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DIFFERENTIAL ALGEBRA FOR ACCELERATOR OPTIMIZATION WITH TRUNCATED GREEN'S FUNCTION

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Abstract

Accelerator optimization is a critical problem in the design of high-performance particle accelerators. The truncated Green's function space charge algorithm is a powerful tool for simulating the effects of space charge in accelerators. However, the truncated Green's function algorithm can be computationally expensive, especially for large accelerators. In this work, we present a new approach to accelerator optimization using differential algebra with the truncated Green's function space charge algorithm. Our approach uses differential algebra to symbolically represent the equations of the truncated Green's function algorithm. This allows us to perform efficient symbolic analysis of the equations, which can be used to identify and optimize the accelerator parameters. We demonstrate the effectiveness of our approach by applying it to the optimization of a linear accelerator. We show that our approach can significantly reduce the computational cost of the truncated Green's function algorithm, while still achieving high accuracy.

INTRODUCTION

Computation of space charge fields in accelerator simulations presents significant challenges. While many accelerator modeling codes incorporate self-consistent space charge solvers to track multiple particles, solving electromagnetic or electrostatic space charge fields self-consistently and analytically is inherently intricate. Consequently, numerous solvers resort to Particle-in-Cell (PIC) methods with open boundary conditions.

During accelerator optimization simulations, gradient-free algorithms are frequently used due to the limited availability of derivative information regarding beam properties in relation to accelerator parameters. To address this constraint, techniques like Differential Algebra (DA) and Truncated Power Series Algebra (TPSA) come into play to bridge this gap.

DA and TPSA have demonstrated their effectiveness in calculating nonlinear maps for lattice elements and are widely embraced in many codes. These techniques hold particular promise in the realm of differentiable space charge simulations, where computational efficiency is paramount for beam dynamics simulations. Proposals for automatic differentiation of space charge simulations using TPSA have emerged, further augmenting their versatility.

DA techniques have become instrumental in solving complex problems in accelerator physics. There have been research contributions where DA methods have significantly enhanced space charge calculations, paving the way for innovative solutions in accelerator science. H. Zhang *et al* applied DA techniques to the Fast Multipole Method (FMM) for space charge calculations. Their research offers valuable insights into the effective use of DA in space charge effect computations [1]. B. Erdelyi *et al* employed the Duffy transformation method to address the Poisson equation with Green's functions. This transformative technique effectively splits integrals into smaller domains, eliminating the singularities associated with Green's functions [2]. Recently, J. Qiang focused on using TPSA techniques to derive local derivatives of beam properties concerning accelerator design parameters. This study investigates the behavior of coasting beams within a rectangular conducting pipe [3].

Collectively, these research contributions demonstrate the widespread adoption of DA techniques to enhance space charge calculations. The combination of DA and related algebraic techniques showcases the versatile and robust nature of these methods, ultimately shaping the future of accelerator science and simulation.

In this work, we have devised a differentiable self-consistent space charge model, harnessing the power of Green's function solvers and implementing the Vico-Greengard-Ferrando algorithms [4]. This approach furnishes several benefits, including enhanced computational efficiency for beam dynamics simulations and the capability to effectively manage differentiable space charge effects [5].

TRUNCATED SPACE CHARGE SOLVER

For a given charge distribution, ρ, the Poisson equation with an open boundary condition can be expressed as:

$$\vec{\nabla}^2\phi = -\frac{\rho}{\epsilon_0},$$

The general solution of the Poisson equation utilizing Green's function is expressed as follows:

$$\begin{aligned}\phi(\vec{r}) &= \frac{1}{\epsilon_0}\int G(\vec{r},\vec{r}')\,\rho(\vec{r}')\,d^3\vec{r}' \\ &= \frac{1}{4\pi\epsilon_0}\int \frac{1}{|\vec{r}-\vec{r}'|}\,\rho(\vec{r}')\,d^3\vec{r}'.\end{aligned}$$

The inclusion of boundary conditions adds a layer of complexity to the problem. In the context of accelerator simulations, open boundary conditions are often the preferred choice, particularly when the pipe radius in an accelerator significantly exceeds the transverse size of the beam bunch.

While the Green's function method provides valuable insights and computational techniques, it also presents challenges: 1) long-range integration: addressing issues

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related to long-range integration is imperative to achieve accurate results. 2) singularities: careful handling and implementation are required due to singularities in the Green's function.

These challenges are at the forefront of considerations when utilizing the Green's function approach for solving Poisson equations in accelerator simulations. The Hockney-Eastwood (HE) algorithm is a prominent method employed in the field of accelerator simulations, facilitating the efficient computation of electric potentials [6]. The HE algorithm is characterized by the following key attributes:

1. use of FFT with zero-padding: the HE algorithm harnesses the power of FFT with zero-padding to enhance computational efficiency. This approach leverages the Convolution Theorem, allowing for the rapid calculation of potentials.

2. potential calculation: the algorithm calculates the electric potential at each mesh point (p, q) as a summation of contributions from all source points (p', q').

The use of Green's function presents a powerful approach to express the electric potential in the context of accelerator simulations. This technique formulates the potential as the convolution of the source distribution ρ with the Green's function of the interaction potential G. The electric potential calculation is mathematically represented as:

$$\phi(\vec{r}) = \frac{h_x h_y h_z}{4\pi\varepsilon_0} \mathcal{F}^{-1}\left\{\sum \mathcal{F}\{G^\wedge\}\mathcal{F}\{\rho^\wedge\}\right\}.$$

Here, $\phi(\vec{r})$ signifies the electric potential, h_x, h_y, and h_z represent grid spacing in the three spatial dimensions, and ε_0 stands for the vacuum permittivity. The various components are computed in the Fourier domain for enhanced efficiency.

The convolution method proves highly advantageous under specific conditions in accelerator simulations. The method effectively addresses periodic systems of sources, accommodating arbitrary interaction forms between particles. It is particularly suitable for scenarios where no conductors or physical boundaries are present within the system. The convolution method excels when the pipe radius in an accelerator significantly exceeds the transverse size of the beam bunch.

In the context of the HE FFT method, certain limitations must be considered. The HE FFT method traditionally relies on Green's function with a long-range definition, introducing singularities at points where $\vec{r} = \vec{r}'$. These singularities can pose challenges in accurate computations.

To address the limitations of the HE FFT method, the concept of a truncated spectral kernel is introduced. This involves the transformation of the Green's function:

$$G(\vec{r}) \to G^L(\vec{r}) = G(\vec{r}) \cdot \mathrm{rect}(\vec{r}/2L).$$

This truncated spectral kernel is applicable when the truncation parameter L is chosen to be greater than the square root of the dimension of the problem ($\sqrt{d}$). In mathematical terms, it is valid when $L > \sqrt{d}$. And the indicator function $\mathrm{rect}(x)$ is defined as follows:

$$\mathrm{rect}(x) = \begin{cases} 1, & \text{if } x < 1/2 \\ 0, & \text{if } x > 1/2 \end{cases}$$

The truncation introduced by the spectral kernel rectifies some of the challenges related to singularities and long-range definitions, allowing for more accurate and manageable computations in the context of the HE FFT method.

One notable advancement in the field of accelerator simulations is the use of analytical Green's functions. This approach offers key advantages that contribute to the efficiency and accuracy of potential calculations.

One of the defining features of analytical Green's functions is their solvability in the Fourier domain. Specifically, the Fourier transform of the truncated spectral kernel, denoted as G^L, can be expressed analytically as:

$$\mathcal{F}\{G^L\} = \frac{2}{\varepsilon_0}\left[\frac{\sin(L|\vec{k}|/2)}{|\vec{k}|}\right]^2.$$

The electric potential $\phi(\vec{r})$ can be computed efficiently using the analytical Green's function. The potential calculation is given by:

$$\phi(\vec{r}) = \frac{2}{(2\pi)^3\varepsilon_0}\int \exp(i\vec{k}\cdot\vec{r})\left[\frac{\sin(L|\vec{k}|/2)}{|\vec{k}|}\right]^2 \mathcal{F}\{\rho(\vec{k})\}\, d^3\vec{k}.$$

The Vico-Greengard-Ferrando (VGF) Poisson Solver can enhance the efficiency and applicability of analytical Green's functions in accelerator simulations. By simplifying potential calculations through the use of analytical Green's functions, this solver streamlines the computational process, making it an invaluable tool in the realm of accelerator physics.

The integration of analytical Green's functions, as facilitated by the VGF Poisson Solver, offers a significant advancement in the field, presenting opportunities for improved efficiency and accuracy in accelerator simulations.

For the Gaussian charge distribution, expressed as:

$$\rho(\vec{r}) = \frac{Q}{\sigma^3\sqrt{(2\pi)^{3/2}}}\exp\left(-\frac{r^2}{2\sigma^2}\right),$$

where Q represents the charge and σ is the standard deviation ot the Poisson equation, which relates the electric potential $\phi(\vec{r})$ can be solved exactly. The solution is expressed as:

$$\phi(\vec{r}) = \frac{Q}{4\pi\varepsilon_0}\frac{1}{r}\mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma}\right)$$

where erf represents the error function.

Efficiently representing and computing the charge distribution necessitates the use of grid domains. In this context, a grid domain with dimensions $N_x \times N_y \times N_z$ is

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employed. To simplify the problem, it is common to assume equal dimensions, resulting in $N = N_x = N_y = N_z$.

The space charge potential $\phi(\vec{r})$ can be also calculated in the Fourier domain, leveraging the analytical Green's function. The potential calculation is given by:

$$\phi(\vec{r}) = \frac{2}{(2\pi)^3 \varepsilon_0} \int e^{i\vec{k}\cdot\vec{r}} \left[\frac{\sin(L|\vec{k}|/2)}{|\vec{k}|} \right]^2 \mathcal{F}\{\rho(\vec{k})\}\, d^3\vec{k}$$

The computation of the Green's function kernel involves several steps, including:

1. Fourier transform of the charge distribution.
2. Inverse Fourier transform of the convolution.

Efficient computation of space charge potentials often necessitates a grid domain with sufficient granularity. Specifically, the requirement is for a grid consisting of $(4N)$ grid domains in each direction. This is in contrast to the HE method, which requires only $(2N)$ grid domains.

ADVANCES IN SPACE CHARGE CALCULATIONS USING DA AND TPSA

DA is an algebraic framework introduced by M. Berz in 1986, designed for solving complex analytical problems. It has achieved widespread adoption in the field of accelerator simulations. Notable accelerator simulation codes, such as Cosy-Infinity, PTC, MAD-X PTC, Bmad, and CHEF (MXYZPTLK), have successfully implemented DA techniques. These codes have benefited significantly from the application of DA, enhancing the precision and efficiency of their simulations.

TPSA complements DA by employing truncated power series expansions. This method approximates functions by retaining a finite number of terms in their power series representations. A distinctive advantage of TPSA is its capability to generate power series with an infinite number of terms, providing a comprehensive framework for precise and accurate calculations. This feature makes TPSA a valuable addition to the toolkit of accelerator physicists.

TPSA excels in handling complex mathematical representations, ensuring the utmost precision and reliability in the calculations. TPSA serves as a critical component in advancing our understanding of accelerator systems and optimizing their performance.

In the PIC method, its numerical nature inherently introduces computational errors. Furthermore, numerical field derivative calculations are susceptible to errors, which can impact the overall accuracy of simulations. In pursuit of higher precision, an alternative approach offers a solution: the direct computation of electric fields using a convolutional method with the truncated Green function. This method presents a promising avenue to mitigate computational errors that are intrinsic to PIC simulations.

Directly calculating the electric fields, the method yields electric field components defined as follows:

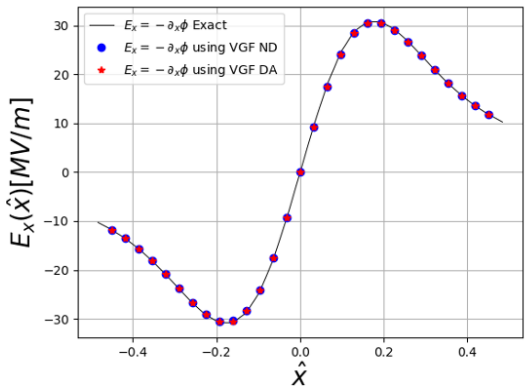

Figure 1: Comparison of electric field components along the x-axis.

$$\begin{aligned}\vec{E}(\vec{r}) &= -\nabla\phi \\ &= \frac{2}{(2\pi)^3\varepsilon_0} \int \left(i\,\vec{k}\cdot\vec{r}'\right) \left(\frac{\sin(L|\vec{k}|/2)}{|\vec{k}|} \right)^2 \rho(\vec{r}')\, \mathrm{d}^3\vec{k}.\end{aligned}$$

For further enhancement in precision, TPSA techniques enable the automatic calculation of higher-order derivatives and provide a systematic and efficient approach to handle such derivatives. This, in turn, allows for precise and reliable computations of space charge field properties with respect to beam properties.

The space charge potential, denoted as $\phi(\vec{r})$, can be expressed as a power series expansion around a reference point $\vec{r}_0$:

$$\begin{aligned}\phi(\vec{r}) =& \phi(\vec{r}_0) + \nabla\phi(\vec{r}_0)\cdot(\vec{r}-\vec{r}_0) \\ &+ \frac{1}{2!}(\vec{r}-\vec{r}_0)\cdot\nabla\nabla\phi(\vec{r}_0)\cdot(\vec{r}-\vec{r}_0) + O(\|\vec{r}-\vec{r}_0\|^2)\end{aligned}$$

To assess higher-order derivatives of the space charge potential accurately and efficiently, we employ DA techniques. Utilizing a DA vector and DA operations, we achieve systematic differentiation of the potential function with respect to the variables of interest.

The DA vector serves as a versatile representation of the potential function, enabling a methodical approach to calculate higher-order derivatives. It facilitates systematic differentiation with respect to the variables of interest, providing a comprehensive understanding of the space charge potential and its associated properties.

The integration of DA techniques enhances the precision and efficiency of space charge potential analysis. This approach allows for a thorough exploration of space charge potential properties and their derivatives, contributing to a deeper understanding of accelerator systems and their performance.

Fig. 1 illustrates a comparative analysis of electric field components along the x-axis. Through the integration of

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DA and the use of truncated Green's function, significant enhancements are observed in the numerical computation of space charge fields.

SUMMARY

In summary, the integration of Differential Algebra (DA) techniques enhances the precision and efficiency of space charge potential analysis. This approach allows for a thorough exploration of space charge potential properties and their derivatives, contributing to a deeper understanding of accelerator systems and their performance. Fig. 1 illustrates a comparative analysis of electric field components along the x-axis. Through the integration of DA and the use of truncated Green's function, significant enhancements are observed in the numerical computation of space charge fields.

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