Smoothed particle hydrodynamics for fluid dynamics

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Homework: you should start

- Hw # 4: Finite difference method + MPI for Helmholtz equations
- If you need a multi-core machine: apply for a CCV account https://www.ccv.brown.edu/

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Conservation law of mass: continuity equation

Total mass flows out of the volume V (per unit time) by surface integral

$$\oint \rho \mathbf{v} \cdot d\mathbf{f}, \tag{1}$$

where ρ density, $\mathbf{v}$ velocity and $d\mathbf{f}$ is along the outward normal.
The decrease of the mass in the volume (per unit time)

$$-\frac{\partial}{\partial t}\int \rho dV. \tag{2}$$

For a mass conservation, we have an equality

$$-\frac{\partial}{\partial t}\int \rho dV = \oint \rho \mathbf{v} \cdot d\mathbf{f} = \int \nabla \cdot (\rho \mathbf{v}) dV, \tag{3}$$

which is valid for an arbitrary V. The continuity equation reads

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \tag{4}$$

Conservation law of momentum: Euler equations

Total pressure force acting on the volume (surface to volume integral)

$$-\oint p d\mathbf{f} = -\int \nabla p dV. \tag{5}$$

For a *unit* of volume, momentum equations in Lagrangian form read

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p \quad or \quad \frac{d\mathbf{v}}{dt} = -\frac{\nabla p}{\rho}. \tag{6}$$

Considering the particle derivative is related to the partial derivatives as

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla, \tag{7}$$

the Euler equations in Eulerian form read

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{\nabla p}{\rho}. \tag{8}$$

Conservation law of momentum: Navier-Stokes equations

For real fluids, we need to add in viscous stress due to irreversible process and assume that the viscous stress depends only *linearly* on derivatives of velocity.
Without derivation, the Navier-Stokes equations read

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho}\left[\nabla p + \eta \triangle \mathbf{v} + (\zeta + \eta/3)\nabla\nabla \cdot \mathbf{v}\right] \tag{9}$$

For an incompressible fluid $\rho = const.$ *and* $\nabla \cdot \mathbf{v} = 0.$
Therefore, the momentum equations simplify to

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho}\left(\nabla p + \eta \triangle \mathbf{v}\right). \tag{10}$$

For a compressible fluid, an equation of state is called for

$$p = p(\rho, T = T_0). \tag{11}$$

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Mesh-based discretizations

Prof. Karniadakis will cover the mesh-based methods in other lectures

- finite difference method
- spectral h/p element method
- ... ...

Mesh-free discretizations: mesh-free = mess-free?

- Some particle methods
  - smoothed particle hydrodynamics (SPH)
  - moving least square methods (MLS)
  - vortex method
  - Voronoi tesselation
  - ... ...
- mesh-free ≈ mess-free
  - no mesh generation
  - Lagrangian, no $\mathbf{v} \cdot \nabla \mathbf{v}$
  - complex moving boundary
  - incorporation of new physics
  - ... ...

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Integral representation of a function

- It was invented in 1970s **(author?)** [12, 8].

Given a scalar function $f(r)$ of spatial coordinate r, its integral representation reads

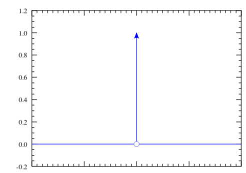
$$f(r) = \int f(r')\delta(r - r')dr', \qquad (12)$$

where the Dirac delta function reads

$$\delta(r - r') \begin{cases} \infty, & r = r' \\ 0, & r \neq r' \end{cases} \qquad (13)$$

and the constraint of normalization is

$$\int_{\infty}^{\infty} \delta(r)dr = 1. \qquad (14)$$



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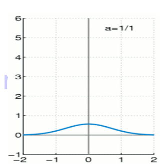


SPH 1^{st} step: smoothing or kernel approximation

(author?) [8]; **(author?)** [12]

Replace δ with another smoothly weighting function w:

$$f(r) \approx f_k(r) = \int f(r')w(r - r', h)dr', \qquad (15)$$

where kernel w has properties

1. smoothness
2. compact with h as parameter
3. $\lim_{h \to 0} w(r - r', h) = \delta(r - r')$
4. $\int w(r - r', h)dr' = 1$
5. symmetric
6. … …

Gaussian: $\frac{1}{a\sqrt{\pi}} e^{-r^2/a^2}$

compact: B-splines, Wendland functions …

(author?) [15, 16, 19]

Compact kernel and its normalization

- a cubic function as reads ($h = 1$ for simplicity)

$$w(r) = \begin{cases} C_D(1-r)^3, & r < 1; \\ 0, & r \geq 1. \end{cases} \quad (16)$$

If we require the constraint of normalization in two dimension

$$\int_0^{2\pi} \int_0^1 C_2(1-r)^3 r dr d\theta = 1 \Longleftrightarrow C_2 = \frac{10}{\pi} \quad (17)$$

- a piecewise quintic function reads

$$w(r) = C_D \begin{cases} (3-s)^5 - 6(2-s)^5 + 15(1-s)^5, & 0 \leq s < 1 \\ (3-s)^5 - 6(2-s)^5, & 1 \leq s < 2 \\ (3-s)^5, & 2 \leq s < 3 \\ 0, & s \geq 3, \end{cases} \quad (18)$$

where $s = 3r/h$ and $C_2 = 7/(478\pi h^2)$ and $C_3 = 1/(120\pi h^3)$.

- $f(r) = f_k(r) + error(h)$

SPH 2^{nd} step: summation or particle approximation

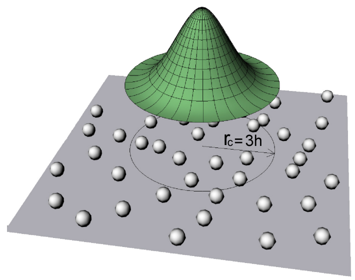
Integral $\Longleftrightarrow$ summation

$$f_k(r) = \int f(r')w(r-r',h)dr' \quad (19)$$

$$f_s(r) = \sum_i^{N_{neigh}} f_i w(r-r_i,h)V_i, \quad (20)$$

where V_i is a distance, area and volume in $1D$, $2D$, and $3D$, respectively. Therefore,

$$f_k(r) \approx f_s(r) \quad (21)$$



summation within compact support

- $f_k(r) = f_s(r) + error(\Delta r, h)$

An example: evaluation of density and arbitrary function

$\forall i$ of particle index, mass m_i, density ρ_i, and $V_i = m_i/\rho_i$.

$$f_s(r) = \sum_i^{N_{neigh}} f_i w(r-r_i,h)V_i = \sum_i^{N_{neigh}} \frac{m_i}{\rho_i} f_i w(r-r_i,h). \quad (22)$$

- What is the density at an arbitrary position r?

$$\rho_s(r) = \sum_i^{N_{neigh}} \frac{m_i}{\rho_i}\rho_i w(r-r_i,h) = \sum_i^{N_{neigh}} m_i w(r-r_i,h). \quad (23)$$

- What is the density of a particle at r_j?

$$\rho_s(r_j) = \sum_i^{N_{neigh}} m_i w(r_j-r_i,h). \quad (24)$$

- What is the value of a function of a particle at r_j?

$$f_s(r_j) = \sum_i^{N_{neigh}} f_i \frac{m_i}{\rho_i} w(r_j-r_i,h) = \sum_i^{N_{neigh}} f_i W_{ji} = f_j \quad (25)$$

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Gradient of a function

$$f(r) \approx f_k(r) = \int f(r')w(r-r',h)dr' \quad (26)$$

$$\Downarrow$$

$$\nabla_r f(r) \approx \nabla_r f_k(r) = \nabla_r \int f(r')w(r-r',h)dr' \quad (27)$$

$$\Downarrow$$

$$\nabla_r f_k(r) = \int \nabla_r f(r')w(r-r',h)dr' + \int f(r')\nabla_r w(r-r',h)dr' \quad (28)$$

$$\Downarrow$$

$$\nabla_r f_k(r) = \int f(r')\nabla_r w(r-r',h)dr' \quad (29)$$

$$\Downarrow$$

$$\nabla_r f(r) \approx \nabla_r f_k(r) \approx \nabla_r f_s(r) = \sum_i^{N_{neigh}} \frac{m_i}{\rho_i} f(r')\nabla_r w(r-r',h) \quad (30)$$

Other first derivatives

$$\nabla_r \cdot f(r) \approx \nabla_r \cdot f_k(r) \approx \nabla_r \cdot f_s(r) = \sum_i^{N_{neigh}} \frac{m_i}{\rho_i} f(r') \cdot \nabla_r w(r-r',h) \quad (31)$$

$$\nabla_r \times f(r) \approx \nabla_r \times f_k(r) \approx \nabla_r \times f_s(r) = \sum_i^{N_{neigh}} \frac{m_i}{\rho_i} f(r') \times \nabla_r w(r-r',h) \quad (32)$$

Second derivatives

Note that we have following identity **(author?)** [4]

$$\int d\mathbf{r}' \left[f(\mathbf{r}') - f(\mathbf{r})\right] \frac{\partial w(|\mathbf{r}'-\mathbf{r}|)}{\partial r'} \frac{1}{r_{ij}} \mathbf{e}_{ij} \left[5\frac{(\mathbf{r}'-\mathbf{r})^\alpha(\mathbf{r}'-\mathbf{r})^\beta}{(\mathbf{r}'-\mathbf{r})^2} - \delta^{\alpha\beta}\right]$$
$$= \quad \nabla^\alpha\nabla^\beta f(\mathbf{r}) + \mathcal{O}(\nabla^4 fh^2). \quad (33)$$

Therefore,

$$\frac{1}{\rho_i}(\nabla^2 \mathbf{v}) = -2\sum_j^{N_{neigh}} \frac{m_j}{\rho_i\rho_j} \frac{\partial w_{ij}}{\partial r} \mathbf{v}_{ij} \quad (34)$$

$$\frac{1}{\rho_i}(\nabla\nabla \cdot \mathbf{v}) = -\sum_j^{N_{neigh}} \frac{m_j}{\rho_i\rho_j} \frac{\partial w_{ij}}{\partial r} (5\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}\mathbf{e}_{ij} - \mathbf{v}_{ij}) \quad (35)$$

$$(36)$$

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Particles for hydrodynamics

- continuity equation is accounted for by

$$\rho_i = \sum_j^{N_{neigh}} m_j W_{ij}, \quad \dot{\mathbf{r}}_i = \mathbf{v}_i \tag{37}$$

- pressure force: $-\nabla p/\rho$

$$\mathbf{F}_i^C = \sum_j^{N_{neigh}} \mathbf{F}_{ij}^C = \sum_j^{N_{neigh}} -m_j \left(\frac{p_j}{\rho_j^2}\right) \frac{\partial w}{\partial r_{ij}} \mathbf{e}_{ij}, \tag{38}$$

  - bad: not antisymmetric by swapping i and j
  - recognize $-\nabla p/\rho = -\frac{p}{\rho^2}\nabla\rho - \nabla\frac{p}{\rho}$

$$\mathbf{F}_{ij}^C = -m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \frac{\partial w}{\partial r_{ij}} \mathbf{e}_{ij}, \tag{39}$$

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viscous force

In general

$$\mathbf{F}_{ij}^D = \frac{m_j}{\rho_i\rho_j r_{ij}} \frac{\partial w}{\partial r_{ij}} \left[\left(\frac{5\eta}{3} - \zeta\right)\mathbf{v}_{ij} + \left(5\zeta + \frac{5\eta}{3}\right)\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\mathbf{e}_{ij}\right] \tag{40}$$

For inompression flows $\nabla\cdot\mathbf{v} = 0$, therefore,

$$\sum_j^N \frac{5}{\rho_i\rho_j r_{ij}} \frac{\partial w_{ij}}{r_{ij}} \mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\mathbf{e}_{ij} \approx \sum_j^N \frac{1}{\rho_i\rho_j r_{ij}} \frac{\partial w_{ij}}{\partial r_{ij}} \mathbf{e}_{ij}. \tag{41}$$

$$\mathbf{F}_{ij}^D = 2\eta \frac{m_j}{\rho_i\rho_j r_{ij}} \frac{\partial w_{ij}}{\partial r_{ij}} \mathbf{v}_{ij} \approx 10\eta \frac{m_j}{\rho_i\rho_j r_{ij}} \frac{\partial w_{ij}}{\partial r_{ij}} \mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\mathbf{e}_{ij}. \tag{42}$$

Either choice is fine, but they are different.

Summary of SPH for isothermal Navier-Stokes equations

- continuity equation:

$$\rho_i = \sum_j^{N_{neigh}} m_j W_{ij}, \quad \dot{\mathbf{r}}_i = \mathbf{v}_i \tag{43}$$

- momentum equations: **(author?)** [4, 11]

$$\dot{\mathbf{v}}_i = \sum_{j \neq i}^{N_{neigh}} \left(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D \right), \tag{44}$$

$$\mathbf{F}_{ij}^C = -m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \frac{\partial w}{\partial r_{ij}} \mathbf{e}_{ij}, \tag{45}$$

$$\mathbf{F}_{ij}^D = \frac{m_j}{\rho_i \rho_j r_{ij}} \frac{\partial w}{\partial r_{ij}} \left[\left(\frac{5\eta}{3} - \zeta \right) \mathbf{v}_{ij} + \left(5\zeta + \frac{5\eta}{3} \right) \mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \mathbf{e}_{ij} \right] \tag{46}$$

- weakly compressible: **(author?)** [2, 13]

$$p = c_T^2 \rho, \quad or \quad p = p_0 \left[\left(\frac{\rho}{\rho_r} \right)^\gamma - 1 \right] \tag{47}$$

p_0 relates to an artificial sound speed c_T

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Density estimate or sampling

Given a set of point particles with mass m_i, what is the density estimate for a position at r.

$$\rho_s(\mathbf{r}) = \sum_i^{N_{neigh}} m_i w(\mathbf{r} - \mathbf{r}_i, h). \tag{48}$$

where kernel w has properties

1. smoothness
2. compact with h as parameter
3. $\int w(r - r', h) dr' = 1$
4. symmetric
5. ... ...

Eq. (48) is more fundamental than the summation form presented early

$$f_s(\mathbf{r}) = \sum_i^{N_{neigh}} f_i \frac{m_i}{\rho_i} w(\mathbf{r} - \mathbf{r}_i, h). \tag{49}$$

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Least action

Define the Lagrangian L as

$$L = T - U, \tag{50}$$

where T and U are kinetic and potential energies, respectively. For a set of particles

$$L = \sum_i^N m_i \left(\frac{1}{2} v_i^2 + u_i(\rho_i, s) \right) \tag{51}$$

Define the action as

$$S = \int L dt. \tag{52}$$

Minimizing S such that $\delta S = \int \delta L dt = 0$, where δ is a variation with respect to particle coordinate $\delta \mathbf{r}$. We have **(author?)** [17]

$$\delta S = \int \left(\frac{\partial L}{\partial \mathbf{v}} \cdot \delta \mathbf{v} + \frac{\partial L}{\partial \mathbf{r}} \cdot \delta \mathbf{r} \right) = 0 \tag{53}$$

Euler-Lagrangian equations

$$\delta S = \int \left(\frac{\partial L}{\partial \mathbf{v}} \cdot \delta \mathbf{v} + \frac{\partial L}{\partial \mathbf{r}} \cdot \delta \mathbf{r} \right) = 0 \tag{54}$$

consider $\delta \mathbf{v} = d(\delta \mathbf{r})/dt$ and $d/dt = \partial/\partial t + \mathbf{v} \cdot \nabla$

$$\Downarrow$$

$$\delta S = \int \left\{ \left[-\frac{d}{dt} \left(\frac{\partial L}{\partial \mathbf{v}} \right) + \frac{\partial L}{\partial \mathbf{r}} \right] \cdot \delta \mathbf{r} \right\} dt + \left[\frac{\partial L}{\partial \mathbf{v}} \cdot \delta \mathbf{r} \right]_{t_0}^{t} = 0 \tag{55}$$

assume variation vanishes at start and end times and furthermore, $\delta \mathbf{r}$ is arbitrary. Therefore, we have the Euler-Lagrangian equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \mathbf{v}_i} \right) - \frac{\partial L}{\partial \mathbf{r}_i} = 0. \tag{56}$$

Equation of motions for particles

From the Lagrangian $L = \sum_i^N m_i \left(\frac{1}{2} v_i^2 + u_i \right)$ we know

$$\frac{\partial L}{\partial \mathbf{v}_i} = m_i \mathbf{v}_i, \quad \frac{\partial L}{\partial \mathbf{r}_i} = -\sum_j^{N_{neigh}} m_j \frac{\partial u_j}{\partial \rho_j} \frac{\partial \rho_j}{\partial \mathbf{r_j}} \tag{57}$$

Some basic thermodynamics: $dU = TdS - PdV$
Since $V = m/\rho$, so $dV = -md\rho/\rho^2$. For per unit mass we have

$$du = Tds - \frac{P}{\rho^2} d\rho. \tag{58}$$

For a reversible process $ds = 0$, therefore $\partial u_i / \partial \rho_i = p/\rho^2$. Put everything known into the Euler-Lagrangian equations, we get

$$\dot{\mathbf{v}}_i = \sum_{j \neq i}^{N_{neigh}} -m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \frac{\partial w}{\partial r_{ij}} \mathbf{e}_{ij}. \tag{59}$$

Conservation laws

Euler hydrodynamics

- total mass $M = \sum_i^N m_i$.
- total linear momentum

$$\frac{d}{dt}\sum_i^N m_i \mathbf{v}_i = \sum_i^N m_i \frac{d\mathbf{v}_i}{dt} = \sum_i^N \sum_j^N -m_i m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \frac{\partial w}{\partial r_{ij}} \mathbf{e}_{ij} = 0. \quad (60)$$

- total angular momentum

$$\frac{d}{dt}\sum_i^N \mathbf{r}_i \times m_i \mathbf{v}_i = \sum_i^N m_i \left(\mathbf{r}_i \times \frac{d\mathbf{v}_i}{dt}\right) \quad (61)$$

$$= \sum_i^N \sum_j^N -m_i m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \frac{\partial w}{\partial r_{ij}} (\mathbf{r}_i \times \mathbf{e}_{ij}) = 0. \quad (62)$$

Similarly for the viscous forces.

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Errors in density estimate: kernel error

Recall the kernel approximation

$$\rho_k(\mathbf{r}) = \int \rho(\mathbf{r}') w(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}', \quad (63)$$

Expanding $\rho(r')$ by Taylor series around $\mathbf{r}$

$$\rho_k(\mathbf{r}) = \rho(\mathbf{r}) \int w(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' + \nabla\rho(\mathbf{r}) \cdot \int (\mathbf{r}' - \mathbf{r}) w(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'$$
$$+ \nabla^\alpha \nabla^\beta \rho(\mathbf{r}) \int \delta\mathbf{r}'^\alpha \delta\mathbf{r}^\beta w(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' + O(h^3). \quad (64)$$

Recall $\int w(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' = 1$ and odd terms vanish due to symmetric w,

$$\rho(\mathbf{r}) = \rho_k(\mathbf{r}) + O(h^2). \quad (65)$$

Errors for a function f: kernel error and summation error

Similarly as for density estimate:

$$f(\mathbf{r}) = f_k(\mathbf{r}) + O(h^2). \quad (66)$$

Recall the particle approximation or summation form

$$f_k(\mathbf{r}_i) \approx f_s(\mathbf{r}_i) = \sum_j^{N_{neigh}} \frac{m_j}{\rho_j} f_j w(\mathbf{r}_i - \mathbf{r}_j, h). \quad (67)$$

Let us do Taylor series on $f(\mathbf{r}_j)$ around $\mathbf{r}_i$

$$f_s(\mathbf{r}_i) = f_i \sum_j^{N_{neigh}} \frac{m_j}{\rho_j} w(\mathbf{r}_{ij}, h) + \nabla f_i \cdot \sum_j^{N_{neigh}} \mathbf{r}_{ji} \frac{m_j}{\rho_j} w(\mathbf{r}_{ij}, h) + O(h^2). \quad (68)$$

To have error of $O(h^2)$, we need

$$\sum_j^N \frac{m_j}{\rho_i} w(\mathbf{r}_{ij}) = 1, \quad \sum_j^N \mathbf{r}_{ji} \frac{m_j}{\rho_i} w(\mathbf{r}_{ij}) = 0, \quad (69)$$

which is not guranteed in practice (depends on configurations, Δx, and h).

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Challenges

- error analysis due to particle configurations
- consistency and conservation at the same time
- convergence for a practical purpose
- coarse-graining from molecular dynamics

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Algorithmic similarity: pairwise forces within short range r_c

- in a nutshell, ∀ particle i in **SPH**, **SDPD**, **DPD**, or **MD**, the EoM:

$$\dot{\mathbf{v}}_i = \sum_{j \neq i} \left(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \right) \tag{70}$$

- options for different components
  - weighting kernel or potential gradient in MD
  - equation of state
  - density field
  - thermal fluctuations
  - canonical ensemble / NVT: thermostat
  - ... ...

SPH: **(author?)** [14]

SDPD: **(author?)** [4]

DPD: **(author?)** [10]; **(author?)** [5]; **(author?)** [9]

MD: **(author?)** [1]; **(author?)** [7]; **(author?)** [6]; **(author?)** [18]

academic toy: several interesting elements

- ∼ 12,000 SDPD particles **(author?)** [3]

academic toy: several interesting elements

- ∼ 12,000 SDPD particles **(author?)** [3]
- hypnotized?

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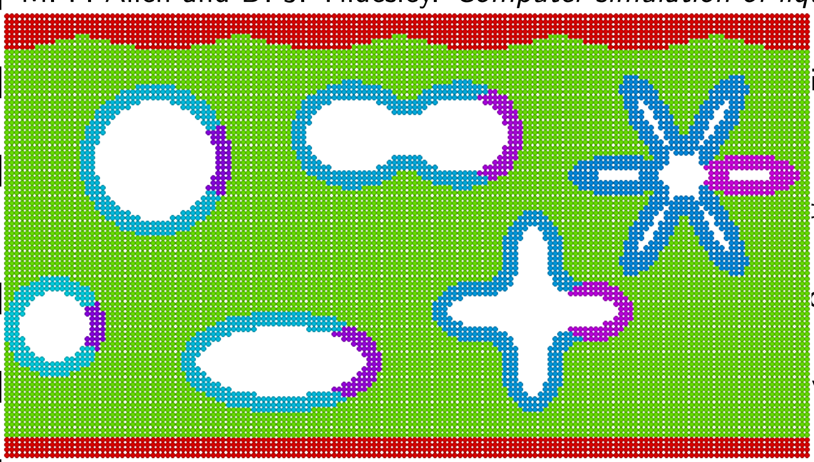

[2] ... idge

[3] ... d

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