A LINEAR SCALING SPACE-CHARGE ROUTINE USING WAVELETS

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Abstract

The present paper proposes a method to solve Poisson's equation in a wavelet basis. To best knowledge this is the first approach to space charge computations that makes use of wavelets. It outlines an efficient discretisation of the discontinuous charge distribution by automatically customising the computational mesh. This is done by including wavelets of the next higher level of resolution if their coefficients are above a certain threshold. For the presented algorithm, the CPU-time scales linearly with the number of mesh points. Moreover, it allows non-uniform grids and does not require any symmetry of the particle distribution.

The motivation for developing the wavelet technique for space-charge simulations in synchrotrons arose from the need to understand the influence of discontinuous charge distributions during multi-turn injection into the CERN PS Booster. The particle distribution during injection is smooth almost everywhere, except for small regions with sharp discontinuities caused by beam loss on the injection septum. Such locally discontinuous functions have sparse representations in a wavelet basis allowing fast computations. Furthermore wavelets allow the detailed examination of the steep gradient regions without causing computational overheads elsewhere. Finally, as the beam distribution evolves in time and loses its discontinuities, the analysing wavelet may be dynamically changed to best match the new situation.

1 INTRODUCTION

The main concern of beam dynamics codes taking into account space-charge effects is an efficient solution of the Poisson equation. Efficient means fast in terms of computing time and precise in terms of quality of the approximation to the true solution. Powerful methods that scale linearly with system size and allow the use of different levels of resolution in different regions of space are therefore highly desirable. These were the main motivations for watching out for new algorithmic trends in computational physics and wavelets, successfully used in various fields of science like geophysics, medicine and biology [1], appeared as promising candidates to fulfil these expectations.

2 WAVELETS AND MULTI-RESOLUTION

The usefulness of wavelets for solving partial differential equations relies on the definition of a Multi-Resolution Analysis (MRA) [2]. An MRA is based on two fundamental concepts: nested subspaces and orthonormal bases. The first permits decomposition of information into different scales, the second allows stable and fast algorithms. On top of these there is a third ingredient, the invariance of the basis functions under translations (in each subspace) and dilation (from one subspace to another).

Wavelets are orthonormal functions which are characterised by the translation and dilation of a single function $\psi(x)$. This function generates a family of basis functions

$$\psi_{mk}(x) = 2^{m/2}\psi(2^m x - k), \quad m, k \in \mathbb{Z}, \qquad (1)$$

where \mathcal{Z} is the set of integer numbers. Any function can be expanded within this level of resolution. Therefore any function f(x) in $L^2(\mathcal{R})$, the space of real square integrable functions, may be represented as

$$f(x) \approx \sum_{m} \sum_{k} d_{mk} \psi_{mk}(x), \qquad (2)$$

with constant coefficients d_{mk} . This expansion becomes more accurate if one goes to a higher level of resolution, i.e. if one increases m, and becomes exact for the limiting case $m \to \infty$.

Wavelets are derived from scaling functions, that is functions that satisfy the recursion

$$\phi(x) = \sum_{k} a_k \phi(2x - k) \tag{3}$$

in which a finite number of the filter coefficients a_k are non-zero. Any $L^2(\mathcal{R})$ function f(x) may be approximated at resolution m by

$$P_m f(x) = \sum_k c_{mk} \phi_{mk}(x) , \qquad k \in \mathcal{Z} , \qquad (4)$$

where $P_m f(x)$ represents the projection of the function f(x) onto the space of scaling functions at resolution m.

$$\phi_{mk}(x) = 2^{m/2} \phi(2^m x - k) , \qquad k \in \mathbb{Z} , \qquad (5)$$

is a scaling function basis for the scale m approximation of $L^2(\mathcal{R})$ and the set of approximations $P_m f(x)$ constitutes a multi-resolution representation of the function f(x).

In two dimensions square integrable functions f(x, y)of $L^2(\mathcal{R}^2)$ may be expressed in terms of the orthonormal basis

$$\psi_{mk}(x)\psi_{nl}(y),\tag{6}$$

with $m, k, n, l \in \mathbb{Z}$. This is simply the tensor product of two one-dimensional bases in the two coordinate directions x and y.

3 GRID GENERATION

Instead of immediately solving Poisson's equation in a wavelet basis, it is possible to optimise the finite difference method using wavelet based dyadic refinement of the computational grid. Considering the horizontal projection of the beam as scraped during injection (Fig. 1), it appears reasonable to invest more computing effort into the steep gradient regions. This corresponds to representing the charge

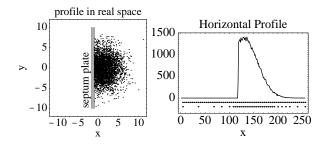


Figure 1: Simulation of the beam at injection into the PSB and its one-dimensional projection. The septum plate introduces a distinct cut. On the bottom of the left figure the equidistant and the wavelet optimised grid is displayed. Daubechies second order wavelet was used for the mesh refinement. The saving in computing time is particularly significant for beams that are small compared to the vacuum vessel.

distribution to be discretised in a wavelet basis. The level of resolution is determined by the number of wavelet coefficients. The two-dimensional generalisation consists in applying the one-dimensional refinement first to all rows, and then to all columns of a two-dimensional mesh.

The advantage of the wavelet transform as compared to the Fourier transform in the case of mesh refinement for discontinuous charge distributions becomes evident in Fig. 2, where the cumulative energy of the development is displayed. This is a measure for the quality of the approximation to the initial function in the considered basis. Unity corresponds to exact representation.

As the beam evolves in the machine the cut in its profile smears out and the analysing wavelet may be adapted to the more continuous distribution. In Fig. 3 the discontinuous second order Daubechies wavelet used for analysing the initial beam distribution is presented. The smooth eighth order Daubechies wavelet is better suited for the later continuous charge distribution.

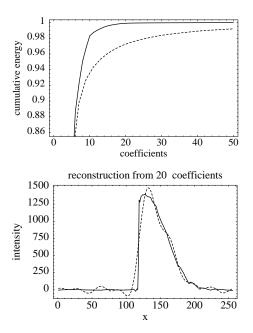


Figure 2: The cumulative energy plot displays the quality of the approximation as a function of the number of coefficients taken into account. Discontinuous functions can be expanded into a wavelet basis (continuous curves) with much higher precision in the steep gradient regions than a Fourier development (dashed curves). The second graph, showing the reconstruction of the charge density of Fig. 1 confirms this.

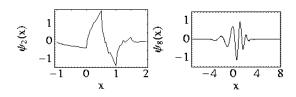


Figure 3: The Daubechies wavelets of order two $\psi_2(x)$ and eight $\psi_8(x)$ used for approximating the early discontinuous and late continuous beam shape.

4 WAVELET-GALERKIN METHOD

The Galerkin method is a special case of the method of weighted residues which expands the solution u of a partial differential equation Lu = f, with $L = \nabla^2$ for the Poisson equation, into a series of linear independent basis functions. The residue $R = L\tilde{u} - f \neq 0$ of the approximate solution \tilde{u} is then minimised introducing weighting functions. The method is called Galerkin method when the same functions are used as basis and weighting functions.

Wavelets have several properties that are useful for representing solutions of partial differential equations [3]. The orthogonality, compact support and exact representation of polynomials of a fixed degree allow the efficient and stable calculation of regions with strong gradients or oscillations. In beam physics, regions with strong gradients appear during multi-turn injection, when the beam hits the septum and suffers losses. This results in a smooth Gaussian beam distribution everywhere, except at the position of the septum cut, where a discontinuity is introduced (cf. Fig.1).

For such a discontinuous charge distribution ρ consider the Poisson problem

$$\nabla^2 u = \rho. \tag{7}$$

The wavelet-Galerkin approximation to the potential u is

$$u(x,y) = \sum_{k} \sum_{l} \tilde{c}_{kl} 2^{m/2} \phi(2^m x - k) 2^{m/2} \phi(2^m y - l)$$
(8)

with $k, l \in \mathbb{Z}$. The integer number m fixes the level of resolution of the approximation. In wavelet space the potential u is defined by its wavelet coefficients \tilde{c}_{kl} and may be translated to physical space using the Fast Fourier Transform (FFT). Therefore one needs to express the wavelet expansion as a discrete convolution. Substituting $X = 2^m x$ and $Y = 2^m y$ gives

$$U(X,Y) = u(x,y) = \sum_{k} \sum_{l} c_{kl} \phi(X-k) \phi(Y-l)$$
(9)

with $c_{kl} = 2^m \tilde{c}_{kl}$. A scale dependent discretisation of u(x, y) is obtained by focusing on the values of u at the dyadic points $x = 2^{-m}X$ and $y = 2^{-m}Y$, where X, Y are allowed to take integer values only. Thus U(X, Y) is discretised on a rectangular mesh $n_x \times n_y$ by

$$U_{ij} = U(i\Delta X, j\Delta Y) \tag{10}$$

where $i = 0, 1, 2, ..., n_x - 1, j = 0, 1, 2, ..., n_y - 1$. Written in matrix form one obtains

$$U = \Phi_{n_x} c \Phi_{n_y}^T. \tag{11}$$

This gives an easy relation between U and its wavelet coefficients c.

An analogous expression is found for the inhomogeneity ρ of the Poisson equation. Inserting both into Eq. (7) one obtains, after some matrix manipulations, the solution in wavelet space that is transformed to the ordinary space solution U using the inverse two-dimensional FFT.

5 BOUNDARY CONDITIONS

Boundary conditions may be taken into account using the capacitance matrix method [4]. In two-dimensional space-charge computations it is required to solve problem (7) on a surface S with Dirichlet boundary conditions

$$u = u_C(x, y) \tag{12}$$

on the boundary $C = \partial S$ that is the vacuum chamber wall. The solution may be found by adding an unknown function w(x, y) to v(x, y)

$$u = v + w . \tag{13}$$

Since $\nabla^2 v = f$ in S, w must satisfy

$$\nabla^2 w = 0 \tag{14}$$

in S, whereas, on the boundary curve C, w must be such as to make u the imposed boundary conditions. This is achieved by distributing image sources along a closed curve C_1 , enclosing the region S. The convolution

$$w = G(x, y) * R_1(x, y)$$
 (15)

$$= \int_{C_1} R_0(p,q) G(x-p,y-q) dC_1, \quad (16)$$

determines the solution to the boundary source problem, where the integral extends over all the boundary points $(p,q) \in C_1$. G(x, y) is the Greens function of the differential equation and may be computed using the method developed in Section 4. Discretisation leads again to a matrix system that can be solved for R and finally w. The solution u is obtained from Eq. (13).

6 CONCLUSIONS

A code is being developed to study space charge problems in the PS Booster. It showed that wavelets provide a natural mechanism for grid selection allowing the computational efforts to be concentrated in regions of steep gradients, diluting parts of the computational domain where the solution is very smooth.

The wavelet method appears to be a powerful numerical tool for the fast and accurate solution of partial differential equations. Although the solution requires slightly more computational effort than the finite difference solution, the gain in accuracy, particularly with higher order wavelets, by far compensates for the increase in computer time. Moreover wavelets have the capability of representing solutions at different levels of resolution, which makes them particularly useful for hierarchical solutions to problems.

7 ACKNOWLEDGEMENTS

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