Voronoi Fluid Particle Dynamics

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Fluid Dynamics

- a very classical theory
- Some names:
  - Bernoullis (Johann, Daniel)
  - Gauss
  - Stokes
  - Euler
  - Lagrange

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  - Lorentz! From `wikipedia`: *In the years 1918-1926, at the request of the Dutch government, Lorentz headed a committee to calculate some of the effects of the proposed Afsluitdijk (Closure Dike) flood control dam on other seaworks in the Netherlands. . . . Lorentz proposed to start from the basic hydrodynamic equations of motion and solve the problem numerically. . . . One of the two sets of locks in the Afsluitdijk was named after him.*

The Laws of Fluid Dynamics

Continuity (aka, matter or charge conservation):

$$\frac{\partial \rho}{\partial t} = -\operatorname{div} \rho \mathbf{v}$$

Notation

$$\operatorname{div} \mathbf{v} \equiv \nabla \cdot \mathbf{v} = \sum_{\alpha=1,2,3} \frac{\partial v_\alpha}{\partial x_\alpha}$$

$$\operatorname{grad} p \equiv \nabla p; \quad (\operatorname{grad} p)_\alpha = \frac{\partial p}{\partial x_\alpha}$$

$$\nabla^2 \mathbf{v} \equiv \Delta \mathbf{v}; \quad (\nabla^2 \mathbf{v})_\alpha = \sum_{\beta=1,2,3} \frac{\partial^2 v_\alpha}{\partial x_\beta^2}$$

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Laws: Navier-Stokes equations

Continuity:

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Momentum density ρv_α, for each coordinate $\alpha = 1, 2, 3$:

$$\frac{\partial \rho v_\alpha}{\partial t} = -\,\mathrm{div}\,\rho v_\alpha \mathbf{v} - \frac{\partial p}{\partial x_\alpha} + \eta \nabla^2 v_\alpha + \frac{\eta}{3} \frac{\partial}{\partial x_\alpha} \mathrm{div}\,\mathbf{v}$$

Entropy density s (this, we will largely neglect today):

$$\frac{\partial s}{\partial t} = -\,\mathrm{div}\,s\mathbf{v} + 2\eta \overline{\nabla \mathbf{v}} : \overline{\nabla \mathbf{v}} + \kappa \nabla^2 T$$

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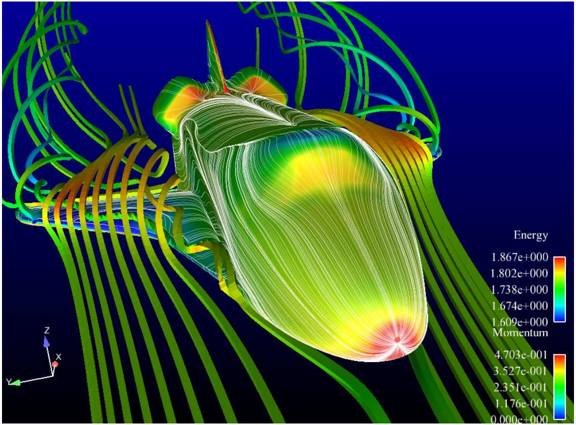
Computational FD

CFD: The hard task of computing numerical solutions to these *non-linear* equations.



From EnSight

Euler's view

Use a grid, and finite differences (or finite elements) for equations that are written in this "frame". E.g., Continuity:

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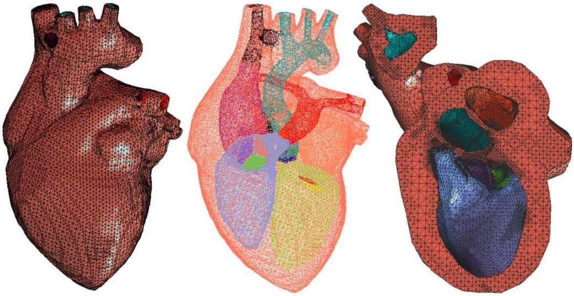

FEM mesh of human heart (Zhang et al. 2004)

Limitations of fixed meshes

Problems arise in many situations.

- When one does not know in advance where more effort (CPU and RAM) will be needed (turbulence, astrophysics. . .)
- When the boundary is also moving, "free boundary problems". E.g. surface waves (what people call "waves"!).

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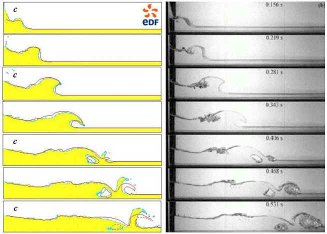

Gate opening in a tank with a wet bed (SPHERIC test case)
SPH (Spartacus-2D, EDF R&D) vs experiments (Janosi *et al.*, 2004)

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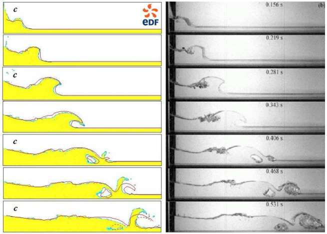

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This calls for a *Lagrangian* approach, and computational methods that will be either *meshless* or have a *moving mesh*.

Lagrange's view

E.g., continuity:

$$\frac{\partial \rho}{\partial t} = -\,\mathrm{div}\,\rho\mathbf{v}$$

means

$$\frac{\partial \rho}{\partial t} + (\mathbf{v}\nabla)\rho = -\rho\,\mathrm{div}\,\mathbf{v}$$

. . . but this is

$$\frac{D\rho}{Dt} = -\rho\,\mathrm{div}\,\mathbf{v},$$

where D/Dt is the substantive derivative: how things change as they flow!

Notation: $D\rho/Dt \equiv d\rho/dt \equiv \dot{\rho}$

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Lagrangian coordinates

They are defined by *pathlines*:

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

with initial condition $\mathbf{R}(t=0)=\mathbf{r}$.

As a valid transformation, it has a Jacobian J, which can be shown to satisfy

$$\frac{DJ}{Dt} = J \operatorname{div} \mathbf{v}.$$

So, it looks like an infinitesimal *volume* that is carried by the flow (e.g., this would be the equation for $v = 1/\rho$).

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Equations in Lagrangian coordinates

Since it looks like a volume, lets call it so: $V = J$. We may introduce extensive particle

- mass $M = \rho V$
- momentum $\mathbf{P} = \rho \mathbf{v} V$
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The resulting equations are

	$$\frac{\partial \mathbf{R}}{\partial t} = \mathbf{v}$$
$$\frac{\partial \rho}{\partial t} = -\operatorname{div} \rho \mathbf{v}$$	$$\frac{DM}{Dt} = 0$$
$$\frac{\partial v_\alpha}{\partial t} = -\operatorname{div} \rho v_\alpha \mathbf{v} - \frac{\partial p}{\partial x_\alpha} + \eta \ldots$$	$$\frac{1}{V}\frac{DP_\alpha}{Dt} = -\frac{\partial p}{\partial x_\alpha} + \eta \ldots$$
$$\frac{\partial s}{\partial t} = -\operatorname{div} s\mathbf{v} + \eta \ldots$$	$$\frac{1}{V}\frac{DS}{Dt} = 0 + \eta \ldots$$

Other forms for the momentum eq.

These will be important later

$$\frac{1}{V}\frac{DP_\alpha}{Dt} = -\frac{\partial p}{\partial x_\alpha} + \eta\nabla^2 v_\alpha + \frac{\eta}{3}\frac{\partial}{\partial x_\alpha}\operatorname{div}\mathbf{v}$$

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With vectors,

$$\frac{1}{V}\frac{D\mathbf{P}}{Dt} = -\operatorname{grad} p + \eta \operatorname{Div} \sigma,$$

Just remember: there is a grad involved in the reversible part, and a Div in the irreversible (viscous) part.

Also, for weak compressions this may suffice:

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Fluid particles

Recall the Lagrangian approach, without a fixed mesh.

- The fluid is described by a set of moving nodes moving according to the velocity field (*convection* is very well described).
- Physically, these are *fluid particles*, a classic concept
- Particles are small subsystems that are, nevertheless large for thermodynamics. (No "particle physics"!).
- If they are quite small ($\sim$ 100 molecules), thermal fluctuations can (and should) be included

H Babinsky

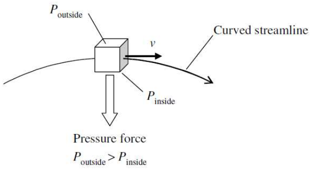

Figure 7. Fluid particle travelling along a curved streamline.

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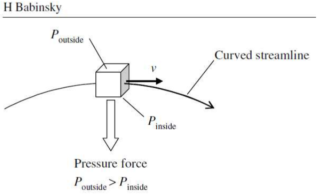

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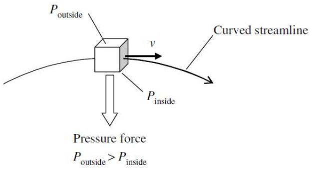

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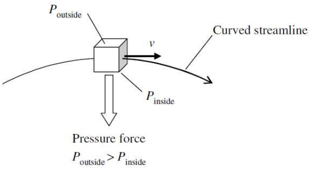

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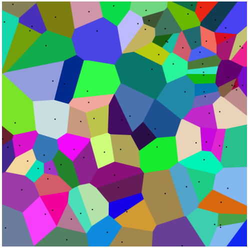
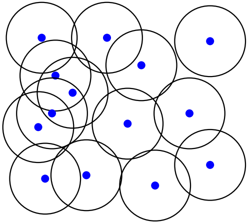
Computational particles

Given a set of point, what are the corresponding fluid particle?

Two methods have been proposed



Voronoi



SPH

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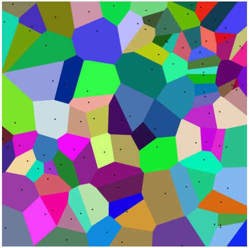

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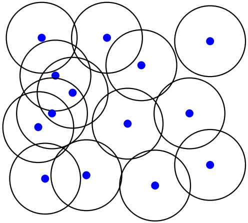


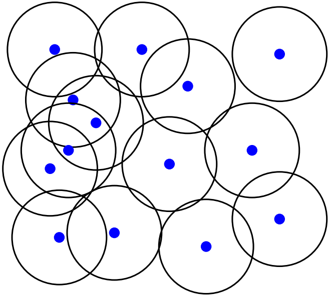
SPH

Smoothed particle hydrodynamics

Rather well established method that does not use any meshes.

Particles are "smooth", since their properties depend on all other within the range (support) of a weight function.

For example, the density of a particle depends on its "neighbours" (the more, the denser), and the volume is its inverse (the more, the smaller).



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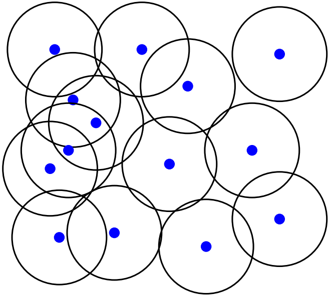

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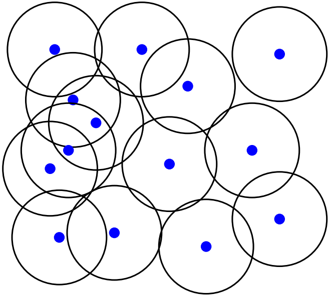
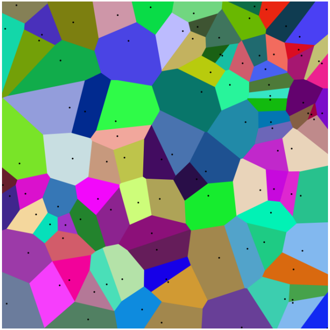


Voronoi particles

The volume of a particle, V_i, is the one of its Voronoi cell.

The Delaunay triangulation is its dual — the particles are the vertices.

This way, “neighbours” are perfectly defined.



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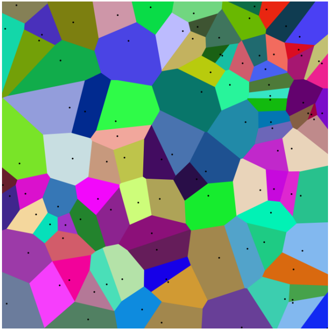

The first equations of motion are easy enough:

$$\frac{\partial \mathbf{R}}{\partial t} = \mathbf{v} \qquad \Rightarrow \qquad \dot{\mathbf{R}}_i = \mathbf{v}_i$$

$$\frac{DM}{Dt} = 0 \qquad \Rightarrow \qquad \dot{M}_i = 0$$

But: the rest involve (many!) space derivative operators: grad p, Div σ ...

$$\frac{1}{V}\frac{D\mathbf{P}}{Dt} = -\operatorname{grad} p + \operatorname{Div}\sigma \qquad \Rightarrow \qquad \frac{1}{V_i}\dot{\mathbf{P}}_i = -(\operatorname{grad} p)_i + (\operatorname{Div}\sigma)_i$$

The main task:

To find expressions for each of these, at particle i, in a "Voronoi discrete vector calculus"! (or, "Delaunay DVC").

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The divergence

Recall the equation for the particle volume (aka Jacobian):

$$\frac{DV}{Dt} \equiv \dot{V} = V \,\mathrm{div}\, \mathbf{v}.$$

Translated to particles:

$$\dot{V}_i = V_i (\mathrm{div}\, \mathbf{v})_i$$

But, the chain rule tells us

$$\dot{V}_i = \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \dot{\mathbf{R}}_j = \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \mathbf{v}_j.$$

Comparing the two:

$$(\mathrm{div}\, \mathbf{v})_i \doteq \frac{1}{V_i} \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \mathbf{v}_j.$$

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$$\dot{V}_i = \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \dot{\mathbf{R}}_j = \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \mathbf{v}_j.$$

Comparing the two:

$$(\operatorname{div} \mathbf{v})_i \doteq \frac{1}{V_i} \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \mathbf{v}_j.$$

(Note: it's actually Div, but it has the same expression.)

The divergence

Recall the equation for the particle volume (aka Jacobian):

$$\frac{DV}{Dt} \equiv \dot{V} = V \operatorname{div} \mathbf{v}.$$

Translated to particles:

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Changes in a Voronoi cell

What is the change of V_i w.r.t. $\mathbf{R}_j$? It can be shown that

$$\frac{\partial V_i}{\partial \mathbf{R}_j} = A_{ij} \left(\frac{\mathbf{u}_{ij}}{2} - \frac{\mathbf{c}_{ij}}{R_{ij}} \right) .$$

- A_{ij} is the area of the facet between i and j
- $\mathbf{u}_{ij}$ is the unit vector from i to j
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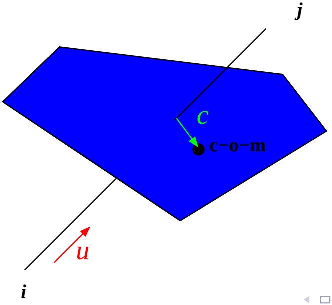

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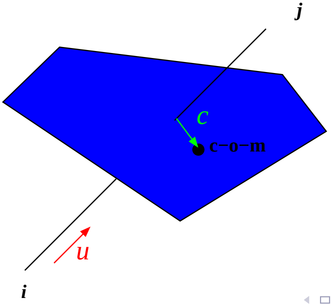

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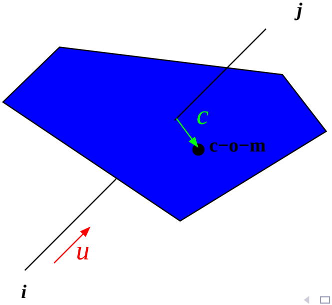

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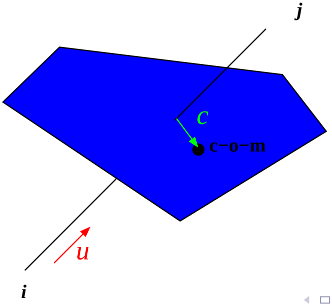
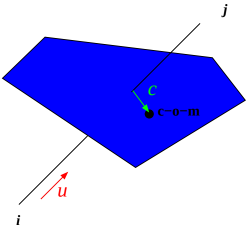


The divergence

We may therefore write:

$$(\operatorname{div} \mathbf{v})_i = \frac{1}{V_i} \sum_{j \neq 1} A_{ij} \left[\frac{\mathbf{u}_{ij}}{2} - \frac{\mathbf{c}_{ij}}{R_{ij}} \right] \cdot (\mathbf{v}_j - \mathbf{v}_i) \,,$$

which "looks" very nice indeed.



Expression for the gradient

This is a bit harder. We may begin with the total internal energy

$$E = \sum_i \frac{1}{2} M_i v_i^2 + \epsilon(\{V_i\}).$$

Let's make sure it does not change:

$$\dot{E} = \sum_i \left(M_i \mathbf{v}_i \dot{\mathbf{v}}_i - p_i \dot{V}_i \right) = 0.$$

(Yes, the pressure $p_i = -\partial\epsilon/\partial V_i$.)
We saw before

$$\dot{V}_i = \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \mathbf{v}_j.$$

Therefore

$$\dot{E} = \sum_i M_i \mathbf{v}_i \dot{\mathbf{v}}_i - \sum_i p_i \sum_j \frac{\partial V_i}{\partial \mathbf{R}_j} \mathbf{v}_j = 0.$$

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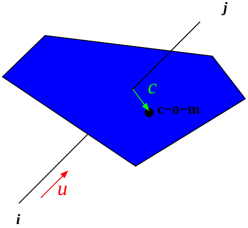
The gradient

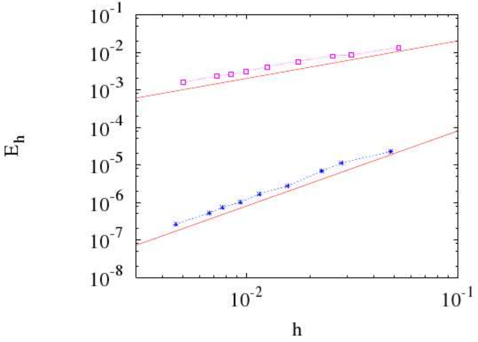
We may therefore write (after some tidying up):

$$(\mathrm{grad}\, p)_i = \frac{1}{V_i} \sum_{j \neq i} A_{ij} \left[\frac{\mathbf{u}_{ij}}{2} (p_i + p_j) - \frac{\mathbf{c}_{ij}}{R_{ij}} (p_i - p_j) \right].$$



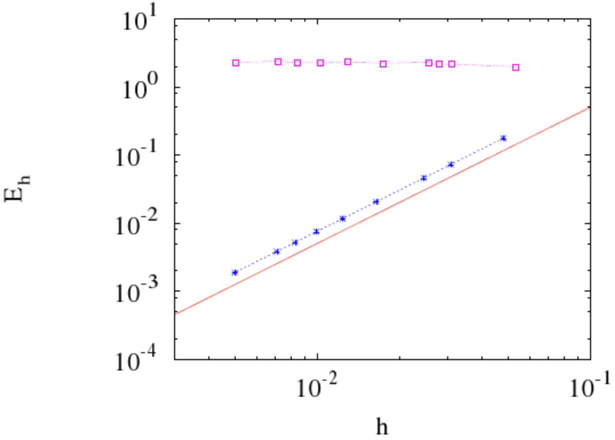
The gradient: good news

- $(\text{grad}\, p)_i = 0$ at all i if p is constant
- $(\text{grad}\, p)_i = \mathbf{a}$ at all i if $p = \mathbf{a} \cdot \mathbf{r}$: *linear fields have the right gradient*!
- The grad operator shows nice convergence, as h^2 for regular lattices, and h^1 for random meshes.



The divergence: bad news

Despite its nice appearance, this div operator convergences as h^1 for regular lattices, and h^0 for random meshes (not at all!).



The divergence issue

The div appears as soon as we include viscosity — we first have to evaluate the stress tensor σ:

$$\sigma_{\alpha\beta} = \left(\frac{\partial v_\alpha}{\partial x_\beta} + \frac{\partial v_\beta}{\partial x_\alpha} \right) - \frac{2}{3} \delta_{\alpha\beta} \operatorname{div} \mathbf{v}.$$

We can expect problems since the divergence of tensor σ appears:

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For small compression, we only need the Laplacian

$$\frac{1}{V}\frac{DP_\alpha}{Dt} = -\frac{\partial p}{\partial x_\alpha} + \eta \nabla^2 \mathbf{v}.$$

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Sure there is: the finite element method!

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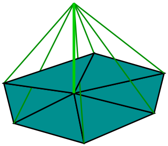
Finite elements

The Laplacian is *very* well studied in the FEM. The steps would be

1. From the existing Delaunay triangulation (which is actually very good for the FEM)
2. On each node i define a pyramid-like weight function Φ_i, with value 1 at the node, 0 at the neighbours, and constant slope in each incident face (triangle)
3. These elements discretize continuous fields:
$$\mathbf{v}_i = \frac{1}{\mathcal{V}_i} \int \Phi_i(\mathbf{r}) \mathbf{v}(\mathbf{r})$$
4. $\mathcal{V}_i$ is the integral of Φ_i. We term it the "Delaunay volume": $1/(D+1)$ of the sum of the areas of the incident triangles



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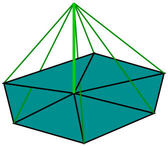

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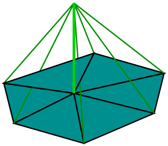

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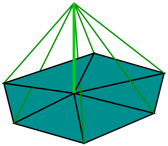

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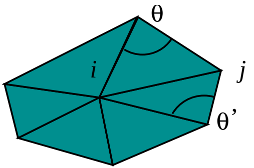
The integral may be evaluated for each pair of nodes. In 1D, one gets the well-known $x_{i-1} + x_{i+1} - 2x_i$. In 2D:

$$\Delta_{ij} = \left(\cot\theta + \cot\theta'\right)/2,$$

the famous *cotangent formula* of the FEM! (FEM people: this would be a "lumped mass" approximation).



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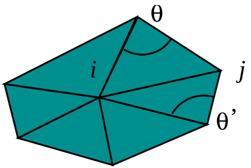

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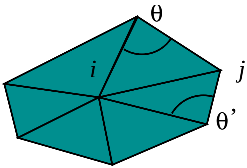

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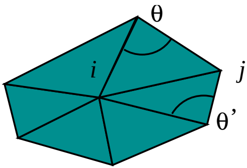

Simulation strategy

Our approach to hydrodynamics is then at two levels:

- For the reversible (Euler) part of the dynamics, just use Voronoi concepts (Voronoi volume, formula for grad. . .)
- For the irreversible (viscous) part, use Delaunay concepts and a FEM expression for the Laplacian (optionally, other features).

Why not use the second approach everywhere?
Simply because the Delaunay volume makes sudden jumps on rearrangements. Not nice at all for the particle volume, tolerable for the force.
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  - the volumes V_i
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Simulation main loop

1. Create initial points, momenta, pressures
2. Build a Delaunay triangulation
3. Calculate info for vertices and edges
4. Apply changes in positions and momenta (Verlet algorithm, predictor-corrector. . .):

$$\dot{\mathbf{R}}_i = \mathbf{v}_i = \mathbf{P}_i / M_i$$

$$\frac{1}{V_i}\dot{\mathbf{P}}_i = -(\operatorname{div} p)_i + \eta(\nabla^2 \mathbf{v})_i .$$

Either:

1. just update all positions and go to 2, or
2. update positions one by one, restoring the Delaunay condition, and go to 3.

Simulation main loop

1. Create initial points, momenta, pressures
2. Build a Delaunay triangulation
3. Calculate info for vertices and edges
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Applications

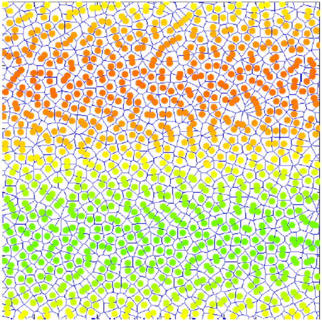
Standard hydrodynamic benchmarks: **Confined fluids**

- Couette flow
- Poiseuille
- Vortex spin-down
- Lamb-Oseen vortex

Applications

Not-so-standard benchmarks: **Periodic bc**

- Kolmogorov flow
- Taylor-Green flow



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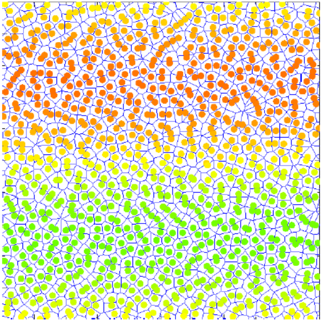

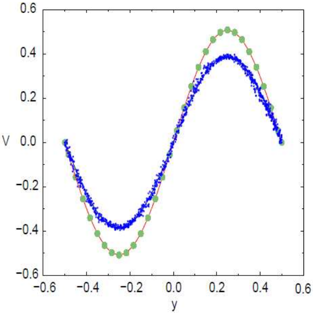

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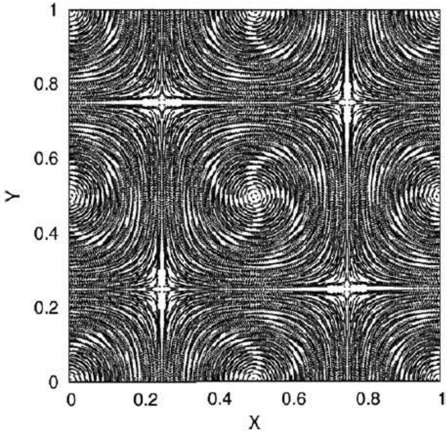

Applications

"Real" applications: **Free surfaces**

- Elliptical drops
- Dam breaking
- Sloshing

Beyond

Other ideas:

- "Delaunay particles" everywhere?
- Centroidal Voronoi tessellation
- Natural coordinates vs FEM interpolation
- Standard (Eulerian) FEM with free surface detection from α-shapes

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- **U. Oslo**: Eirik G Flekkøy

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- The kind audience

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Some references

- Pep Español and Ignacio Zúñiga, for the Delaunay volume and the Laplacian
- Pep Español and Mar Serrano, in "Tessellations in the Sciences Virtues, Techniques and Applications of Geometric Tilings", Eds: Rien van de Weijgaert, Gert Vegter, Jelle Ritzerveld, and Vincent Icke, Kluwer/Springer (2009)
- A good source is Pep Español's references webpage