A link between information theory and SPH

Daniel Duque¹, Pablo Eleazar Merino-Alonso², Javier Calderon-Sanchez¹, Jose Luis Cercos-Pita³

¹CEHINAV - ETSIN, Universidad Politécnica de Madrid ²CoreMarine / Universidad Politécnica de Madrid ³Surgical Sciences Dep, Uppsala Universitet, Sweden

3rd Iberian Congress Advances on SPH







SPH may be derived from a Lagrangian:

$$L = T + \sum_{i} p_i V_i$$

SPH may be derived from a Lagrangian:

$$L = T + \sum_{i} p_i V_i,$$

together with

 \blacktriangleright some definition of V_i

SPH may be derived from a Lagrangian:

$$L = T + \sum_{i} p_i V_i,$$

together with

- \triangleright some definition of V_i
- ▶ some "closure" to get the pressures p_i

In fact, it is easy to show that if

$$V_i = rac{m_i}{
ho_i} \qquad
ho_i = m_j \sum_j W_{ij},$$

In fact, it is easy to show that if

$$egin{aligned} V_i &= rac{m_i}{
ho_i} \qquad
ho_i &= m_j \sum_j W_{ij}, \ egin{aligned} egin{aligned} egin{aligned} egin{aligned} egin{aligned} eta_i &= &- \sum_j \left(rac{m_j^2 p_j}{
ho_j^2} + rac{m_i^2 p_i}{
ho_i^2}
ight)
abla_i W_{ij}. \end{aligned}$$

Forget SPH – SFs

All we have is *particles*. Particle *i* influences particle *j* through a shape function (SF), " $\phi_i(\boldsymbol{r}_j)$ ".



Forget SPH – SFs

All we have is *particles*. Particle *i* influences particle *j* through a shape function (SF), " $\phi_i(\mathbf{r}_j)$ ". Subject to constraints, such as $\sum_i \phi_i(\mathbf{r}_j) = 1$.



Information entropy

Too many possibilities! But, information theory's "unbiased inference" (Jaynes, 1957) says we should maximize

$$S_j = -\sum_i \phi_i(\boldsymbol{r}_j) \log \left[\phi_i(\boldsymbol{r}_j)
ight].$$





The resulting SFs are very wide. Hence, Arroyo and Ortiz (2006) added an **energy** to make SFs more local:

$$E_j = \beta \sum_i \phi_i(\boldsymbol{r}_j) r_{ij}^2.$$



The resulting SFs are very wide. Hence, Arroyo and Ortiz (2006) added an energy to make SFs more local:

$$E_j = \beta \sum_i \phi_i(\boldsymbol{r}_j) r_{ij}^2.$$

If we forget constraints, the extreme of F = E - TS gives

$$\phi_i(\boldsymbol{r}_j) = \exp(-\beta r_{ij}^2).$$

More than enough to drive me(*) nuts at the time (*from* that time, to be precise.)

Building a theory: ideal part

A continuum theory already exists[1], so we may inspire ourselves.

$$-S=c^2\int
ho(oldsymbol{r})\sum_i\phi_i(oldsymbol{r})\left[\log\left(ar
ho(oldsymbol{r})\phi_i(oldsymbol{r})
ight)-1
ight]doldsymbol{r}.$$

Building a theory: ideal part

A continuum theory already exists[1], so we may inspire ourselves.

$$-S=c^2\int
ho(oldsymbol{r})\sum_i\phi_i(oldsymbol{r})\left[\log\left(ar
ho(oldsymbol{r})\phi_i(oldsymbol{r})
ight)-1
ight]doldsymbol{r}.$$

Any integral may be approximated as

$$\int f(\boldsymbol{r}) d\boldsymbol{r} \doteq \sum_{j} \frac{m_{j}}{\rho_{j}} f(\boldsymbol{r}_{j})$$

Building a theory: ideal part

A continuum theory already exists[1], so we may inspire ourselves.

$$-S=c^2\int
ho(oldsymbol{r})\sum_i\phi_i(oldsymbol{r})\left[\log\left(ar
ho(oldsymbol{r})\phi_i(oldsymbol{r})
ight)-1
ight]doldsymbol{r}.$$

Any integral may be approximated as

$$\int f(\boldsymbol{r}) d\boldsymbol{r} \doteq \sum_{j} rac{m_{j}}{
ho_{j}} f(\boldsymbol{r}_{j})$$

Therefore,

$$-S \doteq c^2 \sum_j m_j \sum_i \phi_i(\boldsymbol{r}_j) \left[\log\left(\frac{\rho_j \phi_i(\boldsymbol{r}_j)}{m_j}\right) - 1 \right]$$

Building a theory: energy part, constraint

The energy term is

$$E=eta\int
ho(m{r})\sum_i\phi_i(m{r})|m{r}-m{r}_i|^2dm{r}$$

Building a theory: energy part, constraint

The energy term is

$$E = eta \int
ho(m{r}) \sum_i \phi_i(m{r}) |m{r} - m{r}_i|^2 dm{r}$$

For a Gaussian kernel, $\beta r_{ij}^2 \propto -\log W_{ij}$, so for any kernel

$$E \doteq -c^2 \sum_j m_j \sum_i \phi_i(r_j) \log(m_j W_{ij}).$$

Building a theory: energy part, constraint

The energy term is

$$E = eta \int
ho(m{r}) \sum_i \phi_i(m{r}) |m{r} - m{r}_i|^2 dm{r}$$

For a Gaussian kernel, $\beta r_{ij}^2 \propto -\log W_{ij}$, so for any kernel

$$E \doteq -c^2 \sum_j m_j \sum_i \phi_i(r_j) \log(m_j W_{ij}).$$

Also, a C0 constraint,

$$L_{\mathrm{C0}} = \sum_{j} m_{j} \alpha_{j} \left(\sum_{i} \phi_{i}(\boldsymbol{r}_{j}) - 1 \right)$$

Density, revealed

Before including the pressure: extremezing F = E - S with respect to $\phi_i(\mathbf{r}_j)$ and α_j ,

$$F'' = -c^2 \sum_{j} m_j \left[\log \left(\frac{m_j Z_j}{\rho_j} \right) + 1 \right]$$
$$Z_i := \sum W_{ij}$$

Density, revealed

Before including the pressure: extremezing F = E - S with respect to $\phi_i(\mathbf{r}_j)$ and α_j ,

$$F'' = -c^2 \sum_{j} m_j \left[\log \left(\frac{m_j Z_j}{\rho_j} \right) + 1 \right]$$
$$Z_i := \sum_{j} W_{ij}$$

But, pressure is not included, and we do not want anything happening yet! This fixes the density:

$$\rho_j := m_j \sum_i W_{ij}$$

Building a theory: pressure

Finally, there will be a pressure term

$$E_p = -\sum_i p_i \left(\int \phi_i(m{r}) dm{r} - V_i^0
ight)$$

Finally, there will be a pressure term

$$E_p = -\sum_i p_i \left(\int \phi_i(\boldsymbol{r}) d\boldsymbol{r} - V_i^0
ight)$$
 $V_i = \int \phi_i(\boldsymbol{r}) d\boldsymbol{r} \doteq \sum_j rac{m_j}{
ho_j} \phi_i(\boldsymbol{r}_j).$

The C0 model: shape functions

$$\phi_i(r_j) = rac{W_{ij} z_{i,j}}{Z_j}, \qquad z_{i,j} := \exp\left(rac{p_i}{
ho_j c^2}
ight)$$

The C0 model: shape functions

$$\phi_i(r_j) = \frac{W_{ij} z_{i,j}}{Z_j}, \qquad z_{i,j} := \exp\left(\frac{p_i}{\rho_j c^2}\right)$$
$$Z_i := \sum_j W_{ij} z_{j,i}$$

The C0 model: forces

$$f_i^{(1)} = -c^2 \sum_j \left(\frac{m_j^2}{\rho_j} + \frac{m_i^2}{\rho_i}\right) \nabla_i W_{ij}$$

The C0 model: forces

$$f_i^{(1)} = -c^2 \sum_j \left(\frac{m_j^2}{\rho_j} + \frac{m_i^2}{\rho_i}\right) \nabla_i W_{ij}$$
$$f_i^{(2)} = c^2 \sum_j \left(\frac{m_j z_{i,j}}{Z_j} + \frac{m_i z_{j,i}}{Z_i}\right) \nabla_i W_{ij}$$

The C0 model: forces

$$f_{i}^{(1)} = -c^{2} \sum_{j} \left(\frac{m_{j}^{2}}{\rho_{j}} + \frac{m_{i}^{2}}{\rho_{i}} \right) \nabla_{i} W_{ij}$$
$$f_{i}^{(2)} = c^{2} \sum_{j} \left(\frac{m_{j} z_{i,j}}{Z_{j}} + \frac{m_{i} z_{j,i}}{Z_{i}} \right) \nabla_{i} W_{ij}$$
$$f_{i}^{(3)} = -\sum_{j} \left(\frac{m_{j}^{2} \bar{p}_{j}}{\rho_{j}^{2}} + \frac{m_{i}^{2} \bar{p}_{i}}{\rho_{i}^{2}} \right) \nabla_{i} W_{ij}, \qquad \bar{p}_{i} := \sum_{j} \phi_{j}(r_{i}) p_{j}.$$

The C0 model: pressure closure

Since the volumes explicitly depend on the pressures, $V_i = \sum_j \frac{m_j}{\rho_j} \phi_i(\boldsymbol{r}_j)$, we may look for the pressure field that fixes their values, through a Newton-Raphson method:

$$\sum_{j} \left(\frac{\partial V_i}{\partial p_j}\right)^{(n)} \left[p_j^{(n+1)} - p_j^{(n)}\right] = -\left(V_i - V_i^0\right)^{(n)},$$

The C0 model: pressure closure

Since the volumes explicitly depend on the pressures, $V_i = \sum_j \frac{m_j}{\rho_j} \phi_i(\boldsymbol{r}_j)$, we may look for the pressure field that fixes their values, through a Newton-Raphson method:

$$\sum_{j} \left(\frac{\partial V_i}{\partial p_j}\right)^{(n)} \left[p_j^{(n+1)} - p_j^{(n)}\right] = -\left(V_i - V_i^0\right)^{(n)},$$

this is a Poisson equation to solve for the pressures.

TG vortex sheet

Future: C1 shape functions

$$L_{ ext{C1}} = \sum_{j} m_{j} oldsymbol{\lambda}_{j} \cdot \left(\sum_{i} \phi_{i}(oldsymbol{r}_{j}) oldsymbol{r}_{i} - oldsymbol{r}_{j}
ight)$$

Future: C1 shape functions

$$L_{ ext{C1}} = \sum_j m_j oldsymbol{\lambda}_j \cdot \left(\sum_i \phi_i(oldsymbol{r}_j) oldsymbol{r}_i - oldsymbol{r}_j
ight)$$

SFs are now C1 consistent, there is a new force term, but most importantly, perhaps ...

C1 shape functions

The SFs have a sort of boundary detection, and have a "weak-Kronecker condition".

Thanks for your attention.

[1] Daniel Duque, A unified derivation of Voronoi, power, and finite-element Lagrangian computational fluid dynamics, European Journal of Mechanics - B/Fluids **98**, 268-278 (2023)

Extra: SFs as interpolants

Consider the smoothing

$$ar{f}(m{r}_j) = \sum_i \phi_i(m{r}_j) f_i$$

Consider the smoothing

$$ar{f}(m{r}_j) = \sum_i \phi_i(m{r}_j) f_i$$

Then C0, $\sum_{i} \phi_i(\mathbf{r}_j) = 1$, means constant fields have proper constant smoothing.

Consider the smoothing

$$ar{f}(m{r}_j) = \sum_i \phi_i(m{r}_j) f_i$$

Then C0, $\sum_{i} \phi_i(\mathbf{r}_j) = 1$, means constant fields have proper constant smoothing. While C1, $\sum_{i} \phi_i(\mathbf{r}_j)\mathbf{r}_i = \mathbf{r}_j$ means linear fields have proper linear smoothing.