Resent developments of particle-based methods for CFD, or can we get out of the morass?

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Oct 30, 2014 **Hokkaido Univ.**

Talk Structure

- SPH and its problems
- Contact discontinuity
- "Density-Independent" formulation
- Pseudo-Density formulation
- Weighted-Particle (or normalized weight) approach
- Weak form?
- Summary
- Something not so hopeless (if we have some time left)

SPH and its problems

Advantages of particle-based method for fluid

- **Naturally adaptive (particles moves to where the mass is there)**
- **Naturally gives Lagrange picture. Useful for low-temperature, high-speed objects**
- **Parallelization fairly easy**

However, there are quite a few problems...

An incomplete list of problems of SPH

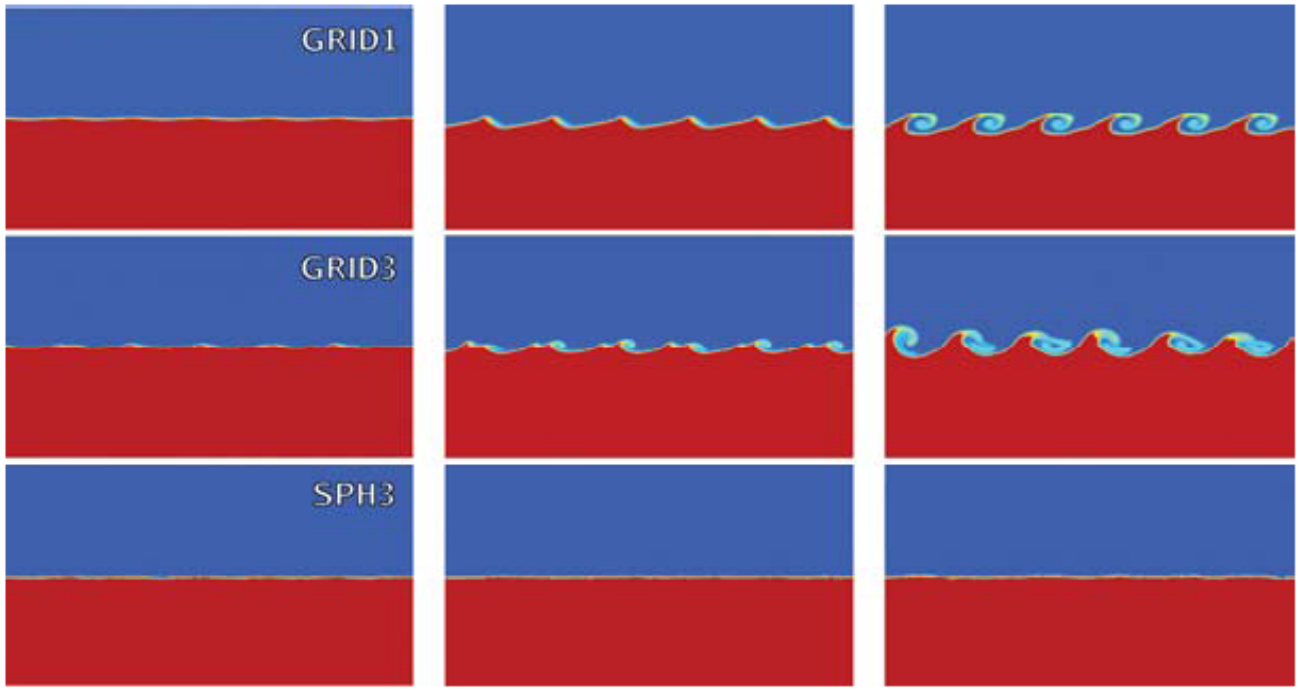
- Known practical problems
  - requires artificial viscosity, cannot easily be used with shock-capturing schemes (I'll not discuss this issue today)
  - cannot handle discontinuities well (contact discontinuity and free surface)
  - does something strange to shear flow (most notably Keplerian disk — the Imaeda problem
  - and more...
- Known theoretical problems
  - lacks "consistency" — does not converges to the original differential equation in the limit of $h \rightarrow 0$
  - I do not think you need more problems here...

SPH and Contact Discontinuity, KH instability

Agertz et al (MN 2007, 380, 963)

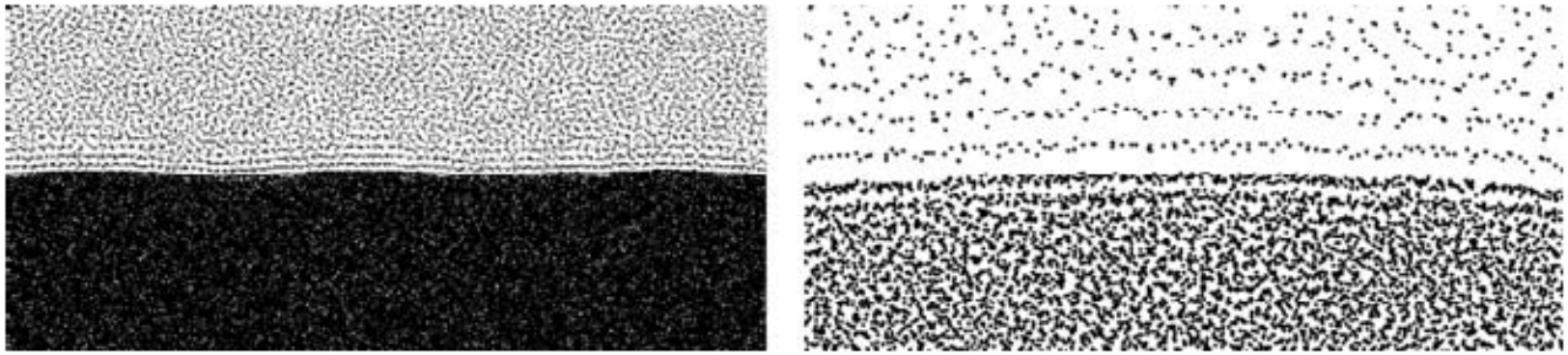
- **Kelvin-Helmholtz Instability is not correctly handled with SPH**
- **Something very bad is occuring at the boundary of two fluids.**
- **Is SPH usable?**

How different? (1)



SPH suppress KHI

How different? (2)



Strange-looking gap of particles at the two-fluid boundary.

Why does this happen?

Fundamental problem with SPH approximation

Density estimate

$$\rho(x) = \sum_j m_j W(x - x_j), \tag{1}$$

Gradient of a quantity f

$$\langle \nabla f \rangle(x) \sim \sum_j m_j \frac{f(x_j)}{\rho(x_j)} \nabla W(x - x_j). \tag{2}$$

ρ must be smooth and differentiable

Not satisfied at the contact discontinuity

Solution?

"Fundamental" reason

Smooth estimate of ρ contains $O(1)$ error at CD.

We could solve the problem by smoothing real ρ.

- **Let u diffuse (artificial conductivity)**
- **Use density which is continuous at CD.**

Sort of working, but not a "true" solution.

Saitoh and Makino 2013: Basic idea

- In SPH, we use m/ρ as "volume element" for numerical integration over smoothing kernel

$$\langle f \rangle(x) = \sum_j \frac{m_j f(x_j)}{\rho(x_j)} W(x - x_j). \tag{3}$$

- We can use other forms of the volume element and derive a consistent set of SPH equations.

Density-Independent SPH

Use the density of the internal energy, instead of mass density, to calculate the volume element. Let U the internal energy of particle, and q its density. We have:

$$q = \sum_j U_j W(x - x_j). \tag{4}$$

We can derive the SPH equation of motion:

$$m_i \dot{v}_i = -\sum_j (\gamma - 1) U_i U_j \left(\frac{1}{q_i} + \frac{1}{q_j} \right) \nabla W(x_i - x_j). \tag{5}$$

- **RHS does not depend on mass – DISPH**
- **This form is symmetric (between i and j particles)**
- **Actual form same as Ritchie and Thomas 2001**

Examples

Standard SPH1

New SPH1

Standard SPH2

New SPH2

Is this the ultimate solution?

- Certainly not.
- Not well behaved at very strong shocks
- Breaks down at liquid surface (near-zero pressure)
- Pressure is continuous, but not always (or almost always not) differentiable at CD. Thus, the estimate for pressure gradient can still contain very large error

Somewhat better treatment for strong shocks

We can use, instead of p, an arbitrary function of p to obtain the volume element. Assume y is a monotonic and differentiable function of p, and Let $Z = yV$, where V is volume.

After some mathematics we have:

Energy equation:

$$\dot{U}_i = \sum_j \frac{p_i Z_i Z_j}{y_i y_j}(v_i - v_j)\nabla W(x_i - x_j). \qquad (6)$$

Equation of motion:

$$m_i \dot{v}_i = -\sum_j \frac{Z_i Z_j}{y_i y_j}(p_i + p_j)\nabla W(x_i - x_j). \qquad (7)$$

How can we calculate y and Z?

What we know is the internal energy U (or entropy if you like that).

For given U, Z is a function of y, through EOS. Therefore

$$y = \sum_j Z_j W(x - x_j). \tag{8}$$

gives implicit equation for y and Z, which we can solve with (under-) relaxation method.

This method works better than the original DISPH

An even better volume element?

One way to define the "volume" of a particle, V_i, in the context of SPH is to use the following implicit equation:

$$\sum_j V_j W(x_i - x_j) = 1. \tag{9}$$

Equation of motion:

$$m_i \dot{v}_i = -\sum_j V_i V_j (p_i + p_j) \nabla W(x_i - x_j). \tag{10}$$

Time evolution of V_i:

$$\dot{V}_i = -V_i \sum_j V_j (v_i - v_j) \nabla W(x_i - x_j). \tag{11}$$

Eq. (12) is implicit, but Eq. (11) is explicit. We do not need to solve the implicit equation during the time integration.

Doesn't this sound good?

Does this actually work?

Short answer — NO

Why not?

This equation

$$\sum_j V_j W(x_i - x_j) = 1. \tag{12}$$

is ill-conditioned, if the Fourier transform of W contains any zero.

Proof: Wave of that wavenumber gives zero to LHS.

One could use kernels that does not contain zeros, but if the distribution of particles is irregular, the resulted equation is still ill-conditioned.

A practical solution for this problem

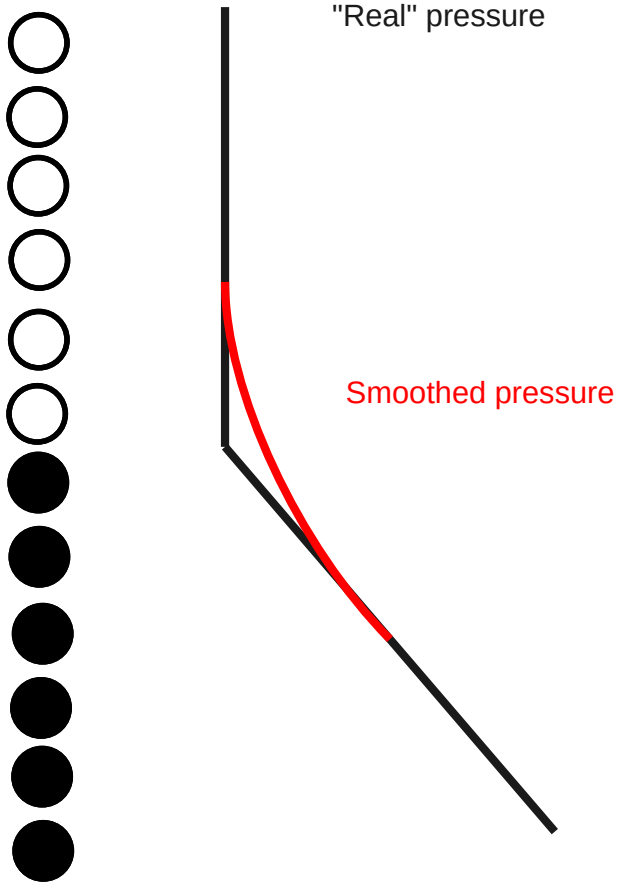
- Introduce a dummy quantity Z and its density y. Here y is not a function of p
- Let Z and y evolve in the same way as the mass and mass density, but add artificial diffusion term.
- We can guarantee that y is smooth everywhere, without introducing any artificial diffusion to physical quantities, unlike the artificial conductivity
- "Smoothed Pseudo-Density" SPH, or SPSPH

To my big surprize, this scheme actually works extremely well.

So, now, have we finally got the ultimate solution?

- Well, we thought so.
- However, as we mentioned some time ago, the discontinuity of pressure gradient still is still problematic.

Thought experiment: air on water



- DISPH assumes the pressure and pressure gradient are continuous
- SPSPH just smooths pressure
- In both cases, large error appears at CD

What do you do with grid schemes?

- **The honest (or the only believable) approach: track the boundary.**
- **Place constraint to the value of the pressure at CD. Use the difference schemes which do not cross CD.**

Can we do something similar with SPH? Sounds unlikely...

Maybe we should forget about SPH?

- There are many ways to express fluid by particles
- SPH is just one of them. There are several new methods which might be better
- In particular, most of new methods are at least consistent, and can be extended to handle discontinuity.

Inconsistency of SPH

We mean, by "consistency", that the numerical scheme converges to the original differential equation in the limit of $h \to 0$.

A necessary condition for the consistency: The estimate for the gradient converges to the true gradient.

SPH gradient estimator

$$\langle \nabla f \rangle(x) \sim \sum_j m_j \frac{f(x_j)}{\rho(x_j)} \nabla W(x - x_j). \tag{13}$$

can always contain $O(1)$ error, unless we do not take the limit of the infinite number of neighbors

Can we construct a consistent gradient estimator?

Yes, but

- We need a completely different mathematical framework
- Some of good properties (or what we believe so) might be lost

Or not?

Hopkins 2014

Or Gaburov and Nitadori 2011, or Lanson and Vila 2008a, 2008b

Use the following volume element for particle i, at any position:

$$\psi_i(\mathrm{x}) = \frac{1}{\omega(\mathrm{x})} W(\mathrm{x} - \mathrm{x}_i, h(\mathrm{x})) \tag{14}$$

$$\omega(\mathrm{x}) = \sum_j W(\mathrm{x} - \mathrm{x}_j, h(\mathrm{x})) \tag{15}$$

With these equations, the estimate of a function f at position x is

$$< f >= \sum_i f(\mathrm{x}_i)\psi_i(\mathrm{x}) \tag{16}$$

Important property:

$$\sum_i \psi_i(\mathrm{x}) = 1 \tag{17}$$

Consistency

The property:

$$\sum_i \psi_i(\mathbf{x}) = 1 \tag{18}$$

gives the consistency.

At least, $< f >(\mathbf{x}_i + \delta\mathbf{x})$ converges to $f(\mathbf{x}_i)$, when we let both h and average distance to near neighbors in the same way.

Hopkins 2014 — continued

- The way H14 derives the discretized equation is quite different from the standard way to derive it through FEM-like Galerkin method.
- In the Galerkin method, the weak form is constructed, using the "shape function" $\psi_i(\mathrm{x})$ (and its spatial derivative) as the test function.
- With the weak form, we do not have to obtain the spatial derivative of the solution, since we eliminate it through partial integration.
- In Hopkins 2014, the second-order-accurate spatial derivative operator is applied to the solution itself, effectively going back to the strong form.

What is achieved by H14?

Achieved:

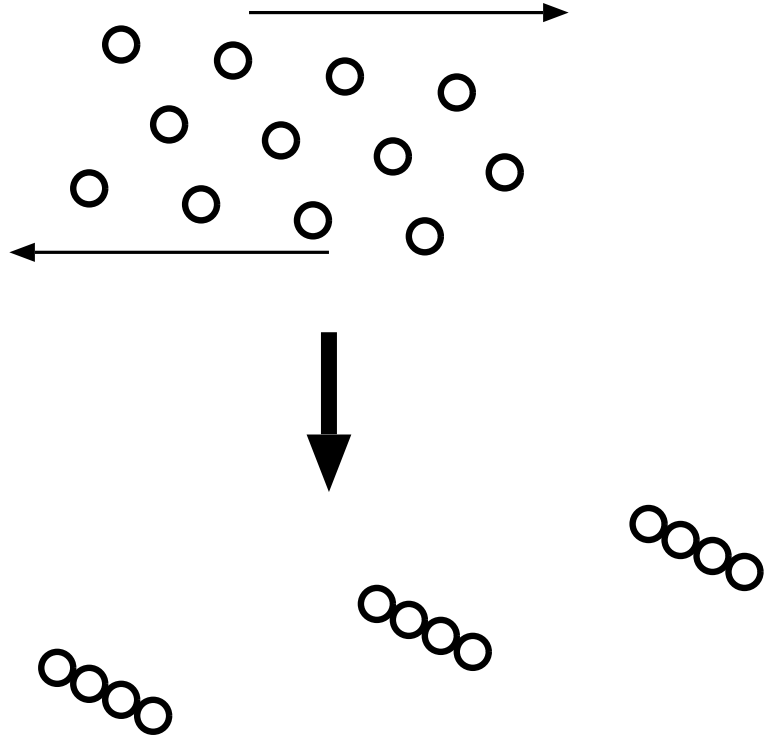
- **Consistency**
- **"reduced" particle noise (not eliminated)**

Not achieved:

- **Sound treatment of free surface or CD**
- **Solution to the "Imaeda" problem**

Imaeda problem

- Particle distribution of SPH: not completely regular
- If one applies shear or differential rotation, one eventually see Poisson noise.
- Something worse can appear in the intermediate stage



Zero-pressure fluid cannot be solved by a fully-Lagrangean scheme

How about more usual Galerkin method?

Consider EFGM (Element-free Galerkin Method)

Some basics:

- **Assume that points in space x have the values of some function u**
- **Use local polynomial basis function $(1, x, y, x^2, xy, y^2, x^3, ...)$**
- **Conceptually, for any point in space, construct the "approximation" by the weighted least square fitting of the polynomial basis, with the weight function with compact support.**
- **The shape function for point i is implicitly defined as the weight which appear in the above approximation**

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Er, sorry, what is "shape function"?

Weak form and Galerkin Method

Assume we want to solve (for simplicity, static equation)

$$\boldsymbol{D f(x) = 0} \tag{19}$$

Where D is some differential operator. The weak form is:

$$\boldsymbol{\int \phi(x) D f(x) dx = 0} \tag{20}$$

Where $\phi(x)$ an arbitrary test function.

With Galerkin Method, we replace $\phi(x)$ with some basis set of functions $\{\phi_i(x)\}$, and solution f by

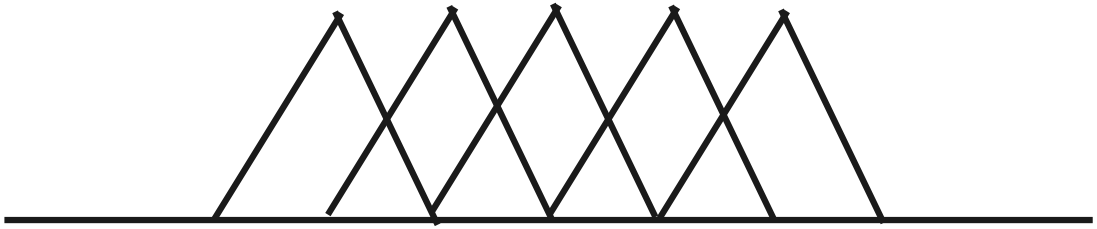
$$\boldsymbol{f \sim \sum_i f_i \phi_i(x)} \tag{21}$$

If the basis set has N basis functions, we end up with N equation.

For whatever reason, FEM people calls the basis function (or part of it) "shape function"

Usual Finite-Element method

Example of the basis set in 1D : linear polylines



Higher-order basis set can be constructed by higher-order fitting polynomials.

Advantage of the weak form:

- We do not need to estimate the derivatives of f itself, since we can eliminate it by partial integration
- The only thing we need is the derivatives of the basis

In the case of EFGM, the basis is defined in a complicated, but still computable, way

Potential advantages of EFGM

- **High-order, consistent schemes can be constructed**
- **Using discontinuous shape functions, CD and free surface can be treated also in a consistent way**
- **Mathematics is straightforward.**

Sounds great, but,

Why I do not like EFGM

Even when we use explicit time stepping, just to obtain the time derivative, we need to solve implicit equation

If this is the only way to go...

Summary

- SPH has too many problems
- We spend some time trying to fix them
- We did fix some of them, but not all
- Second-order Galerkin-like method seems to work reasonably well, for some cases
- EFGM might work better, but...