Lattice Boltzmann-Particle Dynamics
Sims @ Phys/Chem/Bio interface

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iit ISTITUTO ITALIANO DI TECNOLOGIA

IACS Institute for Applied Computational Science
HARVARD SCHOOL OF ENGINEERING AND APPLIED SCIENCES

Sauro Succi,

IIT Rome and IACS Harvard

Indianapolis, May 2018

Plan of the talk

- Basics of Lattice Boltzmann (LB)
- LB+Particle Dynamics (LBPD) across scales
- Extreme LBPD at the Phys/Chem/Bio interface
- LBPD for nanoscale soft meso-materials design
- Towards Exascale LB
- Summary and outlook

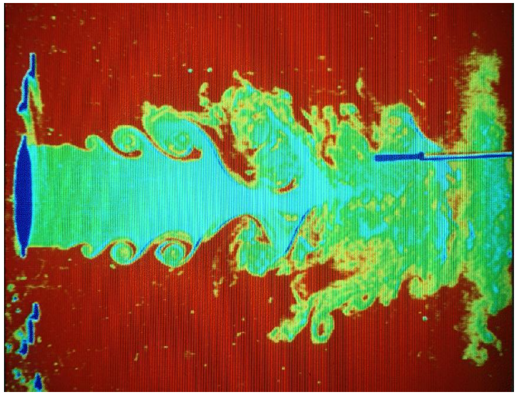
Why Boltzmann for fluids?

Fluids are properly described by the Navier-Stokes equations (NSE),

The NSE's are known for nearly two centuries (1822!), simply ma=F,

but ,,, VVVery HARD to solve:

$$\boxed{\begin{array}{l} \partial_t \vec{u} + \vec{u} \cdot \nabla \vec{u} = \nu \Delta \vec{u} - \nabla p \\ \nabla \cdot \vec{u} = 0, \ \ \rho = 1 \end{array}}$$



Nonlinear advection versus dissipation : ***Turbulence***

$$\mathrm{Re} = \frac{UL}{\nu}$$

$$\mathrm{Re} = \frac{UL}{\nu} = \frac{U}{c_s} \times \frac{L}{\lambda}$$

$$\mathrm{Re} \geq 10^6$$

$$CPU \approx \mathrm{Re}^{13/4}$$

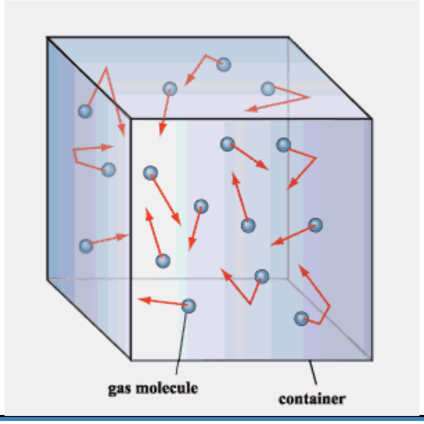
Why a Kinetic Theory of Fluids?

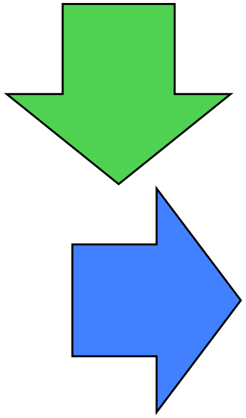
$$f(\vec{r},\vec{p};t) \qquad 2d+1 \quad \mathrm{dim}$$

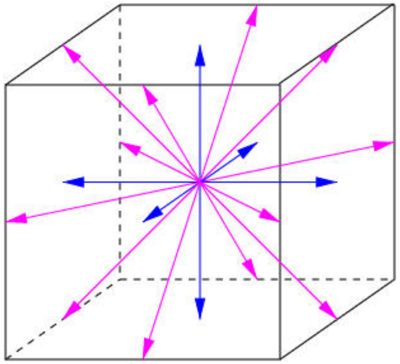
Boltzmann for fluids? Insane!

$$\boxed{\partial_t f + \vec{p}\cdot\nabla_r f + \vec{F}\cdot\nabla_p f = \frac{Q(f,f)}{\tau}}$$

velocity-space is sweet: lattice!







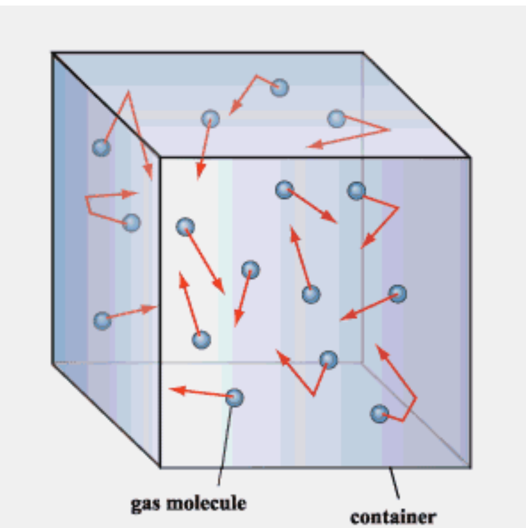
Lattice Boltzmann: crystal hydrodynamics

$$\boxed{f(\vec{r},\vec{p};t) = \sum_{i=0}^{b} f_i(\vec{r},t)\delta(\vec{p}-\vec{c}_i)} \qquad i = 0, b$$

Triple infinity to just 19!

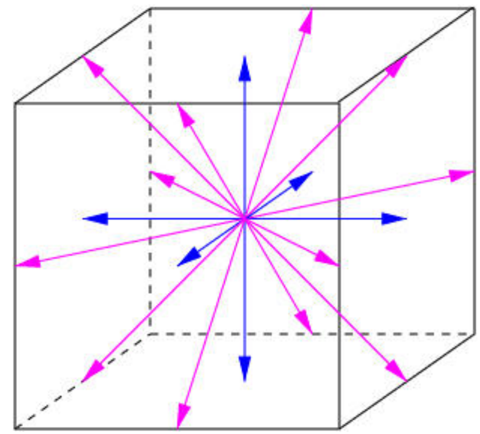
Quasiparticles: magic speeds!

Exact sampling of frequent events



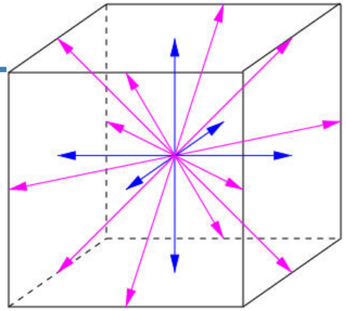
Universality

Individuality



$$\rho(\vec{r};t)\overline{\varphi}(\vec{r};t) \doteq \int \varphi(\vec{p}) f(\vec{r},\vec{p};t)\, d\vec{p} = \sum_{i=0}^{b} \varphi_i f_i(\vec{r};t)$$

LBE: Stream&Collide



Mathematical paradigm for flowing systems:

Free-streaming **Collisions** **Sources**

$$\boxed{f_i\left(\vec{r}+\vec{c}_i,t+1\right)-f_i\left(\vec{r},t\right)=-\Omega_{ij}\left(f_j-f_j^{eq}\right)+F_i}$$

$$f_i^{eq}=\rho w_i\{1+\beta\vec{u}\cdot\vec{c}_i+\frac{1}{2}[(\beta\vec{u}\cdot\vec{c}_i)^2-\beta u^2]\}+\ldots \qquad \beta=1/kT$$ **(EoS)**

$$\{\rho,\rho\vec{u},\overleftrightarrow{P},\ldots\}=\sum_{i=0}^{b}\{1,\vec{c}_i,\vec{c}_i\vec{c}_i,\ldots\}f_i$$ **Conservative (zero modes)** **Mass-Mom-MomFlux**

$$\Omega_{ij}=\Omega(\vec{c}_i\cdot\vec{c}_j)$$ **Transport/Dissipation**

$$F_i=\vec{F}\cdot\vec{c}_i$$ **External/Internal drives**

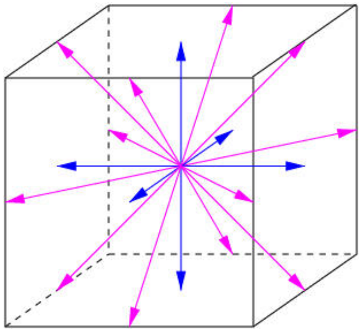
LBE: Stream-Collide paradigm (gather/scatter)

$$f_i(\vec{r};t)$$

HYDRO

$$\rho = \sum_i f_i \qquad \vec{J} = \sum_i f_i \vec{c}_i$$

$$f_i^{eq}(x;t) = w_i[\rho + Jc_i + \ldots]$$



COLLIDE

$$f'_i\,(x;t) = (1-\Omega) f_i + \Omega f_i^{eq}$$

STREAM

$$f_i\,(\vec{r} + c_i; t+1) = f'_i\,(\vec{r};t)$$

LBE assets

- Non-locality is linear and strictly exact

$$\boxed{\vec{c}_i \cdot \nabla f_i} \quad vs \quad \boxed{\vec{u} \cdot \vec{\nabla} \vec{u}}$$

- Non-linearity is local and machine roundoff
  Laplacian-free dissipation, roundoff conservative

$$\boxed{\omega[f_i - f_i^{eq}(u)]} \quad vs \quad \boxed{\nu \Delta \vec{u}}$$

- "Easy" on complex geometries (straight lines)
- $\boxed{\text{Pressure is local}}$ (weakly compressible)
- Excellent for parallel computing
- Emergent complexity at very low programming cost

The dark sides of the LB moon

- Natural-born dynamic:
  Steady-state

- Natural-born cartesian:
  Body-fitted geometries

- Natural born athermal:
  Strong thermal/incompressible flows

- Spurious effects (computer "hallucinations")
  at near-grid scales

LB History

Trailblazers (1988-89)

Mc Namara, Zanetti, PRL 1988

Higuera-SS, Higuera-SS-Benzi,

Higuera-Jimenez, EPL 1989

Key improvements (>1990)

D'Humieres, P. Lallemand, YH Qian, H. Chen,

S. Chen, I. Karlin, X. He, L.S. Luo

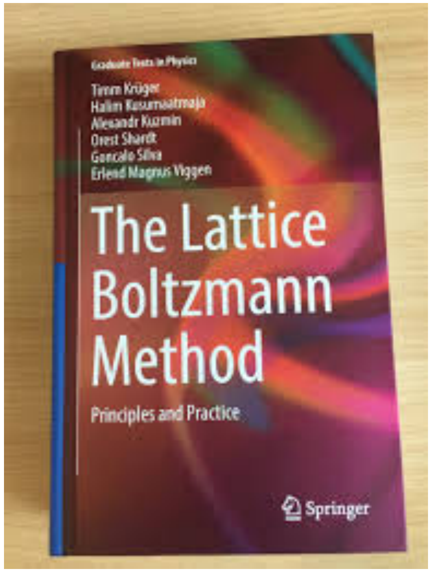
Breakthru spinoffs (1993):

X. Shan, H. Chen (non-ideal fluids)

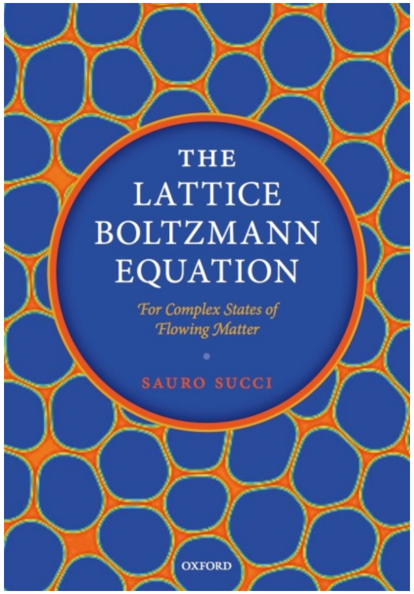
A. Ladd (suspended bodies)

Recent Books

T. Krueger, H. Kusumaatmaja, A Kuzmin, O Shardt, E M Viggen,
The lattice Boltzmann method, principles and practice
Springer 2017



SS: The lattice Boltzmann equation for complex states of flowing matter, Oxford U.P., 2018 (near 800 pages, gasp!)



Is it rrreally NS?

Well, yes, yes … YES!

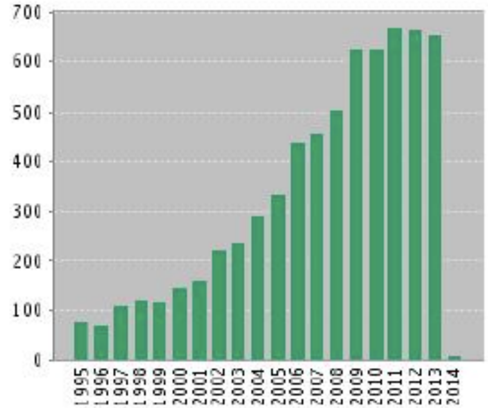
>40 Kpapers, >100Kcites, h=122, as of Dec 2013

Porous Media
Turbulence
Reactive
Multiphase flows
Colloidal flows
Microfluids
Nanofluids
………

Timespan=All years. Databases=SCI-EXPANDED, SSCI, A&HCI, CPCI-S, CPCI-SSH, BKCI-S, BKCI-SSH, CCR-EXPANDED, IC.

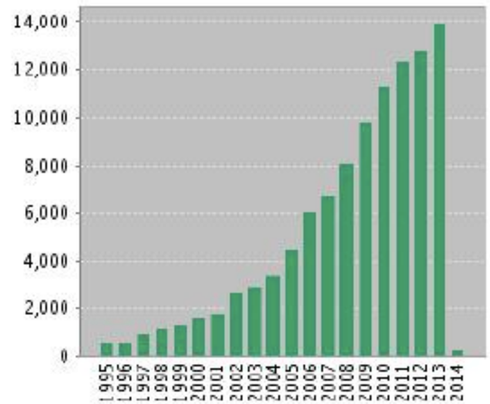
his report reflects citations to source items indexed within Web of Science. Perform a Cited Reference Search to include citations to items not indexed within Web of Science.

Published Items in Each Year



The latest 20 years are displayed.
View a graph with all years.

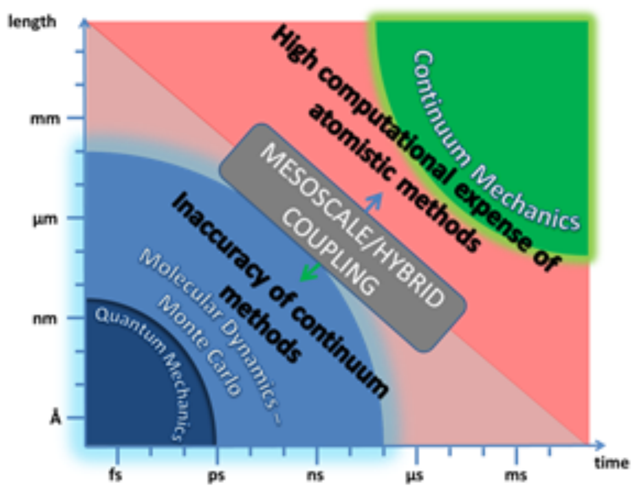
Citations in Each Year

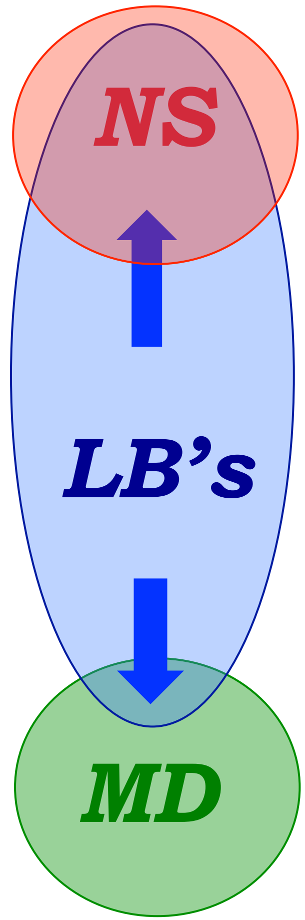


The latest 20 years are displayed.
View a graph with all years.

Results found:	6818
Sum of the Times Cited [?] :	104220
Sum of Times Cited without self-citations [?] :	43419
Citing Articles[?] :	37970
Citing Articles without self-citations [?] :	32015
Average Citations per Item [?] :	15.29
h-index [?] :	122

Multiscale LB-PD



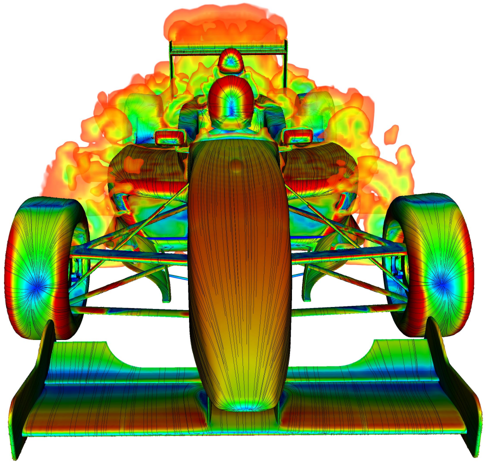


Fields (>mm)

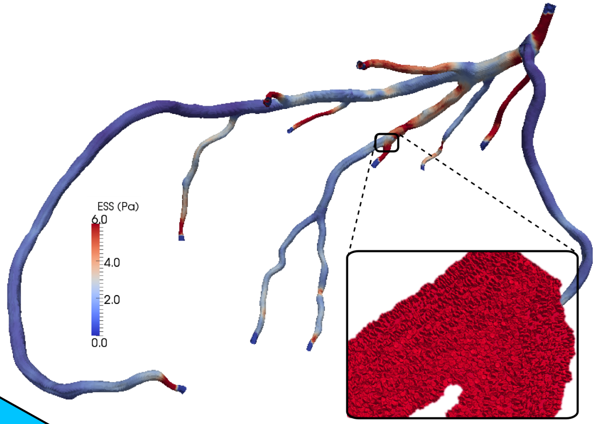
PDF's (micron)

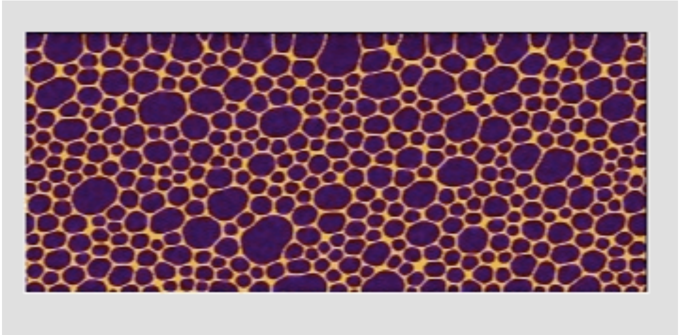
Particles (nm)

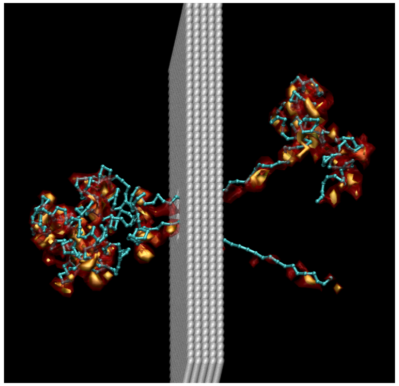
LB across scales:
from turbulence to biopolymers to quark-gluon plasmas (m to fm)



(1m)







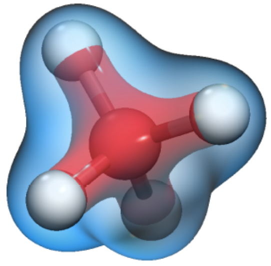
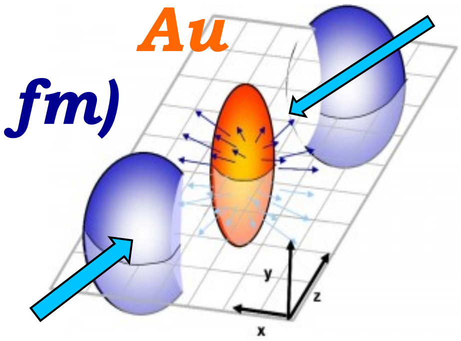


FIG. 1. Methane molecule, CH_4. The blue and red isosurfaces denote low and high electronic density, respectively. Using our model, we have obtained for the angles between bonds, 109.47 degrees, and a C-H bond distance of 108.6 pm.

(1 fm)



Hydrodynamics is universal across scales, and LB goes along with it

The first MUPHY team (2008)

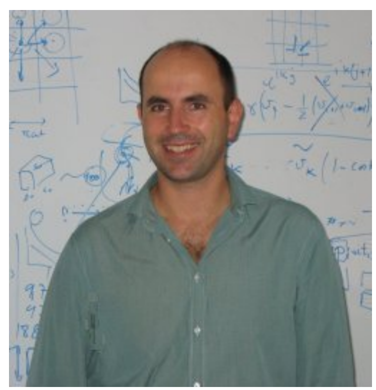
Massimo

Tim

Sauro

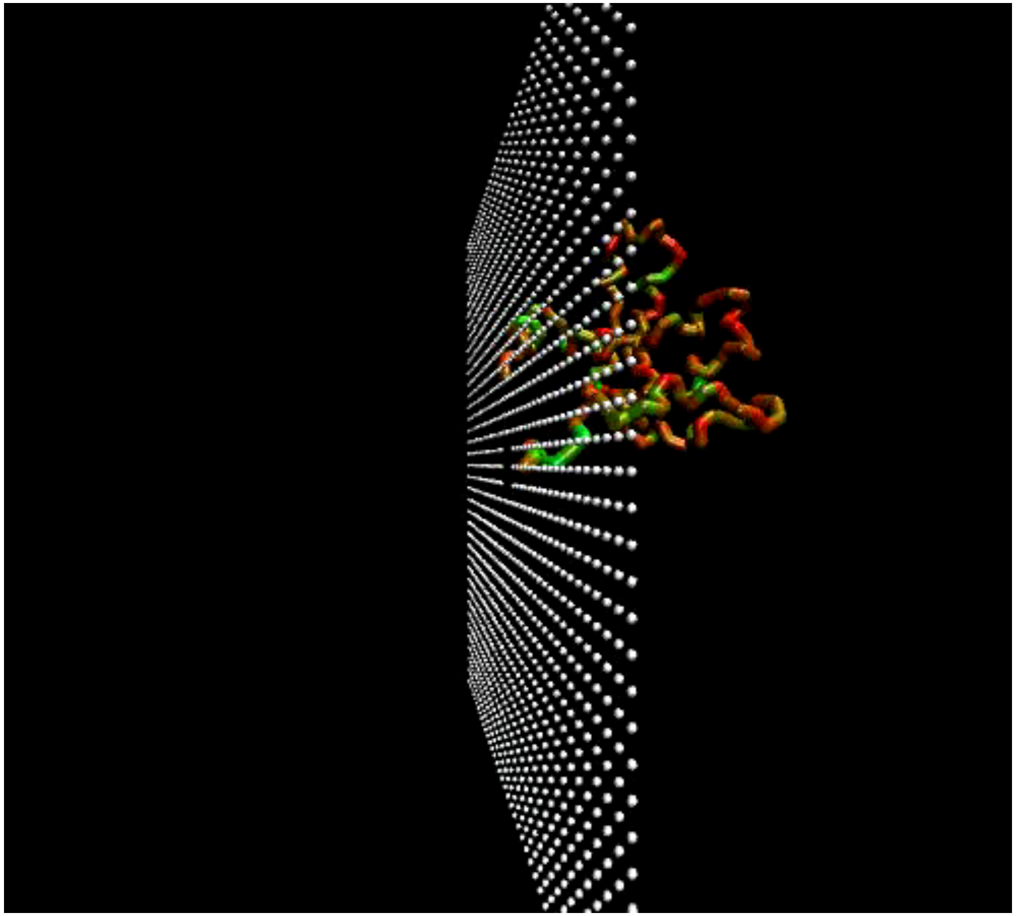
Maria

Simone



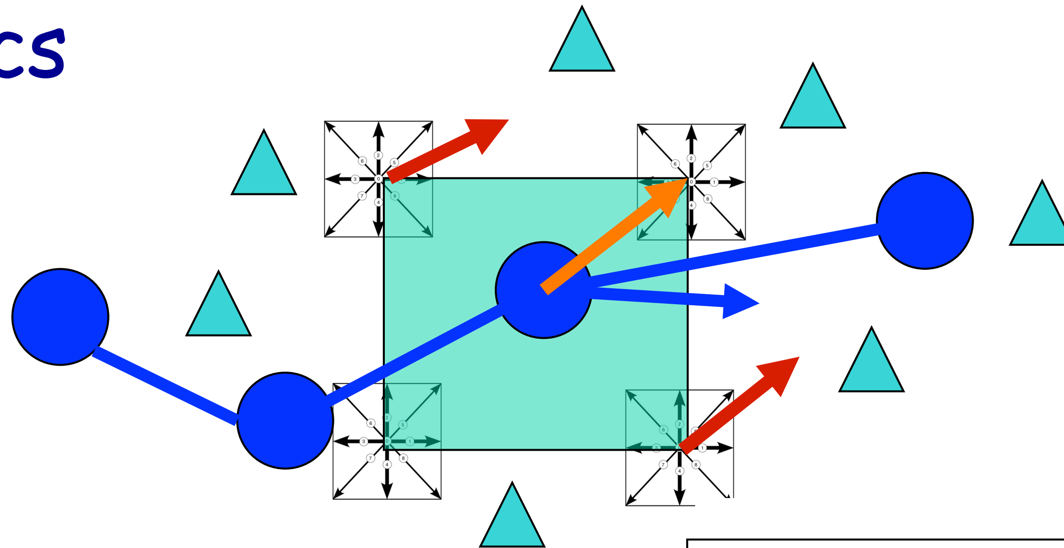
Joy

Biopolymer translocation



Coupling LB with stochastic PD (Langevin-like)

Langevin dynamics (point-particles)



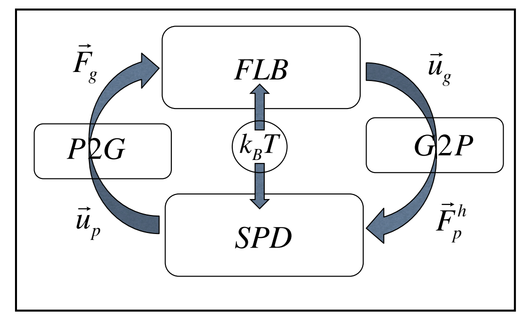
$$
\begin{cases}
\dfrac{d\vec{r}_p}{dt} = \vec{v}_p \\[2ex]
\dfrac{d\vec{v}_p}{dt} = -\gamma(\vec{v}_p - \vec{u}_p) + \vec{\xi}_p + \sum_q \vec{a}_{pq} + \dfrac{\vec{F}_p}{m}
\end{cases}
$$

Friction

Random

Conservative

External



LB added value

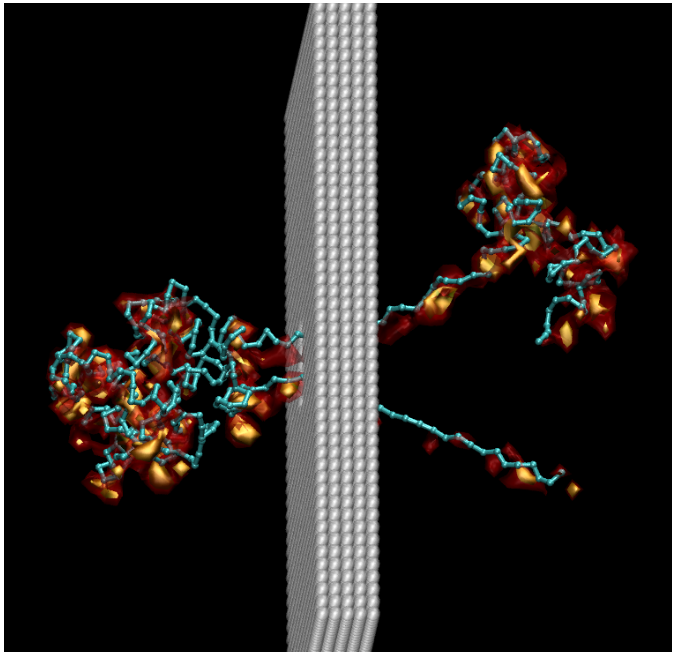
+ Parallel efficiency in complex geos

+ O(N) Particle-Fluid scheme

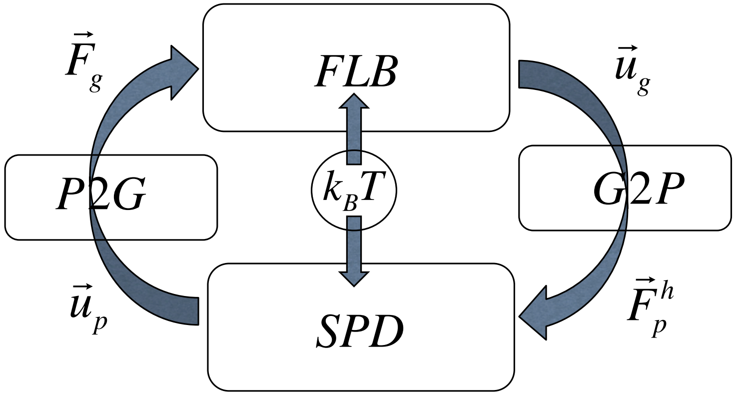
+ Explicit solvent (hydrocorrel)

- Small dt, compressibility ...

DNA translocation: LB/Langevin



Solvent: LB; "DNA": Langevin



294,912 JuGene (L and P) cores

11 TF (Finalist GB 2011)

Multiscale Hemodynamics

The MUPHY team adds on

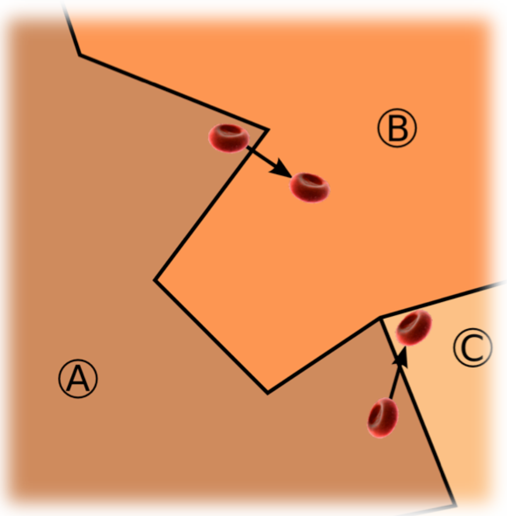
A. Peters-Randles

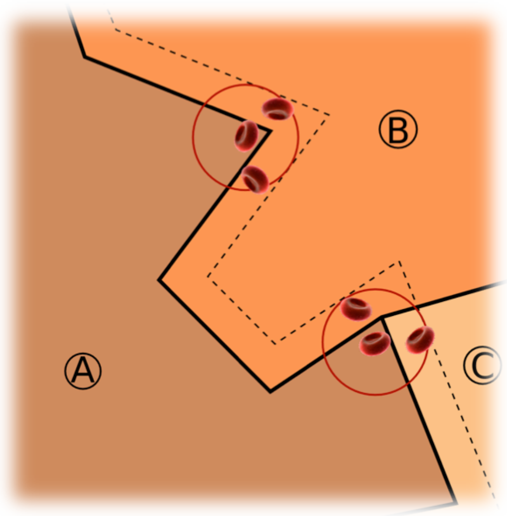
M. Fatica

M. Bisson

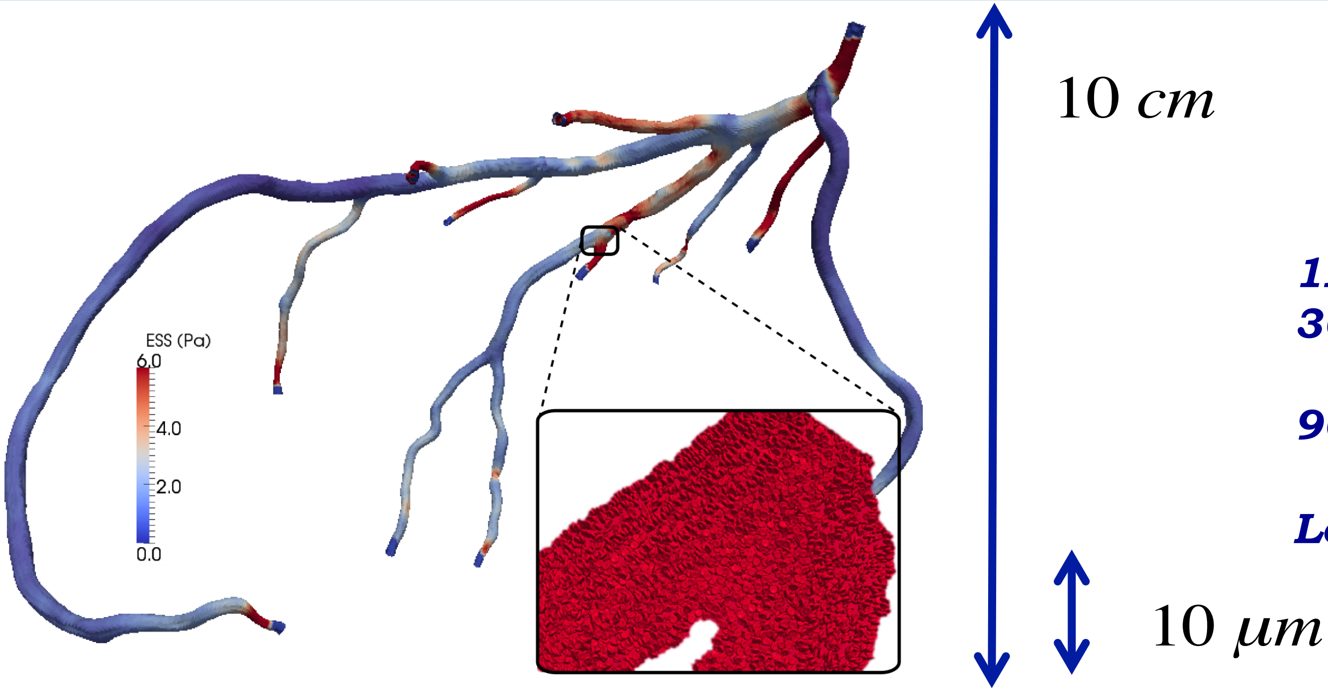
Cell Dynamics on Irregular Domains

Finite-size Rigid Particles in Complex Geometries





Multiscale hemodynamics



1Billion sites
300M particles

90% parallel efficiency

Low watt/flop

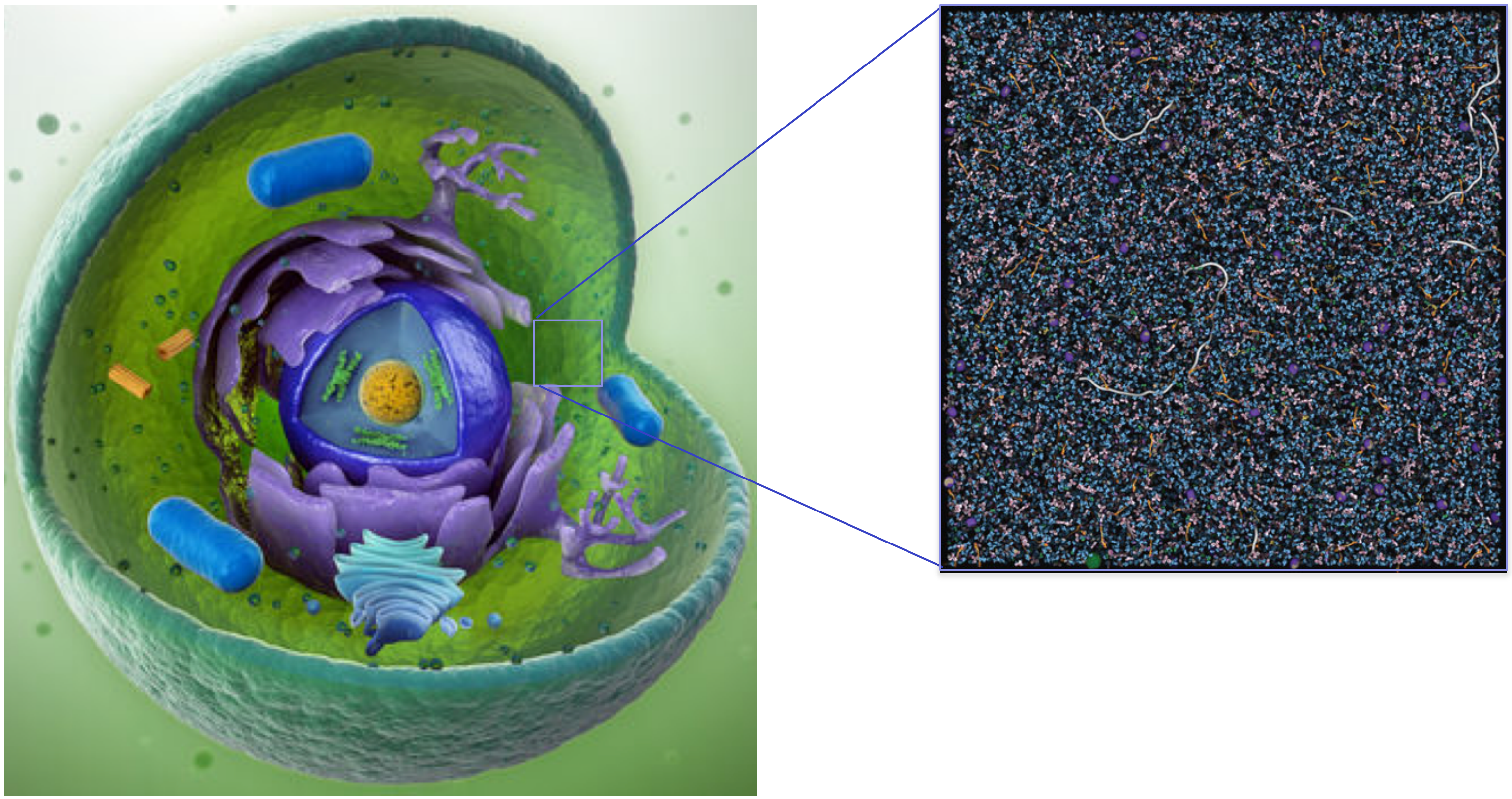
Melchionna, Bernaschi, Bisson, Fatica, Peters, Kaxiras, SS

Honorable mention, Gordon Bell final 2012
0.7 Pflops, 2M cores, multi-GPU (Tsubame2)

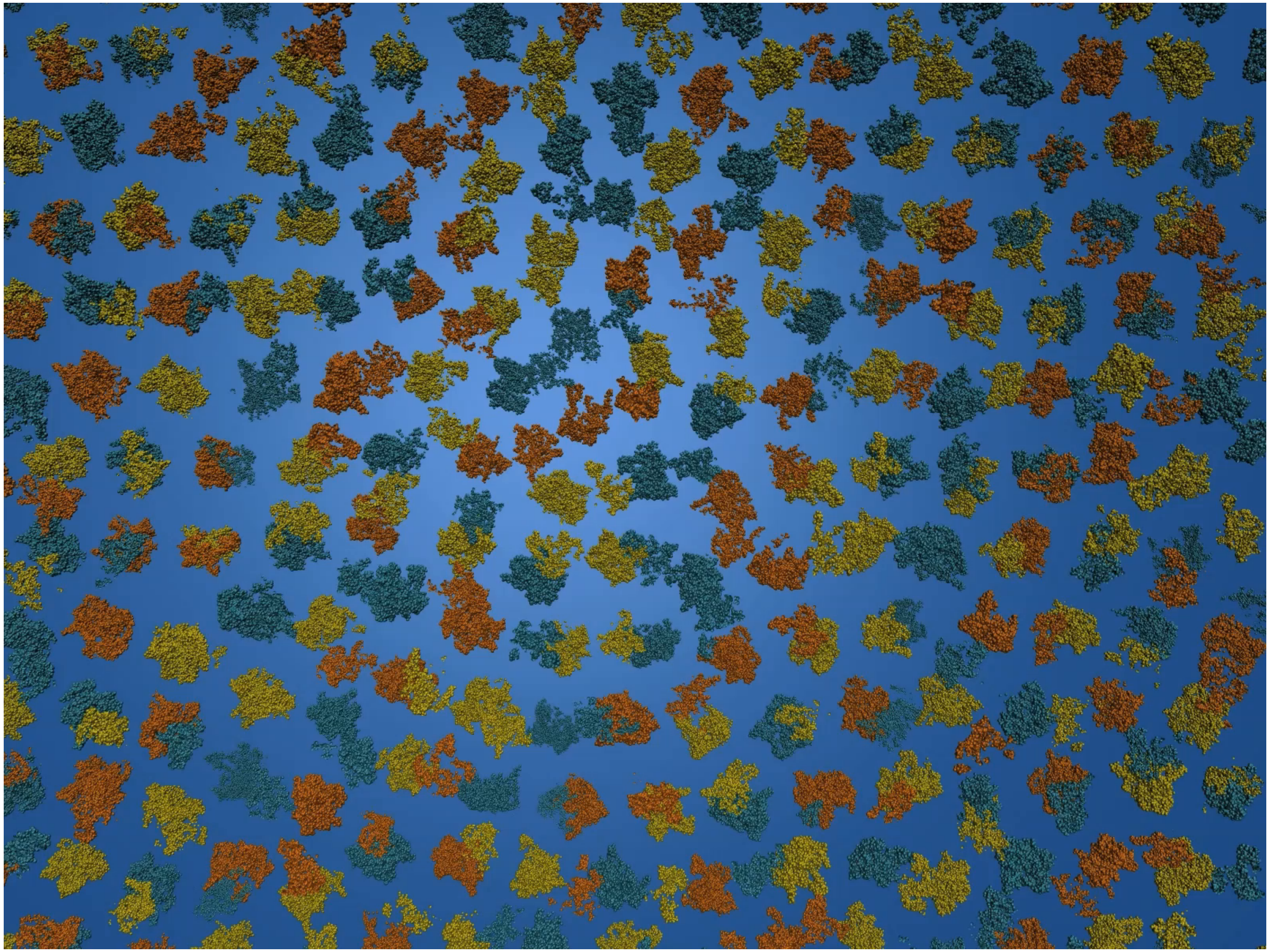
Protein crowding in the cell

Protein Crowding in Cells

Properties of enzymes and proteins in vitro and dilute solutions may differ by orders of magnitude from the true values seen in actual cells.

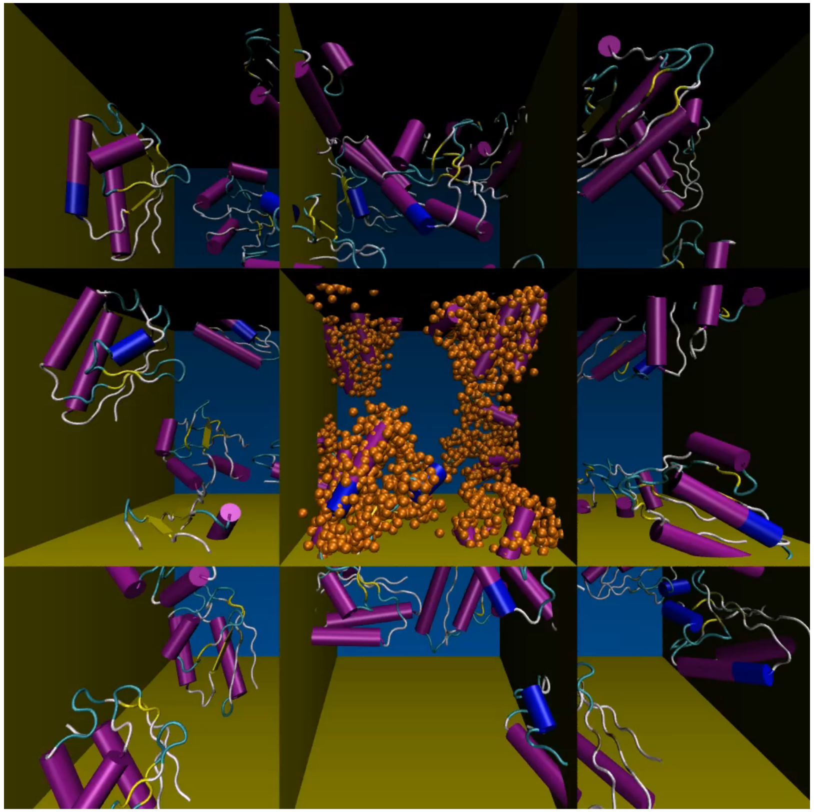


Crowding implies much lower diffusivity



Protein Crowding in Cells

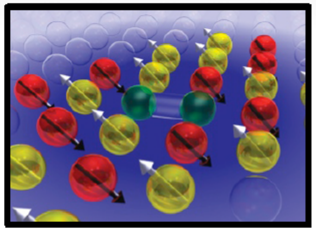
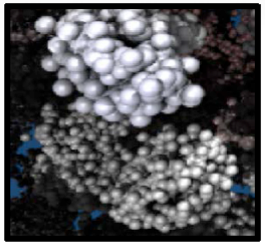
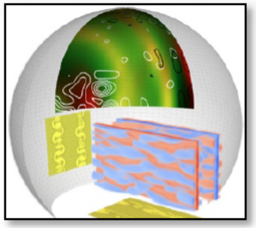
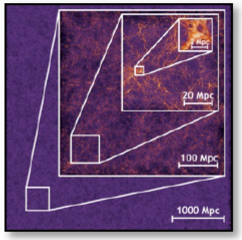
Gordon Bell 2013: *20 Pflops (Titan,ORNL)*
about ½ fold@home



*3K*3K*2K=18G sites*
*18K proteins * 4K particles*
72M particles

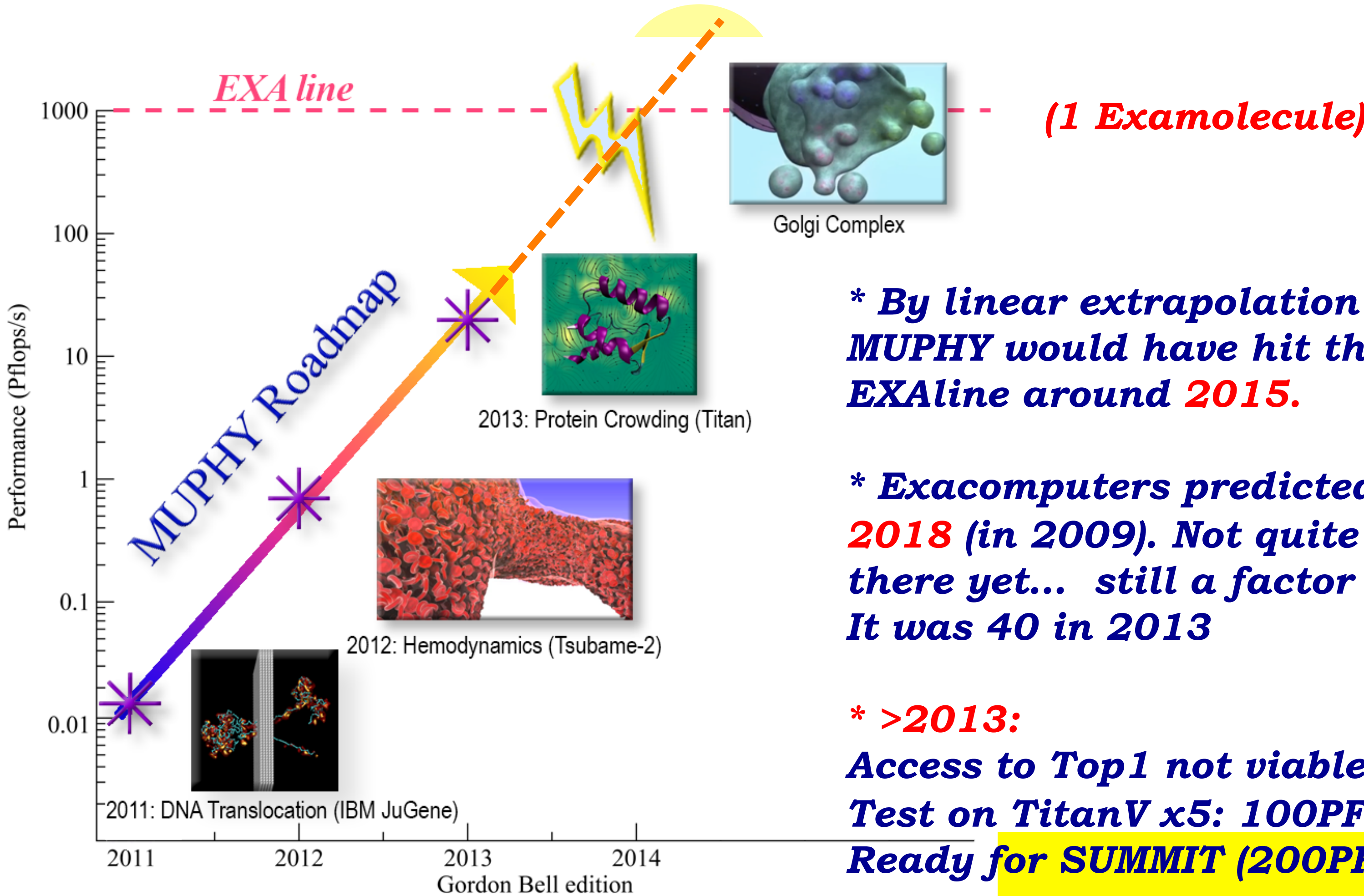
(Courtesy M. Bernaschi, M. Bisson, M. Fatica, S. Melchionna)

High-impact science at OLCF: Four of Six SC13 Gordon Bell Finalists Used Titan

Peter Staar	Massimo Bernaschi	Michael Bussmann	Salman Habib
ETH Zurich	ICNR-IAC Rome	HZDR - Dresden	Argonne
High-Temperature Superconductivity	**Biofluidic Systems**	**Plasma Physics**	**Cosmology**
Taking a Quantum Leap in Time to Solution for Simulations of High-T_C Superconductors	20 Petaflops Simulation of Protein Suspensions in Crowding Conditions	Radiative Signatures of the Relativistic Kelvin-Helmholtz Instability	HACC: Extreme Scaling and Performance Across Diverse Architectures
Titan (15.4 PF)	Titan (20 PF)	Titan (7.2 PF)	Sequoia (13.9 PF), Titan
			

Extreme LBPD computing: The MUPHY roadmap

Gordon Bell editions

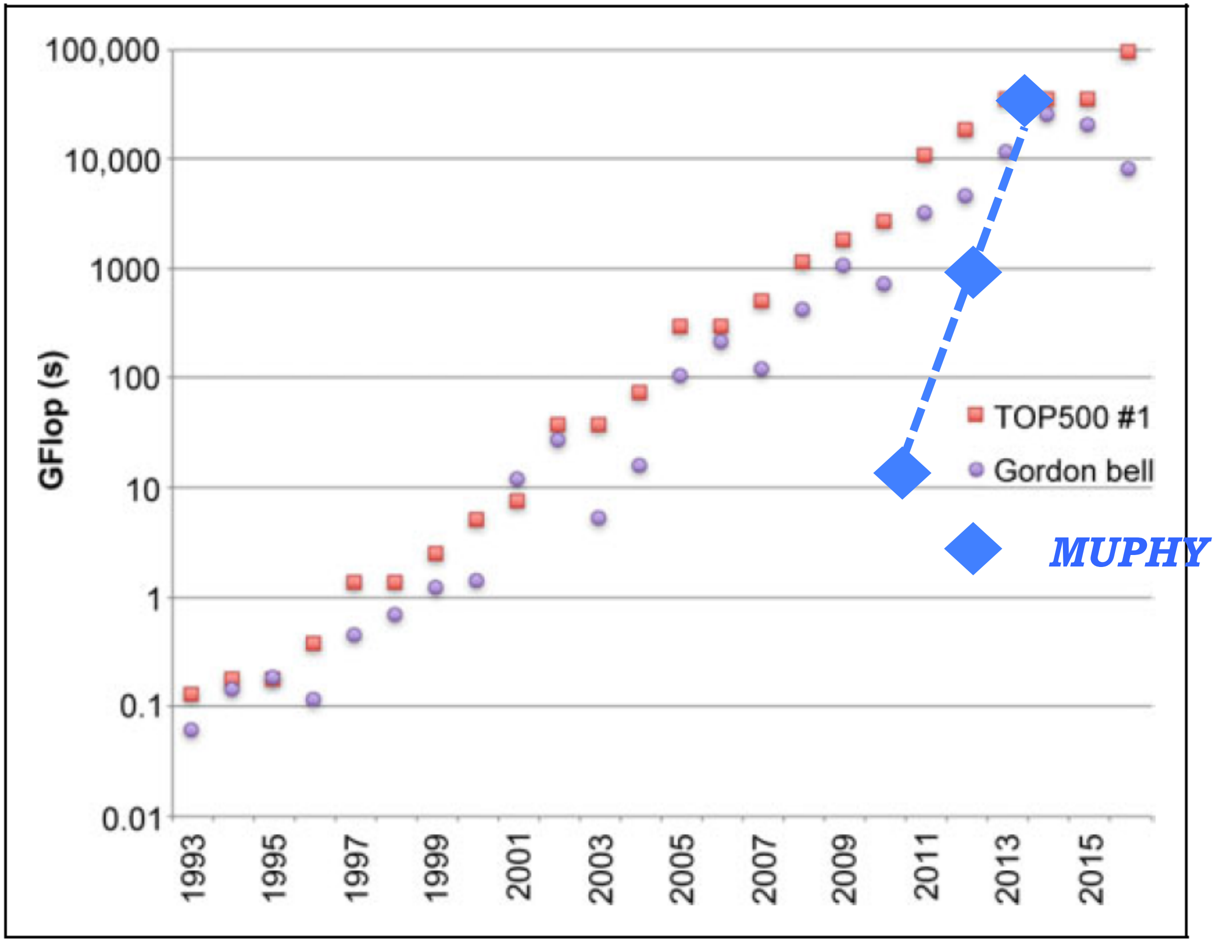


* By linear extrapolation MUPHY would have hit the EXAline around 2015.

* Exacomputers predicted by 2018 (in 2009). Not quite there yet... still a factor 10
It was 40 in 2013

* >2013:
Access to Top1 not viable
Test on TitanV x5: 100PF
Ready for SUMMIT (200PF)

Gordon Bell winners timeline



G. Bell,
D. Payley
J. Dongarra
A. Karp,
K. Walsh,
JHPCA 2017

COPMAT

Full-scale **CO**mputational design of **P**orous mesoscale **MAT**erials

European Research Council

PI: S. Succi

The COPMAT Team

M. Lauricella

Sauro Succi

A. Montessori

M.Bernaschi

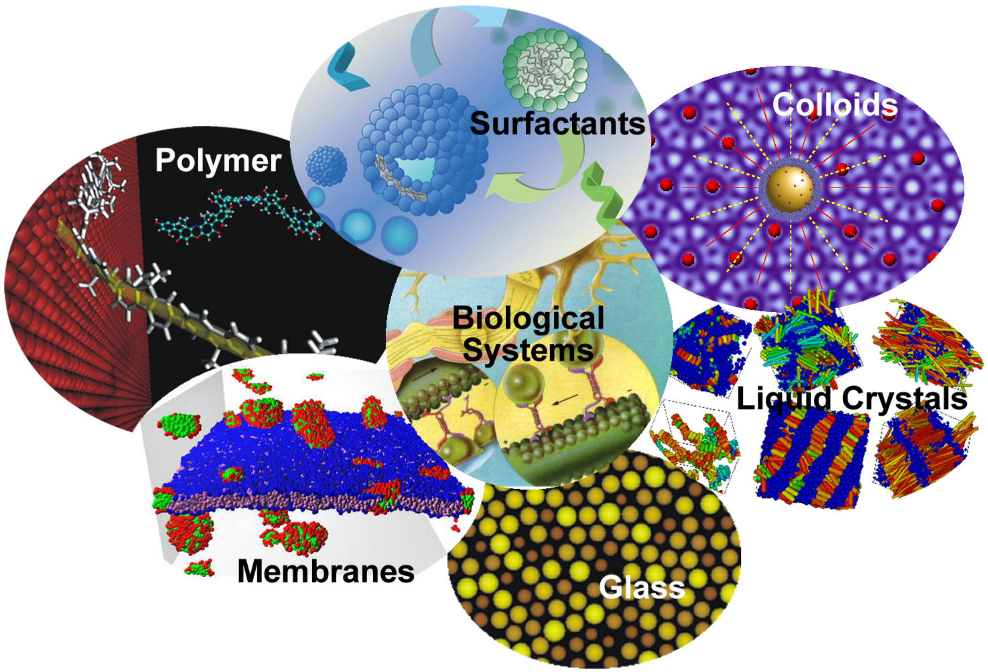
G. Falcucci

A. Scagliarini

G. Amati

Soft Mesoscale Materials

Phys/Chem/Bio = Soft matter



Internal structure: weakly broken universality
Beyond Navier-Stokes (BNS)

Flows with (lot of) interfaces

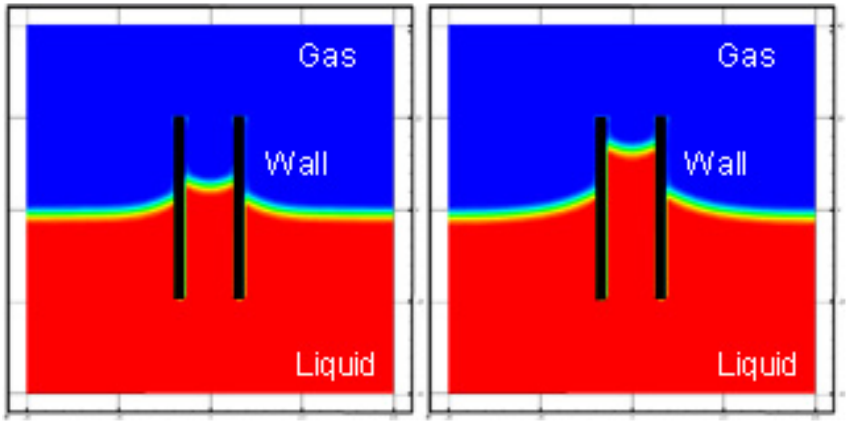
$$h \equiv V / S \to 0$$

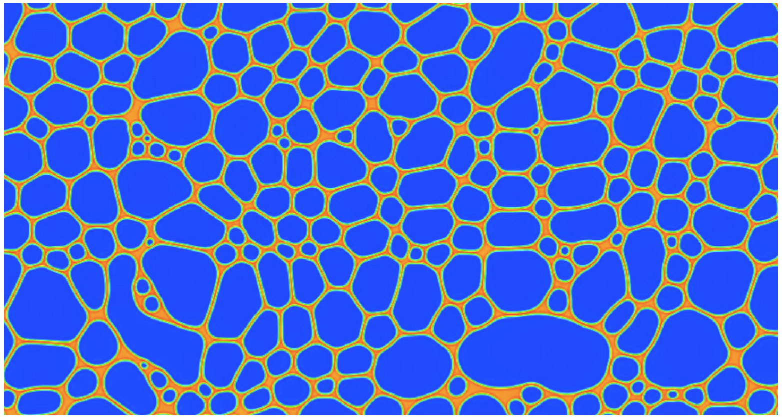
$$h > \lambda_m$$

Complex fluids

$$h \approx \lambda_m$$

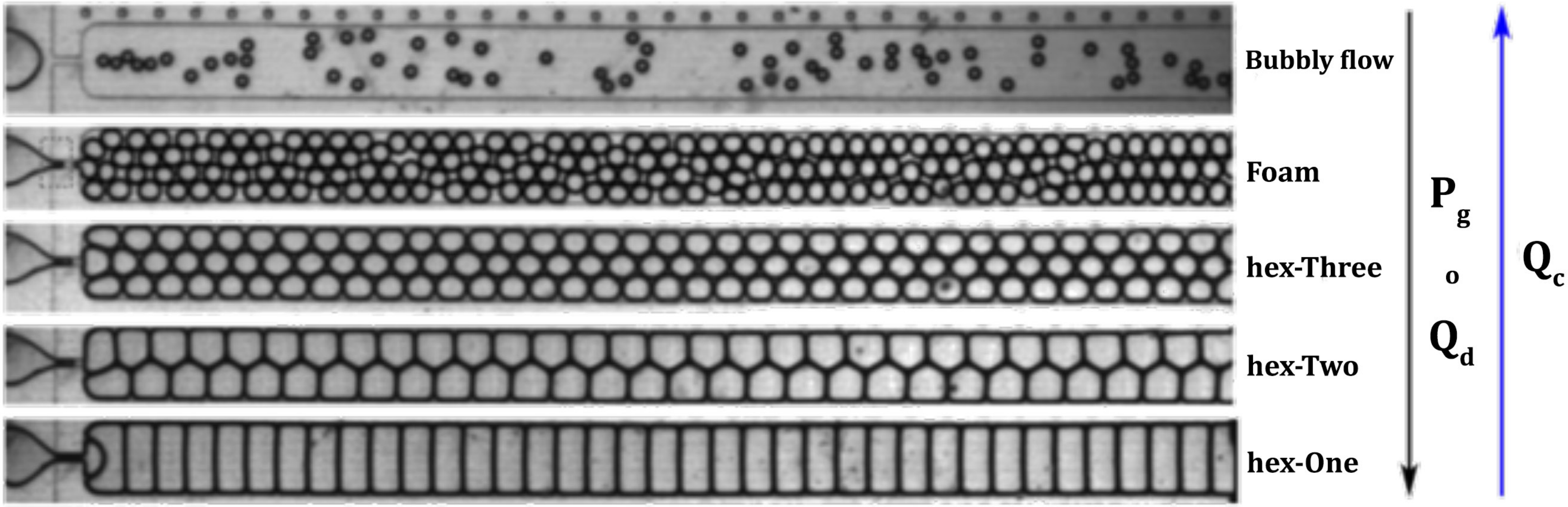
Beyond hydro





Soft-Flowing Crystals

Droplet-based states of matter!



Piotr Garstecki, Howard Stone and George Whitesides, Phys Rev Lett, 2005, 94, 164501(4)

By regulating the flow rate of the dispersed phase Q_d (or gas pressure P in the case of foams) and of the continuous phase Q_c, different pore sizes (different configurations/arrangements can be obtained)

LB requirements BNS

Physical challenges

Non-ideal Equation of State

Tunable (low) surface tension

Tunable disjoining pressure

Near-contact many-body physics

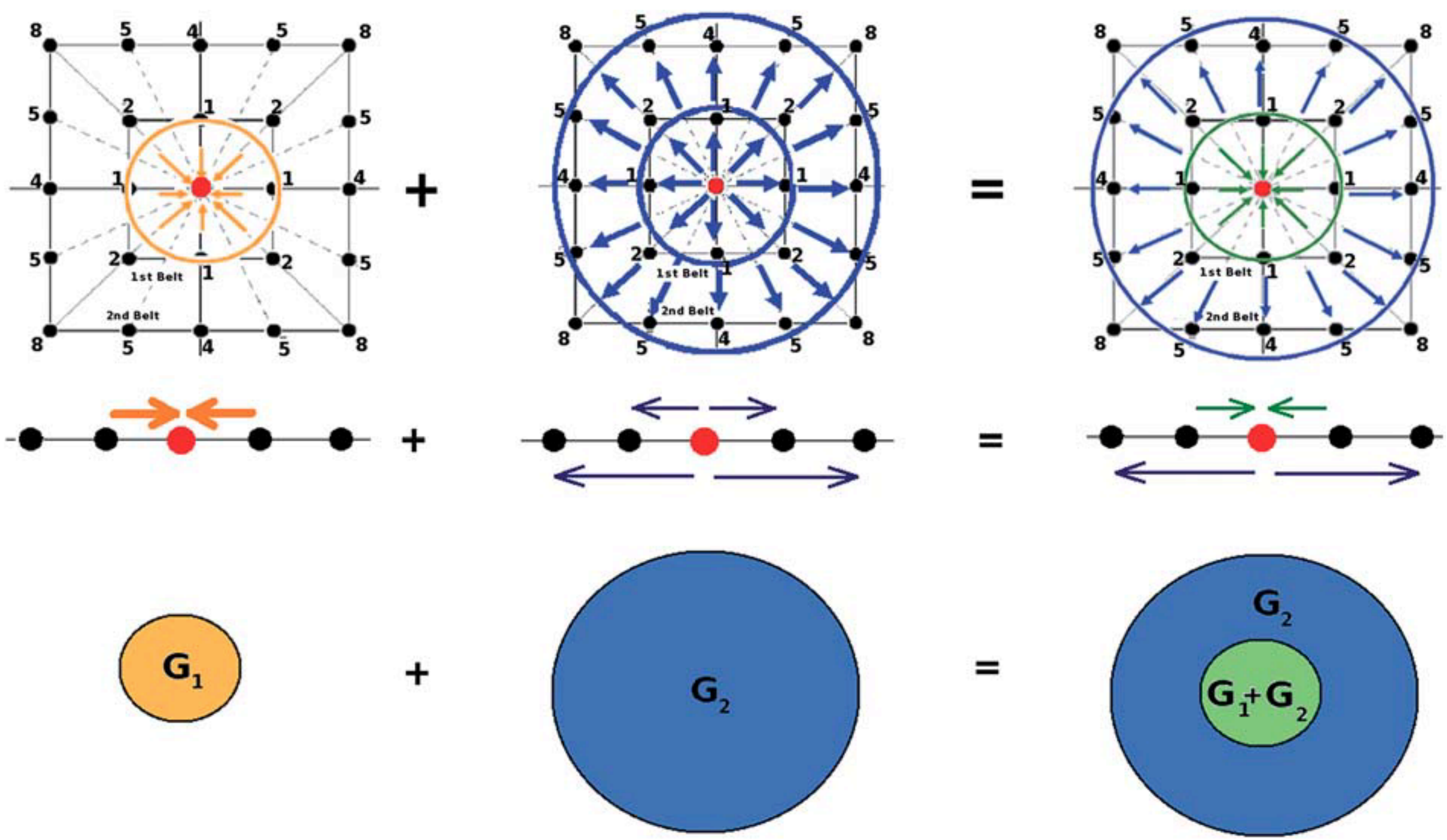
Numerical challenges

Large and sharp density jumps (1:1000 within 1 nm)

Large viscosity ratioes (1:10)

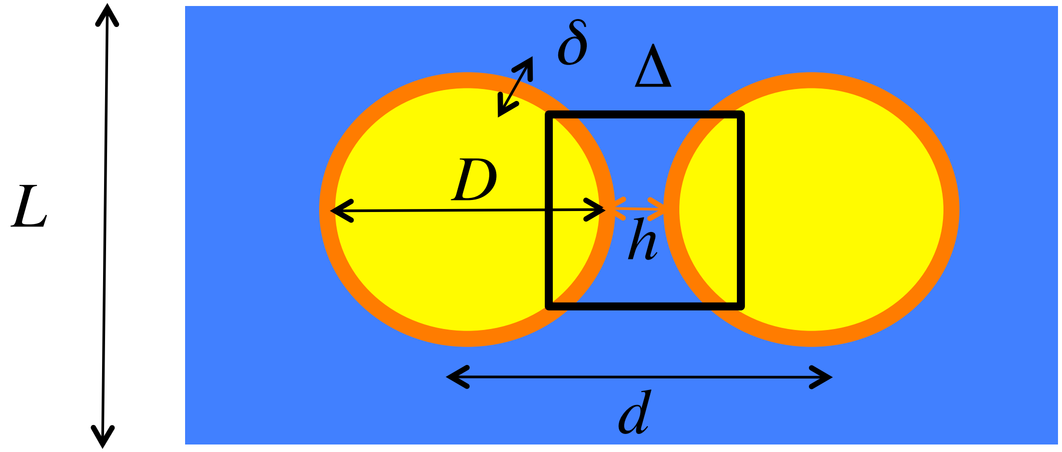
High-order lattices

Multi-range lattice potentials



Major extension of Shan-Chen: Falcucci et al, Sbragaglia et al, 2007

Micro-Meso-Macro connection



$L = 1\,cm$

$D = 10 - 100\,\mu$

Δ

$h = d - D \approx 10\,nm$

$\delta = 1\,nm$

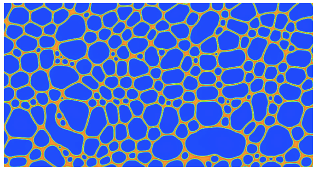
Disjoining Pressure is hydro-singular!

$$F(h) = a/h - b/h^3 + \dots$$

$a < 0$ **Coalescence**

$a > 0$ **Rebound**

Long-lived states

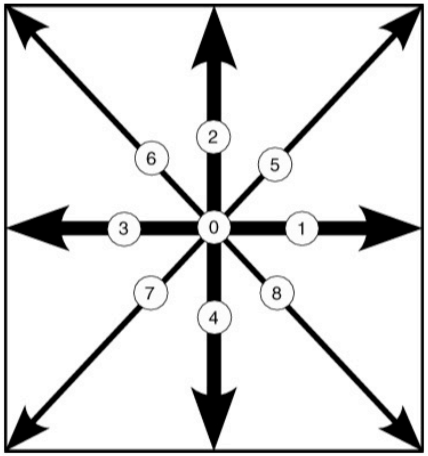


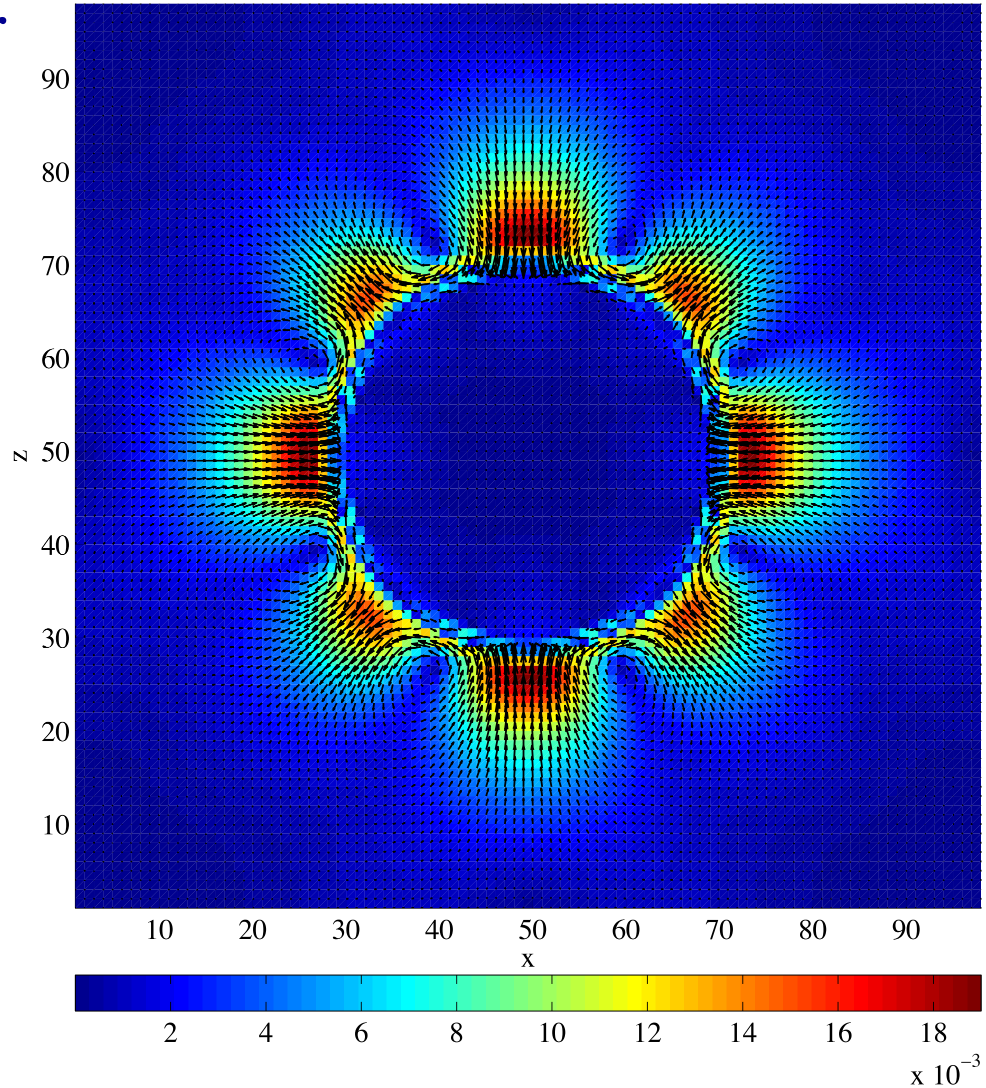
$\delta << \Delta < h << D$	**LB is ok**
$\delta < h < \Delta << D$	**LB subgrid**
$\Delta < \delta \approx h << D$	**LB subnano**

Casimir effects

"Hallucinations": spurious currents

Easy access to major configurational complexity, comes at a price…





These modes have no citizenship in the Continuum!

Near-grid physics always UV exposed

How to go about it?

Hard-way:
Massively Parallel (nm to cm: 7 decades!)
Grid Refinement, Unstructured, Hybrid …
Programming Complexity skyrockets

Beyond EXAscale!

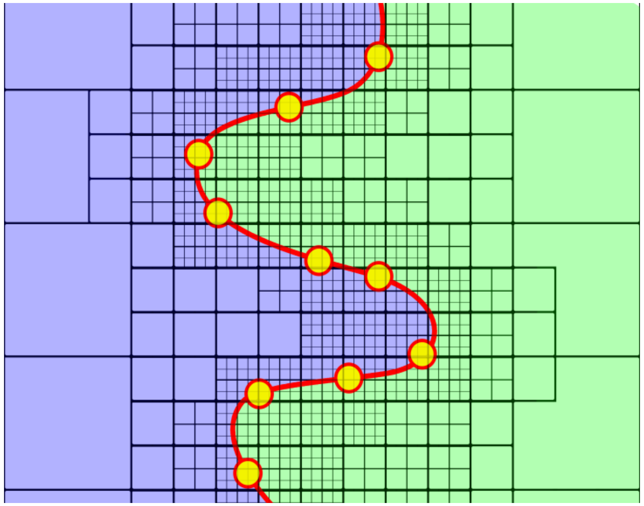
Several groups: Hoekstra,Chopard, Krafczyk, Coveney, Walberla…

Soft way:

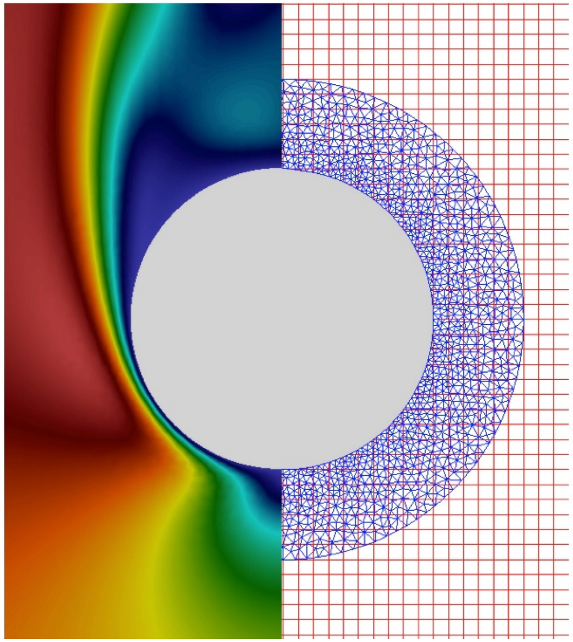
Sub-grid BNS-LB models
(Effective interactions, Renormalized DLVO theory)

Hard-core Computational Tools

- LB/PD: MUPHY (local grid refinement)
- Unstructured LB (LB/ULB instead of LB/DPD)



Adaptive grid-refinement



Hybrid unstructured

(G. Di Ilio et al, PRE 2017, C&F 2018)

Effective interactions on high order lattices

$$\vec{F}(\vec{r}) = \sum_{j=1}^{N_E} G_j \psi[\rho(\vec{r})] \sum_{i=1}^{N_j} w_{ij} \vec{c}_{ij} \psi[\rho(\vec{r} + \vec{c}_{ij}\Delta t)]$$

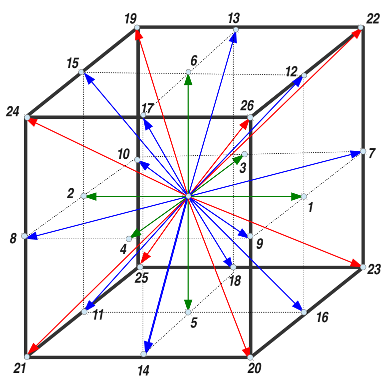
f_i

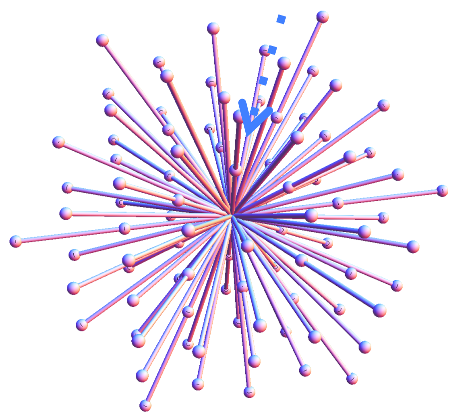
$\{\rho, \vec{J}, \overleftrightarrow{P}\}$

d=3; 27 velocities, 10 macrofields:

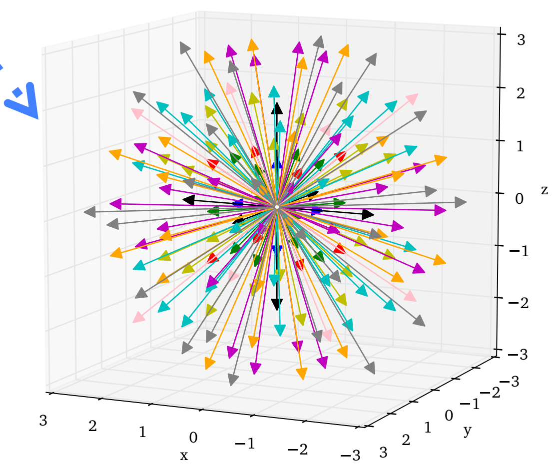
Renormalized couplings G's
Ren potentials psi
Multiple Relaxation
.....

Relativistic lattice:
100+ velocities, order 8+

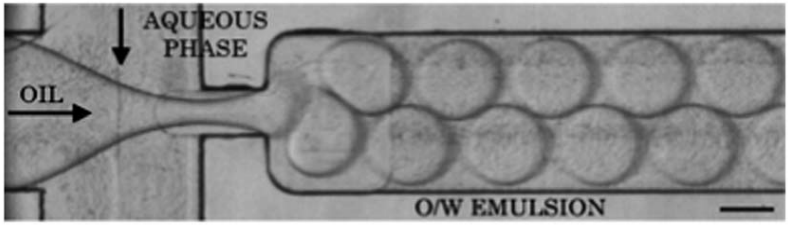




93 vel, order 8

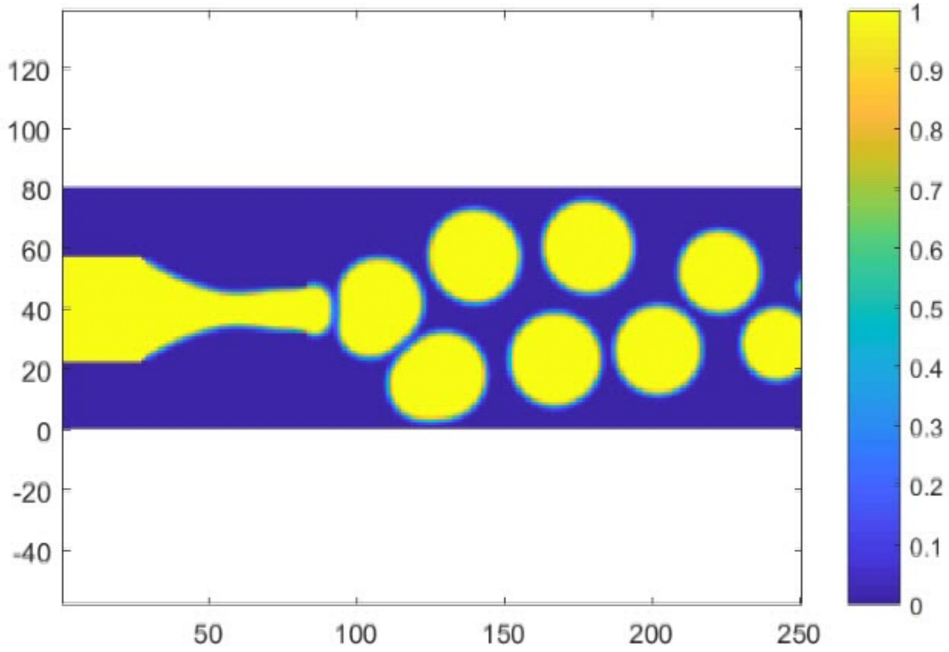


Flow-focuser microfluidics



Costantini, M., et Al.(2016). Materials Science and Engineering: C, 62, 668-677.

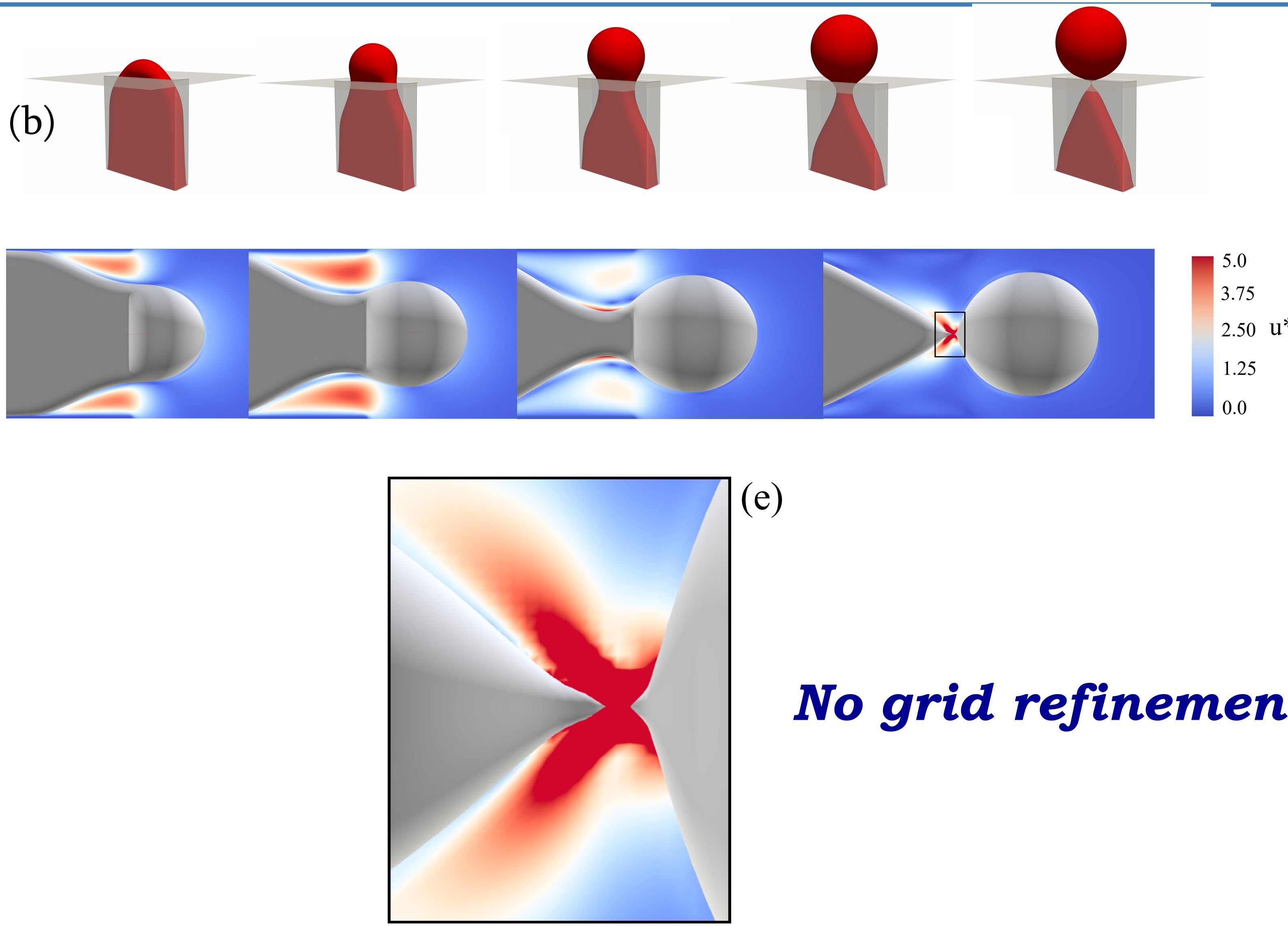
Avoid coalescence



Multirange Color Gradient LB,

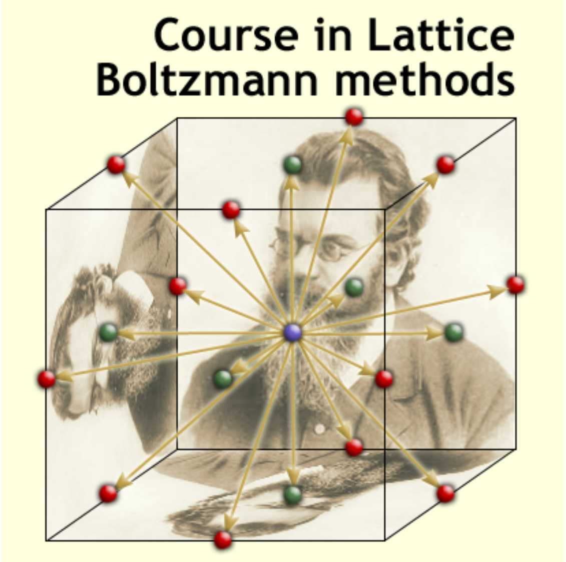
A. Montessori et al C&F, 2018

Step emulsifiers



No grid refinement

Towards Exascale LB computing



M G T P E

1,000000,000,000,000,000

Heat barrier

1 flops / electron transfer!

Large Scale LB simulations

1 MLUPS = 1 Million Lattice UPdates per Second

Updates a 10^6 grid in 1 CPU seconds

LB compute density ~ 200 Flops/site/step

$$1\,MLUPS_{200} \approx 200\,MFlops\,/\,s$$

1 EXAflops/s: 5 PLUPS

LBGK on Marconi KNL (top14)

1 node = 68 cores
(11Pflops, 250K cores)

$$1024 * 512 * 512 = 1/4\ Gsites$$

1	$0.380\ GLUPs \sim 76\ Gflops_{200}$	
8	$2.6\ GLUPs$	0.87
64	$19.3\ GLUPs$	0.79
256	$50.8\ GLUPs$	0.52
512	$117.6\ GLUPs$	0.60

(Courtesy G. Amati)

Extreme-scale LB: WALBERLA

Extreme-scale Block-Structured Adaptive Mesh Refinement

$$110\,Gsites \qquad 155\,GLUPS$$

JUQUEEN, SUPERMUC
32Kcores @ 2.7 GHz

Schornbaum and Rude, SIAM 2016

Major large-scale LB codes

OpenLB: http://optilb.org/openlb/overview
HemeLB: https://github.com/UCL/hemelb
Ludwig: http://ludwig.epcc.ed.ac.uk/software
Palabos: http://www.palabos.org/
waLBerla: http://walberla.net/
DL_MESO: https://www.scd.stfc.ac.uk/Pages/DL_MESO.aspx

Nearing TRILLION fluid sites
(a cube of side 10^4)

Largest turbo: FLASH

FLASH code on SUPERMUC

$$2\ \mu s / cell / step$$

$$10^{12} cells \times 10^{6} steps = 2x10^{12} s / 10^{5} cores \sim 8 months$$

With Exaflop: 3 weeks

Re =10*Re: significant new physics
(Physics ~ Re^9/4: over 2 decades)

ExaScale LB simulation

10^4 lattice side x 10^6 timesteps

$$10^{12} \times 10^{6} = 10^{18} = 1\,ExaLUP$$

$$@500GLUPs \rightarrow 2 \times 10^{6}\,s \approx 3weeks$$

10 times faster than FLASH: but this is too rosy: many more factors must be included

LB Memory and Data Traffic

Memory footprint: $$10^{12} \times 20 \times 8 = 160\,TB$$

CCR: 200 Flops/160 bytes

EXAflop LB: 1 Exabyte/s bandwith!

Memory Access:

Streaming is zero-flops but easily 30% of the CPU

Stream-Free LB (Fused LB)

Stream&Collide -> Non-local Collide

Towards Exascale LB

Optimized memory access

* Organize by energy shells (sum partial sums)
* Crucial with high-order lattices (b~100)

Multi-level parallelism

(core,node,cluster)

Hide communication costs

* Non-blocking send/receive
* Merge stream&collide (fused LB)

Resilience/Fault tolerance

* Check/Restart, Redundant Replicas, Time Parallel

Exascale LB prospects

Multiscale models at the PCB interface

Hemo: One heartbeat/hour at RBC resolution

Millisec intracellular protein dynamics

Direct simulation of biological organelles

Soft Matter (beyond Navier-Stokes)

High S/V fluids (foams, emulsions, soft glasses)

Nanoresolved design of functional materials
(with brainware assistance)

Beyond Exascale: Zepto/Yottascale:

Merge with electronic-atomistic scales (QM/MM)

Biochem-Physio drug-design (QM/MM/LBPD)

Ack's

M. Bernaschi, S. Melchionna, E. Kaxiras, M. Fatica, M.Bisson

G. Amati, A. Montessori, M. Lauricella

R. Benzi, L. Biferale, G. Falcucci, M. Sbragaglia,

And many other colleagues alla around the world….

Ack's

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erc

ISTITUTO ITALIANO DI TECNOLOGIA

IACS Institute for Applied Computational Science
HARVARD SCHOOL OF ENGINEERING AND APPLIED SCIENCES

Consiglio Nazionale delle Ricerche

Thank you!


Parallel CFD 2018
May 14-17, 2018
Indianapolis, Indiana, USA
The 30th International Conference on Parallel Computational Fluid Dynamics
Click on "Schedule" drop-down menu to see the schedule in simple, expanded, grid, or venue mode. Make sure to fill out your SCHED profile completely