* Particle - Particle Approach - Algorithm

Time - stepping loop of the PP method

- compute diagnostics
- compute forces / velocities

```
for k = 1 : Np
    V(k) = 0
end
```

} clean accumulators

```
for k = 1 : Np
    for l = 1 : Np
        if (k ≠ l)
            V(k) = V(k) + F(k,l)
        end
    end
end
```

$\underbrace{F(k,l)}$ evaluation of binary (particle-particle) interactions

- integrate equations of motion

```
for k = 1 : Np
    xnew = xold + dt * V(k)
end
```

end of time-stepping loop

Remark

Using the symmetry of the particle-particle interactions, the computational cost of the main loop can be reduced by half $V(l) = V(l) - F(k,l)$

REGULARIZATION

Using Green's functions, the velocity field can be expressed as

$$\bar{V} = [u, v] = \left[\frac{\partial}{\partial y}, -\frac{\partial}{\partial x}\right] \int_{\Omega} G(\bar{x} - \bar{x}')\, \omega(\bar{x}')\, d\Omega$$

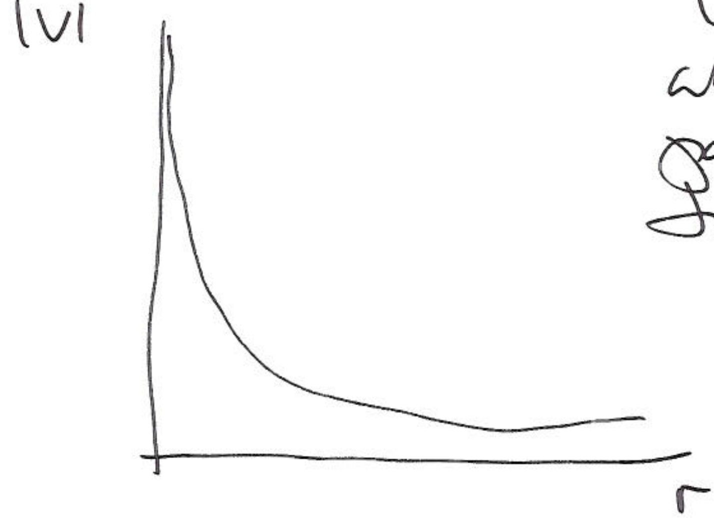
$$= \underbrace{\int_{\Omega} K(\bar{x} - \bar{x}')}_{\text{Biot-Savart kernel}}\, \omega(\bar{x}')\, d\Omega$$

If $G(\bar{x} - \bar{x}') = \frac{1}{2\pi} \ln|\bar{x} - x'|$

then $K(\bar{x} - \bar{x}') = ~~[illegible]~~ \frac{[-(y-y'), x-x']}{2\pi r^2}$

where $r = |\bar{x} - \bar{x}'|$

Analogous expressions can be obtained for forces in the celestial mechanics & electrodynamics problems



Velocity becomes unbounded when $r \to 0$, i.e. two particles get very close together

Issues:

— numerical stability
↳ tighter time-step limitations

<u>Solutions</u>:

* "mollify" the Biot - Savart kernel, so that it does not become singular

* replace the point vortex (mass, charge) with a smoothed distribution

We will show that in principle these two approaches are closely related

Introduce the <u>regularization parameter</u> $\delta > 0$

then the <u>regularized</u> velocity field

$$\bar{V}_\delta(\bar{x}) = \int_\Omega K_\delta(\bar{x}-\bar{x}')\,\omega(\bar{x}')\,d\Omega$$

$$\text{where } \bar{\omega}(\bar{x}') = \sum_{k=1}^{N} \Gamma_k\,\delta(\bar{x}'-\bar{x}_k)$$

$K_\delta \xrightarrow[\delta \to 0]{} K$ is the regularized (mollified) Biot - Savart kernel

For simplicity, set $\underline{\bar{x}'=0}$

then

$$K_\delta(\bar{x}) = K * \omega_\delta(\bar{x}) = \int_\Omega K(\bar{x}-\bar{x}'')\,\omega_\delta(\bar{x}'')\,d\Omega$$

$\omega_\delta(|\bar{x}|)$ - radially symmetric mollifier

$$K_\delta(\bar{x}) = K(\bar{x}) \int_\Omega \omega_\delta(\bar{x})\,d\Omega = \frac{[-y, x]}{2\pi r^2}\, f\!\left(\frac{r}{\delta}\right)$$

where
$$g(r) = 2\pi \int_0^r x' \omega_{\delta=1}(x')\,dx'$$

δ - also called the "cut-off" parameter

K_δ thus may alternatively be interpreted as:

- modified (mollified) velocity field induced by a point vortex
- classical velocity field induced by a smeared (finite-size) ~~???~~ vortex; distribution of vorticity in this regularized vortex is given by $\omega_\delta(x) = \delta^2 \omega_1(\frac{x}{\delta})$

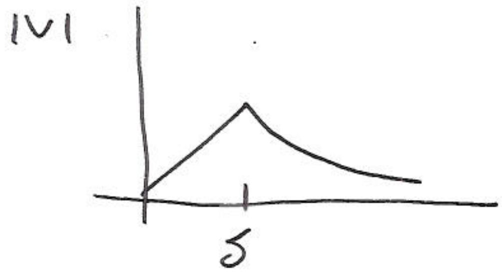
Possible choices:

* Rankine vortex

$$\omega_\delta(\bar{x}) = \begin{cases} \frac{1}{\pi\delta^2}, & 0 < r < \delta \\ 0, & r > \delta \end{cases}$$

The corresponding velocity

$$V(\bar{x}) = \begin{cases} \frac{[-y, x]}{2\pi\delta^2}, & 0 < r < \delta \quad // \text{ solid body rotation} \\ \frac{[-y, x]}{2\pi r^2}, & r > \delta \quad // \text{ potential flow} \end{cases}$$



* other choices — simply desingularize the denominator by including an extra term δ^2

$$V(\bar{x}) = \frac{[-y, x]}{2\pi r^2 + \delta^2}$$

Remarks

* Regularization required for numerical stability in all more complicated computations

* Particle system with mollified Biot-Savart kernels is no longer Hamiltonian; its conservation property may be different

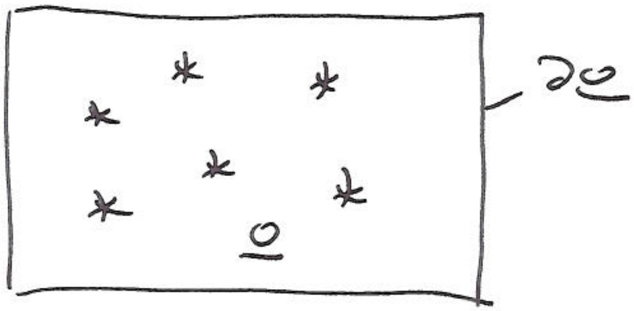
* ———— * ———— *

Particle - Mesh (PM) approach

Time - stepping loop of the PM method

- compute diagnostics
- interpolate particles onto the grid (to obtain the RHS for the Poisson eq.)
- solve the Poisson equation for the potential φ (streamfunction ψ)
- differentiate the potential / streamfunction to obtain the components of force / velocity
- interpolate the force / velocity back to particle locations
- integrate equations of motion

* The Poisson equation $\Delta \psi = -\sum_{k=1}^{N} \Gamma_k \delta(\bar{x}-\bar{x}_k)$



How about the boundary conditions $\psi|_{\partial \underline{\Omega}} = ?$

$\underline{\Omega}$ represents a truncation of an infinite domain $\mathbb{R}^d$, therefore the behaviour of of ψ on the boundary $\partial \underline{\Omega}$ should mimick its behaviour in unbounded domain. Thus, we should use the exact representation

$$\psi|_{\partial \underline{\Omega}} = -\int_{\underline{\Omega}} G(x|_{\partial \underline{\Omega}} - x') \sum_{k=1}^{N} \Gamma_k \delta(\bar{x}' - \bar{x}_k)\, d\underline{\Omega}$$

$$= -\sum_{k=1}^{N} \Gamma_k \ln |\bar{x}|_{\partial \underline{\Omega}} - \bar{x}_k|$$

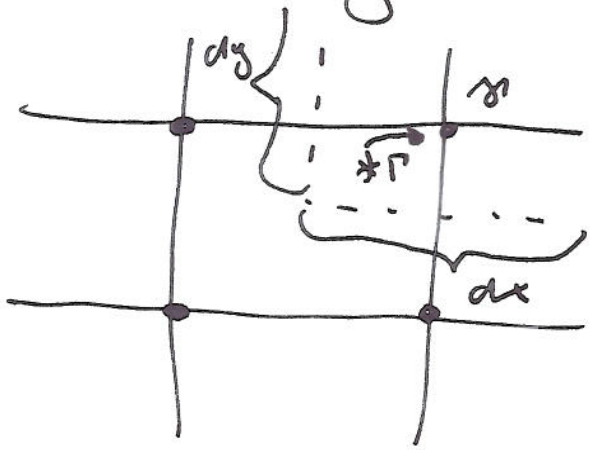
Remark:

* Note that using homogeneous BCs $\psi|_{\partial \underline{\Omega}} = 0$ is equivalent to imposing solid boundaries

$$\psi|_{\partial \underline{\Omega}} = 0 \Rightarrow \frac{\partial \psi}{\partial s}\Big|_{\partial \underline{\Omega}} = \bar{V} \cdot \bar{n} = 0$$

* Interpolation Particles – Mesh

– nearest neighbour (zero-order) interpolation

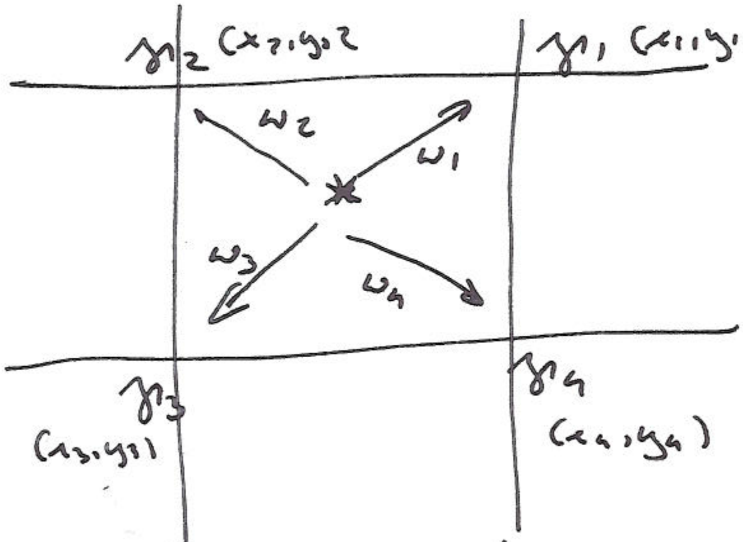


$\int \Gamma dx dy = \Gamma$

– zeroth order conserved

– other moments not conserved
($\int \Gamma x\, dx dy$, $\int \Gamma y\, dx dy$, $\int \Gamma (x^2+y^2) dx dy$)

– first - ~~order~~ order interpolation



How to choose weights $w_1, \dots, w_4$?

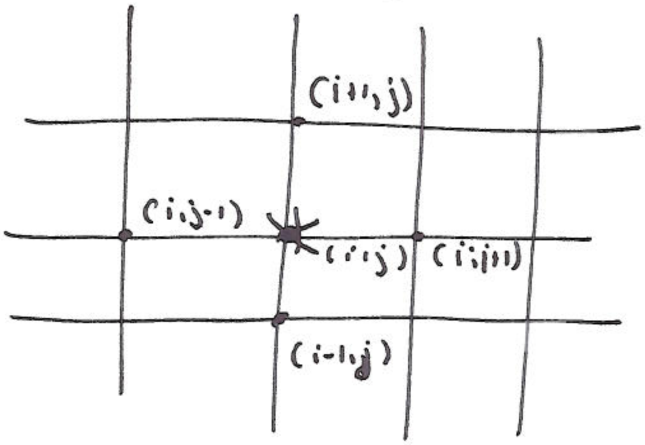
Choose them, so that they satisfy the following moment conditions

Four equations for four unknowns $w_1, \dots, w_4$

all moments up to the second conserved.

$$
\left\{
\begin{aligned}
\sum_{i=1}^{4} w_i &= \Gamma \\
\sum_{i=1}^{4} w_i x_i &= \Gamma x \\
\sum_{i=1}^{N} w_i y_i &= \Gamma y \\
\sum_{i=1}^{N} w_i (x_i^2 + y_i^2) &= \Gamma r^2
\end{aligned}
\right.
$$

* Solution of the Poisson equation



$$\Delta u = \frac{u_{i+1,j} + u_{i-1,j} - 4u_{i,j} + u_{i,j+1} + u_{i,j-1}}{h^2} + O(h^2)$$

u_{ij} put into a vector

$$u_{i,j} = u_{i\cdot(N_m-1)+j}$$

Need to solve a pentadiagonal system

$$\begin{bmatrix} 4 & -1 & \ddots & -1 & \ddots & 0 \\ -1 & \ddots & \ddots & & \ddots & -1 \\ \ddots & \ddots & \ddots & \ddots & & \ddots \\ -1 & & \ddots & \ddots & \ddots & -1 \\ 0 & \ddots & & \ddots & \ddots & \ddots \\ & & -1 & & -1 & 4 \end{bmatrix} \begin{bmatrix} u_1 \\ \\ u \\ \\ u_{N^2} \end{bmatrix} = \begin{bmatrix} \\ RHS \\ \\ \end{bmatrix}$$

Remarks

* in 3D the system is septadiagonal

* BCs (Dirichlet) added to the RHS

* cost of iterative solution (Jacobi, Gauss-Seidel, SOR, ADI, LTDMA, ...) is $O(N_m^3)$
N_m is the number of grid points, not particles
($N_m \ll N$)

* finite-differencing the potential gives force/velocity on a staggered grid