P. Koumoutsakos, M. Troyer
ETH Zentrum, CLT F 12
CH-8092 Zürich

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Set 8 - Particle Methods

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Question 1: Roll-up of 1D Vortex Sheet

Given N point vortices in 2D, the total vorticity field can be expressed as

$$\boldsymbol{\omega}(\mathbf{x}) = \omega(\mathbf{x})\hat{\mathbf{e}}_\mathbf{z} = \sum_{n=1}^{N} \Gamma_n \delta(\mathbf{x} - \mathbf{x}_n)\hat{\mathbf{e}}_\mathbf{z}, \tag{1}$$

where Γ_n and $\mathbf{x}_n$ are the strength and location vector of point vortex n, respectively.

We are interested in finding the velocity $\mathbf{u} = u\hat{\mathbf{e}}_\mathbf{x} + v\hat{\mathbf{e}}_\mathbf{y} \equiv \nabla \times \boldsymbol{\Psi}$ due to this vorticity field, where $\boldsymbol{\Psi} = \Psi\hat{\mathbf{e}}_\mathbf{z}$. We can find the streamfunction Ψ from the vorticity field ω by solving a Poisson equation:

$$\nabla^2\Psi = -\omega. \tag{2}$$

Using the Green's function solution of the Poisson equation we can write down an explicit expression of Ψ in integral form. Taking the curl of that will provide us with the velocity vector $\mathbf{u}$.

From here on we replace our two-dimensional vectors by complex numbers. A spatial coordinate vector $\mathbf{x} = x\hat{\mathbf{e}}_\mathbf{x} + y\hat{\mathbf{e}}_\mathbf{y}$ is represented by a single complex number $Z \equiv x + iy$ where $i^2 = -1$. In this formulation, the real part of Z corresponds to the x-coordinate and the imaginary part of Z corresponds to the y-coordinate. Similarly, we replace the vector $\mathbf{u}$ with a complex formulation $V(Z) \equiv u - iv$ (note the minus!).

The velocity field can then be expressed as

$$V(Z) = -\frac{i}{2\pi}\sum_{n=1}^{N}\frac{\Gamma_n}{Z - Z_n}. \tag{3}$$

We can thus evolve the vortex particles by integrating their position according to the evolution equation

$$\frac{\mathrm{d}Z_j}{\mathrm{d}t} = \bar{V}(Z_j), \tag{4}$$

where the bar denotes the complex conjugate.

a) Consider two vortices with circulations Γ_1 and Γ_2, originally located on the $y = 0$ axis at

$$Z_1(t = 0) = \Delta/2 \tag{5}$$
$$Z_2(t = 0) = -\Delta/2. \tag{6}$$

The vortices now move under their self-induced velocities following Equation 4, where the velocities are computed from Equation 3:

$$V(Z_1) = -\frac{i}{2\pi}\frac{\Gamma_2}{Z_1(t) - Z_2(t)}, \tag{7}$$
$$V(Z_2) = -\frac{i}{2\pi}\frac{\Gamma_1}{Z_2(t) - Z_1(t)}. \tag{8}$$

How do the two particles move, if $\Gamma_1 = \Gamma_2 = \Gamma$?
Substituting $\Gamma_1 = \Gamma_2 = \Gamma$ into the velocity definitions we get

$$V(Z_1, t) = -\frac{i}{2\pi}\frac{\Gamma}{Z_1(t) - Z_2(t)} \tag{9}$$
$$V(Z_2, t) = -\frac{i}{2\pi}\frac{\Gamma}{Z_2(t) - Z_1(t)} = -V(Z_1, t). \tag{10}$$

In Cartesian form, this translates to

$$u_1(t) = -\frac{\Gamma}{2\pi}\frac{y_1 - y_2}{|\mathbf{x}_1 - \mathbf{x}_2|^2} \tag{11}$$
$$v_1(t) = \frac{\Gamma}{2\pi}\frac{x_1 - x_2}{|\mathbf{x}_1 - \mathbf{x}_2|^2} \tag{12}$$
$$u_2(t) = -\frac{\Gamma}{2\pi}\frac{y_2 - y_1}{|\mathbf{x}_1 - \mathbf{x}_2|^2} \tag{13}$$
$$v_2(t) = \frac{\Gamma}{2\pi}\frac{x_2 - x_1}{|\mathbf{x}_1 - \mathbf{x}_2|^2} \tag{14}$$
$$\tag{15}$$

If we introduce the angle of vortex 1 relative to the position of vortex 2 as $\tan\theta = (y_1 - y_2)/(x_1 - x_2)$, we get

$$u_1(t) = -\frac{\Gamma}{2\pi\Delta}\sin(\theta) \tag{16}$$
$$v_1(t) = \frac{\Gamma}{2\pi\Delta}\cos(\theta) \tag{17}$$

Since $V(Z_2, t) = -V(Z_1, t)$, this means that the vortices will move with a constant and equal azimuthal velocity $\Gamma/(2\pi\Delta)$ on a circle with radius Δ.
How does their behavior change if instead we have $\Gamma_1 = -\Gamma_2 = \Gamma$?
Substituting $\Gamma_1 = -\Gamma_2 = \Gamma$ into the velocity definitions we get

$$V(Z_1, t) = -\frac{i}{2\pi}\frac{\Gamma}{Z_1(t) - Z_2(t)} \tag{18}$$
$$V(Z_2, t) = \frac{i}{2\pi}\frac{\Gamma}{Z_2(t) - Z_1(t)} = V(Z_1, t). \tag{19}$$

We see therefore that both particles have the same velocity. Furthermore, because $Z_1(0) - Z_2(0)$ is real, the velocity is complex and therefore the particles will move upward with an equal velocity. The difference $Z_1(t) - Z_2(t)$ does not change with time and the particles will just keep moving upward with constant velocity $V = \Gamma/(2\pi\Delta)$.

b) Based on the equations (1), (3) and (4), implement a double precision, serial N-body solver using a forward Euler time stepping scheme.

Distribute the N particle uniformly on a straight horizontal line ($y = 0$) of length $L = 1$ starting at $x = -0.5$:

$$x_{p_j} = -0.5 + (j + 0.5) \cdot h, \tag{20}$$

where $h = 1/N$ is the initial distance between the particles (N is the number of particles in the simulation) and j is the particle index.

The initial circulation can be computed as:

$$\Gamma(x_p) = \gamma(Z)h, \tag{21}$$

where

$$\gamma(Z) = -\frac{d}{dx}\left[\Gamma_s\sqrt{1 - \left(\frac{x}{0.5}\right)^2}\right]. \tag{22}$$

Assume $\Gamma_s = 1$.

This initial condition should give you a velocity distribution that rolls up the particles at both ends of the line, as a model of a vortex sheet. This is a simplified model of, for instance, the time evolution of a cross-section of an aircraft wake as shown in Figure 1.

Figure 1: Wake behind an aircraft that is visualized because of condensation behind the engines. The vortical structures arise because of the loading on the wings.

Run your vortex code using $10\,000$ particles and show a plot of particle positions at $t = 0.5$, $t = 1.0$ and $t = 2.0$, or, alternatively, create a small animation. Use a timestep $\delta t = 10^{-3}$ to integrate equation (4).

The code is contained in the corresponding solution folder. Figure 2 show the roll-up of the vortex sheet. The singular nature of our point vortices, the limited floating point accuracy and the low-order timestepping cause small perturbations that results in the clustering of particles, and eventually the breaking of symmetry. Several solutions for this problem have been proposed in literature, for instance by regularizing the particle kernel from a Dirac delta function to some smooth function such as a Gaussian.

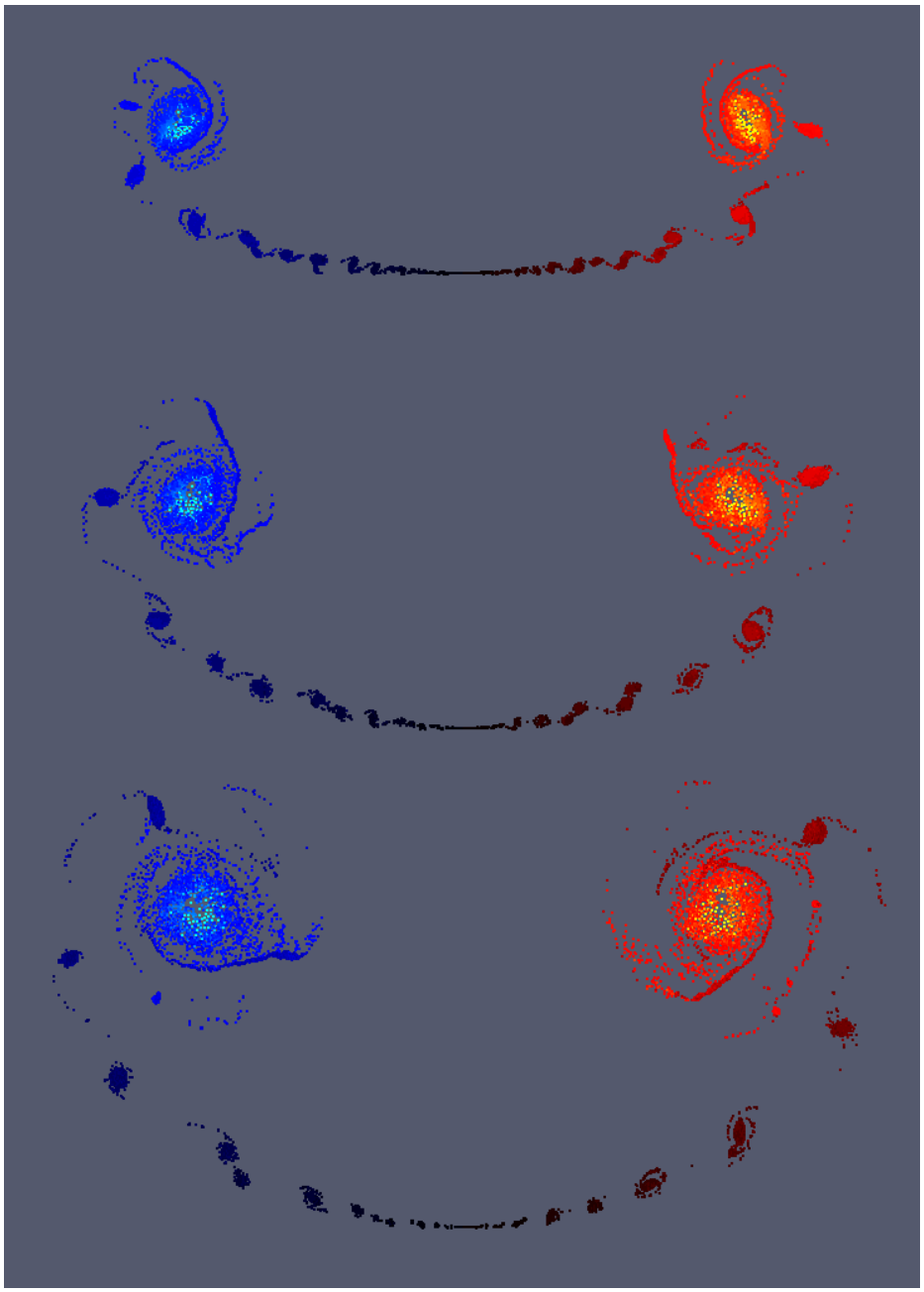

Figure 2: Evolution of the vortex sheet at times $t = 0.5$, $t = 1.0$ and $t = 2.0$, from top to bottom.

		process rank p				
		1	2	$\cdots$	P-1	P
	1	V_1	V_2	$\cdots$	V_{P-1}	V_P
	2	V_2	V_3	$\cdots$	V_P	V_1
pass q	$\vdots$			$\vdots$		
	P-1	V_{P-1}	V_P	$\cdots$	V_{P-3}	V_{P-2}
	P	V_P	V_1	$\cdots$	V_{P-2}	V_{P-1}

Table 1: Multipass approach for the N-body problem.

c) Parallelize your code using MPI and report weak and strong scaling.

You should assume that the N particles do not fit into the memory of a single MPI process. Therefore, you need to split the particles such that each process p has $M = N/P$ particles with positions $\{Z_{p_i}\}_{i=1}^{M}$, where P is the number of processes.

The computation of the interactions of each particle with position Z_{p_i} can be expressed as follows:

$$V(Z_{p_i}) = -\frac{i}{2\pi}\sum_{n=1}^{N}\frac{\Gamma_n}{Z_{p_i}-Z_n} = -\frac{i}{2\pi}\sum_{q=1}^{P}\sum_{n=1+(q-1)M}^{qM}\frac{\Gamma_n}{Z_{p_i}-Z_n} = -\frac{i}{2\pi}\sum_{q=1}^{P}V_q(Z_{p_i}). \quad (23)$$

The above equation will be implemented with a multi-pass approach, where in each pass, each process p computes an internal sum

$$V_q(Z_{p_i}) = \sum_{n=1+(q-1)M}^{qM}\frac{\Gamma_n}{Z_{p_i}-Z_n}. \quad (24)$$

Therefore, for P processes, there will be P passes.

At the end of each pass, the processes will then need to exchange particles with each other.

Table 1 shows the task of each process rank at each pass.

Figure 3 shows the strong scaling and weak efficiency for the implementation given in the solutions. Both show perfect behavior for the case with $N = 10^4$ and $N = 10^5$, where in the first case 100 samples per point have been measured, while in the 2nd, 10 samples are considered.

The reasons for this behavior can be found in the low communication costs, which are negligible compared to the computation ($< 0.2\%$) and due to the small problem size (even with 100000 particles), the problem fits into the caches, so that the effective bandwidth when doing computations is high enough that the problem is computationally bound.

Although, this implementation might look ideal from a computer performance point of view however, the approach taken in this exercise is inefficient and expensive from a mathematical point of view and algorithmic improvements can lead to better time-to-solution (which is actually the objective of performance optimizations), even for worse scaling behaviors.

d) Experiment with different vorticity distributions. How does the behavior of the vortex sheet change?

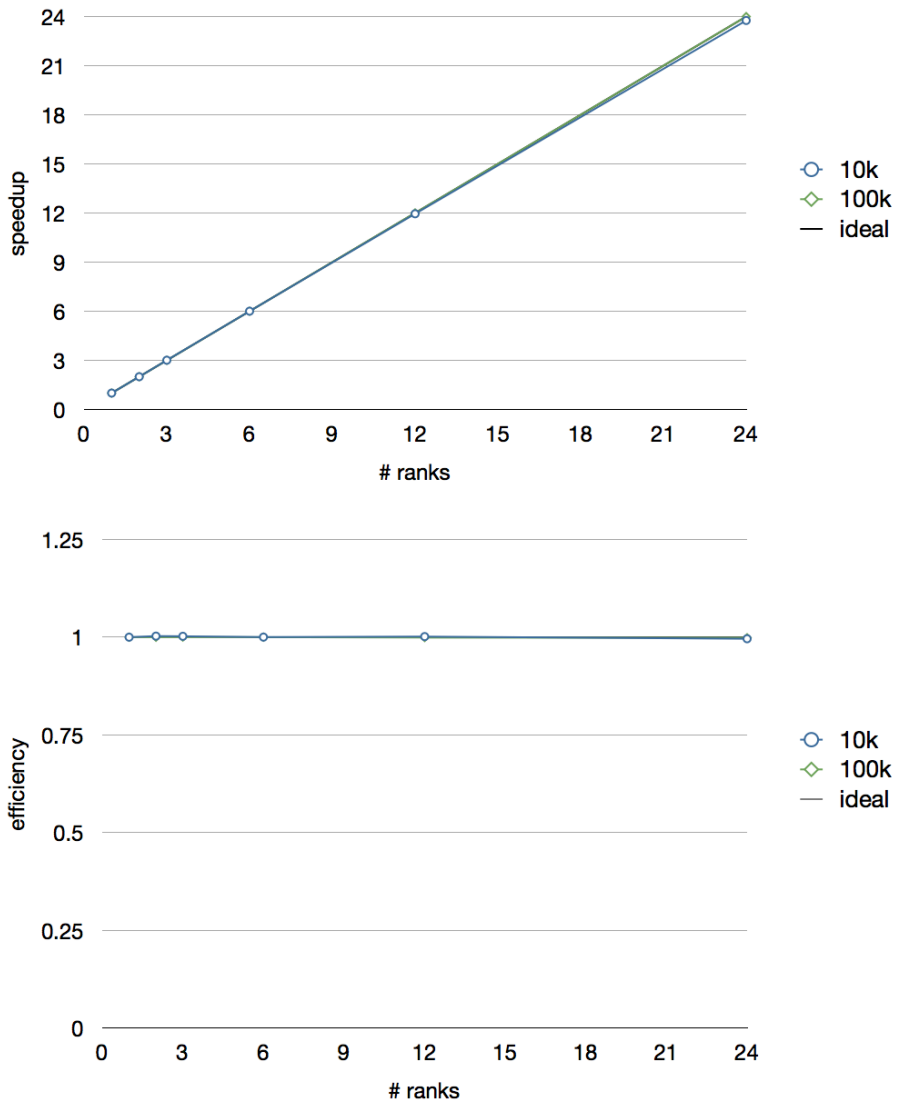

Figure 3: Strong scaling (top) and weak efficiency (bottom).

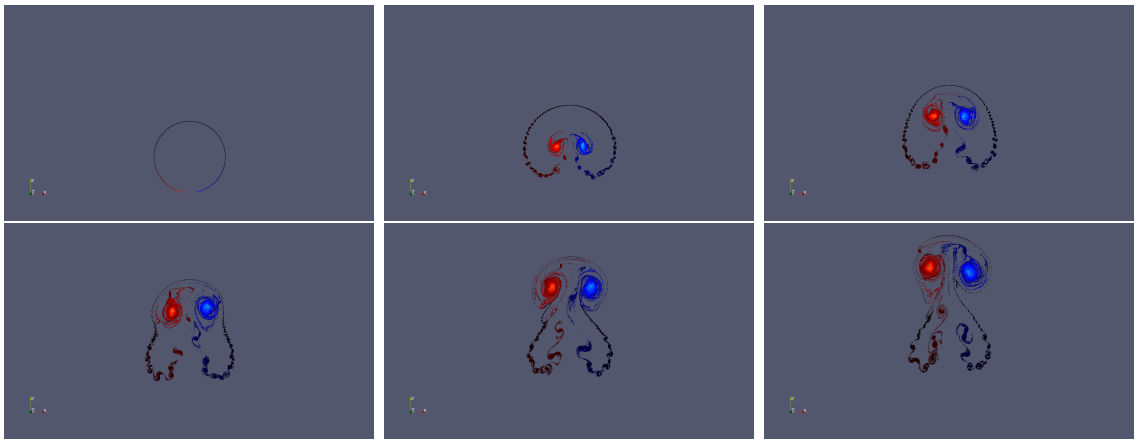

Figure 4: Evolution of a circular vortex sheet.

Figure 4 shows the evolution of a vortex sheet placed in a circular configuration, with the same vorticity distribution but with a higher magnitude $\Gamma_S = 10$.

Summary

Summarize your answers, results and plots into a PDF document. Furthermore, elucidate the main structure of the code and report possible code details that are relevant in terms of accuracy or performance. Send the PDF document and source code to your assigned teaching assistant.