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A high order solver for the unbounded Poisson equation

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ABSTRACT

A high order converging Poisson solver is presented, based on the Green's function solution to Poisson's equation subject to free-space boundary conditions. The high order convergence is achieved by formulating regularised integration kernels, analogous to a smoothing of the solution field. The method is extended to directly solve the derivatives of the solution to Poisson's equation. In this way differential operators such as the divergence or curl of the solution field can be solved to the same high order convergence without additional computational effort. The method, is applied and validated, however not restricted, to the equations of fluid mechanics, and can be used in many applications to solve Poisson's equation on a rectangular unbounded domain.

1. Introduction

The solution of Poisson's equation on an unbounded domain is essential in many physical problems and appears among others in the field of fluid mechanics [1], molecular dynamics [2], and astrophysics [3]. The Poisson equation often describes the energy or potential of a physical system, and is either directly or indirectly governing the dynamics of the system. Particle Methods, techniques that have been extensively applied and validated in the past two decades [4–6], are typically used for simulating such problems.

Particle methods generally provide a solution to Poisson's equation by applying a Green's function solution in the form of the Biot–Savart equation [7] where each particle exerts a force onto every other particle in the system. The direct evaluation of the mutual particle interaction is an N_p-body problem which scales as $\mathcal{O}(N_p^2)$, and tree algorithms such as the Barnes–Hut [8] or the fast multipole method (FMM) [9] have been used to improve the computational scaling of particle methods. The FMM is capable of achieving an optimal scaling of $\mathcal{O}(N_p)$ [9], however, it is subject to a large pre-factor when constructing and traversing the tree data structure. This reduces the efficiency of the FMM and makes it less attractive, particularly for three-dimensional simulations where the translation of multipole expansions becomes expensive. Recent development in large-scale particle methods, such as fluid dynamics applications, has been focused on hybrid particle-mesh methods such as the Vortex-In-Cell (VIC) method by Christiansen [10]. Through interpolation schemes the VIC method applies a mixed

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particle-mesh discretisation of the governing equations and thereby exploits the advantages of both a Lagrangian and an Eulerian frame of reference. Specifically, the vorticity–velocity relation which leads to a Poisson equation, is handled on a uniform mesh. This enables the use of highly efficient fast Fourier transform (FFT) based Poisson solvers that offer a direct solution at a reduced computational cost relative to most iterative solvers. Given the right conditions, the Poisson solver on a square/cubic domain has the capability to scale as $\mathcal{O}(dN^d \log(N))$ where N is the number of grid points in each direction, and d is the number of dimensions.

There are two main strategies for using FFTs to solve Poisson's equation. The first is to exploit the sine/cosine formulated eigenvalues of a finite difference approximation to Poisson's equation, subject to either Dirichlet or Neumann boundary conditions. The order of convergence in this method depends on the finite difference scheme and on the accurate determination of boundary conditions. Methods for accurately determining Dirichlet boundary conditions that corresponds to free-space boundary conditions have been investigated by James [11], Serafini et al. [12] Colonius and Taira [13], and Cocle et al. [14].

The second strategy, which is the focus of the presented work, is to construct the Green's function solution through an integral formulation carried out in a discrete sense by convolving the field with an integration kernel. The convolution is performed efficiently in the Fourier domain by multiplying the discrete Fourier coefficients of the field with the Fourier coefficients of the integration kernel. In a periodic domain, spectral differentiating is obtained in Fourier space simply by multiplying the coefficients with their respective wavenumber. Furthermore, the periodic boundary condition is naturally treated by the periodicity of the Fourier series and a spectral convergence is therefore easily obtained as shown by Rasmussen [15]. For the unbounded free-space problem, the integration kernel cannot be represented exactly in Fourier space due to the inherent periodicity of the Fourier transform. On the same ground the domain must be extended to twice the size, to avoid the periodicity of the discrete convolution operator. Hockney and Eastwood [4] showed that it is possible to impose free-space boundary conditions by zero-padding the vorticity field and convolving this with a free-space integration kernel of equal size.

At first sight, extending the domain size to $2N$ in each unbounded direction increases the computational scaling to $\mathcal{O}(2^d dN^d \log(2N))$ and requires an allocated memory of $(2N)^d$ for a fully unbounded domain. However, an FFT based convolution algorithm, proposed by [4], significantly reduces the computational scaling and the memory needed by exploiting the fact that a multidimensional Fourier transform consists of series of one-dimensional transforms carried out in each direction, sequentially.

The method of [4] is widely used in the field of particle-mesh methods and has been extended in recent work. Mixed periodic and free-space boundary conditions were obtained by Chatelain and Koumoutsakos [16] who solved the extended Poisson equation in the free-space directions leading to a Helmholtz type equation in the periodic directions. A multi-resolution method was developed by Rasmussen et al. [17]. This method exploits the linearity of the problem to obtain local mesh refinement by applying rectangular patches using a buffer-zone to ensure a continuous solution and is similar to the method of Villumsen [18].

The convolution of the density field and the integral kernels are inherently based on a mid-point numerical quadrature and is therefore limited to a second order convergence as shown by [15]. A high order converging, Green's function based Poisson solver has, to this point, not been presented in the literature. Qiang [19] however, used a similar convolution integral method to find the electric potential of a charge density field and reached $\mathcal{O}(h^4)$ convergence by enforcing a quadrature rule correction onto the charge density field. Here, h denotes the discretisation length such as the mesh cell size or particle spacing. Qiang applied the method to cases where the integration kernel is non-singular and does not address the problems of singular integration kernels, which are the most common when solving Poisson's equation by a Green's function.

In the present work the Green's function based Poisson solver is extended to achieve a high order of convergence of the convolution integral for a continuous field by formulating regularised integration kernels. These are based on the work of [20–24] using smoothed particles to achieve high order regularised integration kernels for mesh-free vortex methods. However, unlike mesh-free methods, the mesh-based Poisson solver requires a finite and continuous integration kernel to ensure an accurate numerical solution. Therefore, a great effort is put into defining the centre value of the regularised integration kernels as this is identified, in the present study, as a crucial factor for achieving high order convergence.

As mentioned, Poisson's equation is often encountered when solving a scalar or a vector field potential. The potential is introduced to simplify the mathematical problem, however, it is often the scalar or the vector field itself which is the essential value. On this ground, the presented method is extended to directly calculate the derivatives of the solution of Poisson's equation to an equally high order as the Poisson solver. Further, the evaluation of differential operators such as the gradient, divergence, or the curl of the solution is discussed with consideration to the lowest computational cost.

2. Vorticity–velocity equations and Fourier-based convolution for their solution

In fluid mechanics, the kinematics is defined through the vorticity–velocity equations. The vorticity $\boldsymbol{\omega}$ is defined as the curl of the velocity $\boldsymbol{u}$:

$$\boldsymbol{\omega} \equiv \nabla \times \boldsymbol{u}. \tag{1}$$

Eq. (1) can be inverted to find $\boldsymbol{u}$ by defining a solenoidal vector potential ($\boldsymbol{\psi}$: $\nabla \cdot \boldsymbol{\psi} = 0$) referred to as the stream function

$$\boldsymbol{u} \equiv \nabla \times \boldsymbol{\psi}. \tag{2}$$