Drafts for Project-Particle Methods for Vortex Problems

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We begin with Poisson's equation in continuous form:

$$\nabla^2 \psi(\mathbf{x}) = -\rho(\mathbf{x})$$

The solution using the Green's function is given by:

$$\psi(\mathbf{x}) = \int_{\mathbb{R}^2} G(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x}')\, d\mathbf{x}'$$

Solving Poisson's equation numerically on a discrete grid, means the domain, potential, source, and Green's function are sampled at grid points. To discretize this:

- Let the domain be sampled on a uniform 2D grid with spacing h
- Let $i = (i_x, i_y)$ index the grid points
- Let $\mathbf{x}_i = h \cdot i$ be the physical coordinates
- Define $\rho_j = \rho(\mathbf{x}_j)$ Here, $G(i - j)$ is the Green's function for the Laplacian in 2D (solution to Poisson's equation)

Then, we approximate the integral using a Riemann sum and denote $\omega_j^g = \rho_j$.

$$\psi_i = \sum_{j \in \mathbb{Z}^2} G(i - j)\, \omega_j^g$$

where ω_j represents the value of ρ at the grid point j, and the sum runs over all grid points $j \in \mathbb{Z}^2$. The function $G(i - j)$ gives the influence of the source at point j on the potential at point i.

The potential on the grid is given by ψ_i, and the source on the grid is given by ω_j^g.

Hockney's algorithm utilizes that The Fourier transform of a convolution equals the product of the Fourier transforms.

$$\begin{aligned} \mathcal{F}\left(f * g\right) &= \mathcal{F}(f) \cdot \mathcal{F}(g) \\ f * g &= \mathcal{F}^{-1}\left[\mathcal{F}(f) \cdot \mathcal{F}(g)\right] \end{aligned}$$

You will be implementing parts of a particle-in-cell (PIC) method for vortex dynamics, described below. This is primarily an exercise in more elaborate template programming. Generally speaking, you are integrating an ODE of the form

$$\frac{dX}{dt} = F(t, X) \tag{1}$$

In this problem set our forcing functions will all be independent of time, so you can ignore the `a_time` argument, but it is good to have this form available to you when you use RK4 in other projects. We will be using the 4th-order explicit Runge-Kutta integration technique to evolved this system of ODEs. In this case X is the class `ParticleSet`.

The stages of RK4 all require the calculation of quantities of the form

$$k := \Delta t * F(t + \Delta t, X + k) \tag{2}$$

Your F operator is an evaluation of everything on the right of the equal sign. RK4 is built up by various estimates of what the update to X should be, then recombined to cancel out low order error terms to create a stable method with an error in the solution that is $O(\Delta t)^4$.

Specifically, you will implement the class `ParticlesVelocities`, that has the single member function

```
void operator()(ParticleShift& a_result,
                double a_time,
                double a_deltat,
                const ParticleSet& a_X)
```

The input is the current estimate for k, `a_result`, and the output new estimate for k is returned in `a_result`:

$$k := \Delta t F(t + \Delta t, X + k)$$

Inputs are the time you are to evaluate the function $t + \Delta t$, the timestep to take Δt, the state at the start of the timestep X in this case `ParticleSet`, and the shift to use to this state in this evaluation of F k, represented by the `ParticleShift` class. In the case of our particle method, F has no explicit dependence on the first time argument, but we still have implement our class as if it does, in order to conform to the general RK4 interface.

Specific Instructions

You are to implement in the directory /src/Particles `ParticleVelocities::operator()(ParticleShift& a_k, const double& a_time, const double& dt, ParticleSet& a_state)` : computes the $k's$ induced on a set of particles by all of the particles in the input `ParticleSet` displaced by the input k. In addition, you are to implement a driver program that performs the following calculations.

1. A single particle, with strength $1./h^2$, placed at (i) (.5,.5) , (ii) .4375,5625, (iii) .45,.55 . The number of grid points is given by N = 32, $\Delta t = 1.$; run for 100 time step. In all of these cases, the displacement of the particle should be roundoff, since the velocity induced by a single particle on itself should vanish. In the case of the initial position of (.5,.5) the displacement should be comparable to roundoff. Output: position of the particle after one step

2. Two particles: one with strength $1/h^2$ located at (.5,.5), the other with strength 0, located at (.5,.25). The number of grid points is given by N = 32. Run for 300 time steps, $\Delta t = .1$. The strength 1 particle should not move, while the zero-strength particle should move at constant angular velocity on a circle centered at (.5,.5) of radius .25. Output: graph of the time history of the radius and angle.

3. Two particles: located at (.5,.25) and (.5,.75) both with strength $1/h^2$. The number of grid points is given by N = 32. Both particles should move at a constant angular velocity on a circle centered at (.5,.5) of radius .25. Output: graph of the time history of the radius and angle for both particles.

4. Two-patch problem. For each point $\boldsymbol{i} \in [0 \dots N_p]$, $N_p = 128, 256$, place a particle at the point $\boldsymbol{i}h_p$, $h_p = \frac{1}{N_p}$ provided that

$$||\boldsymbol{i}h_p - (.5, .375)|| \leq .12 \text{ or } ||\boldsymbol{i}h_p - (.5, .625)|| \leq .12.$$

   The strength of each of the particles should be h_p^2/h^2. This corresponds to a pair of patches of vorticity of constant strength. Take the grid spacing $N = 64$. Integrate the solution to time T = 15, plotting the result at least every 1.25 units of time (to make a nifty movie, plot every time step). Set $\Delta t = .025$. We will provide a reference solution against which you can compare yours.

By setting `ANIMATION = TRUE` in your makefile, you can produce a pair of plotfiles every time step (particle locations, vorticity field on the grid). The default is to produce a pair of plotfiles at the end of the calculation for the two-patch case.

Description of Algorithm for Computing the Velocity Field

1. Depositing the charges in the particles on the grid.

$$\omega^g_{\boldsymbol{i}} = \sum_k \omega^k \Psi(\boldsymbol{i}h - \boldsymbol{x}^k)$$

   where the $\boldsymbol{x}^k$'s are the positions of the particles in `a_state` displaces by the input `a_k`'s.

$$\omega^g \equiv 0$$

$$\boldsymbol{i}^k = \left\lfloor \frac{\boldsymbol{x}^k}{h} \right\rfloor$$

$$\boldsymbol{s}^k = \frac{\boldsymbol{x}^k - \boldsymbol{i}^k h}{h}$$

$$\omega^g_{\boldsymbol{i}^k} += \omega^k (1 - s^k_0)(1 - s^k_1)$$

$$\omega^g_{\boldsymbol{i}^k+(1,0)} += \omega^k s^k_0 (1 - s^k_1)$$

$$\omega^g_{\boldsymbol{i}^k+(0,1)} += \omega^k (1 - s^k_0) s^k_1$$

$$\omega^g_{\boldsymbol{i}^k+(1,1)} += \omega^k s^k_0 s^k_1$$

2. Convolution with the Green's function to obtain the potential on the grid, using Hockney's algorithm. The Hockney class will be constructed and maintained in `ParticleSet` - all you have to do is call it at the appropriate time.

$$\psi_{\boldsymbol{i}} = \sum_{\boldsymbol{j} \in \mathbb{Z}^2} G(\boldsymbol{i} - \boldsymbol{j}) \omega^g_{\boldsymbol{j}}$$

3. Compute the fields on the grid using finite differences.

$$\vec{U}^g_{\boldsymbol{i}} = \Big(\frac{\psi_{\boldsymbol{i}+(0,1)} - \psi_{\boldsymbol{i}-(0,1)}}{2h}, - \frac{\psi_{\boldsymbol{i}+(1,0)} - \psi_{\boldsymbol{i}-(1,0)}}{2h} \Big)$$

4. Interpolate the fields from the grid to the particles.

$$\vec{U}^k = \sum_{\boldsymbol{i} \in \mathbb{Z}^2} \vec{U}_{\boldsymbol{i}} \Psi(\boldsymbol{x}^k - \boldsymbol{i}h)$$

$$\begin{aligned} \boldsymbol{i}^k &= \left\lfloor \frac{\boldsymbol{x}^k}{h} \right\rfloor \\ \boldsymbol{s}^k &= \frac{\boldsymbol{x}^k - \boldsymbol{i}^k h}{h} \end{aligned}$$

$$\begin{aligned} \vec{U}^k =& \vec{U}^g_{\boldsymbol{i}} (1 - s^k_0)(1 - s^k_1) \\ &+ \vec{U}^g_{\boldsymbol{i}+(1,0)} s^k_0 (1 - s^k_1) \\ &+ \vec{U}^g_{\boldsymbol{i}+(0,1)} (1 - s^k_0) s^k_1 \\ &+ \vec{U}^g_{\boldsymbol{i}+(1,1)} s^k_0 s^k_1 \end{aligned}$$

Note that the operator`ParticleVelocities::operator()` requires you to return in `a_k` the quantities $\Delta t \vec{U}^k$.