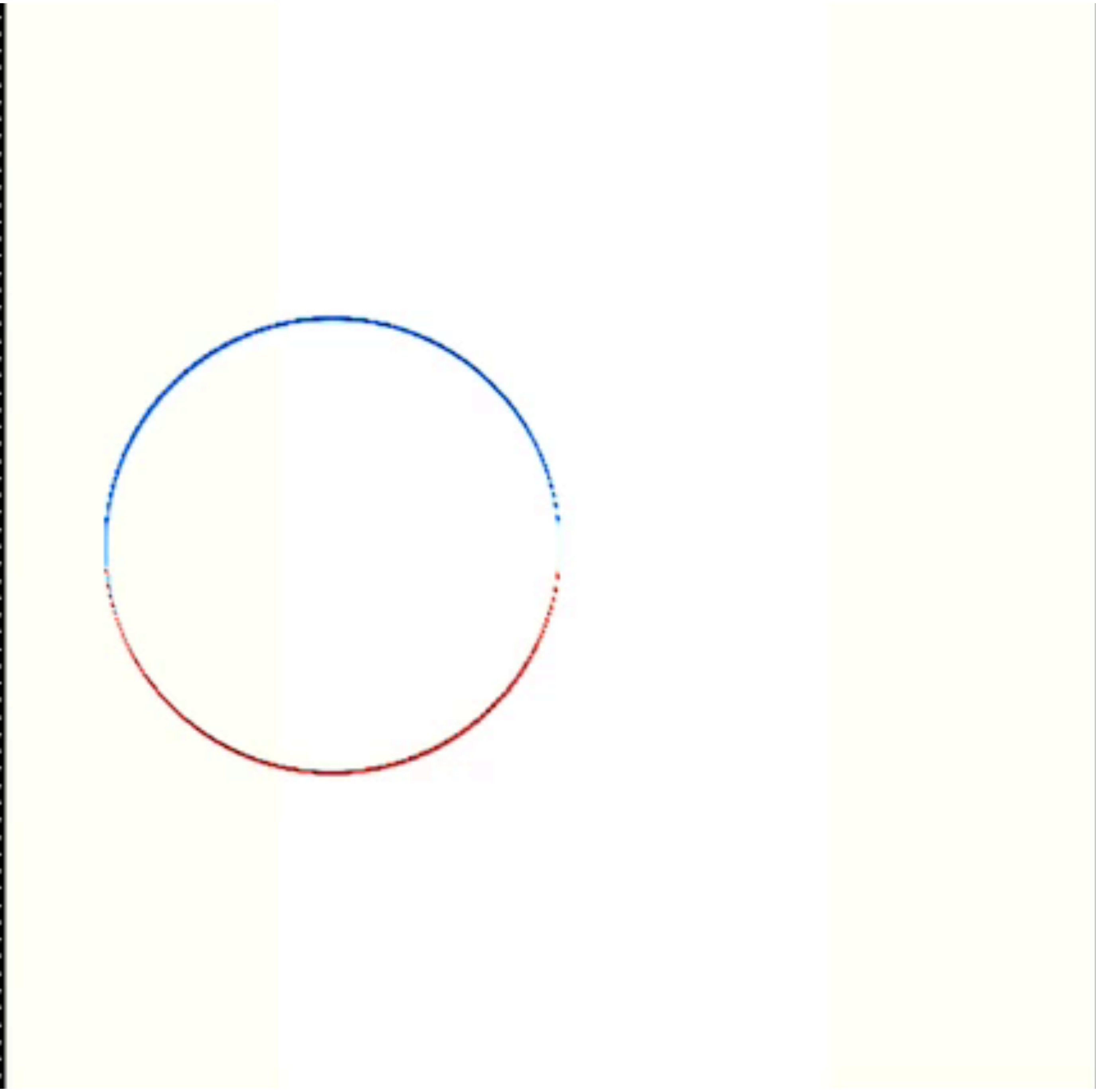
Wavelet-based Block-Adaptivity

IMPULSIVELY STARTED CYLINDER AT RE = 2000, MA = 0.4

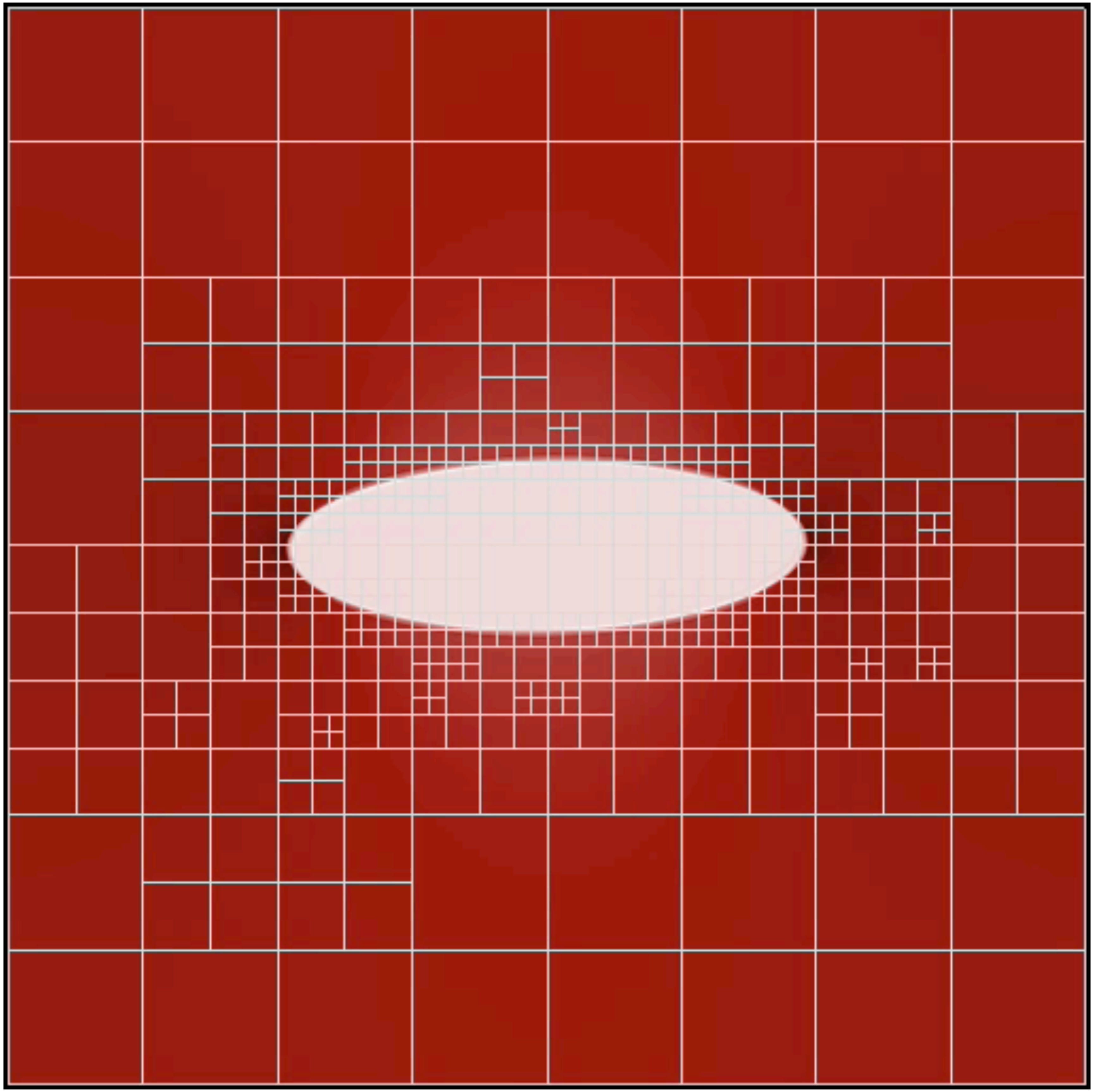


VORTICITY + BLOCKS



VORTICITY

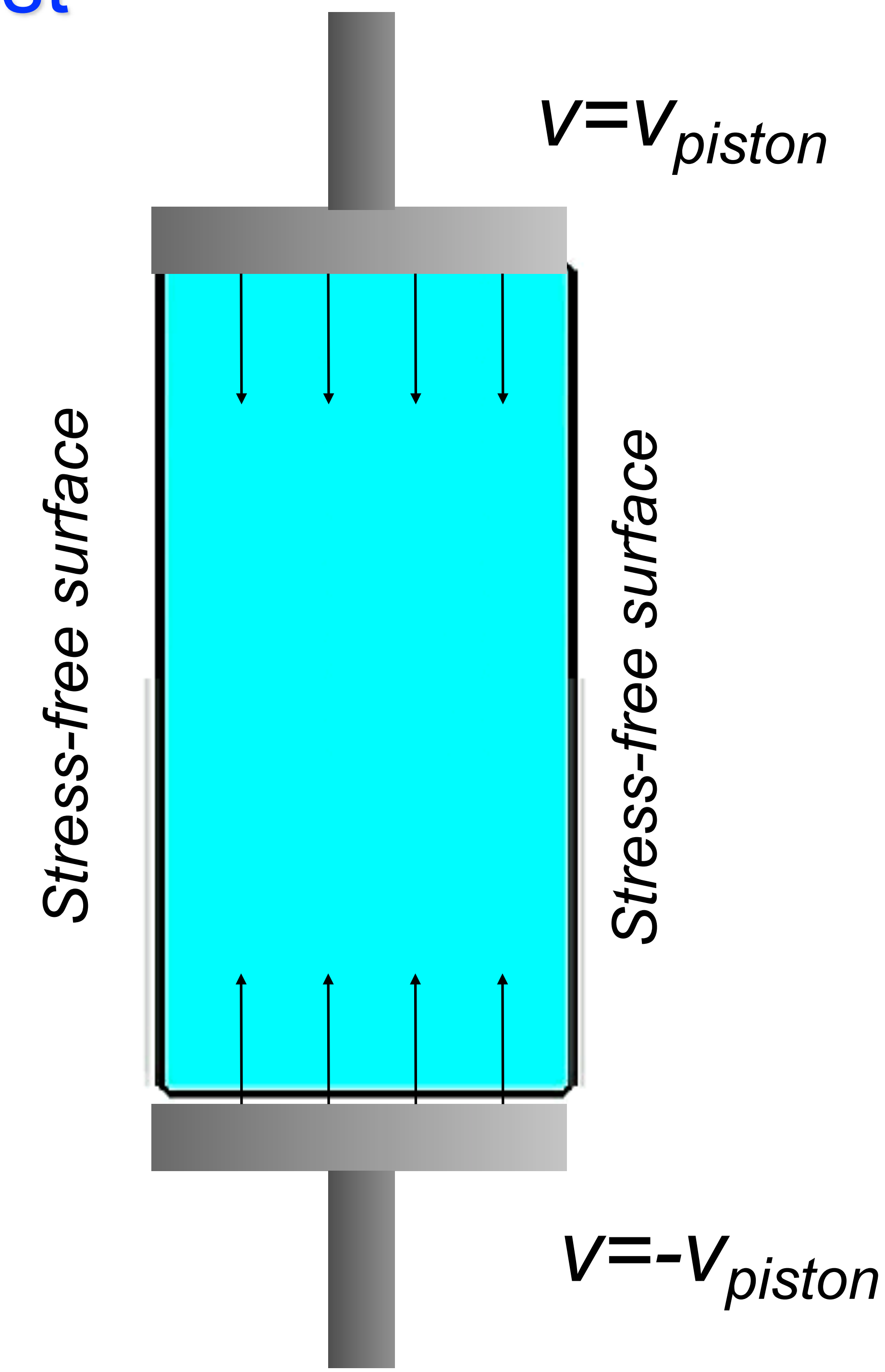
Wavelet-based Block-Adaptivity



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



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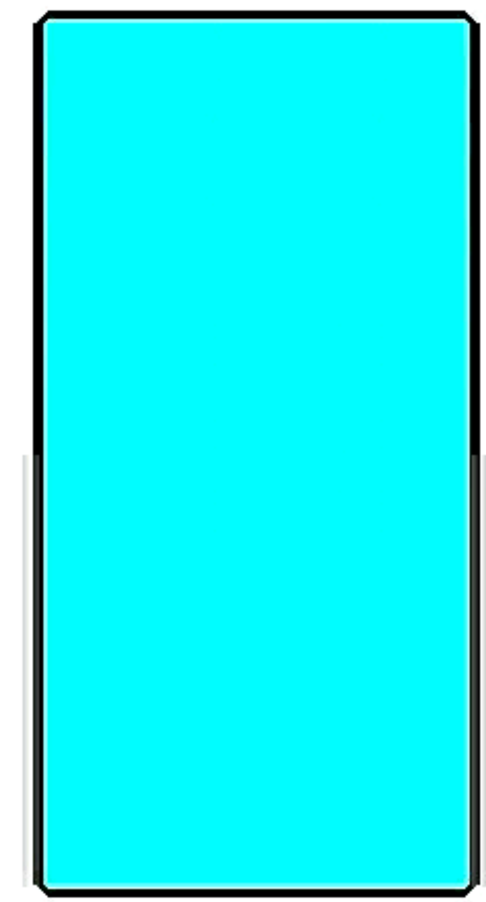
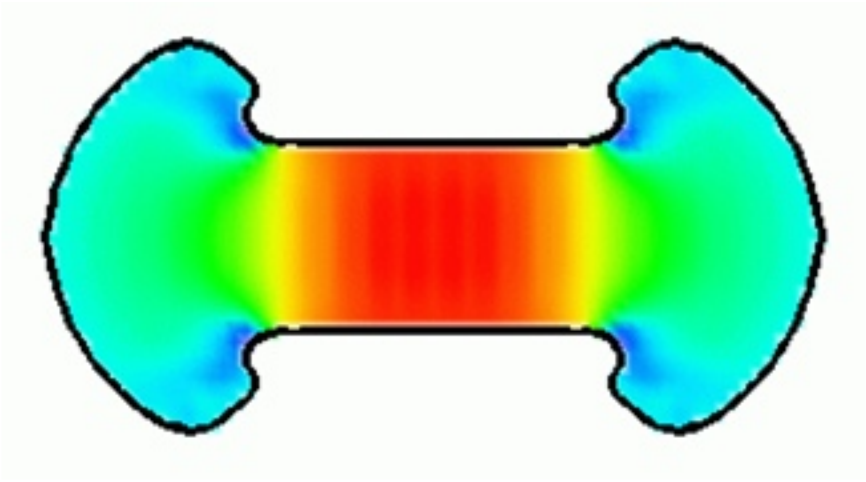


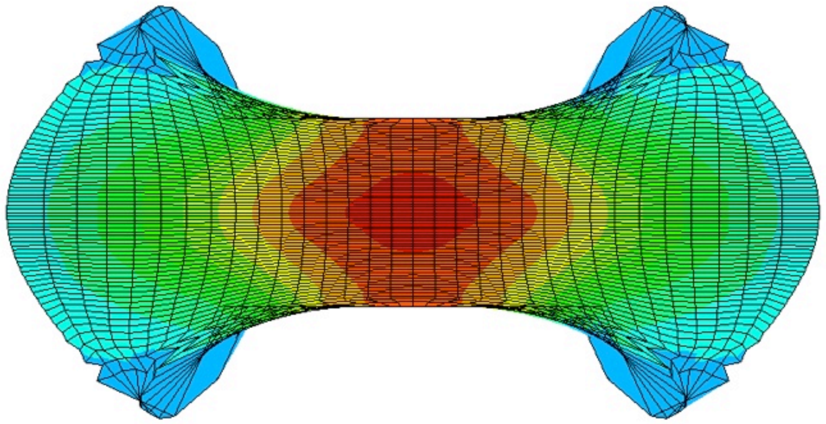
Plane Strain Compression Test

	Redistributed Particle solution	FEM solution (ABAQUS 6.4/Explicit)

Linear Elasticity

Young's Modulus =100
Poisson ratio=0.49 ~2000 particles/nodes



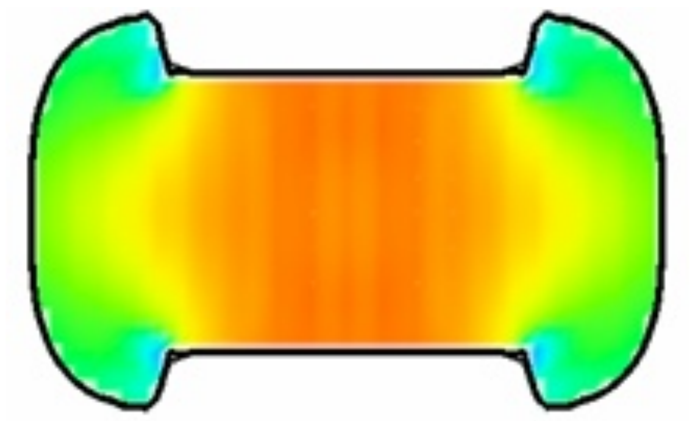


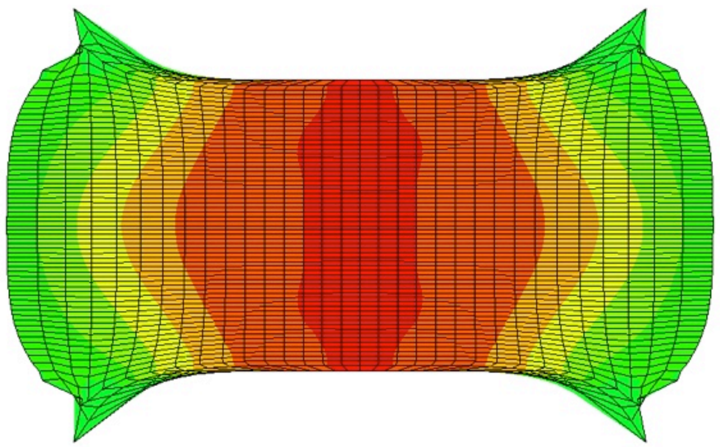
Nonlinear Elasticity

Hyperelastic Material

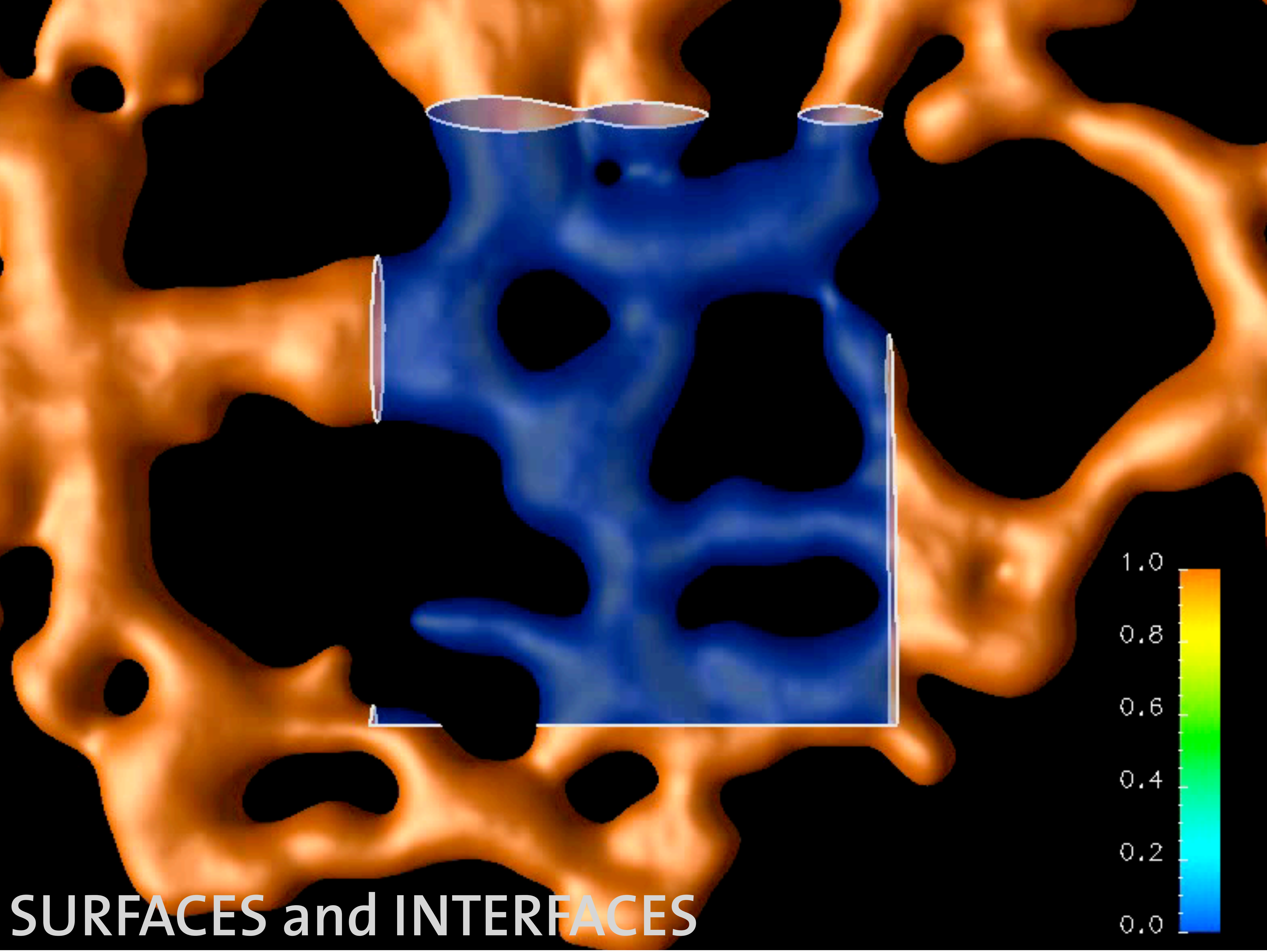
C_{10}=2.2, D=0.001

~2000 particles/nodes

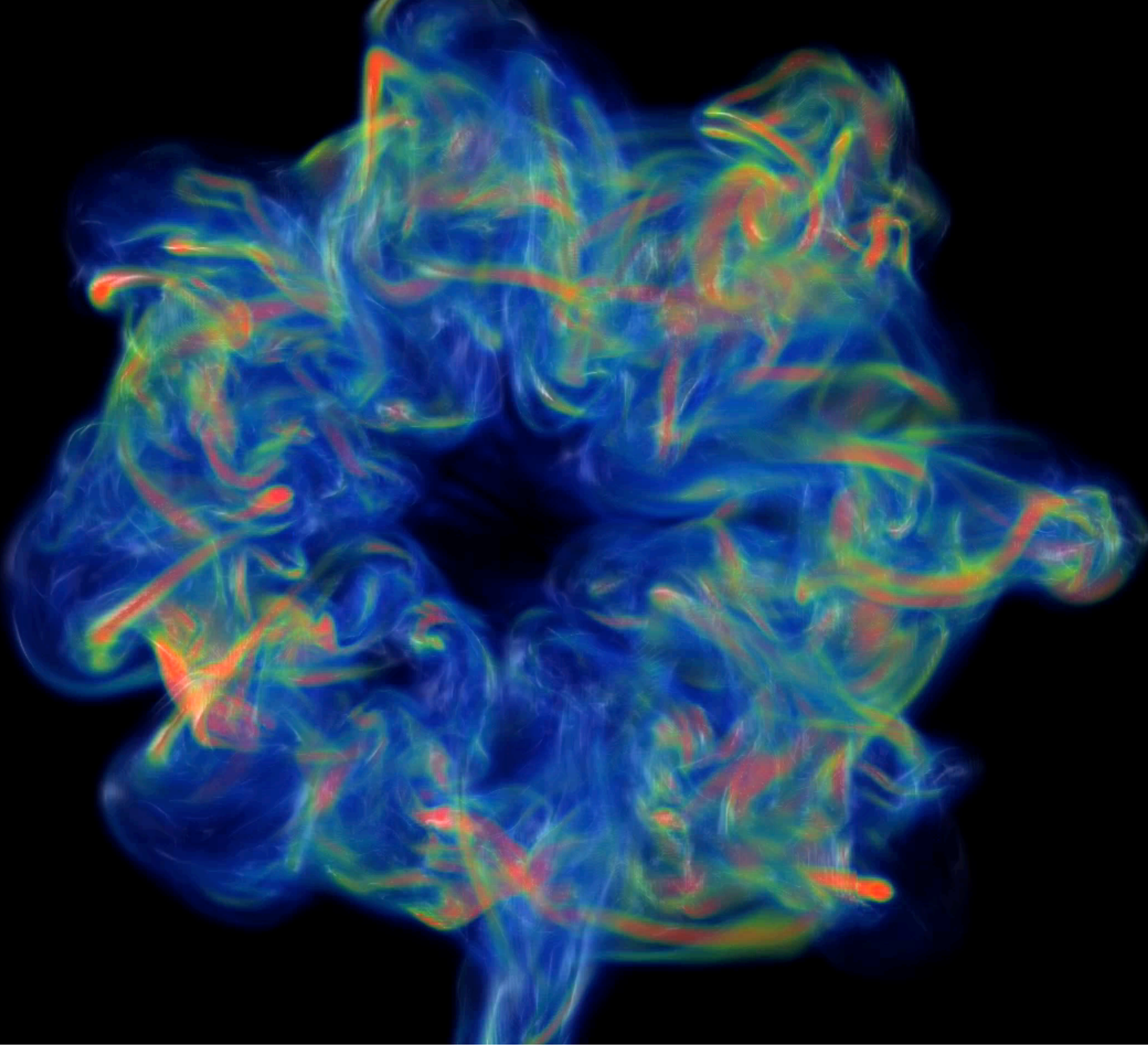




S.E. Hieber and P. Koumoutsakos A Lagrangian particle method for the simulation of linear and nonlinear elastic models of soft tissue. *al., J. Comp. Physics, 2008*



SURFACES and INTERFACES




Walther


Chatelain


Cottet


Bergdorf


Rossinelli


Gazzola


Hedjazialhosseini


van Rees


Milde