Inertial Coupling for blob particle hydrodynamics at different scales

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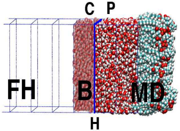
HYBRID2013, Jülich

Multiscale approaches for complex liquids

Domain decomposition

type A

Molecular detail,
interfases, surfaces,
macromolecule -fluid interaction



shear flows ✓
sound, heat
large molecules
multispecies ✗
electrostatics

Eulerian-Lagrangian Solute-solvent hydrodynamic coupling

Suspensions
of colloids or polymers,
small particles in flow

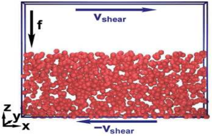


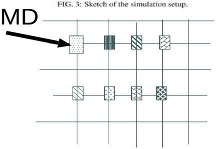
FIG. 3: Sketch of the simulation setup.

Point particle aproximation:
Stokes drag (point particle),
Faxen terms (finite size effects)
Basset memory effects...
Force Coupling
particles of finite size
Direct simulation
Immersed boundaries

Patch dynamics
HMM
Velocity-Stress coupling

type B

Non-Newtonian fluids
Unknown constituve relation
polymer mels...



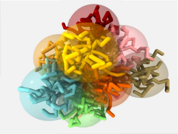
MD nodes used to
evaluate the **local stress**
for the Continuum solver.

Continuum solver provides
the local **velocity gradient**
imposed at each MD node.

how to "lift MD" ✗

Coarse-grained dynamics

How to reduce the degrees of freedom and keep the underlying dynamics



diffusion ✓
viscosity
anisotropy ✗
(nematics...)

Motivation

- Minimal: blob model for particle hydrodynamics
- Fast: large particle numbers $O(10^5)$ over large physical times.
- **Multiregime**: wide range of physical conditions: *lengths* (10*nm*-1 *m*), non-dimensional numbers (Sc, Re, Pe, Ma) and arbitrary fluid eos.
  - Thermal fluctuations
  - Inertia: particle *and* fluid (turbulence)
- Flexible: allow for generalizations
  - Brownian limit
  - Polymers
  - Immersed structures (rigid or flexible)
  - Porous media, chemical reactions, etc.
  - Ultrasound colloidal manipulation original motivation

Hydrodynamic solvers in continuum space

Fluid Reynolds number $Re_F = V\,L/\nu$	Particle Reynolds number $Re_P = Va/\nu$: 0	10^{-1}	$1 - 10^2$
0	Brownian Dynamics	Stokesian Dynamics, SD	-
1	Force Coupling Method, FCM	Stokes Coupling	Inertial Coupling (ICM)
10^3	Point-Particle Methods	-	fully resolved, ICM

Hydrodynamic solvers in continuum space

Particle Reynolds number $Re_P = Va/\nu$

Fluid Reynolds number $\mathrm{Re}_F = V\,L/\nu$

Re_F \ Re_P	0	10^{-1}	$1 - 10^2$
0	**Brownian Dynamics**	Stokesian Dynamics, SD	-

$$0 = \boldsymbol{\xi}\left(\mathbf{u} - \mathbf{v}_0\right) + \mathbf{F} + \mathcal{W}$$ McEmon, 1970

colloidal diffusion time $\tau_D = a^2\xi/kT \sim 10^{-n}$

Re_F \ Re_P	0	10^{-1}	$1 - 10^2$
1	Force Coupling Method, FCM	Stokes Coupling	Inertial Coupling (ICM)
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Hydrodynamic solvers in continuum space

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Fluid Reynolds number $\mathrm{Re}_F = V\,L/\nu$

$\mathrm{Re}_F = V\,L/\nu$	0	10^{-1}	$1 - 10^2$
0	Brownian Dynamics	**Stokesian Dynamics, SD**	-
1	Force Coupling Method, FCM	Stokes Coupling	Inertial Coupling (ICM)
10^3	Point-Particle Methods	-	fully resolved, ICM

$$m\dot{\mathbf{u}} = \boldsymbol{\xi}\left(\mathbf{u} - \mathbf{v}_0\right) + \mathbf{F} + \mathcal{W}$$

Brady, 1990

Friction time $\tau_\xi = m/\xi \sim 10^{-n}$

Hydrodynamic solvers in continuum space

Particle Reynolds number $Re_P = Va/\nu$

Fluid Reynolds number $Re_F = V\,L/\nu$

Re_F \ Re_P	0	10^{-1}	$1 - 10^2$
0	Brownian Dynamics	Stokesian Dynamics, SD	-
1	**Force Coupling Method, FCM**	Stokes Coupling	Inertial Coupling (ICM)

$$\text{fluid: } \rho D_t \mathbf{v} = -\nabla \cdot \mathbf{P} + \mathtt{S}\mathbf{F} \quad \text{Maxey, 2000}$$

$$\text{part.: } 0 = \lambda + \mathbf{F}$$

$\mathtt{S}$: Gaussian kernels   Stokeslet,Stresslet,Rotlet

10^3	Point-Particle Method...	-	fully resolved, ICM...

Particle Reynolds number $Re_P = Va/\nu$

Fluid Reynolds number $\mathrm{Re}_F = V\,L/\nu$	0	10^{-1}	$1 - 10^2$
0	Brownian Dynamics	Stokesian Dynamics, SD	-
1	Force Coupling Method, FCM	**Stokes Coupling**	Inertial Coupling (ICM)
10^3	Point-Particle Methods	-	fully resolved, ICM

$$\rho D_t \mathbf{v} = -\nabla \cdot (\mathbf{P} + \mathcal{W}_\mathrm{f}) + \mathrm{S}\gamma(\mathbf{u} - \mathbf{v})$$

$$\mathbf{u} = -\gamma(\mathbf{u} - \mathbf{v}) + \mathbf{F} + \mathcal{W}_\mathrm{p}$$

Ladd, Dunweg, 2000 Langevin time $\tau_{fric} = 1/\gamma \sim a^2/\nu$

Particle Reynolds number $Re_P = Va/\nu$

Fluid Reynolds number $Re_F = VL/\nu$

Re_F \ Re_P	0	10^{-1}	$1-10^2$
0	Brownian Dynamics	Stokesian Dynamics, SD	-
1	Force Coupling Method, FCM	Stokes Coupling	Inertial Coupling (ICM)

$$
\begin{aligned}
\rho D_t \mathbf{v} &= -\nabla \cdot (\mathbf{P} + \mathcal{W}_{\mathrm{f}}) + \mathsf{S}\lambda \\
m\mathbf{u} &= \lambda + \mathbf{F} \\
\mathbf{v} &= \mathbf{u}\,\text{(no-slip)}
\end{aligned}
$$

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Instantaneous coupling

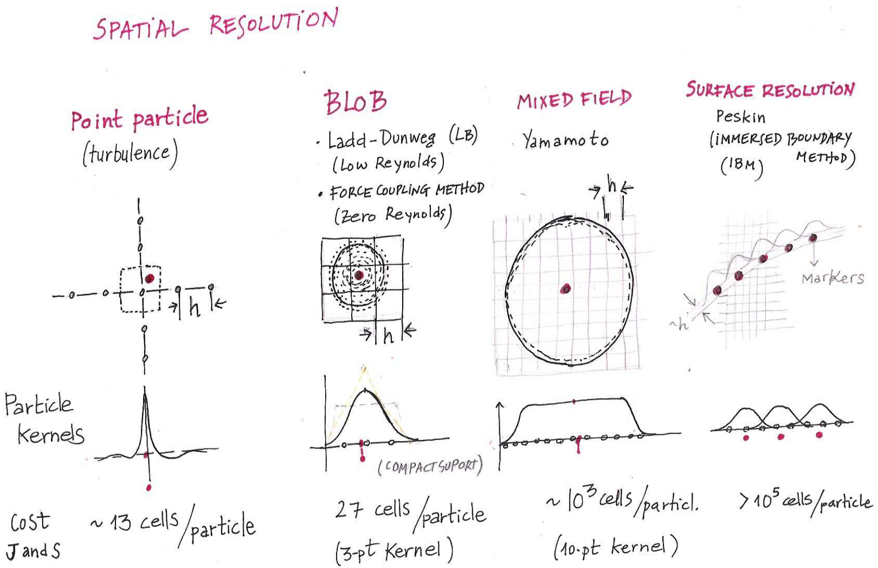
Hydrodynamic solvers in continuum space

Particle Reynolds number $Re_P = Va/\nu$

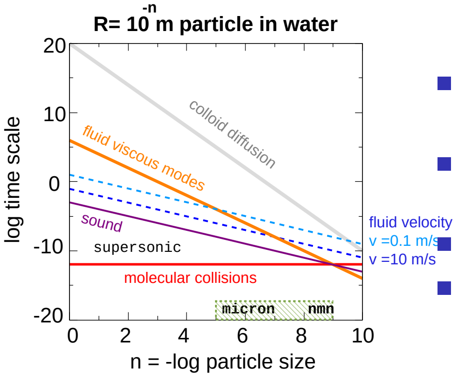
Fluid Reynolds number $\mathrm{Re}_F = V\,L/\nu$

Re_F \ Re_P	0	10^{-1}	$1 - 10^2$
0	Brownian Dynamics	Stokesian Dynamics, SD	-
1	Force Coupling Method, FCM	Stokes Coupling	Inertial Coupling (ICM)
10^3	Point-Particle Methods	-	fully resolved, ICM

Particle spatial resolution: models

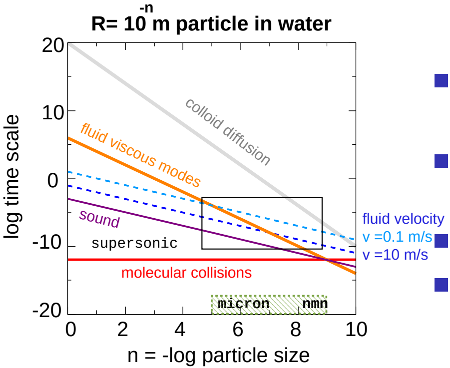


Characteristic times and inertia's relevance



- Colloid diffusion $\tau_D = a^2/D$
- Momentum diffusion $\tau_\nu = a^2/\nu$
- Advection time $\tau_a = a/v$
- Sonic time $\tau_s = a/c$

Characteristic times and inertia's relevance



- Colloid diffusion $\tau_D = a^2/D$
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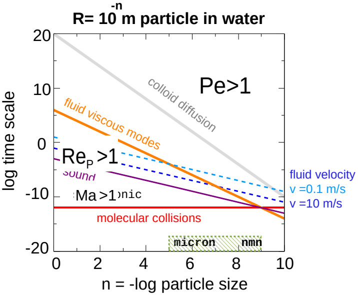
Non-dimensional numbers



		ICM
Schmidt	$\mathrm{Sc} = \frac{\nu}{D}$	arbitrary
Peclet	$\mathrm{Pe} = \frac{av}{D}$	arbitrary
Particle Reynolds	$\mathrm{Re}_p = \frac{a\,v}{\nu}$	< 100
Fluid Reynolds	$\mathrm{Re}_f = \frac{L\,v}{\nu}$	arbitrary
Mach	$\mathrm{Ma} = c/v$	$[0 - 0.3]$

The blob model: Equation of motion

Rigid particle

$$m_p\dot{\mathbf{u}} = -\oint_S \mathbf{P}\cdot\mathbf{n}\mathrm{d}s - \int \chi_a(\mathbf{q}-\mathbf{r})\nabla\cdot\mathbf{P}\mathrm{d}\mathbf{r}$$

with χ_a the characteristic function (1)

Blob model

$$m_p\dot{\mathbf{u}} = -\int \delta_a(\mathbf{q}-\mathbf{r})\nabla\cdot\mathbf{P}\mathrm{d}\mathbf{r}$$

with δ_a smeared delta (soft kernel) (2)

The blob model: Equation of motion

Rigid particle

$$m_p \dot{\mathbf{u}} = -\int_{\mathbb{V}} \nabla \cdot \mathbf{P} d\mathbf{r} - \int \chi_a(\mathbf{q}-\mathbf{r}) \nabla \cdot \mathbf{P} d\mathbf{r} \quad \text{with } \chi_a \text{ the characteristic function} \tag{1}$$

Blob model

$$m_p \dot{\mathbf{u}} = -\int \delta_a(\mathbf{q}-\mathbf{r}) \nabla \cdot \mathbf{P} d\mathbf{r} \quad \text{with } \delta_a \text{ smeared delta (soft kernel)} \tag{2}$$

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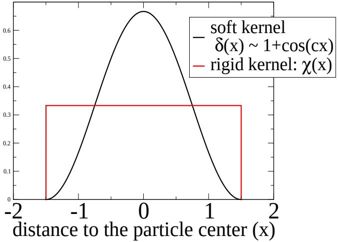
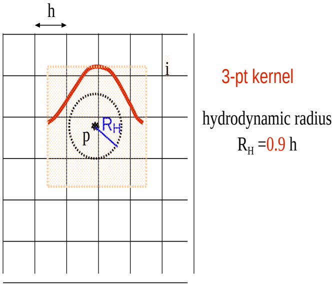
with δ_a smeared delta (soft kernel) (2)

Blob kernel: general idea





The blob model: fluid-particle constraint

Rigid particle (centered at $\mathbf{q} = 0$)

$$\begin{aligned} \mathbf{v}(\mathbf{r}) &= \mathbf{u} + \vec{\Omega} \times \mathbf{r} \ \text{ for } r < a\text{, no-slip, rigid body} \\ \rho(\mathbf{r}) &= 0\ ;\text{for } r < a\text{, no fluid inside the particle} \end{aligned}$$

Blob

$$\begin{aligned} \int \delta_a(\mathbf{r} - \mathbf{q})\mathbf{v}(\mathbf{r})\mathrm{d}\mathbf{r} &= \mathbf{u} \ \textit{ coarse-grained} \text{ no-slip} \\ \rho(\mathbf{r}) &\neq 0 \ \text{ blob is permeable to fluid} \end{aligned}$$

Interpolation and spreading kernels

Interpolation: $\mathtt{J} : \mathbb{L}^2 \to \mathbb{R}$

$$\mathtt{J}_{\mathbf{q}}\mathbf{v} \equiv \int \delta_a(\mathbf{r}-\mathbf{q})\mathbf{v}(\mathbf{r})\mathrm{d}\mathbf{r} \qquad (3)$$

Spreading: $\mathtt{S} : \mathbb{R} \to \mathbb{C}_c$

$$\mathtt{S}_{\mathbf{q}}\mathbf{F}(\mathbf{q}) \equiv \delta_a(\mathbf{r}-\mathbf{q})\mathbf{F}(\mathbf{q})$$

Units: $[\mathtt{J}] = 1$ and $[\mathtt{S}] = 1/\mathrm{volume}]$

Kernel properties

Normalization

$$\int \delta_a(\mathbf{r} - \mathbf{q})\mathrm{d}\mathbf{r} = 1$$

Consistency ($\mathbb{L}_c^2$–norm) $\int \delta_a^2(\mathbf{r} - \mathbf{q})\mathrm{d}\mathbf{r} = 1/\mathbb{V}$, thus

$$\boxed{\mathtt{JS} = 1/\mathbb{V}}$$

S *and* J *are adjoint operators*

$$\mathtt{J}\mathbf{v} \cdot \mathbf{u} = \int \mathbf{v} \cdot \mathtt{S}\mathbf{u}\,\mathrm{d}\mathbf{r} = \delta(\mathbf{r} - \mathbf{q})\mathbf{v} \cdot \mathbf{u}\,\mathrm{d}\mathbf{r}$$

Discrete kernels (Immersed Boundary Method)

Regular (Eulerian) grid mesh widht h,

$$\vec{r}_k = \vec{k}h$$

notation $\mathbf{v}_k = \mathbf{v}(\mathbf{r}_k)$, etc.

Interpolation

$$\mathsf{J}_{\mathbf{q}}\mathbf{v} = \sum_{k \in grid} \delta(\mathbf{r}_k - \mathbf{q})\mathbf{v}$$

Spreading

$$(\mathsf{S}\mathbf{F})_k = \delta(\mathbf{r}_k - \mathbf{q})\mathbf{F}(\mathbf{q})$$

Discrete kernels

IBM kernels

The IBM kernels satisfy the following properties in a regular lattice: **For any** $\mathbf{q} \in \mathbb{R}^3$

- 3D kernels separable in each direction (fast and clean)
- Normalization
- Consistency $\mathtt{JS} = 1/\mathbb{V}$: well defined "volume" $\mathbb{V}$
- Exact linear interpolation (conserve angular momentum)

$$\delta_a(\mathbf{r}_k - \mathbf{q}) = \prod_{\alpha=1}^{3} \phi(r_\alpha - q_\alpha)$$

$$\sum_{k \in \mathrm{grid}} \delta_a(\mathbf{r}_k - \mathbf{q}) = 1$$

$$\sum_{k \in \mathrm{grid}} \delta_a^2(\mathbf{r}_k - \mathbf{q}) = 1/\mathbb{V}$$

$$\sum_{k \in \mathrm{grid}} \mathbf{r}_k \delta_a(\mathbf{r}_k - \mathbf{q}) = \mathbf{q}$$

Equations of motion

Fluid

$$\frac{\partial \mathbf{g}}{\partial t} = -\nabla \cdot (\mathbf{g}\mathbf{v} + \mathbf{P}) - \mathtt{S}(\mathbf{q})\lambda$$

Particle:

$$m_p \dot{\mathbf{u}} = -\mathtt{J}\left(\nabla \cdot \mathbf{P}\right)\mathbb{V} + \mathbf{F} - \mathtt{J}\left[\nabla \cdot (\mathbf{v} - \mathbf{u})\, \mathbf{g}\right]$$

No-slip constraint

$$\mathbf{J}\mathbf{v} = \mathbf{u}$$

Fluid momentum density	$\mathbf{g} = \rho \mathbf{v}$
Pressure tensor	$\mathbf{P} = p(\rho)\mathbf{1} + \boldsymbol{\sigma} + (k_B T \eta)^{1/2} \boldsymbol{\mathcal{W}}^{sym}$
Fluid-Particle force	$\boldsymbol{\lambda}$
Particles (conservative) forces	$\mathbf{F}(\mathbf{q}) = -\nabla U(\mathbf{q})$

Equations of motion

Fluid

$$\mathsf{J}\left(\frac{\partial \mathbf{g}}{\partial t}\right) = -\mathsf{J}\left(\nabla \cdot \mathbf{P}\right) - \mathsf{J}\mathbb{S}(\mathbf{q})\lambda - \mathsf{J}\nabla \cdot (\mathbf{g}\mathbf{v})$$

Particle:

$$m_p \dot{\mathbf{u}} = -\mathsf{J}\left(\nabla \cdot \mathbf{P}\right)\mathbb{V} + \mathbf{F} - \mathsf{J}\left[\nabla \cdot (\mathbf{v} - \mathbf{u})\,\mathbf{g}\right]$$

No-slip constraint

$$\mathsf{J}\mathbf{v} = \mathbf{u}$$

$$\frac{\mathrm{d}\mathrm{J}(\mathbf{q})\mathbf{g}}{\mathrm{d}t} = \mathsf{J}\left(\frac{\partial \mathbf{g}}{\partial t}\right) + \left(\mathbf{u} \cdot \frac{\partial \mathrm{J}}{\partial \mathbf{q}}\right)\mathbf{g}$$

Equations of motion

Fluid

$$\frac{d(\mathsf{J}\mathbf{g})}{\mathrm{d}t} = -\mathsf{J}\left(\nabla\cdot\mathbf{P}\right) - \lambda/\mathbb{V} - \mathsf{J}\left[\nabla\cdot\left(\mathbf{v}-\mathbf{u}\right)\mathbf{g}\right]$$

Particle:

$$m_p\dot{\mathbf{u}} = -\mathsf{J}\left(\nabla\cdot\mathbf{P}\right)\mathbb{V} + \mathbf{F} - \mathsf{J}\left[\nabla\cdot\left(\mathbf{v}-\mathbf{u}\right)\mathbf{g}\right]$$

No-slip constraint

$$\mathsf{J}\mathbf{v} = \mathbf{u}$$

$$\mathsf{J}\left[\nabla\cdot\left(\mathbf{v}-\mathbf{u}\right)\mathbf{g}\right] = \int \mathbf{g}\left(\mathbf{u}-\mathbf{v}\right)\cdot\nabla_{\mathbf{r}}\delta_a(\mathbf{q}-\mathbf{r})\mathrm{d}\mathbf{r}$$

Equations of motion

Fluid

$$\frac{d(\mathsf{J}\mathbf{g})}{\mathrm{d}t} = -\mathsf{J}\left(\nabla \cdot \mathbf{P}\right) - \lambda/\mathbb{V} - \mathsf{J}\left[\nabla \cdot (\mathbf{v} - \mathbf{u})\,\mathbf{g}\right]$$

Particle:

$$m_p \dot{\mathbf{u}} = \frac{\mathrm{d}(\mathsf{J}\mathbf{g})}{\mathrm{d}t}\mathbb{V} + \lambda + \mathbf{F}$$

No-slip constraint

$$\mathsf{J}\mathbf{v} = \mathbf{u}$$

$$\frac{\mathrm{d}(\mathsf{J}\mathbf{g})}{\mathrm{d}t}\mathbb{V} = m_f \frac{\mathrm{d}(\mathsf{J}\mathbf{v})}{\mathrm{d}t} + O(\mathrm{Ma}^2),$$ $m_f = \rho\mathbb{V}$ dragged fluid mass

Equations of motion

Fluid

$$\frac{\partial \mathbf{g}}{\partial t} = -\nabla \cdot (\mathbf{g}\mathbf{v} + \mathbf{P}) - \mathtt{S}(\mathbf{q})\lambda$$

Particle: `Low Mach approximation`

$$m_p \dot{\mathbf{u}} = m_f \frac{\mathrm{d}(\mathbf{J}\mathbf{v})}{\mathrm{d}t} + \lambda + \mathbf{F}$$

No-slip constraint

$$\mathbf{J}\mathbf{v} = \mathbf{u}$$

$$\frac{\mathrm{d}(\mathbf{J}\mathbf{g})}{\mathrm{d}t}\mathbb{V} = m_f \frac{\mathrm{d}(\mathbf{J}\mathbf{v})}{\mathrm{d}t} + O(\mathrm{Ma}^2),$$ $m_f = \rho\mathbb{V}$ dragged fluid mass

Equations of motion

Fluid

$$\frac{\partial \mathbf{g}}{\partial t} = -\nabla \cdot (\mathbf{g}\mathbf{v} + \mathbf{P}) - \mathtt{S}(\mathbf{q})\lambda$$

Particle: `Low Mach approximation`

$$(m_p - m_f)\dot{\mathbf{u}} = \lambda + \mathbf{F}$$

No-slip constraint

$$\mathbf{J}\mathbf{v} = \mathbf{u}$$

$$\frac{\mathrm{d}(\mathbf{J}\mathbf{g})}{\mathrm{d}t}\mathbb{V} = m_f \frac{\mathrm{d}(\mathbf{J}\mathbf{v})}{\mathrm{d}t} + O(\mathrm{Ma}^2),\ m_f = \rho\mathbb{V} \text{ dragged fluid mass}$$

Equations of motion

Fluid

$$\frac{\partial \mathbf{g}}{\partial t} = -\nabla \cdot (\mathbf{g}\mathbf{v} + \mathbf{P}) - \mathtt{S}(\mathbf{q})\lambda$$

Particle: ***excess*** **mass** $m_e = m_p - m_f$

$$m_e \dot{\mathbf{u}} = \lambda + \mathbf{F}$$

No-slip constraint

$$\mathbf{J}\mathbf{v} = \mathbf{u}$$

$$\frac{\mathrm{d}(\mathbf{J}\mathbf{g})}{\mathrm{d}t}\mathbb{V} = m_f \frac{\mathrm{d}(\mathbf{J}\mathbf{v})}{\mathrm{d}t} + O(\mathrm{Ma}^2), \; m_f = \rho\mathbb{V} \text{ dragged fluid mass}$$

Conservation

Momentum field (fluid+particle)

$$\mathbf{p}(\mathbf{r},t) = \rho\mathbf{v} + m_e \mathtt{S}\mathbf{u} = (\rho + m_e \mathtt{SJ})\,\mathbf{v} = \boldsymbol{\rho}_{eff}\mathbf{v}$$

1. Total momentum $\mathtt{P} = \int \mathbf{p} d\mathbf{r}$ is conserved
2. Local momentum is conserved, if $\mathbf{F} = 0$:

$$\partial_t \mathbf{p} = -\nabla \cdot \left(\mathbf{P} + \mathbf{g}\mathbf{v}^T + m_e \mathtt{S}\mathbf{u}\mathbf{u}^T\right)$$

Energy (without fluid viscous dissipation) Hamiltonian:

$$H(\mathbf{v},\mathbf{u},\mathbf{q}) = m_e u^2/2 + U(\mathbf{q}) + \int \rho v^2/2 + \varepsilon(\rho) d\mathbf{r}$$

$$\frac{dH}{dt} = 0, \text{ proof requires } \mathtt{J} \text{ adjoint } \mathtt{S} \qquad (4)$$

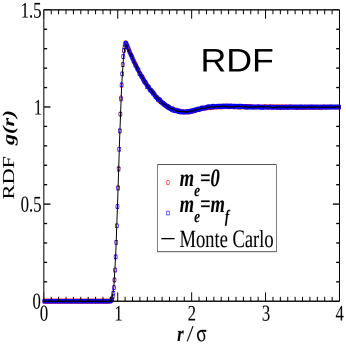
Fluctuation-dissipation and equilibrium

Hamiltonian $H(x)$ with $x = (\mathbf{v}, \mathbf{u}, \mathbf{q})$ for reversible dynamics:
$\mathrm{d}H/\mathrm{d}t = 0$

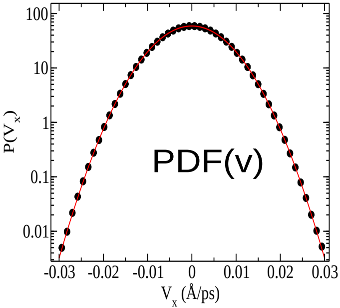
Fluctuation-dissipation balance Particle "noise" is not needed
The fluid-particle coupling is **not dissipative** so, it is enough to add thermal fluctuations in the fluid equations

Gibbs-Boltzmann Equilibrium distribution $Z^{-1}\exp(-\beta\, H(x)]$

Radial distribution Func.



Particle velocity distribution



Gibbs-Boltzmann Equilibrium distribution

Time-stepping: First order algorithm

$t_n = n\Delta t$, $\mathbf{v}^n = \mathbf{v}(t^n)$, $\mathsf{J}^n = \mathsf{J}(\mathbf{q}^n)$, etc,

Unperturbed flow

$$\mathbf{g}_0^{n+1} = \mathbf{g}_0^n - [\nabla \cdot \mathbf{P}]^n \Delta t$$

Particle position

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \mathsf{J}^n \mathbf{v}^n \Delta t$$

Interpolation $\mathsf{J}^{n+1}\mathbf{v}_0^{n+1}$

Particle velocity and fluid-particle force

Spread fluid-particle force

$$\mathbf{v}^{n+1} = \mathbf{v}_0^{n+1} - \mathsf{S}^n \lambda^n \Delta t + O(\Delta t^2)$$

Time-stepping: First order algorithm

$t_n = n\Delta t$, $\mathbf{v}^n = \mathbf{v}(t^n)$, $\mathsf{J}^n = \mathsf{J}(\mathbf{q}^n)$, etc,

Unperturbed flow

$$\mathbf{g}_0^{n+1} = \mathbf{g}_0^n - [\nabla \cdot \mathbf{P}]^n \, \Delta t$$

Particle position

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \mathsf{J}^n \mathbf{v}^n \Delta t$$

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Time-stepping: First order algorithm

$t_n = n\Delta t$, $\mathbf{v}^n = \mathbf{v}(t^n)$, $\mathsf{J}^n = \mathsf{J}(\mathbf{q}^n)$, etc,

Unperturbed flow

$$\mathbf{g}_0^{n+1} = \mathbf{g}_0^n - [\nabla \cdot \mathbf{P}]^n \, \Delta t$$

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Time-stepping: First order algorithm

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Unperturbed flow

$$\mathbf{g}_0^{n+1} = \mathbf{g}_0^n - [\nabla \cdot \mathbf{P}]^n \, \Delta t$$

Particle position

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \mathsf{J}^n \mathbf{v}^n \Delta t$$

Interpolation $\mathsf{J}^{n+1}\mathbf{v}_0^{n+1}$

Particle velocity and fluid-particle force

$$\text{Fluid Eq. } \mathsf{J}^{n+1}\mathbf{v}^{n+1} = \mathsf{J}^{n+1}\mathbf{v}_0^{n+1} - m_f^{-1} \lambda^n \Delta t$$

Spread fluid-particle force

$$\mathbf{v}^{n+1} = \mathbf{v}_0^{n+1} - \mathsf{S}^n \lambda^n \Delta t + O(\Delta t^2)$$

Time-stepping: First order algorithm

$t_n = n\Delta t$, $\mathbf{v}^n = \mathbf{v}(t^n)$, $\mathsf{J}^n = \mathsf{J}(\mathbf{q}^n)$, etc,

Unperturbed flow

$$\mathbf{g}_0^{n+1} = \mathbf{g}_0^n - \left[\nabla \cdot \mathbf{P}\right]^n \Delta t$$

Particle position

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \mathsf{J}^n \mathbf{v}^n \Delta t$$

Interpolation $\mathsf{J}^{n+1}\mathbf{v}_0^{n+1}$

Particle velocity and fluid-particle force

No-slip $\mathbf{u}^{n+1} = \mathsf{J}^{n+1}\mathbf{v}_0^{n+1} - m_f^{-1}\lambda^n \Delta t$

Spread fluid-particle force

$$\mathbf{v}^{n+1} = \mathbf{v}_0^{n+1} - \mathsf{S}^n \lambda^n \Delta t + O(\Delta t^2)$$

Time-stepping: First order algorithm

$t_n = n\Delta t$, $\mathbf{v}^n = \mathbf{v}(t^n)$, $\mathsf{J}^n = \mathsf{J}(\mathbf{q}^n)$, etc,

Unperturbed flow

$$\mathbf{g}_0^{n+1} = \mathbf{g}_0^n - [\nabla \cdot \mathbf{P}]^n \, \Delta t$$

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Time-stepping: Second order algorithm

"position-Verlet-like" (time centered), Crank-Nicholson (Laplacian), Adam-Bashforth (advection)

Position at mid-time

$$\mathbf{q}^{n+1/2} = \mathbf{q}^n + \frac{\Delta t}{2} \mathtt{J}^n \mathbf{v}^n$$

Velocity full step

$$\left(\rho \mathbf{1} + m_e (\mathtt{SJ})^{n+1/2}\right) \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} + \nabla p = -\nabla \cdot \left(\rho \mathbf{v}\mathbf{v}^T + \sigma\right)$$
$$+ \mathtt{S}^{n+1/2} \mathbf{F}^{n+1/2} - \left[m_e \mathtt{SJ} \left(\mathbf{v} \cdot \frac{\partial \mathtt{J}}{\partial \mathbf{q}} \right) \mathbf{v} \right]^{n+1/2}$$

Position end-time

$$\mathbf{q}^{n+1} = \mathbf{q}^{n+} + \frac{\Delta t}{2} \mathtt{J}^{n+1/2} \left(\mathbf{v}^{n+1} + \mathbf{v}^n\right)$$

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Compressible, second order for $m_e = 0$ (neutrally bouyant)

$$
\begin{aligned}
\mathbf{q}^{n+\frac{1}{2}} &= \mathbf{q}^n + \frac{\Delta t}{2}\mathsf{J}^n\mathbf{u}^n \\
\mathbf{g}_0^{n+1} &= \mathbf{g}^n - \nabla\cdot\mathbf{P}\Delta t - (\mathsf{S}\mathbf{F})^{n+\frac{1}{2}} \\
(\mathbf{u})^{n+1} &= (\mathbf{u})^n + \frac{m_f}{m_p}\left[(\mathsf{J}\mathbf{v}_0)^{n+\frac{1}{2}} - (\mathsf{J}\mathbf{v})^n\right] && (5) \\
\mathbf{v}^{n+1} &= \mathbf{v}_0^{n+1} + \mathsf{S}^{n+\frac{1}{2}}\left[\mathbf{u}^{n+1} - (\mathsf{J}\mathbf{v}_0)^{n+1}\right] && (6) \\
\mathbf{q}^{n+1} &= \mathbf{q}^n + \frac{\Delta t}{2}\mathsf{J}^{n+\frac{1}{2}}\left(\mathbf{v}^n + \mathbf{v}^{n+1}\right) && (7)
\end{aligned}
$$

(small) Errors and (large) Courant numbers

$$\text{Courant number CFL} = V \frac{\Delta t}{\Delta x} \lesssim 1$$

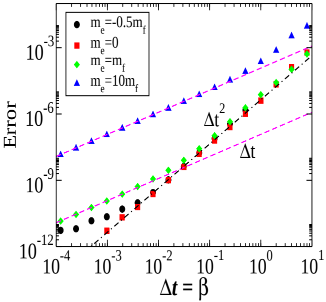
Advective CFL	$V = v$ flow velocity	$\alpha = \frac{v \Delta t}{\Delta x}$
Viscous CFL	$V = \nu / \Delta x$ momentum diffusion	$\beta = \frac{\nu \Delta t}{\Delta x^2}$
Sonic CFL	$V = c$ sound velocity	$\alpha_s = \frac{c \Delta t}{\Delta x}$
Cell Reynolds number		$r = \alpha / \beta$

(small) Errors and (large) Courant numbers

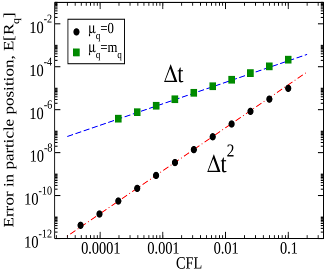
$$\text{Courant number } \mathtt{CFL} = V\frac{\Delta t}{\Delta x} \lesssim 1$$

$$\text{Error: } E(\Delta t) = \frac{1}{N_s}\sum_{n=1}^{N_s}\left|\mathbf{q}_{\Delta t}(n\Delta t) - \mathbf{q}_{\Delta t/2}(2n\Delta t/2)\right|$$

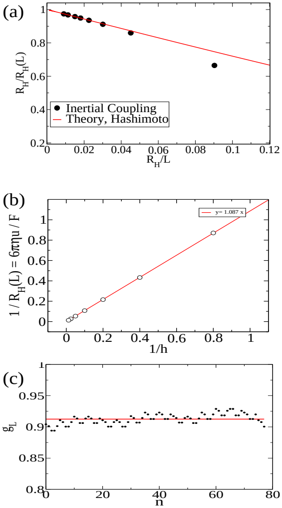
Incompressible formulation



Compressible formulation



Blob hydrodynamic radius



Hydrodynamic radius:

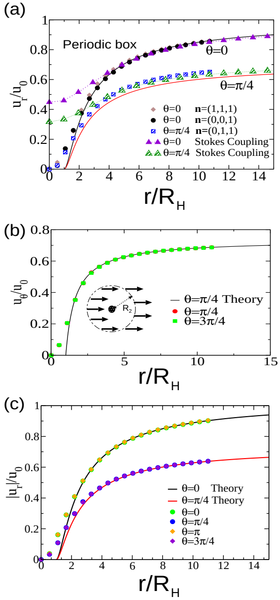
$R_H = 0.90 \pm 0.01$

Very small dependence on the underlying Eulerian grid

Flow past a "blob", at $\mathrm{Re}_P \sim 0$

$\longrightarrow$ ○

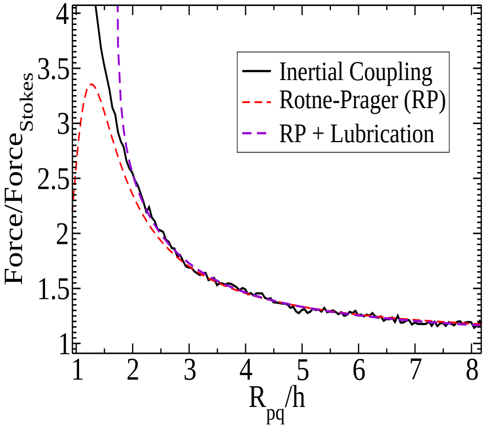
The **no-slip** constraint over the blob gives velocity profiles which agree with theoretical profiles for a rigid particle, for $r > 2R_H$



Two-particles mutual friction and lubrication

○ ⟶ ○

Friction and lubrication forces between two approaching particles. Captured for distances $d > 2\,R_H$ (not divergent at contact)



Velocity autocorrelation function

$$C(t) = \frac{1}{3}\langle \mathbf{u}(t) \cdot \mathbf{u}(0) \rangle$$

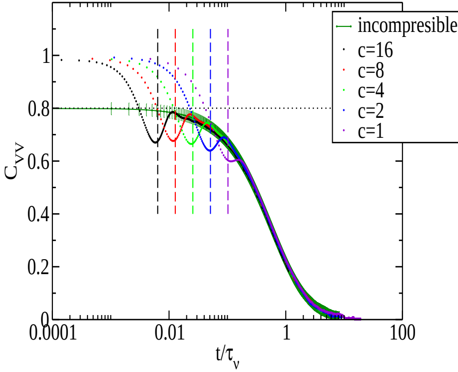
Short times

- $C(0) = \langle u^2 \rangle = \dfrac{kT}{m_p}$
- Compressible flow: sonic "bump" at $t_s = 2R_H/c$

$$C(t_s) \simeq \frac{kT}{m_p + m_f/2}$$

- Incompressible $c \to \infty$. **Added mass effect is ok**

$$C(0) = \frac{kT}{m_p + m_f/2}$$



Velocity autocorrelation function

$$C(t) = \frac{1}{3}\langle \mathbf{u}(t)\cdot\mathbf{u}(0)\rangle$$

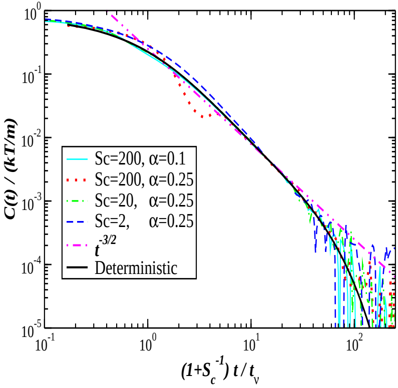
Long times

- Long time tail fluid momentum conservation, ok
- Correct Schmidt depedence at long times $t >> t_\nu$,

$$C(t) = \left[(\nu + D)\, t\right]^{-3/2}$$

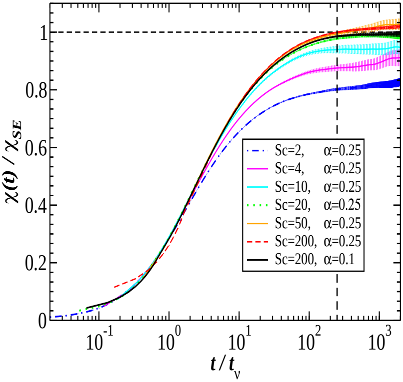
fluctuation-dissipation balance is ok

- Exp. decay at very long times (finite box effect)



Blob diffusive behaviour

- Einstein relation $\chi_E = \dfrac{kT}{\xi}$
- Stokes-Einstein relation
  $\chi_{SE} = \dfrac{kT}{6\pi\eta R_H}$
- Deviations from Stokes-Einstein relation at small $\mathrm{Sc} = \nu/\chi$
- Thermal velocity $v_{th} = (kT/m_f)^{1/2}$
- Thermal particle Reynolds: $Re_{p,th} \sim \mathrm{Sc}^{-1/2}$
- Thermal "advection" becomes relevant at low Sc (e.g. bubbles)



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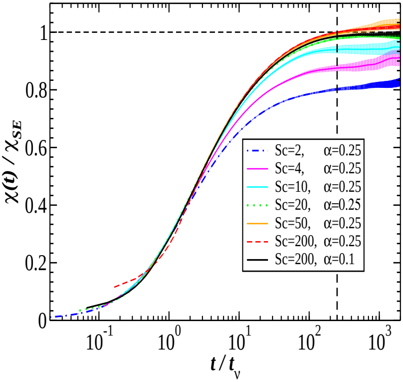

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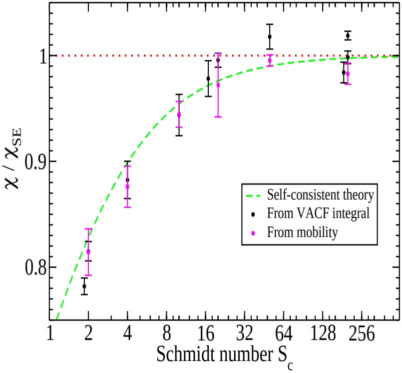

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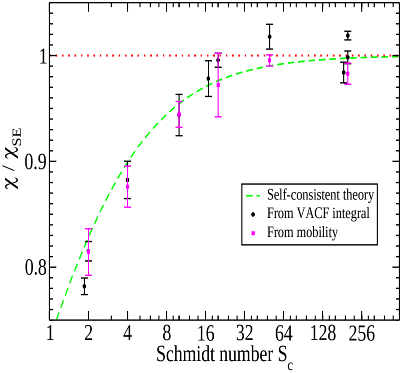

Fluid drag

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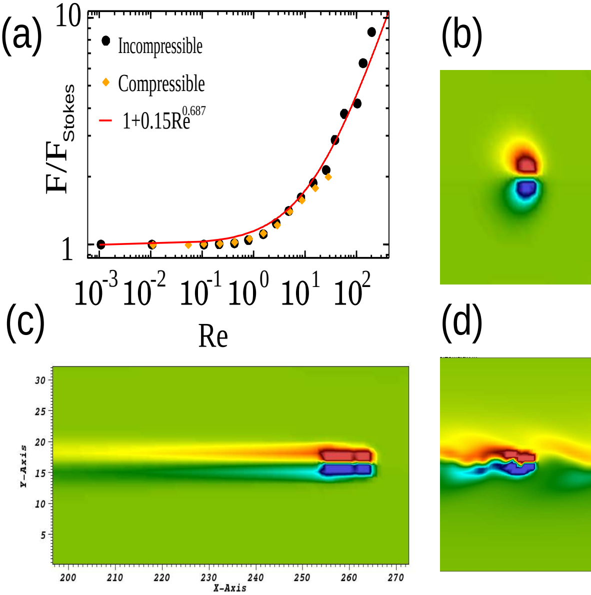
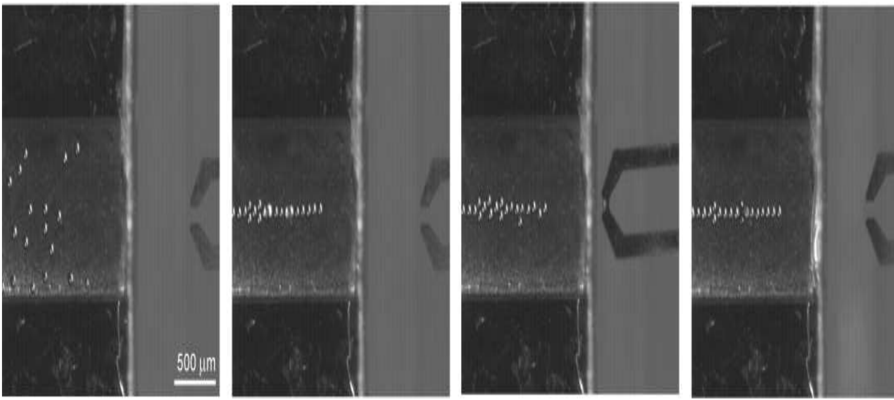
The drag force to the blob is consistent with that of a rigid particle, up to **large** particle Reynolds number $\mathrm{Re_p} = R_H\, v_0/\nu \leq 200$



Sound-particle interaction

Micromanipulation of micron size particles with ultrasound. Jürg Dual group, ETH



(a) (b) (c) (d)

Sound-particle interaction

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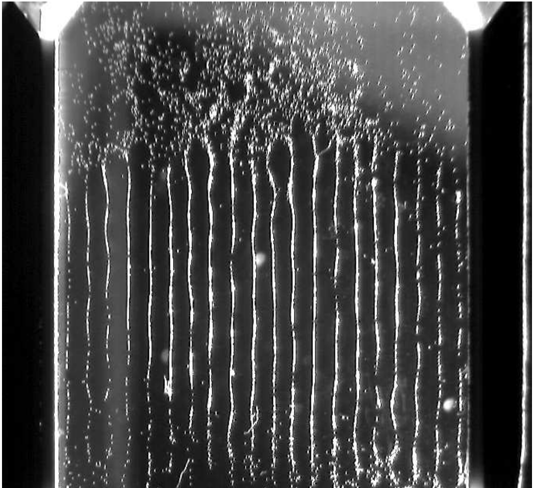

Sound-particle interaction

- A stationary sound wave generates an average force on a particle given by the gradient of a mean potential field $\langle \mathbf{F} \rangle = -\nabla \langle U \rangle$,

$$\langle U \rangle = 2\pi R^3 \rho_f \left(\frac{\langle \delta p^2 \rangle}{3\rho_f^2 c_f^2} f_1 - \frac{1}{2} \langle \delta u^2 \rangle f_2 \right) \tag{8}$$

  - $f_1 = 1 - \rho_f c_f / (\rho_p c_p)$ and $f_2 = 2(\rho_p - \rho_f)/(2\rho_p + \rho_f)$
- Acoustic force for standing plane wave (wavenumber k, amplitude $\Delta\rho$)

$$\langle \mathbf{F} \rangle = \frac{\pi c_f^2 \Delta\rho^2 R^3 k}{\rho_f} \left(\frac{1}{3} f_1 + \frac{1}{2} f_2 \right) \sin(2kz)\hat{\mathbf{z}} \tag{9}$$

- Fit f_1, f_2 and R from simulations: $c_p = c_f$ and $R = 1.19 R_H$

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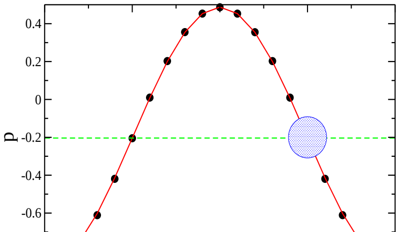
- Fit f_1, f_2 and R from simulations:$c_p = c_f$ and $R = 1.19 R_H$

Sound-particle interaction

- Acoustic boundary layer $\delta = \sqrt{\nu/\omega}$, with $\nu = \eta/\rho$
- Wave number: $\lambda = c\,2\pi/\omega$
- Particle radius: R_H

Simulation

- $R_H/\lambda \simeq 0.06$.
- Viscous effects: $\delta/R_H \simeq 0.2$
- Stokes is **not** valid, as it requires $\delta/R_H >> 1$



Animation

Acoustic force