Fully Resolved Simulation of Particle-laden Flows

Dr. György Tegze

Hungarian Academy of Sciences
Wigner Research Centre for Physics
Budapest

October 26, 2014
Motivation: mixing, particles & crystallization (FP7 EXOMET)

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

The initial distribution defines nucleation rate!

L. Ratkai, T. Pusztai and L. Granasy unpublished
Examples: stirring - 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:

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

- 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

- 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!

J.H.E. Cartwright et al. (2010)
 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, $\nabla \cdot (\mathbb{T} - \rho \mathbb{I})$ must be zero (so that hydrostatic pressure results).

Momentum and mass conservation

- constant density and viscosity
- incompressibility

\[
\begin{align*}
\frac{\partial \mathbf{v}}{\partial t} & = - \mathbf{v} \cdot (\nabla \otimes \mathbf{v}) + \frac{\eta}{2} \nabla \cdot (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \nabla \rho \\
0 & = - \nabla \cdot \mathbf{v}
\end{align*}
\]
The solution strategy: Chorin’s projection method

decomposing pressure as: \( p^{t+1} = p^t + \delta p \)
predicting velocity

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

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

pressure equation

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

correcting velocity

\[
\mathbf{v}^{t+1} = \mathbf{v}^* - \nabla \delta p
\]  (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

**Programming 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 accumulation of trunc. err.!

• CG and variants: $O(N)$ complexity, gradients must be stored

• GMRES, $O(N \log(N))$ complexity, fast convergence, data dependence, complex schemes and compute code

hybrid solvers

• Gauss-Seidel+multigrid: low memory usage + $O(L)$!
The multigrid method for elliptic PDEs

multiresolution discretization

multigrid cycle

- residual is relaxing on multiple wavelength
- faster convergence

Fig. by Marius Sucan

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 arithmetic 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)

<table>
<thead>
<tr>
<th>reference</th>
<th>grid</th>
<th>$u_{max}$</th>
<th>$v_{min}$</th>
<th>$v_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>present work</td>
<td>512 × 512</td>
<td>0.3781</td>
<td>-0.5142</td>
<td>0.3659</td>
</tr>
<tr>
<td>Ghia 1982 JCP</td>
<td>129 × 129</td>
<td>0.3829</td>
<td>-0.5155</td>
<td>0.3710</td>
</tr>
<tr>
<td>Deng 1994 CAF stagg.</td>
<td>128 × 128</td>
<td>0.3805</td>
<td>-0.5173</td>
<td>0.3688</td>
</tr>
<tr>
<td>Bruneau 1990 JCP</td>
<td>256 × 256</td>
<td>0.3764</td>
<td>-0.5208</td>
<td>0.3665</td>
</tr>
<tr>
<td>Vanka 1986 JCP</td>
<td>321 × 321</td>
<td>0.3870</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Botella 1998 CAF spec</td>
<td>160 × 160</td>
<td>0.3886</td>
<td>-0.5271</td>
<td>0.3769</td>
</tr>
</tbody>
</table>
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
Fluid jet mimics a gap in the comb $\rightarrow$ equally spaced jets
eddy size growing
benchmark: 2D turbulence

Boffetta 2009 $32k^2$ pseudo-spectral
The fictitious domain method

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

\[
0 = -\nabla \cdot \mathbf{v} \tag{7}
\]

\[
0 = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \tag{8}
\]

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

computing NS eq. ➔
computing divergence ➔
multigrid pressure solver ➔
velocity correction ➔
computing particle $v_x, v_y, \omega$ ➔
correcting $v_x, v_y$ over the particle ➔
multigrid pressure solver ➔
updating particle position

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

summation for:
- momentum
- mass
- angular momentum
- angular mass

computing particle increment:
- particle velocity
- angular velocity
- displacement
- overwriting velocity fields over the particle

Rough approximation / fixing needed at boundary
particle trajectory

position updated using a first order time integration cell list algorithm

- particle assigned to a coarse grid
- easy to find neighbors
- 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 – exit long range flow – exited fluid domains interact

- Particle rotation

- Particle collision: particles may overlap due to finite resolution of space and time

- Coagulation

- Fragmentation
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: $3872 \times 2192$, $\nu_0 = 0.05$
- 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 interaction

- 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 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
Acknowledgement

- Prof. Laszlo Granasy for support and discussions
- Team members Prof. Tamas Pusztai, Gyula Toth PhD, Frigyes Podmaniczky, and Laszlo Ratkai for sharing ideas
- Mate Nagy, and the Wigner GPU Lab for supporting us with hardware and programming advices

This work has been supported by the EU FP7 Collaborative Project “EXOMET” (contract no. NMP-LA-2012-280421, co-funded by ESA), and by the ESA MAP project “GRADECET” (Contract No. 4000104330/11/NL/KML). G. Tegze is a grantee of the János Bolyai Scholarship of the Hungarian Academy of Sciences.