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A fast solver for Poisson problems on infinite regular lattices

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ABSTRACT

The Fast Multipole Method (FMM) provides a highly efficient computational tool for solving constant coefficient partial differential equations (e.g. the Poisson equation) on infinite domains. The solution to such an equation is given as the convolution between a fundamental solution and the given data function, and the FMM is used to rapidly evaluate the sum resulting upon discretization of the integral. This paper describes an analogous procedure for rapidly solving elliptic *difference* equations on infinite lattices. In particular, a fast summation technique for a discrete equivalent of the continuum fundamental solution is constructed. The asymptotic complexity of the proposed method is $O(N_{\rm source})$, where $N_{\rm source}$ is the number of points subject to body loads. This is in contrast to FFT based methods which solve a lattice Poisson problem at a cost $O(N_\Omega \log N_\Omega)$ independent of $N_{\rm source}$, where Ω is an artificial rectangular box containing the loaded points and N_Ω is the number of lattice points in Ω.

1. Introduction

This paper describes an efficient technique for solving Poisson problems defined on the integer lattice $\mathbb{Z}^2$. For simplicity of presentation, we limit our attention to the equation

$$[\mathsf{A}u](\boldsymbol{m}) = f(\boldsymbol{m}), \quad \boldsymbol{m} \in \mathbb{Z}^2, \tag{1.1}$$

where $f = f(\boldsymbol{m})$ and $u = u(\boldsymbol{m})$ are scalar valued functions on $\mathbb{Z}^2$, and where A is the so-called *discrete Laplace operator*

$$[\mathsf{A}\,u](\boldsymbol{m}) = 4u(\boldsymbol{m}) - u(\boldsymbol{m}+\boldsymbol{e}_1) - u(\boldsymbol{m}-\boldsymbol{e}_1) - u(\boldsymbol{m}+\boldsymbol{e}_2) - u(\boldsymbol{m}-\boldsymbol{e}_2), \quad \boldsymbol{m} \in \mathbb{Z}^2. \tag{1.2}$$

In (1.2), $\boldsymbol{e}_1 = [1, 0]$ and $\boldsymbol{e}_2 = [0, 1]$ are the canonical basis vectors in $\mathbb{Z}^2$. If $f \in L^1(\mathbb{Z}^2)$ (meaning that $\sum_{m\in\mathbb{Z}^2} |f(m)| < \infty$) and $\sum_{\boldsymbol{m}\in\mathbb{Z}^2} f(\boldsymbol{m}) = 0$, Eq. (1.1) is well-posed when coupled with a suitable decay condition for u, see [1,2] for details.

We are primarily interested in the situation where the given function f (the *source*) is supported at a finite number of points which we refer to as *source locations*, and where the function u (the *potential*) is sought at a finite number of points called *target locations*. While the solution technique is described for Eq. (1.1) involving the specific operator (1.2), it may readily be extended to a broad range of lattice equations involving constant coefficient elliptic difference operators. (The method can in principle be extended to elliptic problems with oscillatory solutions, but it can realistically only be used in situations where the support of f is contained in a domain that is not larger than a few dozen or so wavelengths. The lattice FMM is in this regard entirely analogous to the classical FMM in that profound modifications are required to handle the highly oscillatory case, see [3].)

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Variations of Eq. (1.1) are perhaps best known as a set of equations associated with the discretization of elliptic partial differential equations. However, such equations also emerge in their own right as natural models in a broad range of applications: random walks [4], analyzing the Ising model (in determining vibration modes of crystals), and many others in engineering mechanics including micro-structural models, macroscopic models, simulating fractures [5,6] and as models of periodic truss and frame structures [7,8,2,9].

Of particular interest in many of these applications is the situation where the lattice involves local deviations from perfect periodicity due to either broken links, or lattice inclusions. The fast technique described in this paper can readily be modified to handle such situations, see Section 10.1. It may also be modified to handle equations defined on finite subsets of $\mathbb{Z}^2$, with appropriate conditions (Dirichlet/Neumann/periodic) prescribed on the boundary, see Section 10.2 and [10].

The technique described is a descendant of the Fast Multipole Method (FMM) [11–13], and, more specifically, of "kernel independent" FMMs [14–16]. A key application of the original FMM was to rapidly solve the Poisson equation

$$-\Delta u(\boldsymbol{x}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^2, \tag{1.3}$$

which is the continuum analog of (1.1). The FMM exploits the fact that the analytic solution to (1.3) takes the form of a convolution

$$u(\boldsymbol{x}) = \int_{\mathbb{R}^2} \phi_{\text{cont}}(\boldsymbol{x} - \boldsymbol{y}) f(\boldsymbol{y})\, d\boldsymbol{y}, \tag{1.4}$$

where ϕ_{cont} is the fundamental solution of the Laplace operator,

$$\phi_{\text{cont}}(\boldsymbol{x}) = -\frac{1}{2\pi} \log|\boldsymbol{x}|. \tag{1.5}$$

If the source function f corresponds to a number of point charges $\{q_j\}_{j=1}^N$ placed at locations $\{\boldsymbol{x}_j\}_{j=1}^N$, and if the potential u is sought at same set of locations, then the convolution (1.4) simplifies to the sum

$$u_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} \phi_{\text{cont}}(\boldsymbol{x}_i - \boldsymbol{x}_j)\, q_j, \quad i = 1, 2, \ldots, N. \tag{1.6}$$

While direct evaluation of (1.6) requires $O(N^2)$ operations since the kernel is dense, the FMM constructs an approximation to the potentials $\{u_i\}_{i=1}^N$ in $O(N)$ operations. Any requested approximation error ε can be attained, with the constant of proportionality in the $O(N)$ estimate depending only logarithmically on ε.

In the same way that the FMM can be said to rely on the fact that the Poisson equation (1.3) has the explicit analytic solution (1.4), the techniques described in this paper can be said to rely on the fact that the lattice Poisson equation (1.1) has an explicit analytic solution in the form

$$u(\boldsymbol{m}) = [\phi * f](\boldsymbol{m}) = \sum_{\boldsymbol{n} \in \mathbb{Z}^2} \phi(\boldsymbol{m} - \boldsymbol{n}) f(\boldsymbol{n}) \tag{1.7}$$

where ϕ is a fundamental solution for the discrete Laplace operator (1.2). This fundamental solution is known analytically [1,2,17,10] via the normalized Fourier integral

$$\phi(\boldsymbol{m}) = \frac{1}{(2\,\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{\cos(t_1 m_1 + t_2 m_2) - 1}{4\,\sin^2(t_1/2) + 4\,\sin^2(t_2/2)}\, dt_1\, dt_2, \quad \boldsymbol{m} = [m_1,\ m_2] \in \mathbb{Z}^2. \tag{1.8}$$

This paper presents an adaptation of the original Fast Multipole Method that enables it to handle discrete kernels such as (1.8) and to exploit accelerations that are possible due the geometric restrictions present in the lattice case. The method extends directly to any problem that can be solved via convolution with a discrete fundamental solution. The technique for numerically evaluating (1.8) extends directly to other kernels, see Section 3.

While we are not aware of any previously published techniques for rapidly solving the free space problem (1.1) (or, equivalently, for evaluating (1.7)), there exist very fast solvers for the closely related case of lattice Poisson equations defined on rectangular subsets of $\mathbb{Z}^2$ with periodic boundary conditions. Such equations become diagonal when transformed to Fourier space, and may consequently be solved very rapidly via the FFT. The computational time T_{fft} required by such a method satisfies

$$T_{\text{fft}} \sim N_{\text{domain}} \log N_{\text{domain}} \quad \text{as } N_{\text{domain}} \to \infty, \tag{1.9}$$

where N_{domain} denotes the number of lattice nodes in the smallest rectangular domain holding all source locations, and where the constant of proportionality is very small. Similar complexity, sometimes without the logarithmic factor, and with fewer restrictions on the boundary conditions, may also be achieved via multigrid methods [18].

The principal contribution of the present work is that the computational time T_{FMM} required by the method described here has asymptotic complexity

$$T_{\text{FMM}} \sim N_{\text{sources}}, \quad \text{as } N_{\text{sources}} \to \infty, \tag{1.10}$$