HPC for Flow Simulations across Scales and Disciplines

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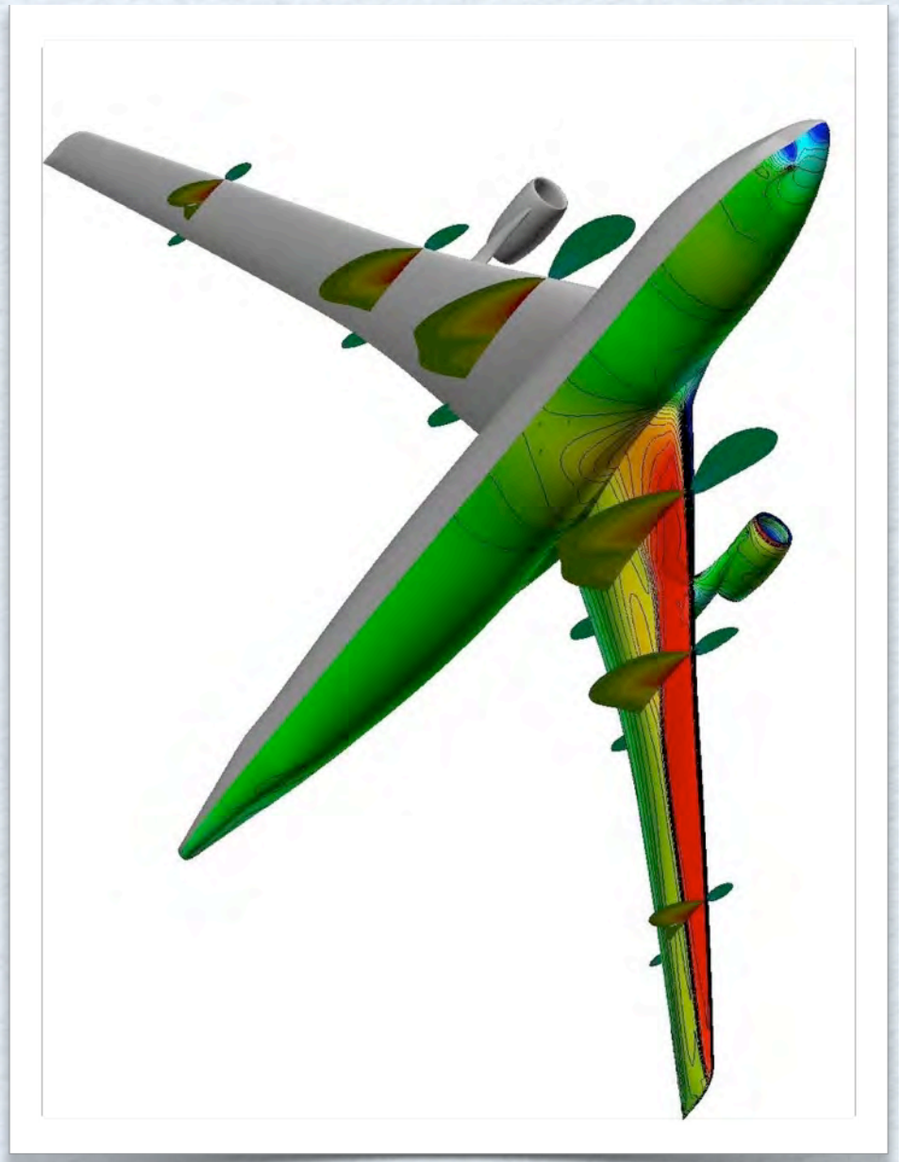
OUTLINE

- **INTRODUCTION**
- **Particles for Continuum Flows**
  - Particle Methods + Grids
  - **Multi**-Resolution for Grids/Particles
  - Multi/Many core Implementations
- **Particles for Atomistic Flows**
  - Uncertainty Quantification + Propagation
- **SUMMARY**

Simulation and Technology

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



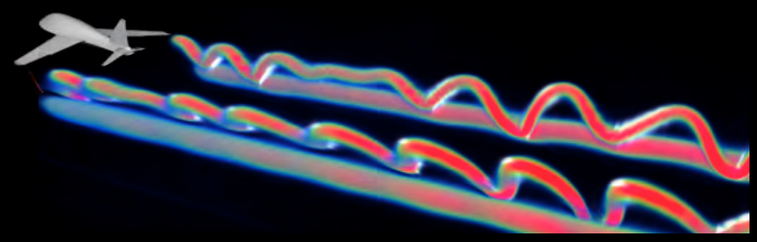
Simulation and Medicine

- Heuristics and Data
- Models ?

Dreamstime.com

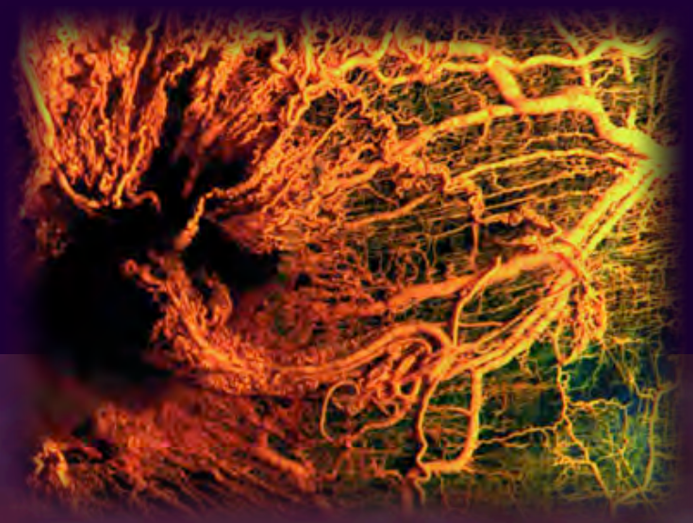
16384 Cores - 10 Billion Particles - 60% efficiency

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



credit : Roche

Multi-scale Modeling of Angiogenesis

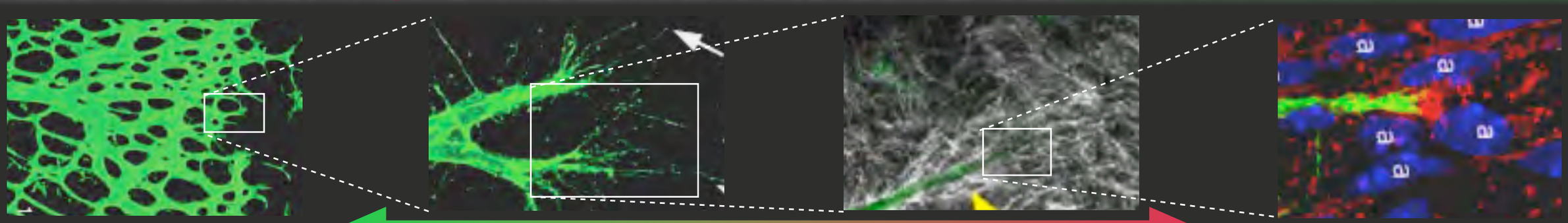
Milde F., Bergdorf M., Koumoutsakos P., A Hybrid Model for 3D Simulations of Sprouting Angiogenesis, **Biophysical J.**,2008

Vasculature

Tip Cell

ECM

Growth Factors



[1] H. GERHARDT, M. GOLDING, M.FRUTTIGER, C. RUHRBERG, A. LUNDKVIST A. ABRAMSSON, M. JELTSCH C. MICHELL, . ALITALO, D. SHIMA AND C. BETSHOLTZ, VEGF GUIDES ANGIOGENIC SPROUTING UTILIZING ENDOTHELIAL TIP CELL FILOPODIA, J. CELL. BIOL., 2003

Angiogenesis : *in silico*

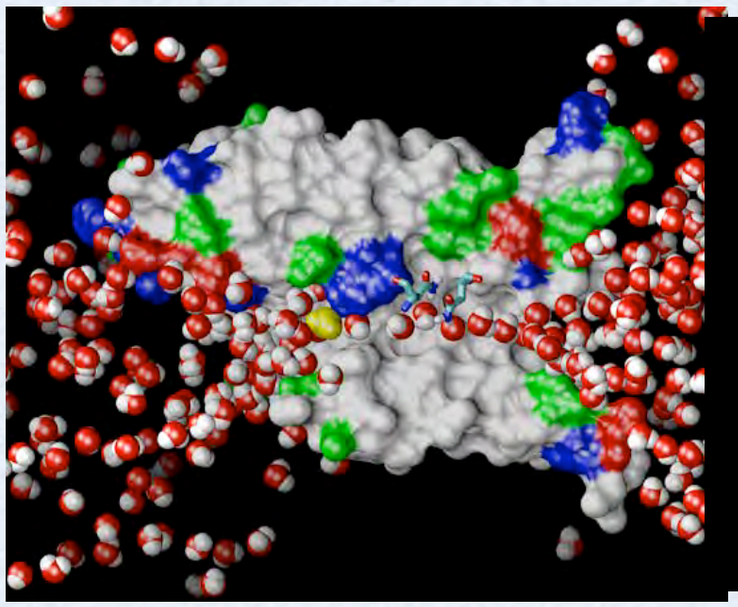
Koumoutsakos et al., The fluid Mechanics of Cancer and its Therapy, Ann. Rev. Fluid Mech. , 2013

Milde F.,et al., A hybrid model of sprouting angiogenesis, Biophysical J.. 2008

PARTICLE METHODS

Molecular Dynamics

-9



Transport in aquaporins
Schulten Lab, UIUC

Vortex Methods

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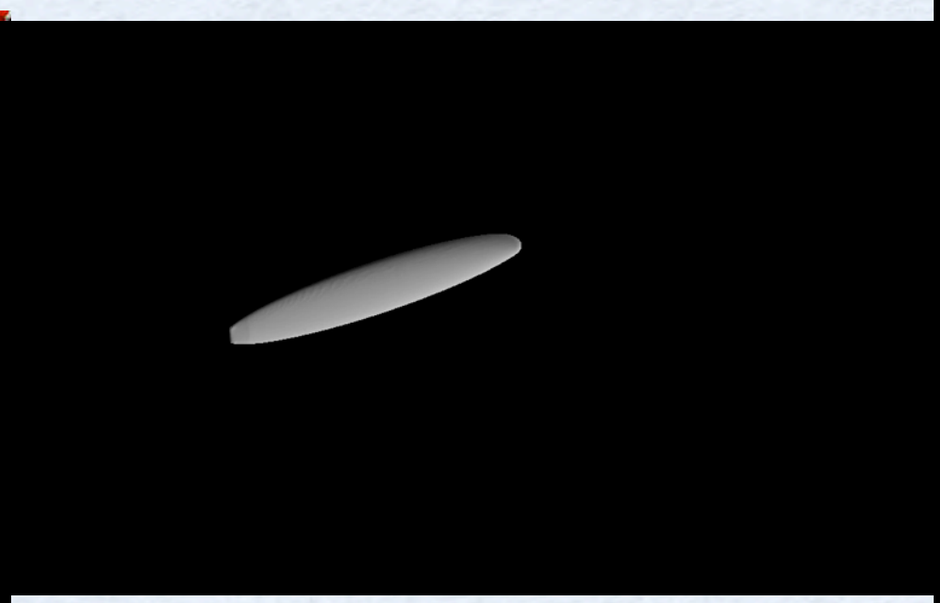
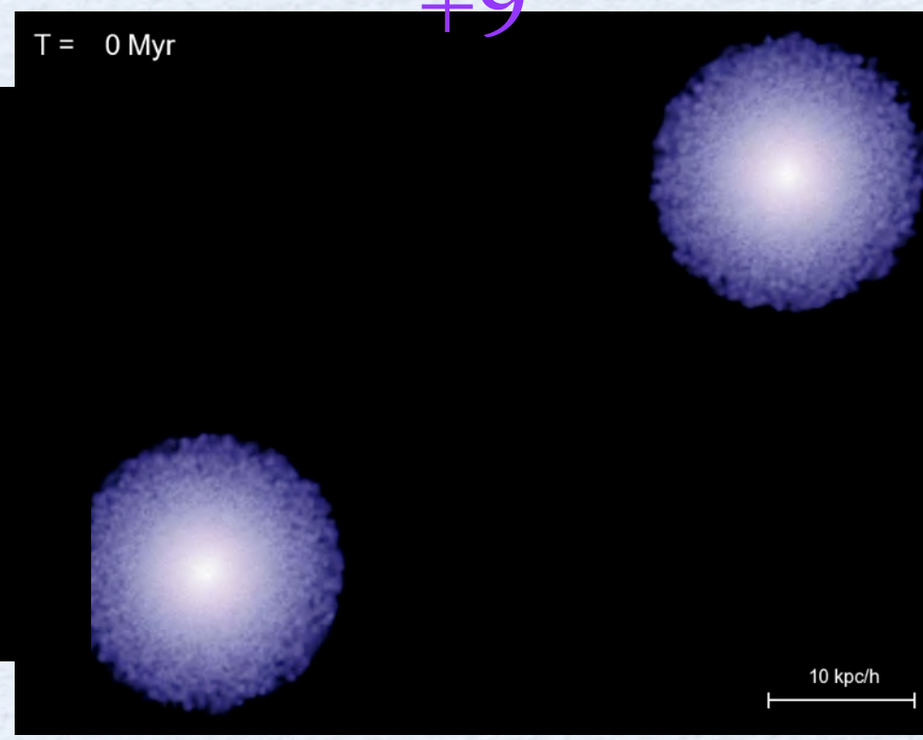


Vortex Dynamics
Koumoutsakos Lab, ETHZ

Smoothed Particle Hydrodynamics

+9



Growth of Black Holes
Springel, MPI - Hernquist, Harvard

PARTICLES : Lagrangian, Conservation and Other Laws

P. Koumoutsakos, Ann. Rev. Fluid Mech., 2005

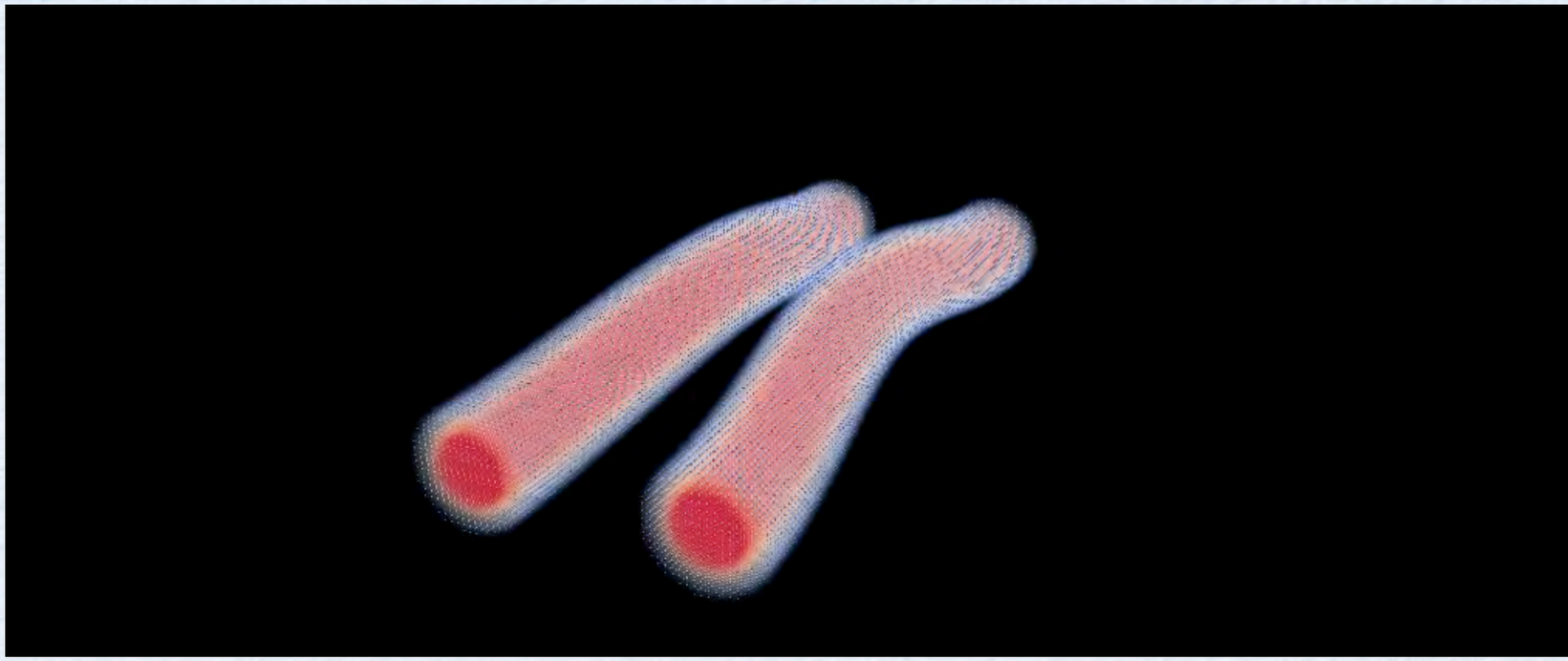
SPH, Vortex Methods

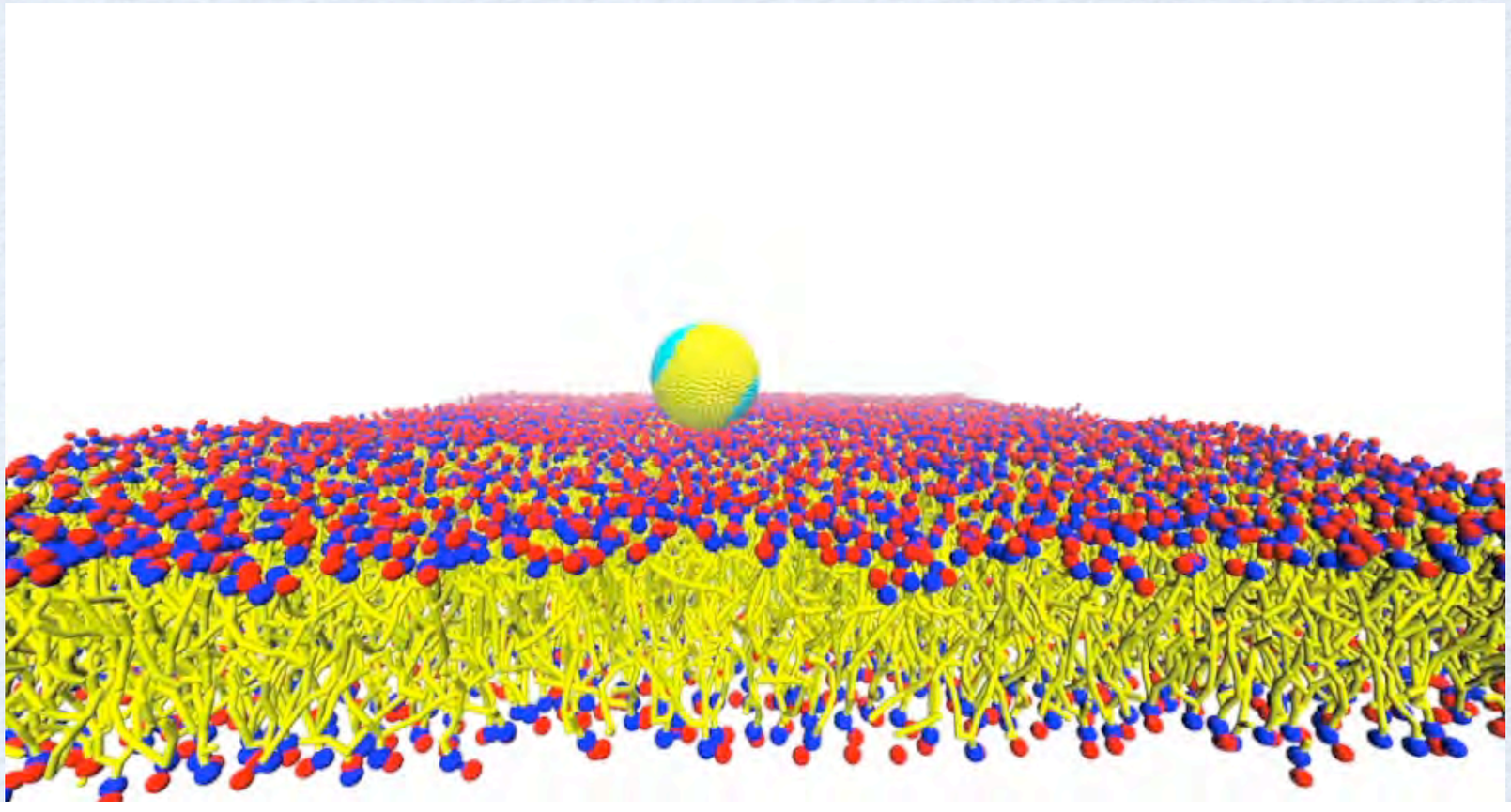
$$\rho_p \frac{D\mathbf{u_p}}{Dt} = (\nabla \cdot \sigma)_p$$

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

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

MD, DPD, CGMD





PARTICLE SIMULATIONS ACROSS SCALES

COMMON MODULES

1. TIME INTEGRATORS
2. NEIGHBOR LISTS : FAR/CLOSE PARTICLES
3. POISSON SOLVERS
4. FAST SUMMATION ALGORITHMS
5. PARTICLE - MESH
6. DERIVATIVES ON GRIDS AND PARTICLES

PART 1 :

Particles for Continuum Flows

van Rees, W.M., Hussain, F. and Koumoutsakos, P., Vortex tube reconnection at Re=10^4. **Physics of Fluids**, 24(7):075105, 2012.

FUNCTIONS and PARTICLES

Integral Function Representation

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

Function Mollification

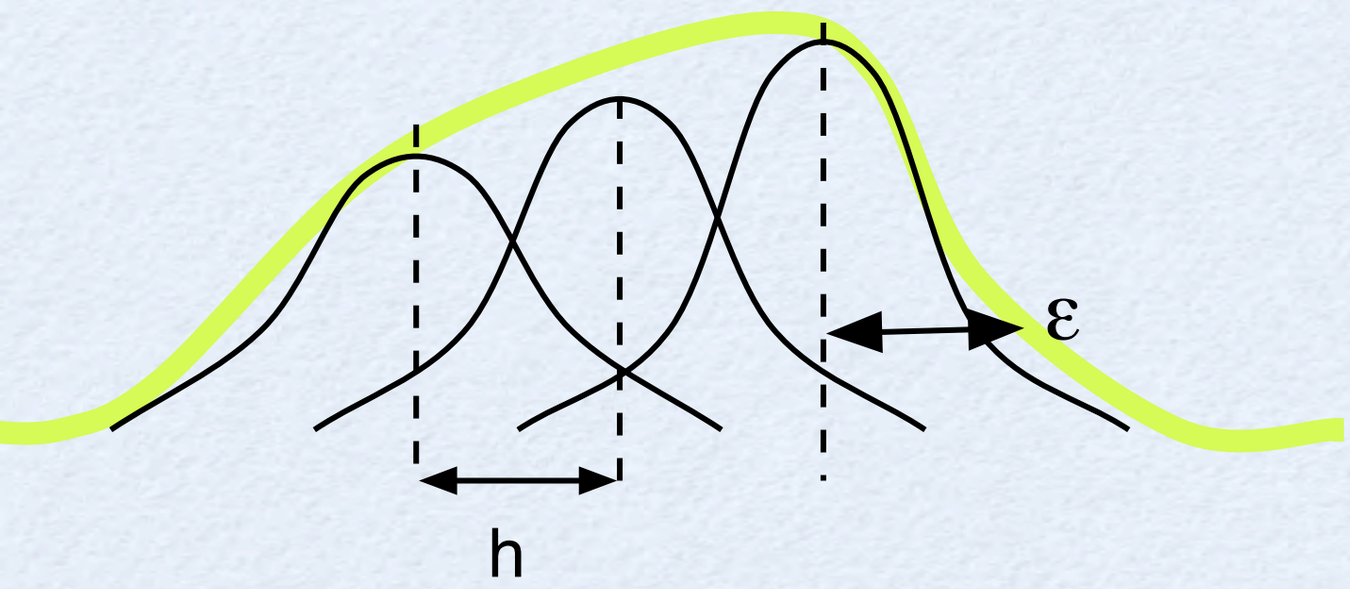
$$\Phi_\epsilon(x) = \int \Phi(y)\,\zeta_\epsilon(x-y)\,dy$$

Point Particle Quadrature

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

Smooth Particle Quadrature

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



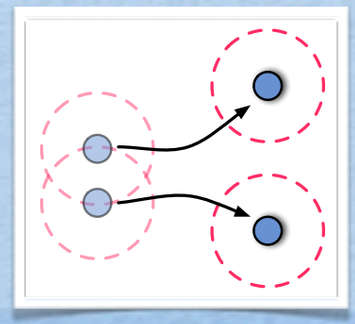
TOTAL ERROR

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

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

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

LAGRANGIAN DISTORTION



- particles location distortion -> loss of overlap -> no convergence

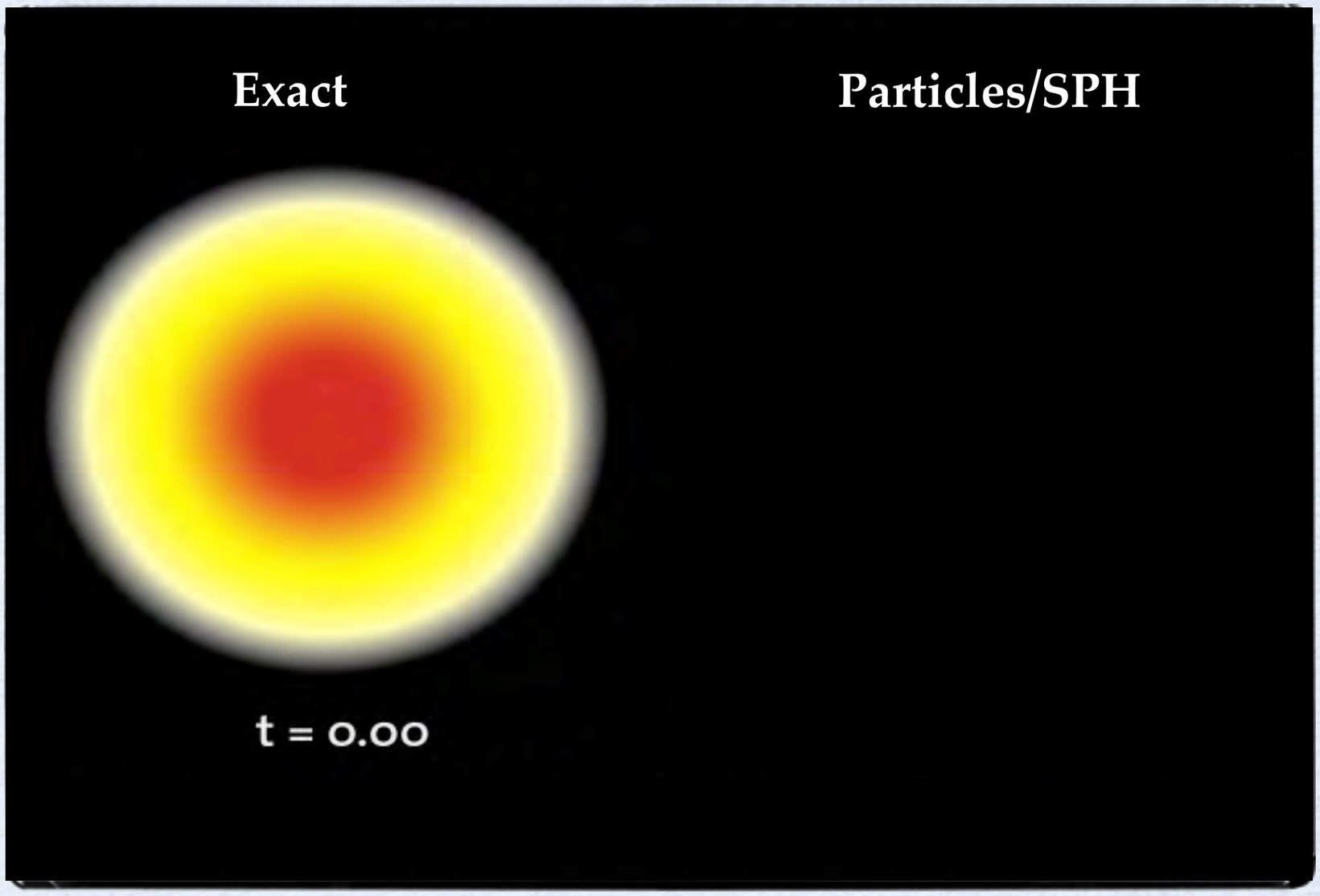
EXAMPLE : Incompressible 2D Euler Equations $\omega = \nabla \times \mathbf{u}$

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

Circular Patch = EXACT soln.

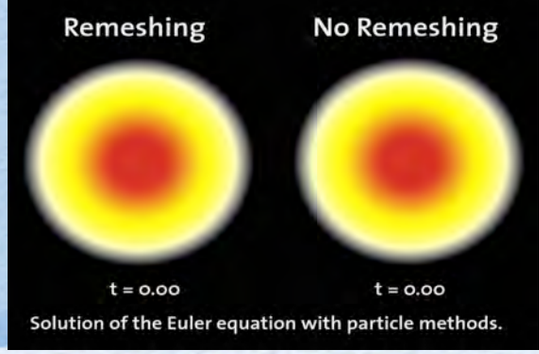
Need $h/\varepsilon < 1$ for accuracy

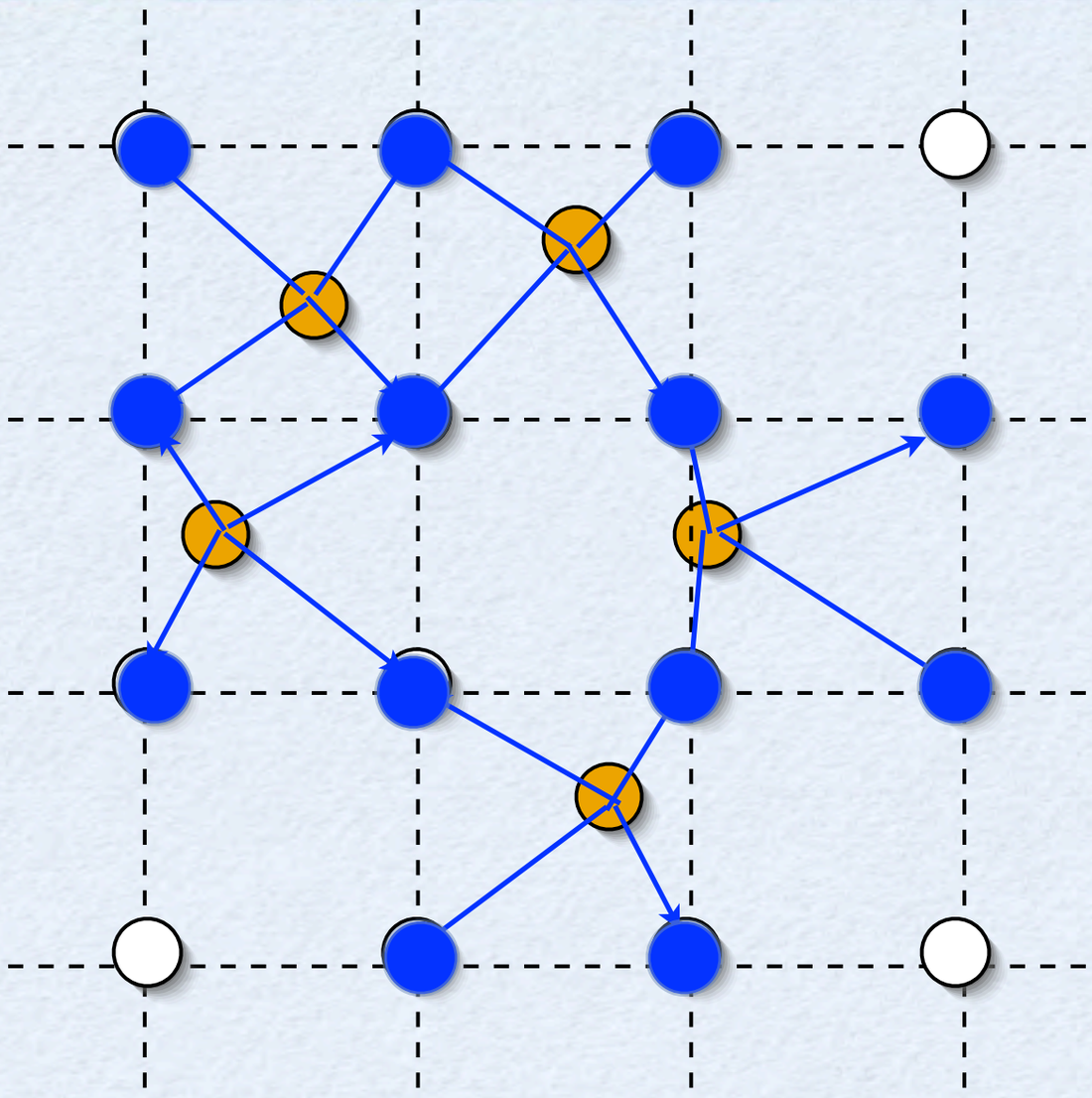
PARTICLES MUST OVERLAP



Particle Remeshing

P. Koumoutsakos, Inviscid axisymmetrization of an elliptical vortex, **J. Comput. Phys.**, 1997





Moment Conserving Interpolation

$$Q_j = \sum_{j=1}^{M} Q_p \; \Lambda(j\,h - x_p)$$

1D : # grid points = # Moments

2/3D : CARTESIAN GRIDS

+

Tensorial products

Finite Differences are a Subset of Remeshed Particle Methods

Rossinelli D., Conti C., Koumoutsakos P., Mesh-particle interpolations on GPUs and multicore CPUs, **Phil. Trans. R. Soc. A**, 369, pp. 2164-2175, 2011

remeshed PARTICLE METHODS (rPM)

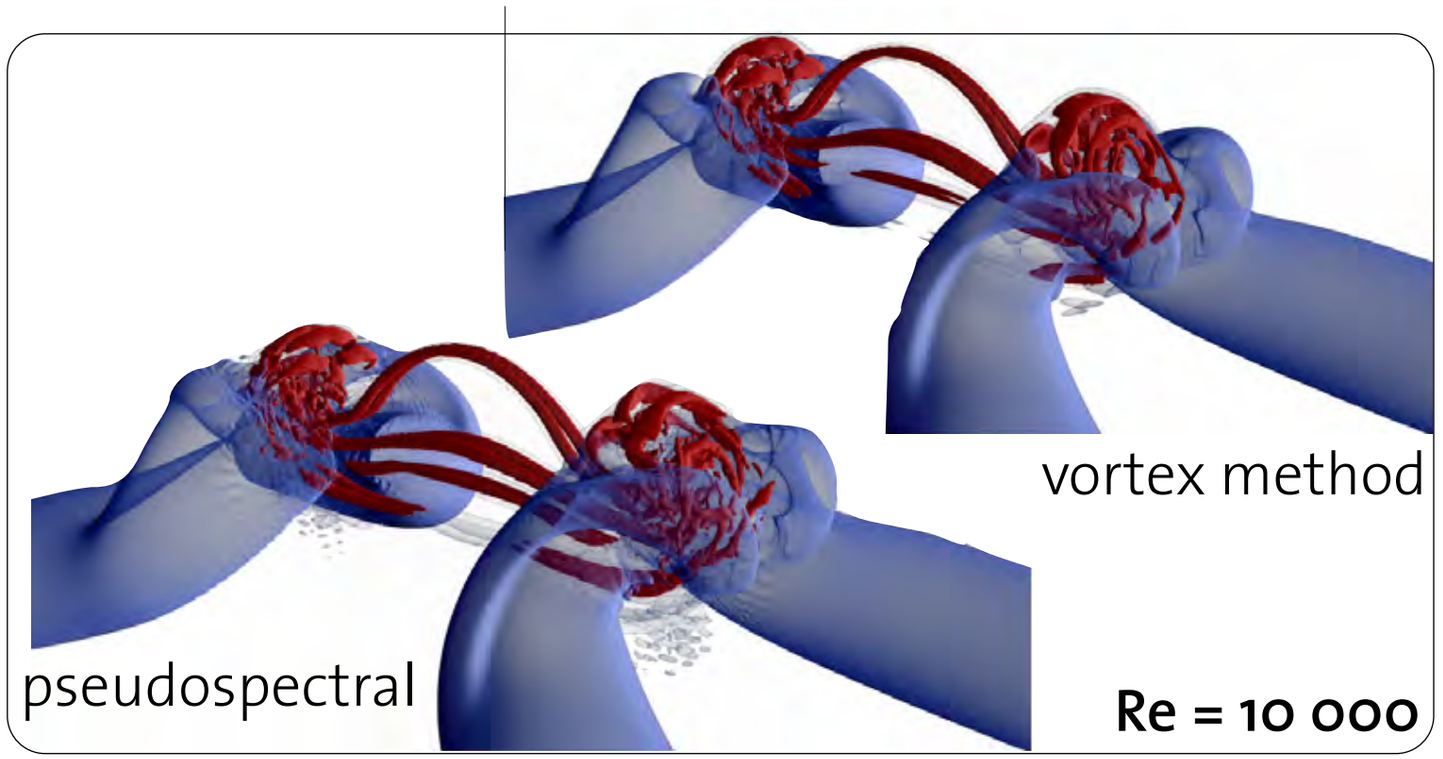
1.ADVECT : Particles ->Large CFL

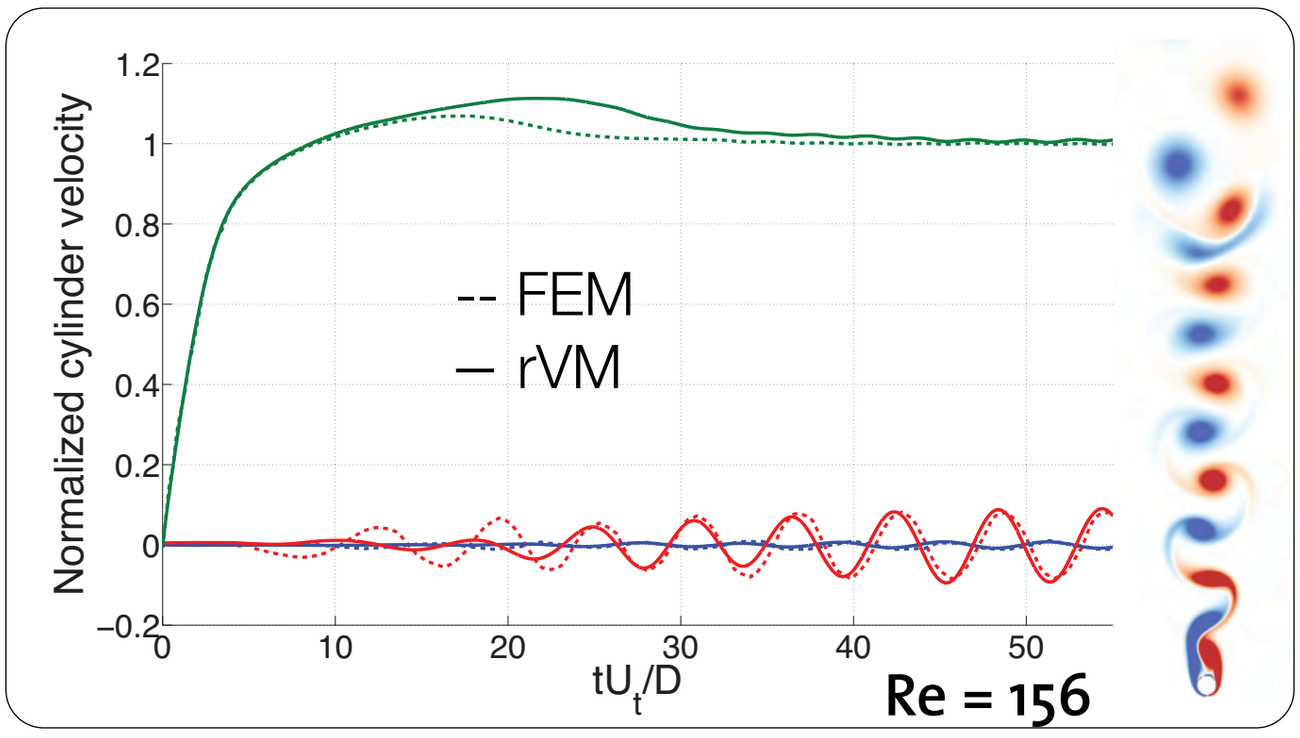
2.REMESH : Particles to Mesh -> Gather/Scatter

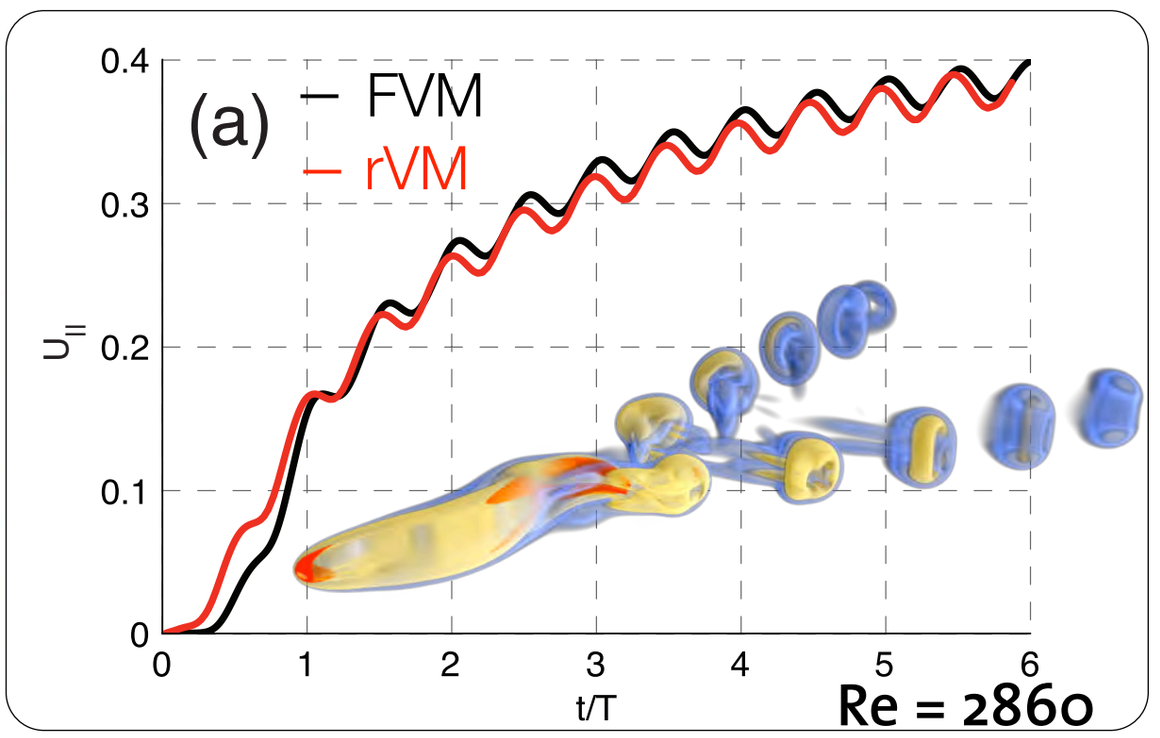
3.SOLVE:Poisson/Derivatives on Mesh ->FFTw/Ghosts

4:RESAMPLE: Mesh Nodes BECOME Particles

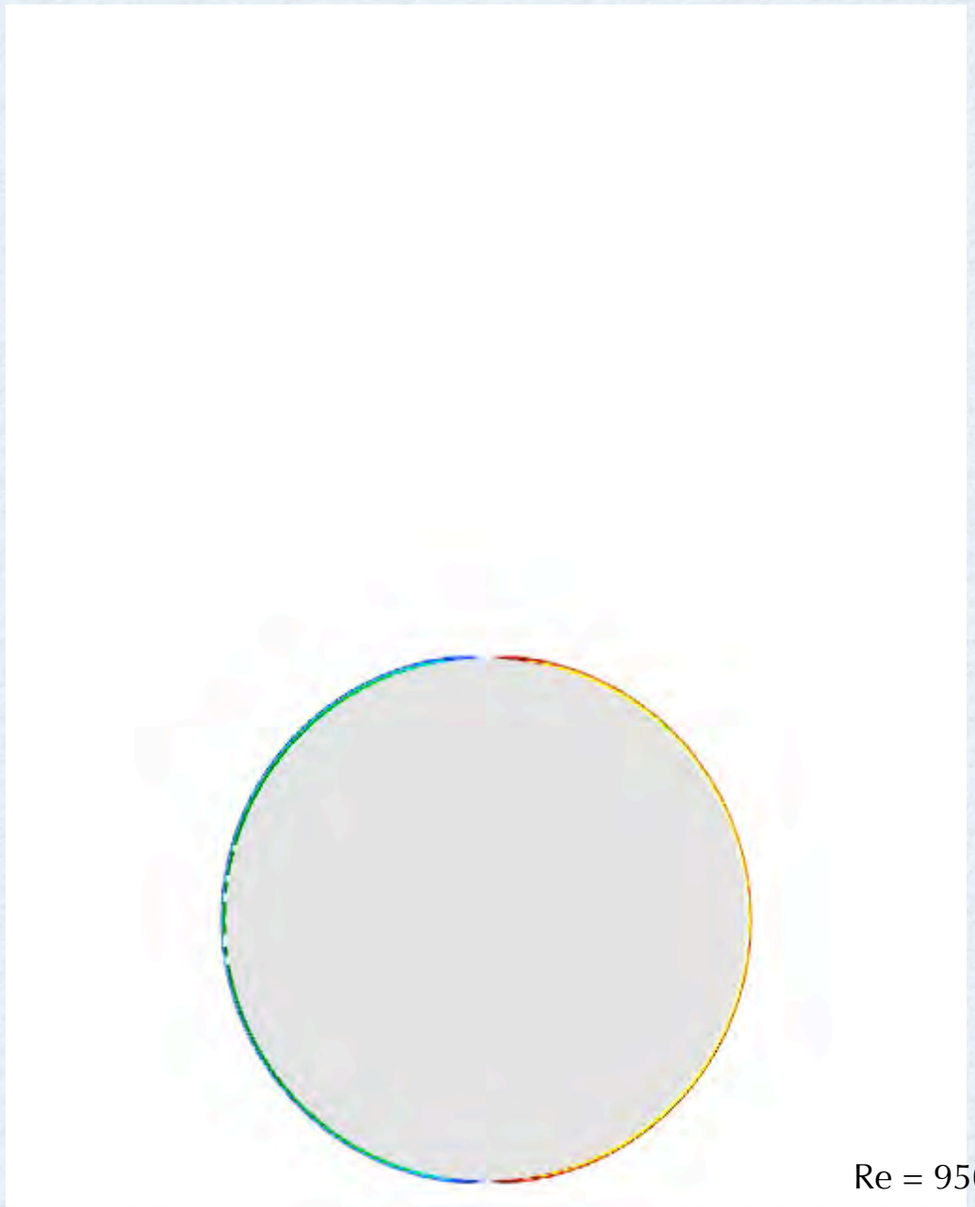
VALIDATION/VERIFICATION

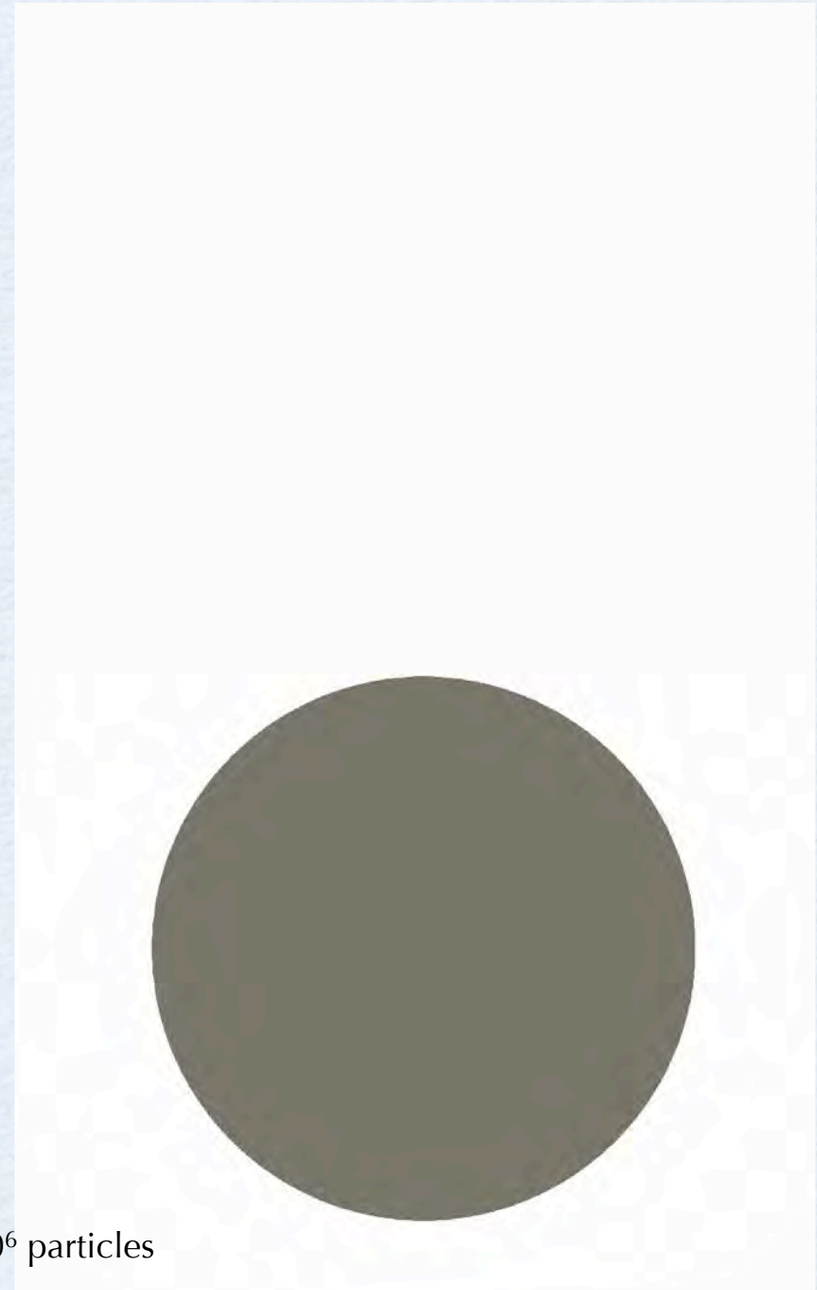






COMPUTERS





Re = 9500 ~ 10^6 particles

1995 **20 Days** on **CRAY YMP**

2011 **100sec** on GPU

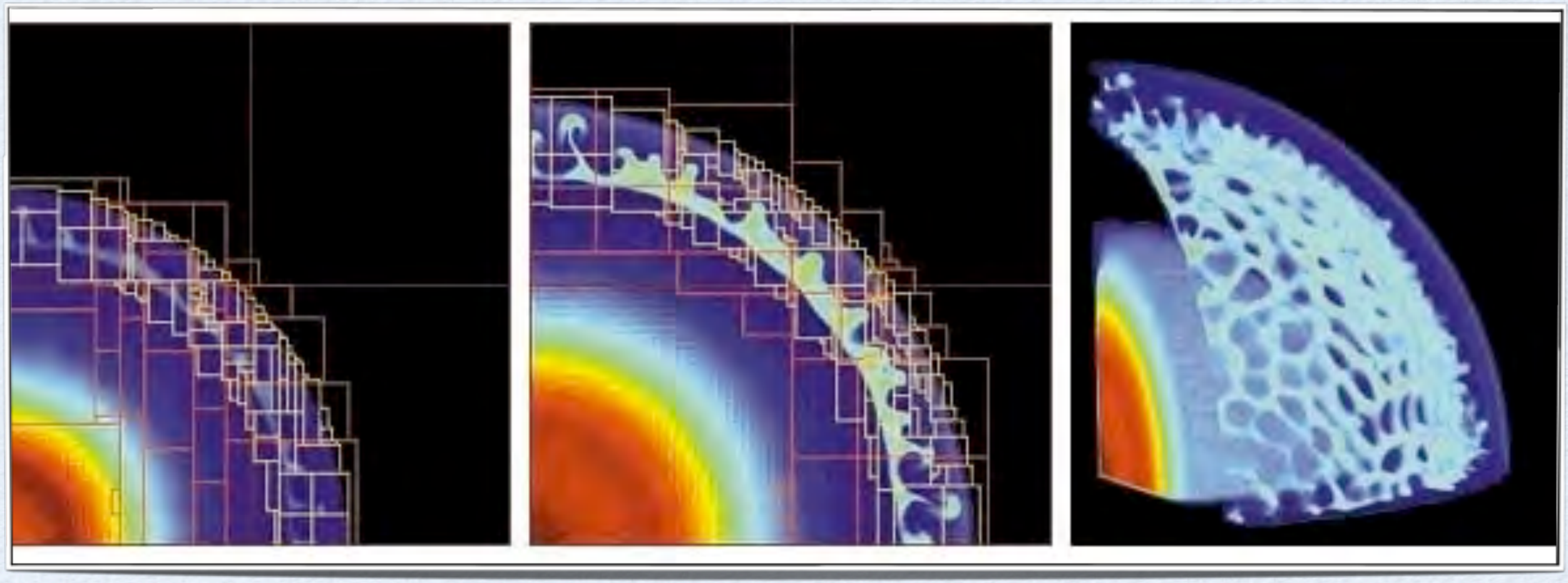
NOTE : ~18,000 speedup BUT ~100 comes out of time alone

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

Remeshed Particles: ADAPTIVE

Adaptive Mesh Refinement

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



- Support of unstructured grids
- Different mesh orientations

- Low compression rate
- No explicit control on the compression error

A better compression : **Wavelets**

50:1

rPM + WAVELET ADPTED GRIDS

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

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

"ground" level

detail coefficients

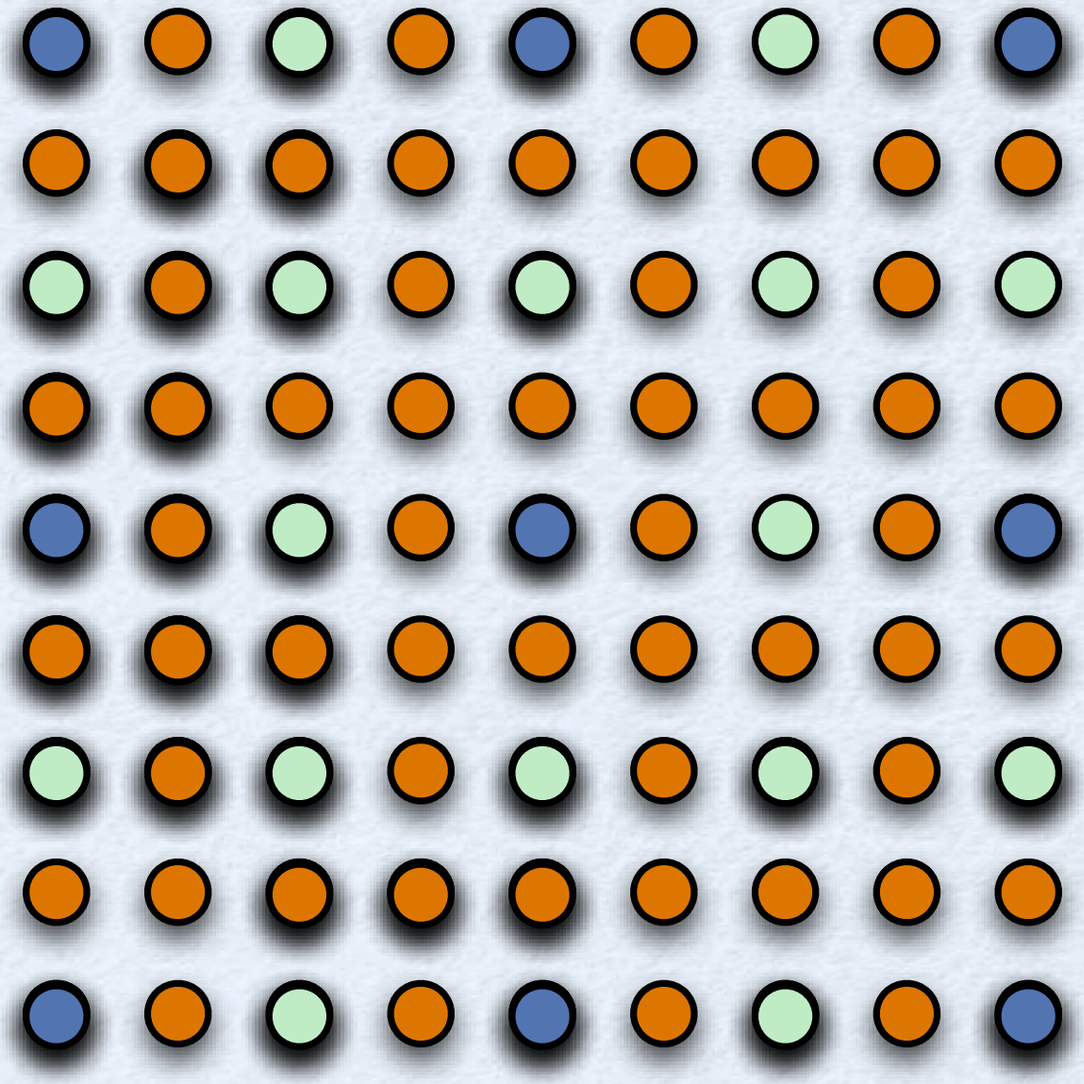
wavelets

Active Wavelet Coefficients

=

Active Grid Points

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

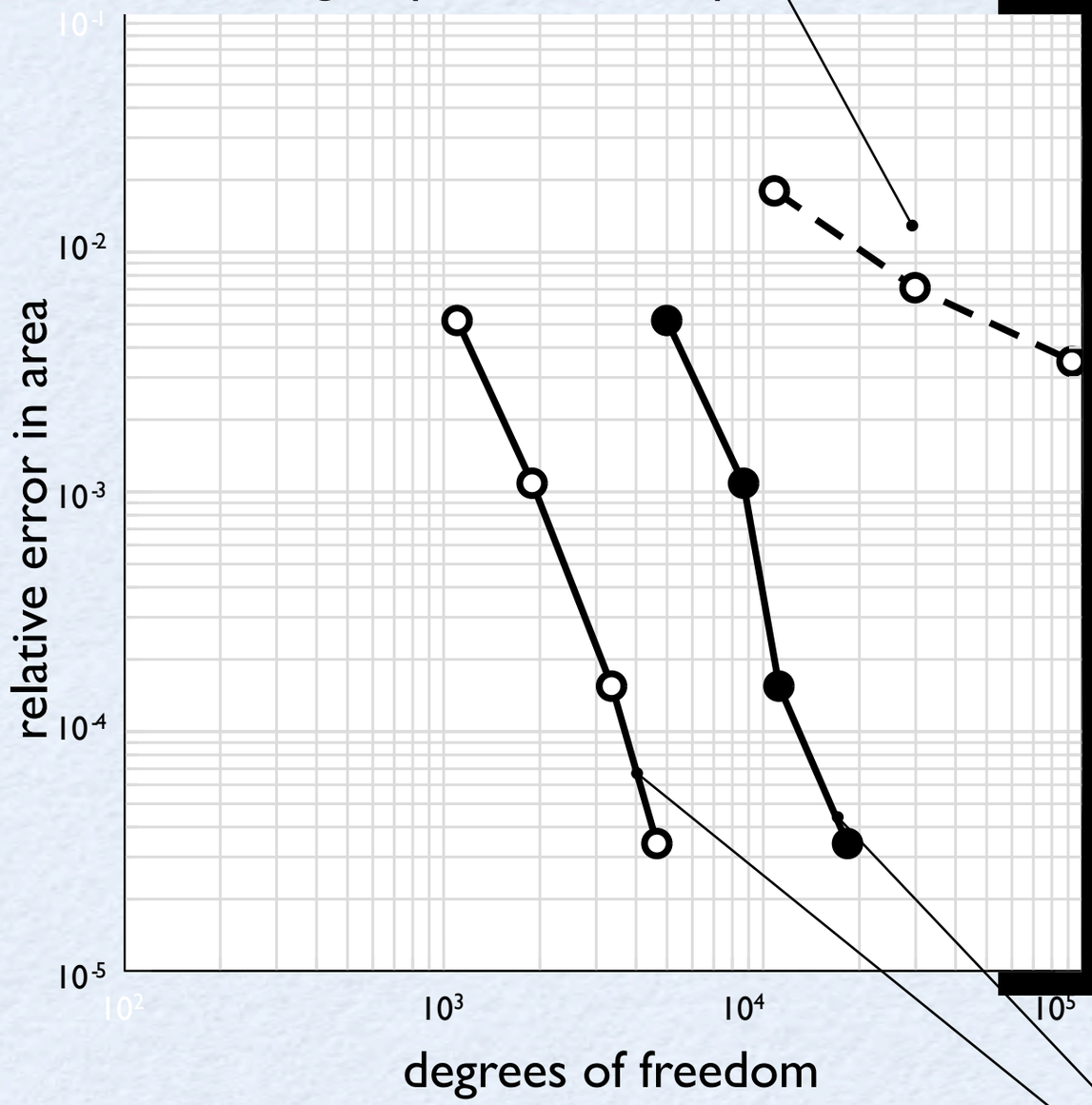


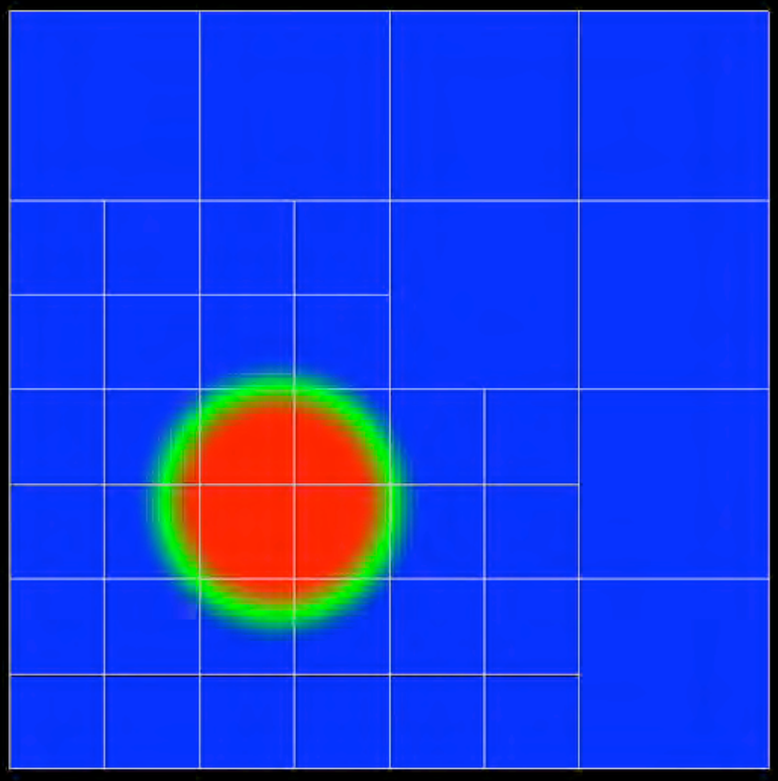
WAVELET ADAPTED LEVEL SETS

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

Enright, Fedkiw et al, 2002

dof = # grid points + aux. particles at t=





Present Method

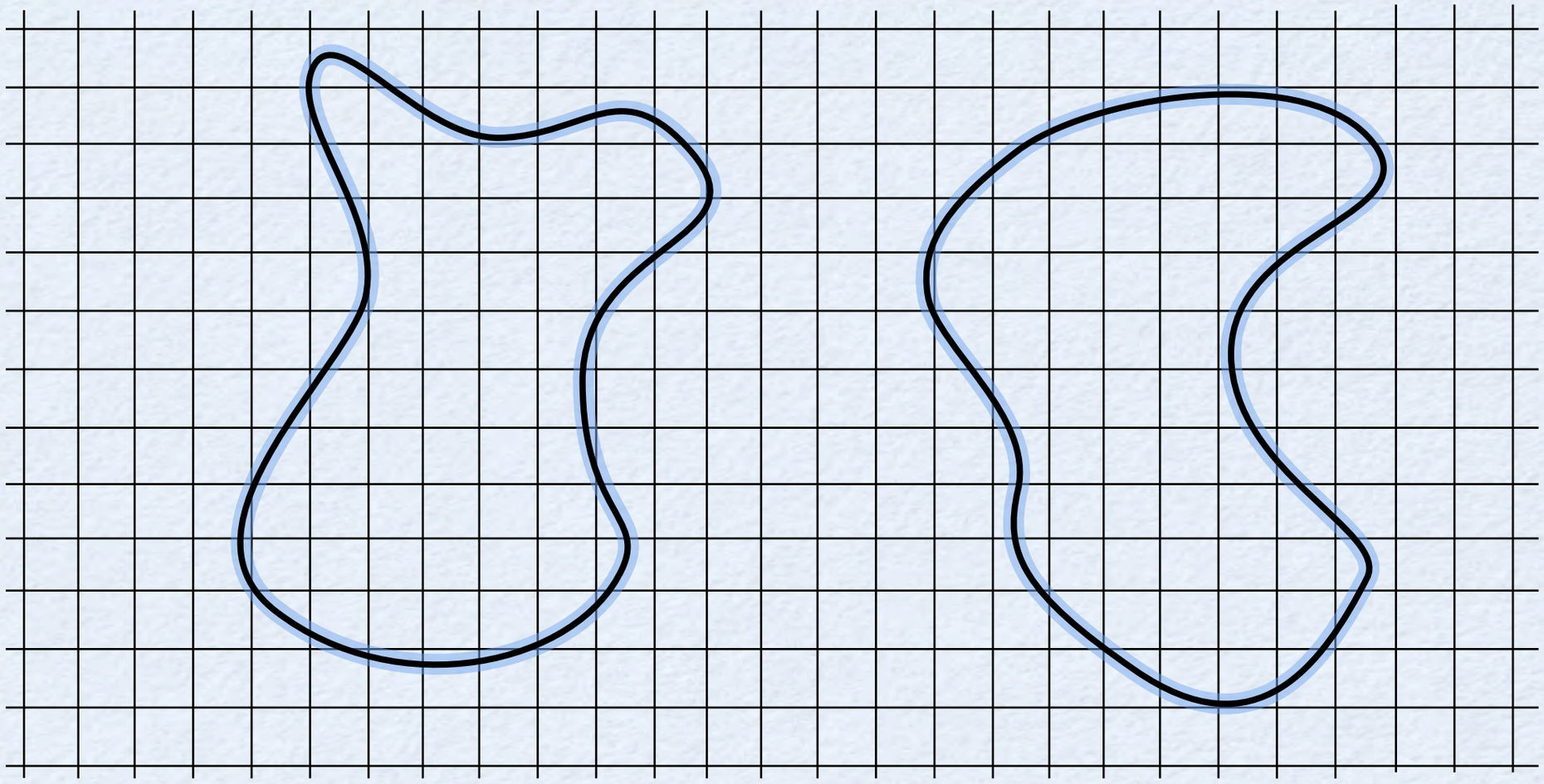
dof = # active gp/particles at t=0.0

dof = # active gp/particles at final time

$CFL_{max} \sim 40$

Boundary Conditions + SIMPLE GRIDS

Dupuis A., Chatelain P., Koumoutsakos P., An Immersed Boundary-Lattice Boltzmann Method, **J. Comput. Physics**, 227, 9, 4486-4498, 2008

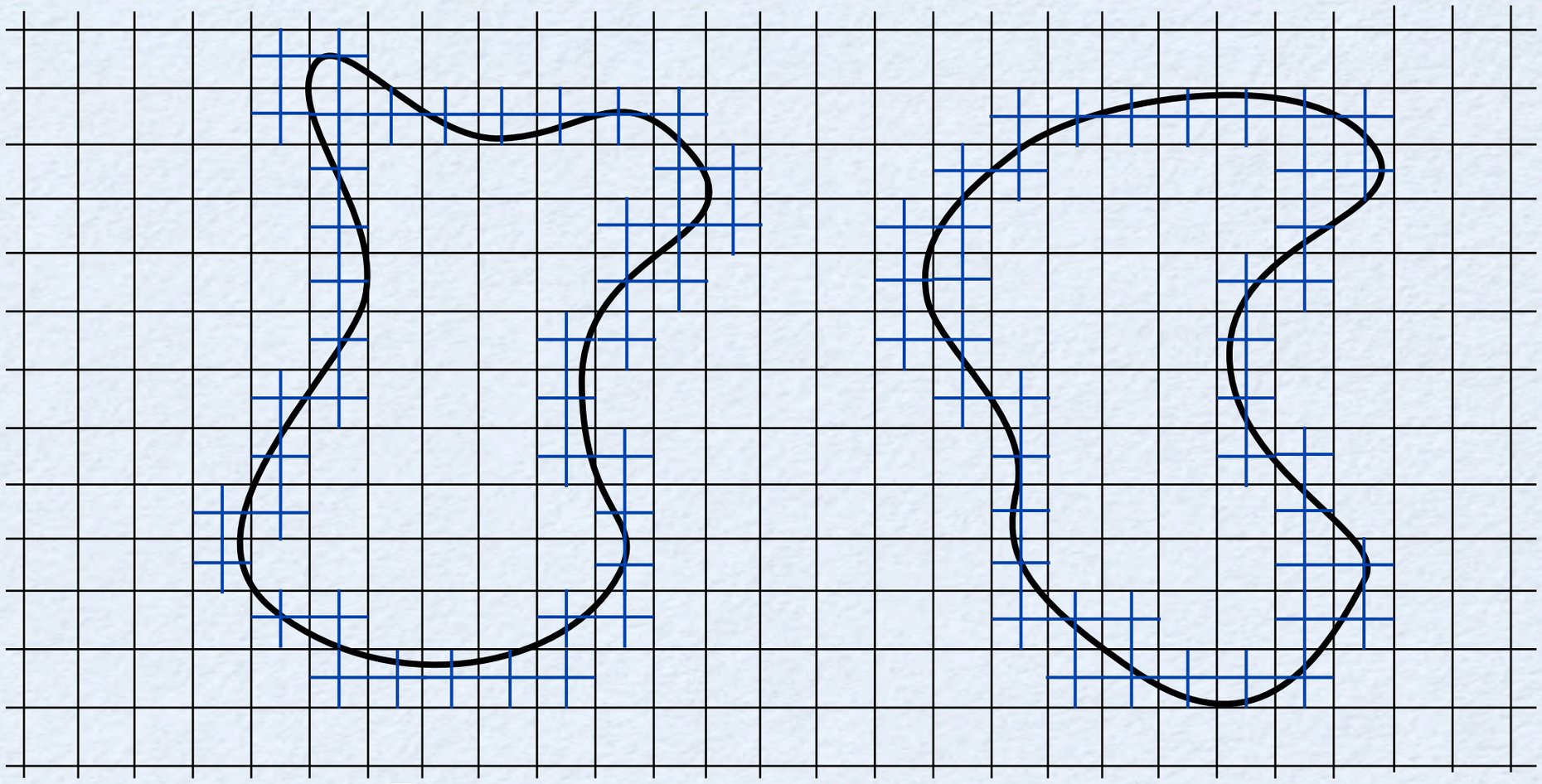


$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + f(\text{enforces b.c.})$$

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

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

Boundary Conditions = Coupling



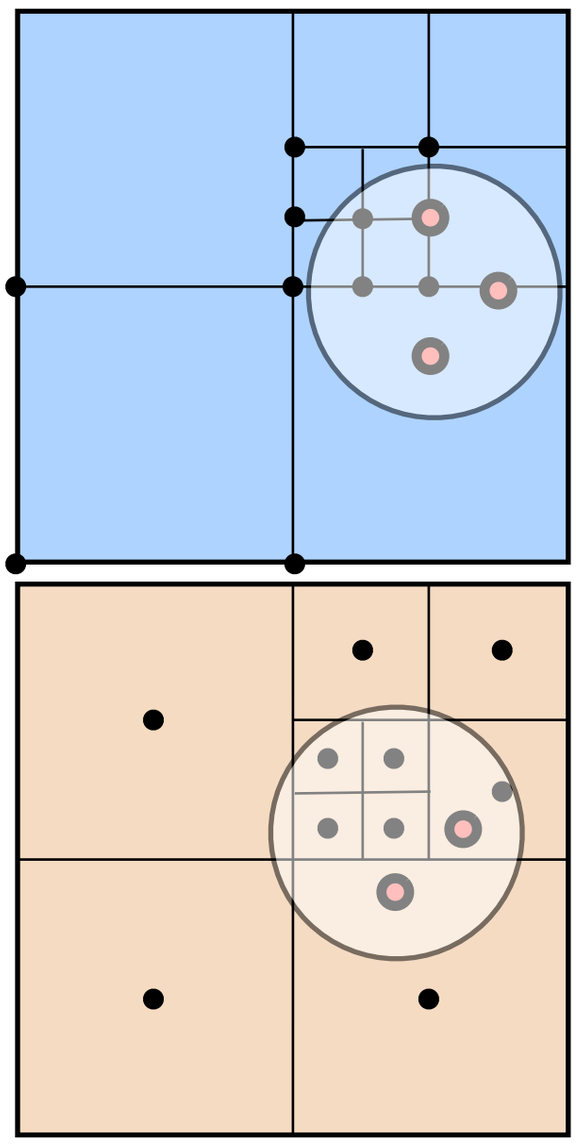
$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + f(\text{enforces b.c.})$$

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

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

Multi-resolution Vortex Methods + Penalization

Wavelet Adapted Grids



PDE:

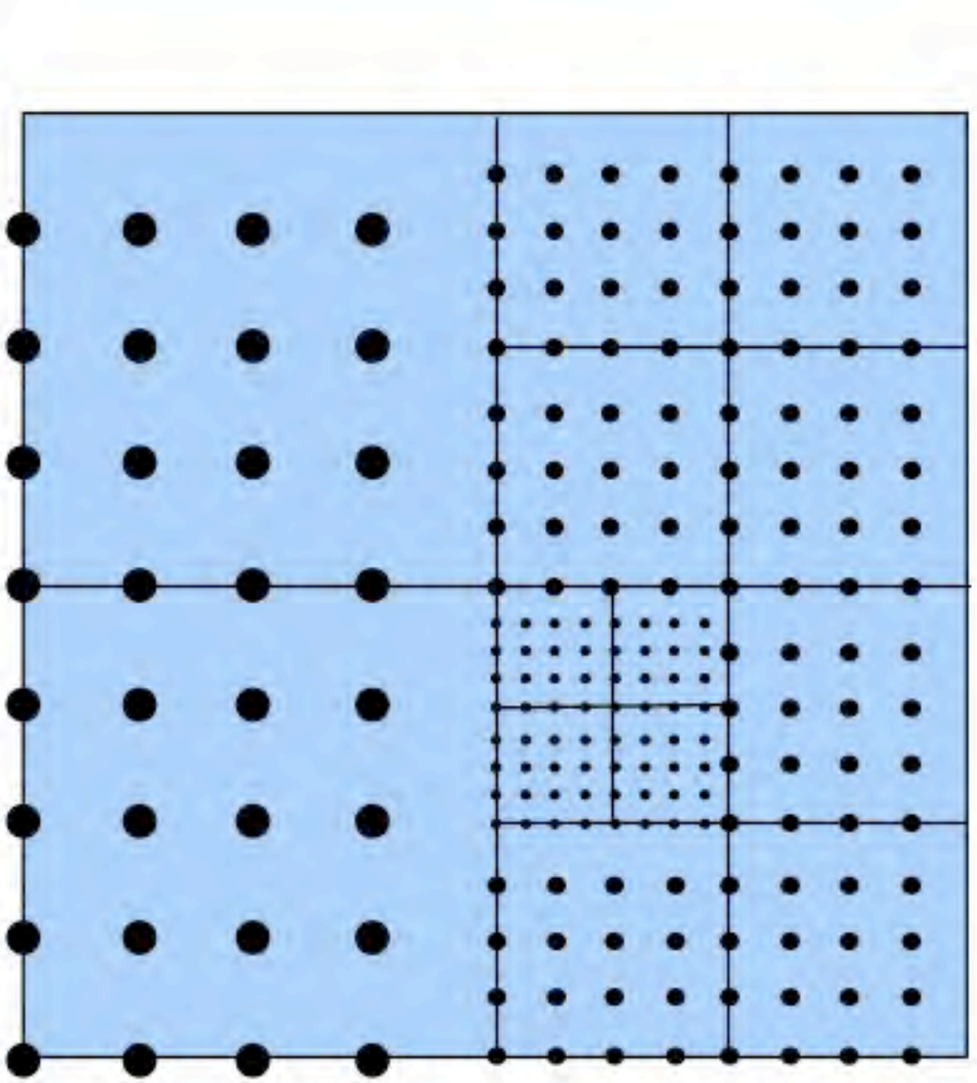
$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0$$

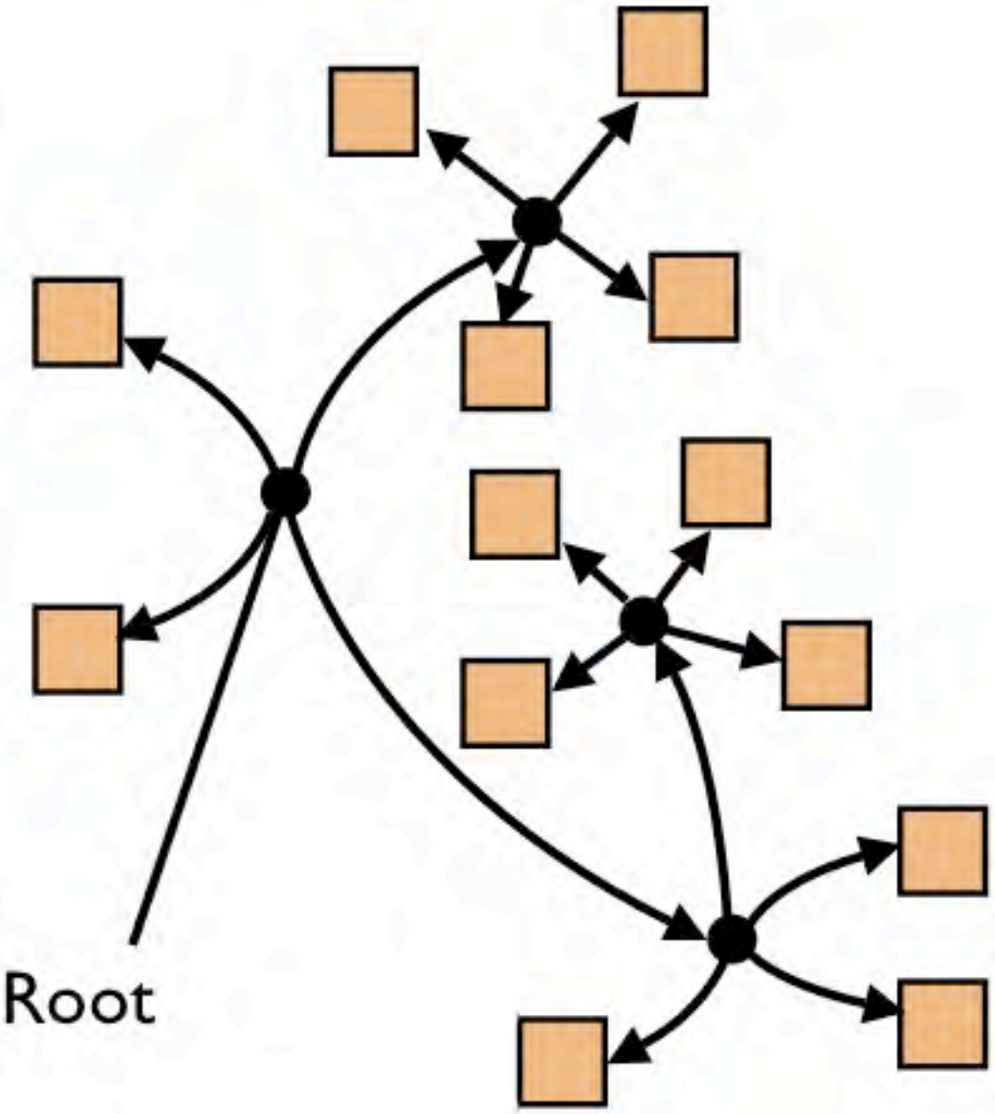
Spatial Differences = filtering operations:

$$F(c_k^l) = \sum_{j=s_f}^{e_f - 1} c_{k+j}^l \beta_j^l, \quad \beta_j^l \text{ function of } \{c_m^l\}$$

GHOSTS : easy to compute – (locally) uniform filtering of the grid

Block Grid for Multi/Many-core:

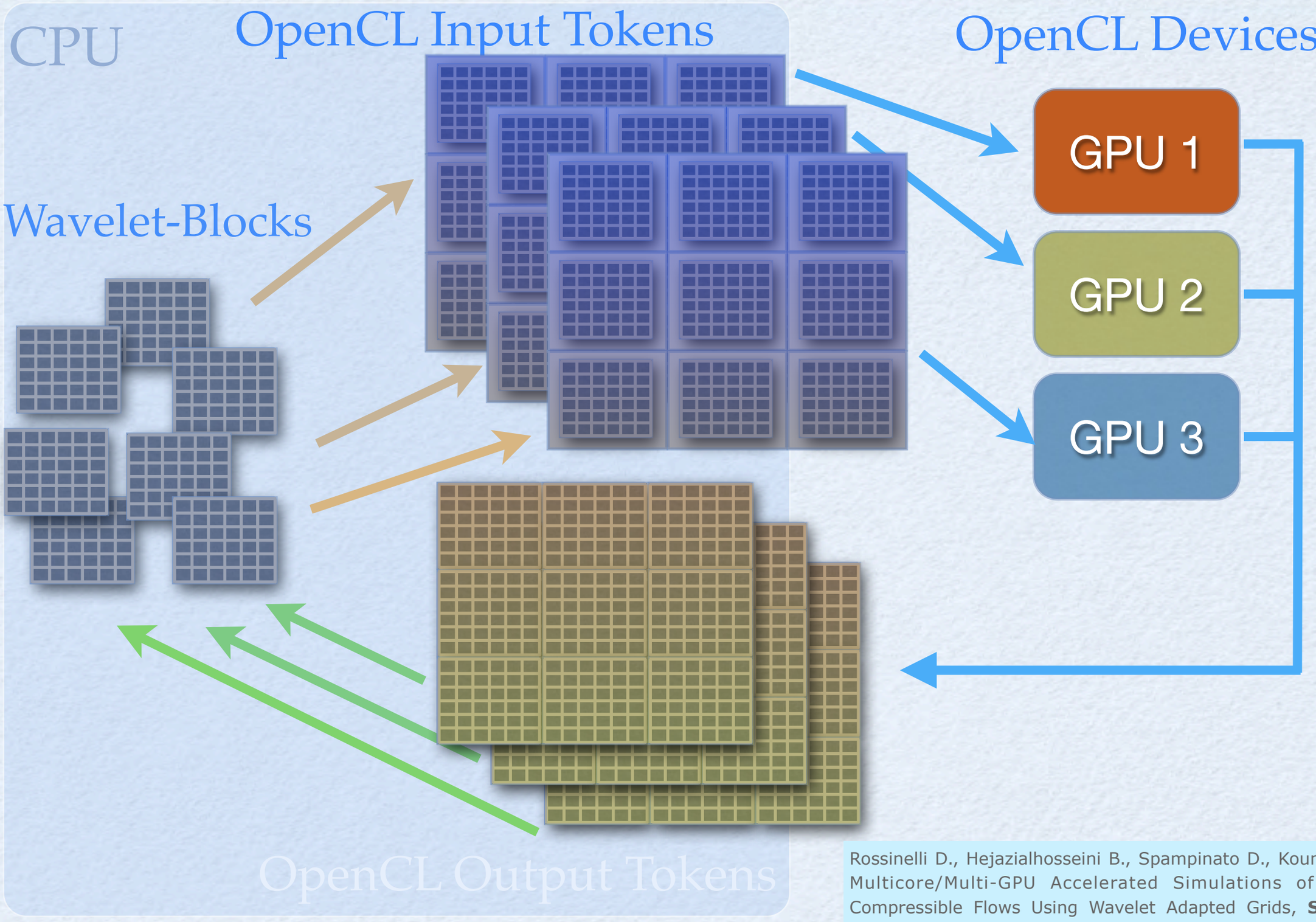




- Neighbors look-up: less memory indirections
- Less #ghosts
- Within a block: random access

Wavelet Blocks on GPUs

- Overall Reduction in time to solution: **~ 1000**



Rossinelli D., Hejazialhosseini B., Spampinato D., Koumoutsakos P., Multicore/Multi-GPU Accelerated Simulations of Multiphase Compressible Flows Using Wavelet Adapted Grids, **SIAM J. Sci. Comput.,** 33, pp. 512-540, 2011

Performance I : Time to Solution

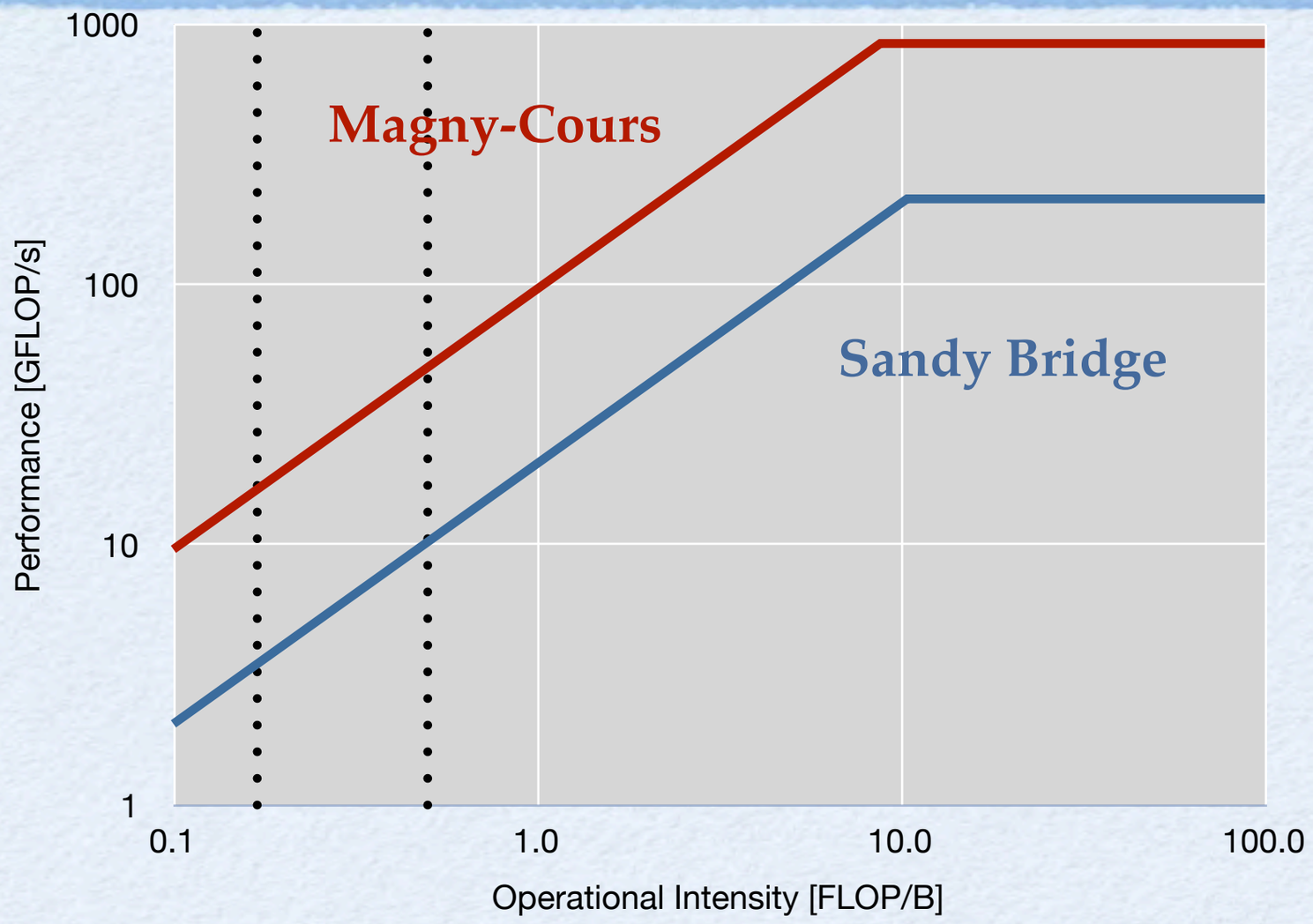
Compared to a space adaptive, single-threaded (CPU) solver:

- **Algorithms :** Local Time Stepping: **24X**
- **Ghost Reconstruction :** CPU optimization (vectorization): **1.8X**
- **Ghost Reconstruction :** Task-based parallelism (via TBB): **8X** (over 12)
- **GPUs** as accelerators: **3X**

Overall Reduction in Time to Solution: ~ 1000

Performance II: The Roofline Model

S. Williams, A. Waterman, D. Patterson - 2009 - Comm. ACM



visual tool

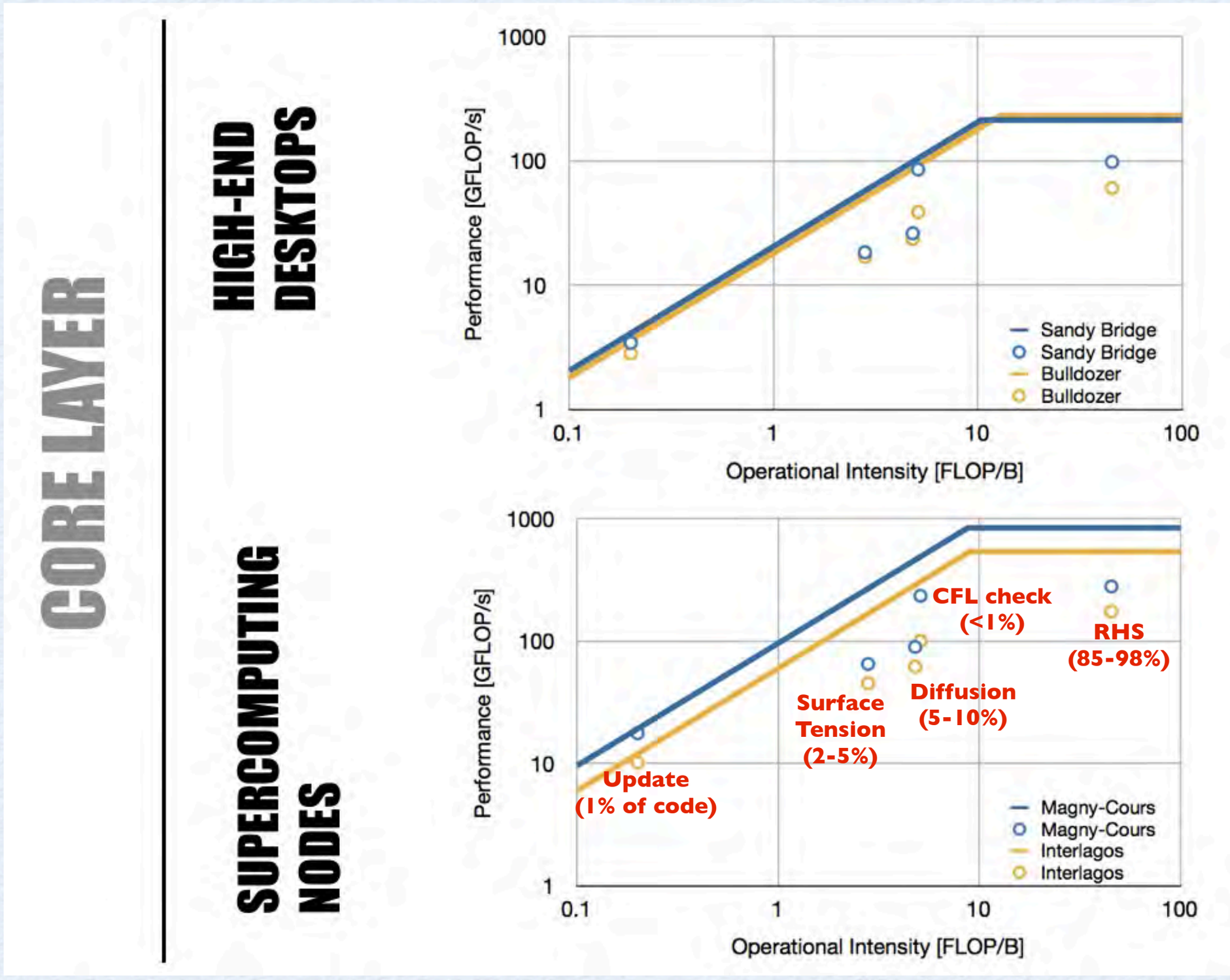
OI for non blocked RHS (right), surface tension and diffusion (left)

tendency of moving even more to the right the ridge point as computing grows faster than memory (HP2C webpage)

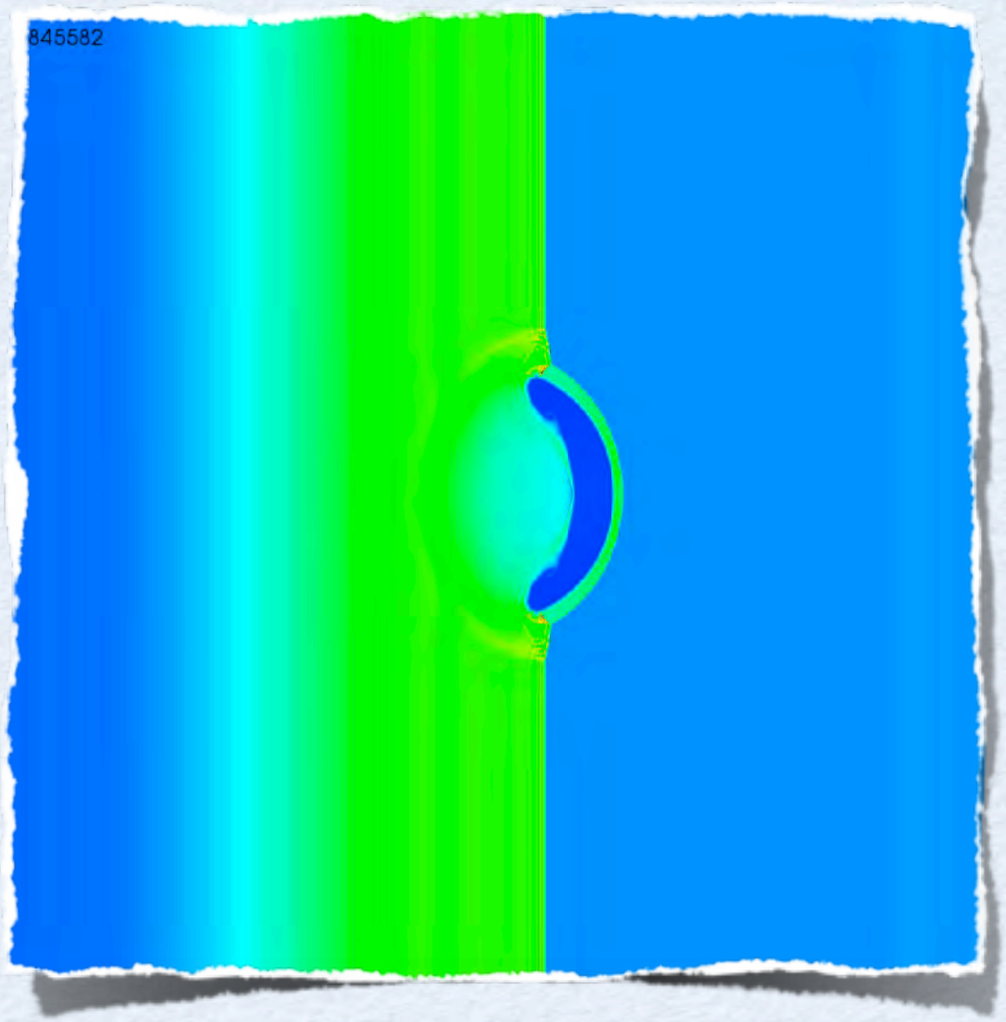
How to predict performance of a compute kernel?

- Performance versus Operational Intensity (OI)
- OI: FLOP/B (off chip) of the kernel
- Low OI: OI < ridge _> A reason for <5% of peak performance

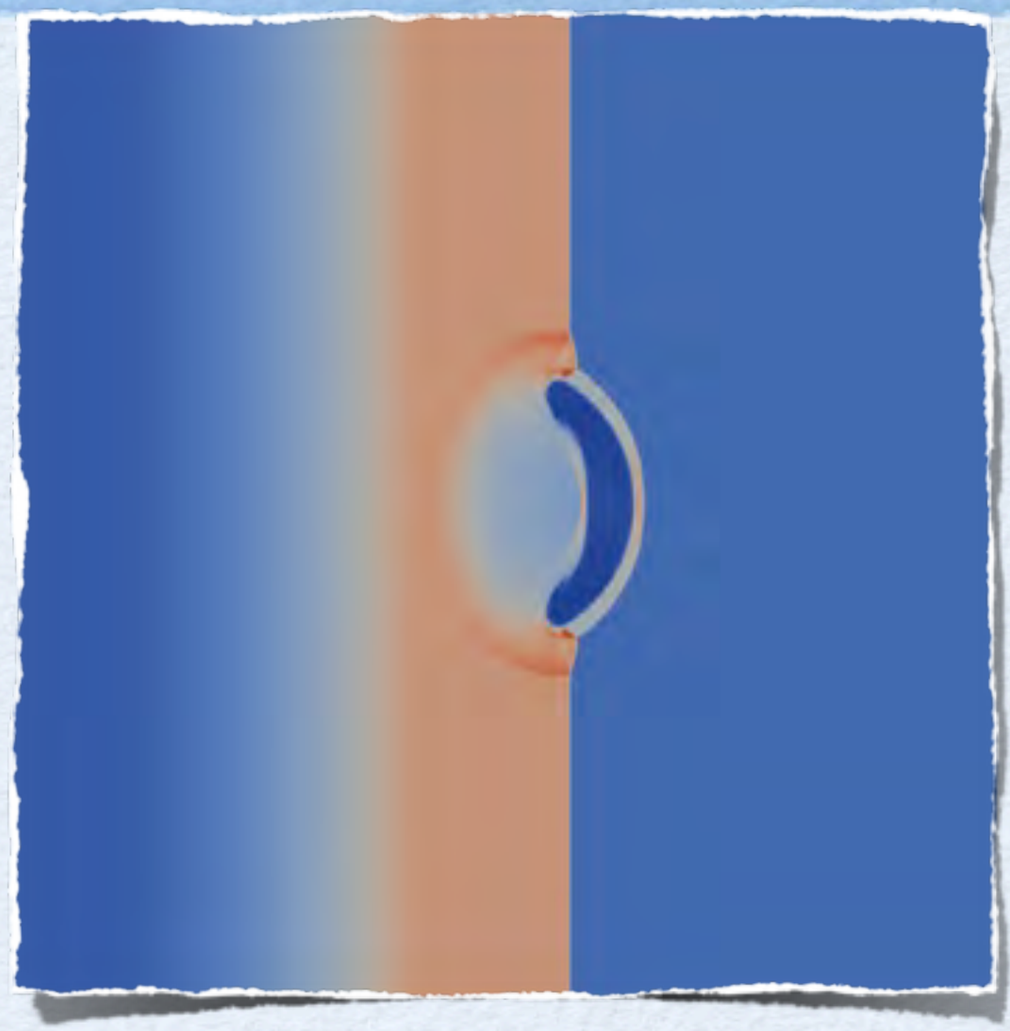
Performance II: The Roofline Model



Performance III : MRAG vs. CHOMBO



density field



CHOMBO – AMR Solver
91 min, 230 MB

single-phase - 2nd order PPM

MRAG
56 min, 244 MB + 1 GPU: 7 min

multi-phase - 5th order WENO

CHOMBO: Colella et al., software package for AMR applications, Technical Report(LBNL), 2000

Rossinelli D., Hejazialhosseini B., Spampinato D., Koumoutsakos P., Multicore/Multi-GPU Accelerated Simulations of Multiphase Compressible Flows Using Wavelet Adapted Grids, **SIAM J. Sci. Comput.,** 33, pp. 512-540, 2011

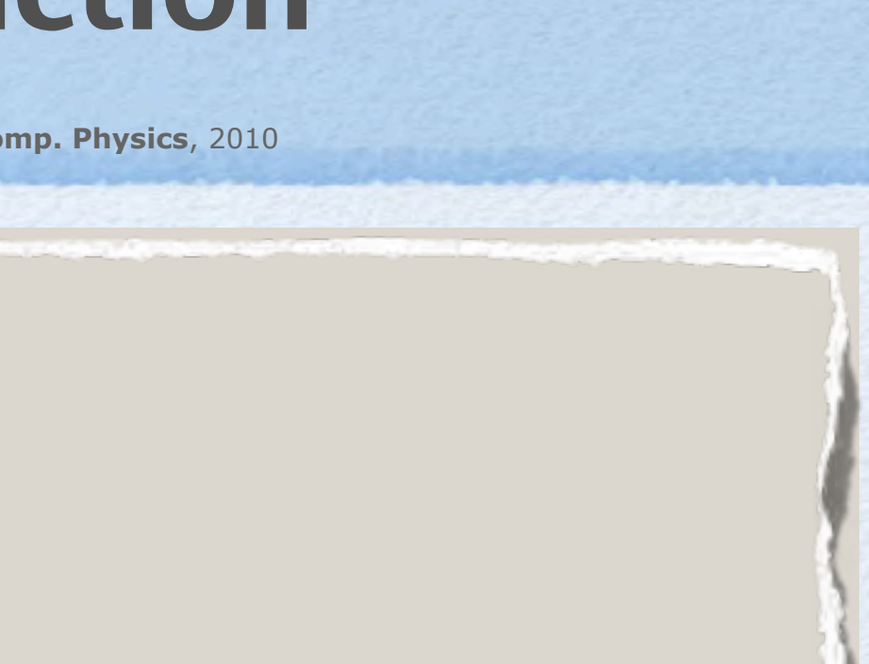
Shock Bubble Interaction

Hejazialhosseini et. al., **J. of Comp. Physics**, 2010

FINEST RESOLUTION EQUIVALENT

8000 x 8000 uniform grid

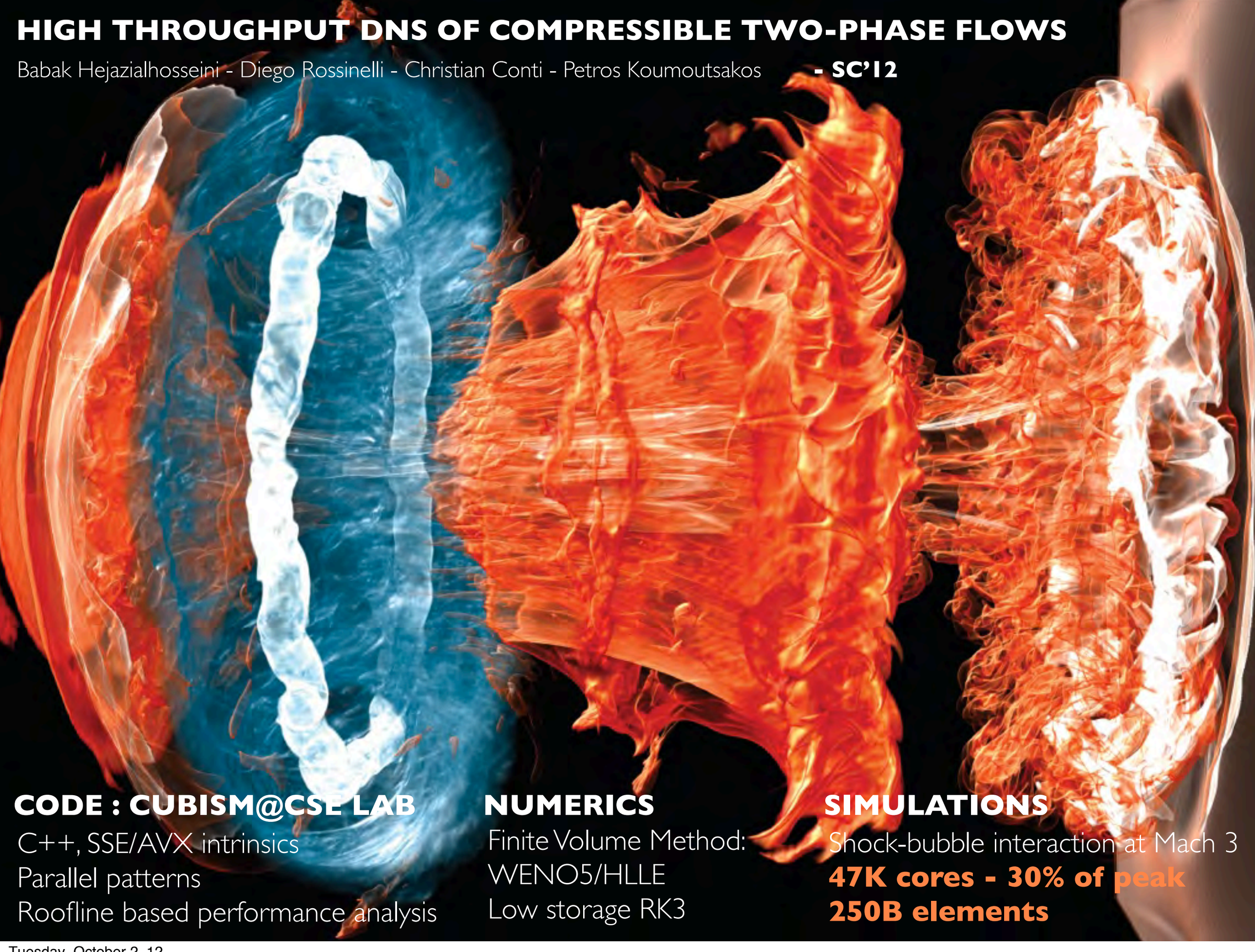
~40 times smaller adaptive



(M=3, At=0.8)

HIGH THROUGHPUT DNS OF COMPRESSIBLE TWO-PHASE FLOWS

Babak Hejazialhosseini - Diego Rossinelli - Christian Conti - Petros Koumoutsakos **- SC'12**



CODE : CUBISM@CSE LAB

C++, SSE/AVX intrinsics
Parallel patterns
Roofline based performance analysis

NUMERICS

Finite Volume Method:
WENO5/HLLE
Low storage RK3

SIMULATIONS

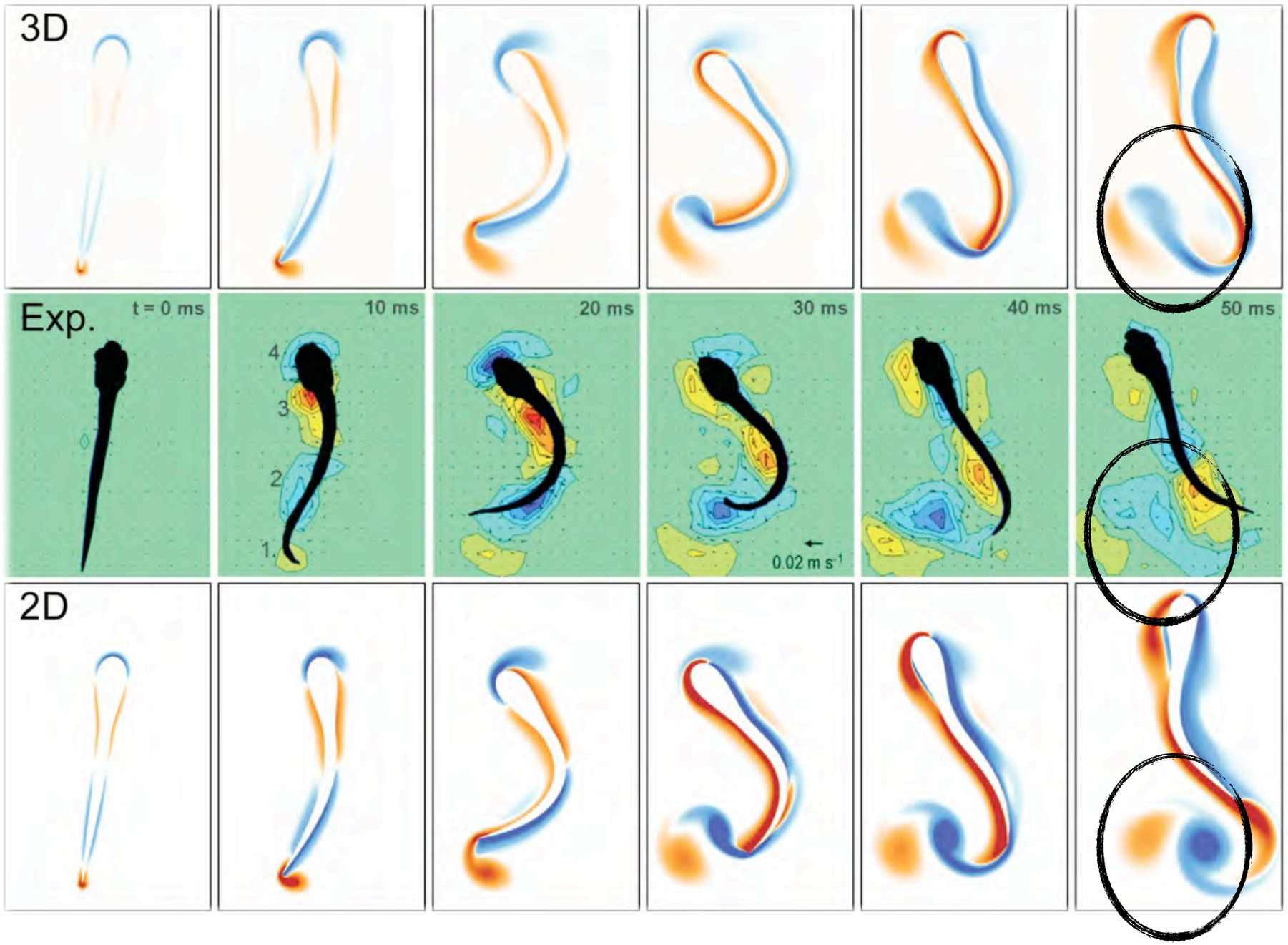
Shock-bubble interaction at Mach 3
47K cores - 30% of peak
250B elements

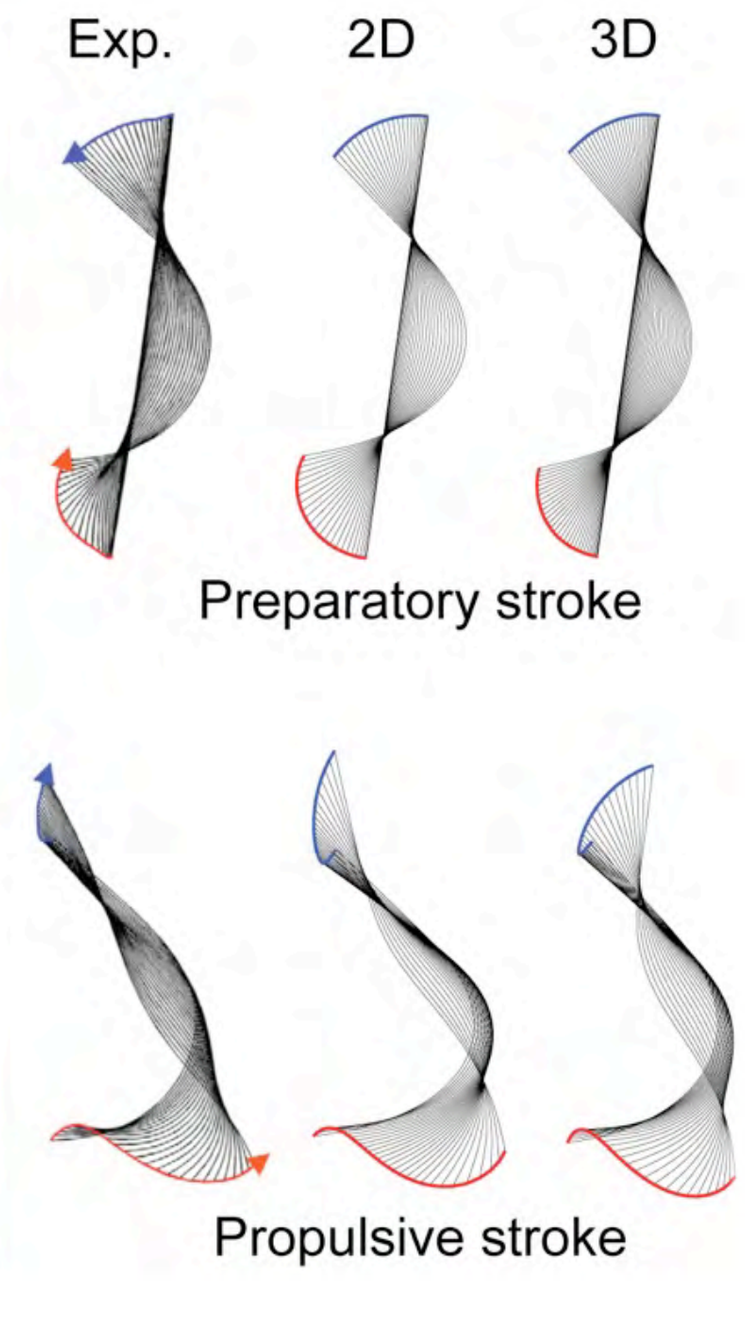
EVOLUTIONARY OPTIMIZATION (~3000 simulations)

C-start is **IS OPTIMAL** ESCAPE response

Gazzola M., van Rees W.M. and Koumoutsakos P., C-start: optimal start of larval fish. **Journal of Fluid Mechanics**, 698:5–18, 2012.

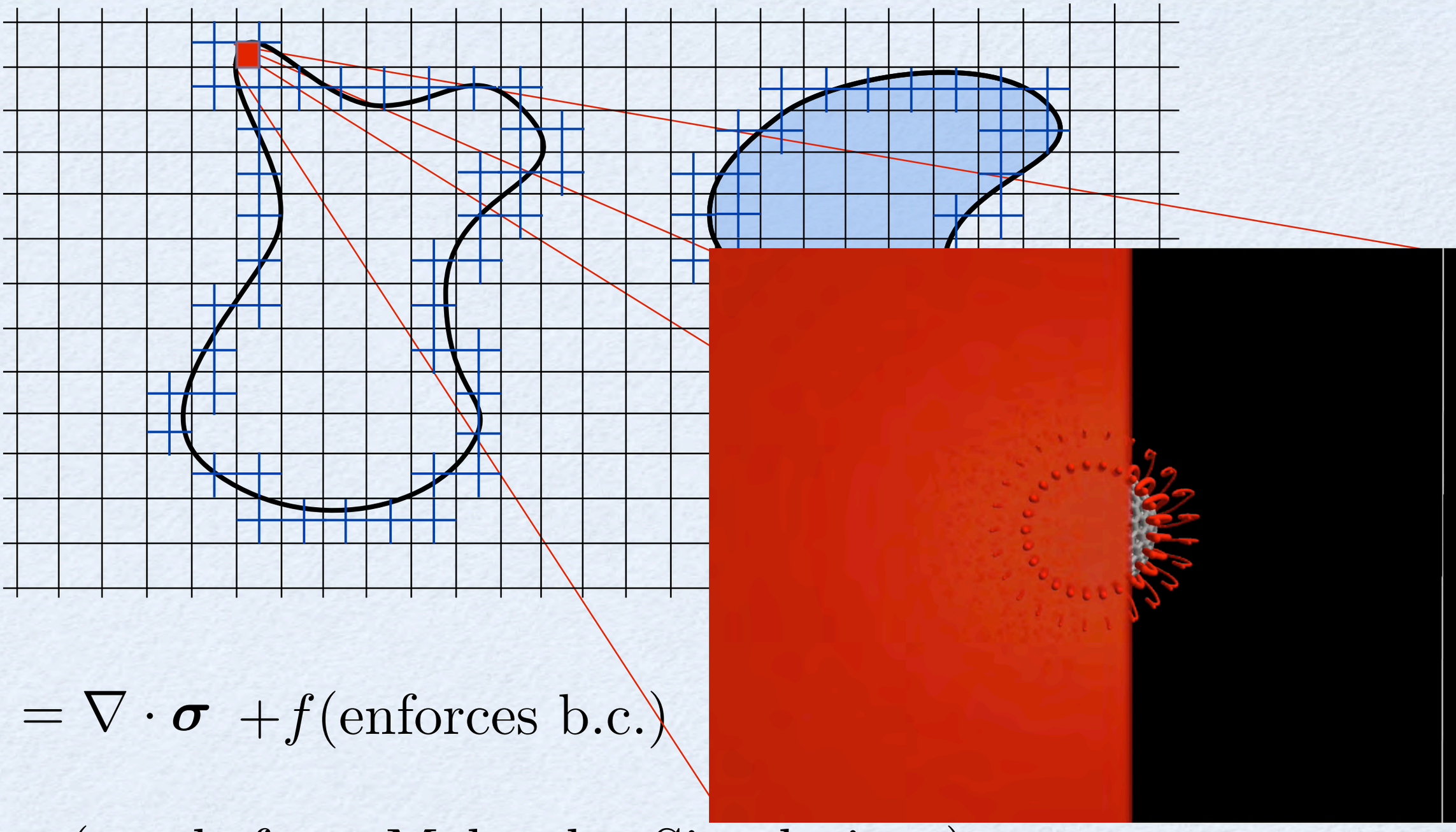
IN VIVO -*IN SILICO*





Experimental data by *Muller, van den Boogaart, van Leeuwen. JEB, 2008.*

Boundary Conditions = Coupling



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

$$f(\mathbf{x}) = (\text{result from Molecular Simulations})$$

Multiphysics/Multiscale

PART 2:

Particles for Discrete Flows

SUPERFAST WATER TRANSPORT IN CNTS

Enhanced flow in carbon nanotubes,

NATURE|Vol 438|3 November 2005

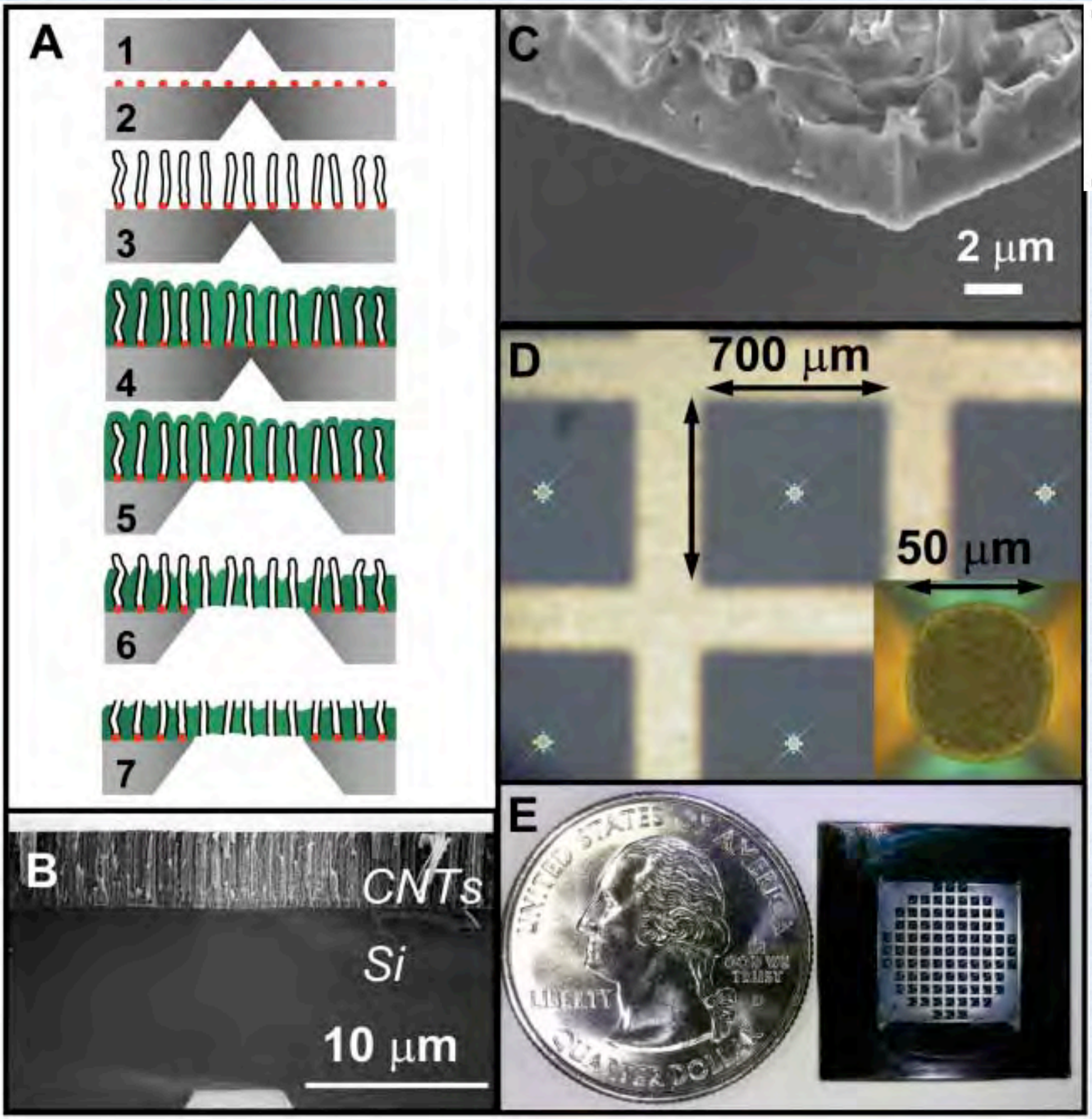
Mainak Majumder*, Nitin Chopra*,Rodney Andrews†, Bruce J. Hinds*

Table 1 | Pressure-driven flow through aligned MWCNT membrane

Liquid	Initial permeability*	Observed flow velocity†	Expected flow velocity†	Slip length (nm)
Water	0.58	25	0.00057	54
	1.01	43.9	0.00057	68
	0.72	9.5	0.00015	39
Ethanol	0.35	4.5	0.00014	28
iso-Propanol	0.088	1.12	0.00077	13
Hexane	0.44	5.6	0.00052	9.5
Decane	0.053	0.67	0.00017	3.4

MWCNT, multiwalled carbon nanotube. For details of methods, see supplementary information. *Units, cm^3 per cm^2 min bar. †Flow velocities in cm s^{-1} at 1 bar. Expected flow velocity is that predicted from conventional flow.

SuperFast Water Transport in CNTs



Fast Mass Transport Through Sub-2-Nanometer Carbon Nanotubes
Jason K. Holt, *et al.*
Science **312**, 1034 (2006);
DOI: 10.1126/science.1126298

Fig. 1. (**A**) Schematic of the fabrication process. Step 1: microscale pit formation (by KOH etching). Step 2: catalyst deposition/annealing. Step 3: nanotube growth. Step 4: gap filling with low-pressure chemical vapor–deposited Si_3N_4. Step 5: membrane area definition (by XeF_2 isotropic Si etching). Step 6: silicon nitride etch to expose nanotubes and remove catalyst nanoparticles (by Ar ion milling); the membrane is still impermeable at this step. Step 7: nanotube uncapping (reactive ion etching); the membrane begins to exhibit gas permeability at this step. (**B**) SEM cross section of the as-grown DWNTs (CNTs). (**C**) SEM cross section of the membrane, illustrating the excellent gap filling by silicon nitride. (**D**) Photograph of the open membrane areas; inset shows a close-up of one membrane. (**E**) Photograph of the membrane chip that contains 89 open windows; each window is 50 μm in diameter.

Fast Mass Transport Through Sub-2-Nanometer Carbon Nanotubes
Jason K. Holt, *et al.*
Science **312**, 1034 (2006);
DOI: 10.1126/science.1126298

Fast Mass Transport Through Sub–2-Nanometer Carbon Nanotubes

Jason K. Holt,[1*] Hyung Gyu Park,[1,2*] Yinmin Wang,[1] Michael Stadermann,[1]
Alexander B. Artyukhin,[1] Costas P. Grigoropoulos,[2] Aleksandr Noy,[1] Olgica Bakajin[1]†

Table 2. Comparisons of experimental air flow rates observed for several DWNT membranes with Knudsen model predictions, and of experimental water flow rates with continuum flow model predictions. The differences among the three DWNT membranes are most likely the result of different numbers of pores opened in the fabrication process. Values for a polycarbonate membrane are provided as a reference. Pore diameters were determined from size exclusion measurements, TEM measurements, and (for polycarbonate) manufacturer's specifications. Pore density values are upper limits, as determined from TEM measurements and (for polycarbonate) manufacturer's specifications.

Membrane	Pore diameter (nm)	Pore density (cm^{-2})	Thickness (μm)	Enhancement over Knudsen model* (minimum)	Enhancement over no-slip, hydrodynamic flow† (minimum)	Calculated minimum slip length‡ (nm)
DWNT 1	1.3 to 2.0	$\leq 0.25 \times 10^{12}$	2.0	40 to 120	1500 to 8400	380 to 1400
DWNT 2	1.3 to 2.0	$\leq 0.25 \times 10^{12}$	3.0	20 to 80	680 to 3800	170 to 600
DWNT 3	1.3 to 2.0	$\leq 0.25 \times 10^{12}$	2.8	16 to 60	560 to 3100	140 to 500
Polycarbonate	15	6×10^{8}	6.0	2.1	3.7	5.1

*From (*18*). †From (*26*). ‡From (*29*).

NOTE: Pressure Gradient = 1 atm

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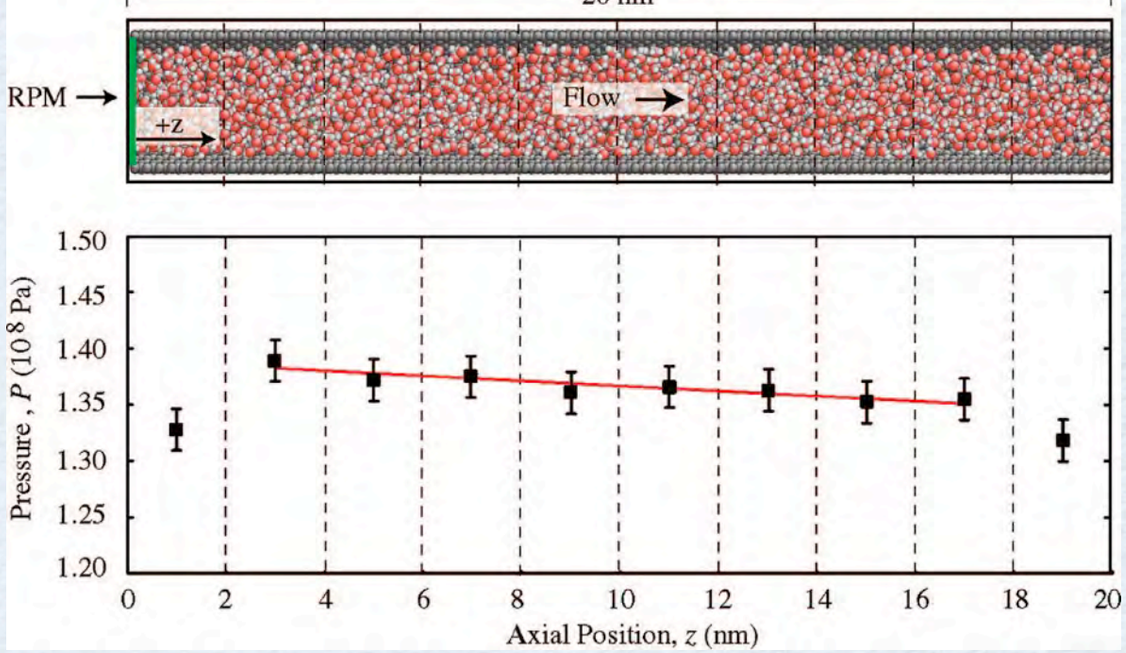
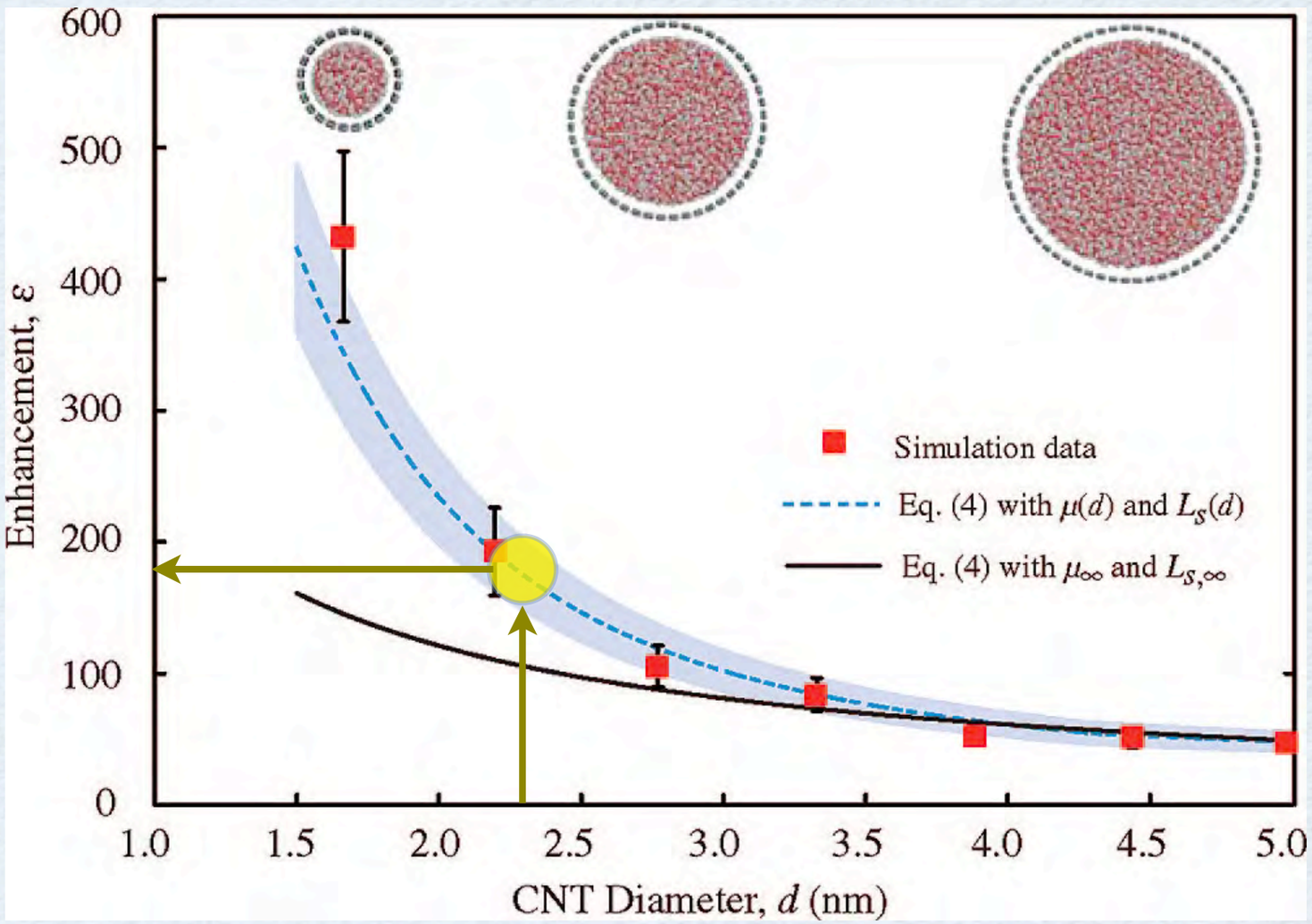
2008
Vol. 8, No. 9
2788-2793

Reassessing Fast Water Transport Through Carbon Nanotubes

John A. Thomas and Alan J. H. McGaughey*
Department of Mechanical Engineering, Carnegie Mellon UniVersity, Pittsburgh, PennsyNania 15213





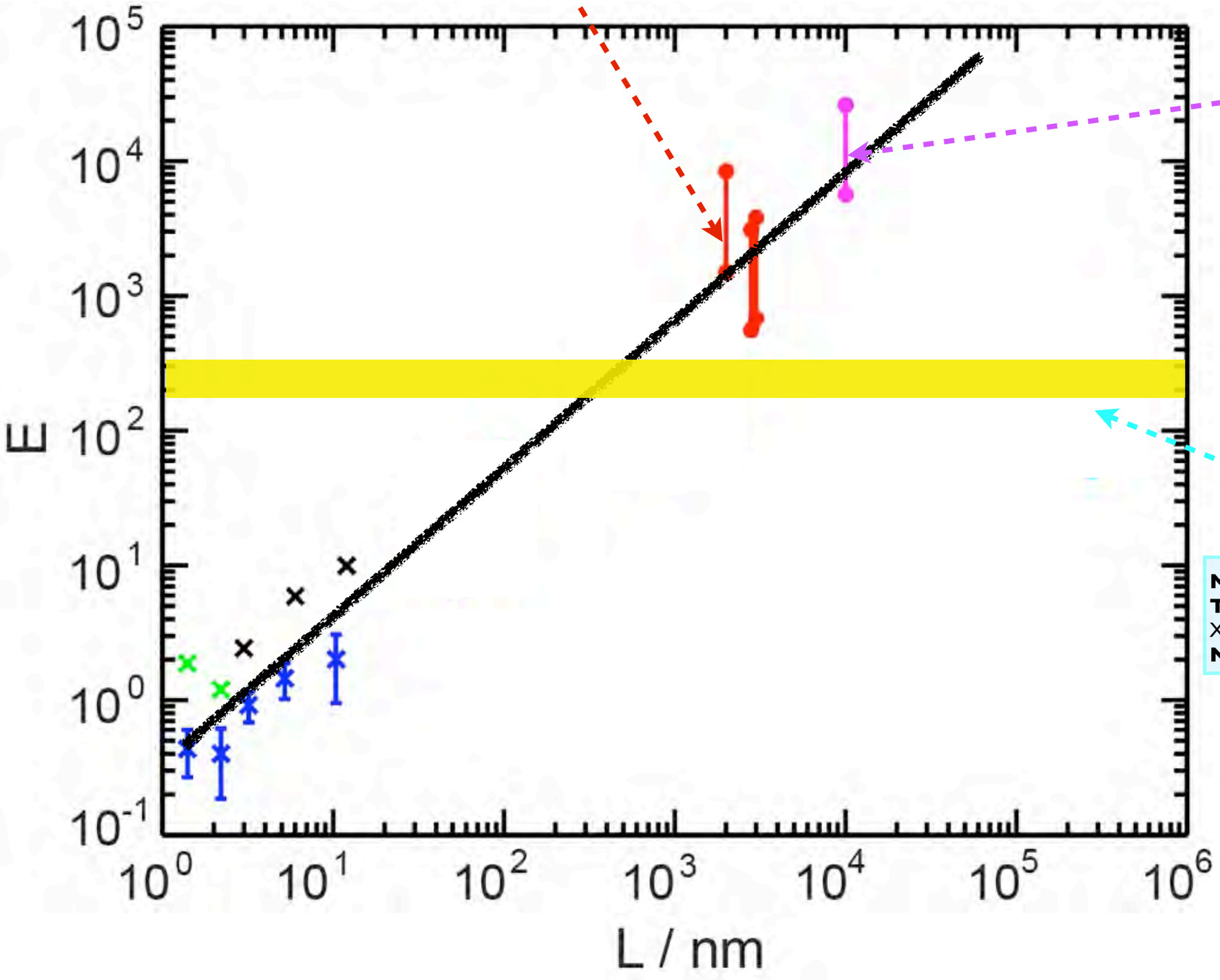
QUESTIONS

i. *How does water enter/exit the CNTs ?*

ii. *Are periodic simulations suitable ?*

MD Simulations at 1μm CNTs

Fast Mass Transport Through Sub-2 Nanometer Carbon Nanotubes
Jason K. Holt, et al.
Science 312, 1034 (2006)



Enhanced Flow in Carbon Nanotubes
Mainak Majumder , et al.
Nature, 438, 2005

Measurement of the Rate of Water Translocation through Carbon Nanotubes
Xingcai Qin, et al.
NanoLetters, 11, 2173, 2011

Uncertainty Quantification for MD

...from WikiPedia

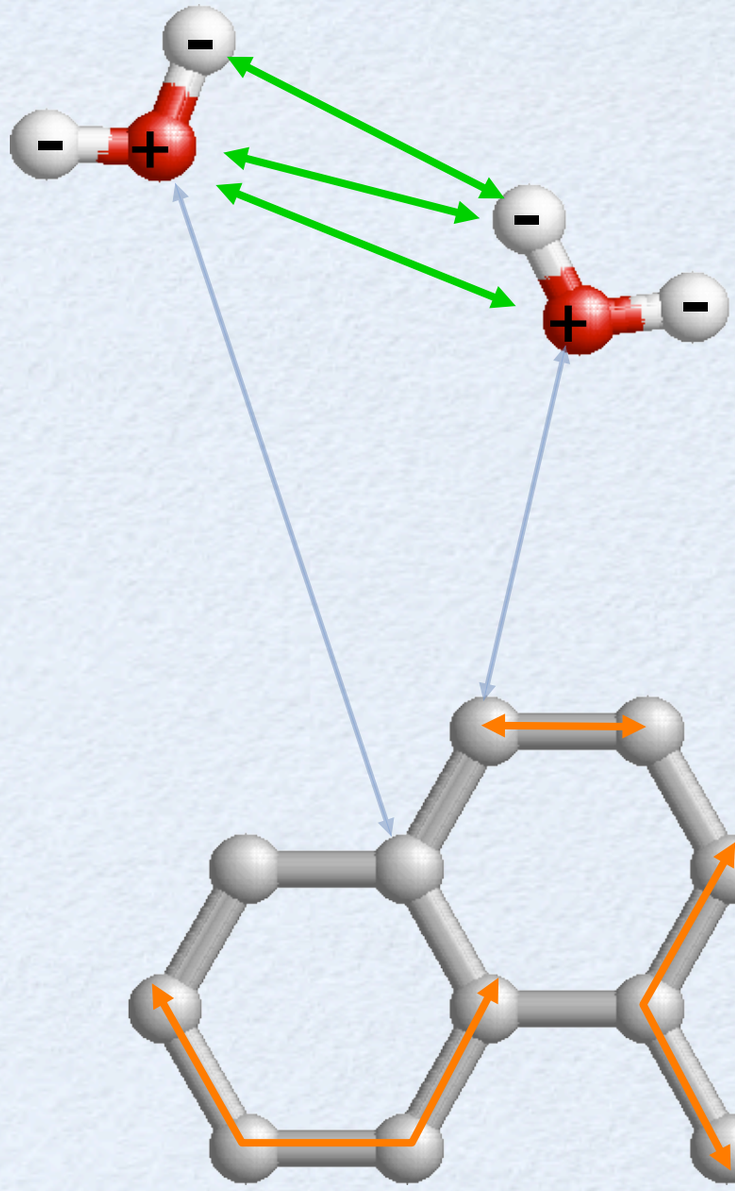
Uncertainty quantification (UQ) is the science of **quantitative characterization** and reduction of **uncertainties** in applications. It tries to determine how likely certain outcomes are if some aspects of the system are not exactly known.

An example would be to predict the acceleration of a human body in a head-on crash with another car: even if we exactly knew the speed, small differences in the manufacturing of individual cars, how tightly every bolt has been tightened, etc, will lead to different results that can only be predicted in a statistical sense. [...]

MD of CNT-Water Systems

- The water potential

  O – O Lennard-Jones
  O – O, O – H Coulomb
  SPC/E : Rigid bonds
  SPCF : O – H bond, H – O – H angle



- The CNT/graphite potential

  C – C Lennard-Jones
  bond, angle, and torsion terms
  (often rigid)

- The carbon-water potential

  C – O Lennard-Jones
  (C – H Lennard-Jones)

Sources of Uncertainty in MD

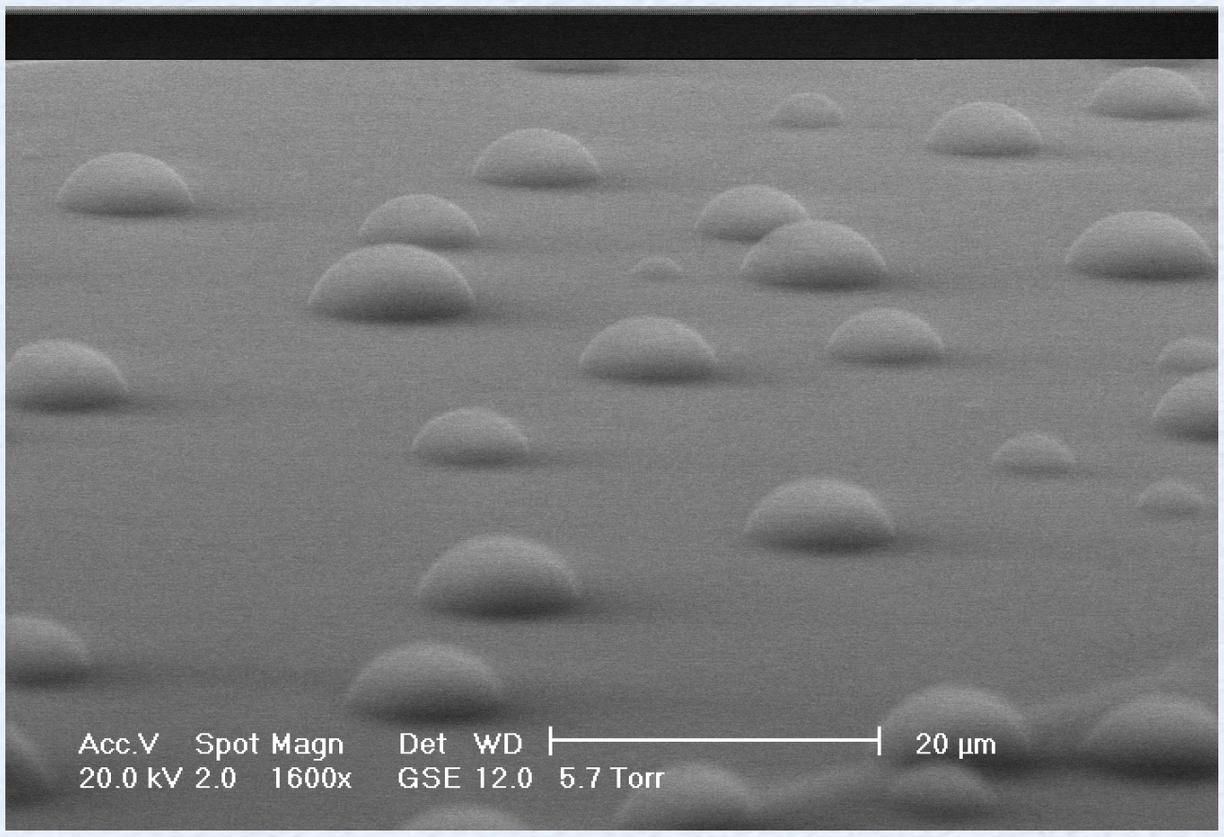
• *MODELING* **Uncertainty-** inadequacy of the mathematical models used to represent the actual system. They arise in postulating **force-field models** to represent the inter-molecular interactions

• *PARAMETRIC* **Uncertainty-** lack of knowledge of the appropriate **values of the parameters** involved in the chosen force-field models and truncation schemes

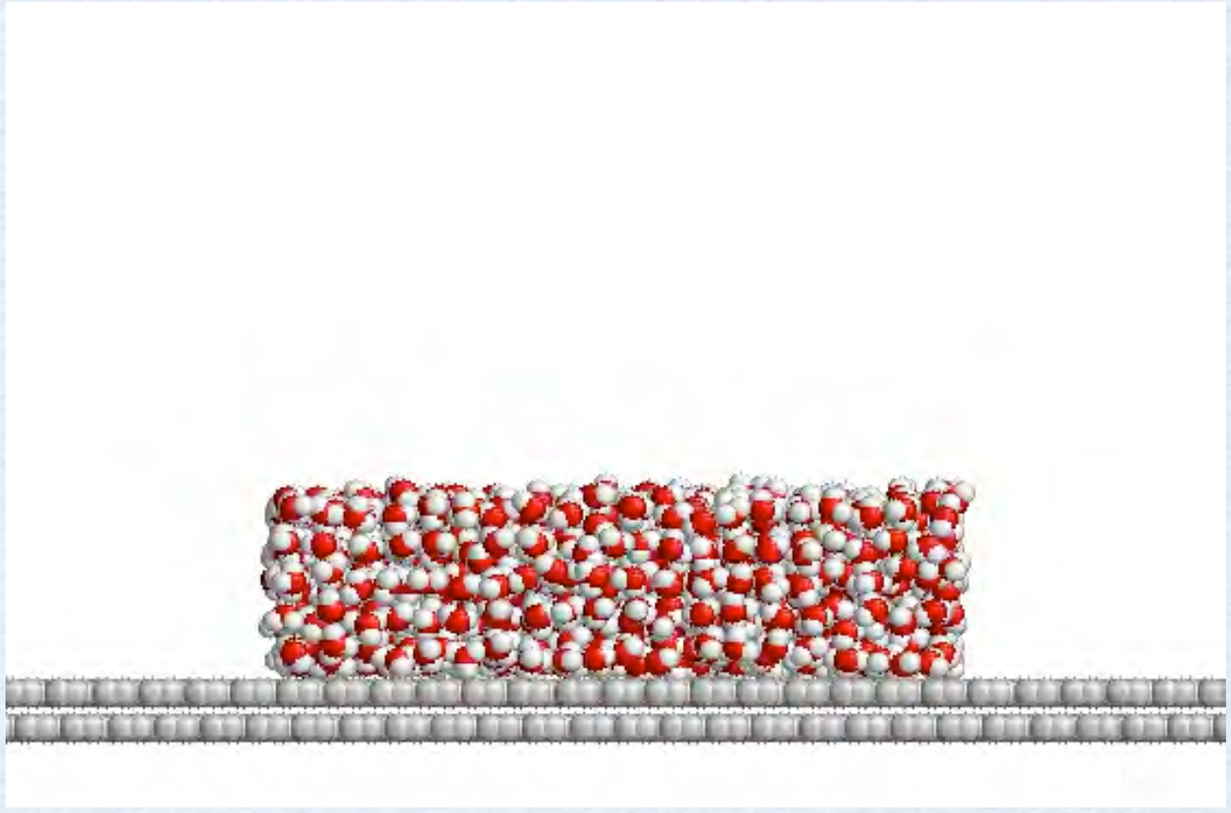
• *COMPUTATIONAL* **uncertainty-** finite size of the simulation box and the values of the **computational parameters** used to evolve the MD equations (e.g. integrate Newton's equations of motion).

• *MEASUREMENT* **uncertainty-** variability in the **values of the experimental properties** due to variability in experimental set, errors in the measuring equipment, and inaccuracies in the data acquisition system.

Wetting of Graphite Sheets by Water Droplets



Microscale Water Micro-droplets condensed over graphite in JPL ESEM (Dr. Flavio Noca)



Nanoscale Water droplets on graphite

Simulations : wetting depends on potentials

NATURE | VOL 414 | 8 NOVEMBER 2001 | www.nature.com

Water conduction through the hydrophobic channel of a carbon nanotube

G. Hummer*, J. C. Rasaiah*† & J. P. Noworyta†

8 April 2002

ELSEVIER

Chemical Physics Letters 355 (2002) 445–448

CHEMICAL PHYSICS LETTERS

www.elsevier.com/locate/cplett

Helical ice-sheets inside carbon nanotubes in the physiological condition

William H. Noon [a], Kevin D. Ausman [b], Richard E. Smalley [b], Jianpeng Ma [a,c,d,*]

ELSEVIER

Chemical Physics 247 (1999) 413–430

Chemical Physics

www.elsevier.nl/locate/chemphys

Scattering of water from graphite: simulations and experiments

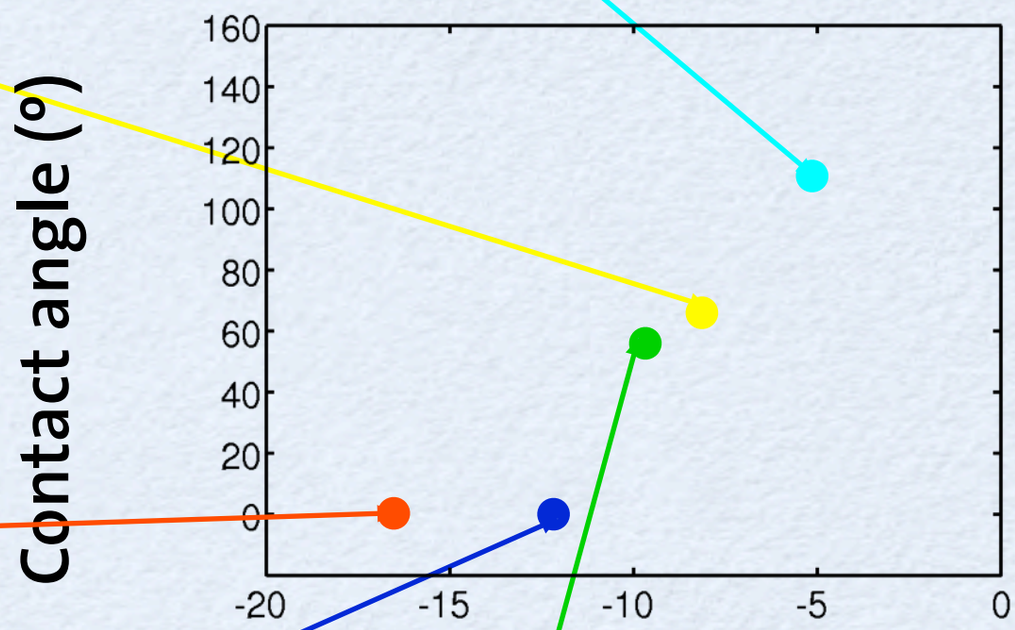
Nikola Marković *, Patrik U. Andersson, Mats B. Någård, Jan B.C. Pettersson [1]

NANO LETTERS

2001
Vol. 1, No. 12
697–702

Molecular Dynamics Simulation of Contact Angles of Water Droplets in Carbon Nanotubes

Thomas Werder,*,† Jens H. Walther,† Richard L. Jaffe,‡ Timur Halicioglu,§ Flavio Noca,|| and Petros Koumoutsakos†,⊥



ELSEVIER

27 October 2000

Chemical Physics Letters 329 (2000) 341–345

CHEMICAL PHYSICS LETTERS

www.elsevier.nl/locate/cplett

Hydrogen bond structure of liquid water confined in nanotubes

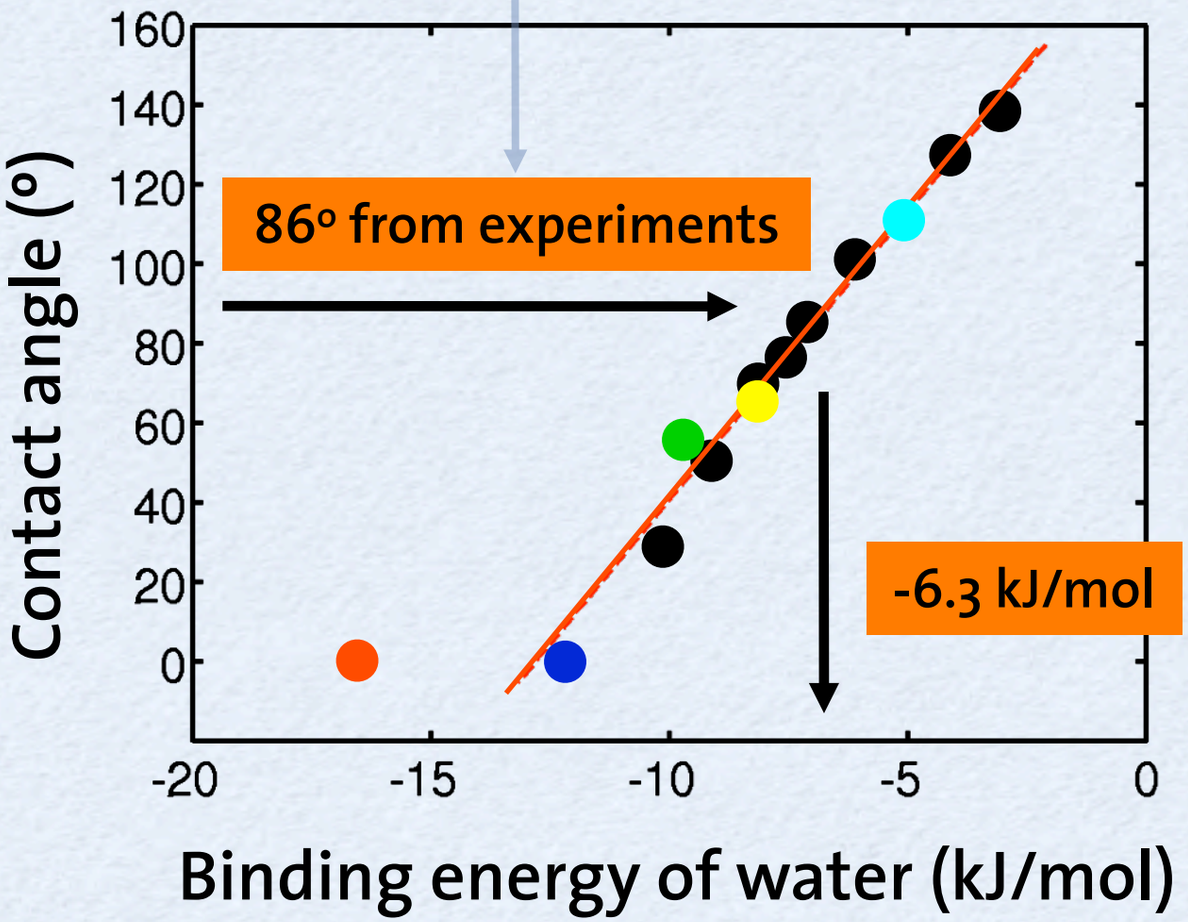
M.C. Gordillo, J. Martí *

CALIBRATE water-graphite potentials from experiments

[CONTRIBUTION FROM THE GEORGE HERBERT JONES CHEMICAL LABORATORY OF THE UNIVERSITY OF CHICAGO]

The State of Monolayers Adsorbed at the Interface Solid–Aqueous Solution

BY FREDERICK M. FOWKES AND WILLIAM D. HARKINS



Lennard-Jones potential

σ_{CO} = 0.319 nm,

ε_{CO} = 0.392 kJ/mol

This value reproduces the *reported* experimental contact angle*

T. Werder, J. H. Walther, R. L. Jaffe, T. Halicioglu, and P. Koumoutsakos, J. Phys. Chem. B, 107:1345-1352, 2003.

Uncertainty Quantification for MD

BAYESIAN UQ+P FRAMEWORK

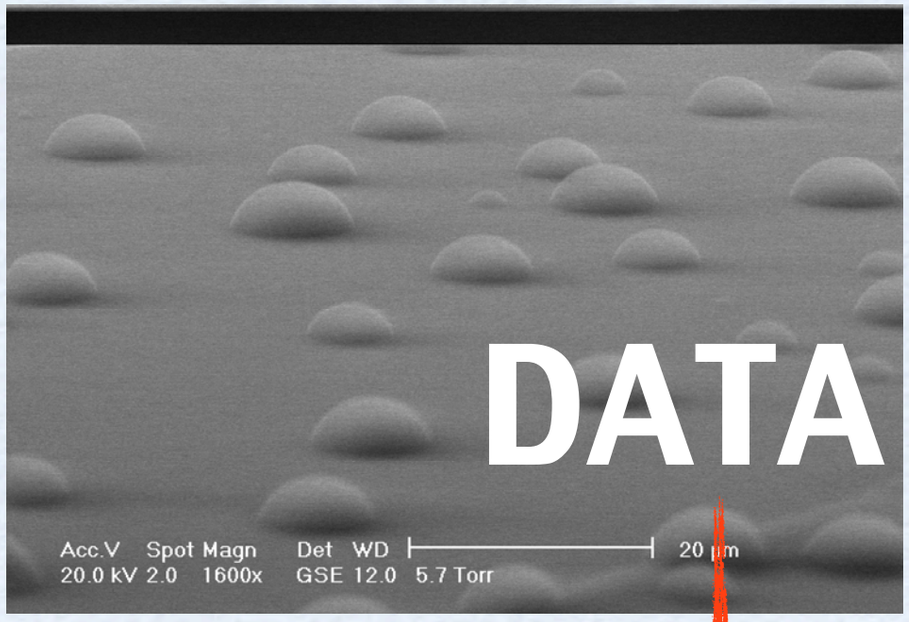
- Bayesian Computational Methods: MCMC and variants
- HPC & Surrogate Models

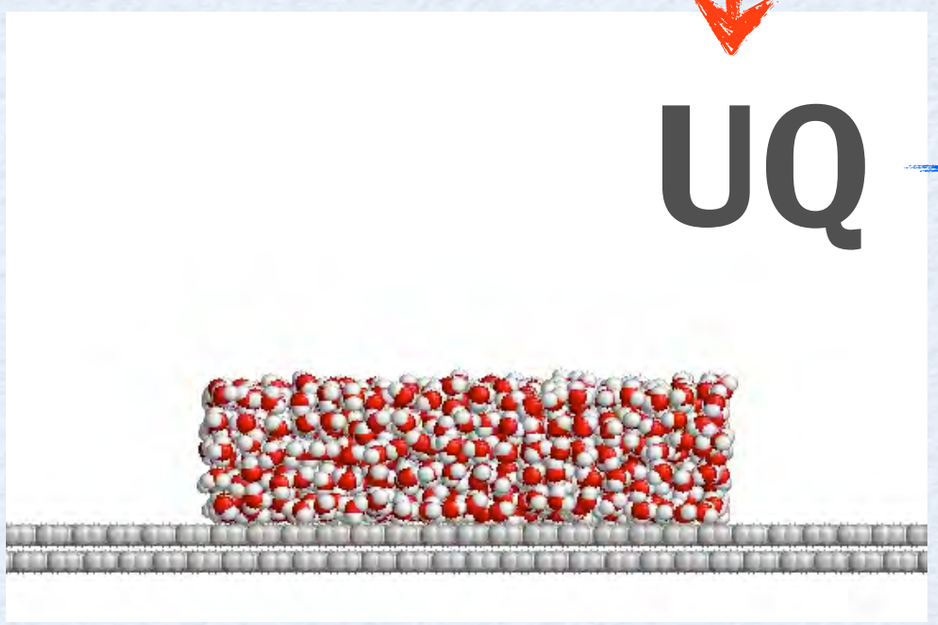
APPLICATIONS IN MOLECULAR DYNAMICS

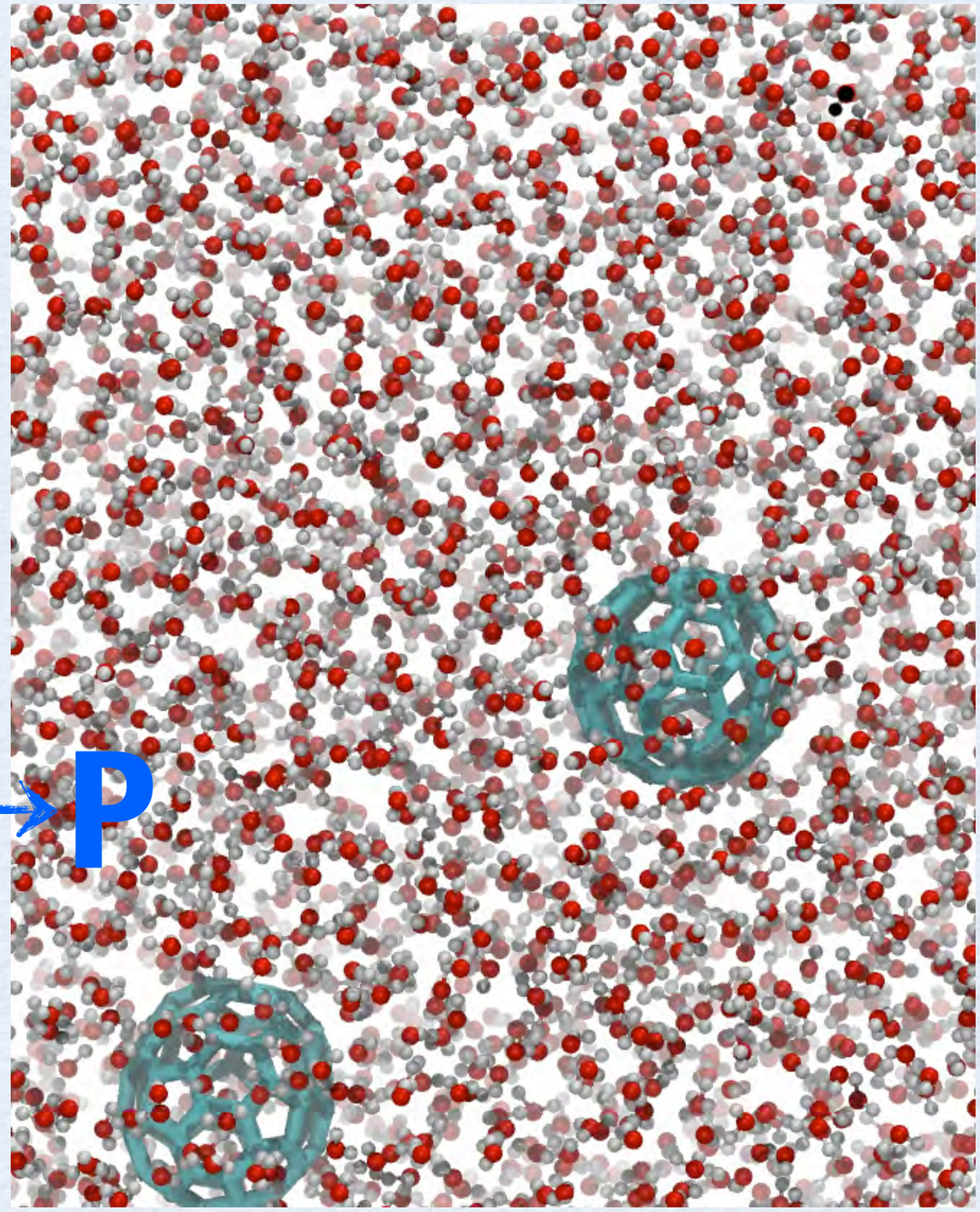
- Argon System
- Water-Carbon Interaction
- Water flow in CNTs

Angelikopoulos et al., Uncertainty Quantification and Prediction in MD Simulations: an HPC framework, J. Chem. Phys. (in press)

UQ (Water Contact Angle) +P (C_{70} Hydration)

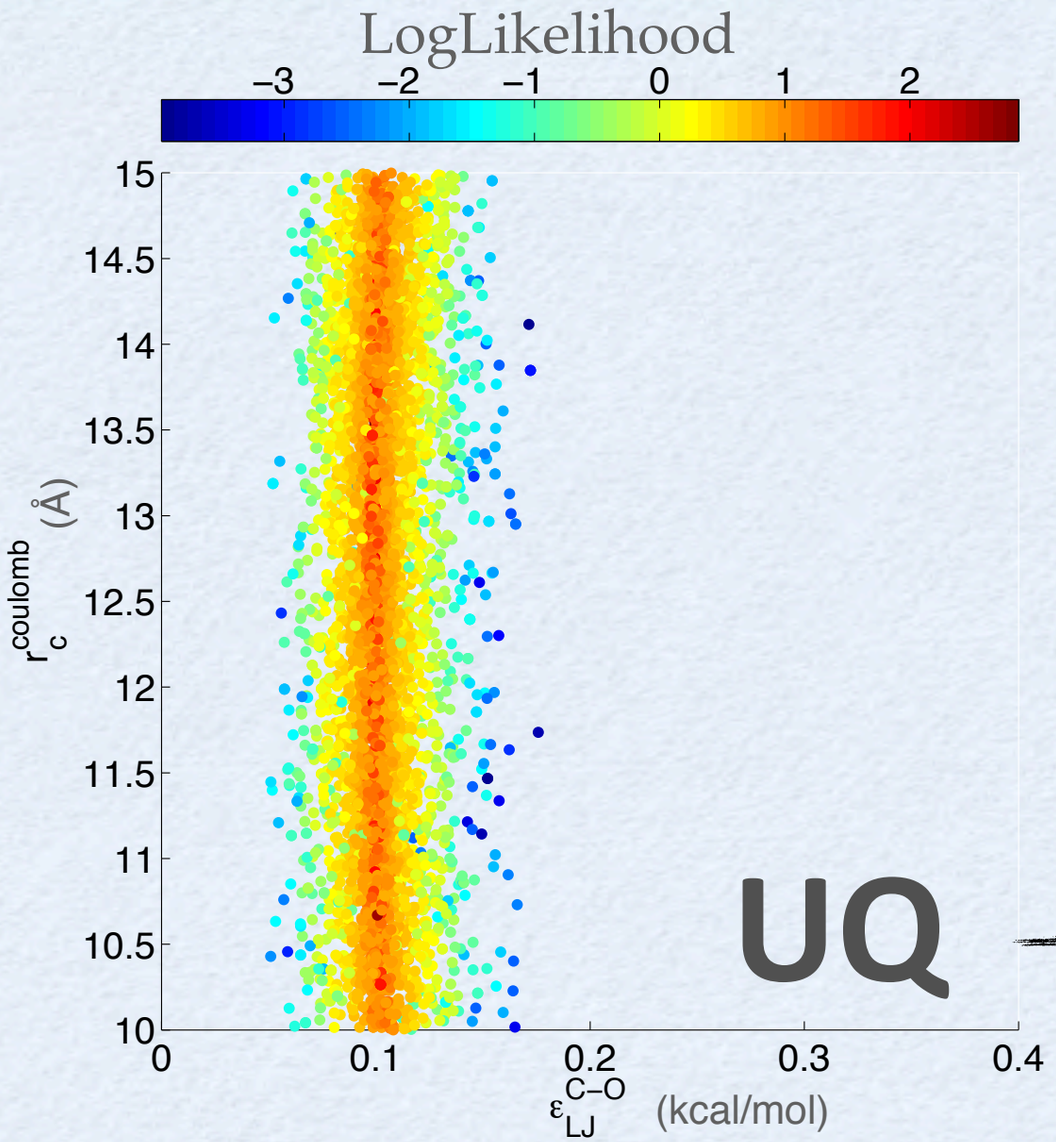




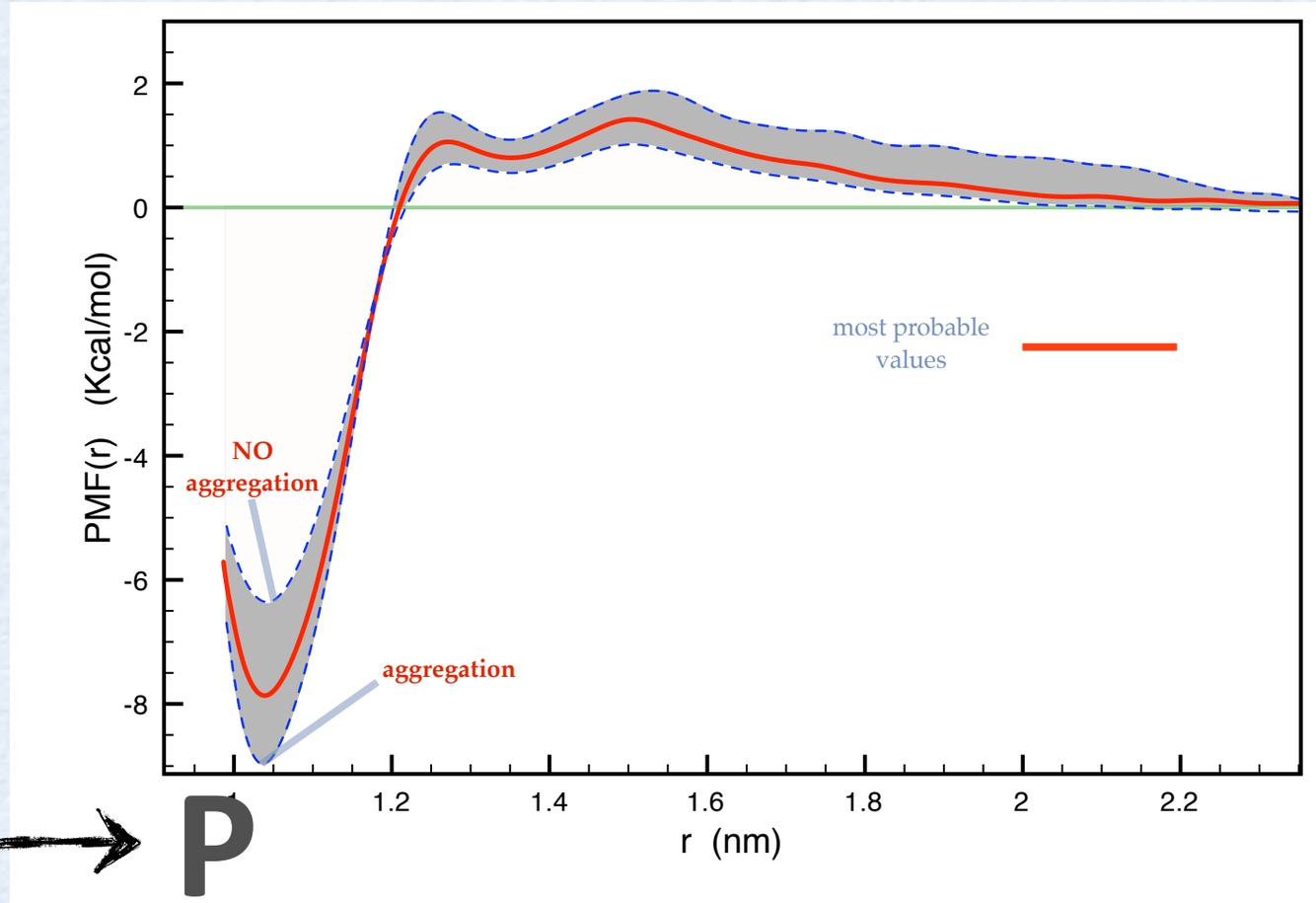


Angelikopoulos et al., Uncertainty Quantification and Prediction in MD Simulations: an HPC framework, J. Chem. Phys. (in press)

UQ (Water Contact Angle) +P (C_{70} Hydration)



UQ



P

Prediction of PMFs including Computational and Modeling Uncertainty.

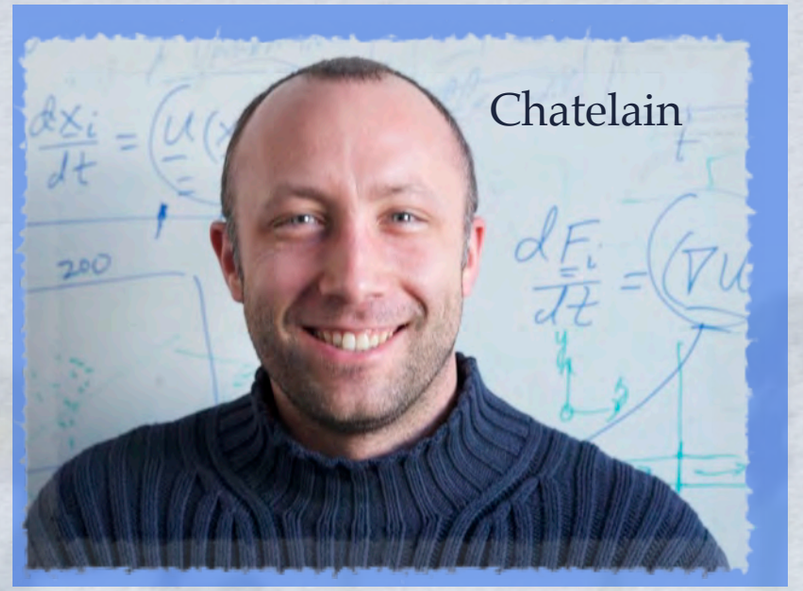
SUMMARY

Particles

- ☑ A robust and Accurate Method for Multi-Physics Simulations
- ☑ Common Computational Modules across Scales
- ☑ Multi-resolution, HPC implementation
- ☑ First steps in Coupling Atomistic-Mesoscale-Continuum
- ☐ **A Particle Programming Language**

- **UQ+P for Particle Based Solvers**


Walther


Chatelain


Bayati


Bergdorf


Rossinelli

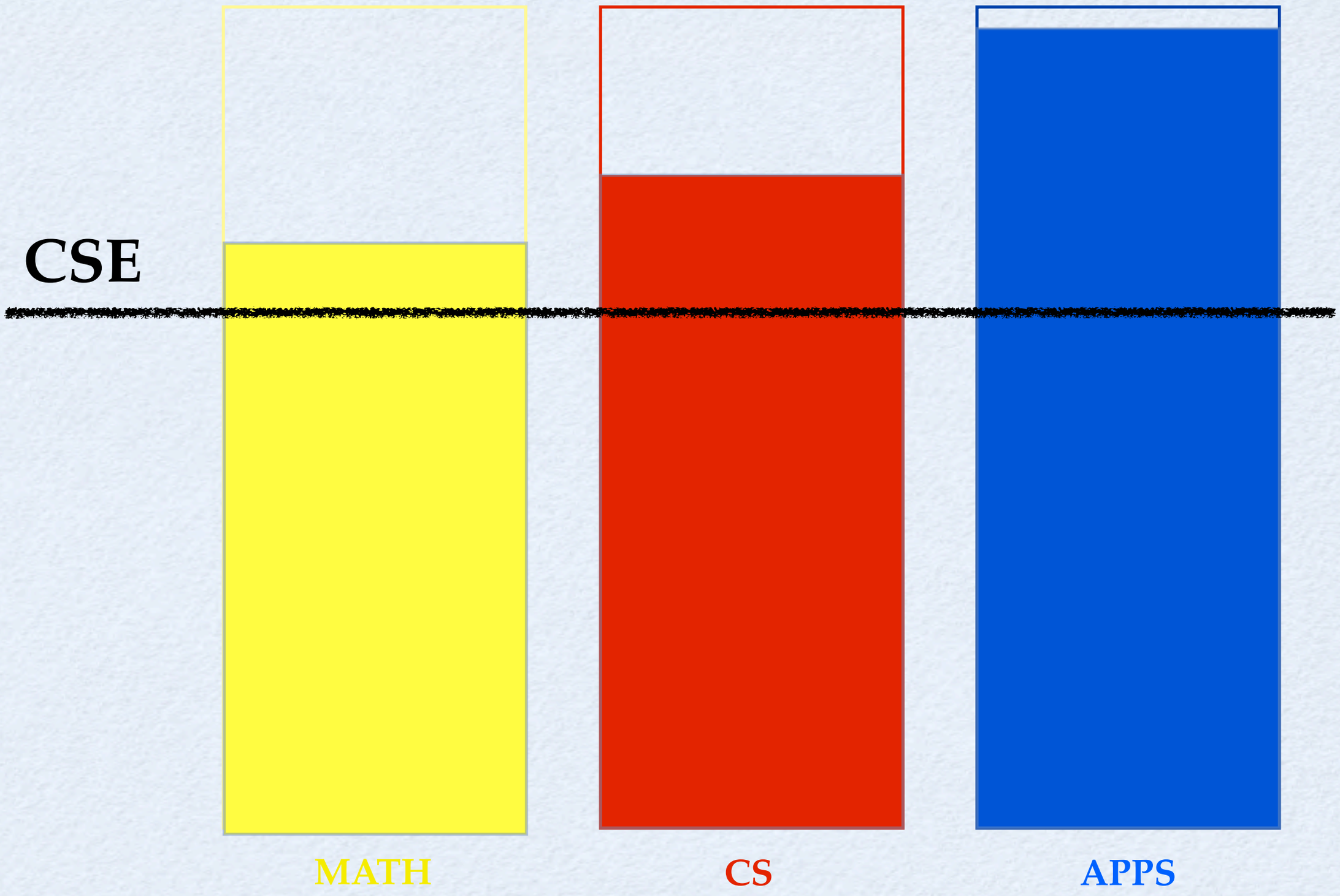

Gazzola


Hedjazialhosseini

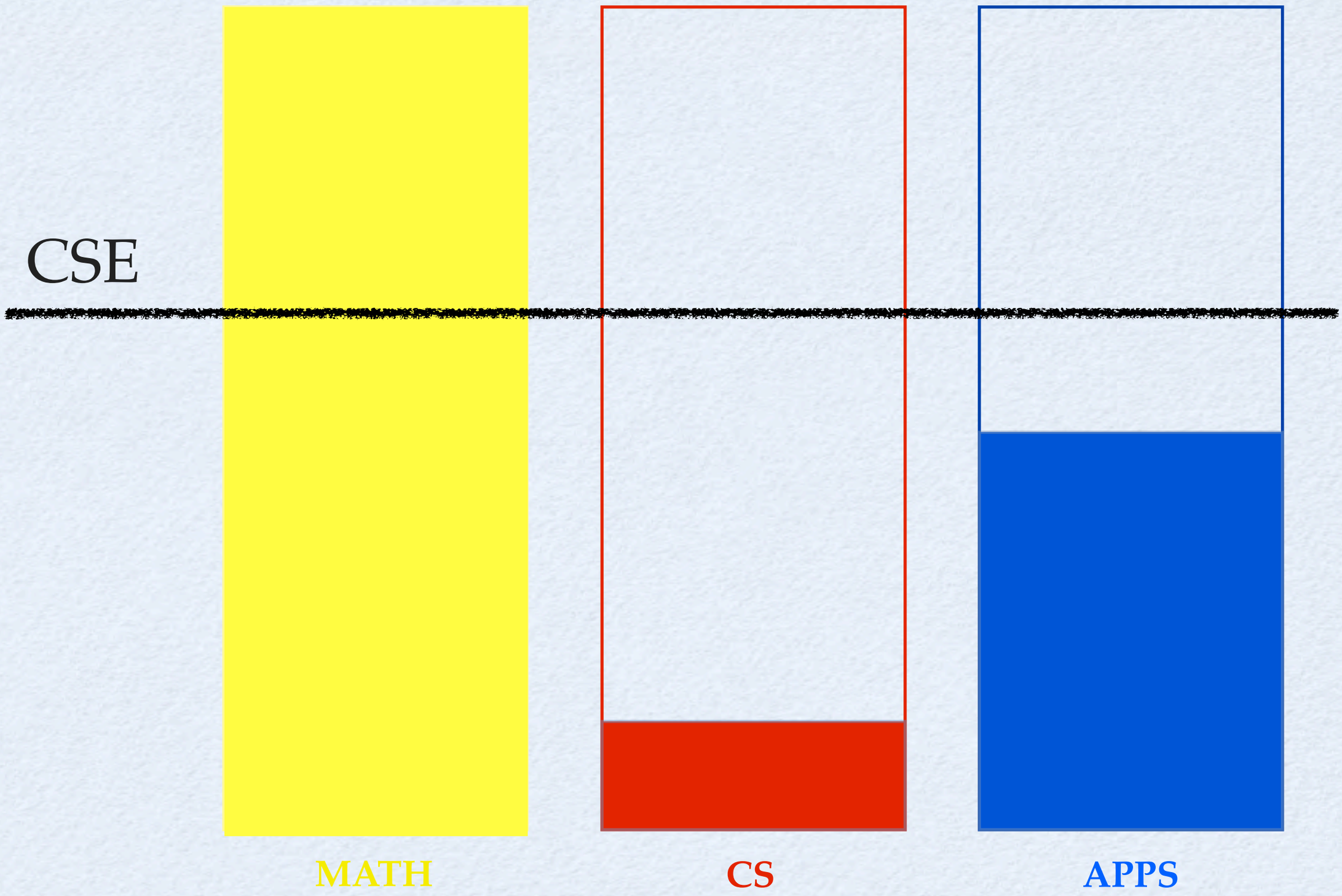

van Rees


Milde

SOME THOUGHTS IN CSE



SOME THOUGHTS IN CSE



SOME THOUGHTS IN CSE

MATHEMATICS - COMPUTER SCIENCE - APPLICATIONS

- A robust and Accurate Method for Multi-Physics Simulations
- Multi-resolution, HPC implementation

MULTISCALE

- First steps in Coupling Atomistic-Mesoscale-Continuum

APPLICATIONS

- **Fluids to Biology and Back**