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CHARACTERISATION OF THE FAST MULTIPOLE APPROXIMATION IN PARTICLE SIMULATIONS

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ABSTRACT

The fast multipole method (FMM) has been listed as one of the top-10 algorithms of the twentieth century [1], due to its dramatic impact on the feasibility of computation of particle pairwise interactions with many particles. It was originally developed for applications in electrostatics and astrophysics, but continues to find new areas of application where N-body problems arise.

When using a global interpolation method on scattered centres such as the radial basis function method, one needs to consider for each evaluation point the contribution of all centres. This translates into an $O(N^2)$ method when both centres and evaluation points are numbered at N. Clearly, the evaluation of a radial basis function expansion becomes prohibitive for many points, when direct evaluation is used. Methods based on the FMM have thus been proposed to alleviate this problem and allow RBF evaluations for thousands or millions of centres [2].

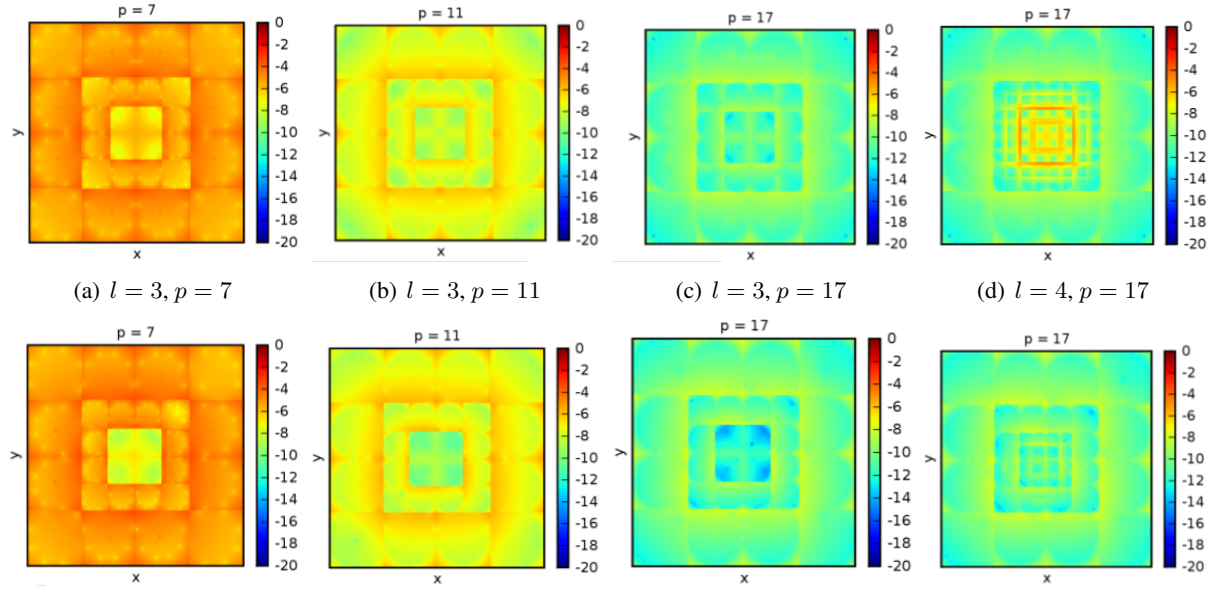
We are interested moreover in another application of the FMM. In the vortex particle method used for computing the flow of an incompressible fluid, the evaluation of the velocity of the particles using the vorticity information results in an N-body problem. The problem is governed by the well-known Biot-Savart law of vorticity dynamics. Here, again, the FMM has allowed the efficient computation of vortex method solutions for thousands or millions of particles. In fact, one of the main reasons for the unpopularity of vortex methods before the late 1990s was the $O(N^2)$ complexity, and thus the FMM has brought this essentially meshless method to a new period of development and usage. And so it is that a vortex method calculation using the FMM was awarded the 1997 Gordon Bell prize in the Price/Performance category (fluid flow problem simulated using 360,000 particles, M. S. Warren, John K. Salmon, Gregoire S. Winckelmans et al.) [3].

In the literature on the application of the FMM it is often cited that the method has an error bound which can be used in computations to achieve a given degree of accuracy with the approximation. However, seldom do authors give any details about how this is achieved in practice, or how do the different parameters of the method affect how the accuracy is achieved. At most, readers are told something like "the first three multipole moments were used", giving an indication of the truncation used on the series expansions involved in the method.

To use the FMM —in addition to the heavy programming effort, as this is a complex algorithm— a researcher should know how the errors of the approximation behave with different choices of parameters. One needs to decide on the number of levels, l, at which the octree spatial structure is constructed, and the number of terms, p, kept in the series expansions (the truncation level). For a given problem size, these parameters will result in different maximum error and structure of the error in space.

We have implemented the FMM for the computation of the Biot-Savart velocity of a set of vortex particles, in addition approximating the kernel by $1/r$, which is accurate at distances of several particle sizes away from each particle. The code will be made publicly available via a website currently under construction, but interested researchers are welcome to email for a copy of the code. It was written entirely using the Python scripting language, but a port to C++ has recently been implemented. In addition, the C++ port is being parallelized and —in collaboration with researchers at Argonne National Laboratories— we expect to provide the FMM as an add-on to the PETSc library.

Using the Python code prototype, more than 900 experiments were performed, for varying N and changing the parameters l and p. We present the maximum errors and the spatial error structure for the FMM approximation for the most illustrative experiments, giving a clear characterisation of the FMM approximation for particle simulations. As an example of the results that will be presented, see the following figures, showing the spatial structure of the error. The behaviour will be explained for varying parameters of the FMM, as well as the impact on efficiency of the calculation, for different problem sizes.



(a) $l = 3, p = 7$ (b) $l = 3, p = 11$ (c) $l = 3, p = 17$ (d) $l = 4, p = 17$

(e) $l = 3, p = 7$ (f) $l = 3, p = 11$ (g) $l = 3, p = 17$ (h) $l = 4, p = 17$

Figure 1: Logarithm of the error incurred when using FMM: (a)–(d) $N = 5776$; (e)–(h) $N = 10201$.

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