Voronoi fluid particles

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Lorentz Center, March 9th, 2006

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Introduction

- Physicist view of fluid modelling.

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- The Voronoi tessellation is a natural framework for the construction of fluid particle models.

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- The Voronoi tessellation is a natural framework for the construction of fluid particle models.
- Discrete differential operators naturally emerge.

Continuum hydrodynamic equations

Inviscid Euler equations (reversible)

$$\begin{aligned}
\partial_t \rho &= -\nabla \rho \mathbf{v} \\
\partial_t \rho \mathbf{v} &= -\nabla \rho \mathbf{v}\mathbf{v} - \nabla P \\
\partial_t s &= -\nabla s \mathbf{v}
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Eulerian point of view.

Continuum hydrodynamic equations

Lagrangian coordinates are the solution of

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

with initial condition

$$\mathbf{R}(\mathbf{r}, 0) = \mathbf{r}$$

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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 $\mathbf{v}(\mathbf{r},t)$.

Continuum hydrodynamic equations

Introduce extensive 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.

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In terms of these extensive fields Euler's equations become

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\qquad \Longrightarrow \qquad
\begin{aligned}
\frac{d}{dt}\mathbf{R} &= \mathbf{v} \\
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Remarkably simple!! Suggests the concept of fluid particle.

Fluid particle dynamics

We divide the fluid in N portions. A fluid particle is a small moving thermodynamic subsystem of the whole system characterised by

$$\mathbf{R}_i, \mathbf{V}_i, \mathcal{V}_i, m_i, S_i, \mathcal{E}_i \quad i = 1, \ldots, N$$

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The independent variables are $x = \{\mathbf{R}_i, \mathbf{V}_i, S_i\}$ because

$$\begin{aligned} M_i &= \text{ctn.} \\ \mathcal{V}_i &= \mathcal{V}_i(\mathbf{R}_1, \cdots, \mathbf{R}_N) \qquad \text{geometry} \\ \mathcal{E}_i &= \mathcal{E}(\mathcal{V}_i, S_i, m_i) \qquad \text{thermodynamics (ideal gas)} \end{aligned}$$

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How to formulate the dynamics for $x = \{\mathbf{R}_i, \mathbf{V}_i, S_i\}$?

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Impose conservation of total energy

$$E = \sum_i \left[\frac{M_i}{2} \mathbf{V}_i^2 + \mathcal{E}(M_i, S_i, \mathcal{V}_i) \right].$$

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

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$$\begin{aligned} M_i \dot{\mathbf{V}}_i &= -\sum_j \frac{\partial \mathcal{E}}{\partial \mathbf{R}_i} = \sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} P_j \\ P_i &\equiv -\frac{\partial \mathcal{E}_i}{\partial \mathcal{V}_i} \qquad \text{Pressure} \end{aligned}$$

The discrete model

$$\begin{aligned} \frac{d}{dt}\mathbf{R} &= \mathbf{v} \\ \frac{d}{dt}M &= 0 \\ \frac{d}{dt}\mathbf{P} &= -\mathcal{V}\nabla P \\ \frac{d}{dt}S &= 0 \end{aligned}$$

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

Symmetries

Any reasonable definition of the volume should be invariant under translations and rotations

$$\begin{aligned}\mathcal{V}_i(\mathbf{R}_1,\cdots,\mathbf{R}_N) &= \mathcal{V}_i(\mathbf{R}_1+\mathbf{a},\cdots,\mathbf{R}_N+\mathbf{a}),\\ \mathcal{V}_i(\mathbf{R}_1,\cdots,\mathbf{R}_N) &= \mathcal{V}_i(\mathbf{\Lambda}\mathbf{R}_1,\cdots,\mathbf{\Lambda}\mathbf{R}_N),\end{aligned}$$

Take derivatives with respect to $\mathbf{a}$ and $\mathbf{\Lambda}$ to obtain

$$\sum_i \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} = 0, \qquad \sum_i \mathbf{R}_i \times \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} = 0.$$

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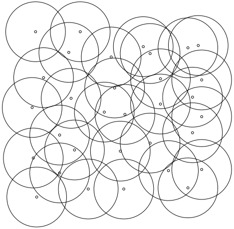
These identities ensure that the discrete equations conserve

$$\begin{aligned}\mathbf{P} &= \sum_i \mathbf{P}_i\\ \mathbf{L} &= \sum_i \mathbf{R}_i \times \mathbf{P}_i\end{aligned}$$

How to define the volume?

We have two possibilities:

SPH



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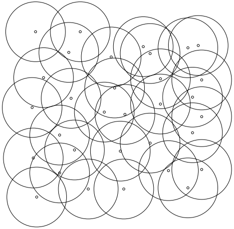
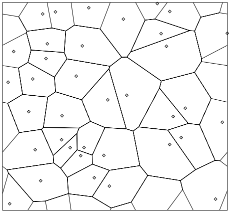


Voronoi tessellation



The Voronoi volume

Consider the Shepard function (Flekkoy-Coveney)

$$\chi_i(\mathbf{r}) = \frac{\Delta(\mathbf{r}-\mathbf{R}_i)}{\sum_j \Delta(\mathbf{r}-\mathbf{R}_j)} \qquad \Delta(\mathbf{r}) = \exp\{-\mathbf{r}^2/\sigma^2\}$$

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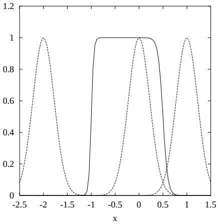

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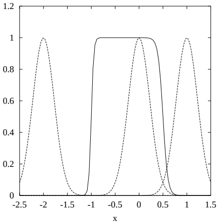

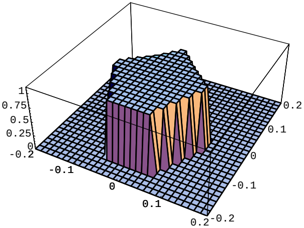

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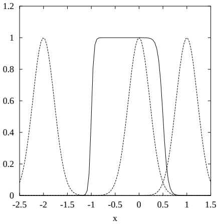

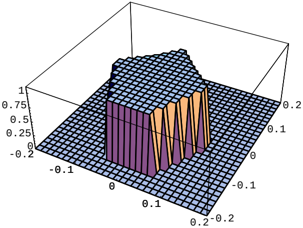

The Voronoi volume is

$$\mathcal{V}_i = \lim_{\sigma\to 0}\int d\mathbf{r}\chi_i(\mathbf{r}) = \lim_{\sigma\to 0}\int d\mathbf{r}\frac{\Delta(\mathbf{r}-\mathbf{R}_i)}{\sum_j \Delta(\mathbf{r}-\mathbf{R}_j)}$$

It satisfies $\sum_i \mathcal{V}_i = \mathcal{V}_T$.

The Voronoi volume

The analytical form of the volume allows to easily compute the derivative of this volume wrt $\mathbf{R}_i$

$$\frac{\partial \mathcal{V}_i}{\partial \mathbf{R}_j} = -A_{ij}\left[\frac{\mathbf{e}_{ij}}{2} - \frac{\mathbf{c}_{ij}}{R_{ij}}\right] \quad \text{for } i \neq j$$

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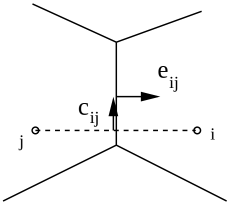

$$M_i \dot{\mathbf{V}}_i = \sum_j A_{ij}\left[\mathbf{e}_{ij} - \frac{\mathbf{c}_{ij}}{R_{ij}}\right](P_i - P_j)$$

Linear consistency

We can prove the following interesting properties for an arbitrary Voronoi tessellation

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Assume a linear pressure field $P_i = P_0 + \mathbf{b}\cdot\mathbf{R}_i$. In this case

$$M_i\dot{\mathbf{V}}_i = \sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i}P_j = -\mathcal{V}_i\mathbf{b} = -\mathcal{V}_i(\mathrm{grad}\ P)_i$$

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Therefore, we have a discrete version of the gradient operator on arbitrary Voronoi meshes!!

Linear consistency

The error for the gradient of $f(\mathbf{r})$ as a function of the resolution

$$\frac{1}{N}\sum_i \left| -\frac{1}{\mathcal{V}_i}\sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{r}_i} f(\mathbf{r}_j) - \nabla f(\mathbf{r}_i) \right|$$

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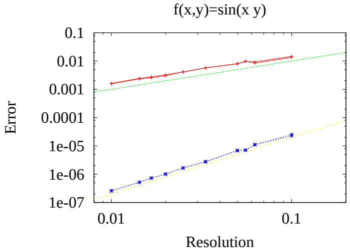

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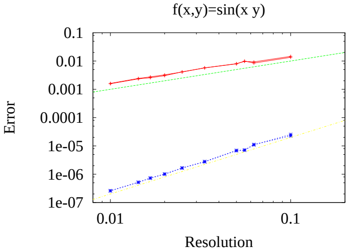


The error scales as λ^{-1} in a random mesh and as λ^{-2} in a regular mesh.

Summary of the inviscid discrete model

$$\begin{aligned}
\dot{\mathbf{R}}_i &= \mathbf{v}_i \\
\dot{M}_i &= 0 \\
\dot{\mathbf{P}}_i &= \sum_j \frac{\partial \mathcal{V}_j}{\partial \mathbf{R}_i} P_j \\
\dot{S}_i &= 0
\end{aligned}$$

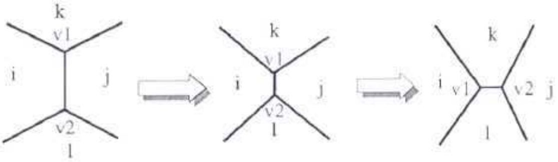
Conserve mass, linear and angular momentum, and energy.

If the flow field is smooth, they converge to Euler equations.

Can be understood as a MD with a many-body potential of interaction.

Computational issues

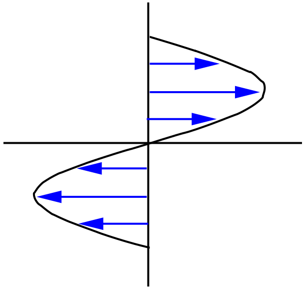
Moving mesh $\rightarrow$ recombination



Yuan X.-F. et al 1993, Albers et al 1998

Shear wave

2D Periodic boundary conditions



movie1.gif

movie2.gif

Shear wave

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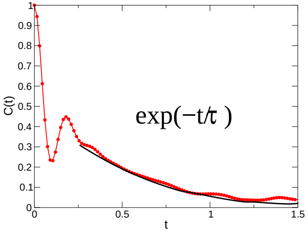
Does the equilibrium state resembles stationary homogeneous turbulence?

Velocity autocorrelation



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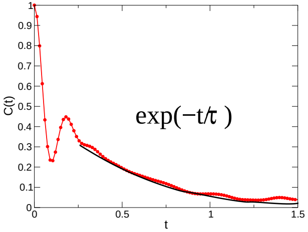
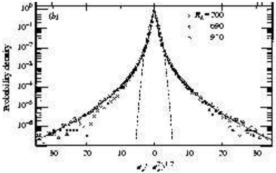


Two time scales:

- Sonic: $\tau_c = \lambda / c$
- Kinetic: $\tau_k = \lambda / v_{\text{thermal}}$

Distribution of accelerations



Mordant et al PRL **87**, 214501 (2001)

Highly non-Gaussian!!

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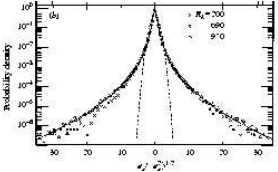

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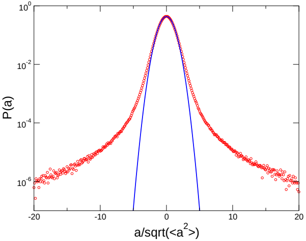

Voronoi Euler model
(non-Gaussian)

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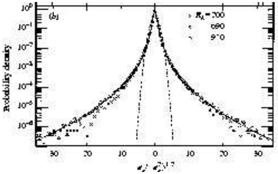

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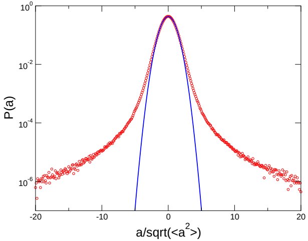
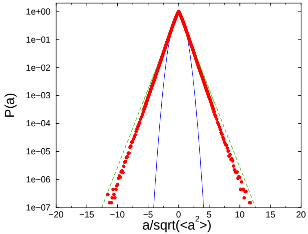


Voronoi Euler model
(non-Gaussian)



Lennard-Jones MD
(exponential)

Conclusion

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