Fully Resolved Simulation of Particle-laden Flows

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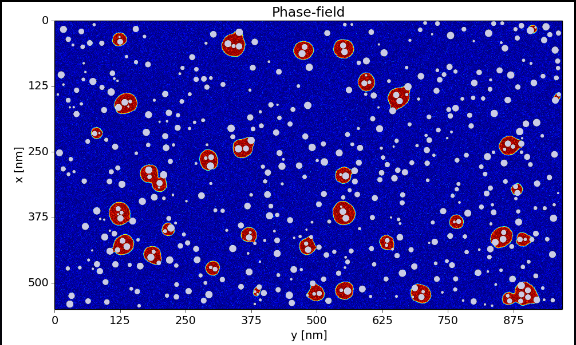
Motivation: mixing, particles & crystallization (FP7 EXOMET)

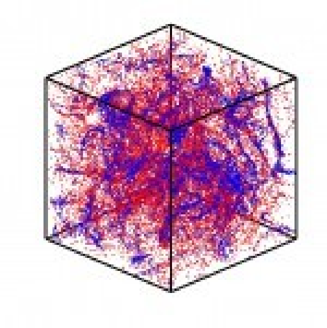


L. Ratkai, T. Pusztai and L. Granasy unpublished

- control crystal nucleation rate
- control mechanical properties (composite materials)

The initial distribution defines nucleation rate!

Examples: stiring - mixing?



turbulent unmixing of phytoplankton (Boffetta Nature Comm. 2013)

Pollutant transport. i.e. The Great Pacific Garbage Patch

Aims

- Strongly turbulent (Re $>$ 1e4) mixing
- solid particles
- nucleation: approx 1% volume fraction (semi-dilute).
- composite materials: up to 20% volume fraction
- Particle trajectories, coagulation and fragmentation.
- Distribution of particles.

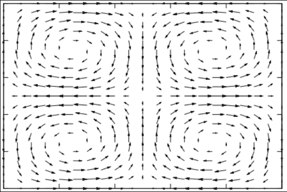
Not resolving particle scale

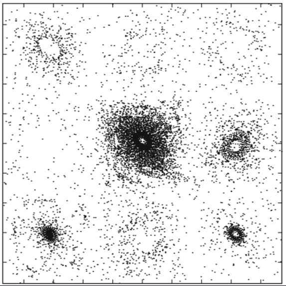
Maxey-Riley equation:

$$m_p \dot{\mathbf{v}} = m_f \frac{D}{Dt}\mathbf{u}(\mathbf{r}(t),t) - \frac{1}{2} m_f \left(\dot{\mathbf{v}} - \frac{D}{Dt}\left[\mathbf{u}(\mathbf{r}(t),t) + \frac{1}{10} a^2 \nabla^2 \mathbf{u}(\mathbf{r}(t),t) \right] \right)$$
$$- 6\pi a \rho_f \nu \mathbf{q}(t) + (m_p - m_f)\mathbf{g} - 6\pi a^2 \rho_f \nu \int_0^t d\tau \frac{d\mathbf{q}(\tau)/d\tau}{\sqrt{\pi \nu (t-\tau)}},$$

- velocity difference across the particle is small!
- dilute (particles do not interact via flow field)
- no inherent agglomeration-fragmentation model
- history force can be computationally expensive

Maxey-Riley predictions





J.H.E. Cartwright et al. (2010)

- Not even neutrally buoyant particle behaves as passive tracer!
- Particles follow chaotic trajectories even in simple time periodic convection
- particles are likely on special manifolds.
- empty voids also can be found!

Fluid structure interaction (FSI) models

Elastic fluid & particle

- Molecular dynamics
- Molecular scale continuum models: (G.I.Toth et al. 2014)
- meso-scale (K. Takae 2011)
- macro-scale (Gene Hou 2012 review)

incompressible fluid & rigid particle

- multiple grid techniques (e.g. overset grid, overlapping grid, immersed boundary method)
- single grid techniques (i.e. method using rigidity constraint over particles)

not resolving acoustic waves, but results in an elliptic PDE

The incompressible NS equation

Assumptions made for Newtonian fluids

- The dissipation is a linear function of the strain rates.
- The fluid is isotropic (comment: rotational invariance)
- For a fluid at rest, $\nabla \cdot (\mathbb{T} - p\mathbb{I})$ must be zero (so that hydrostatic pressure results).

Momentum and mass conservation

- constant density and viscosity
- incompressibility

$$
\begin{aligned}
\frac{\partial \mathbf{v}}{\partial t} &= -\mathbf{v} \cdot (\nabla \otimes \mathbf{v}) + \frac{\eta}{2} \nabla \cdot (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \nabla p && (1) \\
0 &= -\nabla \cdot \mathbf{v} && (2)
\end{aligned}
$$

The solution strategy: Chorin's projection method

decomposing pressure as: $p^{t+1} = p^t + \delta p$

predicting velocity

$$\mathbf{v}^* = \mathbf{v}^t - \Delta t[\mathbf{v}^t \cdot (\nabla \otimes \mathbf{v}^t) + \eta \Delta \otimes \mathbf{v}^t] - \nabla p^t \quad (3)$$

Substituting $\mathbf{v}^{t+1} = \mathbf{v}^* - \nabla \delta p$ into Eq. (2)

pressure equation

$$0 = \nabla \cdot \mathbf{v}^* + \nabla^2 \delta p \quad (4)$$

correcting velocity

$$\mathbf{v}^{t+1} = \mathbf{v}^* - \nabla \delta p \quad (5)$$

Modern hardware & programming

modern hardware

- many scales of parallelism (e.g. instruction scale, threads, cores, compute devices)
- extreme FLOPs count
- limited high speed memory
- throughput/latency limit

programing paradigms

- ”embarrassingly” parallel: explicit declaring independent arithmetics (substituting for loops)
- hiding memory access latency (built in feature)
- compute copy overlap (hand-made feature)

Elliptic PDEs on modern hardware

pseudo-spectral

- exponential convergence
- non dissipative
- easy to ”force” incompressibility
- available system size saturates:
  2002 Earth Simulator Japan $4k^3$,
  2013 Argonne Lab $18k \times 1.5k \times 12k$

FEM,FD,FVM

- polynomial convergence
- numerical dissipation
- huge linear equations from elliptic PDEs
- available system size is linear with compute power:
  compute copy overlap,
  multi level parallelism,
  hiding latency,
  fitting to new paradigms

Solving large linear systems

direct solvers: Gaussian elimination and its variants

- excessive cost for large systems $O(N^3)$

iterative solvers

- Gauss-Seidel, Jacobi, SOR: simple, low memory usage, L^2 iterations, no systematic accumlation of trunct. err.!
- CG and variants: $O(N)$ complexity, gradients must be stored
- GMRES, $O(Nlog(N))$ complexity, fast convergence, data dependence, complex schemes and compute code

hybrid solvers

- Gauss-Seidel+multigrid: low memory usage + $O(L)$! complexity

The multigrid method for elliptic PDEs

multiresolution discretization

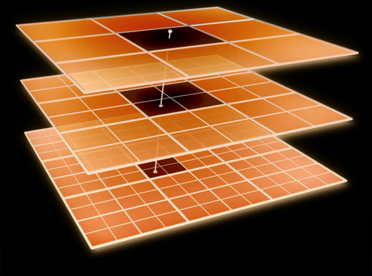
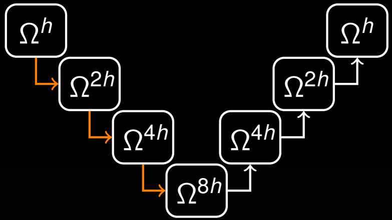


Fig. by Marius Sucan

- residual is relaxing on multiple wavelength
- faster convergence

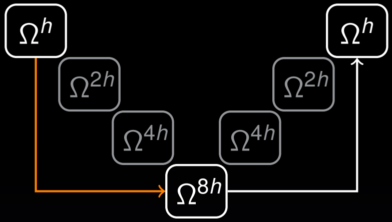
multigrid cycle



1. GS iteration
2. downsampling
3. resampling

Decreasing the number of iterations

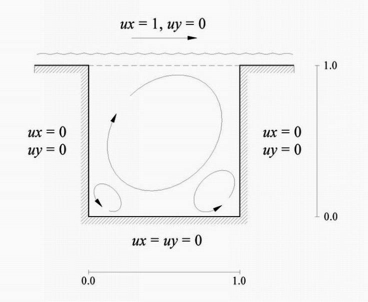
sparse multigrid cycle



- we assume that not all discretization levels are equally important
- we try to bypass some levels

- arithmetic cost slightly increased
- iteration count decreased to $1/5$ of the full cycle
- further tricks to decrease aritmetic cost (G.Tegze & G.I. Toth Arxiv.org)

Test: lid driven cavity



Extrema of v_x, v_y through centerlines , at various Reynolds numbers (table shows values for Re = 1000)

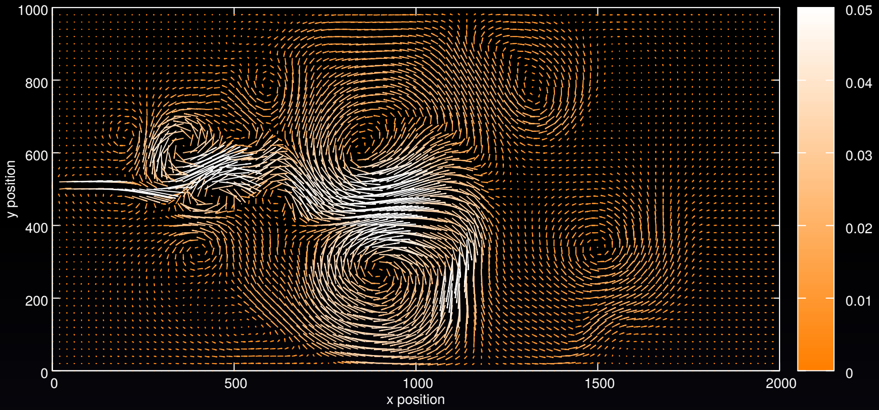
reference	grid	u_{max}	v_{min}	v_{max}
present work	512×512	0.3781	-0.5142	0.3659
Ghia 1982 JCP	129×129	0.3829	-0.5155	0.3710
Deng 1994 CAF stagg.	128×128	0.3805	-0.5173	0.3688
Bruneau 1990 JCP	256×256	0.3764	-0.5208	0.3665
Vanka 1986 JCP	321×321	0.3870	-	-
Botella 1998 CAF spec	160×160	0.3886	-0.5271	0.3769

benchmark: 2D turbulence

- Very large Re numbers and fully resolved particles can be handled.
- No direct extrapolation to 3D! (2D turbulence shows inverse energy cascade, and dissipating on boundaries)

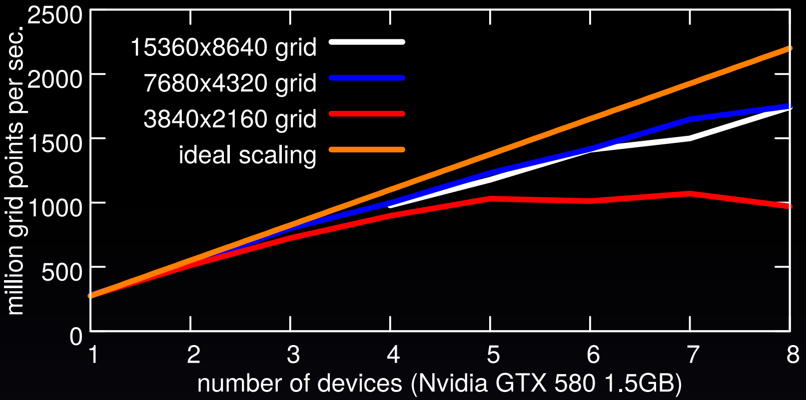
M.A. Rurgers: Soap film turbulence

2D jet



- Fluid jet mimics a gap in the comb $-- >$ equally spaced jets
- eddy size growing

benchmark: 2D turbulence



Boffetta 2009 $32k^2$ pseudo-spectral

The fictitous domain method

$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v}\cdot(\nabla\otimes\mathbf{v}) + \frac{\eta}{2}\nabla\cdot(\nabla\mathbf{v}+\nabla\mathbf{v}^T) - \nabla p \qquad (6)$$

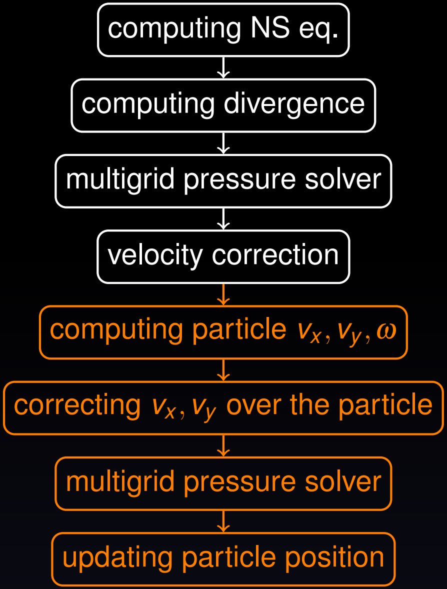
$$0 = -\nabla\cdot\mathbf{v} \qquad (7)$$

$$0 = \frac{1}{2}(\nabla\mathbf{v}+\nabla\mathbf{v}^T) \qquad (8)$$

an extra constraint applies over the particle

- deformation free
- note: dissipation penalizing this term
- distributed Lagrangian multiplier method (looking for a tensor that recovers deformation free velocity)
- solving a set of elliptic PDEs can be excessively demanding

A quick and dirty scheme

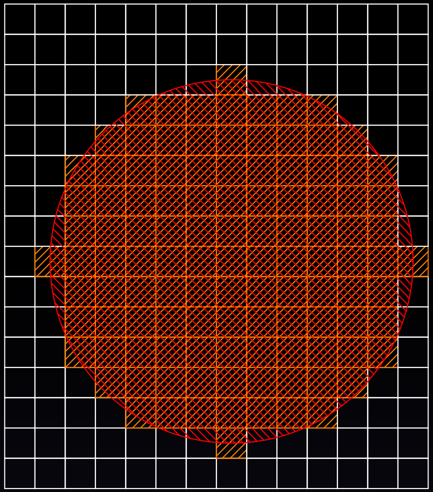


Rigid motion can be written as a sum translating and rotating components:

$$\mathbf{v} = \mathbf{V_p} + \omega_p \times \mathbf{r_p}$$

measuring angular and translational momentum is needed

particle translation and rotation



Rough approximation / fixing needed at boundary

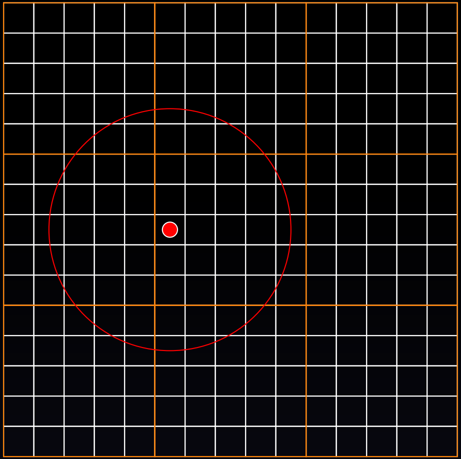
summation for:

- momentum
- mass
- angular momentum
- angular mass

computing particle increment:

- particle velocity
- angular velocity
- displacement
- overwriting velocity fields over the particle

particle trajectory



position updated using a first order time integration

cell list algorithm

- particle assigned to a coarse grid
- easy to find neigbors
- easier data exchange between slices

Extra features (over MR equation)

- two way coupling
- Hydrodynamic interaction between particles: rigid body motion is incompatible with deforming fluid – exite longe range flow – exited fluid domains interact
- Particle rotation
- Particle collision: particles may overlap due to finite resolution of space and time
- Coagulation
- Fragmentation

Testing

simple single particle tests at low Re numbers

Re	Dennis	Takami	Tuann	Fornberg	Toth/Tegze
10	2.85	2.8	3.18	–	2.95
20	2.05	2.01	2.25	2.00	2.01
40	1.522	1.536	1.675	1.498	1.44

Table : Drag coefficient vs. Reynolds number

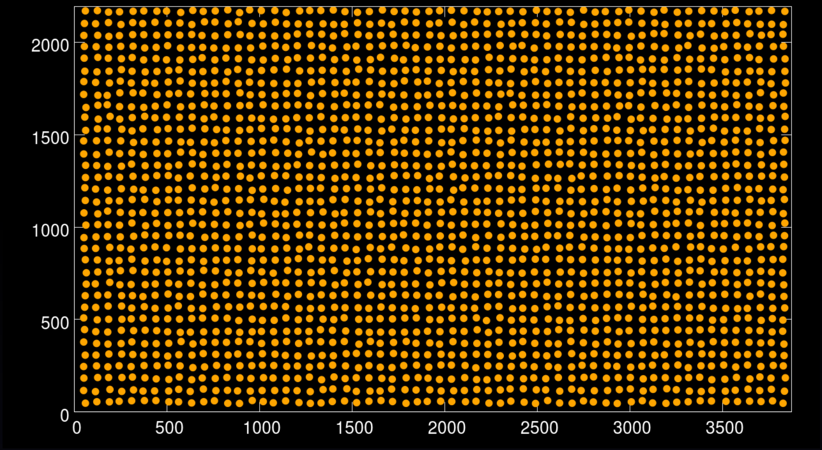
testing of a complex setup is needed

- chaotic nature – error estimates are difficult
- convergence of statistical properties can be tested on large samples

Simulation setup

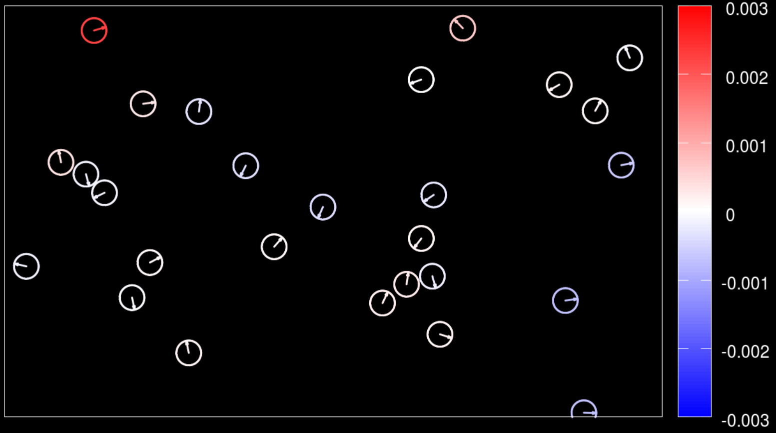
- Lid driven cavity: 3872×2192, $v_0 = 0.05$
- Discretization: $\Delta x = \Delta t = 1$
- Reynolds numbers: 2192,1096,548
- particle Reynolds numbers: ??
- particle radius: 11, 13, 15
- particle number: 2040, 1296, 646
- particle volume fraction: 18.2% – 2.8%

Simulation setup example:



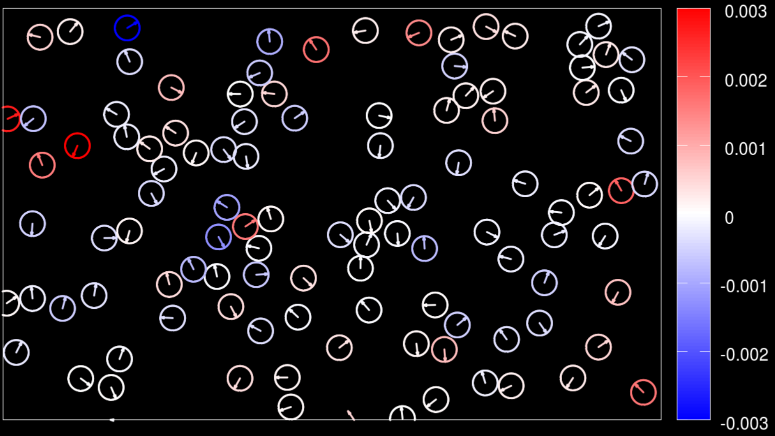
Re=2192,Radius=15, 2040 particles, 18.2% volume fraction

Particle rotation high Re: dilute



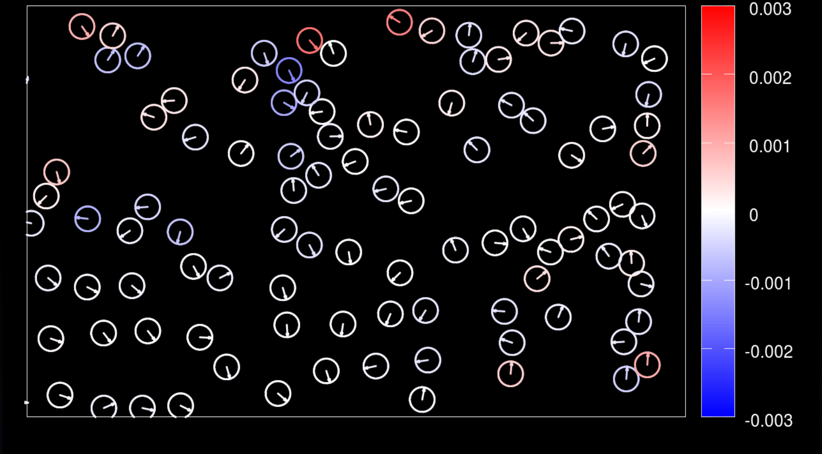
Top right corner: Re=2192,Radius=15, 646 particles

Particle rotation high Re: dense



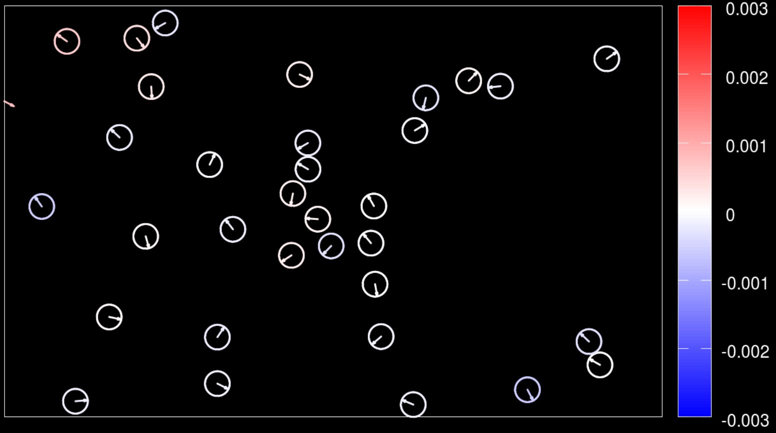
Top right corner: Re=2192,Radius=15, 646 particles

Particle rotation low Re: dense



Top right corner: Re=548, Radius=15, 2040 particles

Particle rotation low Re: dilute



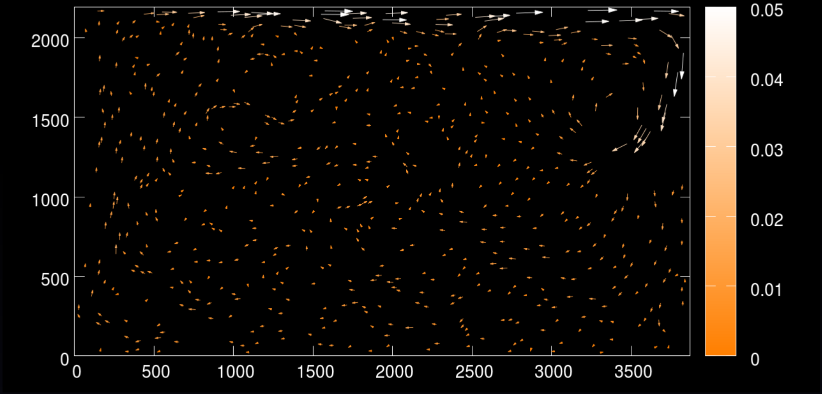
Top right corner: Re=548, Radius=15, 646 particles

Rotation & hydrodynamic interaction

Particle rotation can correlate with hydrodynamic interacton

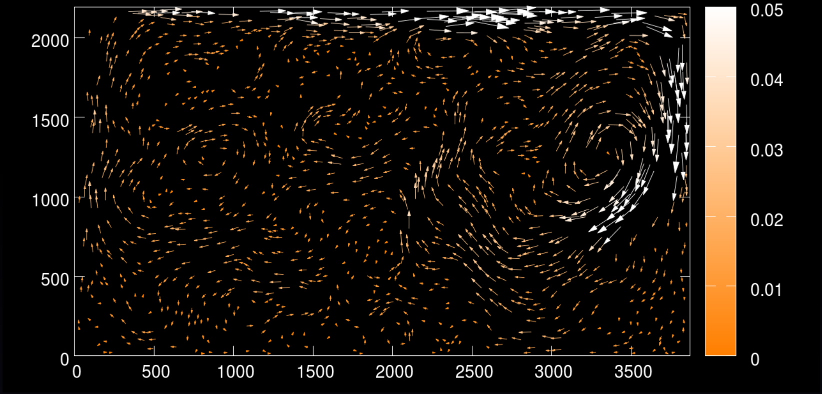
- Dilute rotating near the wall – Dense also inside
- Higher viscosity penalize deformation – more conform to rigid body motion
- Further analysis is needed to understand flip-flop motion (details of fluid flow around particles)
- Convergence study: higher order (in some sense) procedure

Particle velocity high Re: dilute



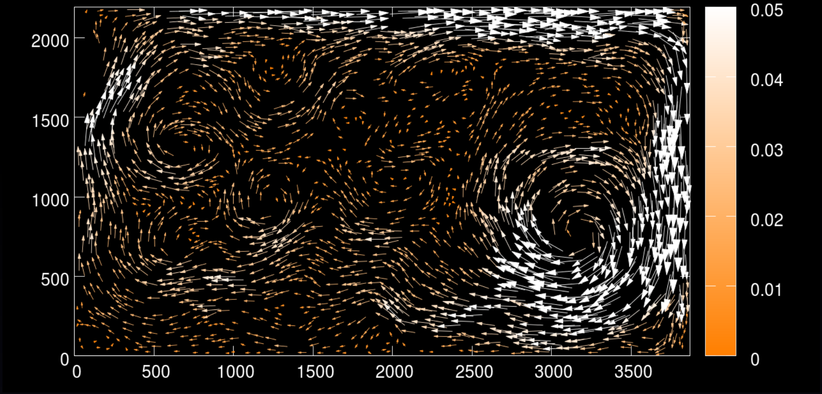
Re=2192, Radius=15, 646 particles

Particle velocity high Re: denser



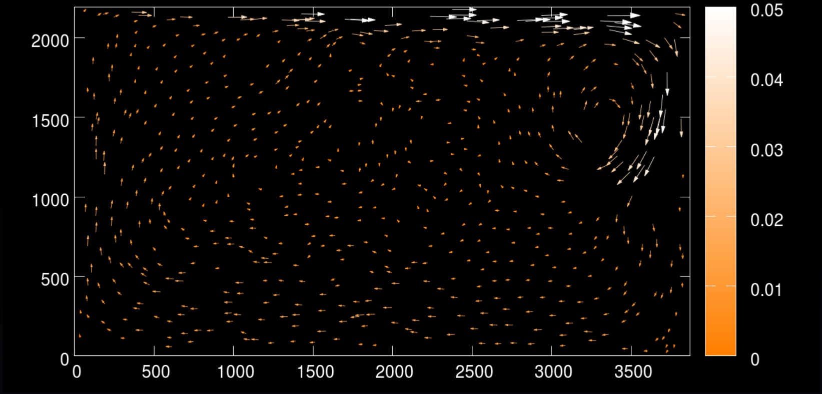
Re=2192, Radius=15, 1296 particles

Particle velocity high Re: crowded



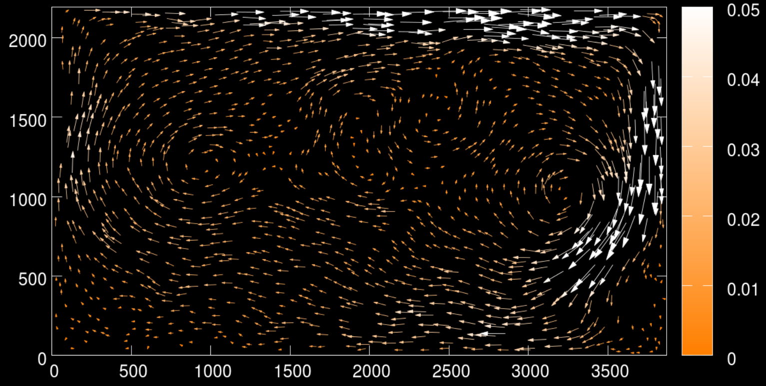
Re=2192, Radius=15, 2040 particles

Particle velocity moderate Re: dilute



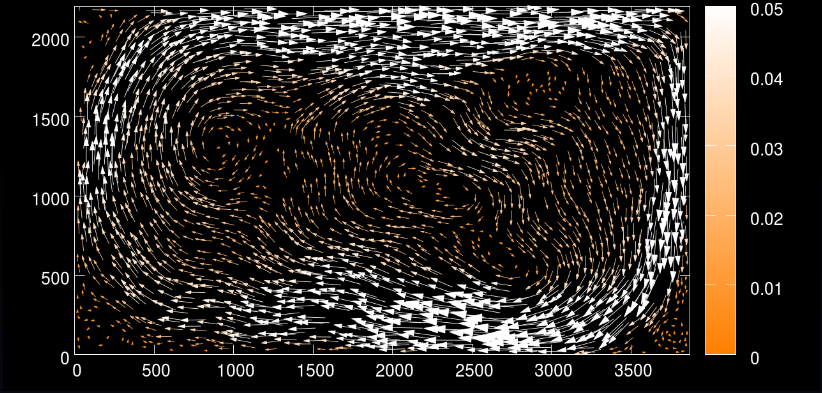
Re=1096, Radius=15, 646 particles

Particle velocity moderate Re: denser



Re=1096, Radius=15, 1296 particles

Particle velocity moderate Re: crowded



Re=1096, Radius=15, 2040 particles

two-way coupling: conclusions

- in crowded systems velocity is picking up very quickly (as if were higher viscosity)
- but remains chaotic
- eddy size is not affected (by naked eye)
- larger system is needed

Questions yet to answer

- particle distribution, radial distribution function etc.
- is averaged model for particle laden flow feasible?
- 2D turbulence in open channel flow, is known to dissipate on duct walls (inverse cascade), but how about disispation due to hi freq. velocity perturbations caused by rigid particles?
- onset of turbulence: role of hydrodynamic interaction between particles

Outlook (rather ambitious todo list)

- fully ”cluster” parallel particle solver $->$ more than 10k particles
- analyzing particle statistics (e.g. pair correlation function)
- collision model (e.g. inelastic) $-->$ very crowded systems
- improving accuracy using higher order schemes
- analyzing two way coupling (e.g. averaged effective viscosity, nonlinear fluidic phenomenon)
- elongated particles
- coupling to to field variables (e.g. temperature, concentration etc.)
- implementing Maxey-Riley eq. for reference
- 3D simulations
- heavy and light particles
- fluctuating hydrodynamics: route to submicron world

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