# SPH in the Mesoscopic World

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- Hydrodynamics apply also to very short scales: Microfluidics and even Nanofluidics.
- However, at these small scales, thermal fluctuations become important!
- They are responsible, for example, for the diffusion of colloidal particles.

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- Show how thermal fluctuations can be introduced in SPH in a thermodynamically consistent way.
- Present a model for colloidal suspensions (i.e. spherical particles inmersed in a fluctuating fluid).
- Present some simulation results that validate the model.

## *Continuum hydrodynamic equations*

Navier-Stokes equations in Eulerian form

$$
\begin{aligned}
\partial_t \rho &= -\nabla \rho \mathbf{v} \\
\partial_t \rho \mathbf{v} &= -\nabla \rho \mathbf{v}\mathbf{v} - \nabla P + \eta \nabla^2 \mathbf{v} + \frac{\eta}{3} \nabla \nabla \cdot \mathbf{v} \\
\partial_t s &= -\nabla s \mathbf{v} + 2\eta \overline{\nabla \mathbf{v}} : \overline{\nabla \mathbf{v}} + \kappa \nabla^2 T
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\end{aligned}$$

Lagrangian coordinates are the solution of

$$\partial_t \mathbf{R}(\mathbf{r}, t) = \mathbf{v}(\mathbf{R}(\mathbf{r}, t), t) \qquad \mathbf{R}(\mathbf{r}, 0) = \mathbf{r}$$

## Continuum hydrodynamic equations

The Jacobian $\mathcal{V}$ of $\mathbf{R} \leftrightarrow \mathbf{r}$ satisfies

$$\frac{d}{dt}\mathcal{V}(\mathbf{R}(\mathbf{r},t),t) = \mathcal{V}(\mathbf{R}(\mathbf{r},t),t)\nabla\cdot\mathbf{v}(\mathbf{R}(\mathbf{r},t),t)$$

$$\frac{d}{dt} = \partial_t + \mathbf{v}\cdot\boldsymbol{\nabla} \qquad \text{substantial derivative}$$

This is the equation for the rate of change of an infinitesimal volume that is transported by a flow field $\mathbf{v}(\mathbf{r},t)$.

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Introduce extensive fields: mass $M(\mathbf{r},t) = \rho(\mathbf{r},t)\mathcal{V}(\mathbf{r},t)$, momentum $\mathbf{P}(\mathbf{r},t) = \rho\mathbf{v}(\mathbf{r},t)\mathcal{V}(\mathbf{r},t)$, and entropy $S(\mathbf{r},t) = s(\mathbf{r},t)\mathcal{V}(\mathbf{r},t)$ fields.

## Continuum hydrodynamic equations

In terms of these extensive fields the NS eqs become

$$
\begin{aligned}
\frac{d}{dt}\mathbf{R} &= \mathbf{V} \\
\frac{d}{dt}M &= 0 \\
\frac{d}{dt}\mathbf{P} &= -\mathcal{V}\ \nabla P \ \ +\eta\mathcal{V}\ (\nabla^2\mathbf{v}) \ + \frac{\eta}{3}\mathcal{V}\ \ \nabla\nabla\cdot\mathbf{v} \\
T\ \frac{d}{dt}S &= 2\eta\mathcal{V}\ \ \overline{\nabla\mathbf{v}} : \overline{\nabla\mathbf{v}} \ \ +\kappa\mathcal{V}\ \ \nabla^2 T
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Constant mass. No convective terms. Suggests the idea of fluid particle.

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T_i\frac{d}{dt}S_i &= 2\eta\mathcal{V}_i(\overline{\nabla\mathbf{v}}:\overline{\nabla\mathbf{v}})_i + \kappa\mathcal{V}_i(\nabla^2 T)_i
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## *Fluid particle dynamics*

A fluid particle is a small moving thermodynamic subsystem of the whole system characterised by $\mathbf{r}_i, \mathbf{v}_i, \mathcal{V}_i, S_i, E_i, T_i, P_i$ $(m_i = \text{ctn.})$

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$$\mathcal{V}_i = \mathcal{V}_i(\mathbf{r}_1, \cdots, \mathbf{r}_N) \qquad E(\mathcal{V}_i, S_i, m_i) \qquad T_i = \frac{\partial E_i}{\partial S_i} \qquad P_i = -\frac{\partial E_i}{\partial \mathcal{V}_i}$$

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The independent variables are $x = \{\mathbf{r}_i, \mathbf{v}_i, S_i\}$

The total energy and entropy of the system are

$$E(x) = \sum_i^N \left[\frac{m_i}{2}\mathbf{v}_i^2 + E(\mathcal{V}_i, S_i, m_i)\right] \qquad S(x) = \sum_i^N S_i$$

## *Fluid particle dynamics*

How far can we go by requiring $\dot{\mathbf{R}}_i = \mathbf{V}_i, \quad \dot{M}_i = 0$

and conservation of total energy $E = \sum_i \left[ \frac{M_i}{2} \mathbf{V}_i^2 + \mathcal{E}(M_i, S_i, \mathcal{V}_i) \right]$?

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$$0 = \dot{E} \quad = \quad \sum_i \frac{\partial \mathcal{E}}{\partial \mathbf{R}_i} \cdot \dot{\mathbf{R}}_i + M_i \cdot \mathbf{V}_i \dot{\mathbf{V}}_i + \frac{\partial \mathcal{E}}{\partial S_i} \dot{S}_i$$

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0 = \dot{E} \quad &= \quad \sum_i \frac{\partial \mathcal{E}}{\partial \mathbf{R}_i} \cdot \dot{\mathbf{R}}_i + M_i \cdot \mathbf{V}_i \dot{\mathbf{V}}_i + \frac{\partial \mathcal{E}}{\partial S_i} \dot{S}_i \\
&= \quad - \sum_{ij} P_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} \cdot \mathbf{V}_i + \mathbf{V}_i \cdot M_i \dot{\mathbf{V}}_i + T_i \dot{S}_i
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0 = \dot{E} &= \sum_i \frac{\partial \mathcal{E}}{\partial \mathbf{R}_i}\cdot\dot{\mathbf{R}}_i + M_i\cdot\mathbf{V}_i\dot{\mathbf{V}}_i + \frac{\partial \mathcal{E}}{\partial S_i}\dot{S}_i \\
&= -\sum_{ij} P_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i}\cdot\mathbf{V}_i + \mathbf{V}_i\cdot M_i\dot{\mathbf{V}}_i + T_i\dot{S}_i \\
&= -\sum_{ij} P_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i}\cdot\mathbf{V}_i - \mathcal{V}_i(\nabla P)_i\cdot\mathbf{V}_i \\
&+ \sum_i \mathbf{V}_i\cdot\left(\eta\mathcal{V}_i(\nabla^2\mathbf{v})_i + \frac{\eta}{3}\mathcal{V}_i(\nabla\nabla\cdot\mathbf{v})_i\right) \\
&+ 2\eta\mathcal{V}_i(\overline{\nabla\mathbf{v}} : \overline{\nabla\mathbf{v}})_i + \sum_i \kappa\mathcal{V}_i(\nabla^2 T)_i
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## Fluid particle dynamics

Therefore, we have

$$
\begin{aligned}
\mathcal{V}_i(\nabla P)_i &= -\sum_j P_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} \\
\sum_i \mathcal{V}_i 2(\overline{\nabla \mathbf{v}} : \overline{\nabla \mathbf{v}})_i &= -\sum_i \mathcal{V}_i \mathbf{V}_i \cdot \left( (\nabla^2 \mathbf{v})_i + \frac{1}{3}(\nabla\nabla \cdot \mathbf{v})_i \right) \\
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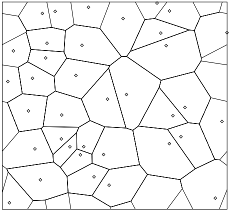
Two basic problems of a fluid particle model:

- How to define the volume $\mathcal{V}_i$ (that gives correct gradients!).
- How to define second derivatives (satisfying both $\dot{E} = 0$ and $\dot{S} > 0$).

## *How to define de volume $\mathcal{V}_i$?*

We have two possibilities:

Voronoi tessellation



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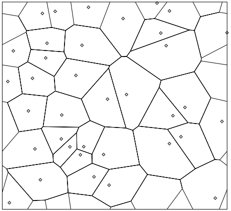
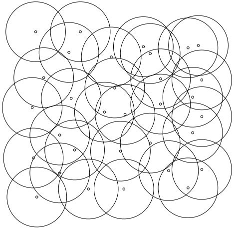


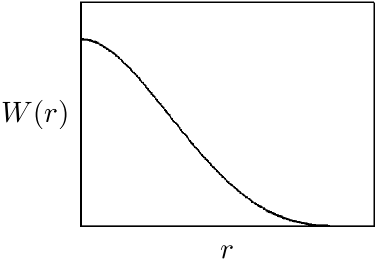
SPH



## The SPH volume

$$W(r) = \frac{105}{16\pi h^3}\left(1+\frac{r}{h}\right)\left(1-\frac{r}{h}\right)^3$$

$$1 = \int d\mathbf{r} W(r)$$



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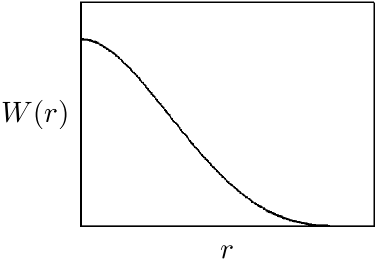


Define the density and the volume by

$$d_i = \sum_j W(r_{ij}) \qquad \mathcal{V}_i = \frac{1}{d_i}$$

## *The* SPH *gradient*

In this way, the pressure gradient is

$$\mathcal{V}_i(\nabla P)_i = -\sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{r}_i} P_j = -\sum_j \left[ \frac{P_i}{d_i^2} + \frac{P_j}{d_j^2} \right] F_{ij} \mathbf{r}_{ij}$$

# SPH *second derivatives*

After Cleary and Monaghan

$$\int d\mathbf{r}'[A(\mathbf{r}') - A(\mathbf{r}_i)]\frac{W'(|\mathbf{r}' - \mathbf{r}|)}{|\mathbf{r}' - \mathbf{r}_i|}\left[\delta^{\alpha\beta} - 5\frac{(\mathbf{r}' - \mathbf{r}_i)^{\alpha}(\mathbf{r}' - \mathbf{r})^{\beta}}{(\mathbf{r}' - \mathbf{r}_i)^2}\right]$$

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$$\approx \quad \nabla^\alpha \nabla^\beta A(\mathbf{r}_i) + \mathcal{O}(\nabla^4 A h^2)$$

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$$\approx \quad \nabla^\alpha\nabla^\beta A(\mathbf{r}_i) + \mathcal{O}(\nabla^4 A h^2)$$

$$\approx \quad \sum_j \frac{1}{d_j}[A_j - A_i]\frac{W'_{ij}}{r_{ij}}\left[\delta^{\alpha\beta} - 5\mathbf{e}_{ij}^\alpha\mathbf{e}_{ij}^\beta\right]$$

## SPH *second derivatives*

2nd derivatives in terms of the values of the function in neighbour points

$$
\begin{aligned}
\frac{1}{d_i}(\nabla^2 \mathbf{v})_i &= -2\sum_j \frac{F_{ij}}{d_i d_j}\mathbf{v}_{ij} \\
\frac{1}{d_i}(\nabla\nabla\cdot\mathbf{v})_i &= -\sum_j \frac{F_{ij}}{d_i d_j}\left[5\mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij} - \mathbf{v}_{ij}\right] \\
\frac{1}{d_i}(\nabla^2 T)_i &= -2\sum_j \frac{F_{ij}}{d_i d_j}T_{ij} \\
F_{ij} &\equiv -\frac{W'(r_{ij})}{r_{ij}} > 0
\end{aligned}
$$

## *The* SPH *fluid particle model*

The SPH equations are (Español and Revenga, PRE)

$$\begin{aligned}
\dot{\mathbf{r}}_i &= \mathbf{v}_i \\
m\dot{\mathbf{v}}_i &= \sum_j \left[\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right] W'_{ij}\mathbf{e}_{ij} - \frac{5\eta}{3}\sum_j \frac{F_{ij}}{d_i d_j}\left[\mathbf{v}_{ij} + \mathbf{e}_{ij}\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right] \\
T_i\dot{S}_i &= \frac{5\eta}{6}\sum_j \frac{F_{ij}}{d_i d_j}\left[\mathbf{v}_{ij}^2 + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})^2\right] - 2\kappa\sum_j \frac{F_{ij}}{d_i d_j} T_{ij}
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\end{aligned}
$$

The discrete equations conserve exactly, mass, momentum, energy and have positive entropy production.

## The GENERIC framework

General Equation for Non-Equilibrium Reversible-Irreversible Coupling

All dynamic equations that comply with the First and Second Laws have a universal structure Öttinger, Grmela Phys. Rev. E **56**, 6633 (1997)

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$$\frac{dx}{dt} = L \cdot \frac{\partial E}{\partial x} + M \cdot \frac{\partial S}{\partial x}$$

$$L(x) = -L^T(x) \qquad M(x) = M^T(x) \geq 0$$

$$L(x)\frac{\partial S}{\partial x} = 0 \qquad M(x)\frac{\partial E}{\partial x} = 0$$

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These properties ensure $\dot{E}(x) = 0 \qquad \dot{S}(x) \geq 0$

## Can we cast the SPH equations in GENERIC format?

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# *Can we cast the* SPH *equations in* GENERIC *format?*

$$\frac{dx}{dt} = L \cdot \frac{\partial E}{\partial x} + M \cdot \frac{\partial S}{\partial x}$$

$$\begin{pmatrix} \dot{\mathbf{r}}_i \\ \dot{\mathbf{v}}_i \\ \dot{S}_i \end{pmatrix} = \qquad \begin{pmatrix} \sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{r}_i} P_j \\ m\mathbf{v}_j \\ T_j \end{pmatrix}$$

$$+ \qquad \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ 1 \end{pmatrix}$$

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$$+ \sum_j \begin{pmatrix} 0 & \mathbf{0}^T & 0 \\ \mathbf{0} & M_{ij}^{vv} & M_{ij}^{vS} \\ 0 & M_{ij}^{vS} & M_{ij}^{SS} \end{pmatrix}\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ 1 \end{pmatrix}$$

# *Can we cast the* SPH *equations in* GENERIC *format?*

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$$+ \sum_j \begin{pmatrix} 0 & \mathbf{0}^T & 0 \\ \mathbf{0} & M_{ij}^{vv} & M_{ij}^{vS} \\ 0 & M_{ij}^{vS} & M_{ij}^{SS} \end{pmatrix}\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ 1 \end{pmatrix}$$

$$\begin{aligned}
M_{ij}^{vv} &= \frac{5\eta}{3}\delta_{ij}\sum_k \frac{F_{ik}}{d_i d_k}\left(\mathbf{1} + \mathbf{e}_{ik}\mathbf{e}_{ik}\right) + \frac{5\eta}{3}\frac{F_{ij}}{d_i d_j}\left(\mathbf{1} + \mathbf{e}_{ij}\mathbf{e}_{ij}\right) \\
M_{ij}^{vS} &= \frac{5\eta}{3}\delta_{ij}\sum_k \frac{F_{ik}}{d_i d_k}\left(\mathbf{v}_{ik} + \mathbf{v}_{ik}^{||}\right) + \frac{5\eta}{3}\frac{F_{ij}}{d_i d_j}\left(\mathbf{v}_{ij} + \mathbf{v}_{ij}^{||}\right) \\
M_{ij}^{SS} &= \frac{5\eta}{3}\delta_{ij}\sum_k \frac{F_{ik}}{d_i d_k}\left(\mathbf{v}_{ik}^2 + \mathbf{v}_{ik}^{||2}\right) + \frac{5\eta}{3}\frac{F_{ij}}{d_i d_j}\left(\mathbf{v}_{ij}^2 + \mathbf{v}_{ij}^{||2}\right) \\
&+ \delta_{ij}\sum_k 2\kappa\frac{F_{ik}}{d_i d_k} - 2\kappa\frac{F_{ij}}{d_i d_j}
\end{aligned}$$

## *The* GENERIC *framework*

Why we need to use the GENERIC framework at all...?

## *The* GENERIC *framework*

Why we need to use the GENERIC framework at all...?

... because thermal fluctuations are easily and elegantly introduced.

$$dx = \left[ L \cdot \frac{\partial E}{\partial x} + M \cdot \frac{\partial S}{\partial x} + k_B \frac{\partial}{\partial x} \cdot M \right] dt + d\tilde{x}, \quad \text{(Ito SDE)}$$

## *The* GENERIC *framework*

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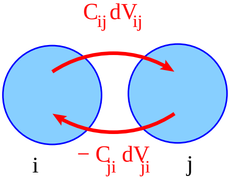
The noises satisfy:

$$\frac{\partial E}{\partial x} \cdot d\tilde{x} = 0 \qquad \text{Energy conserving}$$

$$d\tilde{x} d\tilde{x}^T = 2 k_B M dt, \qquad \text{Fluctuation-Dissipation}$$

## *Physics of noise*

The noise reflects each elementary transport process!!



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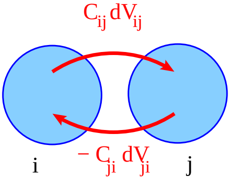


We postulate (satisfying $\sum_i m d\tilde{\mathbf{v}}_i \cdot \mathbf{v}_i + T_i d\tilde{S}_i = 0$)

$$
\begin{aligned}
d\tilde{\mathbf{r}}_i &= 0 \\
m d\tilde{\mathbf{v}}_i &= \sum_j A_{ij} d\mathbf{W}_{ij} \cdot \mathbf{e}_{ij} \\
T_i d\tilde{S}_i &= \sum_j C_{ij} d\mathbf{V}_{ij} - \frac{1}{2} \sum_j A_{ij} d\mathbf{W}_{ij} : \mathbf{e}_{ij} \mathbf{v}_{ij}
\end{aligned}
$$

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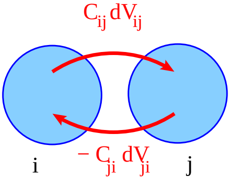


If we choose the following amplitudes ...

$$
\begin{aligned}
A_{ij} &= \left( \frac{8 k_B T_i T_j}{T_i + T_j} \frac{F_{ij}}{d_i d_j} \frac{5}{3} \eta \right)^{1/2} \\
C_{ij} &= \left( 2 k_B T_i T_j \frac{F_{ij}}{d_i d_j} \kappa \right)^{1/2}
\end{aligned}
$$

... then the $d\tilde{x} d\tilde{x} = 2 k_B M dt$.

## Summary of SPH+thermal fluctuations

For the dissipative forces proposed, simply add the following stochastic forces to the SPH equations

$$
\begin{aligned}
\tilde{\mathbf{F}}_i &= \sum_j \left( \frac{8k_B T_i T_j}{T_i + T_j} \frac{F_{ij}}{d_i d_j} \frac{5}{3} \eta \right)^{1/2} \frac{d\mathbf{W}_{ij}}{dt} \cdot \mathbf{e}_{ij} \\
T_i \tilde{J}_i &= \sum_j \left( 2k_B T_i T_j \frac{F_{ij}}{d_i d_j} \kappa \right)^{1/2} \frac{d\mathbf{V}_{ij}}{dt} \\
&- \frac{1}{2} \sum_j \left( \frac{8k_B T_i T_j}{T_i + T_j} \frac{F_{ij}}{d_i d_j} \frac{5}{3} \eta \right)^{1/2} \frac{d\mathbf{W}_{ij}}{dt} : \mathbf{e}_{ij} \mathbf{v}_{ij}
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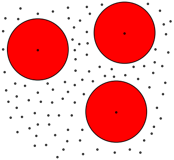
# SPH model for colloidal suspensions

Two types of particles: colloids and fluid particles.



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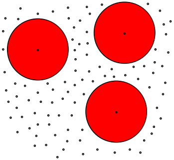

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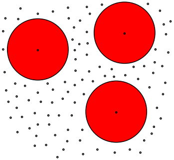

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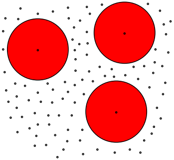

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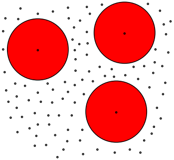

Three types of forces:

- $\mathbf{F}_{ij}^{FF}$, which we take from $\mathrm{SPH}$.
- $\mathbf{F}_{ij}^{CC}$, assumed to come from a repulsive potential.
- $\mathbf{F}_{ij}^{FC}$, which arise from boundary conditions.

## Boundary conditions

We treat immersed solid objects and walls as being made of "wall fluid particles" that interact in prescribed ways with the real fluid particles. At the end, a continuum limit is taken, and only "effective" interactions remain.

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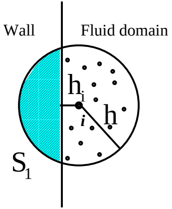
We treat immersed solid objects and walls as being made of "wall fluid particles" that interact in prescribed ways with the real fluid particles. At the end, a continuum limit is taken, and only "effective" interactions remain.

The issues to consider are:

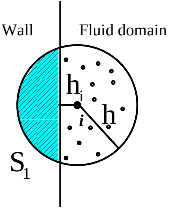
- Density deficit.
- Impenetrability.
- Stick boundary conditions.

# Boundary conditions: Density deficit




$$\overline{d}_i = \sum_{j \in \text{fluid}} W(r_{ij}) + \sum_{j \in \text{wall}} W(r_{ij})$$

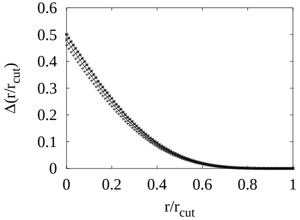
# Boundary conditions: Density deficit




$$\bar{d}_i = \sum_{j\in\text{fluid}} W(r_{ij}) + \sum_{j\in\text{wall}} W(r_{ij})$$

$$= \sum_{j\in\text{fluid}} W(r_{ij}) + d_0\Delta(h_i)$$

$$\Delta(h_i) = \int_S d\mathbf{r} W(|\mathbf{r}_i - \mathbf{r}|)$$



# Boundary conditions: Density deficit

The new pressure gradient is now

$$\mathcal{V}_i(\nabla P)_i = -\sum_i \frac{\partial \overline{\mathcal{V}}_j}{\partial \mathbf{r}_i} P_j = \sum_j \left[ \frac{P_i}{\overline{d}_i^2} + \frac{P_j}{\overline{d}_j^2} \right] F_{ij}\mathbf{r}_{ij} + \frac{P_i}{\overline{d}_i^2} d_0 \Delta'(h_i)\mathbf{n}$$

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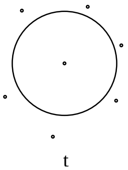
The last term is the pressure that a "continuum" of fluid particles inside the wall would exerted on $i$.

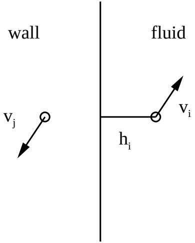
## Boundary conditions: Impenetrable walls




The bounce back transformation

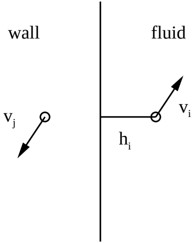
$$
\begin{aligned}
\mathbf{v}_i - \mathbf{V} &= -(\mathbf{v}_i' - \mathbf{V}') \\
m\mathbf{v}_i + M\mathbf{V} &= m\mathbf{v}_i' + M\mathbf{V}' \\
\frac{m}{2}\mathbf{v}_i^2 + \frac{M}{2}\mathbf{V}^2 &= \frac{m}{2}\mathbf{v}_i'^2 + \frac{M}{2}\mathbf{V}'^2
\end{aligned}
$$

## Boundary conditions: Stick




$$\mathbf{v}_j = \mathbf{v}_i + \frac{h_j + h_i}{h_i}(\mathbf{V}_{\text{wall}} - \mathbf{v}_i)$$

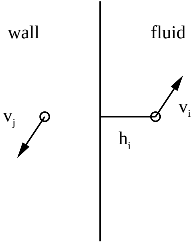
# Boundary conditions: Stick




$$\mathbf{v}_j = \mathbf{v}_i + \frac{h_j + h_i}{h_i}(\mathbf{V}_{\text{wall}} - \mathbf{v}_i)$$

$$\begin{aligned} m\dot{\mathbf{v}}_i\big|_{\text{wall}} &= -\frac{5\eta}{3}\sum_{j\in\text{wall}}\frac{F_{ij}}{d_i d_j}\left[(\mathbf{v}_i - \mathbf{v}_j) + \mathbf{e}_{ij}\mathbf{e}_{ij}\cdot(\mathbf{v}_i - \mathbf{v}_j)\right] \\ &= -\frac{5\eta}{3}\left(\sum_{j\in\text{wall}}\frac{F_{ij}}{\overline{d}_j}\mathbf{r}_{ij}\cdot\mathbf{n}\right)\left[\frac{(\mathbf{v}_i - \mathbf{V}_{\text{wall}})}{\overline{d}_i h_i} - \cdots\right] \\ &\approx -\frac{5\eta}{3}\left(\psi(h_i)\mathbf{1} + \mathbf{\Psi}(h_i)\right)\cdot\frac{(\mathbf{v}_i - \mathbf{V}_{\text{wall}})}{\overline{d}_i h_i} \end{aligned}$$

## Boundary conditions: Stick




$$\mathbf{v}_j = \mathbf{v}_i + \frac{h_j + h_i}{h_i}(\mathbf{V}_{\text{wall}} - \mathbf{v}_i)$$

$$\mathbf{F}_{ij}^{FC} = -\frac{5\eta}{3}\left(\psi(h_i)\mathbf{1} + \mathbf{\Psi}(h_i)\right)\cdot\frac{(\mathbf{v}_i - \mathbf{V})}{\bar{d}_i h_i}$$

$$\mathbf{\Psi}(h_i) \equiv \int_{\mathrm{S}} d\mathbf{r} F(|\mathbf{r}-\mathbf{r}_i|)\frac{\mathbf{r}_i-\mathbf{r}}{|\mathbf{r}_i-\mathbf{r}|}\frac{\mathbf{r}_i-\mathbf{r}}{|\mathbf{r}_i-\mathbf{r}|}(\mathbf{r}_i-\mathbf{r})\cdot\mathbf{n}$$

It has the same structure as the $\mathbf{F}_{ij}^{FF}$ force, only the coefficients change.

# SPH model for colloidal suspensions

Energy and entropy

$$
\begin{aligned}
E(x) &= \sum_i \left[\frac{m}{2}\mathbf{v}_i^2 + \mathcal{E}(s_i, \overline{\mathcal{V}}_i)\right] + \sum_i \left[\frac{M}{2}\mathbf{V}_i^2 + \mathcal{E}^C(S_i)\right] \\
&+ \frac{1}{2}\sum_{ij} \phi^{\mathrm{CC}}(|\mathbf{R}_i - \mathbf{R}_j|) \\
S(x) &= \sum_i s_i + \sum_i S_i
\end{aligned}
$$

We follow the GENERIC route to construct a thermodynamically consistent model for colloids

# SPH model for colloidal suspensions

The final equations are

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = \sum_{j=N_C+1}^{N_T}\left(\mathbf{F}_{ij}^{\mathrm{FF}} + \boldsymbol{F}_{ij}^{\mathrm{FF}} + \tilde{\boldsymbol{F}}_{ij}^{\mathrm{FF}}\right) + \sum_{j=1}^{N_C}\left(\mathbf{F}_{ij}^{\mathrm{FC}} + \boldsymbol{F}_{ij}^{\mathrm{FC}} + \tilde{\boldsymbol{F}}_{ij}^{\mathrm{FC}}\right)$$

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T_i\dot{s}_i &= -\frac{1}{2}\sum_{j=N_C+1}^{N_T}\left(\boldsymbol{F}_{ij}^{\mathrm{FF}} + \tilde{\boldsymbol{F}}_{ij}^{\mathrm{FF}}\right)\cdot(\mathbf{v}_i - \mathbf{v}_j) - \frac{1}{2}\sum_{j=1}^{N_C}\left(\boldsymbol{F}_{ij}^{\mathrm{FC}} + \tilde{\boldsymbol{F}}_{ij}^{\mathrm{FC}}\right)\cdot(\mathbf{v}_i - \mathbf{V}_j) \\
&+ \sum_{j=N_C+1}^{N_T}\left(\mathcal{Q}_{ij}^{FF} + \tilde{\mathcal{Q}}_{ij}^{FF}\right) + \sum_{j=1}^{N_C}\left(\mathcal{Q}_{ij}^{FC} + \tilde{\mathcal{Q}}_{ij}^{FC}\right) \\
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T_i^C\dot{S}_i &= \sum_{j=N_C+1}^{N_T}\left(\mathcal{Q}_{ij}^{CF} + \tilde{\mathcal{Q}}_{ij}^{CF}\right) - \frac{1}{2}\sum_{j=N_C+1}^{N_T}\left(\boldsymbol{F}_{ij}^{\mathrm{CF}} + \tilde{\boldsymbol{F}}_{ij}^{\mathrm{CF}}\right)\cdot(\mathbf{V}_i - \mathbf{v}_j)
\end{aligned}
$$

## *Units and scales*

The basic units we chose are

$$\rho_F = 1 \qquad T_F = 1 \qquad R_C = 1 \qquad V_C = \sqrt{\frac{k_B T_F}{M_C}} = 1$$

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In these units, the crucial parameters are

$$\begin{aligned} c^* &= \frac{c_0}{V_C} = \frac{1}{\mathrm{Ma}} \\ \eta^* &= \frac{\eta}{\rho_F V_C R_C} = \frac{1}{\mathrm{Re}} \end{aligned}$$

## Units and scales

For water, $c = 1500$m/s and $\nu = 10^{-6}\mathrm{m}^2/\mathrm{s}$.

| $R_C$ | $V_T$ | $c^*$ | $\eta^*$ |
|---|---|---|---|
| $10^{-6}$m | $10^{-3}$m/s | $10^6$ | $10^3$ |
| $10^{-8}$m | 1 m/s | $10^3$ | 1 |
| $10^{-9}$m | 31m/s | 31 | 0.03 |

I will be presenting results at $c^* = 60$, $\eta^* = 1$

## *Brownian motion?*

Brownian motion of single colloidal particle in a periodic box.

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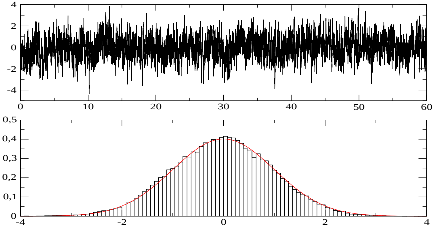


$$\langle V^2 \rangle = \frac{k_B T_F}{M_C} = 0.998$$

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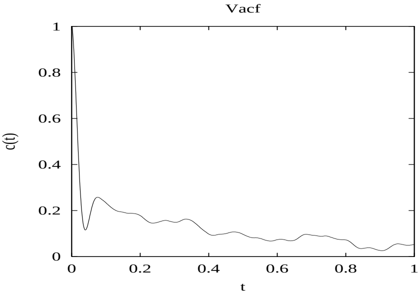
$$c(t) = \langle V V(t) \rangle$$



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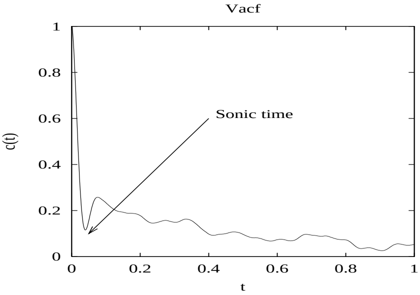

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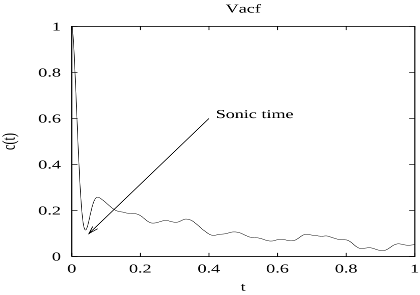


Wouldn't we expect exponential decay??

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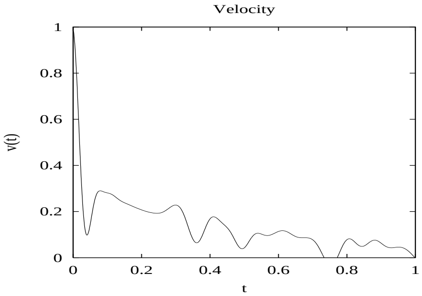

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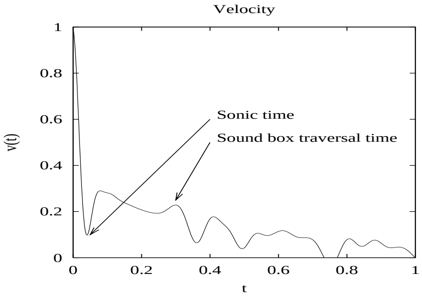

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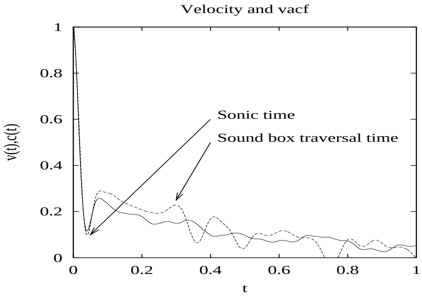

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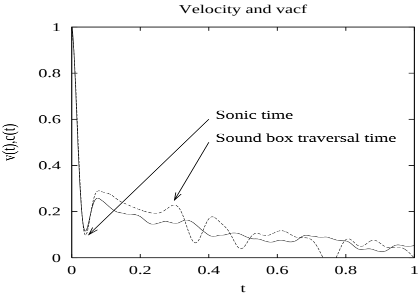


$$\frac{\langle VV(t)\rangle}{\langle V^2\rangle} = \frac{V(t)}{V(0)}$$

Onsager regression of fluctuations hypothesis is fullfilled.

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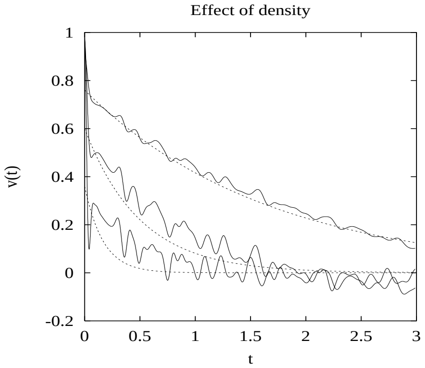

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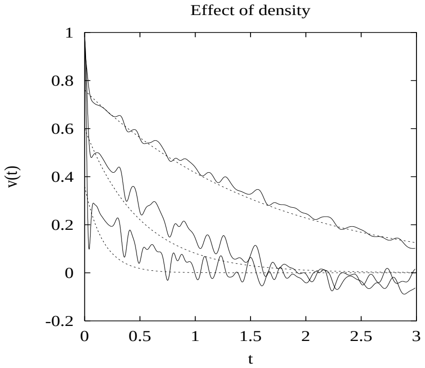


- The dashed line is $V_0 \exp\{-t/\tau_B\}$ with $\tau_B = \frac{M_C}{6\pi\eta R_C}$

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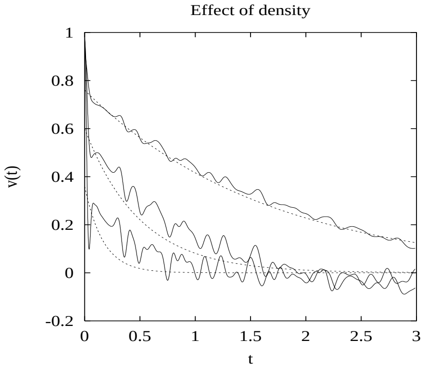


- The dashed line is $V_0 \exp\{-t/\tau_B\}$ with $\tau_B = \frac{M_C}{6\pi\eta R_C}$
- As $M_C \to \infty$ the decay is exponential, agreeing with Langevin.

# *Conclusions*

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# *Conclusions*

- We have shown how thermal noise can be introduced in SPH in a thermodynamically consistent way.
- We have constructed a model of colloidal particles.
- Preliminary basic test show that the simulation model works.

## *For the future*

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- Non-isothermal effects in Brownian motion.