CES 712 – PARTICLE METHODS

* Continuous vs. discrete description of a physical system
  - continuous – state variable $\phi \in X$

$$\underbrace{\phi : [0,t] \times \underline{\Omega}}_{\text{infinite number of degrees of freedom}} \rightarrow \mathbb{R} \; (\mathbb{R}^d)$$

ϕ satisfies a PDE

- discrete description – parameters (position, velocity, etc.) of N discrete objects such as point charges (electrodynamics) point masses (celestial mechanics), point vortices (hydrodynamics)

$$\{x_1(t), \ldots, x_N(t)\} : [0,T] \longrightarrow \mathbb{R}^{dN}$$

$\downarrow$ not independent $\qquad\qquad d = 2,3$

$$\{v_1(t), \ldots, v_N(t)\} : [0,T] \longrightarrow \mathbb{R}^{dN}$$

Characterization of particles' strength:

- charge : q_i
- mass : m_i $\qquad m_i > 0 \ \forall i$
- circulation : Γ_i

Particle parameters $(x_i, v_i, q_i / m_i / \Gamma_i)_{i=1}^{N}$ satisfy a system of coupled ODEs.

First we will be interested in systems admitting a discrete description. Later we will see how continuous systems can be modelled using particles.

* Particle evolution

System configuration:

$$\bar{x}(t) = \left[\bar{x}_1(t), \ldots, \bar{x}_N(t)\right]$$

// molecule, galaxy, ~~vortex~~ tube

Assume the particle a potential field (electrostatic / gravitational / hydrodynamic, etc.)

Potential field — force given by the negative gradient of a scalar field (potential)

Electrostatic / gravitational / hydrodynamic potentials have different physical meaning, but a very similar mathematical expression which depends on the dimension only (2D vs. 3D).

$$\dot{\bar{x}}_i = \bar{v}_i \quad , i=1, \ldots, N \qquad \text{(Kinematic)}$$

$$m_i \dot{\bar{v}}_i = \bar{F}(x_i) \quad , i=1, \ldots, N \qquad \text{(dynamic – Newton's second law of mechanics)}$$

$$\bar{F}(x) = -\nabla \phi(x) \qquad \text{(potential interaction)}$$

$$\dot{m}_i = 0 \quad , i=1, \ldots, N \qquad \text{(particle properties do not change)}$$

$$(\dot{r}_i = 0, \; \dot{q}_i = 0)$$

Remark – in most conservative ~~pro~~ problems we assume that particle properties do not change, however, in general non-conservative problems ~~the~~ this assumption may be relaxed (e.g. $\dot{\Gamma}_i \neq 0$) to account for dissipative effects.

Combining the evolution equations we get:

$$\left\{ \begin{array}{l} m_i \ddot{\bar{x}}_i = -\nabla \phi(\bar{x}_i) \quad , \; i = 1, \dots, N \\ m_i, q_i, \Gamma_i \; - \; \text{const.} \\ \bar{x}_i(0) = \bar{x}_i^0 \\ \dot{\bar{x}}_i(0) = \bar{v}_i^0 \end{array} \right. \qquad (*)$$

The potential ϕ

$$\phi = \underbrace{\phi_{par}(\bar{x}_1, \dots, \bar{x}_N)}_{\substack{\text{potential energy} \\ \text{due to particle} \\ \text{interactions in infinite} \\ \text{space}}} + \underbrace{\phi_{ex}}_{\substack{\text{externally imposed} \\ \text{field (e.g.} \\ \text{presence of boundary} \\ \text{effects)}}}$$

In most situations we will be interested in

$$\phi \equiv \phi_{par}$$

(unless needed for clarity, we will ~~[illegible]~~ skip the subscript "par")

Example – charged particles in 3D

potential : $\phi(x_1, \dots, x_N) = V(x_1, \dots, x_N) =$
(potential energy)

$$= \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{q_i q_j}{|x_i - x_j|}$$

electric force:
field

$$E_j(x_1, \dots, x_N) = -\nabla_j V(x_1, \dots, x_N),$$

where $\nabla_j \stackrel{\Delta}{=} \nabla_{x_j} = \left[\frac{\partial}{\partial (x_j)_1}, \frac{\partial}{\partial (x_j)_2}, \frac{\partial}{\partial (x_j)_3} \right]$

Newton's equation:

$$m_i \ddot{x}_i = - \sum_{\substack{j=1 \\ j \neq i}}^{N} q_i q_j \frac{x_i - x_j}{|x_i - x_j|^3}, \quad i = 1, \dots, N$$

Remarks:

* ~~[illegible]~~ to avoid singularity ($\phi \to \infty$), the singular term $i=j$ is subtracted in the potential ϕ; this can actually be rigorously justified
* in the gravitational problem of celestial mechanics we replace the charges q_i with (scaled) masses $\sqrt{G}\, m_i$ (G ensures dimensional consistence)

Note that then the force between two point masses

$$F \propto \frac{m_1 m_2}{r^2}$$

consistently with Newton's theory of universal gravitation.

* in 2D hydrodynamics things tend to be slightly more complicated: instead of potential ϕ we often use the streamfunction ψ such that velocity is given by $\bar{v}(x) = \nabla \times (\psi \bar{e}_z) = \left[\frac{\partial \psi}{\partial y}, -\frac{\partial \psi}{\partial x}\right]$ ($\bar{e}_z$ is the unit vector normal to the plane of motion)

Thus, the equations of motion:

$$\dot{x}_i = \frac{\partial}{\partial y} \psi(\bar{x}_1, \dots, \bar{x}_N)$$

$$\dot{y}_i = -\frac{\partial}{\partial x} \psi(\bar{x}_1, \dots, \bar{x}_N)$$

However, the general mathematical structure remains the same

* We will often use the notation $\sum_{j=1}^{N}{}' \triangleq \sum_{\substack{j=1 \\ j\neq i}}^{N}$

* All of the above are examples of N-body (N-vortex) problems

* There are other types of potential interactions with a different mathematical structure, e.g., the Lennard-Jones potential for neutral atoms and molecules; time-permitting, we may discuss them as well

Remarks about N-body problems

* computational cost $O(N^2)$ is often prohibitive (every particle interacts with the remaining $(N-1)$ particles)

* Invariants (conserved quantities)
  - center of mass (3)
  - linear momentum (3)
  - angular momentum (3)
  - energy (1)

  useful for benchmarking numerical codes

* N-body problem has 6N variables in 3D and 4N variables in 2D

* 3-body problem is nonintegrable in 3D
* ~~2~~4-body ——— in ——— 2D
* restricted problems – the mass of one object is vanishing

PDE for the potential ϕ

$$\bar{F}(x) = -\nabla\phi(x)$$

The force field should be source-free (divergence-free) everywhere in Ω away from the particle location $\bar{x}_0$. In other words, the particle at $\bar{x}_0$ should be the only source of the field $\bar{F}$.

Thus: $\nabla \cdot \bar{F} = -\nabla \cdot \nabla \phi = -\Delta \phi = \delta(x - \bar{x}_0)$

The potential induced by a particle at $\bar{x}_0$ satisfies the Laplace equation with a Dirac delta on the RHS.

This potential ("impulse response") has the form (in 3D):

$$\phi(\bar{x}, \bar{x}_0) = \frac{1}{4\pi |\bar{x} - \bar{x}_0|}$$

Proof:

Assume $\bar{x}_0 = 0$, $|\bar{x} - \bar{x}_0| = r$, $\phi(r) = \frac{1}{4\pi r}$

for $r \neq 0$

$$\Delta \phi(r) = \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \phi}{\partial r}\right) = \frac{1}{r^2} \frac{\partial}{\partial r}\left(-\frac{1}{4\pi}\right) = 0$$

(can be shown (using the theory of weak solutions) that

$$\phi(r) \xrightarrow[r \to 0]{} \delta(r)$$

$\phi(r) = \phi(|x - x_0|)$ is the fundamental solution of the Laplace equation corresponding to a single point-source (particle) on the RHS

If there are N such point sources, the resulting potential will be a superposition of the fundamental solutions corresponding to each source:

$$\phi_N(\bar{x}) = \sum_i \phi_i(\bar{x}, x_i), \quad \{x_i\}_{i=1}^{N} \text{ - position of point sources.}$$

* Behavior at infinity (3D)

$$\phi(x) \xrightarrow[|x|\to\infty]{} 0 \quad (\text{as } O(|x|^{-1}))$$

(This may be regarded as the BC for the Laplace equation)

* Fundamental solution in 2D

$$\phi(\bar{x}, \bar{x}_0) = -\frac{1}{2\pi}\ln|\bar{x}-\bar{x}_0|$$

<u>Proof</u>

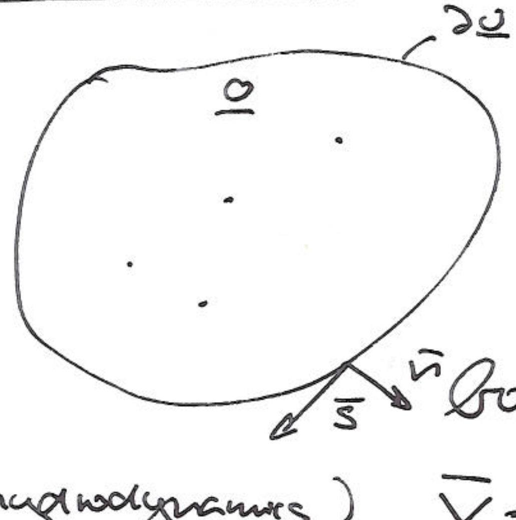
Assume $\bar{x}_0 = 0$, $|\bar{x}-\bar{x}_0| = r$, $\phi(r) = -\frac{1}{2\pi}\ln|\bar{x}-\bar{x}_0|$

For $r \neq 0$

$$\Delta\phi(r) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\phi}{\partial r}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(-\frac{1}{2\pi}\right) = 0$$

Using the theory of weak solutions it can be shown that $\phi(r) \xrightarrow[r\to 0]{} \delta(r)$ ∎

* <u>Problems in bounded domains</u> (for the sake of completeness)



What can we require of the potential on the domain boundary $\partial\Omega$?

Particles ~~may~~ should not penetrate boundaries

-(hydrodynamics) $\bar{V}\cdot\bar{n}|_{\partial\Omega} = 0 \Rightarrow \frac{\partial\psi}{\partial s}\Big|_{\partial\Omega} = 0$

Integrating w.r.t. arc-length

$$\Psi(s) = \Psi_0 + \int_0^s \frac{\partial \Psi}{\partial s}(s')\,ds' = \Psi_0 + \underbrace{\int_0^s \bar{V}\cdot\bar{n}(s')\,ds'}_{\triangleq\, \Psi_b}$$

Thus we have

Dirichlet boundary conditions

– (celestial mechanics / electrodynamics) – problems in bounded domains occur much less frequently & treatment of the potential BCs is less obvious

Since $m_i \frac{dv_i}{dt} = -\nabla\phi(x_i)$, it's not clear what assumptions on the potential ϕ on the boundary will ensure that $\bar{V}\cdot\bar{n}|_{\partial\Omega} = 0$

Assuming, to fix attention, that <u>normal</u> forces should vanish on the boundary, we would have

$$\bar{n}\cdot\nabla\phi|_{\partial\Omega} = \frac{\partial\phi}{\partial n} = 0$$

Neumann Boundary conditions

<u>Remark</u> – no assumptions are made regarding tangential velocities (hydrodynamics) and forces (celestial mechanics / electrodynamics). Tangential ~~interactions~~ interactions are a signature of frictional (dissipative) effects which are not included

* Behavior at infinity in <u>unbounded domains</u>

$$\underline{\Omega} = \mathbb{R}^d, \ d = 2, 3 \qquad \phi \xrightarrow[|x|\to\infty]{} \ ?$$

- in 3D $\quad \phi(x) \xrightarrow[|x|\to\infty]{} 0$

- in 2D the behavior of the potential at infinity depends on the sign of $\sum_{i=1}^{n} \Gamma_i$

$$\sum_{i=1}^{n} \Gamma_i < 0 \quad \Rightarrow \quad \phi(x) \xrightarrow[|x|\to\infty]{} +\infty$$

$$\text{—''—} = 0 \quad \Rightarrow \quad \text{—''—} \quad 0$$

$$\text{—''—} > 0 \quad \Rightarrow \quad \text{—''—} \quad -\infty$$

<u>Proof</u>

$\cdot \bar{x}_i$

$\{x_i\}$ - particle positions

$$\phi_{total}(\bar{x}) = \underbrace{\sum_{i=1}^{n} \phi(\bar{x}, \bar{x}_i)}$$

superpositions of the potentials (fundamental solutions) due to individual particles.

~~Proof:~~

~~Transformation~~

~~Transform the potential due to any individual particle by adding a constant~~

$$\cancel{-\frac{1}{2\pi}\ln|\bar{x}-\bar{x}_i| = -\frac{1}{2\pi}\ln|\bar{x}| \ldots = -\frac{1}{2\pi} \ldots}$$

Use methods of complex analysis $\quad z = x + iy$

$$\phi_i = - \operatorname{Im}\left[\frac{\Gamma}{2\pi i} \ln(z - z_i)\right]$$

$$= - \operatorname{Im}\left[\frac{\Gamma}{2\pi i} \ln(z - z_0) + \frac{\Gamma}{2\pi i} \ln \frac{z - z_i}{z - z_0}\right]$$

$$= - \operatorname{Im}\left[\frac{\Gamma}{2\pi i} \ln(z - z_0) + \frac{\Gamma}{2\pi i} \ln\left(1 - \frac{z_0 - z_i}{z - z_0}\right)\right]$$

Since $|z - z_0| \gg |z_0 - z_i|$, $\left|\frac{z_0 - z_i}{z - z_i}\right|$ is small

and we can use the expansion

$$\ln(1 - \varepsilon) = - \varepsilon - \frac{1}{2}\varepsilon^2 - \frac{1}{3}\varepsilon^3 - O(\varepsilon^4)$$

Therefore

$$\phi_i(z) = - \operatorname{Im}\left[\underbrace{\frac{\Gamma}{2\pi i} \ln(z - z_0)}_{\substack{\text{These terms go to } \infty, \\ \text{but they are independent} \\ \text{of } z_i \text{ and are} \\ \text{therefore the same for} \\ \text{all vortices}}} - \underbrace{\frac{\Gamma}{2\pi i} \sum_{p=1}^{\infty} \frac{1}{p}\left(\frac{z_0 - z_i}{z - z_0}\right)^p}_{\substack{\text{These terms vanish} \\ \text{for } |z| \to \infty}}\right]$$

$$\phi(z) = - \operatorname{Im}\left[\frac{1}{2\pi i}\left(\sum_{k=1}^{n} \Gamma_k\right) \ln(z - z_0) - \frac{1}{2\pi i} \sum_{k=1}^{n} \Gamma_k \sum_{p=1}^{\infty} \frac{1}{p}\left(\frac{z_0 - z_i}{z - z_0}\right)^p\right]$$

Equation for the potential

$$(*)\quad \begin{cases} \Delta\psi = \sum_{k=1}^{n} \Gamma_k \, \delta(x - \bar{x}_k) & \text{in } \underline{\Omega} \subset \mathbb{R}^d \\ & (\underline{\Omega} \equiv \mathbb{R}^d) \\ \psi\big|_{\partial\underline{\Omega}} = \psi_b & \end{cases}$$

Solution of (*) using <u>Green's functions</u>

Green's function $G(x, x')$ allows one to solve the equation $Lu(x) = g(x)$ for some linear operator L in the form of a convolution

$$u(x) = \int_{\underline{\Omega}} G(x, x') \, g(x') \, dx'$$

Green's functions have the following properties:

- $G(x, x')$ continuous in x and x'
- $L\,G(x, x') = \delta(x - x')$

  $G(x, \cdot)$ satisfies also the BCs associated with the operator L

- symmetry: $G(x, x') = G(x', x)$

Finding Green's functions:

- problems in unbounded domains $\underline{\Omega} \equiv \mathbb{R}^d$

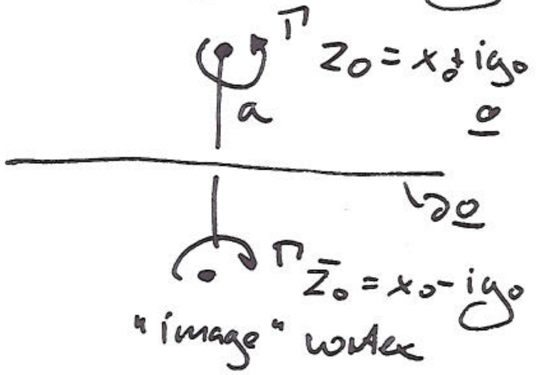
  Green's function $\equiv$ fundamental solution

- problems in bounded domains $\underline{\Omega} \subset \mathbb{R}^d$

  Green's function $\equiv$ [fundamental solution] + [terms chosen to ensure that BCs are satisfied]

Example — construction of Green's functions in bounded domains using the method of images

$\underline{\Omega} = \{(x,y),\ y>0\}$



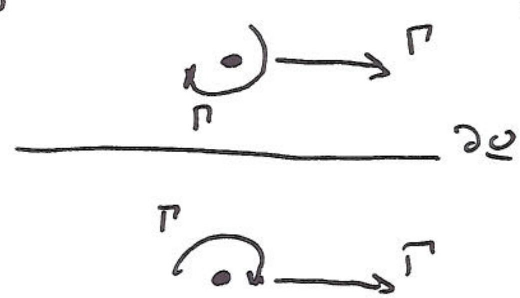
$$\psi(z) = -\frac{\Gamma}{2\pi}\ln|z-z_0| + \frac{\Gamma}{2\pi}\ln|z-\bar{z}_0|$$
$$= -\frac{\Gamma}{2\pi}\ln\frac{|z-z_0|}{|z-\bar{z}_0|}$$

Note that for $z|_{\partial\underline{\Omega}} = x + i0 = x$ (point on the boundary $\partial\underline{\Omega}$)

$$\psi(z)\Big|_{\partial\underline{\Omega}} = \psi(x) = -\frac{\Gamma}{2\pi}\ln\frac{\sqrt{(x-x_0)^2+y_0^2}}{\sqrt{(x-x_0)^2+y_0^2}} = -\frac{\Gamma}{2\pi}\ln 1 = 0 = \psi_b$$

Remarks

* Thus constructed Green's function (streamfunction) satisfies the BC $\psi|_{\partial\underline{\Omega}} = \psi_b$
* The image vortex moves together with the original vortex



* finding image vortices is straightforward in simple geometries only; otherwise it can be quite difficult

* in ~~[illegible]~~ general situations other methods may be preferable (continuous distribution of vorticity on the boundary)

<u>Problem</u> – Given N particles with strengths $\{\Gamma_i\}_{i=1}^N$ and positions $\{\bar{x}_i\}_{i=1}^N$, how to compute the force (velocity) at each particle's location?

Particle – Particle (PP) approach

Use Green's function to solve the problem

$$\Delta \phi = \sum_i \Gamma_i \delta(\bar{x} - \bar{x}_i)$$

$$\phi(\bar{x}) = \int_\Omega G(\bar{x}, \bar{x}') \sum_{i=1}^{N} \Gamma_i \delta(\bar{x}' - \bar{x}_i) \, dx'$$

$$= \sum_{i=1}^{N} \Gamma_i G(\bar{x}, \bar{x}_i)$$

To evaluate at $\bar{x} = \bar{x}_i$ we omit the undefined self-induction term $\Gamma_i G(\bar{x}_i, \bar{x}_i)$

(~~[illegible]~~ this step can be justified more rigorously)

~~Thus we have:~~

$$\cancel{m_i \ddot{x}_i = \sum_{j=1}^{N} q_i q_j \nabla_{x_i} G(\bar{x}_i, \bar{x}_j)} \quad \cancel{(\Gamma_i \to q_i)}$$

~~and~~

$$\cancel{\ddot{x}_i = \sum_{j=1}^{N} [illegible]}$$

Thus we have

$$m_i \ddot{\bar{x}}_i = -\sum_{j=1}^{N}{}' q_i q_j \nabla_{x_i} G(\bar{x}_i, \bar{x}_j)$$

$$(\Gamma_j \to q_j)$$

$$\dot{\bar{x}}_i = \sum_{j=1}^{N}{}' \Gamma_j \underbrace{\left[\frac{\partial}{\partial y}, -\frac{\partial}{\partial x}\right] G(\bar{x}_i, \bar{x}_j)}_{\text{Biot - Savart kernel}}$$

equations derived previously in an ad-hoc manner

Approach is accurate (exact), but slow - $O(N^2)$

Particle - Mesh (PM) approach

Obtain ϕ (or ψ) by solving the Poisson equation

$$\begin{cases} \Delta \phi = \sum_i q_i \delta(\bar{x} - \bar{x}_i) \\ + \\ BC \end{cases} \quad \text{OR} \quad \begin{cases} \Delta \psi = -\sum_i \Gamma_i \delta(\bar{x} - \bar{x}_i) \\ + \\ BC \end{cases}$$

using a mesh - based technique, then differentiate numerically to obtain $\nabla \phi$

Approach potentially much faster, but less accurate. Sources of error:

- interpolation from particle locations onto the grid to determine a mass density distribution
- interpolation of $\nabla \phi$ from the fixed grid onto the particle locations.