Particle hydrodynamics: from molecular to colloidal fluids

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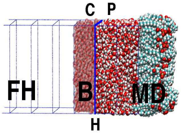
Universidad Autónoma de Madrid

von Neumann Symposia, Snowbird. July 2011

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

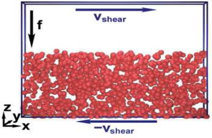
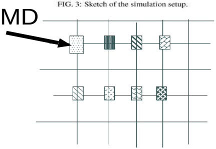


FIG. 3: Sketch of the simulation setup.

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...



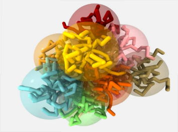
MD nodes used to
evaluate the **local stress**
for the Continuum solver.

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...)

- Particle hydrodynamics
  - Florencio Balboa (Univ. Autonoma Madrid)
  - Aleks Donev (Courant Institute, New York)
  - Ignacio Pagonabarraga (Univ. Barcelona)
- Open flutuating hydrodynamics
  - Anne Dejoan (CIEMAT)
- Hybrid molecular-continuum hydrodynamics
  - Gianni De Fabritiis (U. Pompeu Fabra, Barcelona)
  - P. V. Coveney (UCL, London)
  - E. Flekkoy (Oslo Univ.)
  - Jason Reese (U. StrathClyde, Glasgow) (new)
- Adaptive resolution in HybridMD
  - Matej Praprotnik (National Inst. Chem. Ljubljana)
  - Kurt Kremer (Max-Plank, Mainz)
- Coarse-grained dynamics
  - Pep Español (UNED)
  - Eric vanden-Eijnden (Courant Institute, NY)

Outline of the talk

- **Domain decomposition**
  - OpenMD: generalized open boundary conditions for MD
  - HybridMD: Particle-continuum hybrid
  - AdResS: Adaptive Resolution *mesoscopic layer*.
- **Particle hydrodynamics: an Eulerian-Lagrangian approach**
  - Direct Forcing theoretical background
  - Tests: manipulation of colloidal particles using ultrasound

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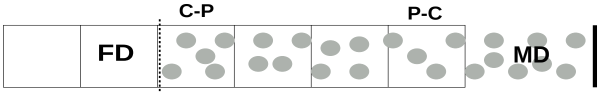
  - Tests: manipulation of colloidal particles using ultrasound

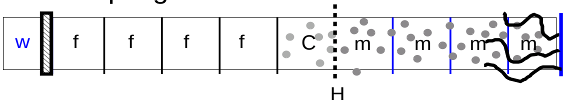
Hybrid particle-continuum schemes

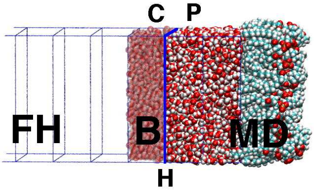
Recent review: R. Delgado-Buscalioni, in "Numerical Analysis and Multiscale Computations", Lect. Notes Comput. Sci. Eng., Volume 82, Springer Verlag (to appear)"

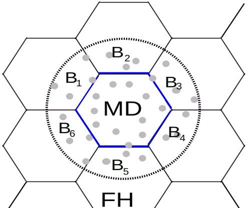
State-coupling



Flux-coupling



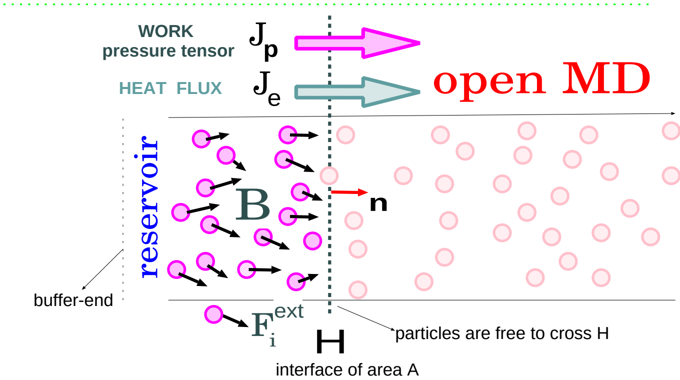




Open Molecular Dynamics

Open MD
via external forces

$$m\ddot{\mathbf{r}}_i = \mathbf{f}_i(\{\mathbf{r}\}) + \mathbf{f}_i^{\text{ext}}$$



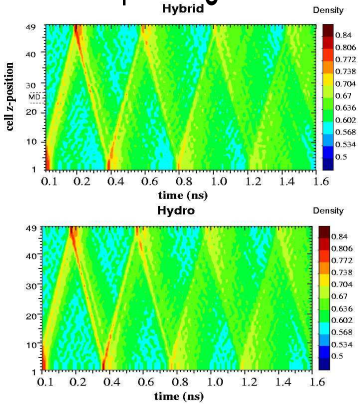
Hybrid MD-FH: Sound

De Fabritiis, R.D-B and P. Coveney, PRL, 97 (2006)

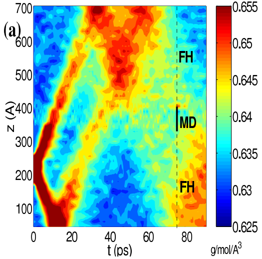
RDB and De Fabritiis PRE 76, 036709 (2007)

Important: Mass conservation and similar sound velocities (EOS) across H

liquid argon

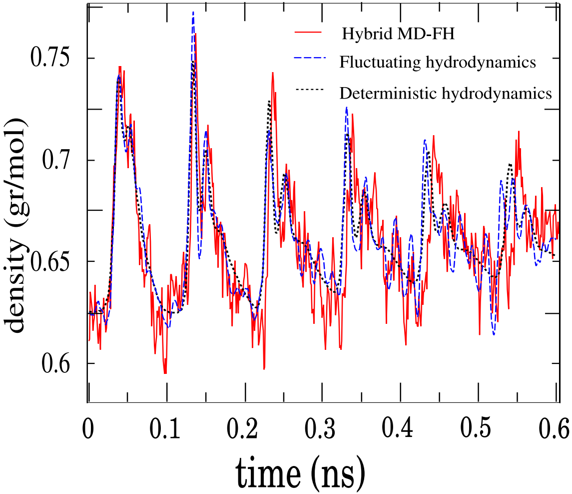


water



Hybrid MD-Fluctuating Hydrodynamics
Some test cases: sound

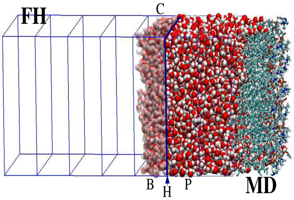
RDB and De Fabritiis PRE 76, 036709 (2007)

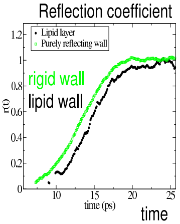


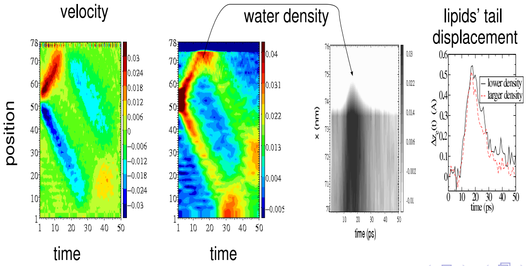
Hybrid MD-Fluctuating Hydrodynamics
Collision of sound waves against DMPC lipid layer

De Fabritiis, R.D-B and P. Coveney, PRL, 97 (2006)

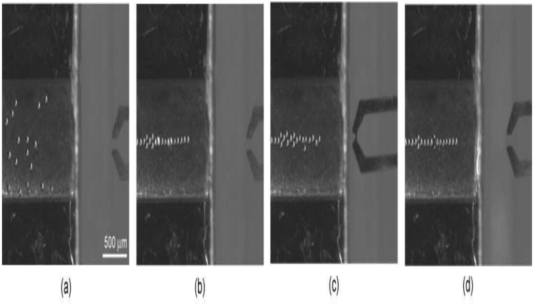
RDB et al, Proc IMechE, Part C: J Mech. Eng. Sci. **222** (2008)







The Direct Forcing Method for particle hydrodynamics



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

Direct Forcing for Point particle hydrodynamics.

Motivation

- **The Immersed Boundary method** $\dot{\mathbf{R}}_p = \mathbf{u}_p$
  - Fluid-structure interaction. $\mathbf{F}_{fp} = \mathbf{F}(\{\mathbf{R}_p\})$
  - No inertial forces
- **The Stokes coupling method** $\ddot{\mathbf{R}}_p = (\xi/M)(\mathbf{u}_p - \mathbf{V}_p)$
  - A practical relaxation method to achieve $\mathbf{u} = \mathbf{v_p}$ [Ladd, Dünweg].
  - Limitted to low Reynolds and small velocity gradients [Maxey, Riley]
  - Response time τ limitted by the friction time $\tau > M/\xi$
  - Cannot solve ultrasound-matter interaction [Mazur, Bedeaux] or fast inertial forces (turbulence).
- **Direct Forcing method** $M_p\ddot{\mathbf{R}}_p = \mathbf{F}_p(\mathbf{V}_p, \mathbf{u})$
  - The fluid-particle force ensures no-slip at the particle site.
  - Instantaneous momentum transfer: particle inertia, fast forcing (ultrasound, etc).
  - Straightforward implementation from Stokes

Equations of motion

- Particle

$$\dot{\mathbf{R}}_p = \mathbf{V}_p \quad (1)$$

$$M_p \frac{d\mathbf{V}_p}{dt} = -\int_{\mathcal{V}_p} \nabla \cdot \mathcal{P} \mathrm{d}\mathbf{r}^3 + \mathbf{F}_{\text{ext}} \quad (2)$$

$$I_p \frac{d\mathbf{\Omega}_p}{dt} = -\oint_S (\mathbf{r} - \mathbf{R}_p) \times \mathcal{P} \cdot \mathbf{n}\mathrm{d}\mathbf{r}^2 + \mathbf{F}_{\text{ext}} \times \mathbf{r} \quad (3)$$

- Fluid (fluctuating hydrodynamics)

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{g} \quad (4)$$

$$\frac{\partial \mathbf{g}}{\partial t} = -\nabla \cdot \mathbf{\Pi} + \mathbf{f}. \quad (5)$$

Stress tensor $\mathbf{\Pi} = \mathbf{g}\mathbf{u} + \mathcal{P}$ with $\mathcal{P} = \pi \mathbf{1} + \eta [\nabla \mathbf{u}]^{\mathtt{sym}} + \tilde{\mathcal{P}}$

Boundary conditions

- **Particle surface resolved**

$$\mathbf{u} = \mathbf{V}_p + \Omega \times (\mathbf{r} - \mathbf{R}_p) \quad (6)$$

$$\rho = 0 \forall \mathbf{r} \in \mathcal{V}_p \quad (7)$$

where $\mathbf{r} - \mathbf{R}_p = R\,\mathbf{n}$

- **Single site approach (pointwise)**

$$\mathbf{u} = \mathbf{V}_p \text{ at } \mathbf{r} = \mathbf{R}_p \quad (8)$$

Momentum balance

- Integrate momentum eq. over the whole domain

$$\frac{d}{dt}\int \mathbf{g}\,\mathrm{d}\mathbf{r}^3 = \int \nabla\cdot\mathcal{P}\,\mathrm{d}\mathbf{r}^3 + \int \mathbf{f}\,\mathrm{d}\mathbf{r}^3 \tag{9}$$

- Fluid-particle interaction is short (microscopic) ranged

$$\int \mathbf{f}\mathrm{d}\mathbf{r}^3 = \int_{\cup\mathcal{V}_p} \mathbf{f}\mathrm{d}\mathbf{r}^3 \tag{10}$$

- *Non-overlapping* particle volumes

$$\int_{\cup\mathcal{V}_p} \mathbf{f}\mathrm{d}\mathbf{r}^3 = \sum_p \int_{\mathcal{V}_p} \mathbf{f}\mathrm{d}\mathbf{r}^3 = \sum_p \mathbf{F}_p \tag{11}$$

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Momentum balance and particle eq. motion

- Integrating over one particle volume:

$$\frac{d}{dt}\int_{\mathcal{V}_p} \mathbf{g}\,\mathrm{d}\mathbf{r}^3 = \int_{\mathcal{V}_p} \nabla\cdot\mathcal{P}\,\mathrm{d}\mathbf{r}^3 + \mathbf{F}_p \quad (12)$$

$$\text{recall } M_p\frac{d\mathbf{V}_p}{dt} = -\int_{\mathcal{V}_p} \nabla\cdot\mathcal{P}\mathrm{d}\mathbf{r}^3 + \mathbf{F}_{\text{ext}} \quad (13)$$

- Particle equation of motion

$$M_p\frac{d\mathbf{V}_p}{dt} = \frac{d}{dt}\int_{\mathcal{V}_p} \mathbf{g}\,\mathrm{d}\mathbf{r}^3 - \mathbf{F}_p + \mathbf{F}_{\text{ext}} \quad (14)$$

- Incompressible fluid: $\int_{\mathcal{V}_p} \mathbf{g}\,\mathrm{d}\mathbf{r}^3 = \rho\mathcal{V}_p\langle\mathbf{u}\rangle_p = \rho\mathcal{V}_p\mathbf{V}_p$

$$\Delta M_p\frac{d\mathbf{V}_p}{dt} = -\mathbf{F}_p + \mathbf{F}_{\text{ext}} \quad (15)$$

Archimedes Eureka: **Particle mass excess** $\Delta M_p = M_p - m_p$ with $m_p = \rho\mathcal{V}_p$ (evacuated fluid mass).

Momentum balance and particle eq. motion

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The particle-fluid force

- Impose zero relative velocity at particle site: $\langle \mathbf{u} \rangle_p = \mathbf{V}_p$
- Incompressible case
  Integrate momentum $\mathbf{g} = \rho \mathbf{u}$ over particle volume $\mathcal{V}_p$ and time Δt:

$$\rho \langle \mathbf{u} \rangle_p (t + \Delta t) = \rho \tilde{\mathbf{u}}_p + \frac{1}{\mathcal{V}_p} \int_t^{t+\Delta t} \mathbf{F}_p(t') \mathrm{d}t'. \qquad (16)$$

- **Pointwise approach:** volume averaged quantities: $\langle \mathbf{u} \rangle_p \mathcal{V}_p \equiv \int_{\mathcal{V}_p} \mathbf{u} \mathrm{d}\mathbf{r}^3$
- The *unperturbed* fluid velocity field is

$$\rho \tilde{\mathbf{u}}_p = \rho \langle \mathbf{u} \rangle_p (t) - \int_t^{t+\Delta t} \langle \nabla \cdot \boldsymbol{\pi} \rangle_p (t') \mathrm{d}t', \qquad (17)$$

- The "stick" constraint $\langle \mathbf{u} \rangle_p = \mathbf{V}_p$ in Eq. (16) yields

$$\int_t^{t+\Delta t} \mathbf{F}_p(t') \mathrm{d}t' = \rho \mathcal{V}_p \left[\mathbf{V}_p(t + \Delta t) - \tilde{\mathbf{u}}_p \right]. \qquad (18)$$

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Eulerian-Lagrangian transformations

- Particles move in continuum (Lagrangian) space $\mathbf{R}_p \in \mathbb{R}$.
- Fluid solved at discrete set of Eulerian nodes $\mathbf{r}_i$.
- Communication requires two operations:
  - Interpolation of the unperturbed fluid velocity at particle site
- Operators in discrete form: $\delta_{ip} = \delta_h(|\mathbf{r}_i - \mathbf{R}_p|)$

$$\text{Interpolation} \quad \phi_p^I = \sum_i \delta_{ip}^I \phi_i \ \text{note} : \langle\phi\rangle_p \to \phi_p^I \quad (19)$$

$$\text{Spreading} \quad \phi_i^S = \sum_p \delta_{ip}^S \phi_p \quad (20)$$

with $\phi_i = \phi(\mathbf{r}_i)$ and $\phi_p = \phi[\mathbf{R}_p]$.

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with $\phi_i = \phi(\mathbf{r}_i)$ and $\phi_p = \phi[\mathbf{R}_p]$.

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- Particles move in continuum (Lagrangian) space $\mathbf{R}_p \in \mathbb{R}$.
- Fluid solved at discrete set of Eulerian nodes $\mathbf{r}_i$.
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Consistency: spreading + interpolation = identity

- It will soon be clear why we need **adjoint operations:** spreading ϕ_p gives $\phi_i^S = \sum_p \phi_p \delta_{ip}^S$ and interpolation back $\phi_p^{SI} = \sum_q [\sum_i \delta_{ip}^I \delta_{iq}^S] \phi_q$.

$$\text{Therefore } \phi_p^{SI} = \phi_p \text{ if } \sum_i \delta_{ip}^I \delta_{iq}^S = \delta_{pq}^{\text{kr}} \tag{21}$$

  where δ_{pq}^{kr} is the Kronecker delta.
  Note that Interpolation+Spreading is **not** the identity

- However IB kernels satisfy a weaker property

$$\sum_i \delta_{ip}^I \delta_{ip}^S = 1 \tag{22}$$

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Immersed Boundary (IB) Kernels *(Peskin)*

- Constructed with a soft function of compact support: $\delta_h(\mathbf{r}) = \phi(x/h)\phi(y/h)\phi(z/h)$

$$\phi(u) = \begin{cases} \frac{1}{3}(1+\sqrt{1-3u^2}) & 0 \leq |u| \leq \frac{1}{2} \\ \frac{1}{6}(5-3|u|-\sqrt{-2+6|u|-3u^2}) & \frac{1}{2} \leq |u| \leq \frac{3}{2} \\ 0 & \frac{3}{2} \leq |u| \end{cases}$$

- Satisfying

$$\sum_i \delta_h(\mathbf{r}_i - \mathbf{R}) = 1 \quad (23)$$

$$\sum_i \delta_h^2(\mathbf{r}_i - \mathbf{R}) = 1/\mathsf{c} \quad (24)$$

$$\sum_i (\mathbf{r}_i - \mathbf{R})\delta_h(\mathbf{r}_i - \mathbf{R}) = 0 \quad (25)$$

where $\mathsf{c} = 8$ for the three point base kernel ϕ.

Interpolation/Spreading pair properties

- Interpolation and spreading based on the same IB kernel:

$$\delta_{ip}^{I} \equiv \delta_h(\mathbf{r}_i - \mathbf{R}_p) \tag{26}$$

$$\delta_{ip}^{S} \equiv \mathtt{c}\,\delta_{\mathtt{h}}(\mathbf{r}_{\mathtt{i}} - \mathbf{R}_{\mathtt{p}}) \tag{27}$$

- **Normalization**

$$\sum_i h^3 \delta_{ip}^{I} = h^3 \tag{28}$$

$$\sum_i h^3 \delta_{ip}^{S} = \mathcal{V}_p \tag{29}$$

Particle effective volume: from (29) and (27): $\mathcal{V}_p = \mathtt{c}\,\mathtt{h}^3$

For the 3 point kernel $\mathtt{c} = 8$

Time integration, some notations

- System evolving in discrete times $t_n = n\,\Delta t$.
- The time integral is noted as

$$\overline{\phi} \equiv \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \phi(t)\mathrm{d}t \tag{30}$$

- The interpolator and spreading operators depend on time via the particle position.

$$\delta^I_{ip^n} \equiv \delta^I(|\mathbf{r}_i - \mathbf{R}_p(t_n)|) \tag{31}$$

- Interpolation at equal times: $\mathbf{u}_p^n = \sum_i \delta^I_{ip^n}\mathbf{u}_i^n$
- Interpolation at *unequal* times: $\mathbf{u}^n_{p^{n+1}} = \sum_i \delta^I_{ip^{n+1}}\mathbf{u}_i^n$

Time integration: the algorithm

1) Unperturbed Eulerian velocity $\rho \tilde{\mathbf{u}}_i = \rho \mathbf{u}_i^n - \overline{[\nabla \cdot \mathbf{\Pi}]}_i \Delta t$

2) Particle positions $\mathbf{R}_p^{n+1} = \mathbf{R}_p^n + \overline{\mathbf{V}}_p \Delta t$

3) Unperturbed Lagrangian velocity $\tilde{\mathbf{u}}_p = \sum_i \delta^I_{ip^{n+1}} \tilde{\mathbf{u}}_i$

4) Particle velocity $M_p \equiv \delta M_p + m_p$ $\mathbf{V}_p^{n+1} = \frac{\delta M_p}{M_p} \mathbf{V}_p^n + \frac{m_p}{M_p} \tilde{\mathbf{u}}_p + \frac{\overline{\mathbf{F}_{\text{ext}}} \Delta t}{M_p}$

5) Force spreading $\overline{\mathbf{f}}_i \Delta t = \rho \sum_p \left[\mathbf{V}_p^{n+1} - \tilde{\mathbf{u}}_p \right] \delta^S_{ip^{n+1}}$

Check:

$$\mathbf{u}_p = \tilde{\mathbf{u}}_p + \sum_q (\mathbf{V}_q - \tilde{\mathbf{u}}_q) \sum_i \delta^I_{ip} \delta^S_{iq} = \tilde{\mathbf{u}}_p + \sum_q (\mathbf{V}_q - \tilde{\mathbf{u}}_q) \delta^{Kr}_{pq} = \mathbf{V}_p$$

Lagrangian dynamics of a fluid parcel $(\delta M_p = 0)$

Eulerian discretized momentum eq.

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

Lagrangian: interpolate at p site: $(\sum_i \delta^I_{ip^{n+1}} \square)$

$$\Delta \mathbf{g}_p = \mathbf{g}_p^{n+1} - \mathbf{g}_p^n = \left(\mathbf{g}^n_{p^{n+1}} - \mathbf{g}^n_{p^n}\right) - \nabla \cdot \left[\overline{\mathbf{gu}}_p + [\overline{\nabla \cdot \mathcal{P}}]_p\right] \Delta t$$

where $\delta \mathbf{g}_p \equiv \left(\mathbf{g}_{p^{n+1}} - \mathbf{g}_{p^n}\right) = \Delta \mathbf{R}_p \cdot \nabla_{\mathbf{R}} \mathbf{g}_{p^n} = \Delta t \overline{\mathbf{V}}_p \cdot \nabla_{\mathbf{R}} \mathbf{g}_{p^n}$

Explicit scheme (Euler):

$$\rho_p^{n+1} \frac{\Delta \mathbf{u}_p}{\Delta t} + \nabla \cdot \mathcal{P}_p^{n+1} =$$

$$\delta \mathbf{u}_p \nabla \cdot \mathbf{g}^n_{p^{n+1}} + \rho^n_{p^{n+1}} \left(\mathbf{V}_p^n - \mathbf{u}^n_{p^{n+1}}\right) \cdot \nabla \mathbf{u}^n_{p^{n+1}} = O(\rho u^3 \Delta t / l^2)$$

Semi-implicit (Crank-Nicholson):

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Accuracy: differences in total fluid momentum gain
in Eulerian and Lagrangian variables

- **Eulerian momentum** $\Delta \mathbf{W}_{\mathrm{E}} = h^3 \sum_i \left(\Delta \mathbf{g}_i + \overline{[\nabla \cdot \mathbf{\Pi}]_i}\Delta t\right)$

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Fluid+particle (*Eulerian*) momentum exactly conserved

- **Lagrangian momentum**

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Explicit scheme: limited to Re< 1/CFD (Courant no.)
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Higher order schemes (open problem).

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Compressible fluid at low Mach number

- Trivial generalization of the spread force density

$$\overline{\mathbf{f}_{ip}}\Delta t = \rho_i \left[\mathbf{V}_p - \tilde{\mathbf{u}}_p\right] \delta^S_{ip} \tag{34}$$

- Particle-fluid force:
  - **Eulerian**

$$\sum_i \overline{\mathbf{f}_{ip}} h^3 \Delta t = \rho_p \mathcal{V}_p \left[\mathbf{V}_p - \tilde{\mathbf{u}}_p\right] = \overline{\mathbf{F}_p}\Delta t \tag{35}$$

  - **Lagrangian**

$$\sum_i \delta^I_{ip} \overline{\mathbf{f}_{ip}} h^3 \Delta t = \rho^*_p \mathcal{V}_p \left[\mathbf{V}_p - \tilde{\mathbf{u}}_p\right] = \overline{\mathbf{F}^*_p}\Delta t \tag{36}$$

with $\rho^*_p = \sum_i \rho_i \delta^I_{ip}\delta^S_{ip}$. recall that $\sum_i \delta^I_{ip}\delta^S_{ip} = 1$ so $\rho^*_p \simeq \rho_p$

Force inconsistency: $\delta F = |F - F^*|/F < 0.17\text{Ma}^2$.

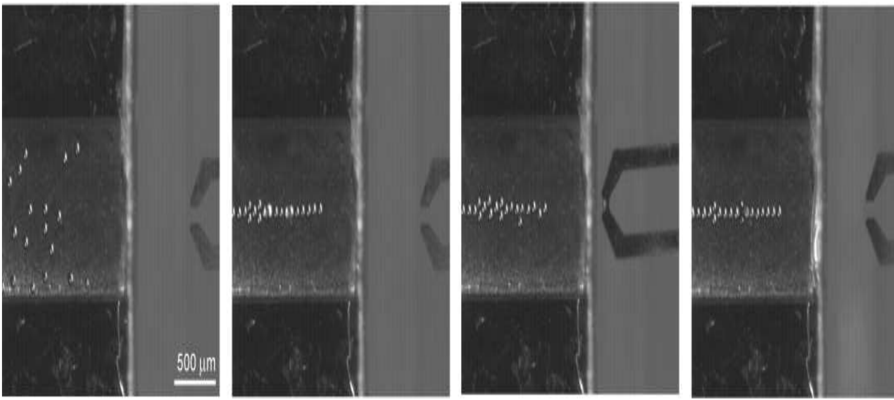
Scheme valid at low Mach number

Tests

- **Hydrodynamic radius**: $R_H = 0.9\,h$ (translational invariance: Std[R_h]$\simeq 1\%$)
- **Drag force**: valid up to Re ~ 10 (equivalent to slippery sufaces)
- **Velocity profiles**
- **Hydrodynamic forces: Oseen and Lubrication**
- **Fluctuations**
- **Velocity autocorrelation**: long time tails
- **Acoustic force**

Sound-particle interaction

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



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

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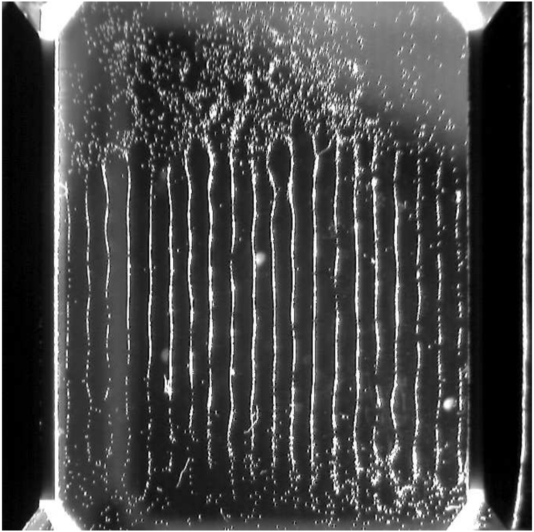

Sound-particle interaction

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

$$\langle U \rangle = 2\pi R^3 \rho_f \left(\frac{\langle \delta p^2 \rangle}{3\rho_f^2 c_f^2} f_1 - \frac{1}{2} \langle \delta u^2 \rangle f_2 \right) \qquad (37)$$

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

$$\langle \mathbf{F} \rangle = \frac{\pi c_f^2 \Delta\rho^2 R^3 k}{\rho_f} \left(\frac{1}{3} f_1 + \frac{1}{2} f_2 \right) \sin(2kz)\hat{\mathbf{z}} \qquad (38)$$

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

Sound-particle interaction

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

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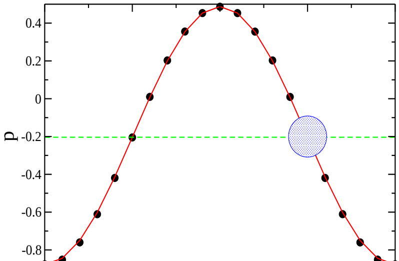
Sound-particle interaction

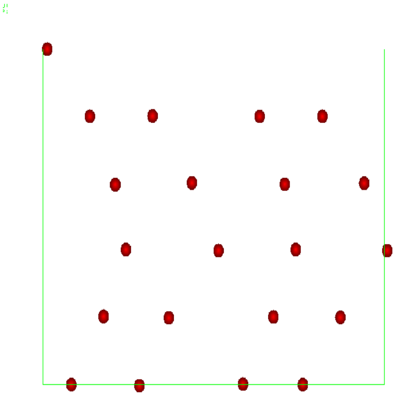
- Acoustic boundary layer $\delta = \sqrt(\nu/\omega)$, with $\nu = \eta/\rho$
- Wave number: $\lambda = c\, 2\pi/\omega$
- Particle radius: R_{NS}

Simulation

- $R_{NS}/\lambda \simeq 0.06.$
- Viscous effects: $\delta/R_{NS} \simeq 0.2$
- Stokes limit $\delta/R_H >> 1$ is **not** valid. (Stokes coupling not suited)

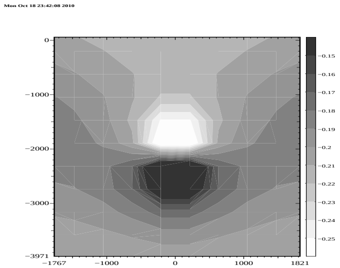


Sound-particle interaction



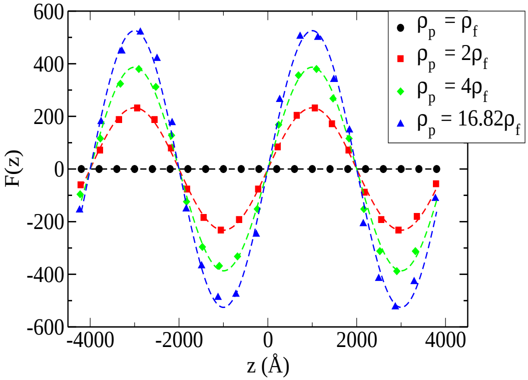
Animation

Direct forcing: pressure perturbation around particle



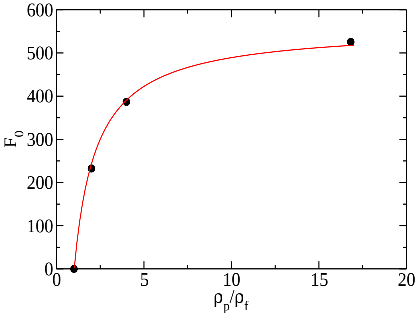
Acoustic force

Force of a standing wave at different positions



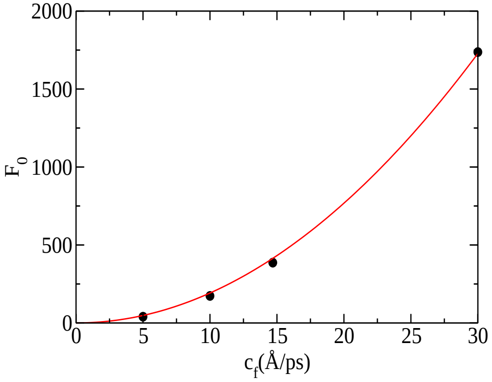
Acoustic force

Maximum force versus density ratio



Acoustic force

Maximum force versus fluid sound velocity



Stokes approximation for point particles

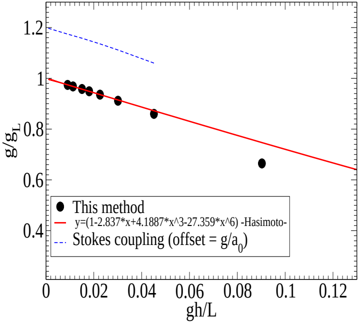
Review: Dünweg and Ladd Adv. Polym. Sci, 2008

Particle moving in an otherwise quiescent fluid, $\mathbf{u}_\infty = 0$

- Fluid-Particle force
$$\mathbf{F} = \xi_{bare}(\mathbf{V}_p - \mathbf{u}_p)$$
- Fluid velocity: $\mathbf{u}_p = T^{av}\mathbf{F}$
- Effective friction: $\mathbf{F} = \xi_{ef}\mathbf{V}_p$
$$\frac{1}{\xi_{ef}} = \frac{1}{\xi_{bare}} + \frac{1}{\xi_{hydro}}$$
- Efective hydrodynamic radius: $R_H = 6\pi\eta/\xi_{ef}$
$$\frac{1}{R_H} = \frac{1}{a_0} + \frac{1}{g\,h}$$
with $a_0 = \xi_{bare}/(6\pi\eta)$ and $g\,h = \xi_{hydro}/(6\pi/\eta)$.

Finite size effects on $R_H = g\,h$

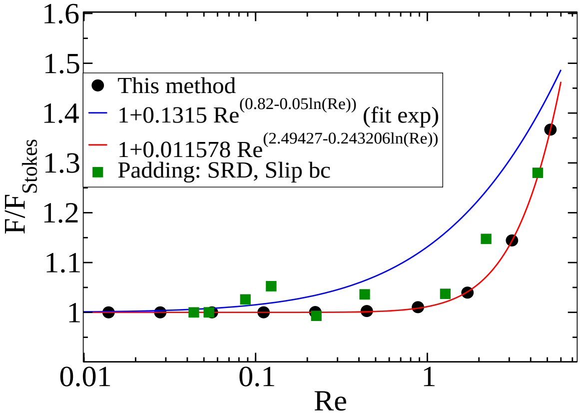
- Direct Forcing: $\dfrac{g}{g_L} = 1 - 2.84\dfrac{gh}{L} + \ldots$
- Stokes coupling: $\dfrac{g}{g_L} = \dfrac{6\pi\eta\, gh}{\xi_{bare}} + 1 - 2.84\dfrac{gh}{L} + ..$



Direct Forcing: strong coupling limit, instantaneous relaxation

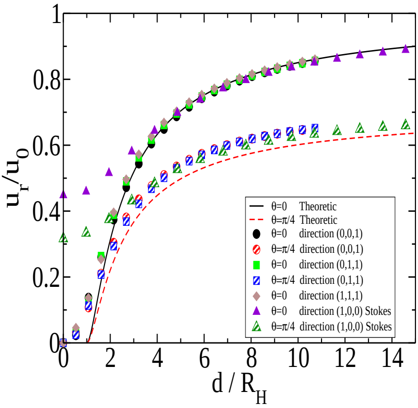
$$1/\xi_{bare} = 0$$

Drag at finite Reynolds number



Velocity profile around particle: PBC

Deviations at large distances are due to finite size effects.



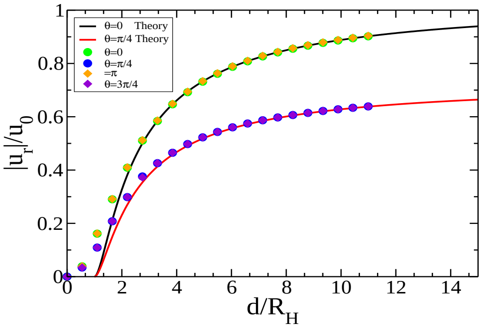
(Lines: analytic solution for $Re = 0$)

Velocity profile around particle: fixed velocity BC

To check for finite size effects we fix the fluid velocity $\mathbf{u}_0$ at the core of a spheric shell around the particle of radius r_s

$$\mathbf{u}(|\mathbf{r} - \mathbf{R}_p| = r_s) = \mathbf{u}_0$$

.



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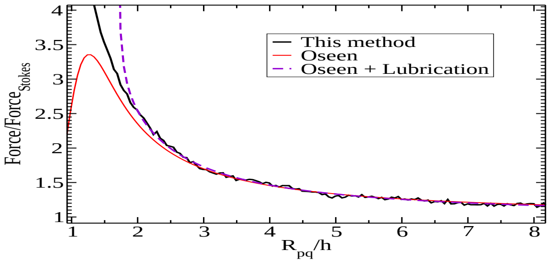
Forces between two particles: Oseen and Lubrication forces

Particles with same hydrodynamic radius

Oseen force: $R_H = 0.9h$
Lubrication: best fit with $R_L = 0.92R_H$

$$F^l = -6\pi\eta \frac{R_1^2 R_2^2}{(R_1 + R_2)^2} \left(\frac{1}{s} - \frac{1}{s_c}\right) (\mathbf{V}_1 - \mathbf{V}_2)\hat{\mathbf{R}}_{12}\hat{\mathbf{R}}_{12} \text{ for } s < s_c$$

with $s = |R_{12}| - R_1 - R_2$



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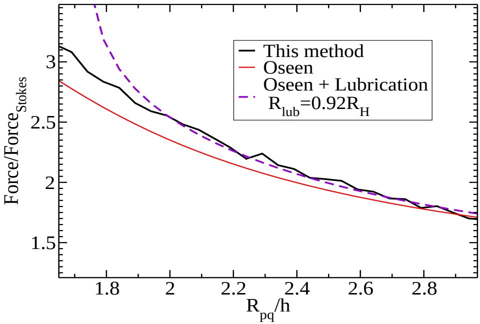
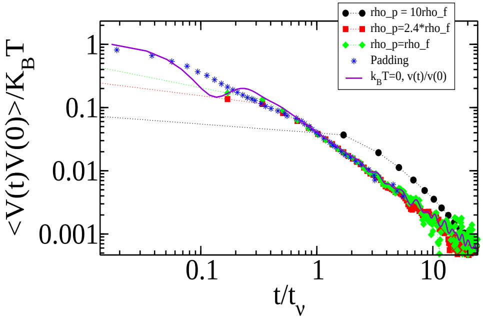
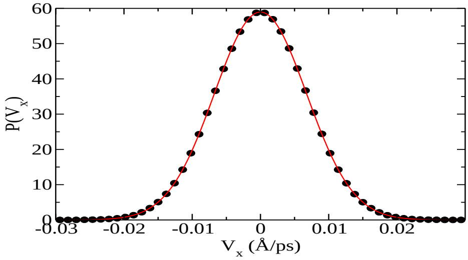


Direct forcing: Velocity decay and long-time tail



Particle within Fluctuating Hydrodynamics

- Particle kinetic temperature thermalizes with fluid
- There is no dissipative channel in the particle motion, as happens in Stokes coupling
- **No need** for Langevin force in the particle motion



Conclusions

Direct forcing for pointwise particles

- Fluid-Particle force from imposition of no-slip at particle site.
- Generalization of Stokes coupling method (strong coupling limit)
- Processes involving fast momentum transfer friction time
  - Ultrasound-particle interaction

- Particle inertia is taken into account
- Wall b.c. of arbitrary shape (first order accuracy). Easily generalized to elastic boundaries (IB with inertia)
- *Fluctuating hydrodynamics*: Fluid momentum fluctuation are transmitted to the particles without dissipation: " particle thermostat" is not required.

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Implementation

- No-slip implemented in **one-step** (no iterations).
- **The algorithm**: easy to implement from a Stokes code
- Parallelizable and written in `CUDA` (GPU): (50-100 faster than in a single CPU)

Formalization (in colab. Aleks Donev)

- Proyection operators
- Fluctuation-dissipation balance

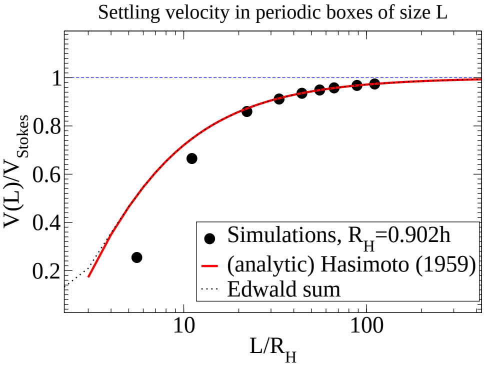
Applications (too many)

- Manipulation of colloids using ultrasound
- Particle dispersion in turbulent flow: memory effects, finite particles
- Effects of hydrodynamics on colloidal fluid gelation (E. Del Gado, ETH)

Calculation of g: finite size effects

- Settling velocity of a periodic array of particles with interparticle distance L (Hasimoto, 1959)

$$\frac{V_L}{V_\infty} = 1 - 2.84\frac{R_H}{L} + 4.1887\frac{R_H}{L}^3 - 27.359 * \frac{R_H}{L}^6 + ..$$



Calculation of g: finite size effects

- If the Stokes relation is assumed in PBC, $R_H = gh$ has to be redefined, $R_H^L \equiv g_L h$, with

$$\frac{g}{g_L} = \frac{V_L}{V_\infty} = 1 - 2.84\frac{gh}{L} + \ldots$$

Hydrodynamic Radius in Direct forcing

- Simulations:
  - PBC box of size L.
  - Particle: constant external force $\mathbf{F}_{ext} = F_{ext}\mathbf{k}$
  - Fluid: external pressure gradient $\partial p_{ext}/\partial z = F_{ext}/L^3$
  - Total momentum conserved
  - Steady state $F_{ext} = F_{drag}$, $\mathbf{V}_p = \mathbf{V}_p^{lim}$ and $\mathbf{u}_\infty = \mathbf{u}_\infty^{lim}$.
  - The hydrodynamic radius R_H is defined via the Stokes drag

$$\mathbf{F}_{drag} = 6\pi\eta R_H(\mathbf{V}_p - \mathbf{u}_\infty)$$

- Results
  - $R_H = g\,h$
  - $g = (0.89 \pm 0.05)$

Translational invariance: g

Quite small variation of g in mesh: $Std[g] \leq 0.01\bar{g}$