Projects for Grant Holders
Scientific Computing Advanced Training (SCAT) Mobility Programme

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1 Development of a completely meshless method for CFD

In Computational Fluid Dynamics (CFD), the "mainstream" methods used are: finite difference methods, finite element methods, finite volume methods, spectral methods. All of these rely on first constructing a *mesh* on the domain of computation, and then writing out discrete versions of the governing equations that solve for the quantities of interest on the nodes of this mesh.

There is a new "wave" in some areas of computational science where people are interested in finding alternative ways of doing computations without using a computational mesh. This is a very challenging and new field.

Some of the reasons why a *meshless* method might be useful are:

- the work required to actually construct a mesh is many times too large, even larger than actually solving the equations;
- there are errors associated with computing things on a mesh that one may be able to get rid of if a meshless method is used;
- many problems have complicated geometries and many scales on which things are happening, and a computational mesh is awkward to deal with these things.

In my research, I have produced improvements on one special meshless method used in fluid dynamics that relies on vortex particles to solve the equations. This method has proved to be very accurate, and useful to solve problems for example in high-Reynolds number vortex dynamics, where accuracy is crucial (in addition to low numerical diffusion, which is another advantage of the particle approach). But there are a number of further improvements that can be made, which could be the topic of your project; see Topics further below.

The formulation of the vortex method is as follows. Let $\mathbf{u}(\mathbf{x}, t)$ be the velocity field and $\boldsymbol{\omega}(\mathbf{x}, t) = \nabla \times \mathbf{u}(\mathbf{x}, t)$ the vorticity field. Taking the curl of the momentum equation and considering an incompressible fluid for which $\nabla \cdot \mathbf{u}(\mathbf{x}, t) = 0$, the vorticity transport equation is obtained. This is the governing equation in vortex methods, which for three-dimensional flow corresponds to the following vector equation,

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\omega} = \boldsymbol{\omega} \cdot \nabla \mathbf{u} + \nu \Delta \boldsymbol{\omega}. \tag{1}$$

The assumptions in the above equation are: constant density flow, conservative body forces, an inertial frame of reference and unbounded domain. In the case of a two dimensional and inviscid flow the right-hand side of (1) is zero and the governing equation reduces to the simple form $\frac{D\omega}{Dt} = 0$, where $\frac{D}{Dt}$ stands for the material derivative. This corresponds to the basic formulation of vortex methods, for which clearly a Lagrangian method based on elements of vorticity is natural and ideal.

In the vortex blob discretization, the elements are identified by a position vector, $\mathbf{x}_i$; a strength vector (vorticity×volume) of circulation; and a core size, σ_i. The discretized vorticity field is expressed as the sum of the vorticities of the vortex elements in the following way:

$$\boldsymbol{\omega}(\mathbf{x}, t) \approx \boldsymbol{\omega}^h(\mathbf{x}, t) = \sum_{i=1}^{N} \boldsymbol{\Gamma}_i(t) \zeta_{\sigma_i} \left(\mathbf{x} - \mathbf{x}_i(t)\right), \tag{2}$$

where $\boldsymbol{\Gamma}_i$ corresponds to the vector circulation strength of particle i (scalar in 2D). In the blob version of the vortex method —in contrast to point vortices, the elements have a non-zero core size σ_i and a characteristic distribution of vorticity ζ_{σ_i}, commonly called the cutoff function. Frequently, the blob cutoff function is a Gaussian distribution and the core sizes are uniform ($\sigma_i = \sigma$), which means that in two dimensions one has

$$\zeta_\sigma(\mathbf{x}) = \frac{1}{k\pi\sigma^2} \exp\left(\frac{-|\mathbf{x}|^2}{k\sigma^2}\right), \tag{3}$$

where the constant k determines the width of the cutoff and is chosen by different authors as either 1, 2 or 4.

In the majority of vortex methods (almost all), the Lagrangian formulation is expressed by assuming that the vortex elements convect without deformation with the local velocity. The velocity is obtained from the vorticity using the Biot-Savart law:

$$\begin{aligned} \mathbf{u}(\mathbf{x}, t) &= \int (\nabla \times \mathbf{G})(\mathbf{x} - \mathbf{x}')\omega(\mathbf{x}', t) d\mathbf{x}' \\ &= \int \mathbf{K}(\mathbf{x} - \mathbf{x}')\omega(\mathbf{x}', t) d\mathbf{x}' = (\mathbf{K} * \omega)(\mathbf{x}, t) \end{aligned} \tag{4}$$

where $\mathbf{K} = \nabla \times \mathbf{G}$ is known as the Biot-Savart kernel, $\mathbf{G}$ is the Green's function for the Poisson equation, and $*$ represents convolution. For example, in two dimensions the Biot-Savart law is written explicitly as

$$\mathbf{u}(\mathbf{x}, t) = \frac{-1}{2\pi} \int \frac{(\mathbf{x} - \mathbf{x}') \times \omega(\mathbf{x}', t)\hat{\mathbf{k}}}{|\mathbf{x} - \mathbf{x}'|^2} d\mathbf{x}'. \tag{5}$$

For the customary case of an axisymmetric cutoff function $\zeta = \zeta(r)$, $r = |\mathbf{x}|$, the velocity kernel can be obtained analytically. The velocity regularization function is defined as the integral

$$q(r) = \int_0^r \zeta(r)\, r\, dr. \tag{6}$$

The regularized Biot-Savart kernel is expressed as follows, where $\times$ represents cross product (with the vorticity vector, or $\omega\hat{e}_{\mathbf{z}}$ in the 2D case) and d is the dimension:

$$\mathbf{K}_\sigma(\mathbf{x})\times = -\frac{q(|\mathbf{x}|/\sigma)}{|\mathbf{x}|^d}\cdot\mathbf{x}\times \tag{7}$$

Therefore, for the 2D Gaussian blob with $k=2$ one has

$$\mathbf{K}_\sigma(\mathbf{x}) = \frac{1}{2\pi r^2}(-y,x)\left(1-\exp(-\frac{r^2}{2\sigma^2})\right). \tag{8}$$

The formula for the discrete Biot-Savart law in two dimensions gives the velocity as follows,

$$\mathbf{u}(\mathbf{x},t) = -\sum_{j=1}^{N}\Gamma_j\;\mathbf{K}_\sigma(\mathbf{x}-\mathbf{x}_j). \tag{9}$$

Finally, the Lagrangian formulation of the (viscous) vortex method in two-dimensions is expressed in the following system of equations:

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{u}(\mathbf{x}_i,t) \tag{10}$$

$$\frac{d\omega}{dt} = \nu\nabla^2\omega + \text{B.C.} \tag{11}$$

The complete numerical method is defined by Equations (10) and (11) which express that the method is to be implemented by integrating the particle trajectories due to the local fluid velocity, while the velocity is obtained from the vorticity using the Biot-Savart law. The vorticity field evolves due to the effects of viscosity, both in the free-stream and on the boundaries (no-slip condition, denoted by B.C.). The viscous effects in the free-stream are enforced by one of a variety of viscosity schemes available for vortex methods, while the effects due to solid boundaries are traditionally accounted for by generation of vorticity implemented in a version of the boundary element method. This is based on the physical mechanism by which the solid wall is a source of vorticity that enters the flow, so a vorticity flux $\frac{\partial\omega}{\partial n}$ may be determined at the wall to satisfy the boundary condition of no-slip at the surface.

Topic 1.1 Adding a consistent and accurate treatment of the boundary conditions in the meshless vortex method. This could be a very interesting and challenging project, involving what is called "geometric modelling" (coming up with a mathematical expression describing a surface in 3D or curve in 2D), and theoretical issues of appropriately prescribing boundary conditions for flow simulation. I have a few ideas that can get you started if you choose this project. The goal would be to describe the boundary (surface, or curve in 2D) without resorting to a surface mesh (again). For example, using scattered points to reconstruct the geometry. Successful progress in this project would in fact be a publishable result.

Topic 1.2 Implementing a fast algorithm for obtaining field information from the computational particles. The use of particles for flow simulation has a number of advantages, but the disadvantages are that it is usually computationally expensive to get information from them (for example, the velocity at any point in the domain, or the vorticity). There are ways around this, but they involve very creative algorithms. One of these is the so-called fast multipole method, which was developed originally in the field of astrophysics to calculate the influence of many stars on each other. This project would involve working with my meshless vortex method to find ways to make it faster, more efficient, based on algorithms developed in other fields (or your own!).

Topic 1.3 Extend the meshless vortex method to include variable resolution in the domain. When using vortex particles for flow computation, practically everyone that uses this method has a set of particles of the same exact size (a small size that determines the resolution of the computation). It would be very convenient to be able to carry out computations where one uses particles of varying sizes. For example, if one has a problem of flow around a solid object, very small particles are needed to resolve the boundary later, but larger particles can be used away from the body, thereby saving computational effort. In my present vortex method, particle sizes are uniform; but I have several ideas on how to modify it to allow variable sizes. Your project would be to explore these ideas, and your own, and try them out on test problems.

Topic 1.4 Add the capability of computing flows where there is barotropic generation of vorticity. The vortex method is based on using a form of the equations for fluid flow where the vorticity replaces the velocity as the main variable. In this formulation, one usually assumes that the fluid is incompressible, to obtain a simpler form of the vorticity equation. If we want to add back the neglected term, i.e., the barotropic generation of vorticity, we now need to find how to compute this term with the vortex particles. There are a few attempts of this in the literature, and we could draw on these to come up with an extension to my vortex method for problems with variations of density in the domain. One very interesting application of such an extended method is the study of Rayleigh-Taylor instability, which occurs in supernova remnants (See: `http://tinyurl.com/83bbd`)

2 Topics in vortex flows

Vortex flows have fascinated scientists since the time of Leonardo (maybe even before?). Leonardo observed and made detailed drawings of the vortices that form in the wake of blunt objects in a stream, and the vortical structures formed when a jet of water falls in a pool. Vortices exhibit very complex behavior and interact in sometimes unexpected ways. Classical phenomena in vortex dynamics include: the formation of vortex rings, the merging of like-signed vortices, vortex breakdown, the formation of so-called "vortex streets" behind objects, the appearance of "coherent structures" of vorticity, and many more.

What is most interesting is that even though the dynamics of vorticity has been studied for many years, there are numerous problems that remain unsolved. Also, many times vortices produce patterns and structures that are dazzling and very attractive to observe. Other times, an aura of mystery is attached to vortices; consider for example the case of the Red Spot of Jupiter, which is just a huge vortex in the atmosphere of the giant planet.

In my research, I've studied some peculiar phenomena that occur in two-dimensional vortex dynamics. These are relevant for atmospheric and oceanographic applications (as both the oceans and atmosphere are very nearly two-dimensional fluids). I've studied the self-organization of vorticity, to form a structure called a *tripole*. This is an arrangement of three vortices, one in the center, and two so-called satellites of opposite sign vorticity than the core. You can find some nice pictures and more details

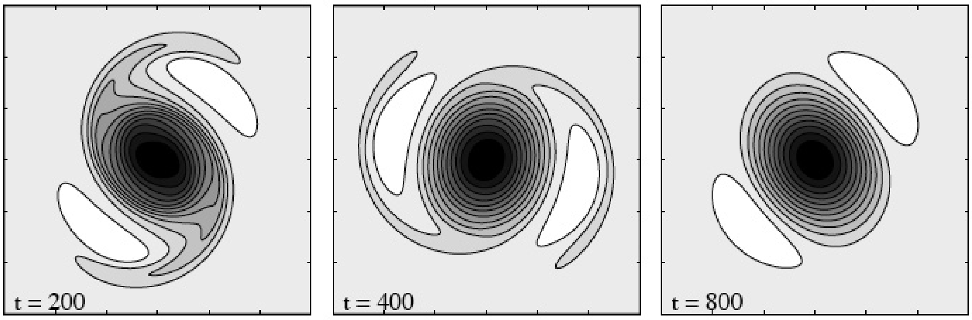

Figure 1: Self-organization of the tripole: 14 equally-spaced contour levels of vorticity. The dark gray and black represents positive vorticity (the fluid turns anti-clockwise), and the white represents negative vorticity (fluid turning clockwise).

in my website `http://www.maths.bris.ac.uk/~aelab/` and also see an example of self-organization of a tripole in Figure 1. There are many interesting questions that you may like to pursue as your project. For example, there are some studies, but no definitive answer to whether the vortex tripole is really a stable object. I suspect that it is, but maybe under certain conditions only. Then there are other structures where the central core is surrounded by three, four, even five satellites. These all seem to be unstable objects, except possibly the one with three satellites, called a triangular vortex; one is shown in Figure 2.

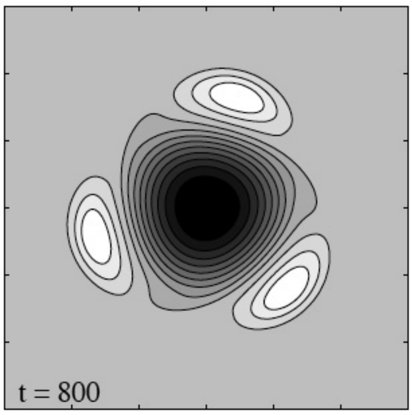

Figure 2: A triangular vortex.

There are other intriguing things that vortices do that would make good topics for projects. For example, sometimes vortices tend to form lattices, that is, arrangements of vortices that remain isolated and just dance around each other. These are called 'vortex crystals'. Also, small and strong vortices tend to travel down or up a slight vorticity gradient (depending on their sign), which is known as 'transverse drift'. All of these effects may be working together sometimes, which contributes to the self-organization of vorticity. Come to see me if you want to know more about these things, and to see some more pretty pictures.

Topic 2.1 Study the stability of the vortex tripole. This is not a straightforward analytical exercise, because there is no analytic solution to the fluid equations that represents a vortex tripole. There is such an analytic solution representing a monopole or a dipole, in contrast, so these objects have been studied in detail. For the tripole, we need to do numerical experiments, and possibly use approximate representations. Sometimes a tripole can go unstable and the core splits, forming two dipoles that travel away from each other. Why? When? How? These are the types of questions you will be looking at.

Topic 2.2 Stability of higher multipoles. Is the triangular vortex stable? We know that a square vortex, having four satellites around a square core, organizes back into a tripole by the merging of pairs of satellites. A pentagon vortex also exists, and is unstable. In this case the satellites merge resulting in a tripole with one larger satellite than the other. What is the difference between this asymmetric tripole and the symmetric counterpart? What are the similarities? There are many interesting questions that you may choose to pursue in this project.

Topic 2.3 Transverse drift and its influence in multipole formation. We know that a positive vortex will travel up a vorticity gradient, and a negative vortex will travel down the vorticity gradient. Is this effect present when vortices re-organize and form multipoles? Can we show other examples of transverse drift? Can we come up with interesting initial conditions that will demonstrate this effect?

Note: This is not an exhaustive list of possible projects, but only a selection of ideas from my notebooks under the "to do" heading. Several other projects are possible, and indeed the grant-holder may want to suggest his own. This list, however, does give a framework of my current interests and expertise.