SCAT APPLE PRIZE ENTRY

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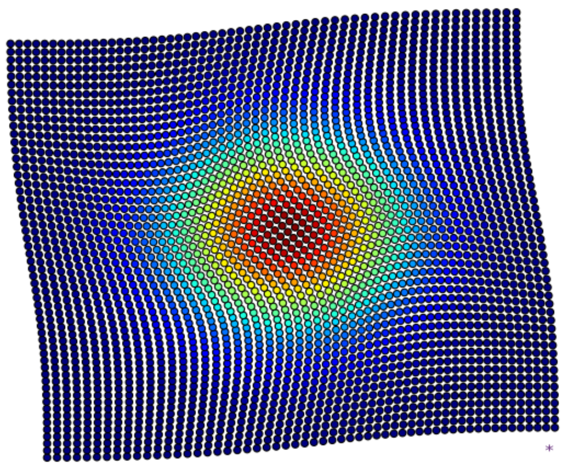
Fast Multipole Methods Applied to Viscous Vortex Method



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* This image shows 3136 blobs simulating the evolution of the Lamb-Oseen vortex (test problem that I use for numerical experiments.) The blobs were initially rendered in a square lattice but at the moment of the snapshot the particles are already moving with the flow. The color of each blob represents the strength of the blob.

1. Summary of the research carried out during the SCAT visit

1.1. Introduction

A big set of problems of great interest to the scientific community involve calculations that are usually too great, and the computational resources too small, to complete them in a sensible time frame. This is the motivation behind the development of clever algorithms that make an efficient use of the available resources in order to find a solution in a shorter time.

This research have its focus on the development of a 'clever' algorithm that can speed up the calculations performed by the Vortex Blob Method (VBM). The VBM is a Lagrangian, grid-free approach to solving Navier-Stokes equations in vorticity formulation, this method is based on spatially discretizing the vorticity field with elements (vortex blobs) that move with the local fluid velocity.

The VBM requires the calculation of all pairwise inter-blob interactions, which by direct evaluation performs $O(N^2)$ operations. In order to solve problems for large N values within reasonable times it is necessary to utilize a computational method which requires fewer than $O(N^2)$ operations. This research explores the use of the Fast Multipole Method [4](FMM) -a highly accurate $O(N)$ algorithm- to speed up the inter-blob interactions. The FMM relies on approximations and factorizations to accelerate the computations, therefore these method trade computational accuracy for computational efficiency.

1.2. Vortex Method

The vortex method is a grid-free approach to solve the Navier-Stokes equations in vorticity formulation. This is achieved by discretizing the continuum vorticity field into Lagrangian elements that move in the flow field which they create. Let,

$$u(z,t) : \text{the velocity field} \tag{1}$$

$$\omega(z,t) = \nabla \times u(z,t) : \text{the vorticity field} \tag{2}$$

The governing equation in the Vortex Method is the vorticity transport equation for flow at constant density and with conservative body forces:

$$\frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = \omega \cdot \nabla u + \nu \nabla^2 \omega \tag{3}$$

In two-dimensions there is no vortex stretching and considering the inviscid case (3) reduces to the form

$$\frac{\mathrm{D}\omega}{\mathrm{D}t} \equiv \frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = 0 \tag{4}$$

Therefore, the Vortex Method discretizes the vorticity field into Lagrangian elements that carry vorticity and move with the local fluid velocity.

In the Vortex Blob Method the elements that carry the vorticity are called blobs. Each blob have a compact core and a characteristic distribution of vorticity (given by the cutoff function ζ_{σ_i}). A blob can be identified by: position z_i, strength Γ_i, and core size σ_i. Now the vorticity field discretized by the blobs is expressed as:

$$\omega(z,t) \approx \omega_h(z,t) = \sum_{i=1}^{N} \Gamma_i(t) \zeta_{\sigma_i}(z - z_i(t)) \tag{5}$$

The most often cutoff function is a Gaussian distribution:

$$\zeta_\sigma(z) = \frac{1}{k\pi\sigma^2} \exp\left(\frac{-|z|^2}{k\sigma^2}\right) \tag{6}$$

Now, the velocity can be obtained from the vortex blob elements using the Biot-Savart law

$$u(z,t) \approx u_h(z,t) = \sum_{i=1}^{N} \Gamma_i \mathbf{K}_\sigma(z - z_i(t)) \tag{7}$$

$$\mathbf{K}_\sigma(z) = -\frac{1}{k\pi|z|^2} \begin{pmatrix} y \\ -x \end{pmatrix} \left(1 - \exp\left(\frac{-|z|^2}{k\sigma^2}\right)\right) \tag{8}$$

The Lagrangian formulation of the viscous vortex method in two dimensions can be expressed in the following equations:

$$\frac{\mathrm{d}z_i}{\mathrm{d}t} = u(z_i, t) \tag{9}$$

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = \nu\nabla^2\omega \tag{10}$$

As it can be seen from the VBM formulation, in the computation of the velocity of a blob (7) it is required to evaluate the velocities induced on that particle by each of the other particles, if there are N particles interacting, the computation of the velocity of a single particle requires $O(N)$ operations, thus the computations of the velocities for all N particles requires $O(N^2)$ operations.

1.3. Viscous Scheme for Vortex Method: Core Spreading Method

The viscous scheme under research is the Core Spreading Method, which changes the core size of the vortex blobs to exactly solve the diffusion equation. When using this method, the use of a correction scheme is needed for this method to converge to the Navier-Stokes equations. The correction scheme can be explained as an spatial adaptation procedure which assures that the core sizes of the vorticity elements are kept small enough to control the convection error.

1.4. Fast Multipole Method

In [4] an algorithm for the evaluation of Coulombic interactions in a system of N particles which requires $O(N)$ operations is presented, this algorithm known as the Fast Multipole Method is also accurate to certain error that can be selected.

The Fast Multipole Method (FMM) is an $O(N)$ fast summation method, which employs approximations to reduce computations and to control the accuracy for N-body type problems. The main idea of the FMM is to group the particles into clusters, in order to calculate an approximation of the interaction with distant (well-separated) clusters. To construct the particle clusters the FMM makes use of a hierarchical grid, using its cells to define the hierarchy of the clusters.

Some of the main concepts of the Fast Multipole Method can be better explained in the next example, concepts of the FMM are applied to speed up a matrix vector product of the form $\sum_i \Phi_{ij} u_i = v_j$

Let,

$$\begin{aligned}
\Phi_{ij} &= \phi(x_i, y_j) \\
&= \sum_{l=1}^{p} \beta_l \Psi_l(x_i - x_*) \psi(y_j - x_*)
\end{aligned}$$

so,

$$\begin{aligned}
v_j &= \sum_{i}^{N} u_i \sum_{l}^{p} \beta_l \Psi_l(x_i - x_*) \psi(y_j - x_*) \\
&= \sum_{l}^{p} \beta_l \psi(y_j - x_*) \sum_{i}^{N} u_i \Psi_l(x_i - x_*)
\end{aligned}$$

where the number of terms retained, p, is related to the accuracy.

$$A_l = \sum_{i}^{N} u_i \Psi_l(x_i - x_*)$$

now, the A_l terms will need to be evaluated only once for all the v_j terms, the computation of the A_l term requires only $O(Np)$ operations. This factorization leads to a problem with this form

$$v_j = \sum_{l}^{p} A_l \beta_l \psi(y_j - x_*)$$

If we have M number of v_j elements, the problem will require $O(Mp + Np)$ operations instead of the $O(M * N)$ operations required by the initial formulation. From this example it is possible to grasp some of the main ideas that support the Fast Multipole Method:

- Factorization of common terms. (known as Multipole Expansions)
- Approximation of functions. (Truncation of the Multipole Expansions)
- Translation and space partitioning. (Use of data structures as quadtree)
- Error bounds. (Calculate the error incurred in the truncation step)

A complete introduction to the Fast Multipole Method would require more than a few pages but I expect that this brief introduction is enough to grasp the main concepts behind the FMM. The next point explains the essence of how the FMM is applied to the VBM.

The FMM speed up the calculations performed by the VBM by breaking the calculations of the velocity field into a near field (with particles near the evaluation point) and a far field (with the particles not included on the near field),

$$\begin{aligned}
u_h(z) &= u_h^{near} + u_h^{far} \\
&= \sum_{z_i \; near \; z} \Gamma_i \mathbf{K}(z - z_i) + \sum_{z_i \; far \; from \; z} \Gamma_i \mathbf{K}(z - z_i) \qquad (11)
\end{aligned}$$

The first summation of (11) is computed directly. The second summation of (11) is replaced by a Multipole Expansion, and by retaining a given number of terms from the expansion we reduce the number of computations and we can achieve any desired accuracy.

2. Description of the research to be carried out

2.1. Study the effects of hierarchical partitioning based on clustering

In the core of the Fast Multipole Method a hierarchical partitioning algorithm is used to sort and access the blob's data during the computation of the blob's interactions, to construct the hierarchical partitioning the blobs must be pre-processed in a computationally efficient way otherwise the magnitude of this computations can even excede the ones of the Multipole calculations, the most common algorithm used to create a hierarchical partitioning is the quad-tree, which have a computational order of $O(NlogN)$ operations. Due to the way that the FMM works, changing the data structures that it use can significantly repercute on the method, a structure that takes advantage of the way that the Multipole Expansions works and the approximations are made could impact on the order of the algorithm and improve the accuracy of the method.

2.2. Parallel implementation of the proposal

A parallel implementation of the Fast Multipole Method Applied to the Vortex Blob Method with Core Spreading Scheme is a mayor goal behind this research. The computational requirements of the Vortex Blob Method is one of its mayor issues and the parallel implementation of this work will be a step forward on the search of an efficient implementation that makes better use of the current technologies available.

2.3. Study the effects of partial regridding based on partitioning the particles

Given the Lagrangian formulation of the Vortex Blob Method, the blobs (due to the interactions with the other blobs) start to gradually cluster in some areas and to separate in others. As the blobs cease to overlap they loose the ability to recover the smooth vorticity field and the accuracy is lost. The widespread solution to this problem is to remesh the whole particle field to control the error due to Lagrangian distortion. A proposed solution is to only remesh reduced areas where the clustering problems appears, this areas can be related to the hierarchical partitioning structure used on the FMM. This study can significally improve the performance of the method for large simulation where millions of particles are interacting and remeshing the whole particle field is computationally expensive.

3. Personal goals for the future

I believe Scientific Computing is on one of its best moments, the advances in computing technology that are occurring sets the scenario for mayor advances in Scientific Computing . Technologies such Cluster-computing and Grid-computing are becoming widely available and this open the door to expand our knowledge of nature and to advance our ability to tackle complex scientific and engineering problems.

I have high expectations of my SCAT visit. One of my big motivations behind the research that I am currently carrying out is to be able to contribute to the further development of the Vortex Blob Method and to achieve this goal I expect in around one year to polish the research carried out during my SCAT visit to a publishable level (with the support of my SCAT supervisors - Dr. L. Barba and Dr. L. Salinas.)

Once back to Chile I will continue working on this research and I will present it as my thesis project to opt for the degree in MSc in Informatics at the Universidad Tcnica Federico Santa Maria.

My personal goals for the future turn around Scientific Computing, one of the only things in the world with which I really do not mind to spend hours and hours in front of a computer is to work right in it. I am a complete passionate/enthusiastic on trying to be able of improving different scientific methods and then, see the positive result of them in the real life. Under my point of view is exiting that through research we can better understand, and possibly solve, real-life problems that can impact the way we develop machines, motors... for everyday, or to produce better predictions for the weather conditions, global warming, etc.

In short words, what I am looking for in my stay in this world is to contribute a little bit to live in a nicer way.

4. Why do I want a MacBook?

Beside of the beautiful machines (impeccable design) and the beautiful interface of Mac OS X there are several good reasons why I want a Mac OS X computer (specifically a MacBook):

- The UNIX foundations plus more: A solid OS design based on UNIX and enhanced to be more friendly and usable (a philosophy in Apple products.) The outcome is Mac OS X an extremely reliable, stable and efficient system that is also easy to use and administrate.

- Mac OS X embraces Open Standards: Mac OS X use guidelines and best practices that increase its compatibility. Mac OS X support a wide variety of standards and protocols, this means freedom for the user because the system is not tied to technologies or vendors, making the system a very versatile tool that is able to work in different kinds of infrastructures.

- Extensive software collection: You can find for Mac OS X an extensive collection of software that it is optimized to run on Mac OS X for every kind of task that you may need. But if required a Mac also let you run Windows software and UNIX-based applications (Virtual Machines, emulators, dual boot, virtualization.)

- MacBook Mobility: a MacBook delivers performance and mobility at the same time. A MacBook enables you to work in group in a more efficient and effective way. This point is really important for me because I use to collaborate intensively with other people and I'm constantly moving from one place to another and I need to access my work wherever I am.

- Mac OS X is a great Scientific Platform: you can find excellent tools for producing papers and graphics in Mac OS X. But it is not only limited to this, it is also possible to find a huge amount of software libraries, mathematics tools, data analysis tools, programming languages, documentation tools, version control tools, editors, compilers, and much more is available for you to accomplish your research work. And all the tools that I personally use on my work are available for Mac OS X!

- Intel Powered: The new MacBook delivers more processing power and an impressive battery life (up to 6 hours.) The processing power and tools that comes from Intel gives you superior performance for number crunching tasks. Combining the power-efficient chip from Intel and the power management from Mac OS X gives you great performance and mobility.

I think that a MacBook would be of much help on my daily life and research life. I am more than ready to enjoy the MacBook stylish design, the powerful Core Duo processors, the multimedia experience, the great scientific platform, the easy-of-use and reliability of Mac OS X, the amazing software that comes with every Mac, the growing communities and to experience a system that just works out of the box. I sure that I want a Mac and I am ready to make the switch!

Referencias

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