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A regularization method for solving the Poisson equation for mixed unbounded-periodic domains

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ABSTRACT

Regularized Green's functions for mixed unbounded-periodic domains are derived. The regularization of the Green's function removes its singularity by introducing a regularization radius which is related to the discretization length and hence imposes a minimum resolved scale. In this way the regularized unbounded-periodic Green's functions can be implemented in an FFT-based Poisson solver to obtain a convergence rate corresponding to the regularization order of the Green's function. The high order is achieved without any additional computational cost from the conventional FFT-based Poisson solver and enables the calculation of the derivative of the solution to the same high order by direct spectral differentiation. We illustrate an application of the FFT-based Poisson solver by using it with a vortex particle mesh method for the approximation of incompressible flow for a problem with a single periodic and two unbounded directions.

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1. Introduction

The Poisson equation is an elliptic equation that most commonly appears in physics when solving potential fields. Examples are the potential of gravitational or electrical charge interactions, or the velocity field induced by a vortex in a potential flow. In this work we propose a high order solver for the Poisson equation for mixed unbounded-periodic domains, which are domains having a mixture of unbounded and periodic directions based on a Green's function approach. In terms of boundary conditions we may use the phrase mixed periodic and free-space boundary conditions.

Using Green's functions is the preferred method for solving linear differential equations in an unbounded domain. The Green's function represents a homogeneous solution which is derived analytically with the appropriate boundary conditions, and then used to obtain the particular solution by a convolution with the right-hand-side field of the Poisson equation.

For triple periodic systems it is widely used within the field of electrostatics to decompose the electrostatic potential into a singular short-range term and a smooth long-range term. This technique is known as Ewald summation [1]. It constitutes an N-body problem, where N is the number of charged particles contained within the unit domain. The summation may be calculated using particle-particle particle-mesh like methods [2], where the long-range term is computed in Fourier space using an FFT-based particle-mesh method with computational efforts scaling $\mathcal{O}(N \log N)$ (see e.g., [3,4]). Likewise, expressions for the Ewald sums for the cases of mixed periodic and free-space boundary conditions have been derived

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in [5] also applicable for fast summation methods [6,7]. The Ewald summation technique, however does not provide an explicit Green's function, which may be discretized and used with a generic solution procedure such as the FFT-based solver presented in the following.

A high-order FFT solver for the unbounded Poisson equation has recently been presented in references [8–10]. Here the high order is achieved by deriving regularized Green's functions by removing their singularity through the introduction of a minimum resolved length scale. The method is based on the work of references [11–15] who employ regularized particles for mesh free particle interactions. We note that solvers based on the adaptive Fast Multipole Method (FMM) [16,17] are alternatives to the FFT-based solvers. The FMM based solvers have an advantage in systems with highly non-uniform particle distributions, since they are not restricted to uniform meshes (see [18] for a detailed comparison of computational efforts required for the two methods). For details on higher-order FMM methods for partial differential equations in general the reader is referred to the references [19,20].

A simple approach to obtain a Green's function for unbounded-periodic domains is to use the method of repeating domains where the unbounded Green's function is summed to implicitly account for a specified number of repeated fields and thus obtain a semi-periodic solution [21]. With the FMM this is effectively employed, since only a local multipole expansion of the unit domain need to be summed to account for the well-separated repeated domains with insignificant additional computational efforts [16]. For a mesh-based FFT-solver however, the method impose a growth of the efforts associated with the precomputation of the convolution kernel, that scales linearly with the number of repeated domains. In both cases it introduces an additional parameter in the algorithm which influences the overall accuracy of the method. The high order regularized Green's functions for unbounded domains derived in references [8–10] may be used together with the method of repeating domains. For this approach the error due to the semi-periodic approximation convergences with respect to the number of repeated domains as first and third order in two- and three-dimensions (2D and 3D), respectively [10]. This corresponds to the rate of decay of the free-space Green's functions in the two spatial dimensions. Hence it may be well worth to look for analytic Green's functions which implicitly account for the periodicity.

A more formal approach to achieve a Green's function for unbounded-periodic domains was proposed by Chatelain and Koumoutsakos [22]. Here the Poisson equation was solved directly in the periodic directions yielding a modified Helmholtz equation for the unbounded directions which in turn is solved by deriving the appropriate real space Green's functions.

In the present work we adopt the approach of Chatelain and Koumoutsakos [22] by deriving Green's functions which are functions of Fourier space variables in the periodic directions and real space variables in the unbounded directions. Combined with the regularization method presented in [8–10] we derive regularized Green's functions for unbounded-periodic domains. The regularized unbounded-periodic Green's functions are implemented in an FFT-based Poisson solver using the zero-padding method of Hockney and Eastwood [2] to obtain a linear convolution in the unbounded directions. We show that the solver obtains a convergence rate corresponding to the regularization order of the Green's function.

For a single free-space and one or more periodic boundary conditions, we note that solving the Poisson equation essentially reduces to solving a one-dimensional modified Helmholtz equation with free-space boundary conditions for each wave number set (when having Fourier transformed the problem in the periodic directions). A spectrally accurate procedure for doing this has been outlined in [23,24]. This procedure is not applicable when the system has more than one free-space condition.

2. Methodology

The Poisson equation is formally stated as

$$\nabla^2 A(\boldsymbol{x}) = -B(\boldsymbol{x}), \tag{1}$$

where $B(\boldsymbol{x})$ is a known bounded field and $A(\boldsymbol{x})$ is the desired solution field. As $B(\boldsymbol{x})$ is bounded we may state for the unbounded domains, that

$$A(\boldsymbol{x}) \to 0 \quad \text{for} \quad |\boldsymbol{x}| \to \infty \tag{2}$$

and for the periodic domains that

$$A(\boldsymbol{x}) = A(\boldsymbol{x} + n\boldsymbol{L}). \tag{3}$$

Here $\boldsymbol{L}$ is the length of the domain and $n \in \mathbb{Z}$. In this work we seek the solution of Eq. (1) for an unbounded-periodic domain which is subject to the conditions of Eqs. (2) and (3) for the unbounded and periodic directions, respectively.

In many applications such as astrophysics, electrodynamics and vortex dynamics, the vector field to be solved $\boldsymbol{v}(\boldsymbol{x})$ is described by potential functions using the Helmholtz decomposition

$$\boldsymbol{v}(\boldsymbol{x}) = \nabla \times \boldsymbol{\psi}(\boldsymbol{x}) - \nabla \phi(\boldsymbol{x}) \qquad \text{where} \qquad \nabla \cdot \boldsymbol{\psi}(\boldsymbol{x}) = 0. \tag{4}$$

The fundamental operations describing the conservation of the flux and circulation of the vector field $\boldsymbol{v}$ is the divergence $\vartheta(\boldsymbol{x}) = \nabla \cdot \boldsymbol{v}(\boldsymbol{x})$ and the curl $\boldsymbol{\omega}(\boldsymbol{x}) = \nabla \times \boldsymbol{v}(\boldsymbol{x})$, respectively. From Eq. (4) it follows that these may be expressed by the potential functions as

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