Particles and Meshes I

Re-meshing and Multi-resolution

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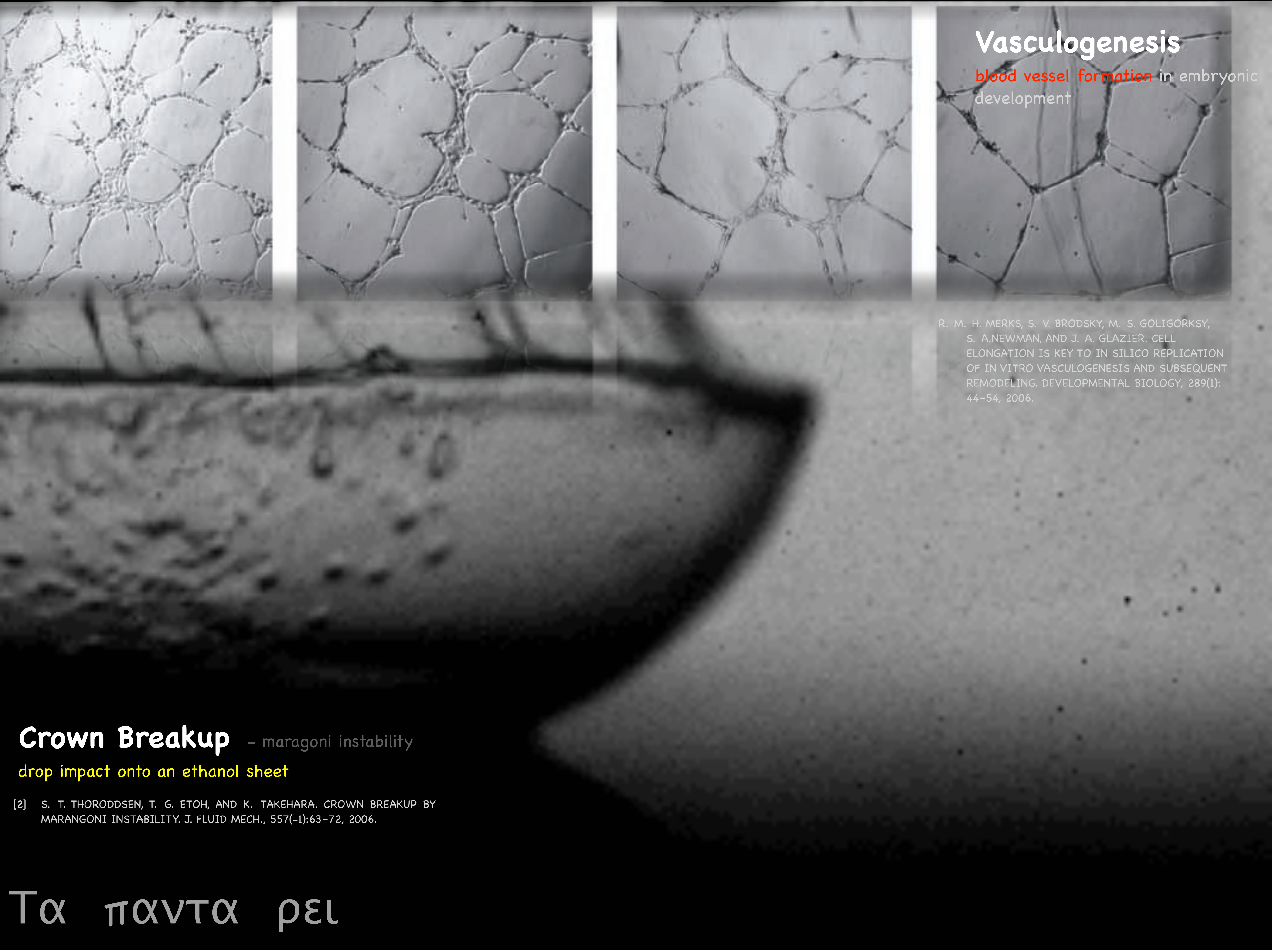
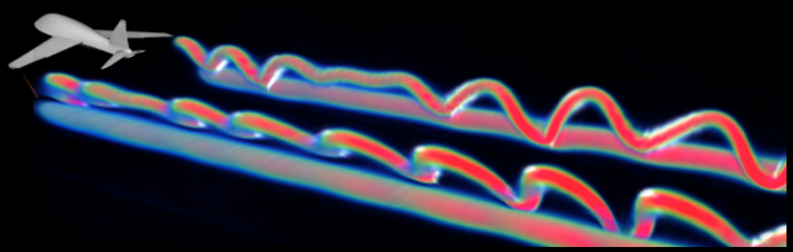
OUTLINE

- why PARTICLES
- necessary REMESHING
- worthy MULTIRESOLUTION
- uniting BOUNDARY CONDITIONS / COUPLING PHYSICS
- fishy RESULTS
- ? OUTLOOK


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

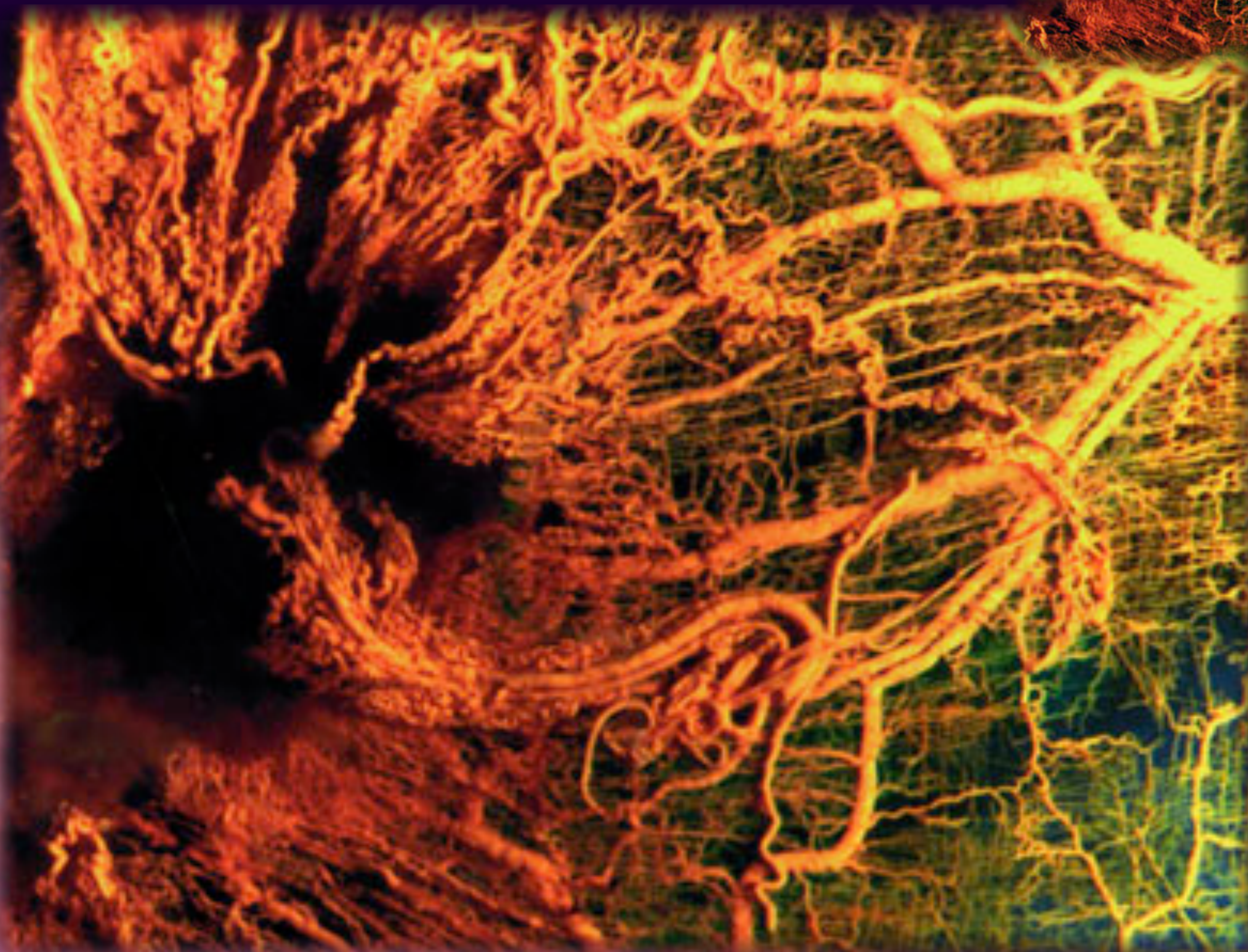
16384 Cores - 10 Billion Particles - 60% efficiency

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

Cancer Growth and Flow

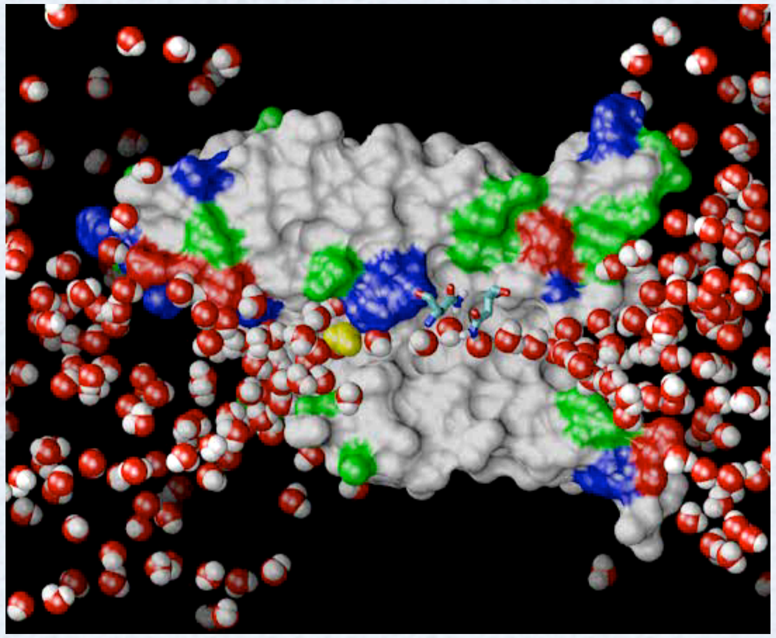


credit : Roche

PARTICLE METHODS ARE UNIQUE

Molecular Dynamics

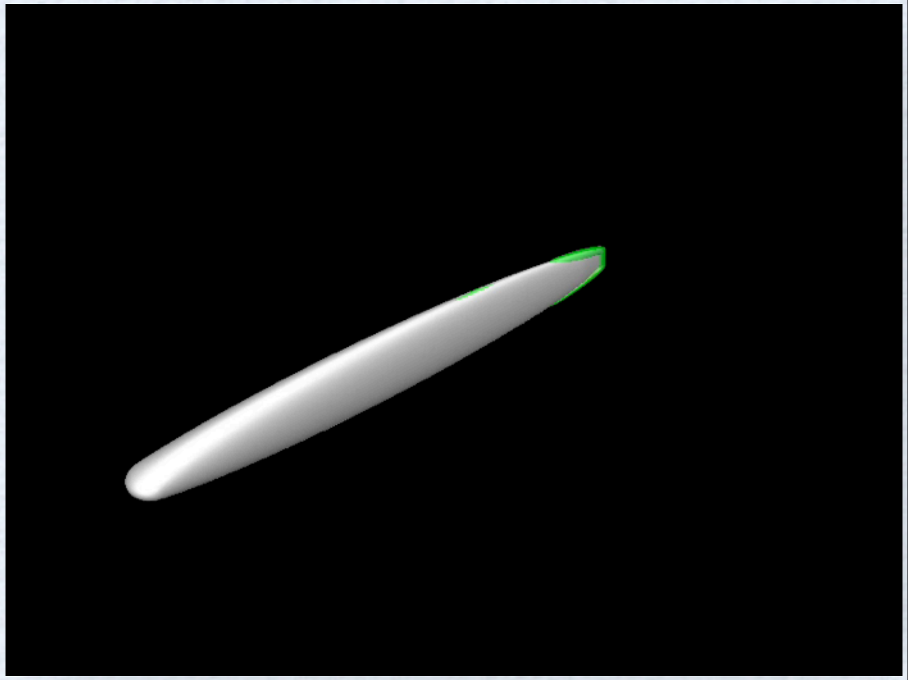
-9



Transport in aquaporins
Schulten Lab, UIUC

Vortex Methods

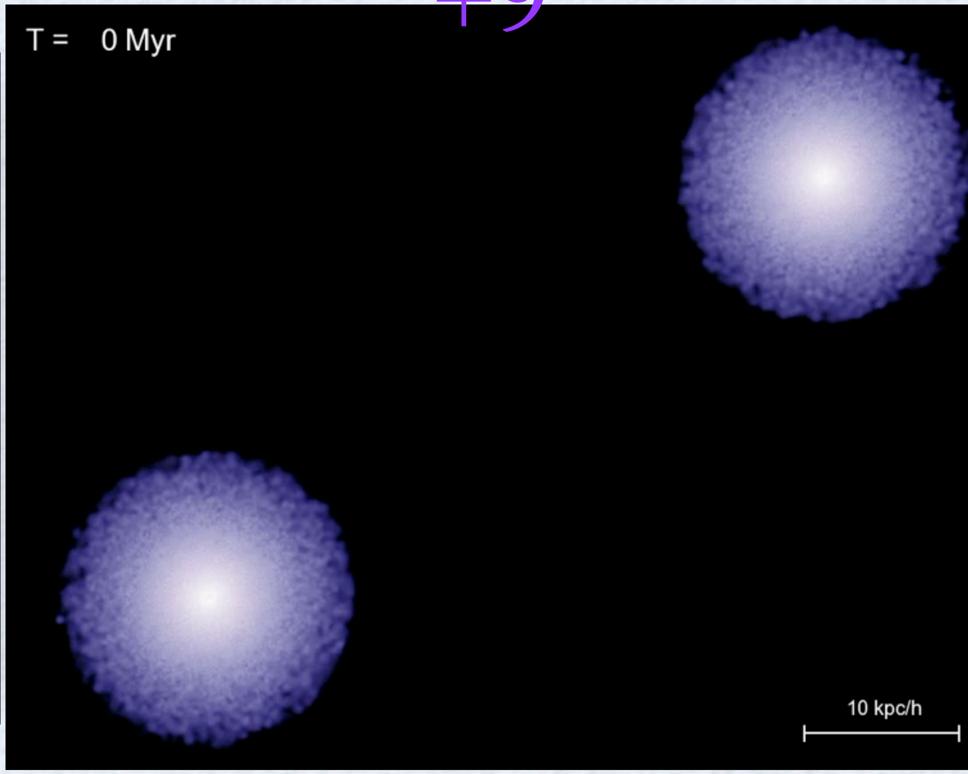
0



Vortex Dynamics
Koumoutsakos Lab, ETHZ

Smoothed Particle Hydrodynamics

+9



Growth of Black Holes
Springel, MPI - Hernquist, Harvard

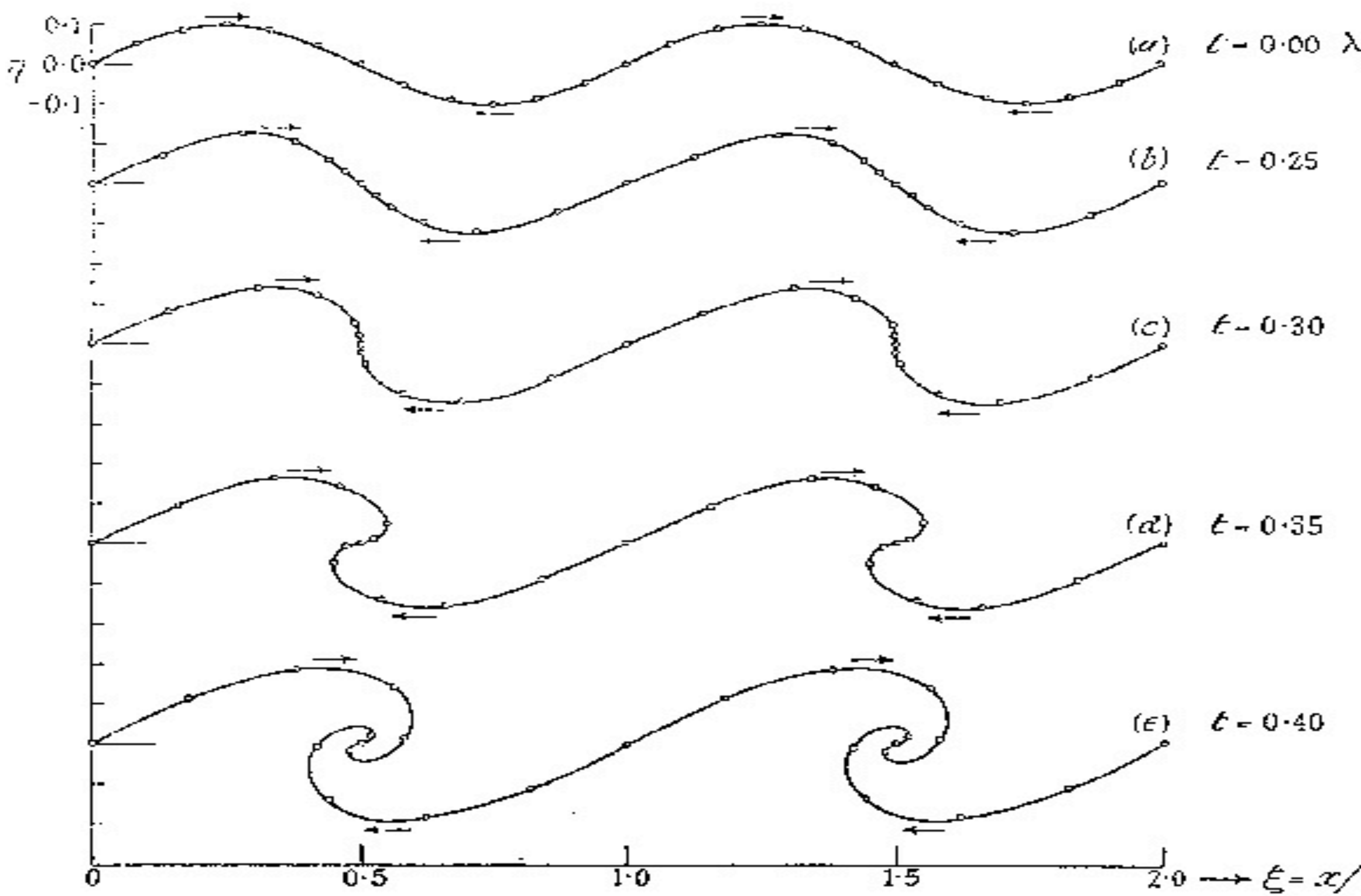
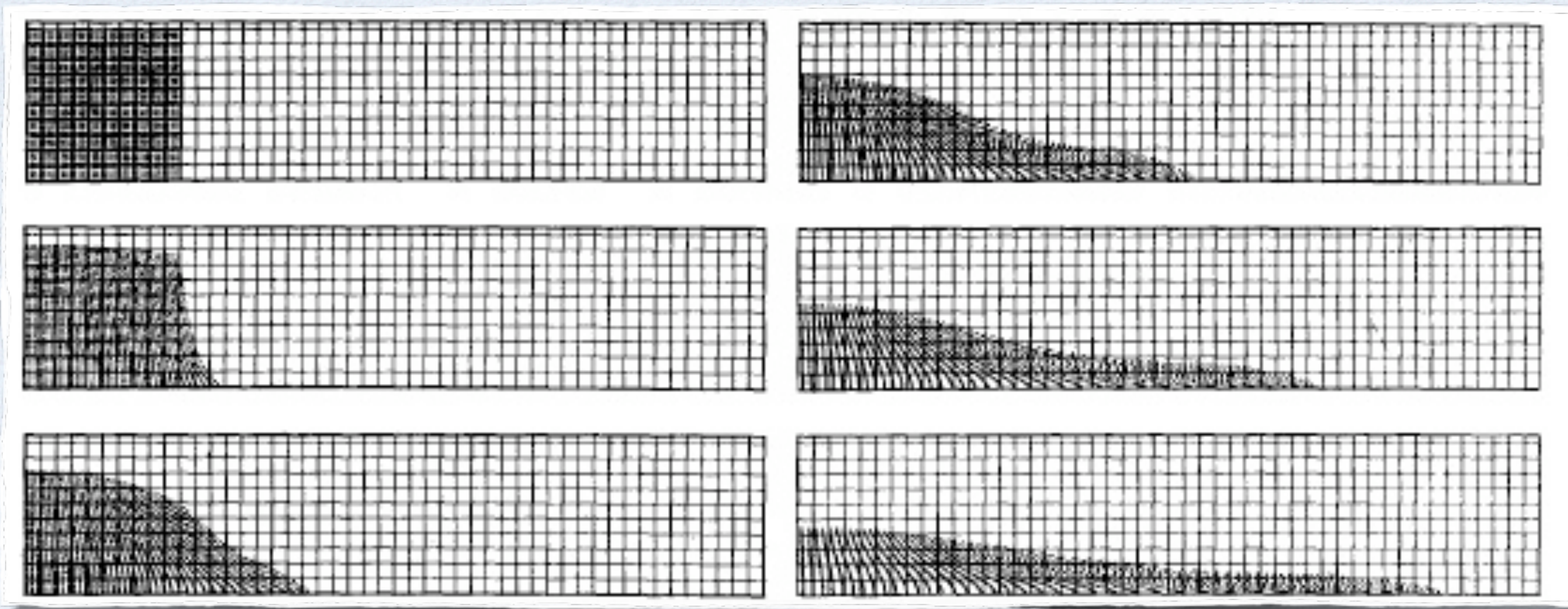


FIG. 4.

A BRIEF HISTORY of PARTICLE METHODS

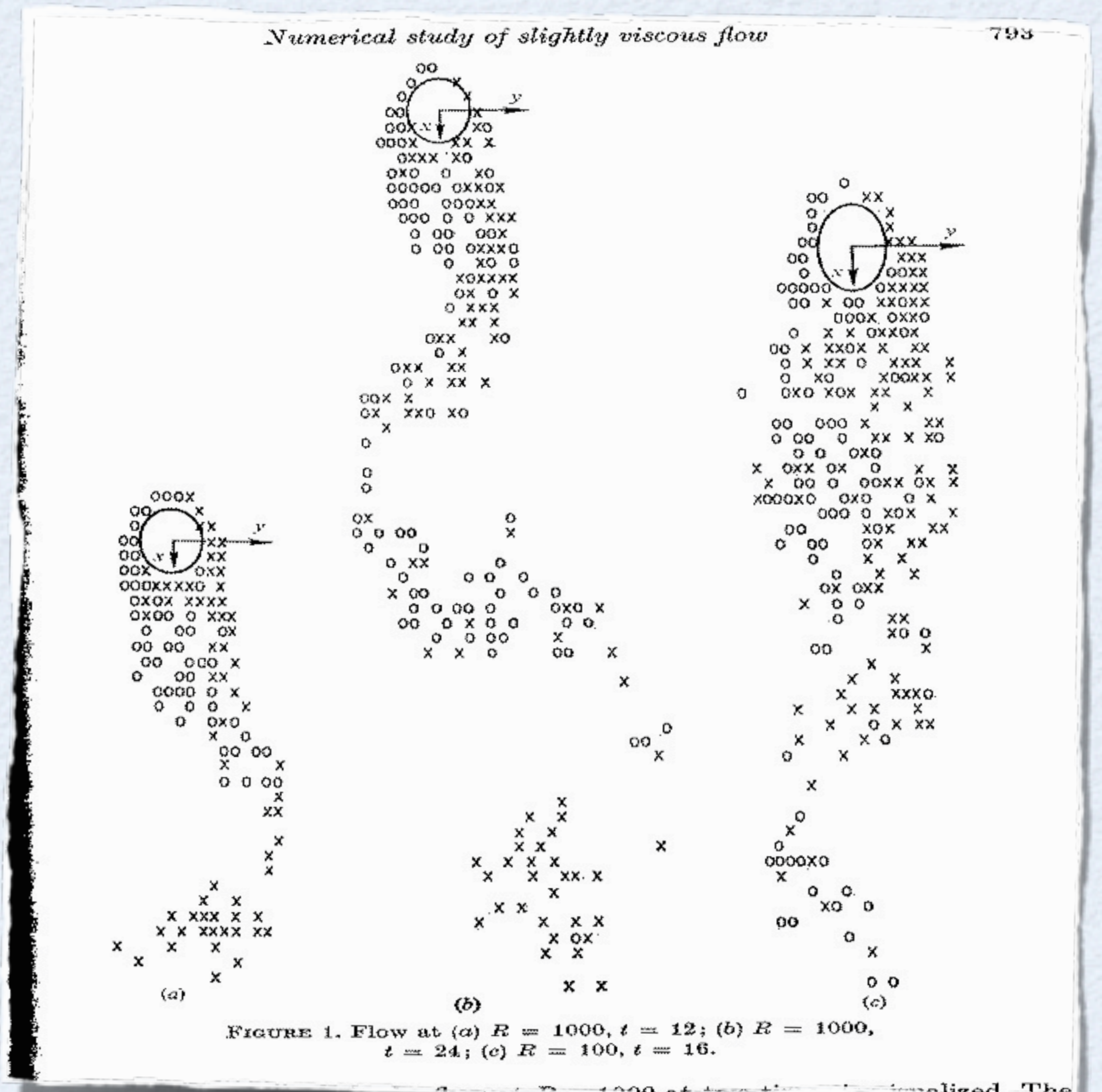
The 60’s : Marker And Cell (MAC) -(velocity – pressure)

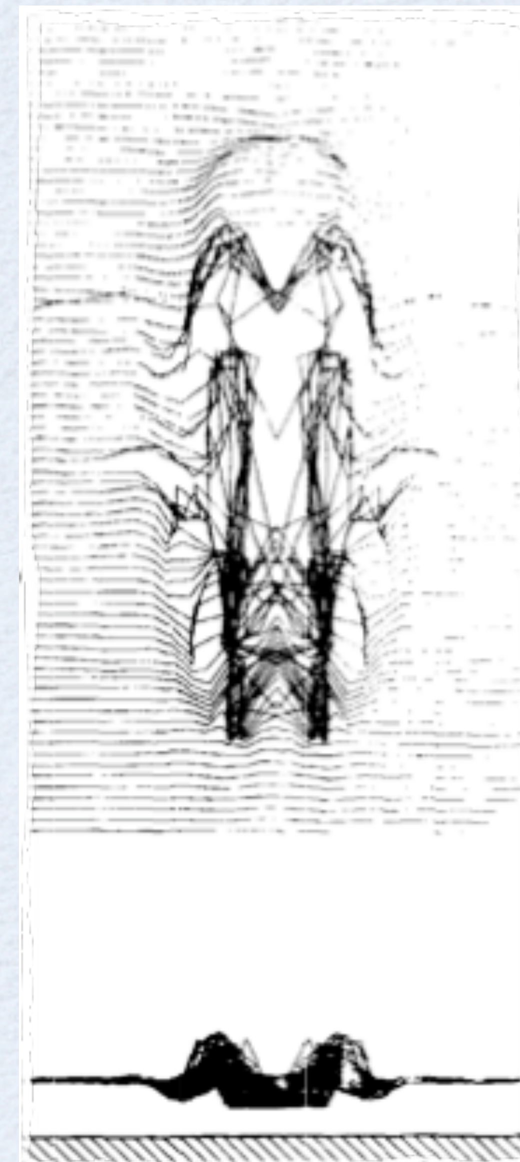
F.H. Harlow and E.J. Welch



***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

CFD genesis : Vortex Particle Methods

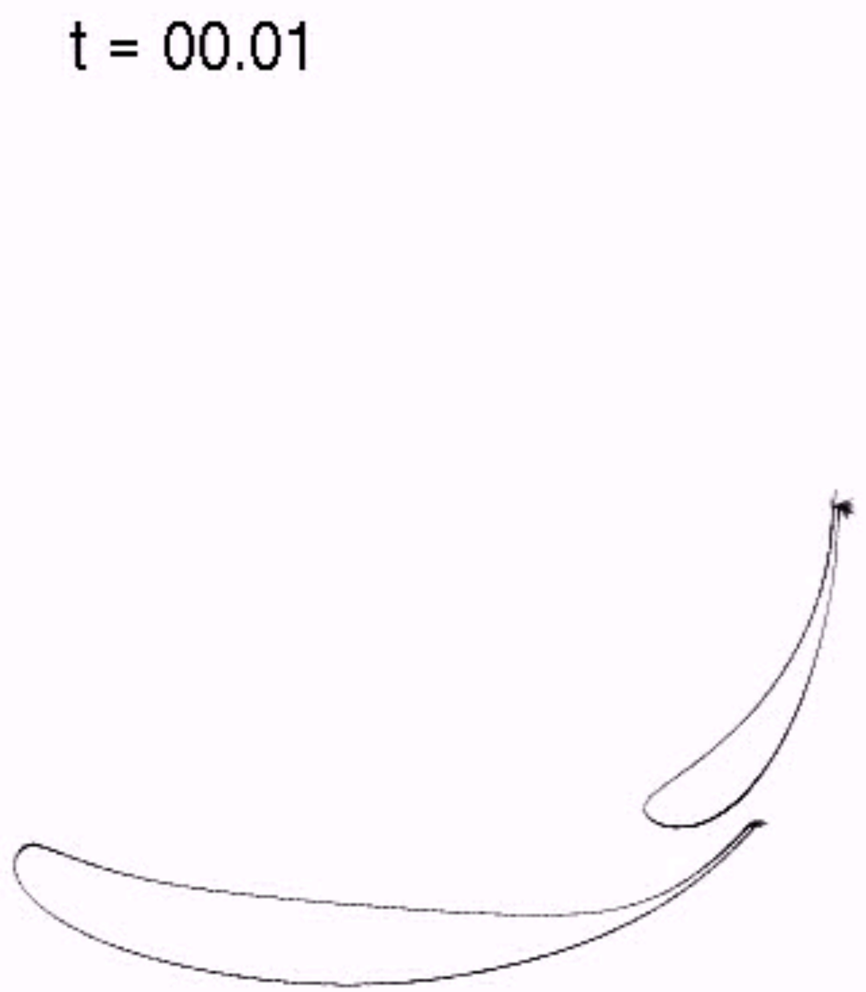
$$\nabla \times \left(\frac{\partial u}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} \right)$$

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

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

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

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



3D - Boundaries

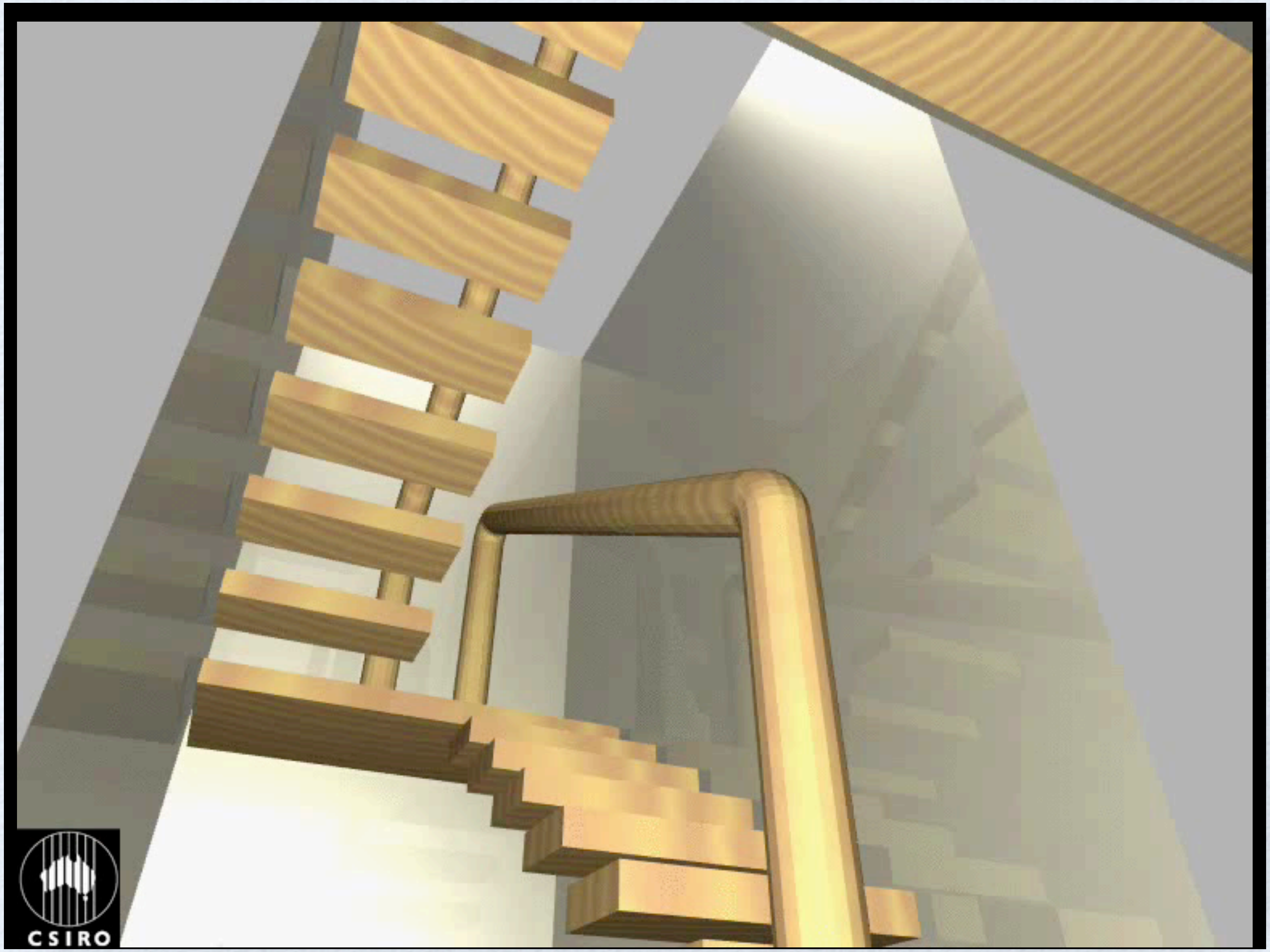
Cost

No theory of convergence

....

What PAUSED Vortex Methods ?

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



Growth of Black Holes
Springel, MPI -
Hernquist, Harvard

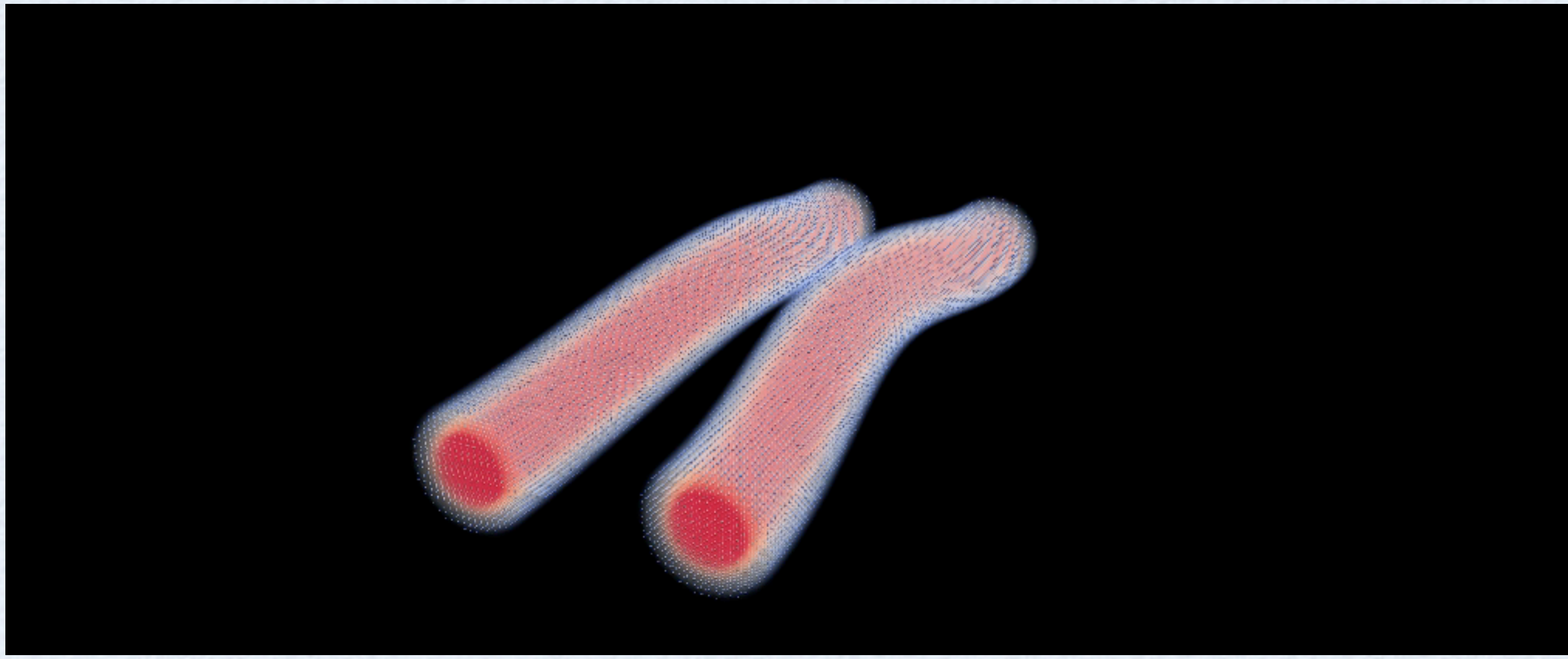
GRID FREE + LAGRANGIAN / ADAPTIVE + NO POISSON EQUATION

PARTICLES : Lagrangian Form of Conservation Laws

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

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

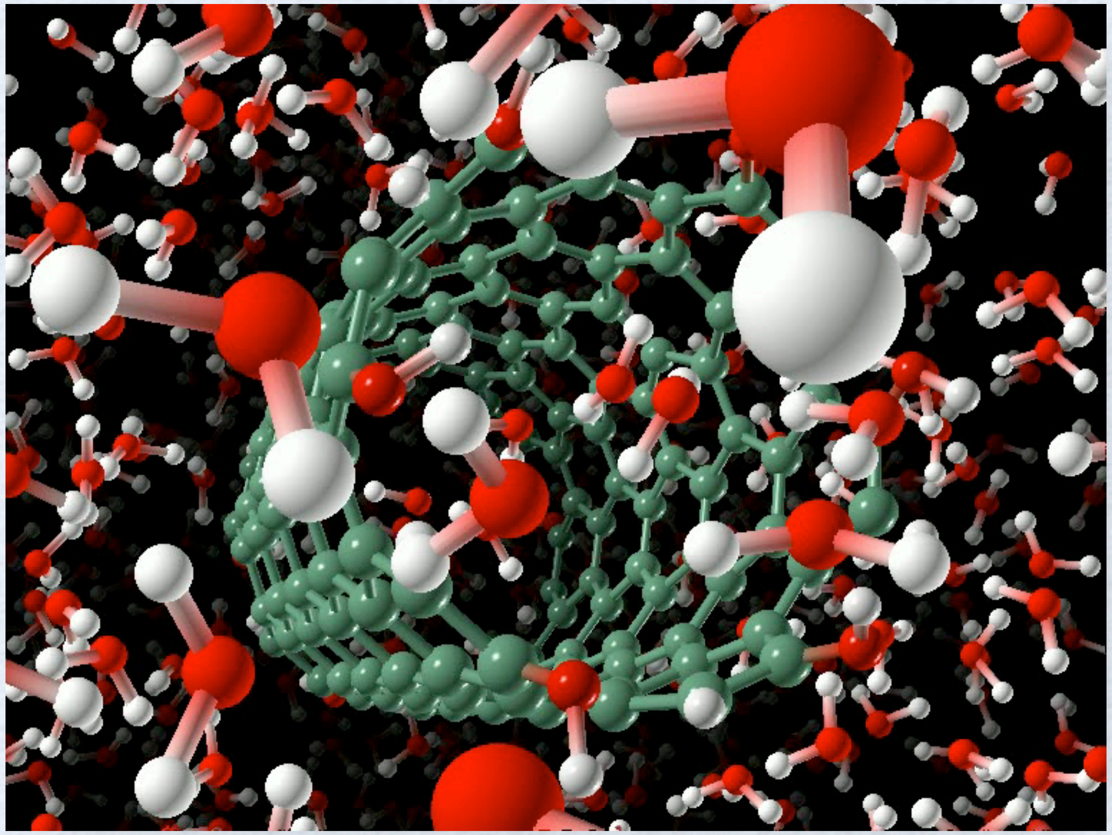
SPH, Vortex Methods



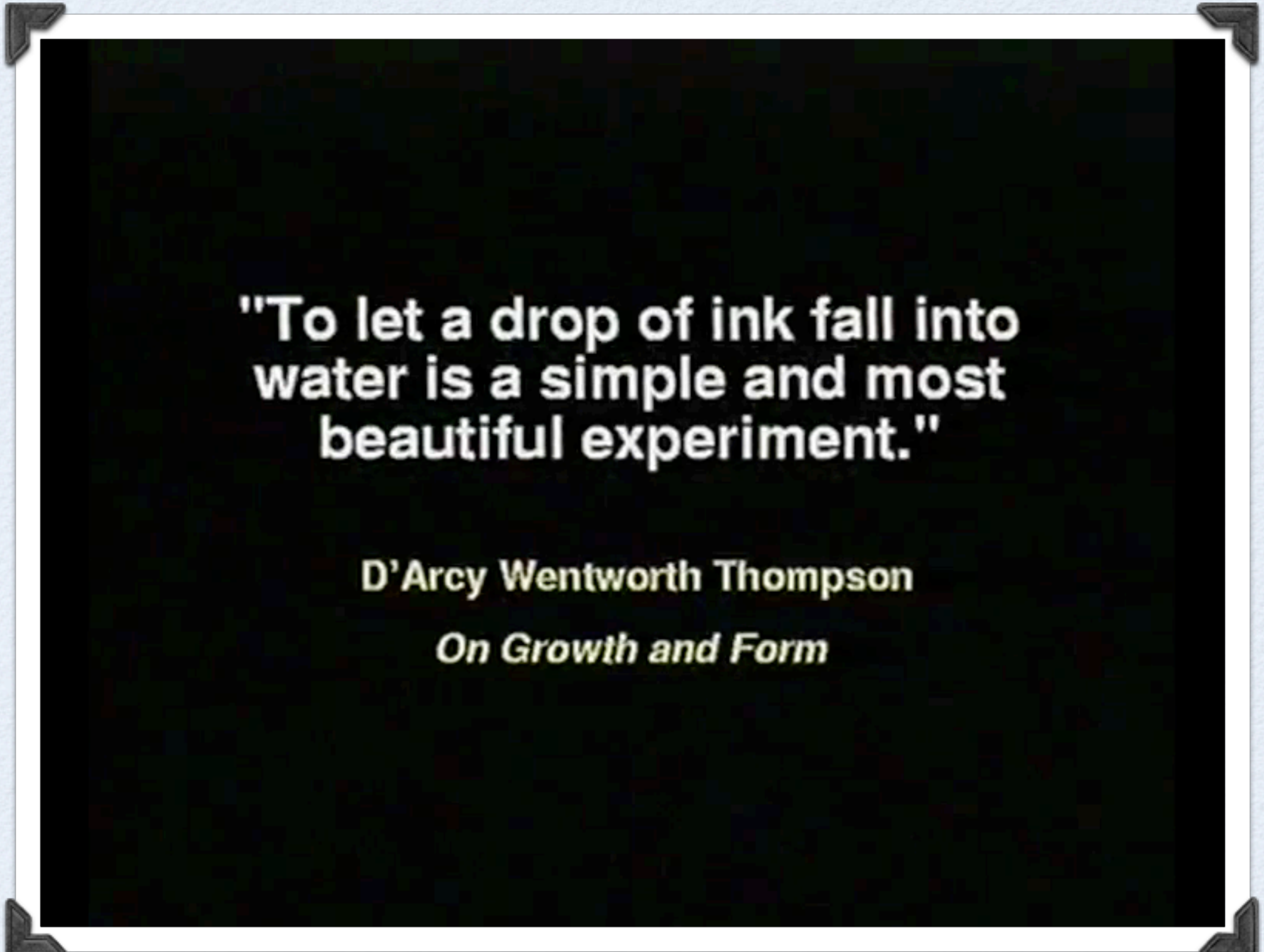
$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u}_p$$

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

Molecular Dynamics, DPD



Particle Approximations + Particle Models



J. H. Walther, P. Koumoutsakos, Three-dimensional vortex methods for **particle-laden flows with two-way coupling**, J. Comput. Phys., 2001

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

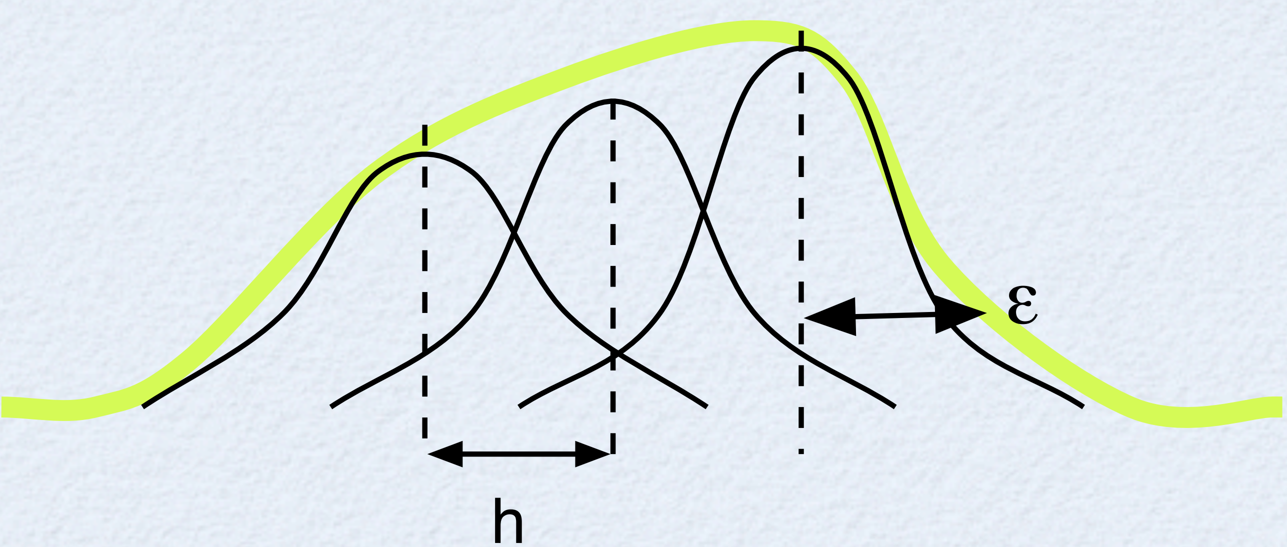
FUNCTIONS and PARTICLES

Integral Function Representation

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

Function Mollification

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



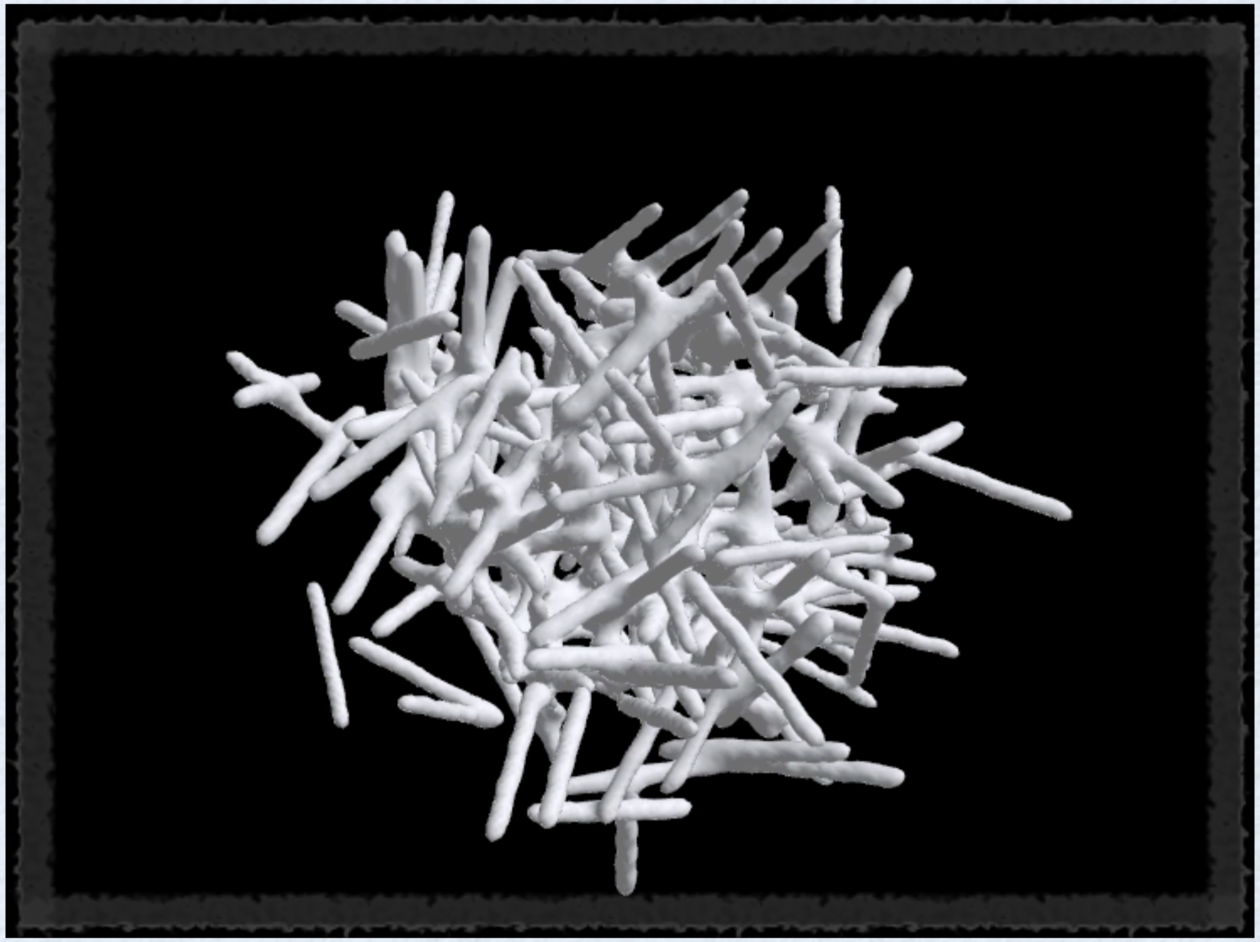
Particles are "mesh" free

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

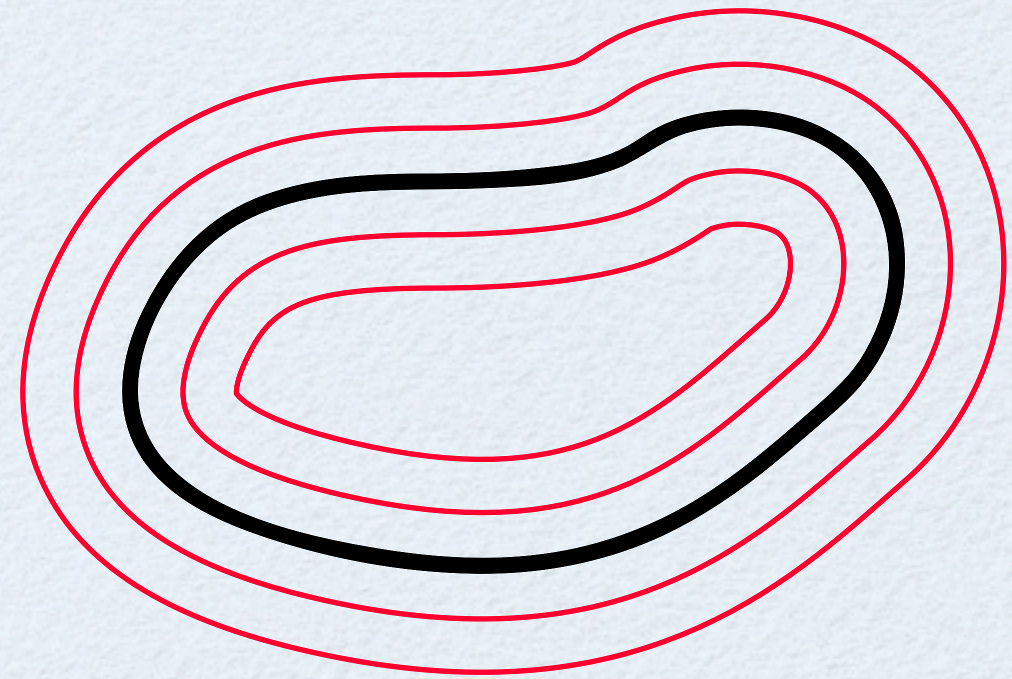
$$\Phi^h_\epsilon(x,t) \;=\; \sum_{p=1}^{N_p} h_p^d\,\Phi_p(t)\,\zeta_\epsilon(x-x_p(t))$$



SURFACES AS LEVEL SETS

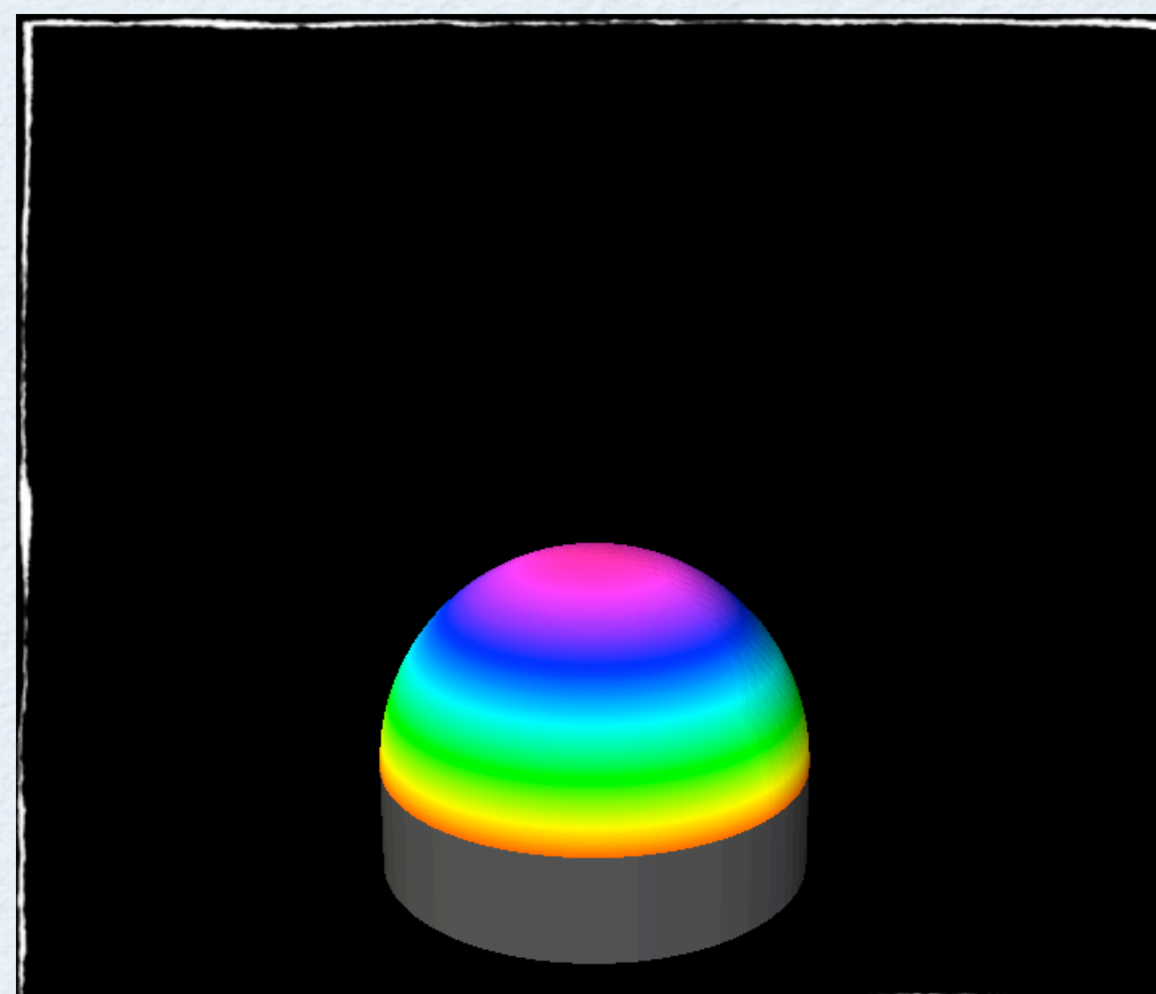
$$\Gamma(t) = \{\mathbf{x} \in \Omega \mid \phi(\mathbf{x}, t) = 0\}$$

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



EVOLVING THE LEVEL SETS

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



PARTICLE APPROXIMATION

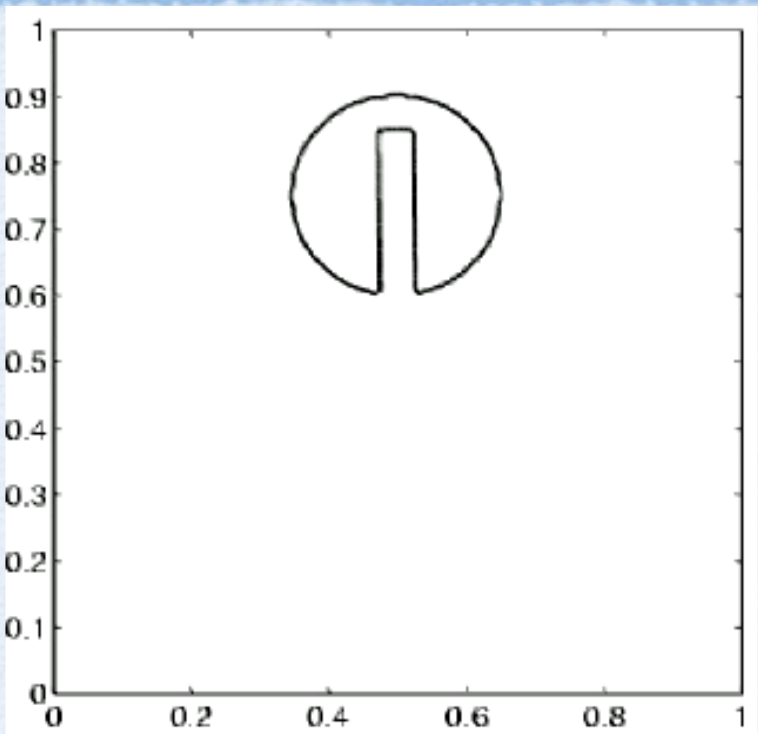
$$\Phi^h_\epsilon(x,t) = \sum_{p=1}^{N_p} h_p^d \, \Phi_p(t) \, \zeta_\epsilon(x - x_p(t))$$

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

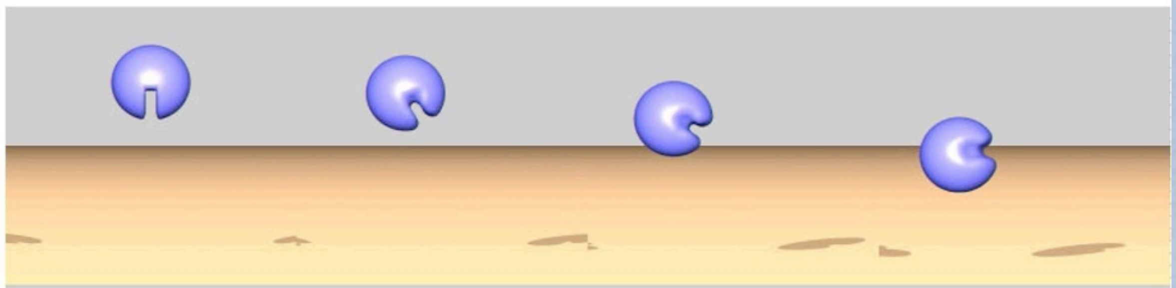
Lagrangian vs Eulerian Descriptions



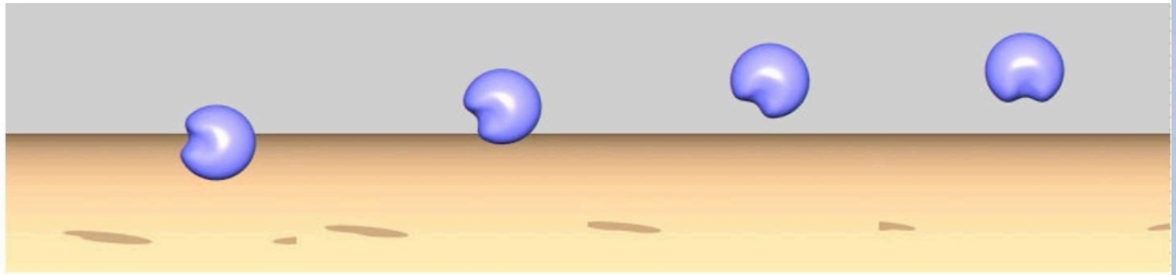
- **PARTICLE LEVEL SETS** exact for rigid body motion

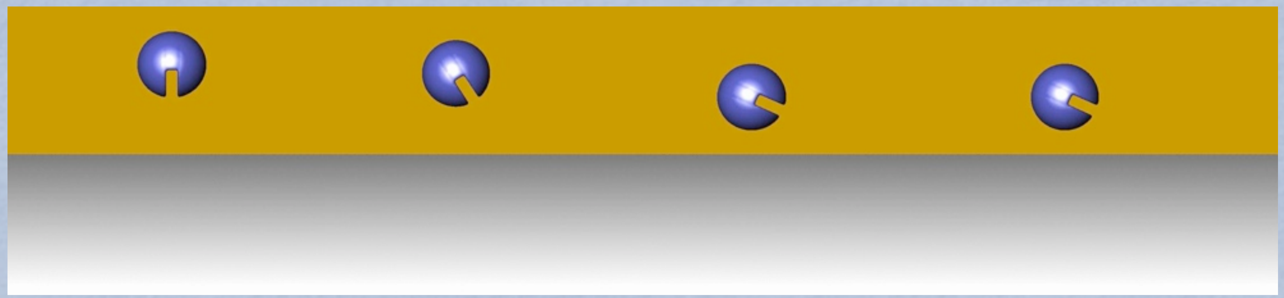
$$\Phi(\mathbf{x}, t) = \Phi_0(\mathbf{x} - \mathbf{u}t)$$

Lagrangian Particle methods
good for **linear** advection

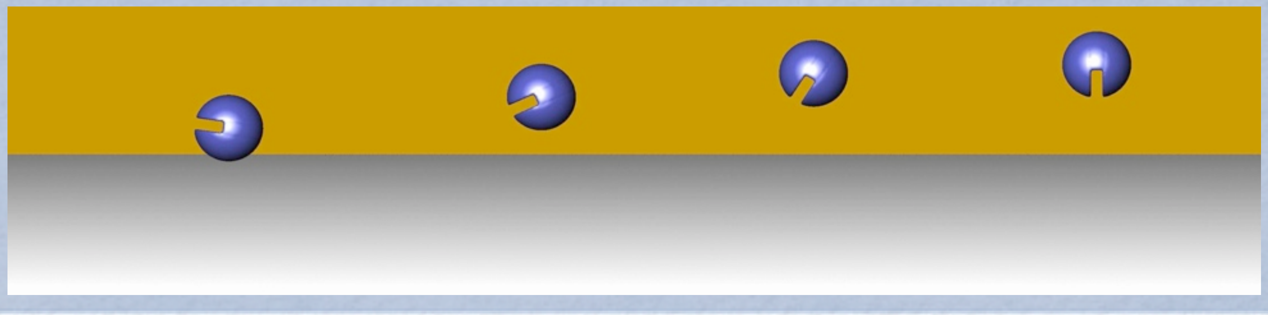


Hubrid Particle-Grid Level Sets
(Enright and Fedkiw, 2002)



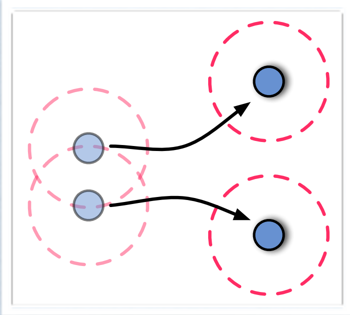


Lagrangian Particle Level Sets
(Hieber and Koumoutsakos, 2005)



LAGRANGIAN DISTORTION

- loss of overlap -> loss of convergence



Particles follow flow trajectories - Location distortion

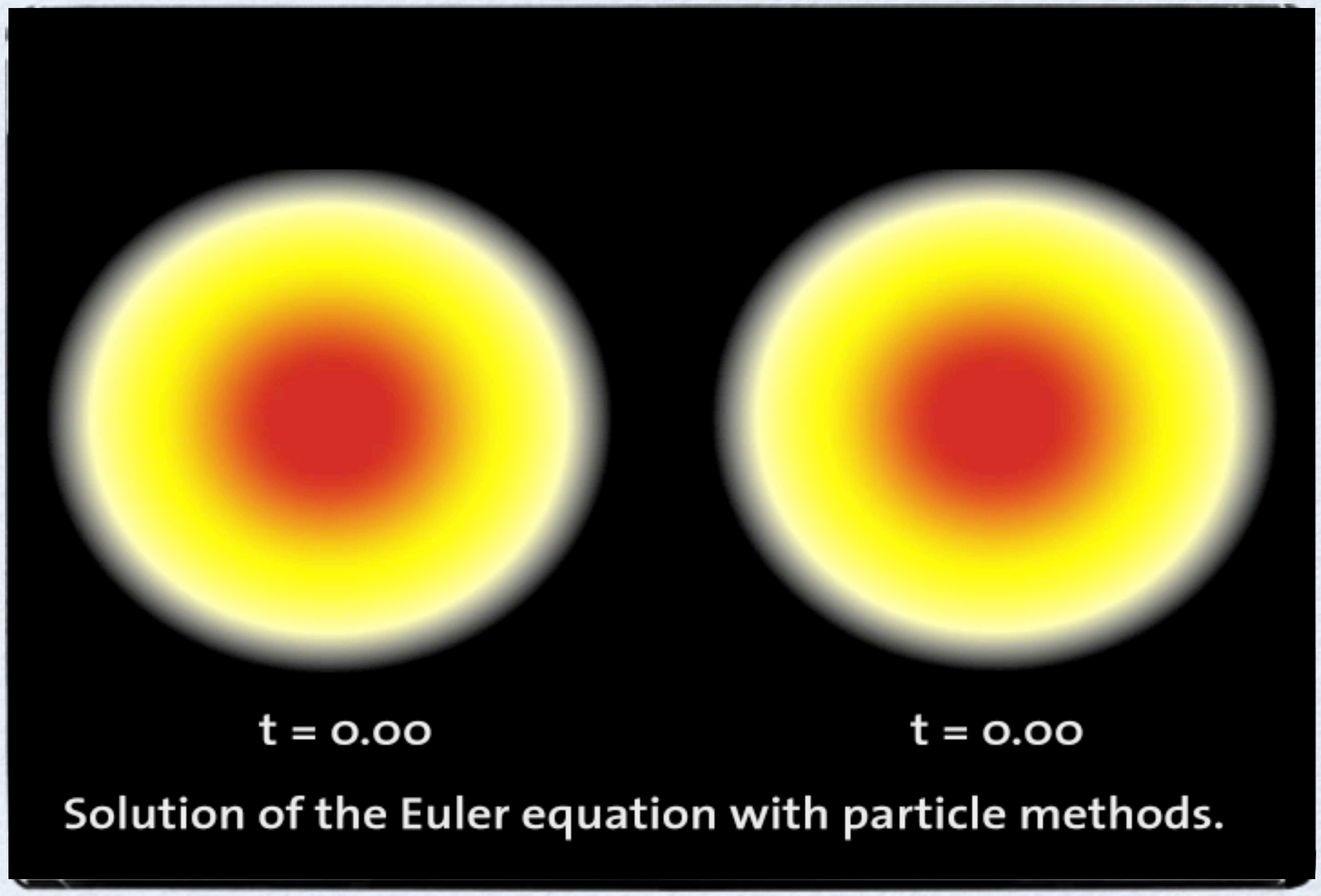
EXAMPLE :

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

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

Smooth Particle Quadrature

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

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

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 ?

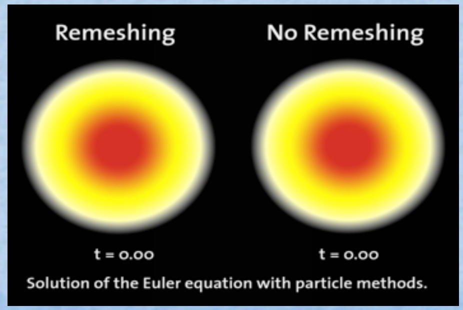
How to fix it ?

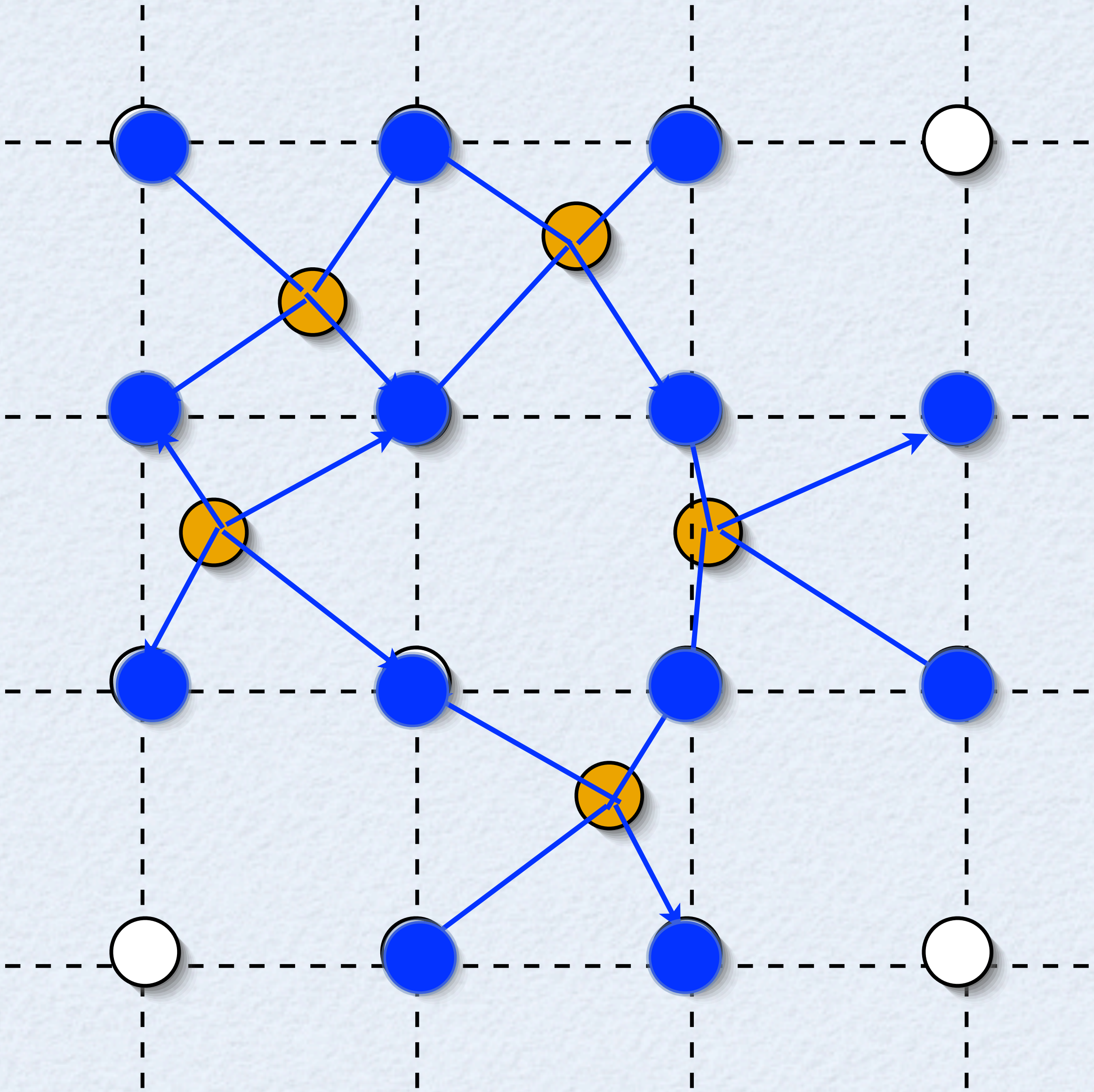
- Modify the smoothing kernels (SPH - Monaghan) — DOES NOT WORK
- Re-distribute particles with Voronoi Meshes (ALE - Russo) — EXPENSIVE - UNSTABLE
- Re-initialise particle strengths (WRKPM - Liu, Belytchko) — EXPENSIVE

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
- ....

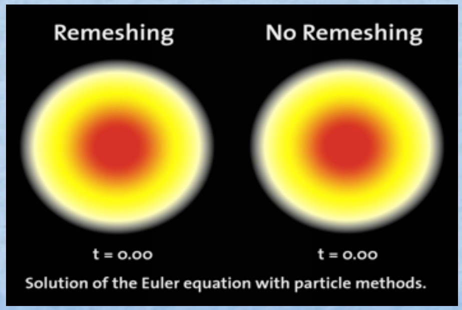
Particle Remeshing = Resampling





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

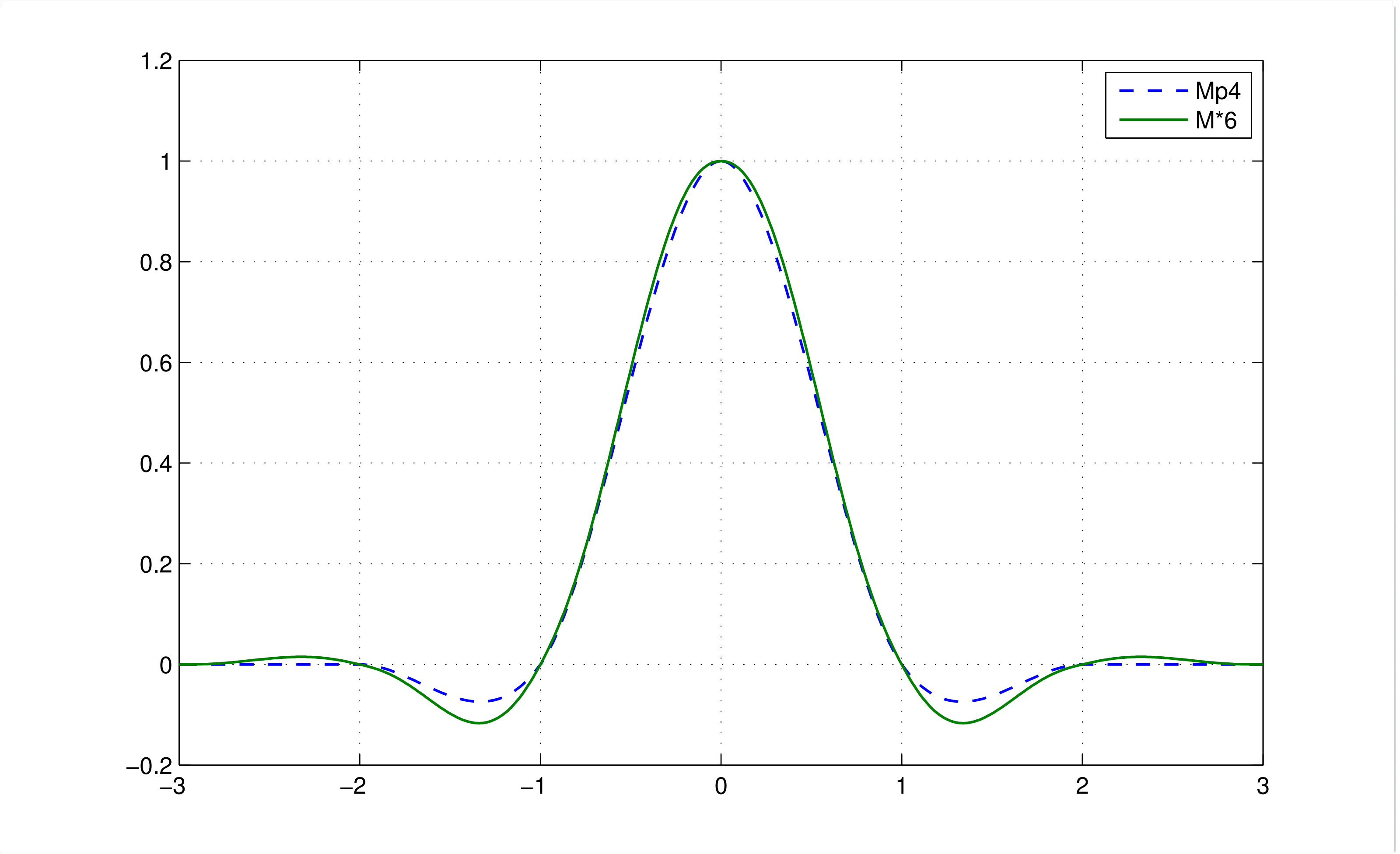
Particle Remeshing = Resampling



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

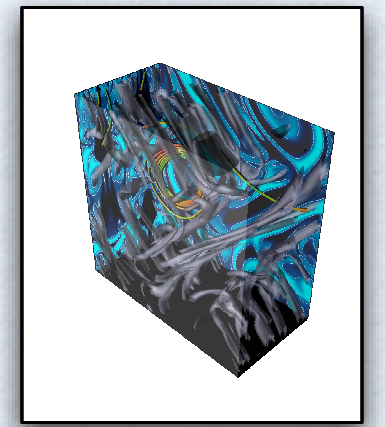
$$M_6^*(x) = \begin{cases} -\frac{1}{12}(|x|-1)(24\,|x|^4+38\,|x|^3-3\,|x|^2+12\,|x|+12) & |x|<1 \\ \frac{1}{24}(|x|-1)(|x|-2)(25\,|x|^3-114\,|x|^2+153\,|x|-48) & 1\le|x|<2 \\ -\frac{1}{24}(|x|-2)(|x|-3)^3(5\,|x|-8) & 2\le|x|<3 \\ 0 & 3\le|x| \end{cases}$$

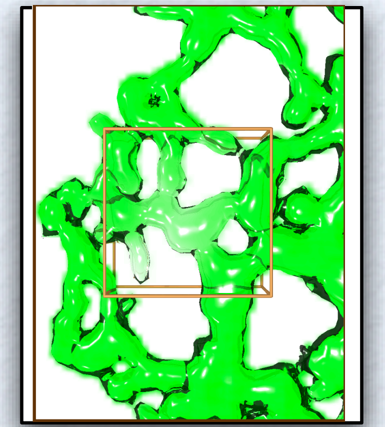
PPM : Parallel Particle Mesh library

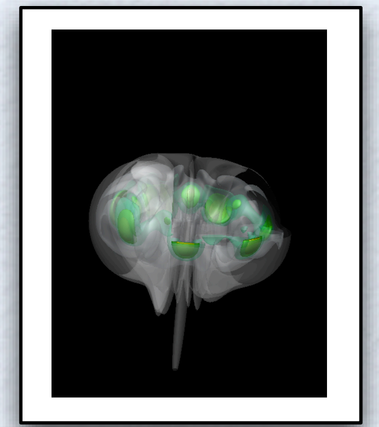
www.ppm-library.org

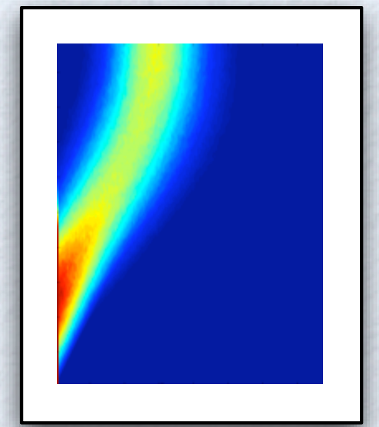
OPEN SOURCE www.cse-lab.ethz.ch/software.html

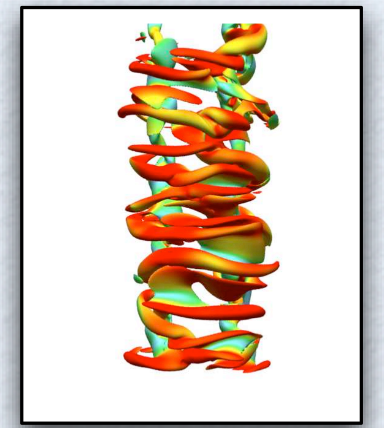
Library for MPI parallel Particle-Mesh simulations











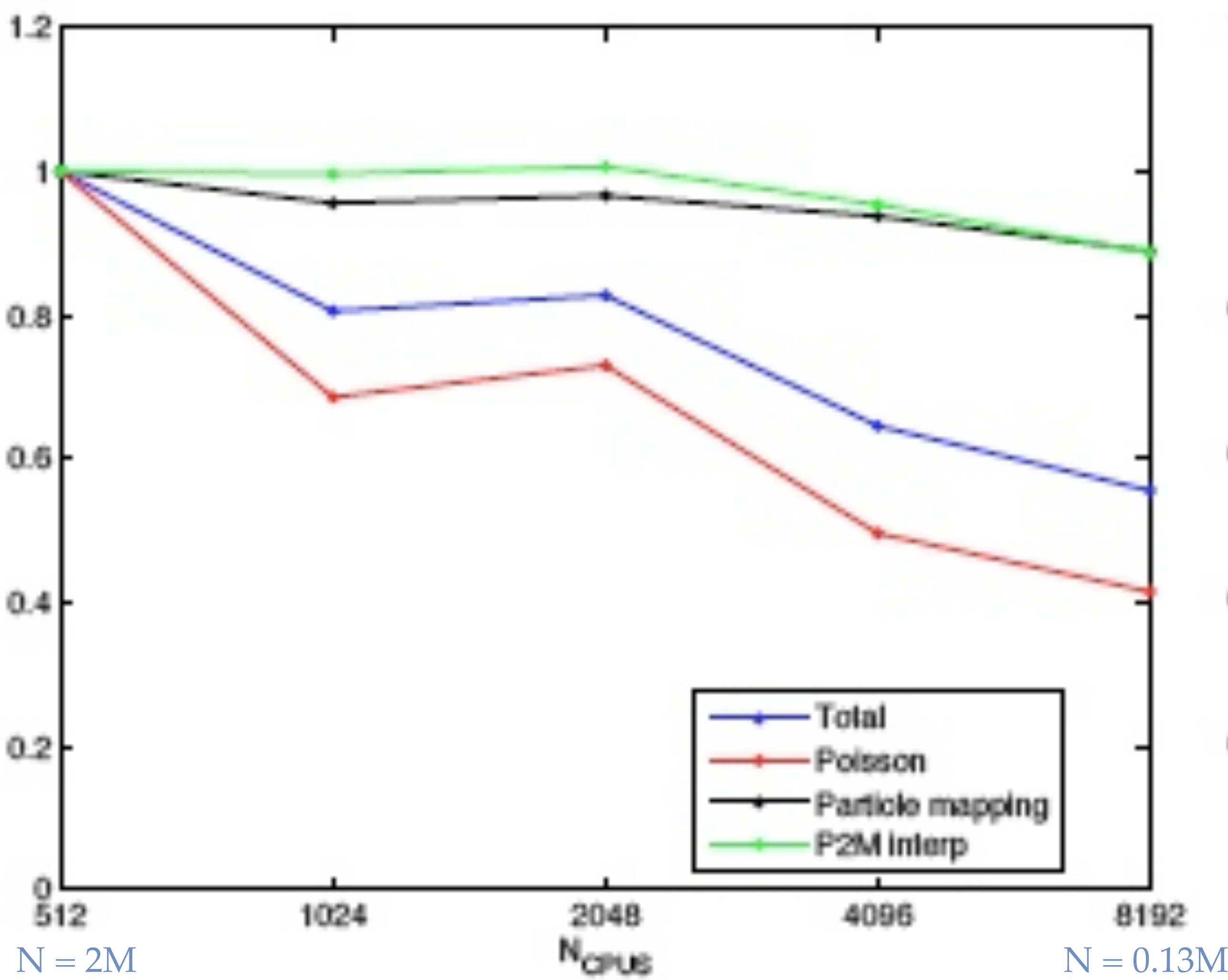
Parallel Particle Mesh Library (PPM)

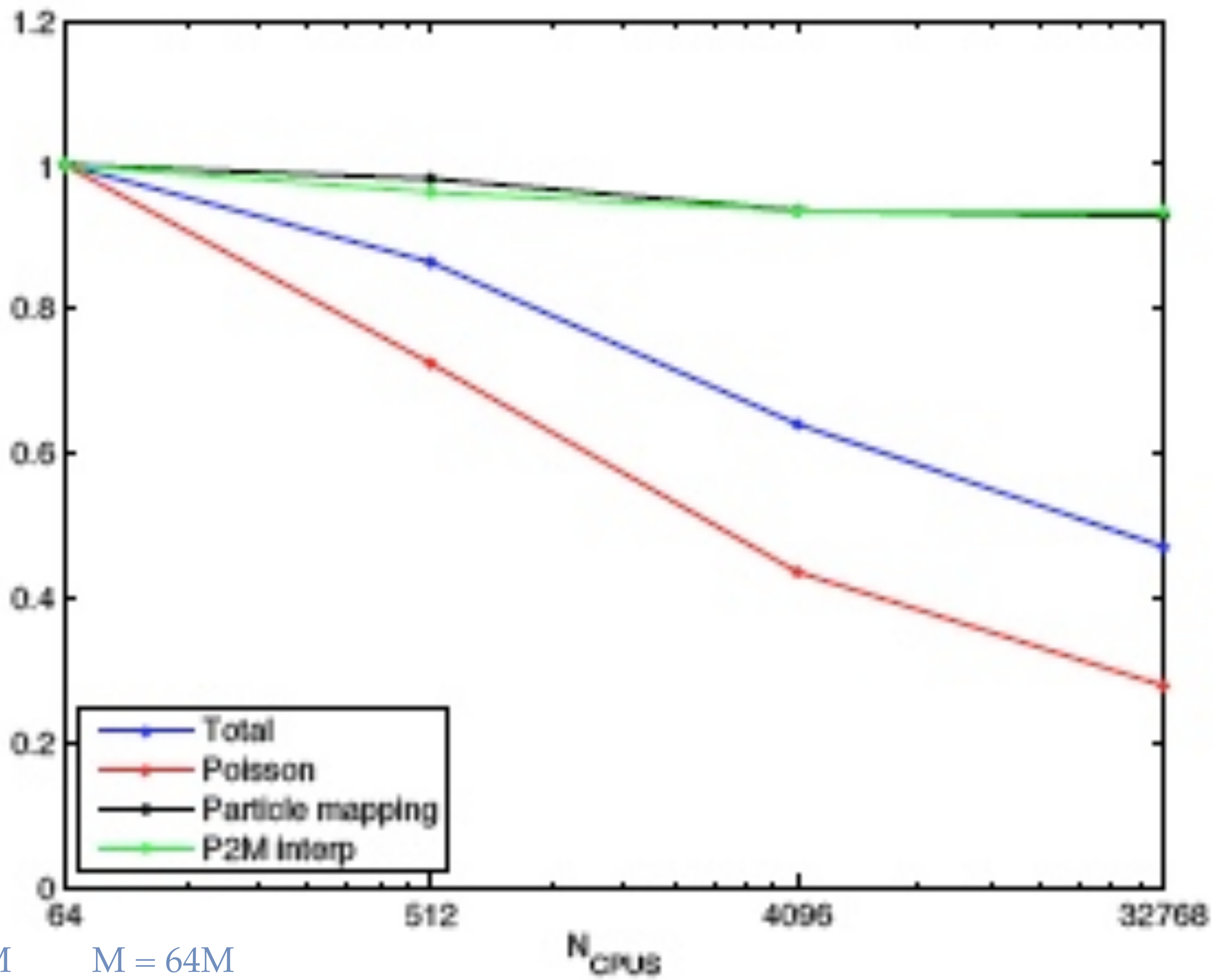
Message Passing Interface (MPI) | METIS | FFTW

vector | shared memory | distributed memory | single processor

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

Scalability – CRAY XT5





Strong

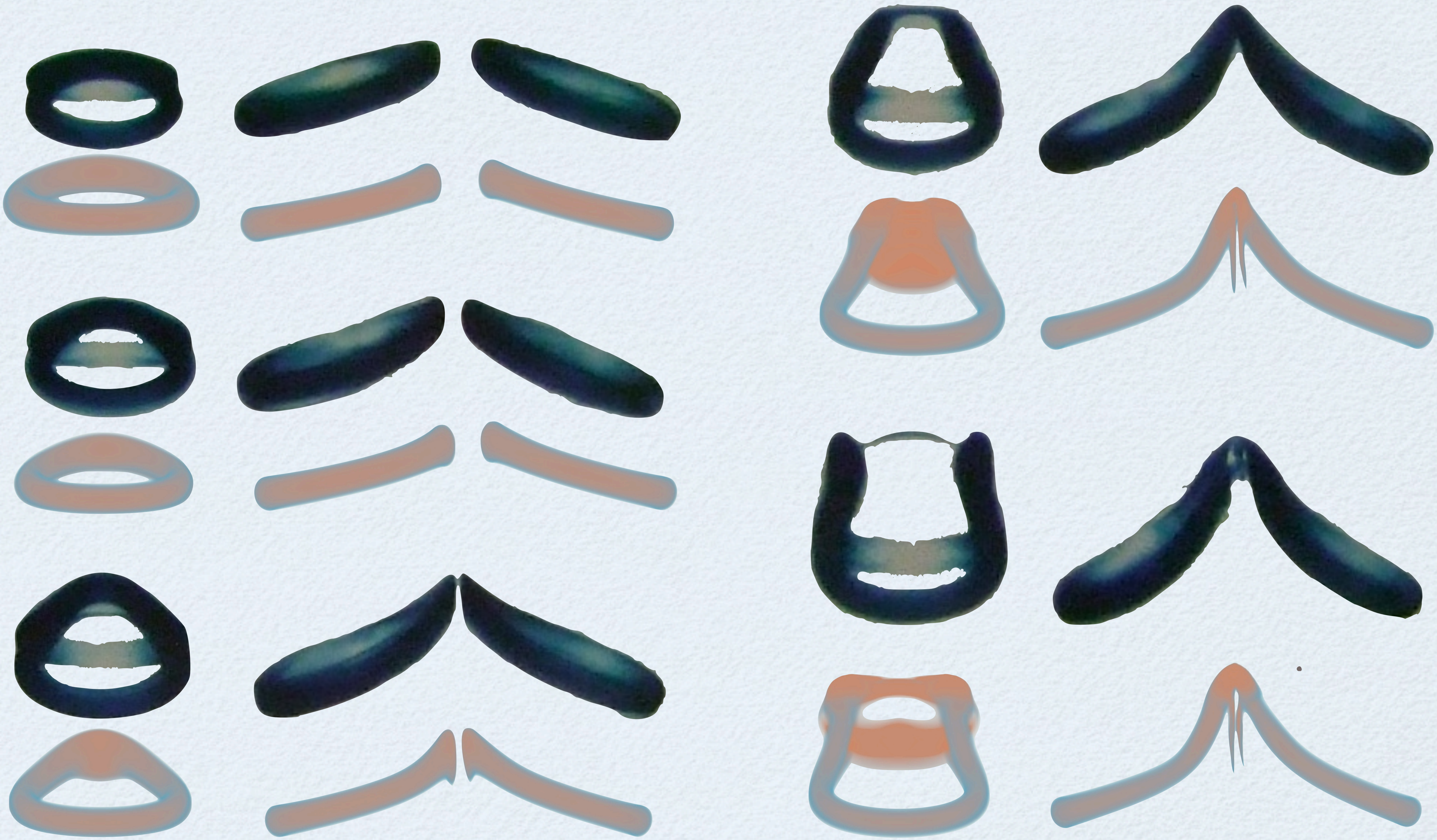
Size : 1280x1280x640

time : 512 / 90s - 8192 / 10s

Weak

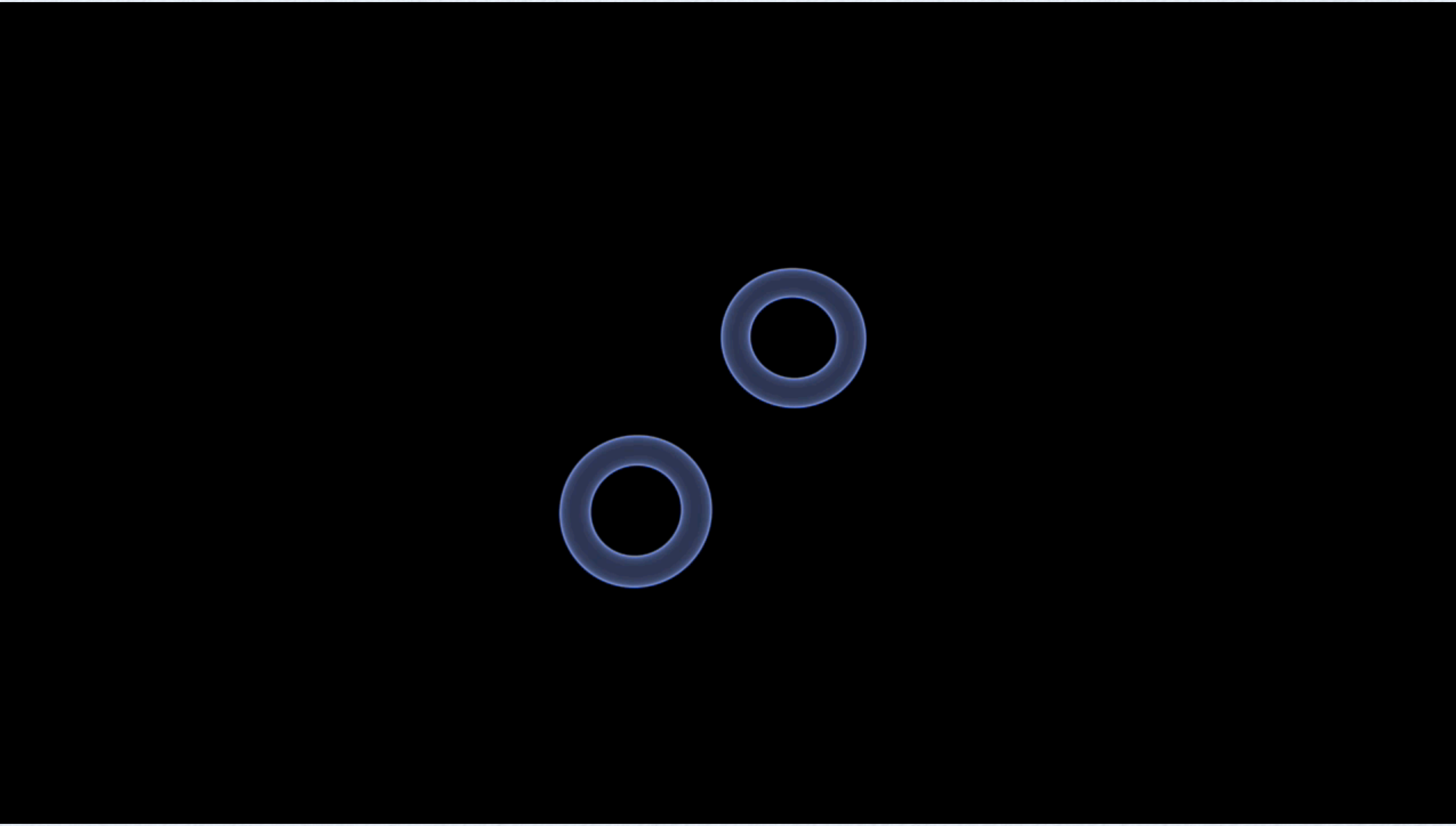
time : 64 / 40s - 32768 / 85s

VORTEX RING COLLISION, Re = 1800

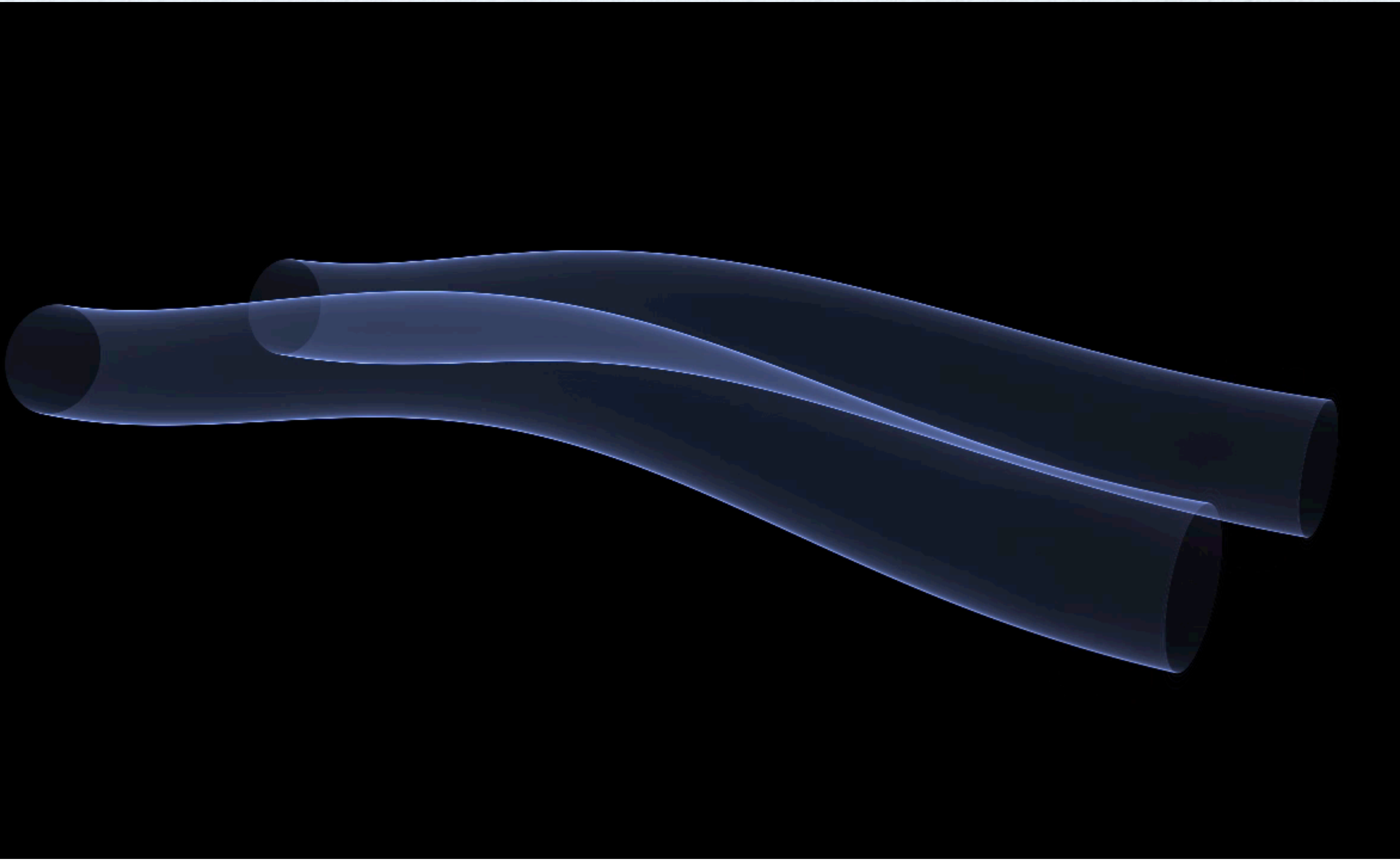


Experiments : P. Schatzle & D. Coles (1986)

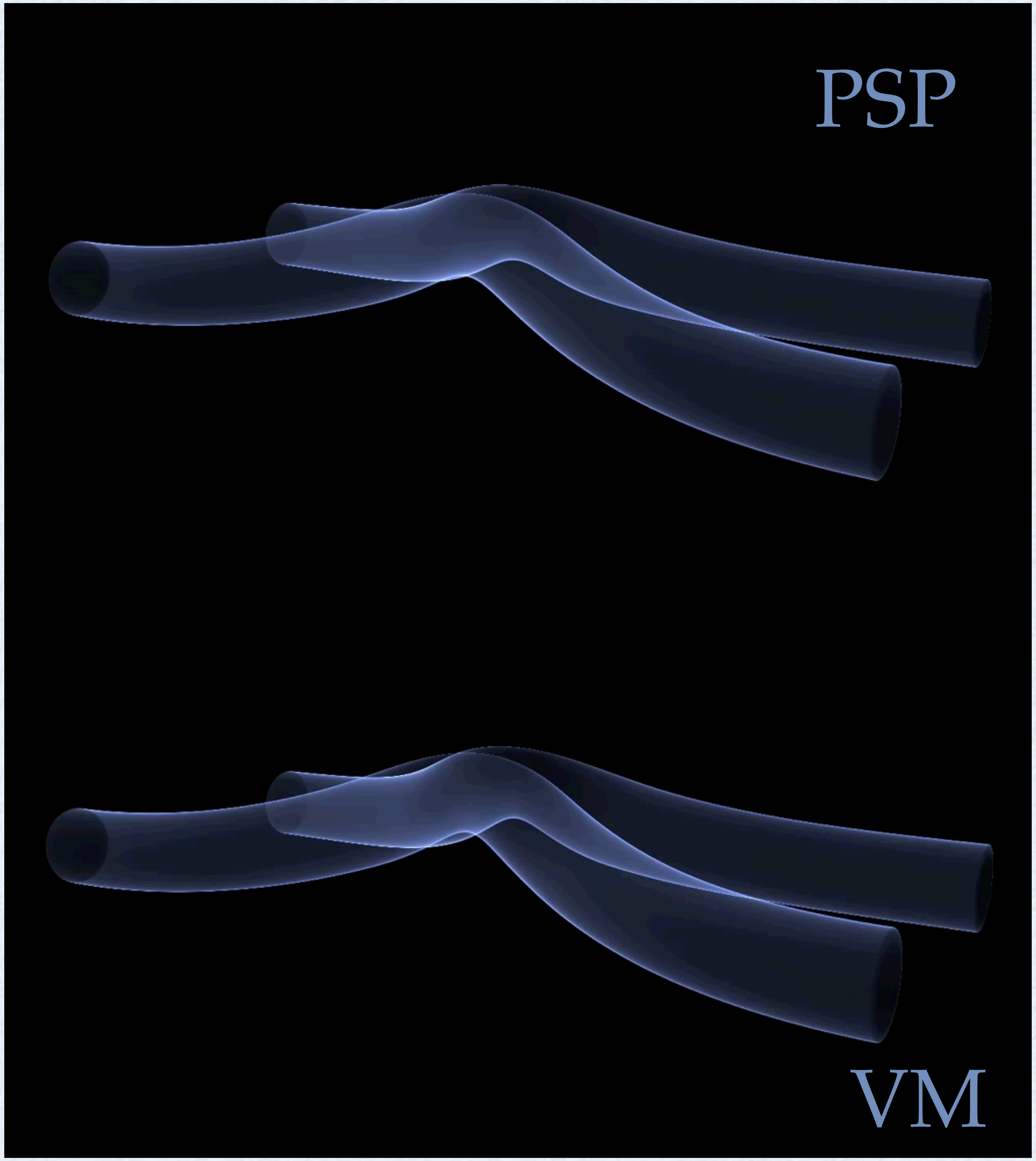
Vortex Ring Collision - Re = 10,000

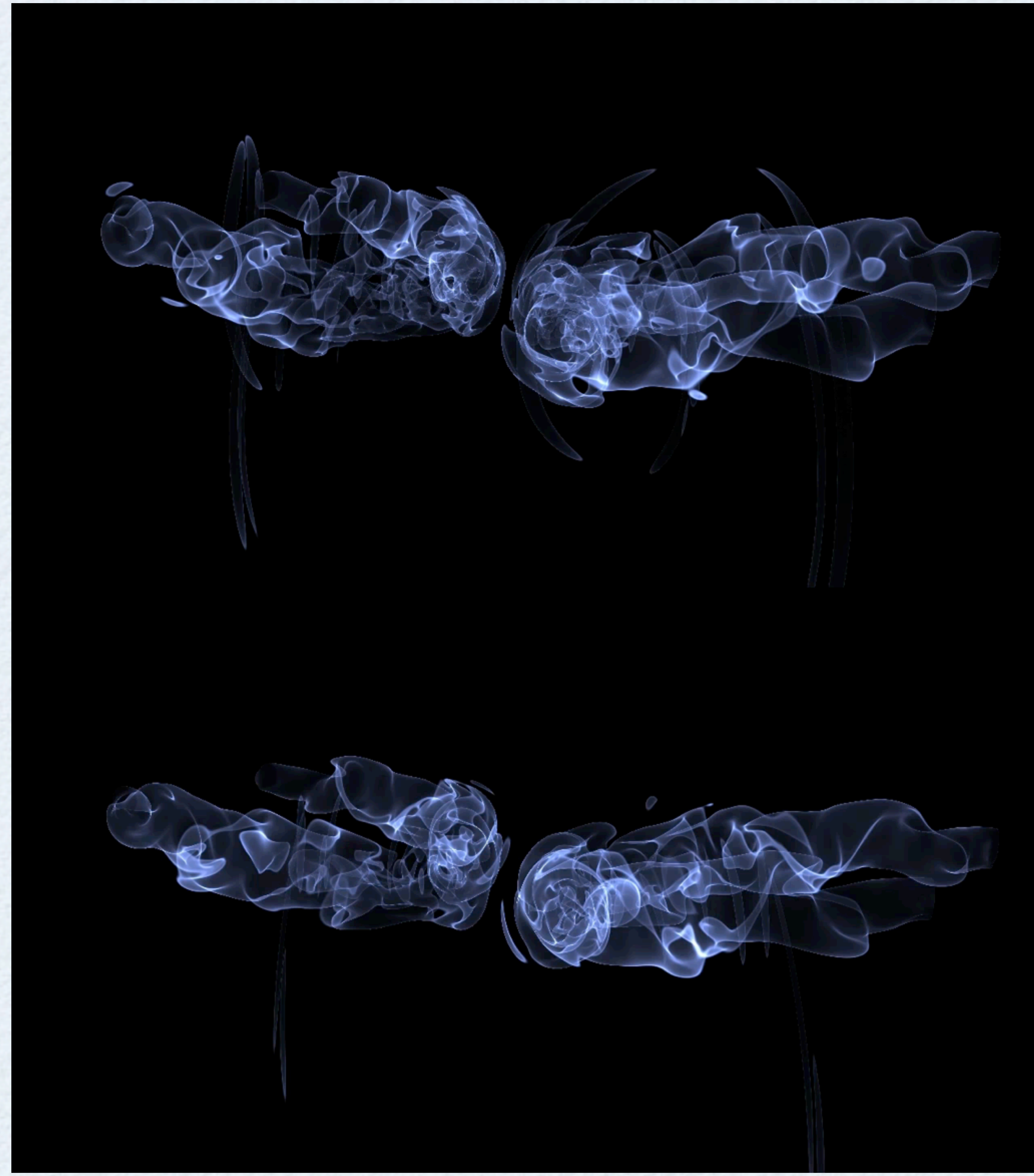


VORTEX DYNAMICS at High Re



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 ?

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

REMESHED PARTICLE METHODS

1. ADVECT : Particles ->Large CFL

2. REMESH : Particles to Mesh -> Gather/Scatter

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

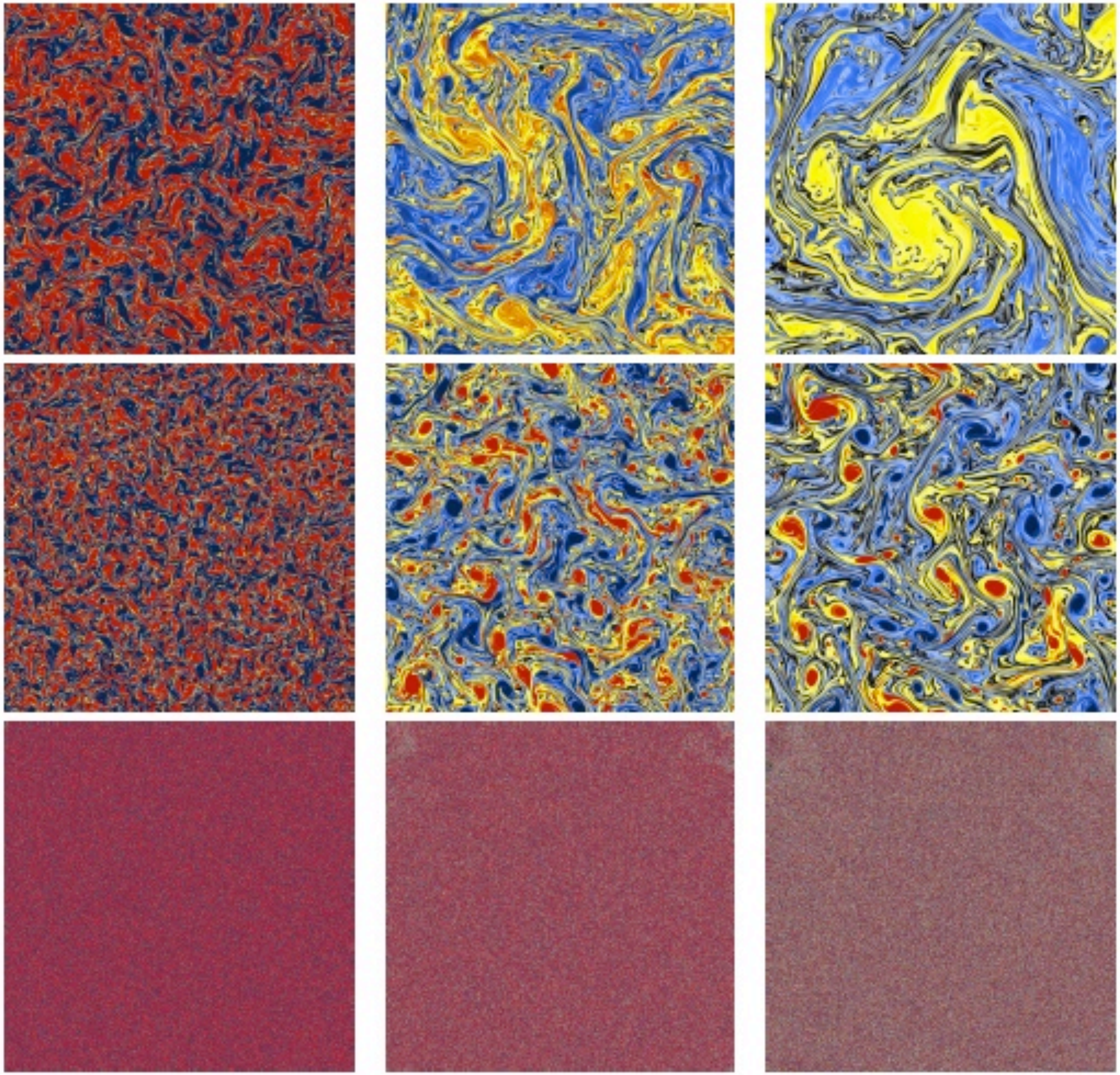
4: RESAMPLE: Mesh Nodes BECOME Particles

Are grid-free Particle Methods Accurate ?

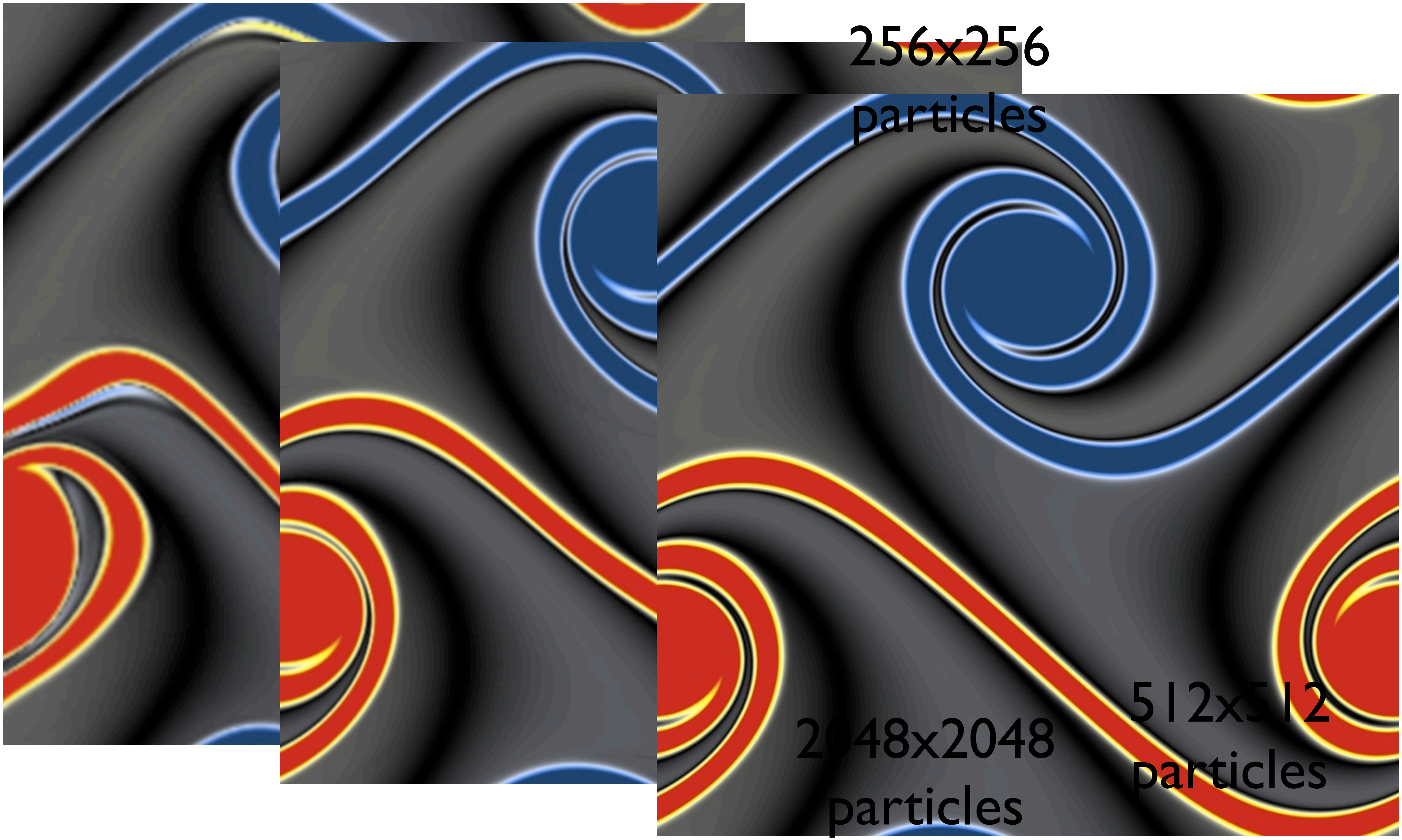
Remeshing Euler

Remeshing RK4

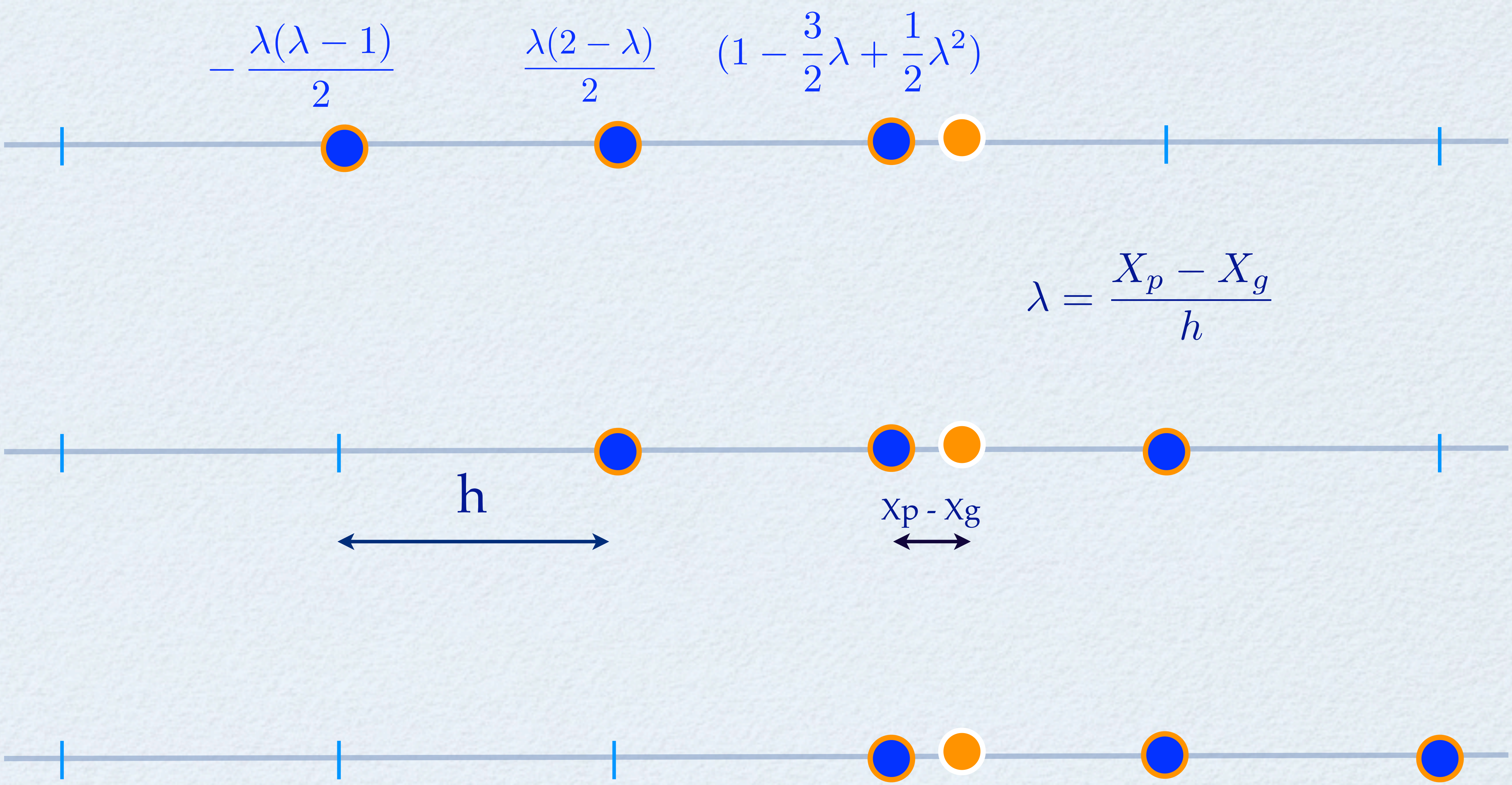
NO Remeshing



Double Shear-Layer (Minion and Brown, JCP, 1997)



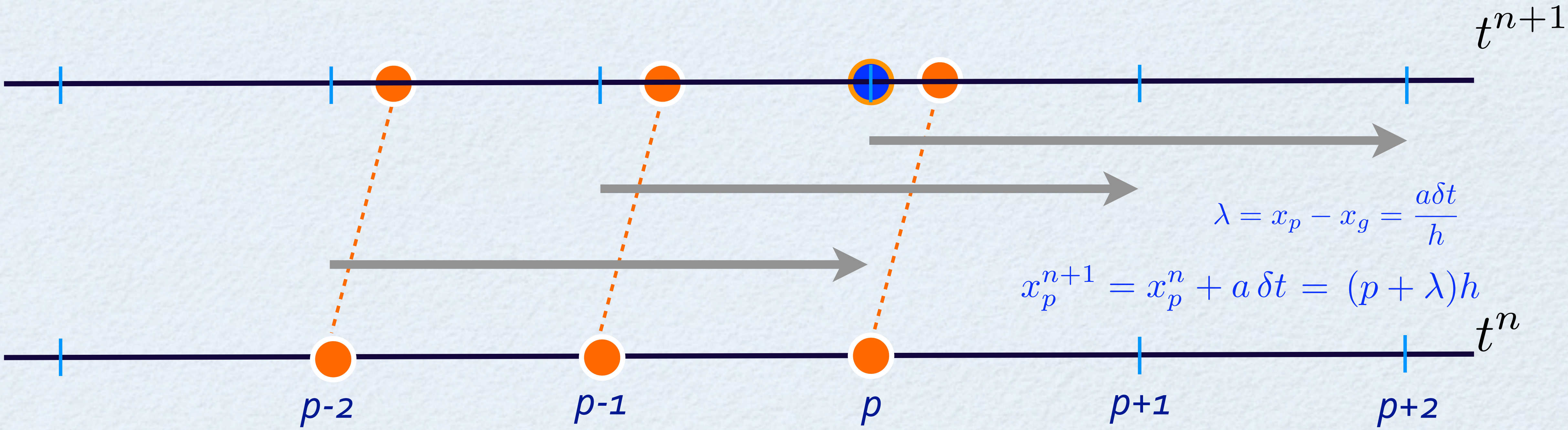
Size of Remeshing Stencil = # Conserved Moments



Bergdorf et. al., MMS,2005

Cottet et.al., CRAS, 2008

$$u_p^{n+1} = -\frac{\lambda(\lambda-1)}{2}u_{p-2}^n + \frac{\lambda(2-\lambda)}{2}u_{p-1}^n + (1-\frac{3}{2}\lambda+\frac{1}{2}\lambda^2)u_p^n$$



$$\lambda = x_p - x_g = \frac{a\delta t}{h}$$

$$x_p^{n+1} = x_p^n + a\,\delta t = (p+\lambda)h$$

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$u_p = u(x_p)h$ →

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

+ REMESH

$$u_p^{n+1} = u_p^n - \frac{\lambda}{2}(3u_p^n - 4u_{p-1}^n + 4u_{p-2}^n) + \frac{\lambda^2}{2}(u_p^n - 2u_{p-1}^n + u_{p-2}^n)$$

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

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

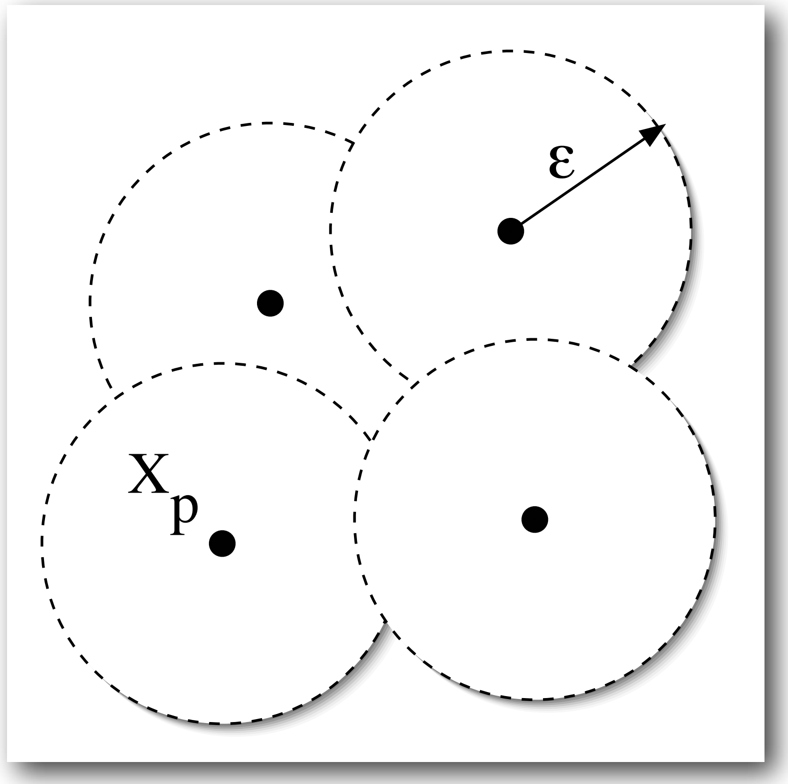
PARTICLE METHODS (flavors)

So far, fields required to advance particles and update their strength (velocity, pressure, diffusion ..) supposed available.

Recovering these fields from the particle strengths is the main challenge in particle methods.

Two possible approaches:

- ONLY Particles - grid-free methods
- rely on an underlying Eulerian grid - particle-grid methods



OPERATION COUNT

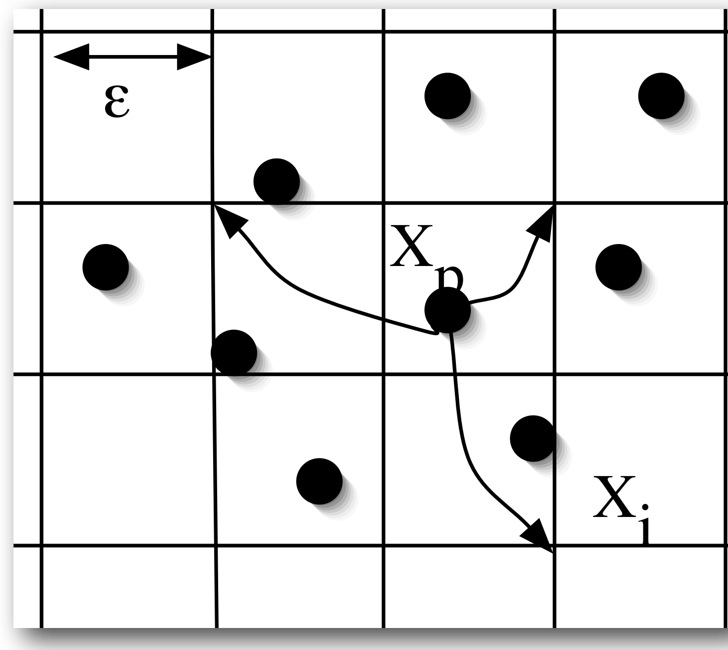
- O(N) for *local* operations (multiplication, differentation ..)
- complexity increases if non-local quantities need to be recovered

(typically : velocity fields from vorticity-carrying particles)

HYBRID Particle-Grid Methods

Hybrid particle-grid methods : values are assigned to grid points by interpolation

$$u_i = \frac{1}{\epsilon^d} \sum_p \phi_i(\mathbf{x}_p)$$



Set up, initial conditions, *etc.* , $t = 0$;

```
/* Particle quantities stored in arrays,
   e.g. vorticity:  ω ∈ R^{∋×N}.  For the ODE solver we
   need two temporary variables:  u0, and dω0          */
```

while $t \leq T$ **do**

  for $l = 1$ *to* 3 *;* `/* stages of the ODE Solver */`

  do

    Interpolate ω onto the grid ($\omega \to \omega_{ijk}$);

    Compute velocity u_{ijk} from ω_{ijk};

    $u0 \leftarrow$ Interpolate u_{ijk} onto the particles;

    $u0 \leftarrow u + \alpha_l\, u0;\ d\omega 0 \leftarrow d\omega + \alpha_l\, d\omega 0$; `/*` $\alpha = (0, -\frac{5}{9}, \frac{153}{128})$ `*/`

    $x \leftarrow x + \delta t\, \beta_l\, u0;\ \omega \leftarrow \omega + \delta t\, \beta_l\, d\omega 0$;

  end

end

Complexity of grid-free vs hybrid methods differ mostly when *non-local* quantities must be recovered.

Typically: compute velocity field from vorticity-carrying particles

Problem to be solved : div $\mathbf{u} = \mathbf{0}$, $\nabla \times \mathbf{u} = \omega = \sum \alpha_{\mathbf{p}}\, \delta(\mathbf{x}-\mathbf{x_p})$ and prescribed behavior at infinity

Grid-free methods rely on Bio-Savart integral representation:

$$u(x,t) = \int \mathbf{K}(x-y) \times \omega(y)\, dy$$

with $\mathbf{K} = (1/4\pi)\, (\mathbf{x}/|\mathbf{x}|^3)$

Remove singularity of K by replacing particle by blobs to obtain : $u(\mathbf{x_p}) = \sum \alpha_{\mathbf{p}}\, K_\varepsilon(\mathbf{x_p}-\mathbf{x_q})$

Fast Summation Algorithms

O(N^2) complexity can be reduced to O(NLogN) with Fast Summation Algorithms:
The key idea is to replace kernel by algebraic expansions:

THEOREM 2.1. (Multipole expansion). *Suppose that m charges of strengths $\{q_i, i = 1, ..., m\}$ are located at points $\{z_i, i = 1, ..., m\}$, with $|z_i| < r$. Then for any $z \in \mathbb{C}$ with $|z| > r$, the potential $\phi(z)$ is given by*

$$\phi(z) = Q \log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k}, \tag{2.2}$$

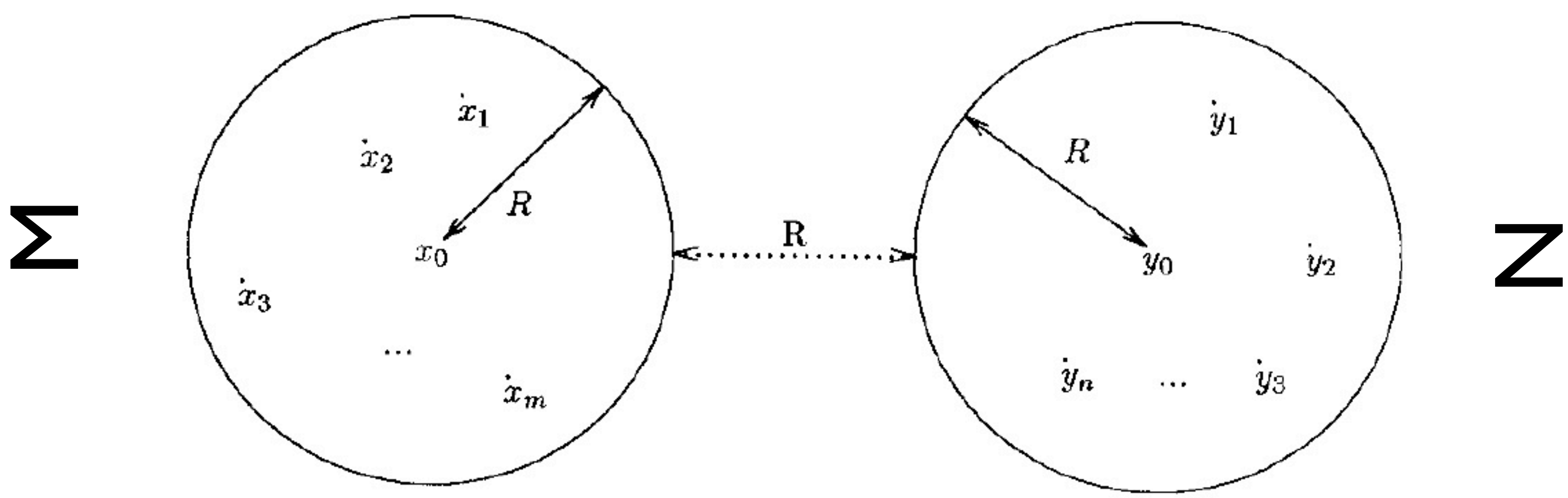
where

$$Q = \sum_{i=1}^{m} q_i, \quad a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k}. \tag{2.3}$$

(from Greengard-Rocklin 1982, for logarithmic kernel)

Fast Summation Algorithms

Gain over direct summation can be explained on simple example



Field of M particles on N particles:

- direct summation: O(MN) operations
- Fast summation with p terms: O(Mp+Np)
    - O(Mp) calculations to compute expansion coefficients from sources
    - 0(Np) calculations to evaluate expansions on receivers

Tree Codes and Fast Multipole Methods

Divide recursively into boxes containing about the same number of particles

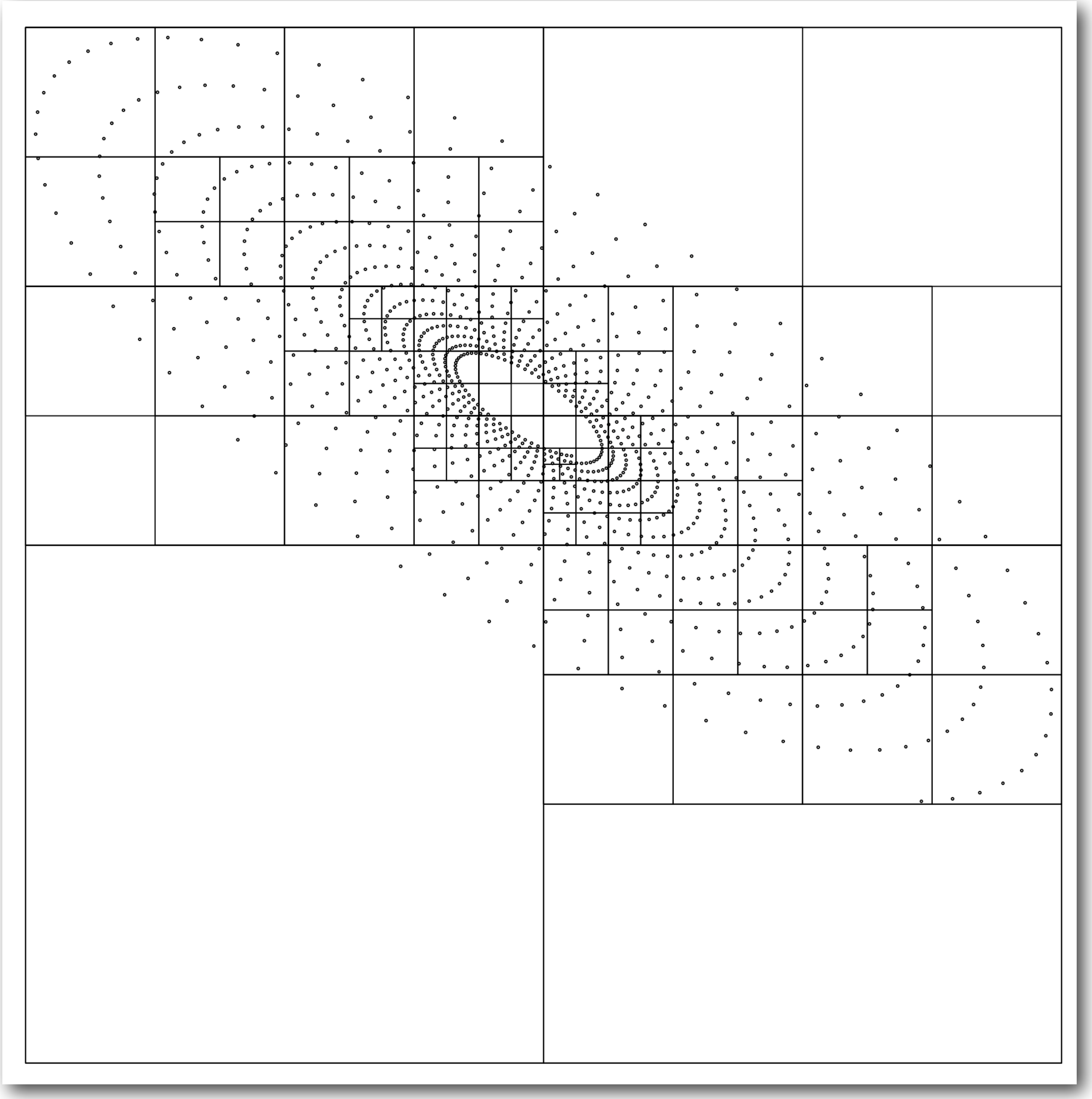
Upward pass:

form mulipole expansions, from finer to coarser level (using shifts of previously computed expansions)

Downward pass:

accumulate contributions of well-separated boxes, from coarser to finer level

At finest level, complete with direct summation of nearby particles



Hybrid - Particle Methods

Hybrid particle-grid for field calculations (also called Particle-In-Cell/Vortex-In-Cell method):

- Project particle strength on grid points
- Use a Poisson solver on that grid
- Differentiate on the grid to get grid field values
- Interpolate back fields on particles

Typically, a formula that conserves 4 first moments of particle distributions is used
-> 4x4x4= O(64N) algorithm
splitting formula reduces to O(12N)

Hybrid vs. Grid-free

DRAWBACKS

•against Lagrangian features of particles (and possible loss of information in grid-particle interpolations)

•require far-field artificial boundary conditions

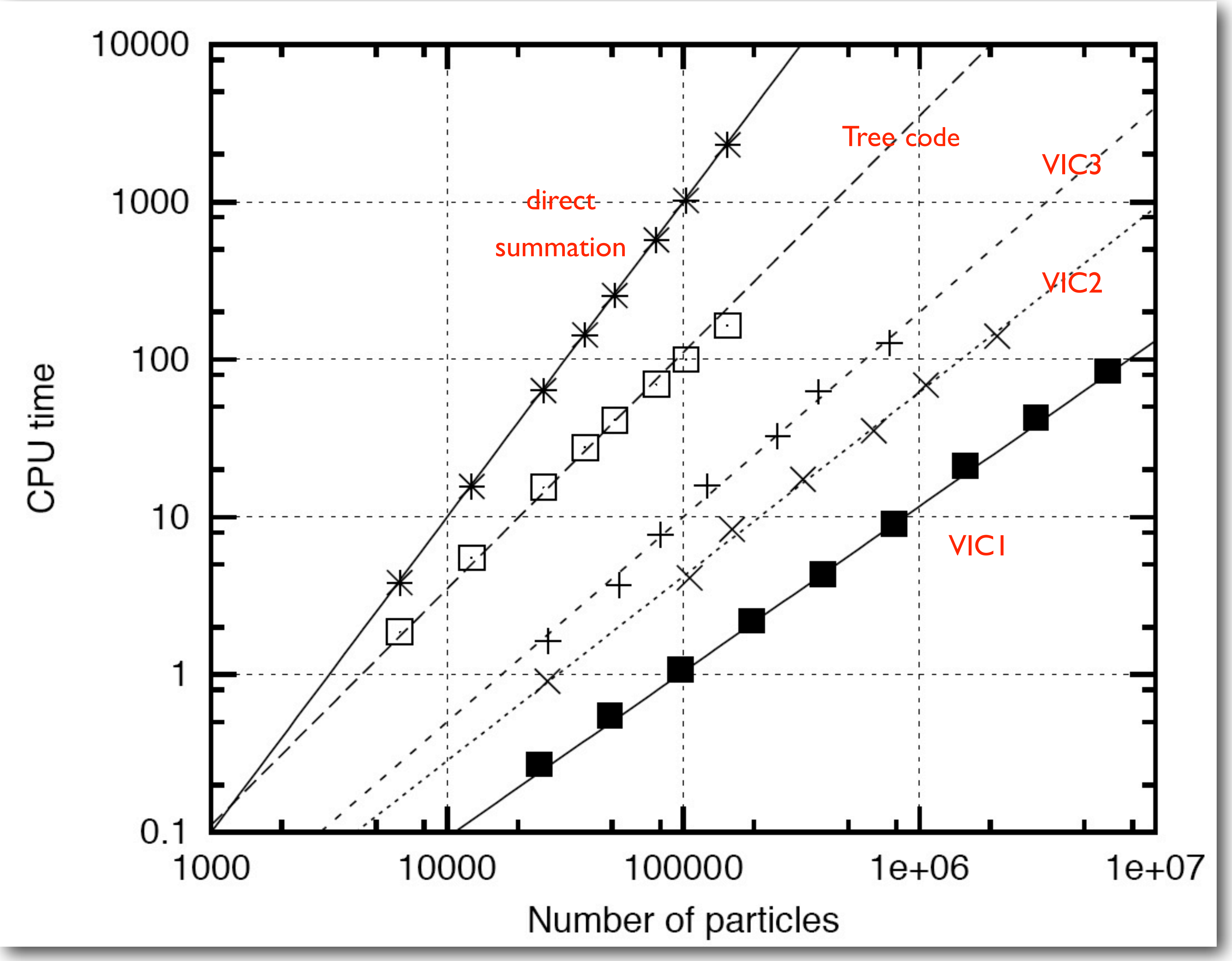
ADVANTAGES

•cheap (for relatively simple geometries)

•relying on a grid also useful/needed for remeshing and adapting local resolution
(come back later on this important issue)

•allows to add subgrid (turbulent) effects on passive tracers by simple interpolations

Computational Cost



Comparison of CPU times for velocity evaluations in 3D

(Krasny tree-code vs VIC with Fishpack and 64 points interpolation formulas)

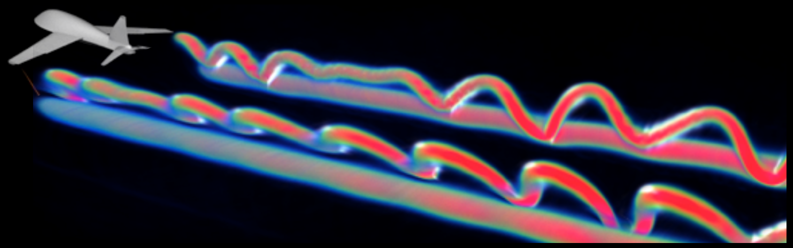
VIC1: cartesian grid with 100% particles

VIC2: polar grid with 65% particles

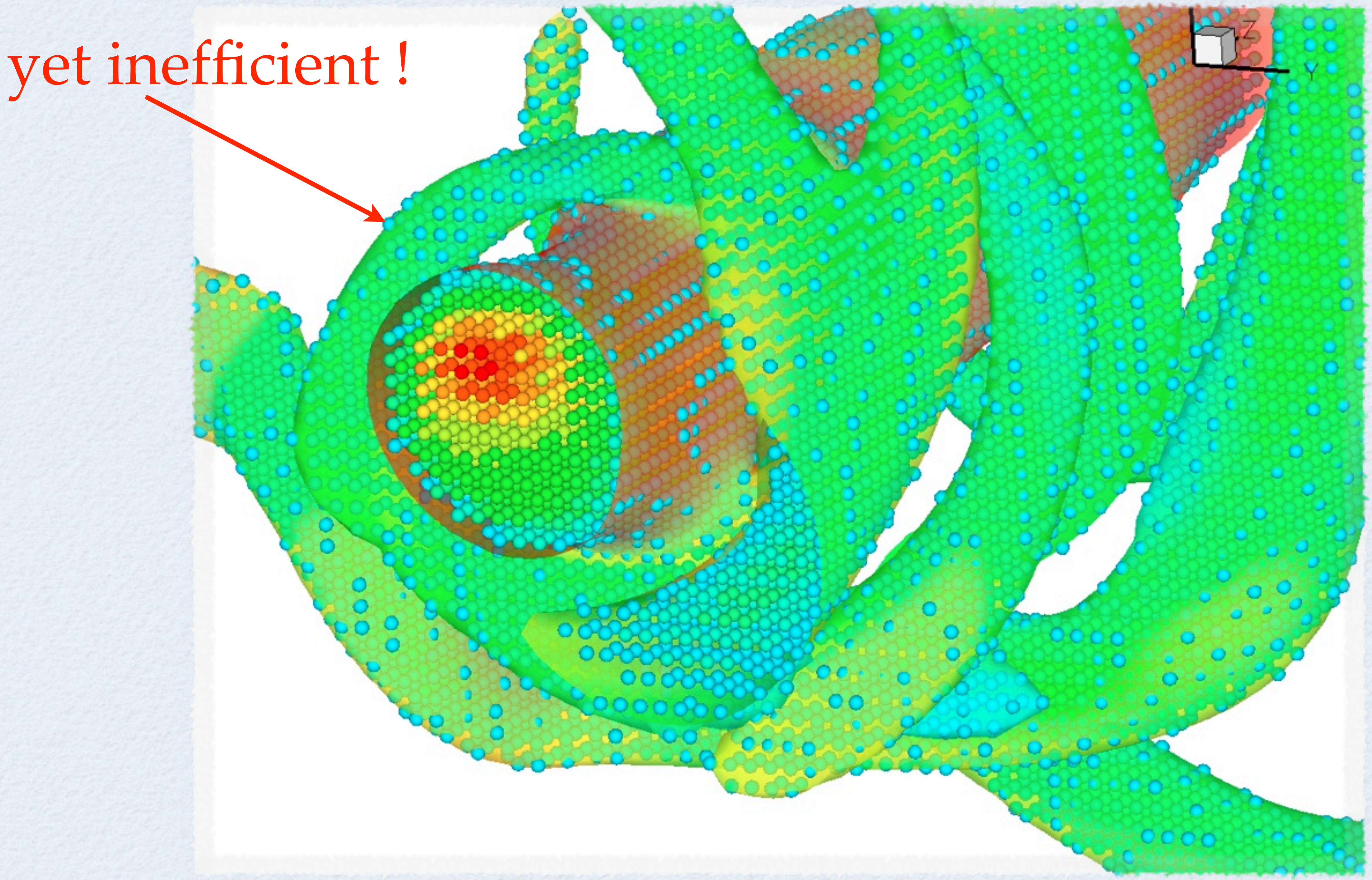
VIC3: polar grid with 25% particles

16384 Cores – 10 Billion Particles - 60% efficiency

Runs at IBM Watson Center - BLue Gene/L

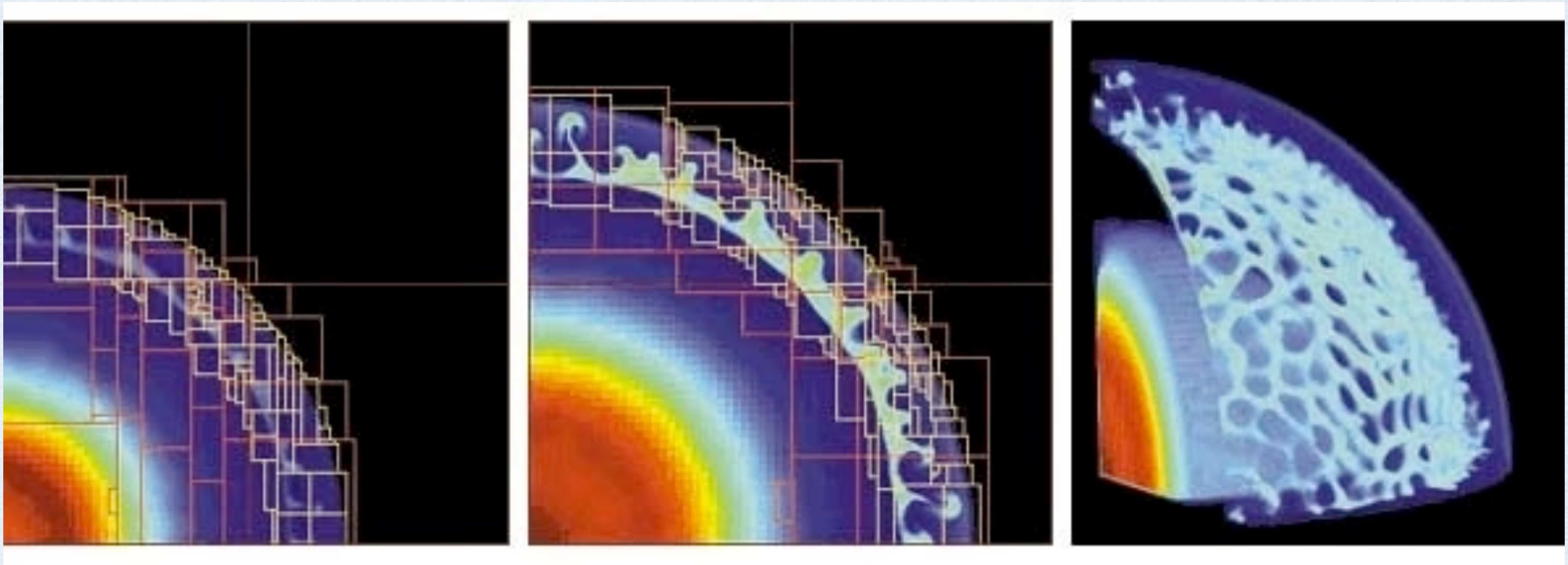


PARTICLES ARE ADAPTIVE



THE COMPETITION: Adaptive Mesh Refinement

References: Berger, Oliger, Colella, Quirk, ...

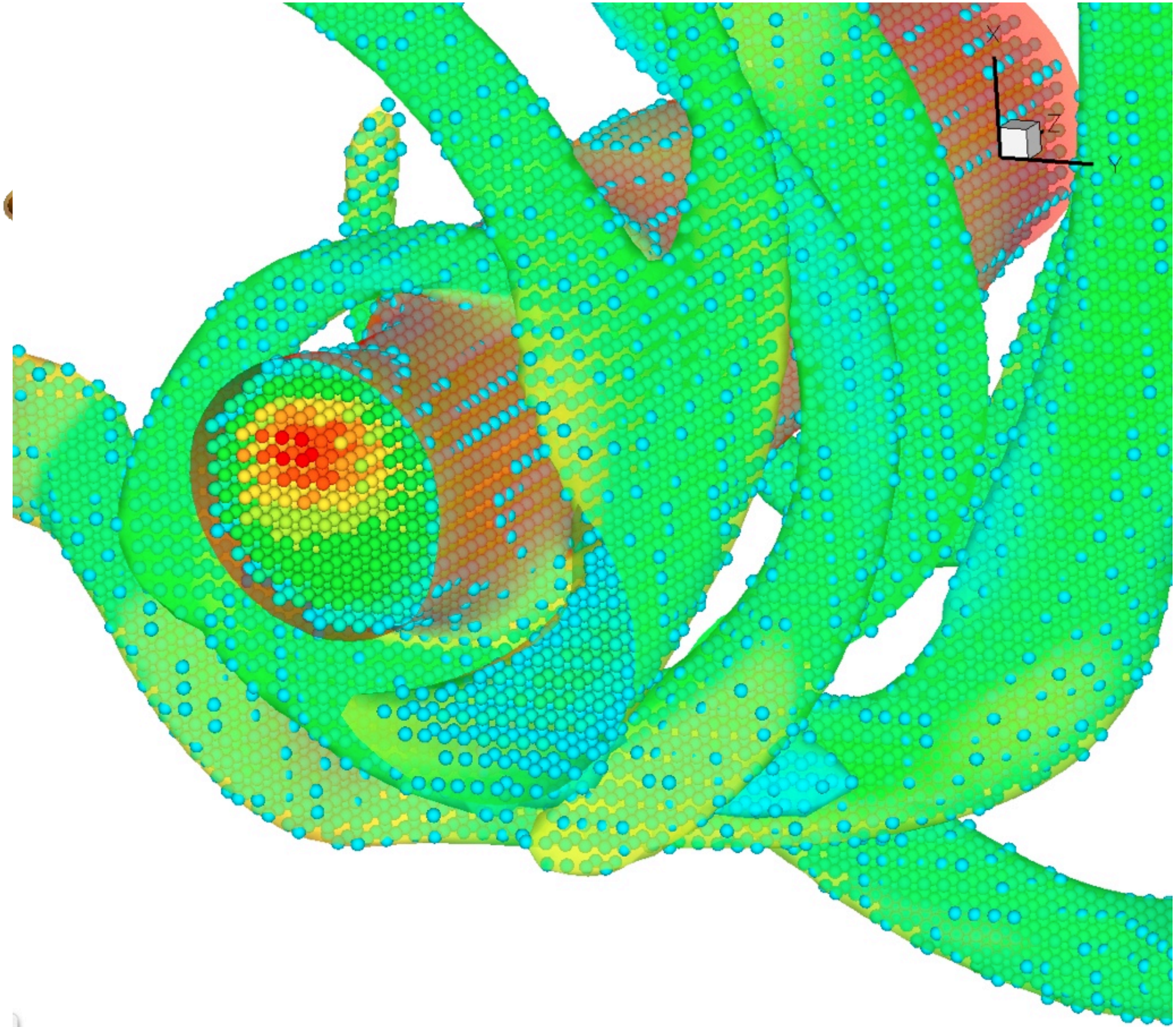


- Support of unstructured grids
- Different mesh orientations

- Low compression rate
- No explicit control on the error

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

Particle Methods are Adaptive yet Inefficient



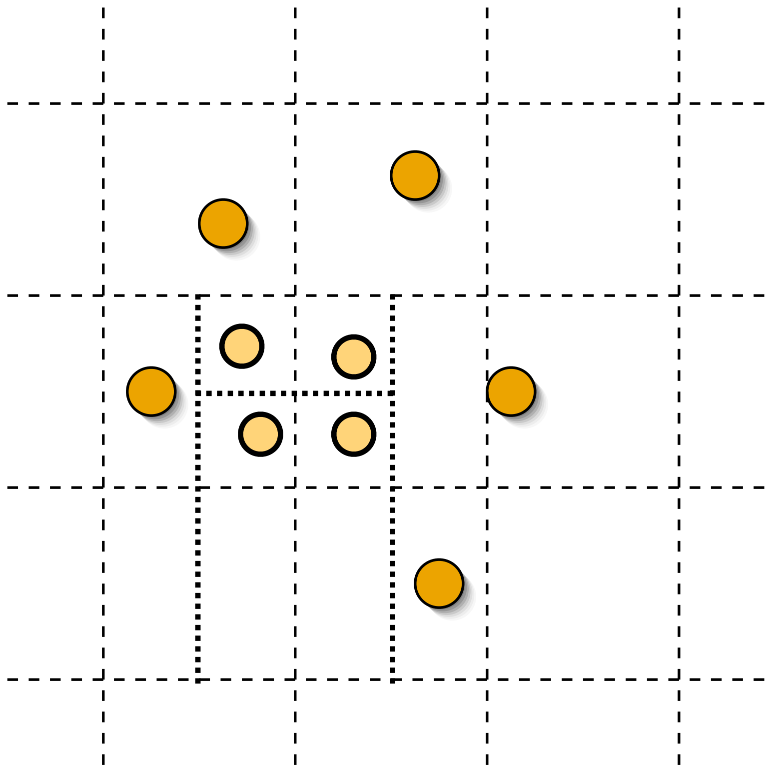
Chatelain P., Curioni A., Bergdorf M., Rossinelli D., Andreoni W., Koumoutsakos P., Billion Vortex Particle Direct Numerical Simulations of Aircraft Wakes, Computer Methods in Applied Mechanics and Engineering, 197/13-16, 1296-1304, 2008

MULTI-RESOLUTION

Wavelet based Particle Methods

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**

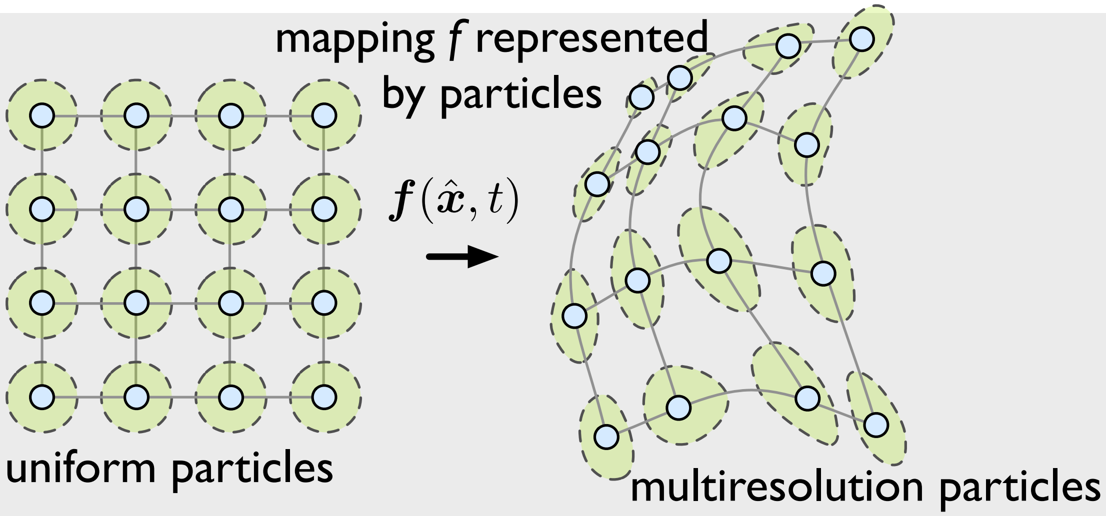
Key Issue : Introduction of a **grid - The old "magic" is gone**

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

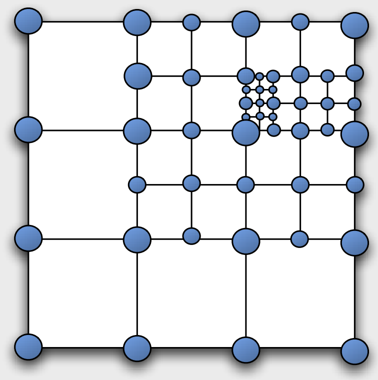
Keypoints: Adaptive mapping represented by particles



AMR-based

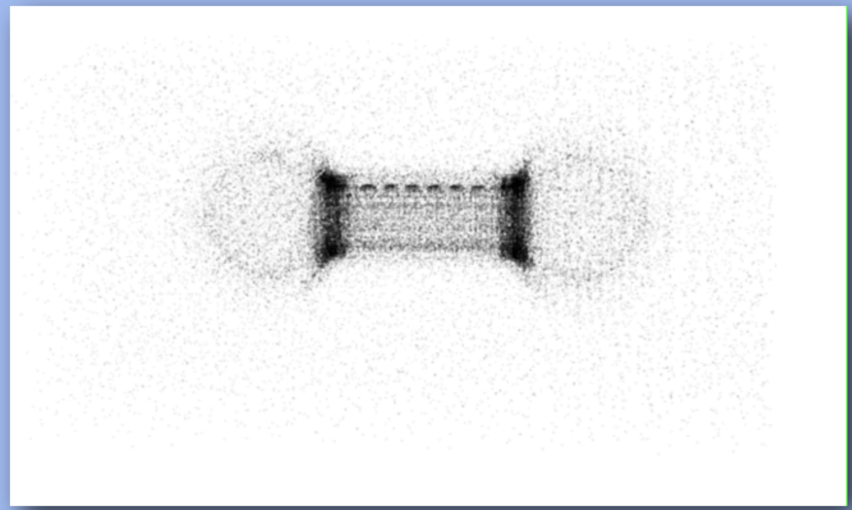
Keypoints: High-resolution particles are created on patches of refinement

\+ Multilevel remeshing

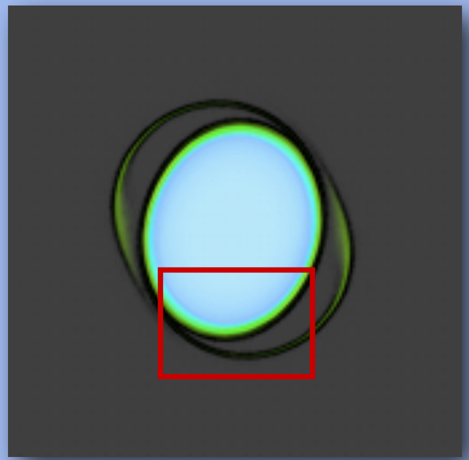


Particle-Wavelet Method

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



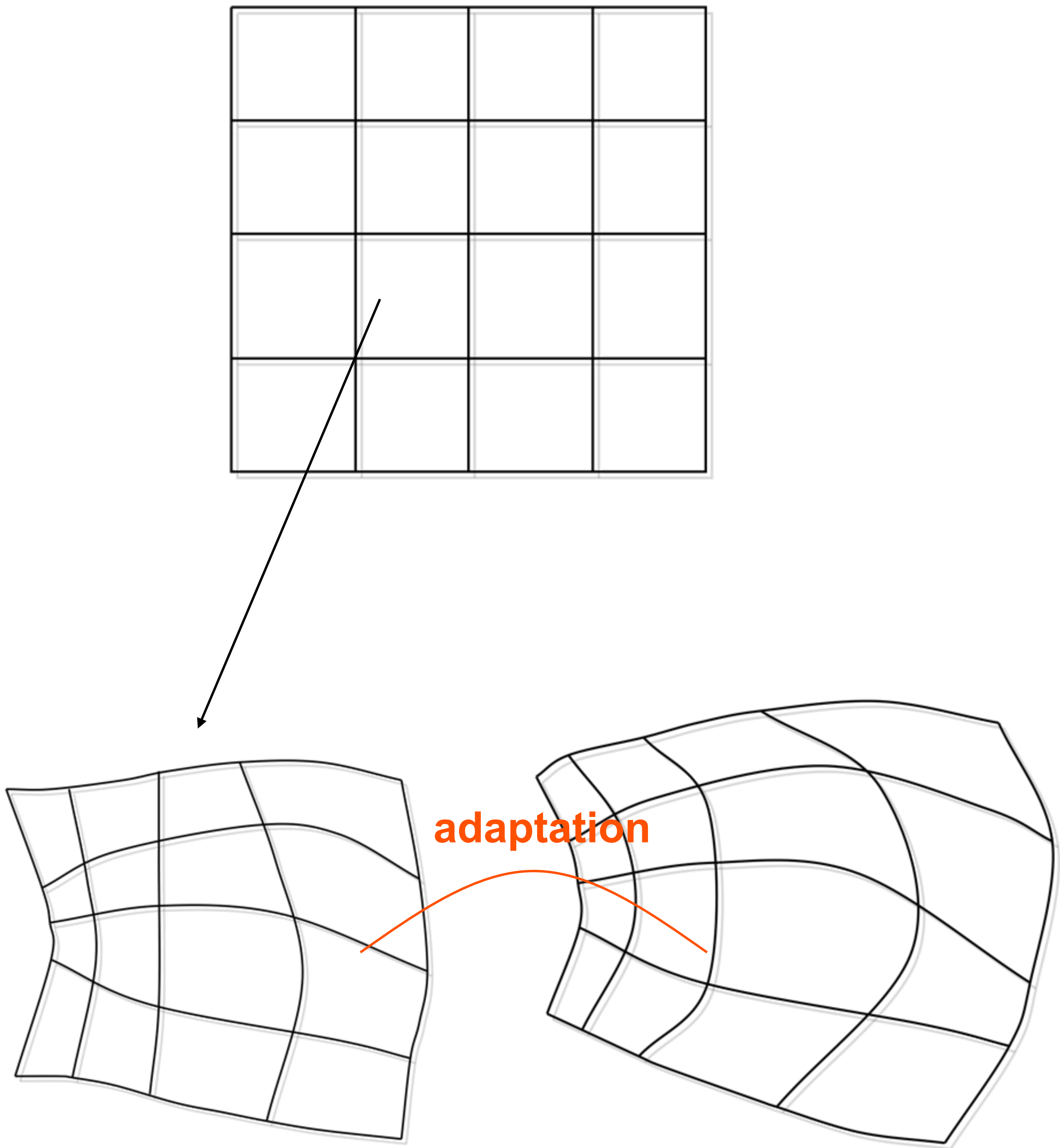
3D curvature driven collapse of a level set dumbbell



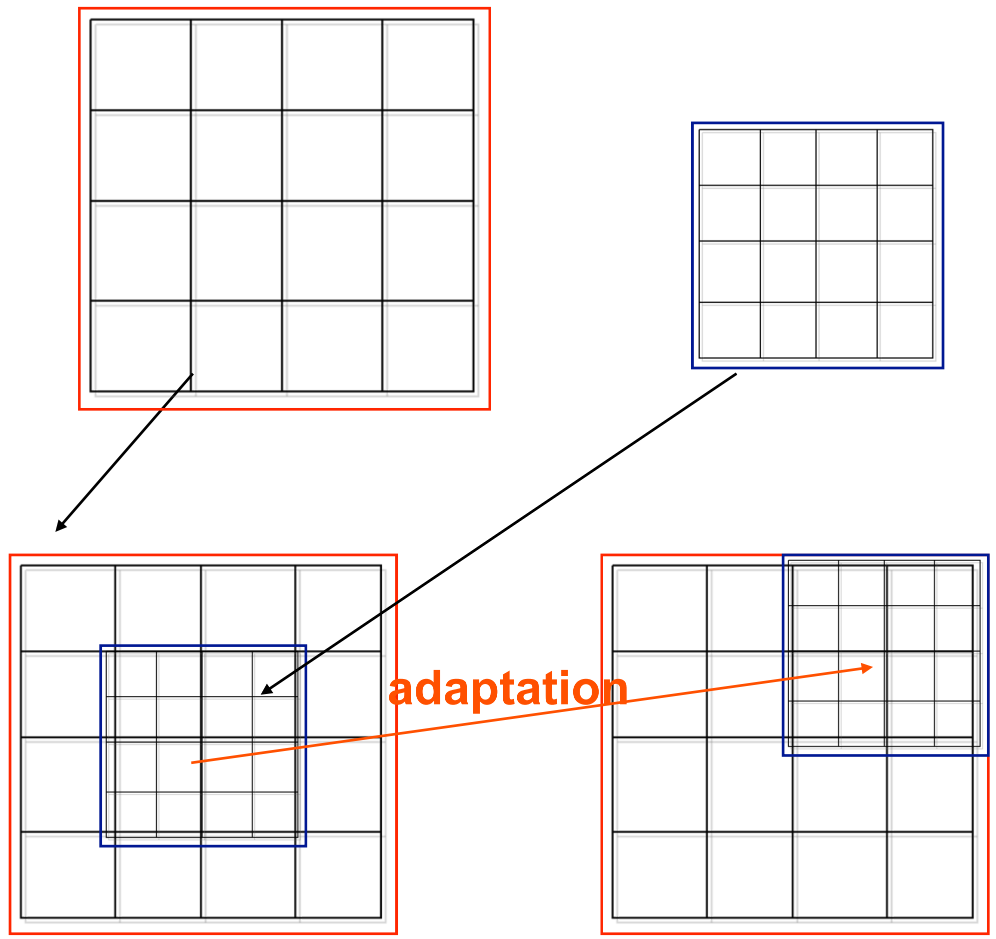
Axisymmetrization of an elliptical vortex (2D Euler)

Adaptive Multiresolution Particle Methods

Adaptive Global Mapping



Adaptive Mesh Refinement



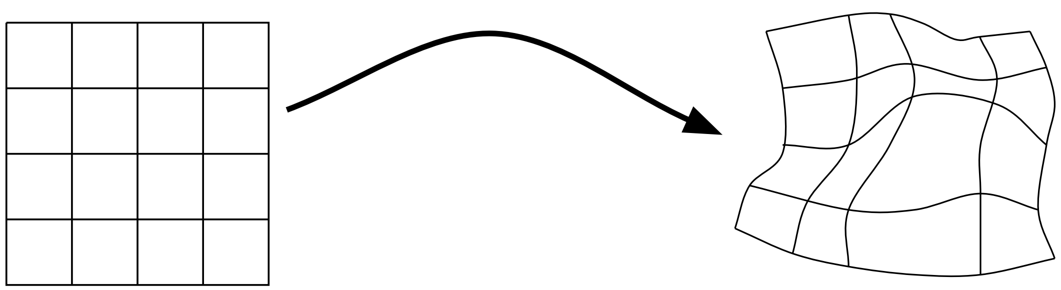
Adaptive Global Mappings

Particles are mapped from a '**reference**' space with uniform particle sizes to the '**physical**' space with varying particle sizes

$$f : \hat{x} \mapsto x$$

Reference space
uniform particle size/shape

$$\hat{x} \in \hat{\boldsymbol{\Omega}}$$



Physical space
distorted particle sizes/shapes

$$x \in \boldsymbol{\Omega}$$

Key Point : Transient Particle approximation of the map

smooth in space & time

$$\boldsymbol{x} = \boldsymbol{f}(\hat{\boldsymbol{x}}, t) = \sum_j \boldsymbol{\chi}_j(t)\, \varphi(\hat{\boldsymbol{x}} - \boldsymbol{\xi}_j)$$

Convection-Diffusion equation

Physical space
$$\frac{\partial q}{\partial t} + \nabla \cdot (\boldsymbol{u}\, q) = \nu\, \Delta q$$

Reference space
$$\frac{\partial \hat{q}'}{\partial t} + \hat{\nabla}\,(\tilde{\boldsymbol{u}}\,\hat{q}') = \nu \hat{\nabla}\left(\boldsymbol{\Phi}\hat{\nabla}\,(\boldsymbol{\Phi}\hat{q}')\right)$$

$$\hat{q}' = \boldsymbol{\Phi}^{-1}\hat{q}$$
$$q(\boldsymbol{x},t) \leftrightarrow q(\hat{\boldsymbol{x}},t)$$

$\tilde{\boldsymbol{u}} = \boldsymbol{\Phi}\,(\hat{\boldsymbol{u}} - \boldsymbol{\mathcal{U}})$
convection velocity
in reference space

$\boldsymbol{\Phi} = \dfrac{\partial \hat{\boldsymbol{x}}}{\partial \boldsymbol{x}}$
Jacobian

positions	$\dfrac{d\hat{x}_p}{dt} = \tilde{u}_p$
strengths	$\dfrac{d\hat{Q}_p}{dt} = \frac{\nu}{\hat{\varepsilon}^2}\sum_q \dfrac{\Phi_p+\Phi_q}{2}\left[\hat{Q}_q\hat{v}_p\Phi_q - \hat{Q}_p\hat{v}_q\Phi_p\right]\eta^{\hat{\varepsilon}}(\hat{x}_p-\hat{x}_q)$
volumes	$\dfrac{d\hat{v}_p}{dt} = \frac{1}{\hat{\varepsilon}}\sum_q\left[\tilde{u}_p+\tilde{u}_q\right]\hat{\nabla}\zeta^{\hat{\varepsilon}}(\hat{x}_p-\hat{x}_q)\,\hat{v}_q\,\hat{v}_p$
map	$\dfrac{d\chi_i}{dt} = \mathcal{U}(\xi_i)$

$$\hat{Q}_p = \hat{q}'_p\,\hat{v}_p$$

Choice of map adaptation in case > 1D

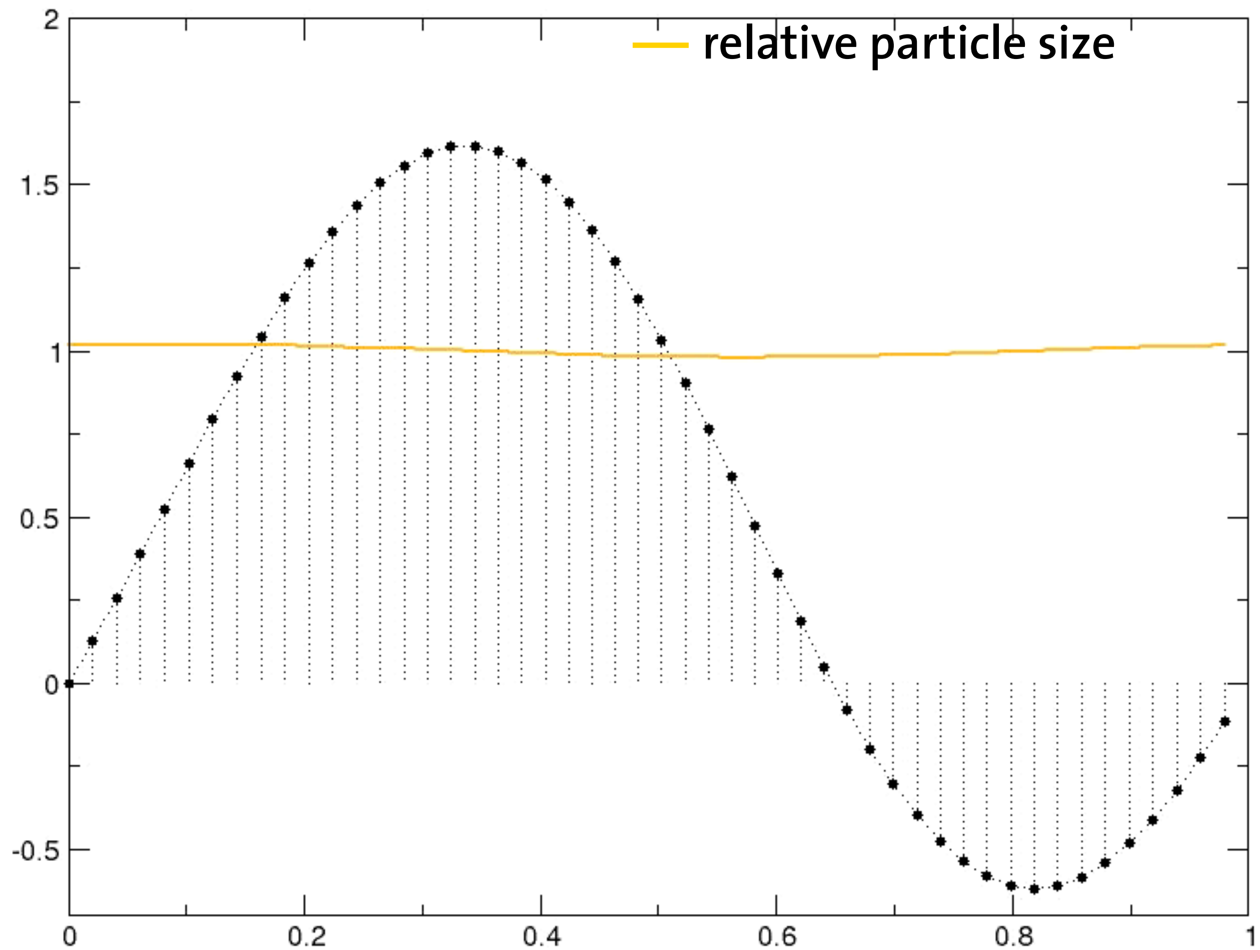
Monitor function $\mathcal{M}(\hat{x},t)$ $\quad \mathcal{M}(\hat{x},t)\Phi^{-1} = \text{const}$

$$\mathcal{U} = C\hat{\nabla}\cdot\left(\mathcal{M}\hat{\nabla}\boldsymbol{x}\right)$$
nonlinear diffusion operator

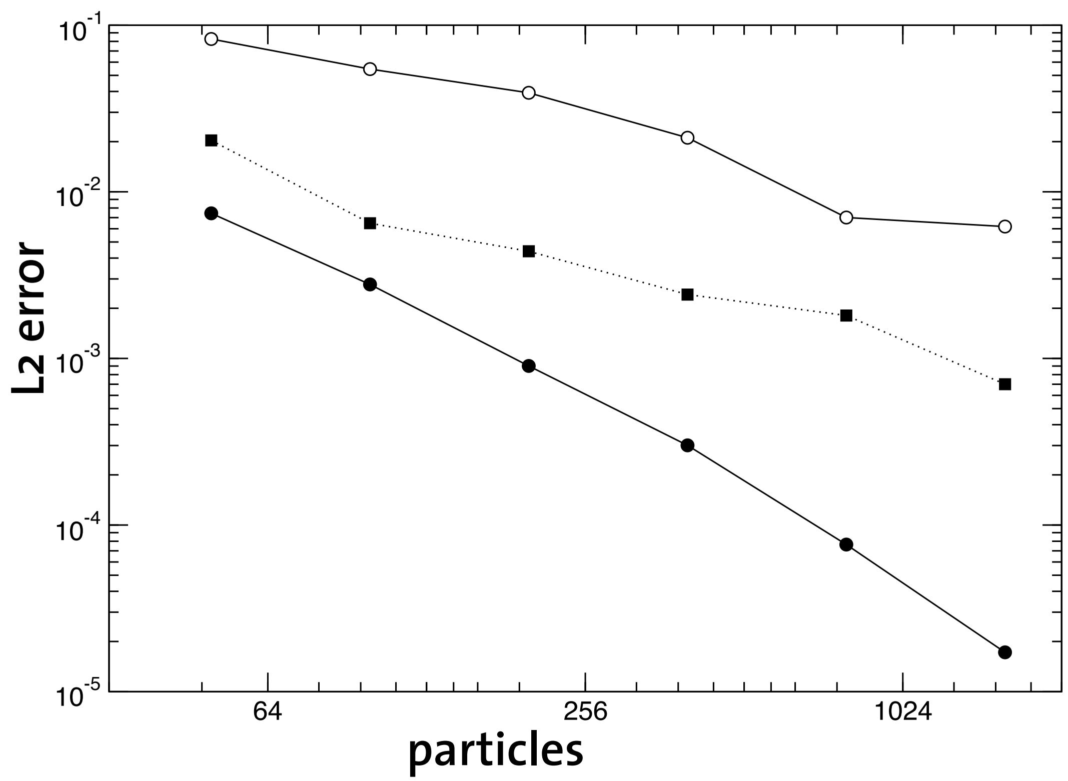
Burger's equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(u^2\right) = \nu \frac{\partial^2 u}{\partial x^2}$$

$$\mathcal{U} = \frac{1}{2}\,u$$



● adaptive
o non-adaptive

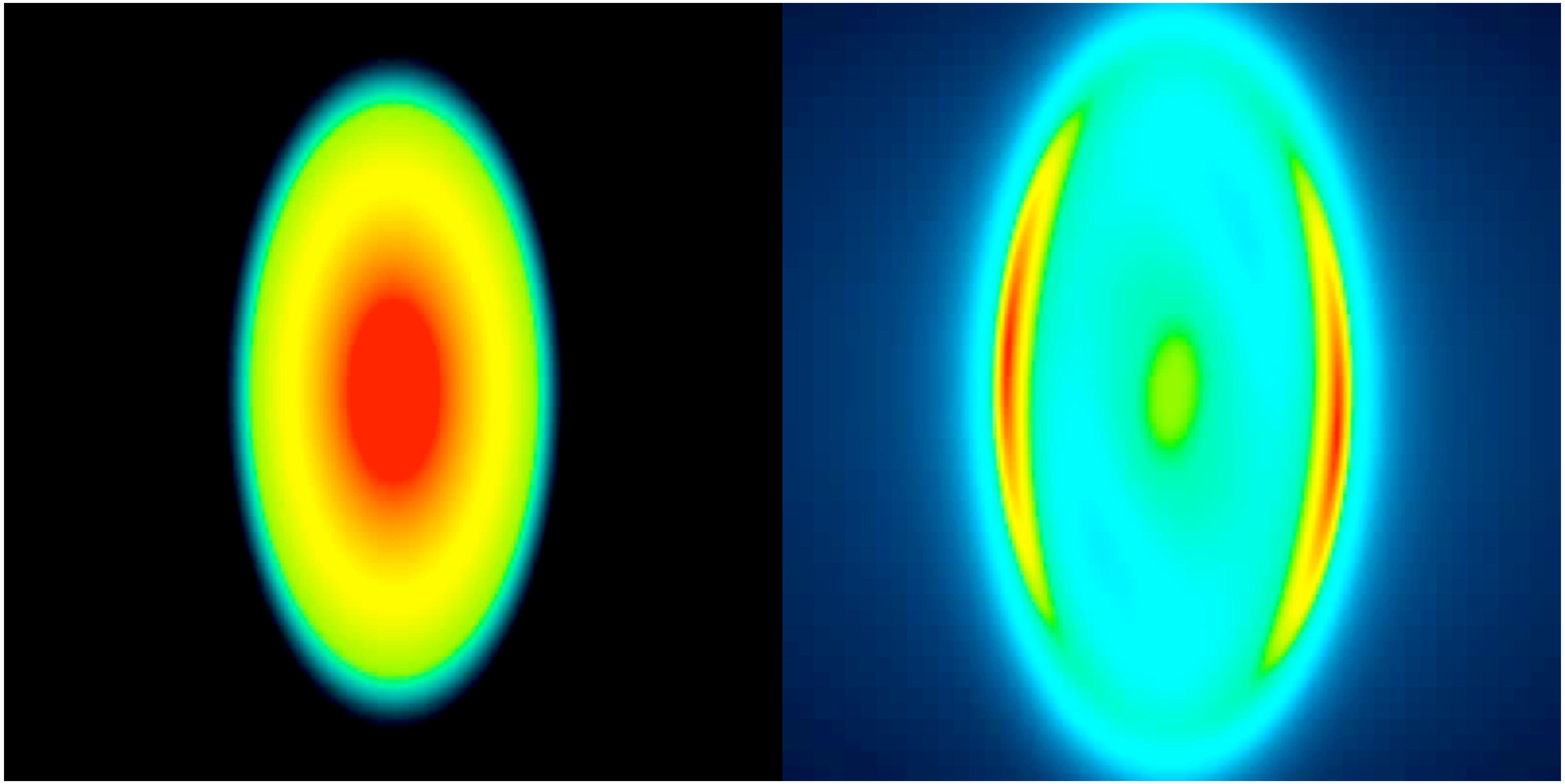


L2 error for the moving shock problem

Evolution of Elliptical Vortex

2D Euler equations

Vorticity | Particle size

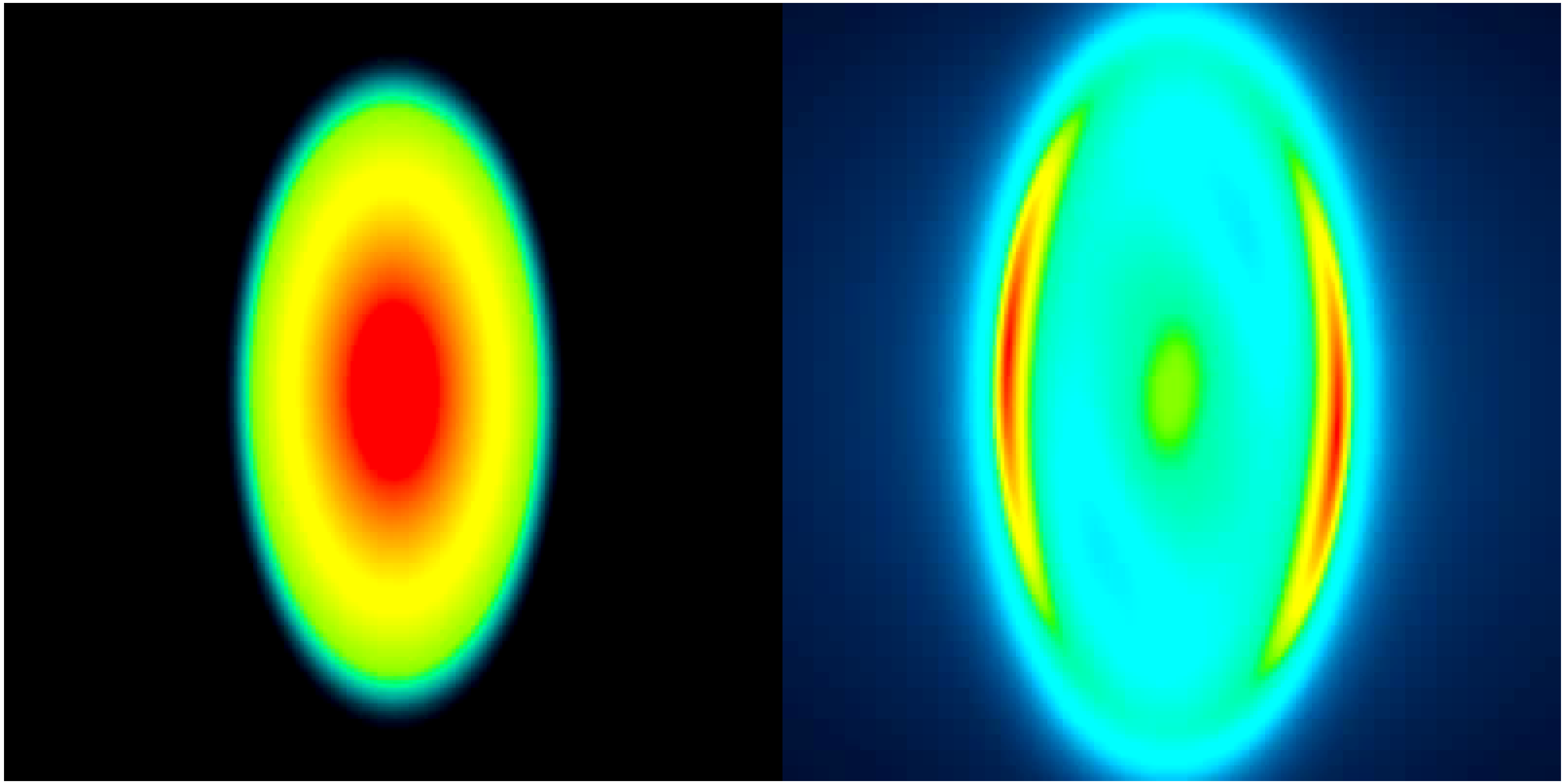


Bergdorf, Cottet & Koumoutsakos, MMS, 2005

Evolution of Elliptical Vortex

2D Euler equations

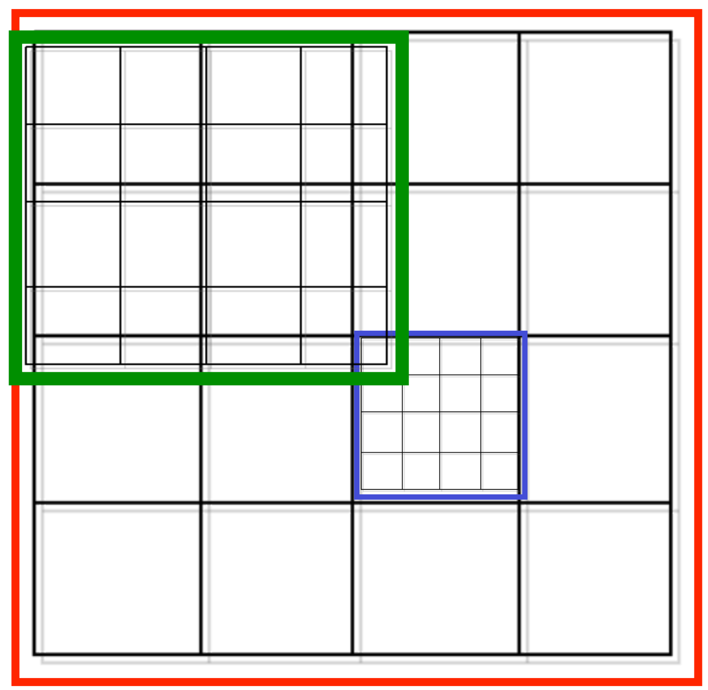
Vorticity | Particle size



Bergdorf, Cottet & Koumoutsakos, MMS, 2005

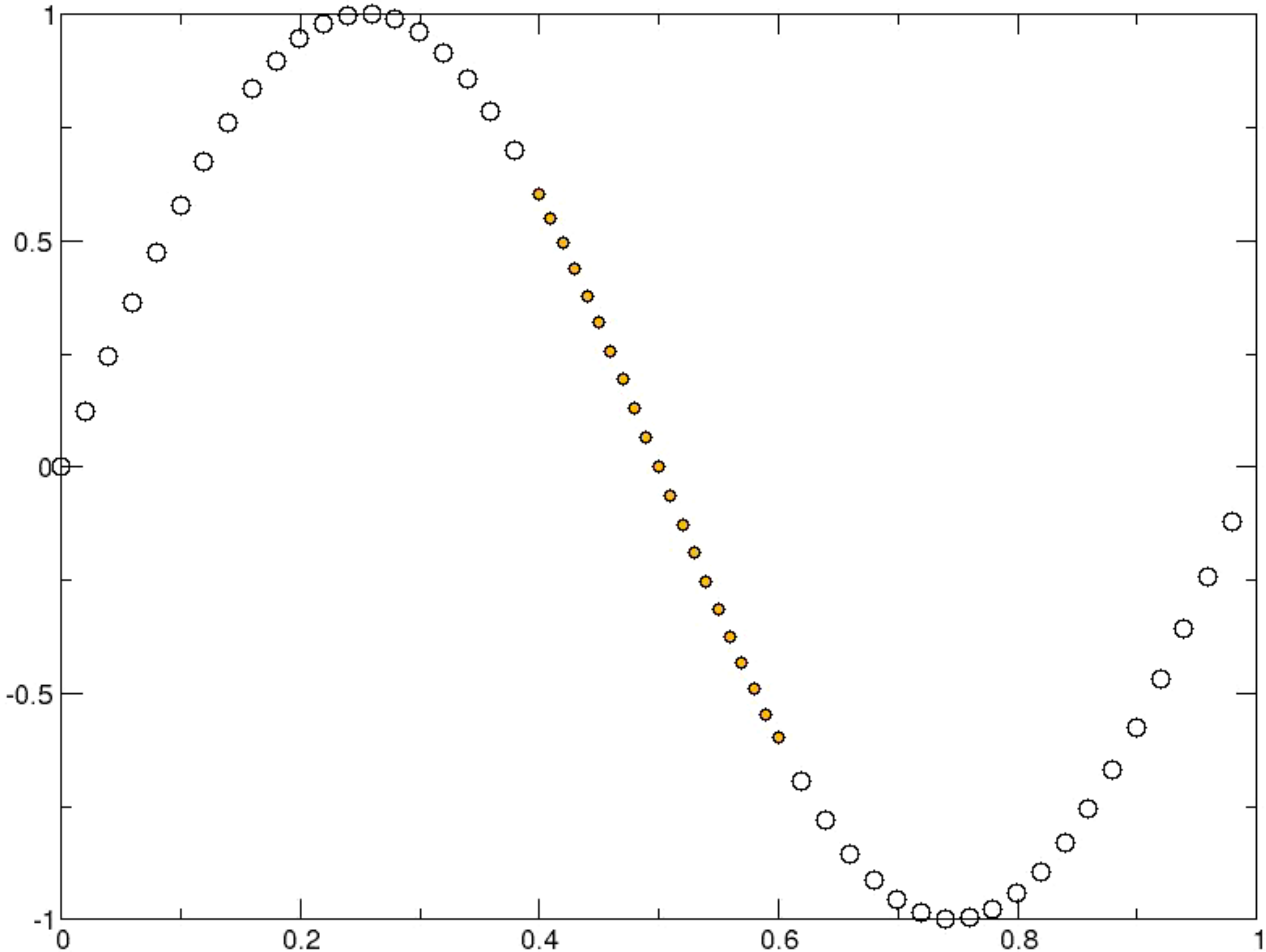
Adaptive Multiresolution Particle Methods (AMR)

Different maps which are piecewise constant are used in different parts of the domain leading to different core-/grid-sizes



Remeshing is used to **communicate boundary conditions** between levels of different core-sizes

AMR Particle Methods



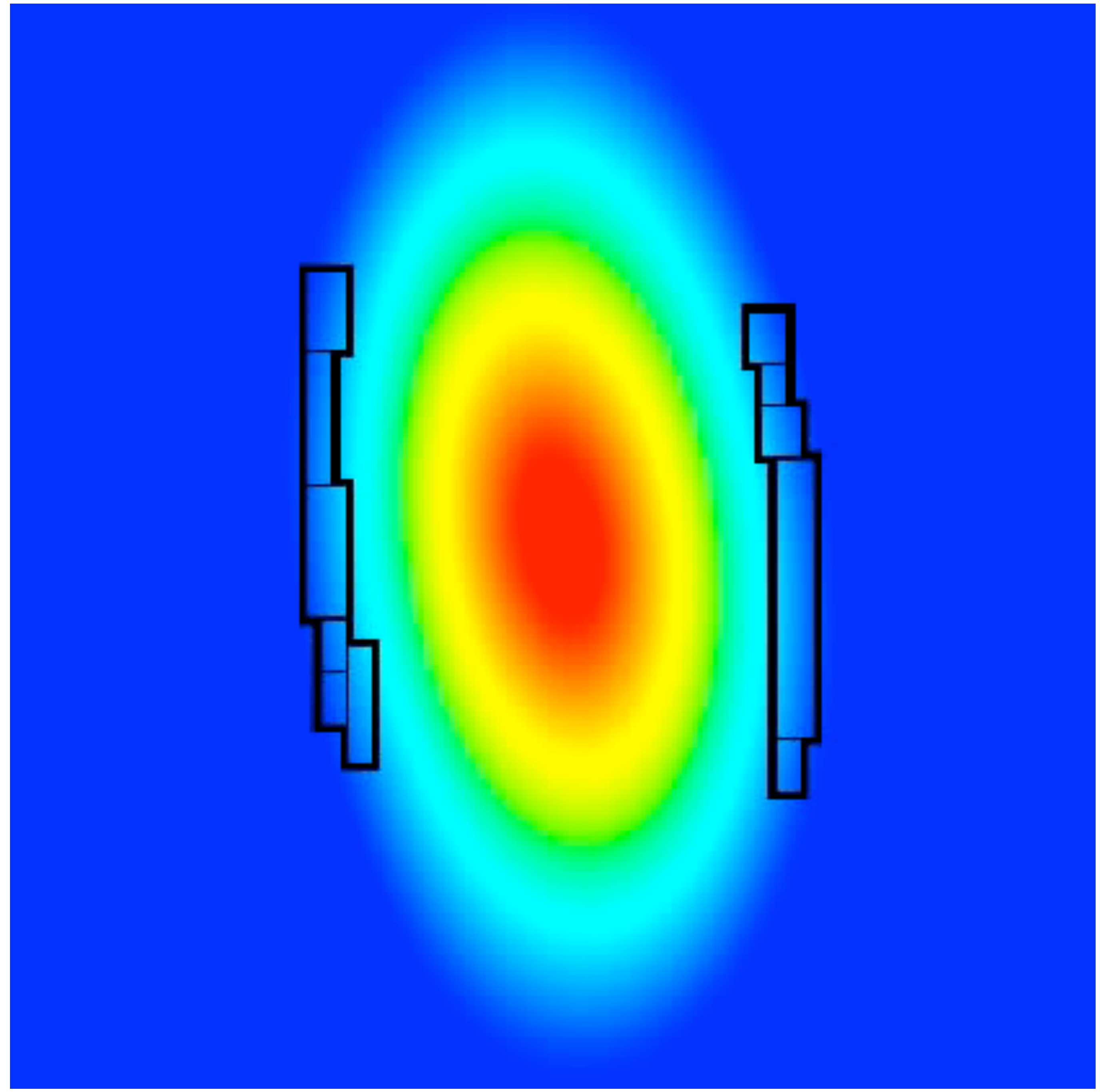
$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(u^2\right) = \nu \frac{\partial^2 u}{\partial x^2}.$$

- periodic boundary conditions
- viscosity coefficient (1e-3)
- initial condition leading to steady "shock"

Evolution of Elliptical Vortex - AMR

2D Euler equations

Vorticity



Bergdorf, Cottet & Koumoutsakos, MMS, 2005

ENHANCED (Dynamic)

AGM - Adaptive Global Mappings

Transient adaptive mapping from a mono-scale reference space to physical space.

Moving Mesh PDEs

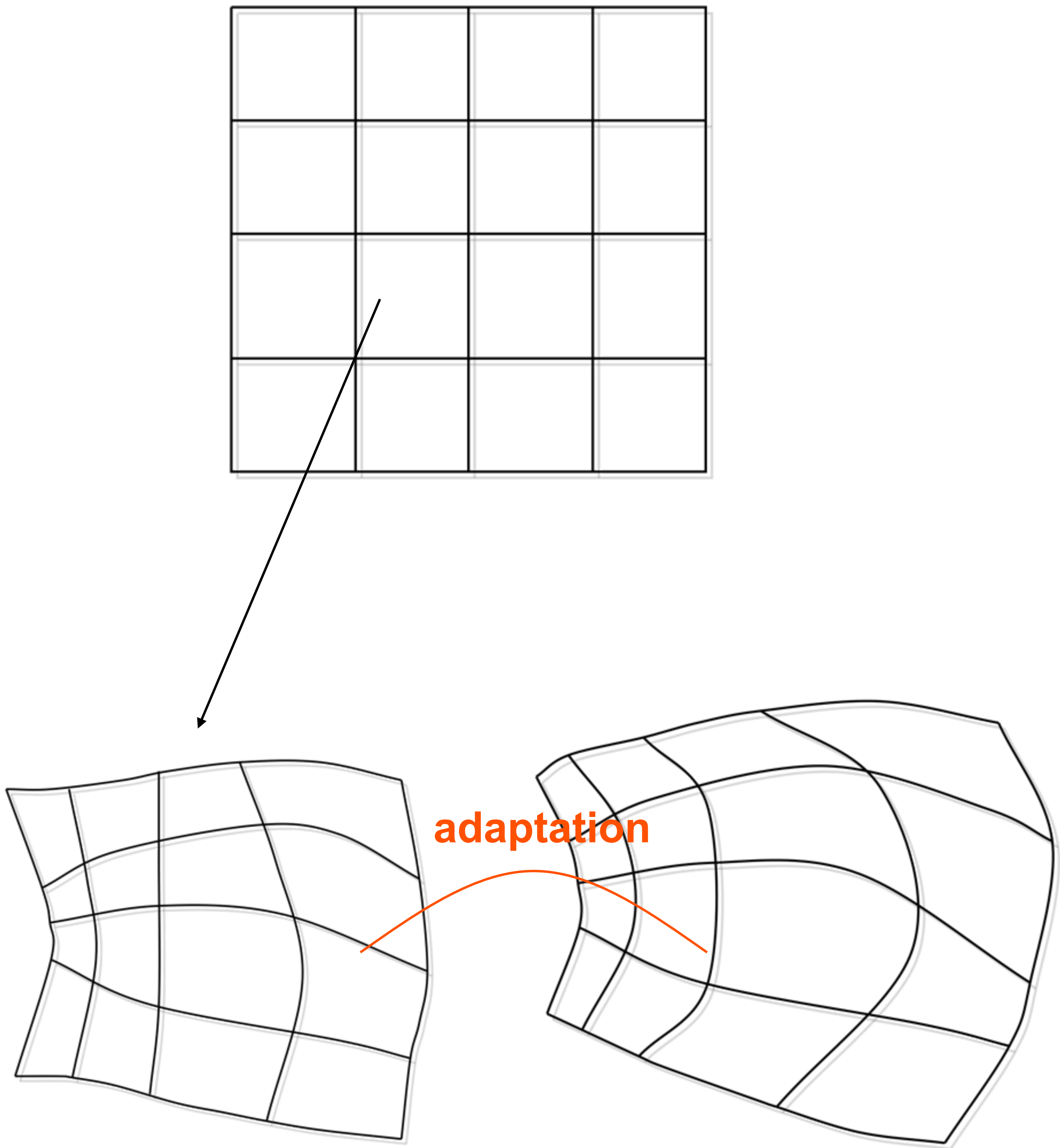
AMR - Grid-Particle Methods

PMW - Particle - Wavelet-based Multiresolution

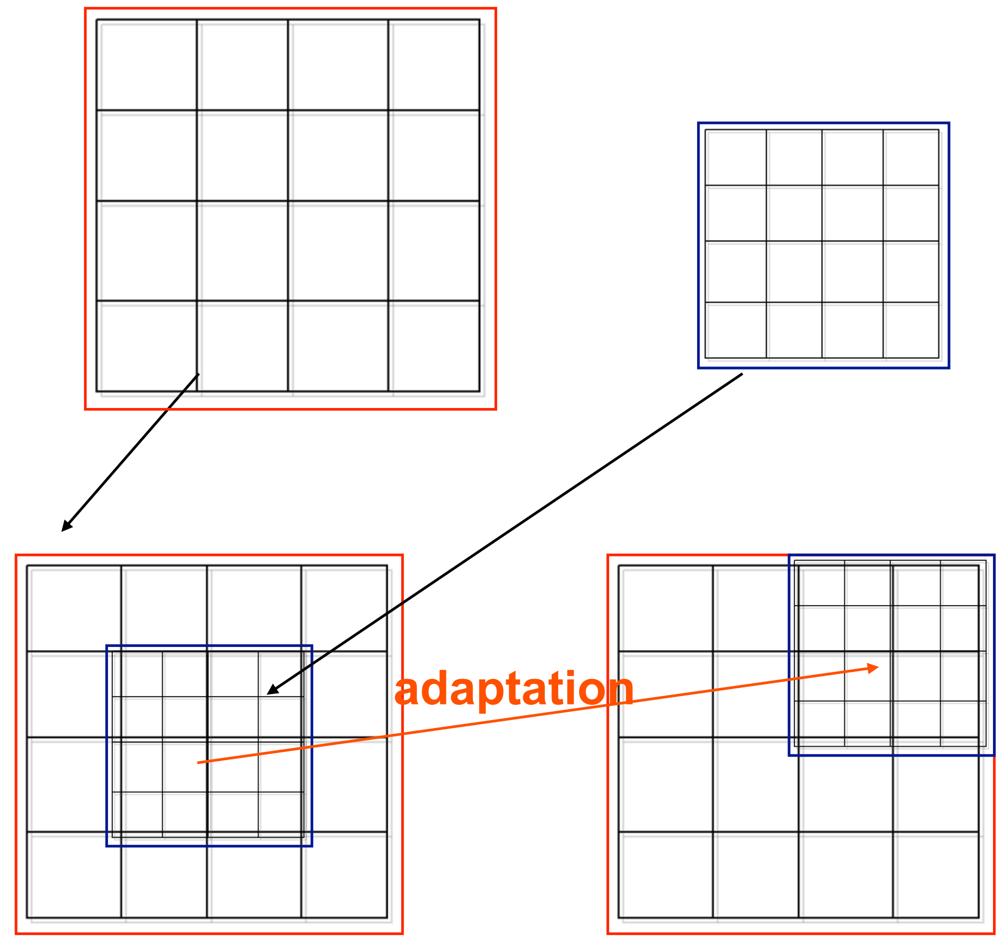
Multiresolution Analysis (MRA) of particle function representation.
Lagrangian convection of the scale distribution.

Adaptive Multiresolution

Adaptive Global Mapping



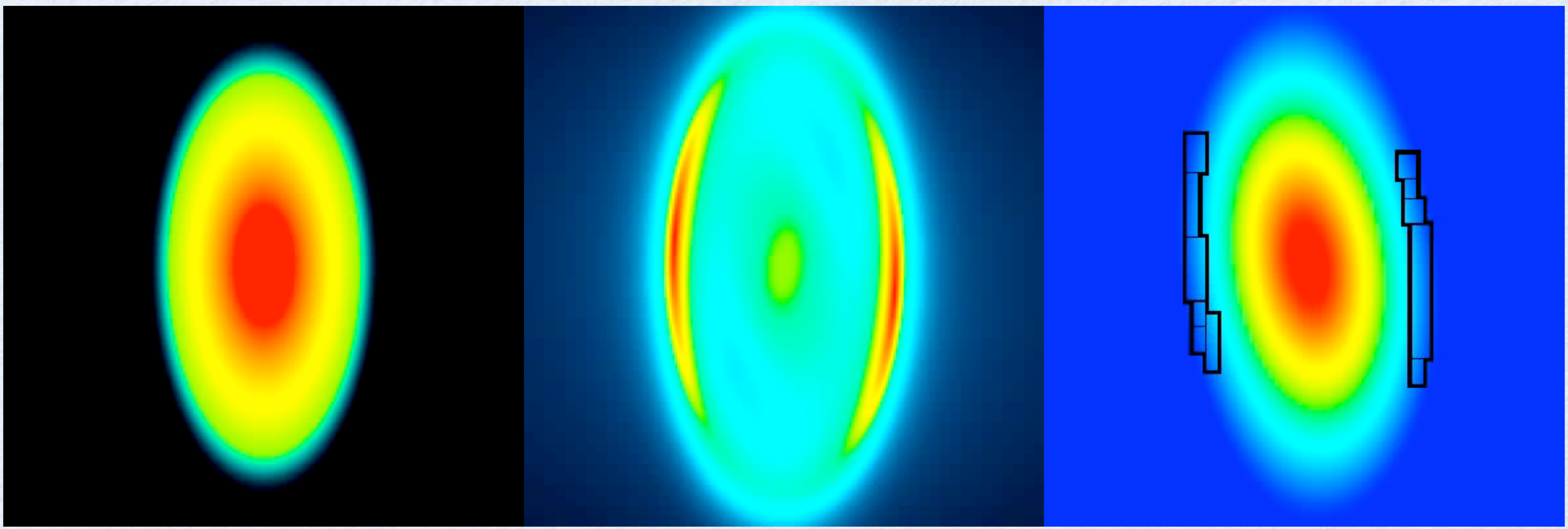
Adaptive Mesh Refinement



Adaptive Global Mappings and AMR

2D Euler equations

Vorticity | **Particle size** | **PARTICLES + AMR**



M. Bergdorf, G.-H. Cottet, P. Koumoutsakos, Multilevel adaptive particle methods for convection-diffusion equations, **Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, 4(1), 328-357, 2005**

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

PARTICLETS : Particles and Wavelets

Wavelet Compression

50:1

WAVELET PARTICLE METHOD

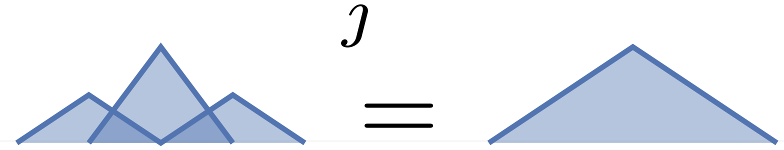
While particles are on grid locations

mollification kernel ⟷ basis/scaling function

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

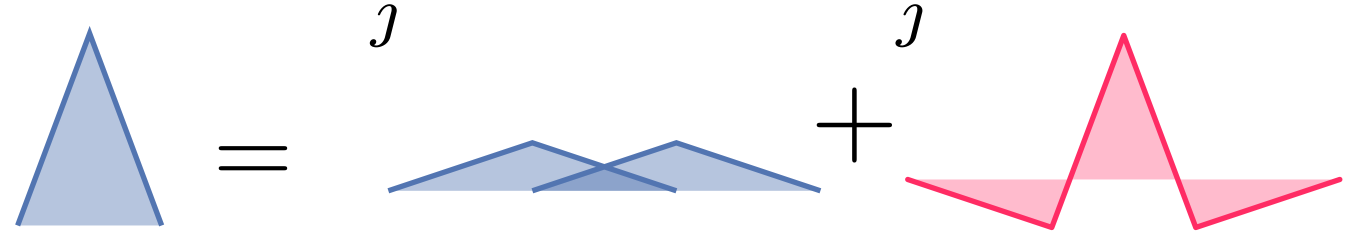
Refineable kernels as basis functions of $\mathcal{V}^l$

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



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

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



Multiresolution function representation:

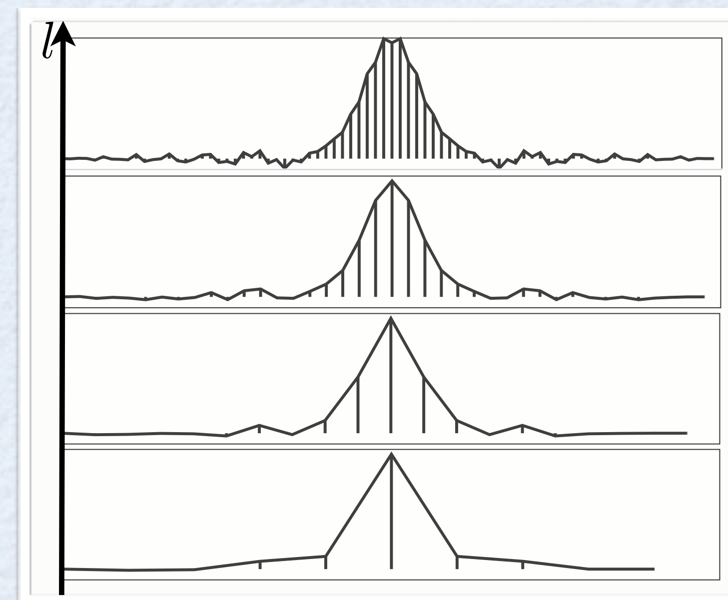
Analysis (collocation): d_k^l ~ | fine - Prediction(coarse) |

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

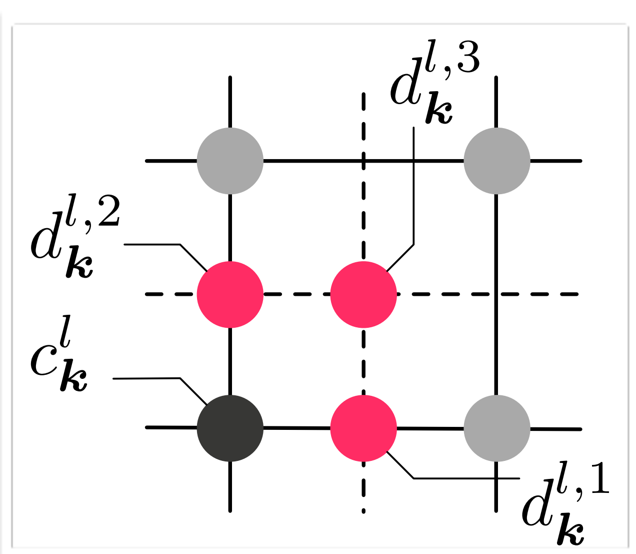
GROUND LEVEL

WAVELETS

DETAIL COEFFICIENTS



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



Compression / Adaptation:

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

Compressed function representation:

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

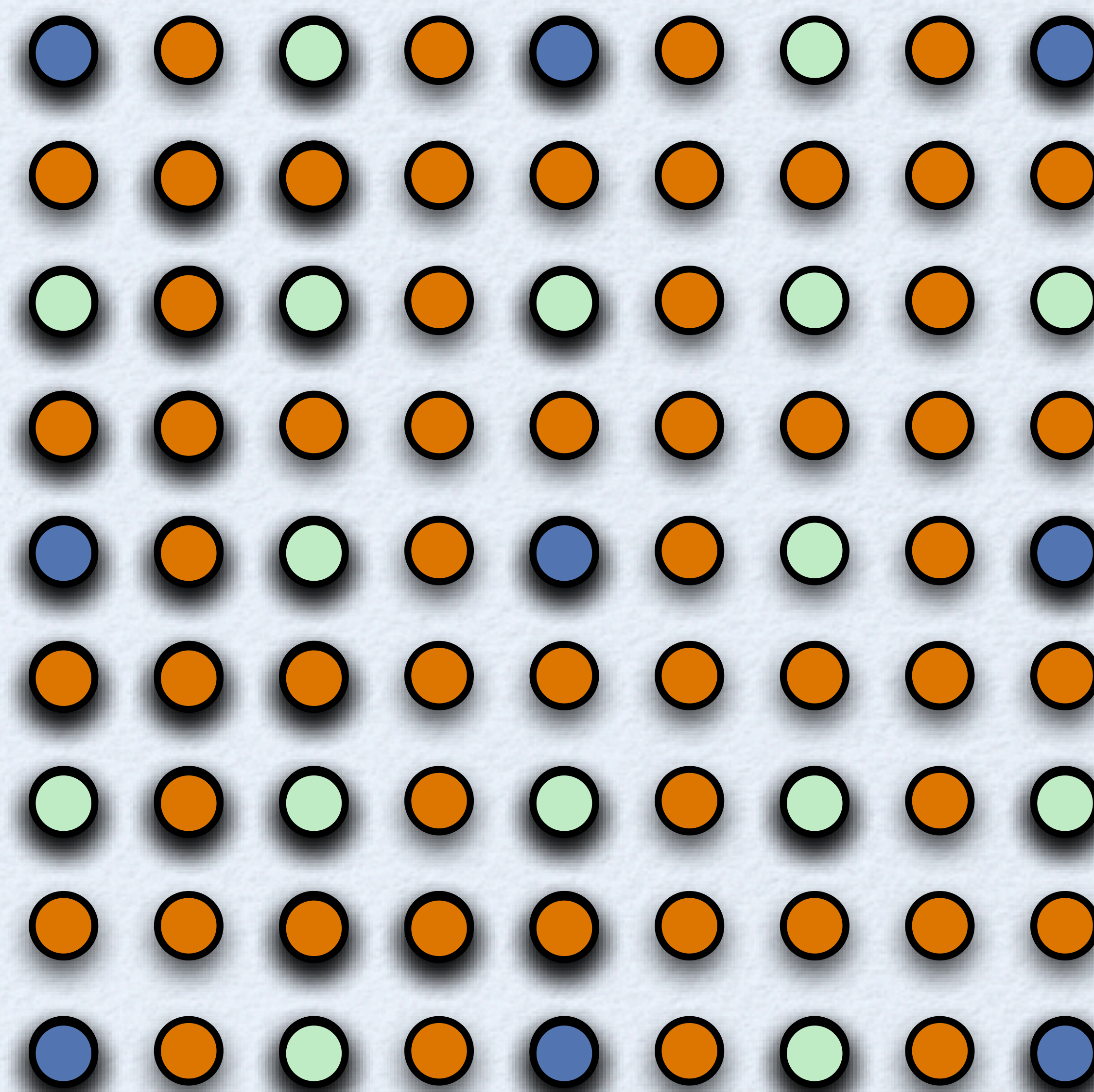
PARTICLETS : REMESHED PARTICLES + WAVELETS

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

"ground" level

detail coefficients

wavelets

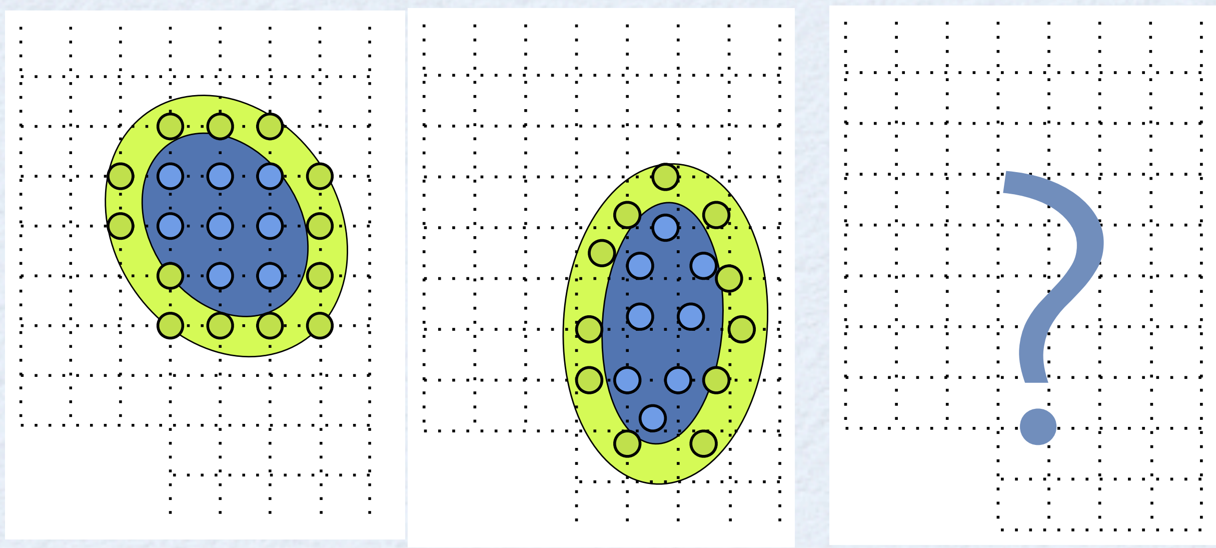


1. Remesh
2. Wavelets- Compress/Adapt
3. Convect
4. Wavelets Reconstruct
5. GOTO 1

Multilevel P2M

Basic concept: Interpolate particles of level l onto grid points of level l by buffer particles

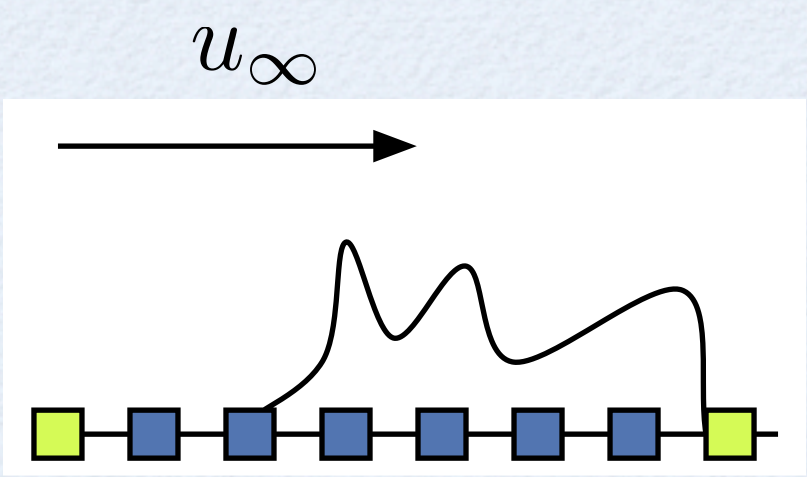
Algorithm:



How to chose the target set?

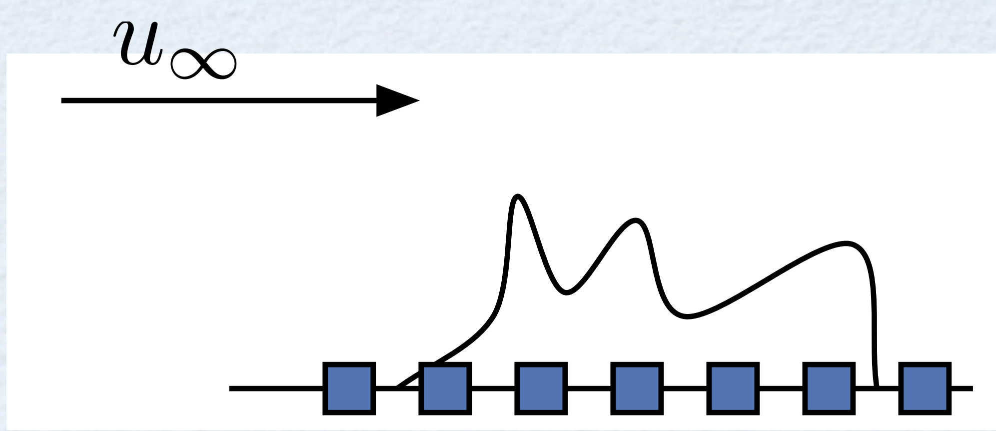
Key points: Get buffer values from l - 1
Size of buffer depends on kernel and "target set"

grid-based method, CFL < 1



Convection of the Scale Distribution

Key idea: Account for the convection of small scales in a Lagrangian way



In multidimensions the scale distribution (≈grid) can become amorphous, complex ...

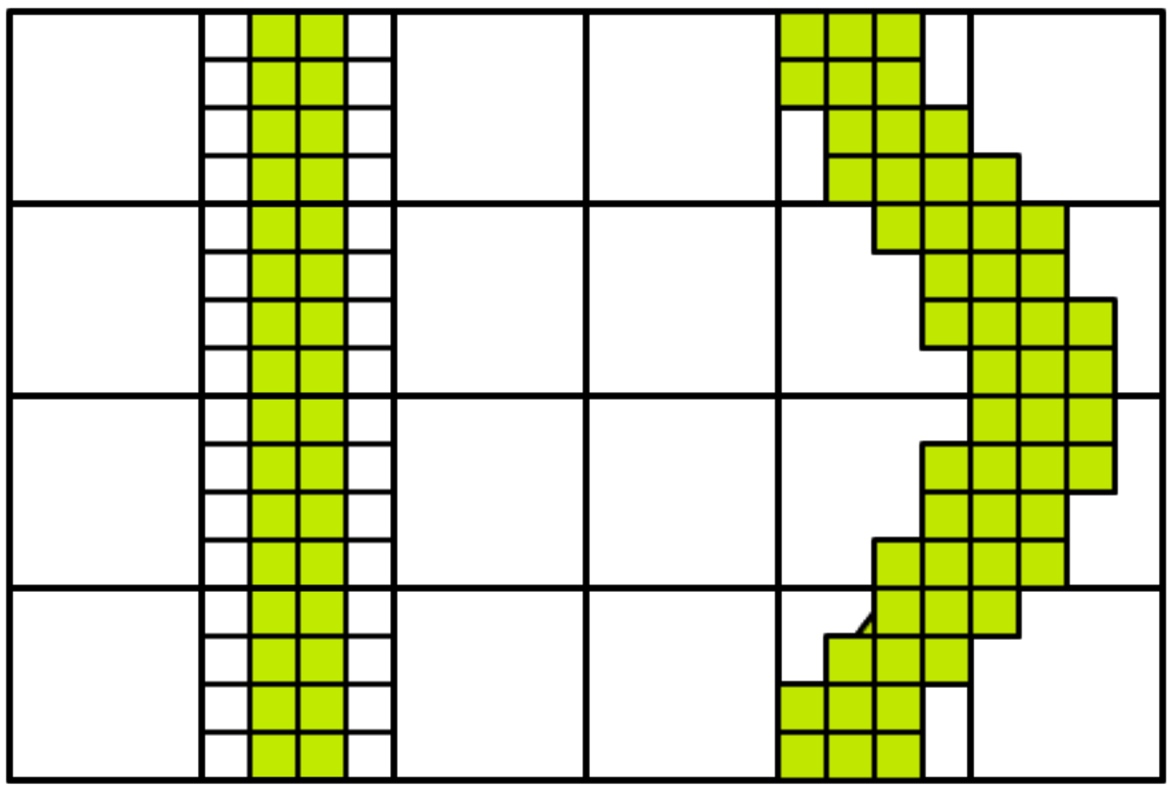
Indicator function: $\chi_{\boldsymbol{k}}^{l}$ $\quad \frac{d\chi_p^l}{dt} = 0\,.$

1 for grid points/particles that have been selected by the FWT
0 for buffer grid points/particles

target set = remeshed indicator function > 1.0-ε

Lagrangian transport of multiscale information

Particle methods: possibly **CFL >> 1** → Traditional approaches become **inefficient**



1) Grid points/particles selected by MRA

2) Indicator function alongside particle properties

3) Convect indicator and properties

4) mark grid points where Remeshing is consistent (indicator)

5) Remesh particle properties onto selected grid points

-> perform MRA on new set of active grid points

Benefit:

- the whole **adaptivity structure** of the grid is convected by the flow map in a **Lagrangian** way.
- independence of **CFL**

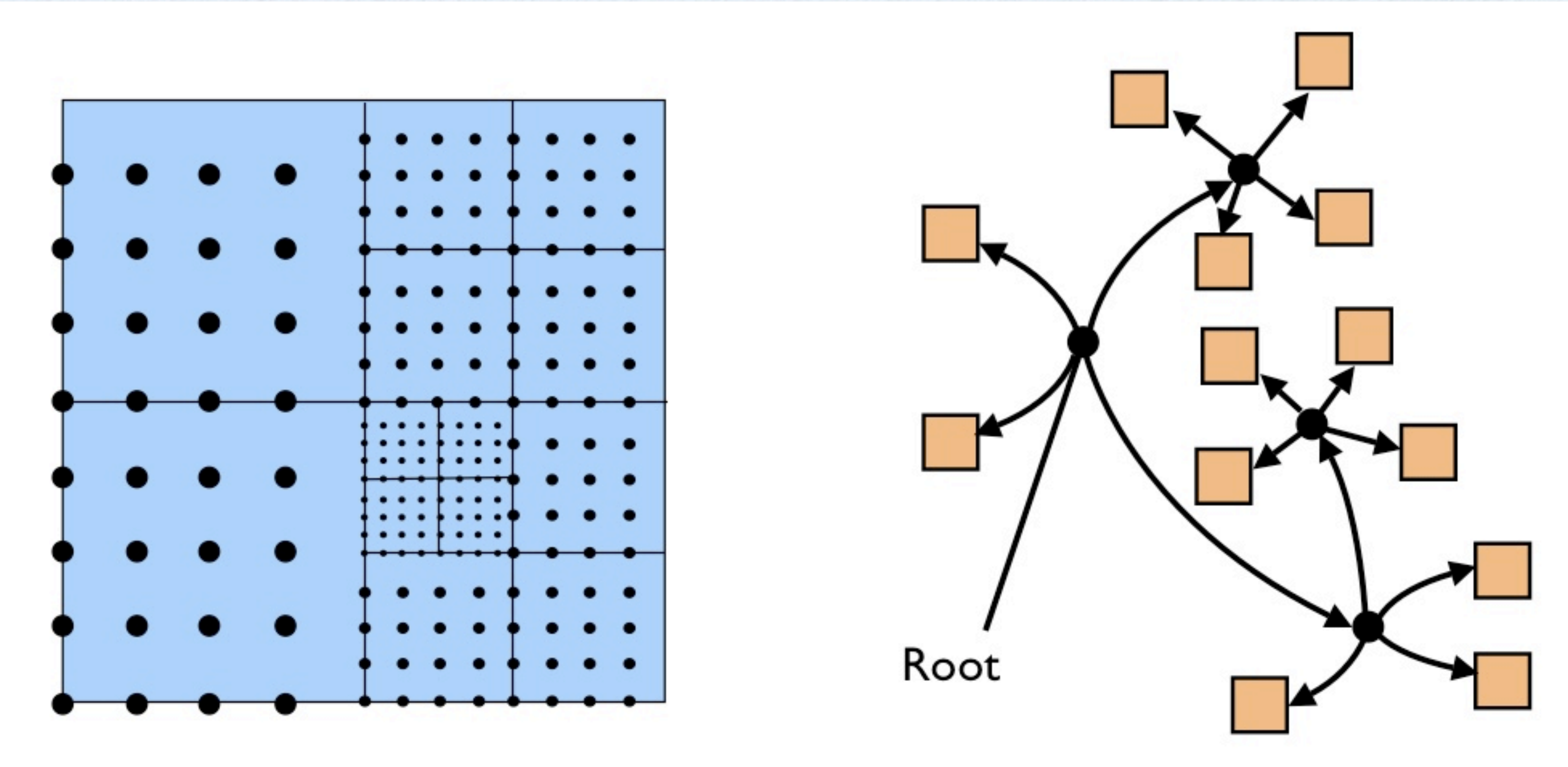
Convection of the Scale Distribution

- The scale distribution, i.e. the whole **adaptivity** structure of the grid is convected by the flow map in a **Lagrangian** way

- Buffer sizes are bounded by $\lceil \frac{1}{2}\, supp(M) + \mathrm{LCFL} \rceil$

- Independence of CFL

Multi-core: Blocked Grid



- Neighbors look-up: less memory indirections
- Less #ghosts

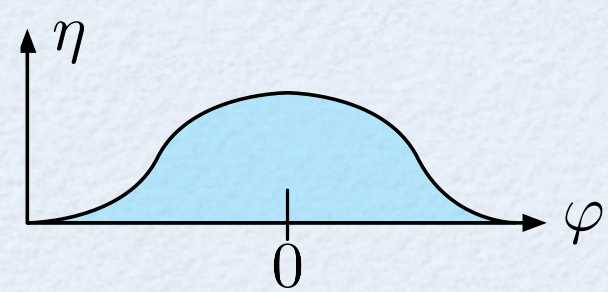
Wavelet Adapted Particle Level Sets

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

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0\,.$$

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

OFTEN "Narrow Band" formulation (Adalsteinsson & Sethian, 1995)

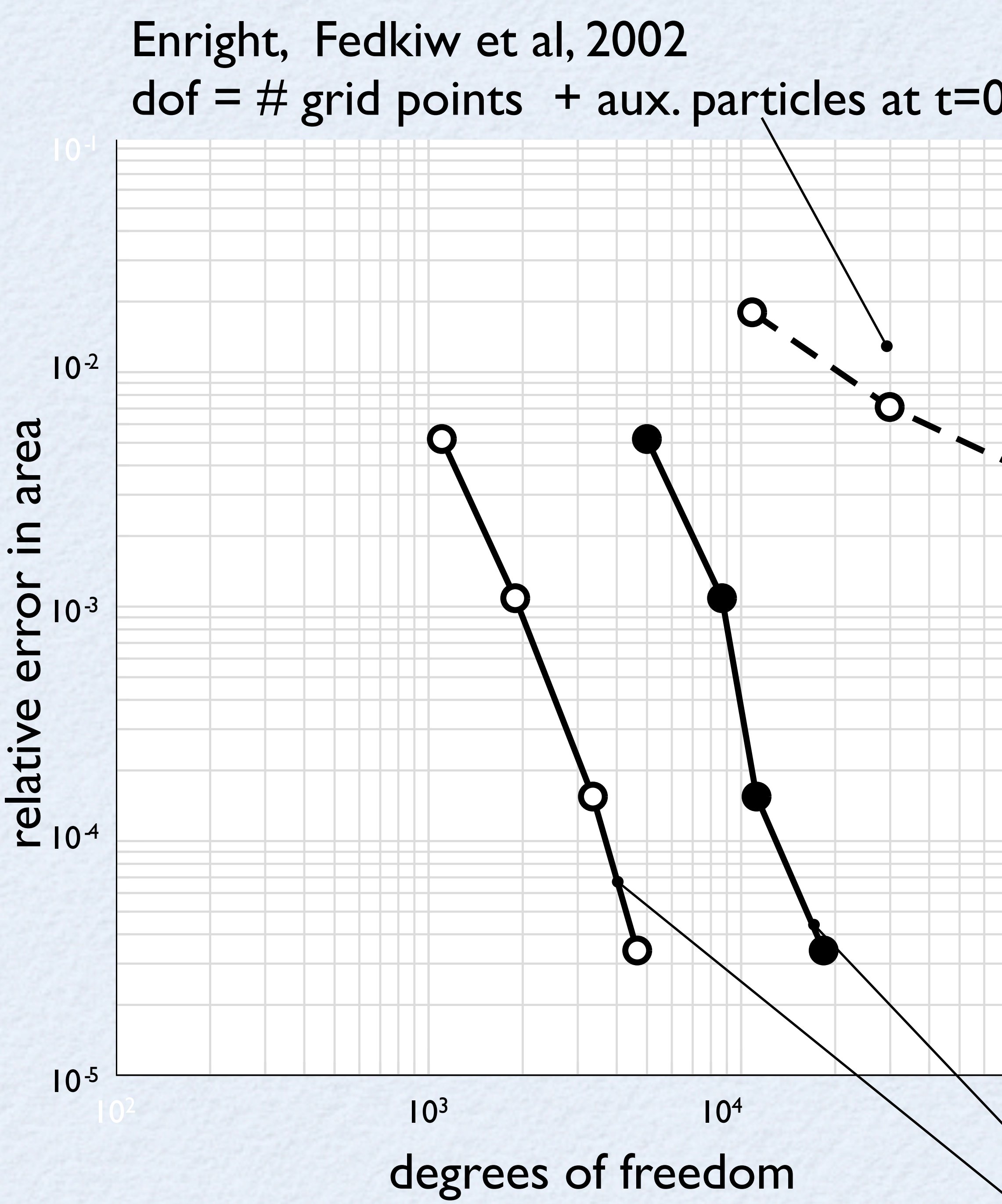


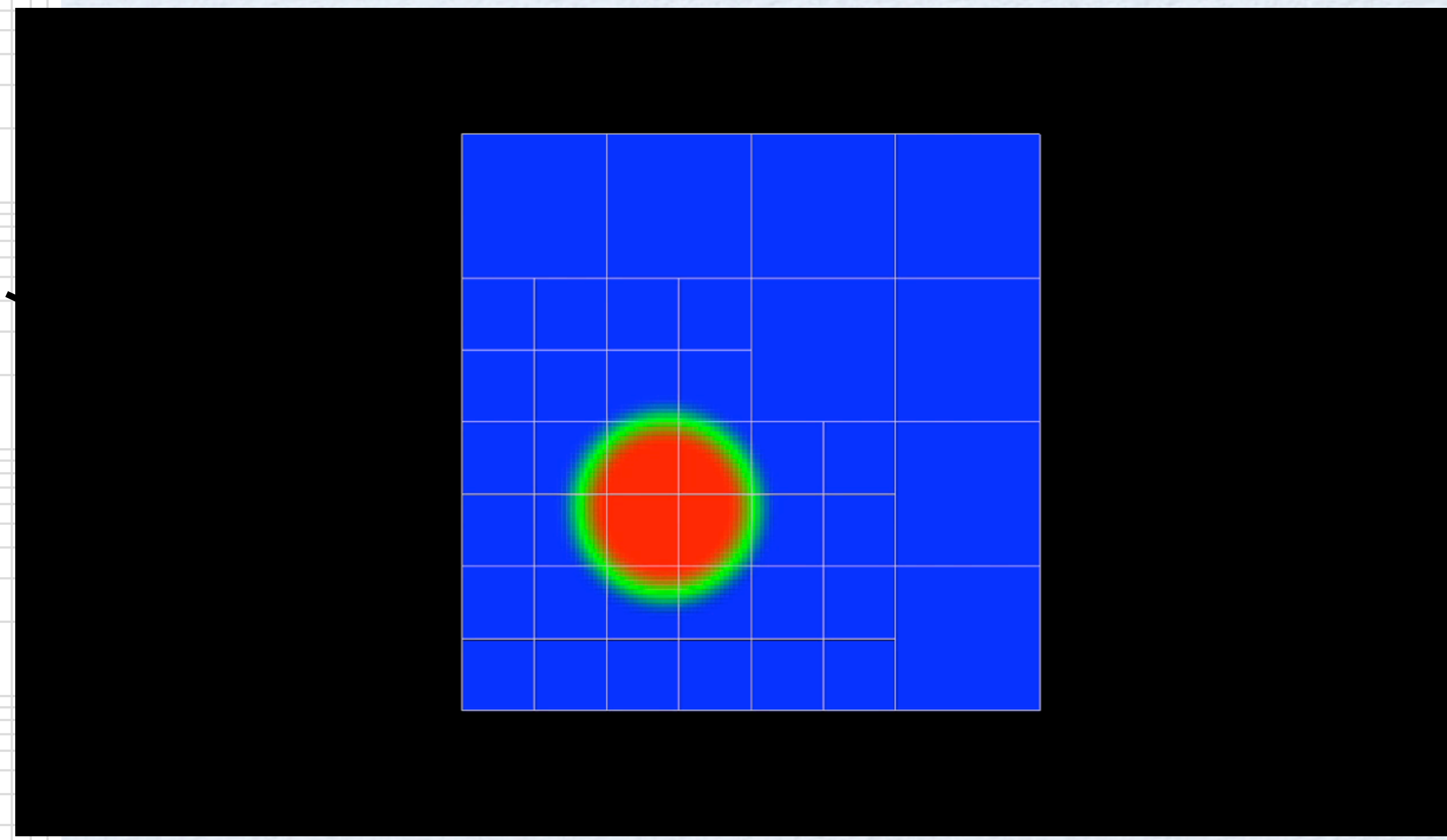
FREE by virtue of adaptivity
Smooth truncation of detail coefficients: $d_{\boldsymbol{k}}^{l,m} \leftarrow d_{\boldsymbol{k}}^{l,m}\, \eta\left(\phi\left(h^{l+1}\right)^{-1}\right)$

Reinitialization: $$\frac{\partial \phi}{\partial \tau} + sign\,(\phi)(|\nabla \phi| - 1\,) = 0$$

(Sussman et al. 1994)

MULTIRESOLUTION LEVEL SETS





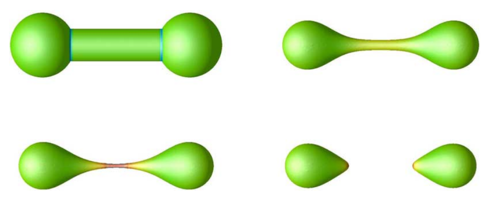
$CFL_{max} \sim 40$

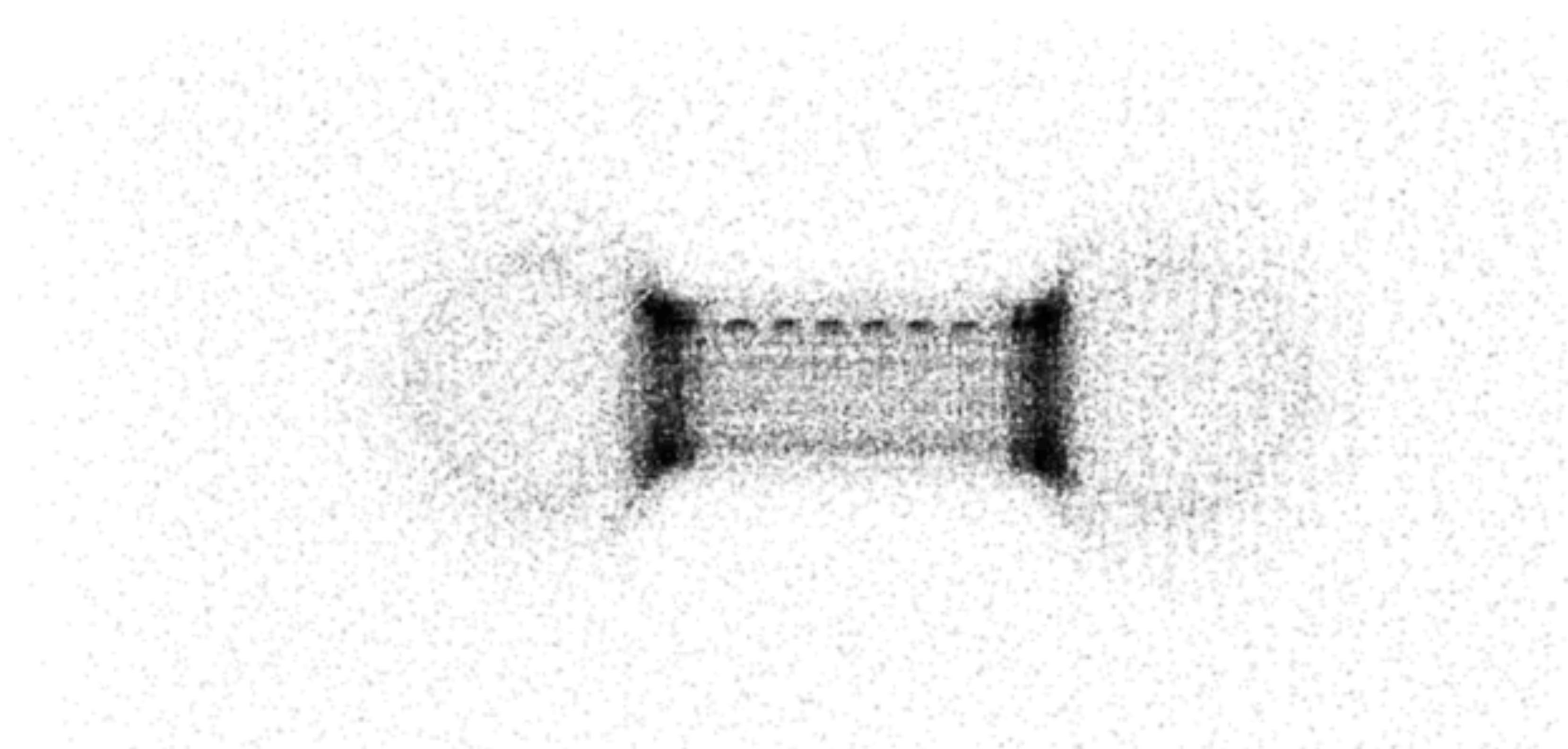
Results: Level sets

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

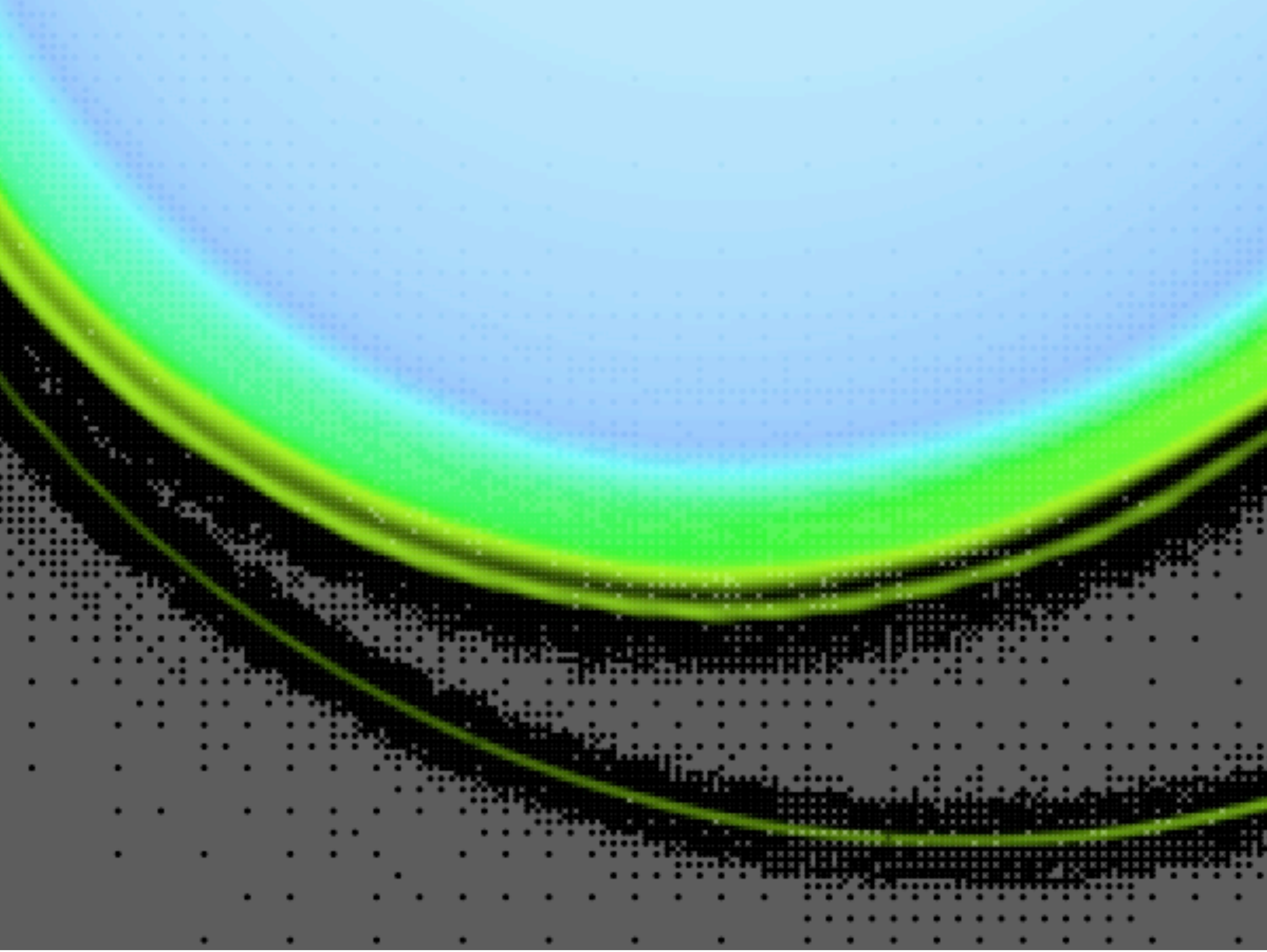
$$\frac{\partial \phi}{\partial t} + \kappa\, \boldsymbol{n} \cdot \nabla \phi = 0.$$

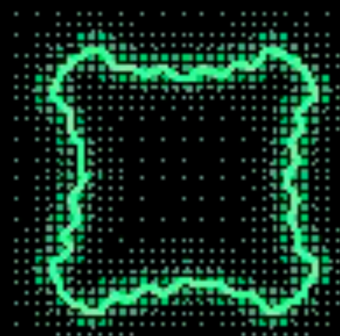
$$\kappa = \nabla \cdot \boldsymbol{n}$$



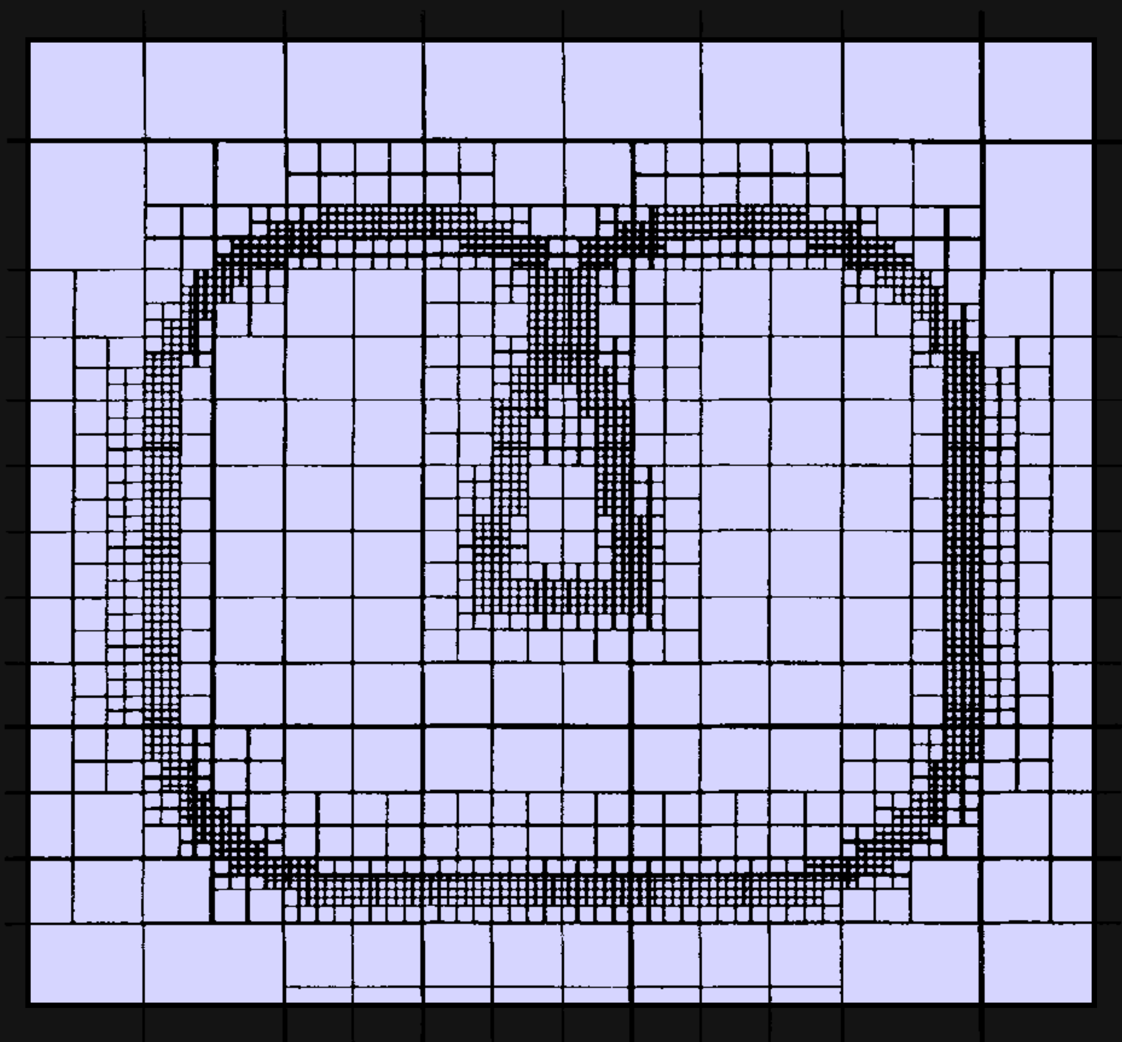


distribution of active particles

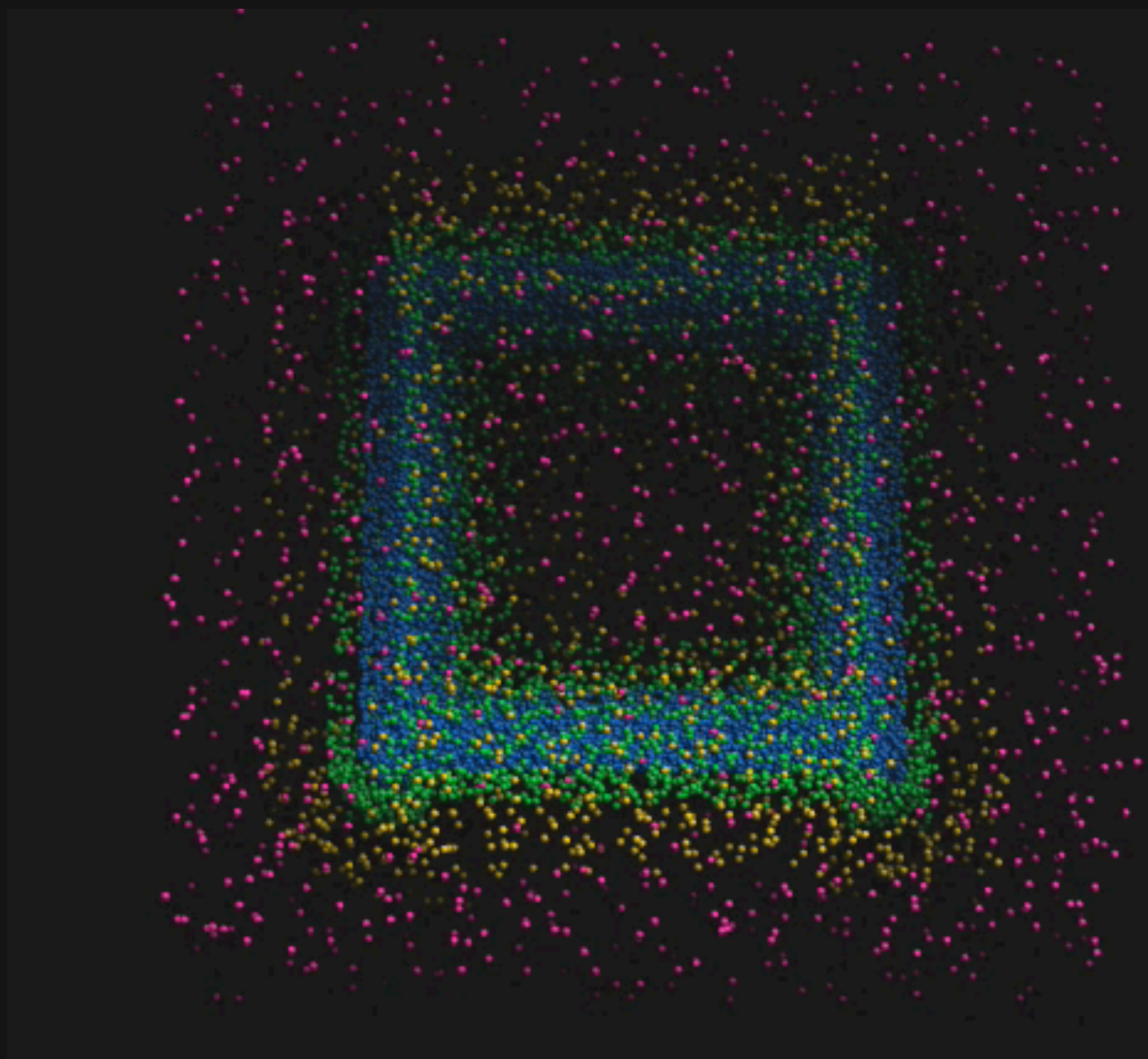




Multiresolution Level sets



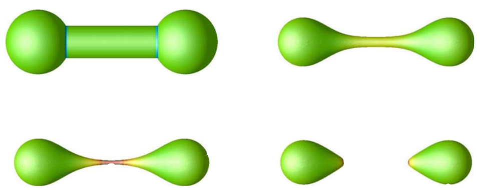
Losasso, Fedkiw et al.

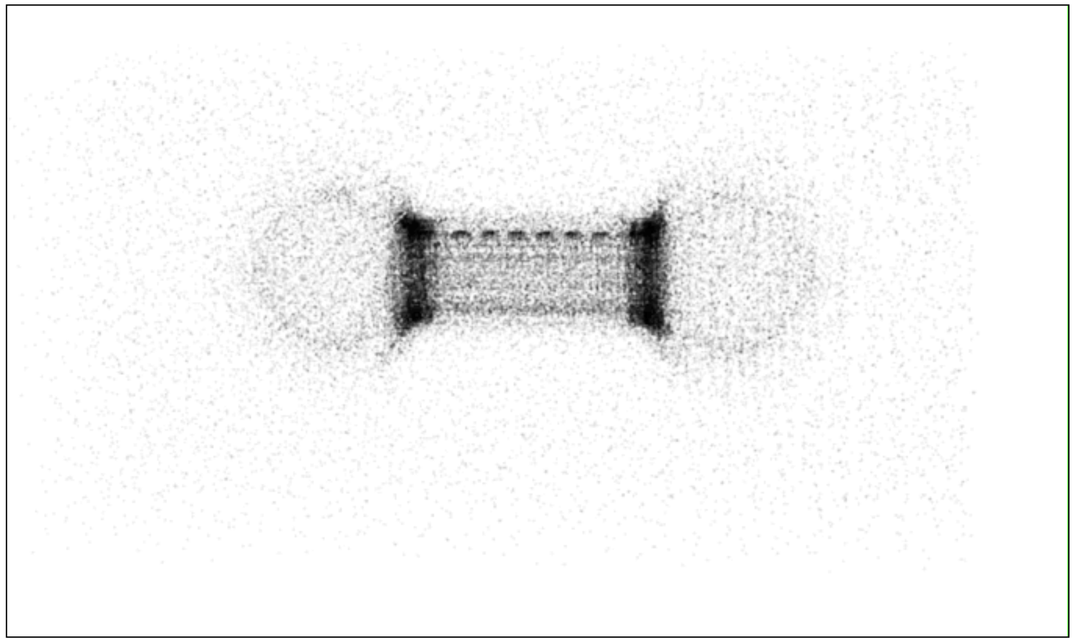


Simulation of 3D curvature-driven flow

Collapsing Dumbbell

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

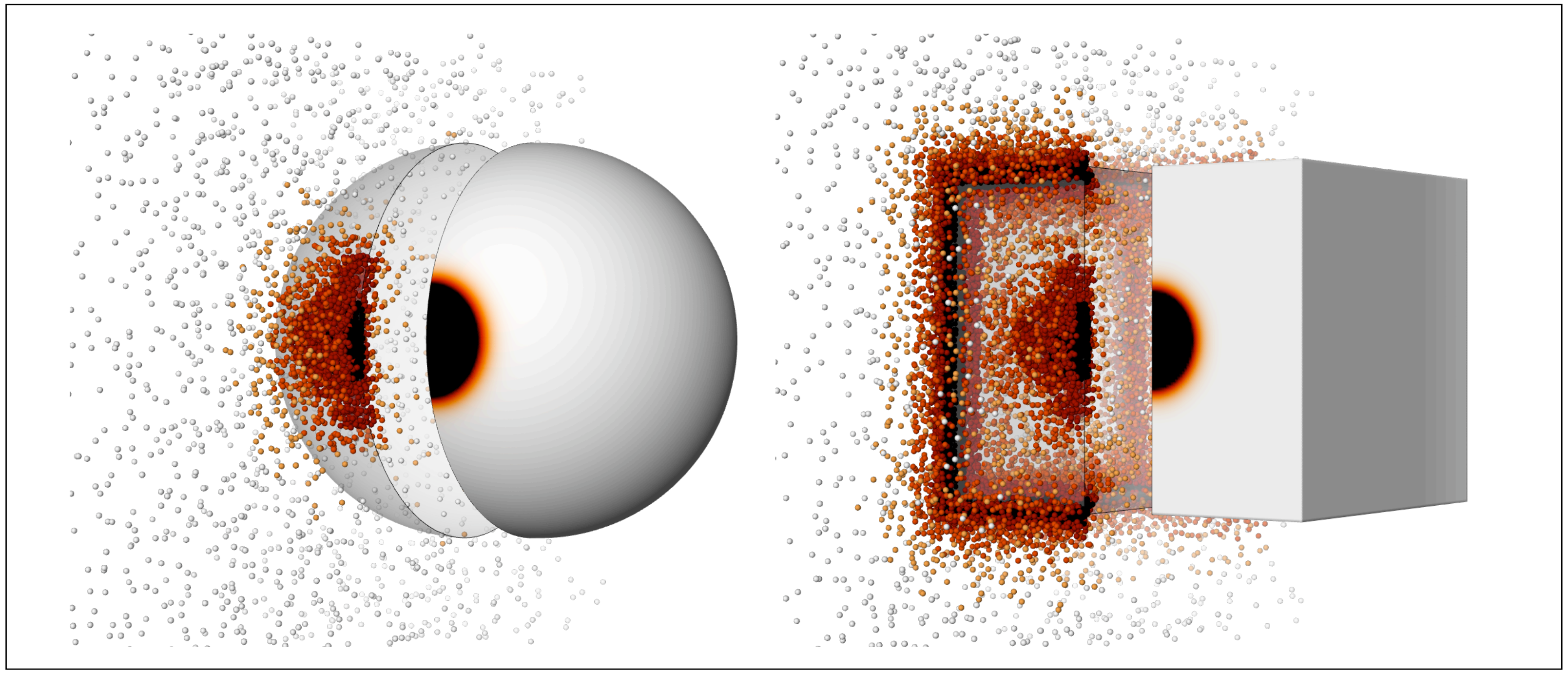




“Surfactant” dynamics

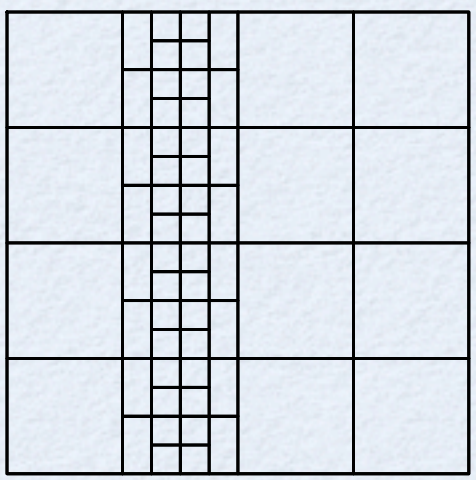
Adapt to:

- complex geometric features of Γ
- small scales of functions defined on Γ



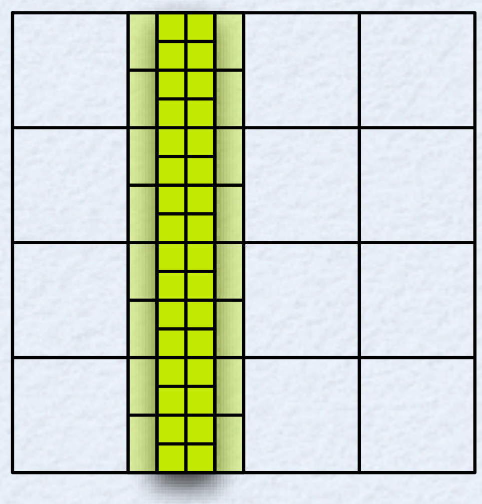
Lagrangian transport of multiscale information

Particle methods: possibly **CFL >> 1** ⇒ Traditional approaches become **inefficient**

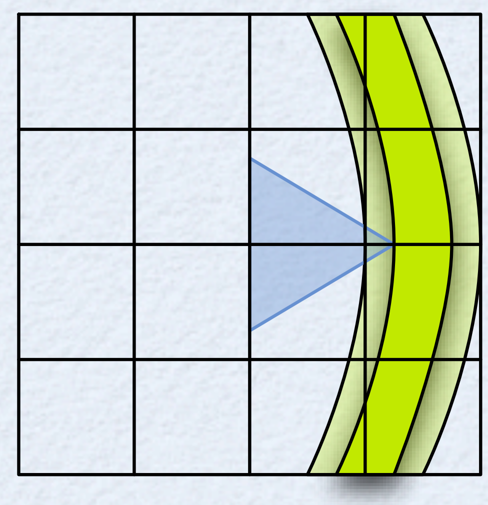


MRA adapts grid

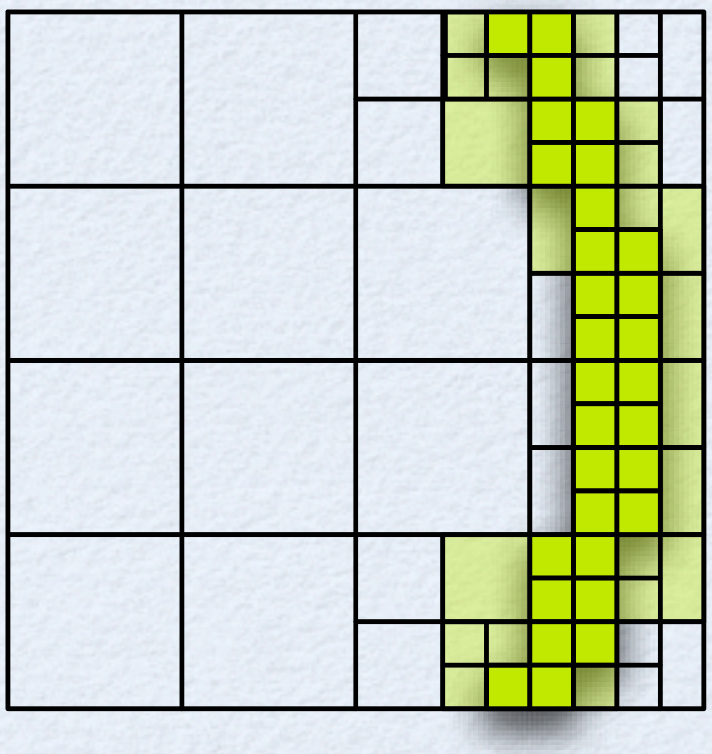
$\mathcal{K}_>(t)$



Create particles with indicator



Interpolate indicator onto grid



Indicator defines new grid $\mathcal{K}_>(t+\delta t)$

Interpolation of particle quantities onto this is **consistent**

MRA on $\mathcal{K}_>(t+\delta t)$