Leveraging Differential Algebraic Methods for Enhanced Beam Dynamics Simulation with Machine Learning

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Outline

Accelerator Modeling with Space Charge Effects

Analytical and Numerical Methods for Space Charge Calculation

Algorithm Implementation and Comparative Analysis

Differentiable Simulation in Accelerator Optimization

Differential Algebra, TPSA, and Their Applications in SC Calculations

Summary

Accelerator Modeling with Differentiable Simulations

- **Accelerator Modeling or Design**
  - Running (space charge) simulations multiples times
  - Examine hundreds of thousands of simulations for hundreds of thousands of machine parameters
- **Differentiable Simulation** can be effectively used in beam dynamics simulations for particle accelerators
  - The key to differentiable simulation is the ability to compute gradients of beam properties, such as emittance, beam size, orbit, w.r.t input parameters (initial beam conditions and accelerator configuration)
- However, **Space Charge Effects** in beam dynamics introduces complexity
  - Modeling space charge effects accurately is crucial for predicting and optimizing the performance of high intensity particle accelerators
  - The nonlinear nature of space charge effects makes the problem the computation resource intensive

Equations of Motion for Charged Particle System

- The Hamiltonian of N_p charged particle system in an accelerator element can be split into $H = H_1 + H_2$ where

$$H_1 = \frac{1}{2m}\sum_i^{N_p}\left[p_{xi}^2 + p_{yi}^2 + (p_{zi} - qA_{z,ext})^2\right] \text{ and } H_2 = q\phi_{self}$$

- Using the split operator method, a state of the system at time τ,

$$\underline{X}(\tau) = \mathcal{M}(\tau)\underline{X}(0) = \mathcal{M}_1(\tau/2)\mathcal{M}_2(\tau)\mathcal{M}_1(\tau/2)\underline{X}(0) + O(\tau^3)$$

- $\mathcal{M}_1$ is a well-known single step transfer map for a (non)linear element.
- For the space charge Hamiltonian H_2, the transfer map $\mathcal{M}_2$ can be derived from

$$\vec{r}(\tau) = \vec{r}(0) \text{ and } \vec{p}(\tau) = \vec{p}(0) - \tau\vec{\nabla}H_2 = \vec{p}(0) - \tau q\vec{\nabla}\phi$$

Space Charge Solvers with Green's Function Method

- **General Solution of the Poisson Equation with Green's function**

$$\phi(\vec{r}) = \frac{1}{\varepsilon_0}\int G(\vec{r},\vec{r}')\rho(\vec{r}')d^3\vec{r}' = \frac{1}{4\pi\varepsilon_0}\int \frac{1}{|\vec{r}-\vec{r}'|}\rho(\vec{r}')d^3\vec{r}'$$

- **Consideration of Boundary Conditions**
  - Inclusion of boundary conditions adds complexity.
  - Open boundary conditions are preferred.
  - This is true if the pipe radius in an accelerator is much larger than the beam bunch transverse size
- **Challenges in Green's Function Approach**
  - Green's function offers valuable insights and computational techniques: Hockney-Eastwood Algorithm
  - Long-range integration and singularities require careful consideration and implementation.

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Hockney-Eastwood Algorithm

- **Hockney-Eastwood Algorithm (HE):**
  - Utilizes Fast Fourier Transform (FFT) with zero-padding of distribution.
  - Leveraging the Convolution Theorem
- **Calculation of Potential:**
  - Potential at mesh point (p, q) as a sum of contributions from all source points (p', q')

$$\phi(p,q) = \frac{h_x h_y h_z}{\varepsilon_0} \sum G(p,q;p',q')\rho(p',q')$$

- **Using Convolution Theorem:**
  - Expresses the potential as the convolution of the source distribution ρ with the Green's function of the interaction potential G.

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

- **Applicability of the Convolution Method:**
  - Solves a periodic system of sources with arbitrary interaction forms.
  - No conductors or boundaries allowed.
  - Ideal for situations where the pipe radius in an accelerator significantly exceeds the beam bunch transverse size.

Truncated Green's Function (TGF) Method

Vico-Greengard-Ferrando Poisson Solver

- **Limitation of HE FFT Method**
  - Utilizes Green's function with long-range definition and singularities at $\vec{r} = \vec{r}'$
  - Has been improved with Integrated Green's Function Method and Shifted Green's Function Method
- **Introducing Truncated Spectral Kernel**
  - Vico *et al*, https://doi.org/10.1016/j.jcp.2016.07.028

$$G(\vec{r}) \Longrightarrow G^L(\vec{r}) = G(\vec{r})\mathrm{rect}\left(\frac{r}{2L}\right),$$

- **Conditions for Truncation**
  - Truncated spectral kernel applies when $L > \sqrt{d}$ (with dimension d) and compactly support distribution
  - The indicator function $\mathrm{rect}(x)$ is defined as

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

- **Analytical Green's Function**
  - The Fourier transform of the Green's function is solvable analytically for a radially symmetric charge distribution
- **Fourier Transform of G^L**

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

- **The potential:**

$$\phi(\vec{r}) = \frac{1}{\varepsilon_0}\frac{1}{(2\pi)^3}\int e^{i\vec{k}\cdot\vec{r}}2\left[\frac{\sin\left(\frac{L|\vec{k}|}{2}\right)}{|\vec{k}|}\right]^2 \mathcal{F}\{\rho\}(\vec{k})d^3\vec{k}$$

- **Efficiency and Applicability**
  - The TGF Poisson Solver simplifies potential calculation with analytical Green's function, enhancing computational efficiency.

Implementation of Algorithms and Benchmarking

Benchmarking

- **Gaussian Charge Distribution:**

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

- **Grid Domain**
  - Utilize $N_x \times N_y \times N_z$ grid domain
  - Simplifying the problem: $N = N_x = N_y = N_z$
- **The Exact Poisson Solution:**

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

Implementation

- **Space Charge Potential**

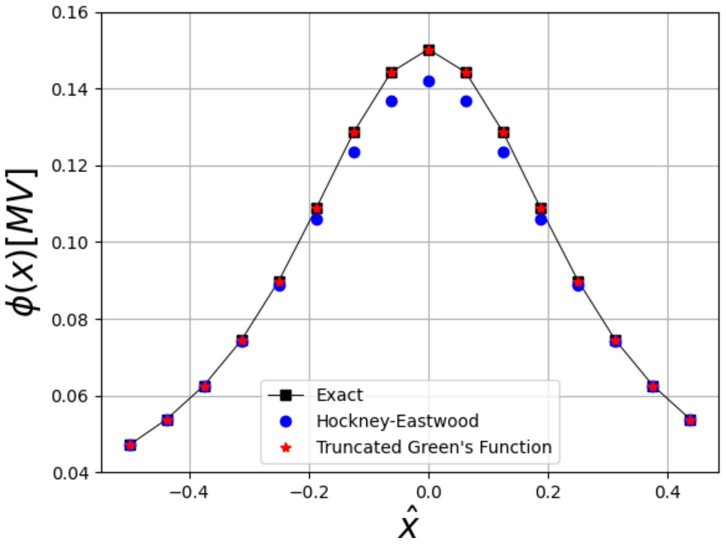
$$\phi(\vec{r}) = \frac{1}{\varepsilon_0} \frac{1}{(2\pi)^3} \int e^{i\vec{k}\cdot\vec{r}} 2 \left[\frac{\sin\left(\frac{L|\vec{k}|}{2}\right)}{|\vec{k}|}\right]^2 \mathcal{F}\{\rho\}(\vec{k}) d^3\vec{k}$$

1. Green's function kernel computation
2. Fourier Transform of the charge distribution
3. Inverse Fourier Transform of the convolution

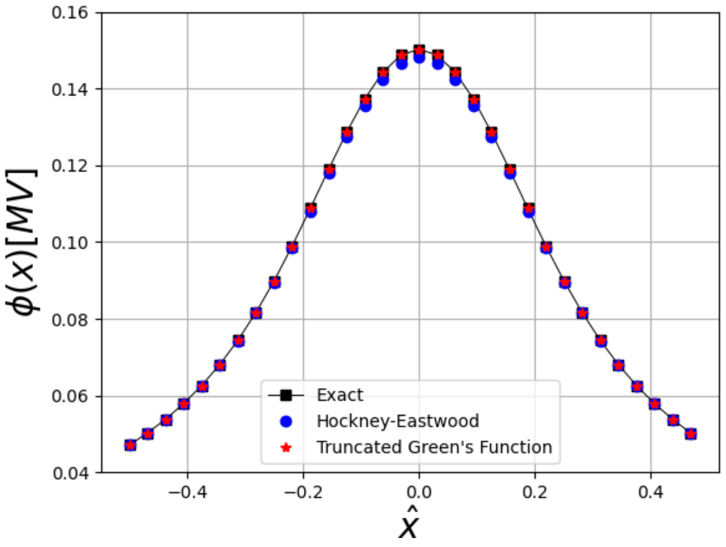
- **Grid Domain for Efficient Computation**
  - (4N) grid domains are needed in each direction.
  - *cf. (2N) number of grid domains is needed for HE*

Comparison of Space Charge Solvers

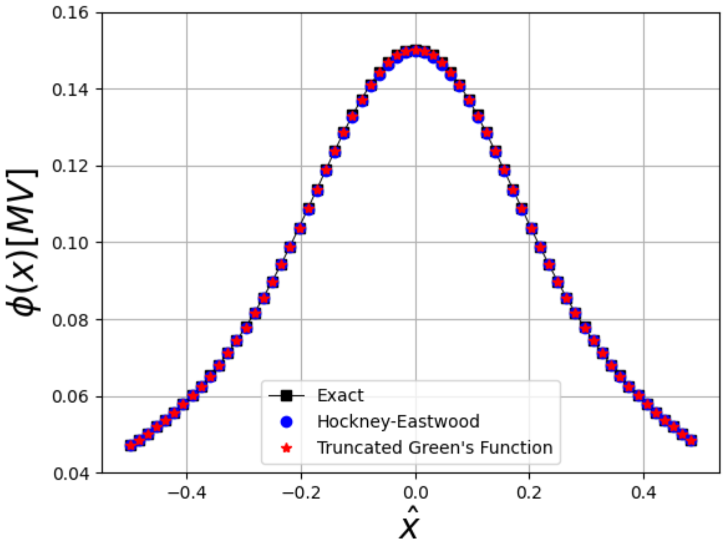
Potentials along the x-axis for a different number of grids



N = 16



N = 32



N = 64

- With a small value of N, the Hockney-Eastwood (HE) algorithm may exhibit significant deviations, especially at the beam center.
- Increasing the value of N, this observed deviation is reduced.
- Unlike HE, the accuracy of the TGF algorithm is not significantly influenced by the number of grid sizes.

Leveraging AD for Simulation Optimization

- **Automatic Differentiation Tool**:
  - Utilize advanced differentiation tools like TensorFlow, PyTorch, or JAX for computational flexibility.
- **Model Implementation**:
  - Within the selected framework, compute the charge distribution, Green's function, and numerical integrations. For convolution operations, apply the Fourier transform method.
- **Gradient Computation**:
  - Harness the AD tool to calculate gradients concerning parameters of interest, streamlining objective analysis.
- **Optimization**:
  - Deploy gradient-based optimization techniques to refine parameters, steering results toward optimal outcomes.

Differential Algebra and TPSA

- **Differential Algebra (DA)**
  - DA: Algebraic methods for analytic problem solving, introduced by M. Berz in 1986.
  - Wide Adoption: Implemented in accelerator simulation codes like COSY-Infinity, PTC, MAD-X PTC, Bmad, and CHEF(MXYZPTLK).
- **Truncated Power Series Algebra (TPSA)**
  - TPSA employs truncated power series expansions.
  - Approximates functions by retaining a finite number of terms in power series.
  - Advantages: Generates infinite order power series, offering comprehensive and accurate calculations.
- **Practical Use in Accelerator Simulations**
  - TPSA is a vital tool in beam dynamics analysis.
  - It handles complex mathematical representations, ensuring precision and reliability.

Basics of Truncated Power Series Algebra

Basic Operations in TPSA, ${}_1D_1$

- $(a_0, a_1) + (b_0, b_1) = (a_0 + b_0, a_1 + b_1)$
- $c(a_0, a_1) = (ca_0, ca_1)$
- $(a_0, a_1) \cdot (b_0, b_1) = (a_0 b_0, a_0 b_1 + a_1 b_0)$
- $(a_0, a_1)^{-1} = \left(\frac{1}{a_0}, -\frac{a_1}{{a_0}^2}\right)$
- Any special functions can be decomposed into a finite number of vector additions and multiplications
- DA can be expanded into higher order n with multiple variables, v: ${}_nD_v$

Examples of TPSA in ${}_1D_1$

- For a given function,
  - $f(x) = \frac{1}{x+1/x}$
- We know that
  - $f'(x) = -\frac{1-1/x^2}{(x+1/x)^2}$
- Therefore, $f(3) = \frac{3}{10}, f'(3) = -\frac{2}{25}$
- If we use TPSA with the DA vector $v = (3,1) = 3 + (0,1)$
  - $f(v) = f\big((3,1)\big) = \frac{1}{(3,1)+1/(3,1)} = \left(\frac{3}{10}, -\frac{2}{25}\right)$

Advancements in SC Calculations Using DA

- **H. Zhang et al: FMM Application (**Nucl. Inst. Meth. A 645 (2011) 338-344)
  - Applied DA techniques to the Fast Multipole Method (FMM) for space charge calculations.
  - Their work offers valuable insights into the effective use of DA in space charge effect computations.
- **B. Erdelyi et al: Duffy Transformation (**Comm. Comp. Phys. 17 (2015), pp 47-78)
  - Employed the Duffy transformation to solve the Poisson equation with Green's functions.
  - This method splits integrals into smaller domains, eliminating singularities associated with Green's functions.
- **J. Qiang: TPSA for Local Derivatives (**Phys. Rev. Accel. Beams 26, 024601 (2023))
  - Focuses on using TPSA techniques to derive local derivatives of beam properties with respect to accelerator design parameters.
  - Investigates coasting beam behavior within a rectangular conducting pipe.
- **Collective Impact of DA Techniques**
  - These three research contributions collectively demonstrate how DA techniques are leveraged to enhance space charge calculations.
  - They offer innovative methods and solutions that contribute to the advancement of accelerator physics.

Enhancing Precision in SC Field Computations

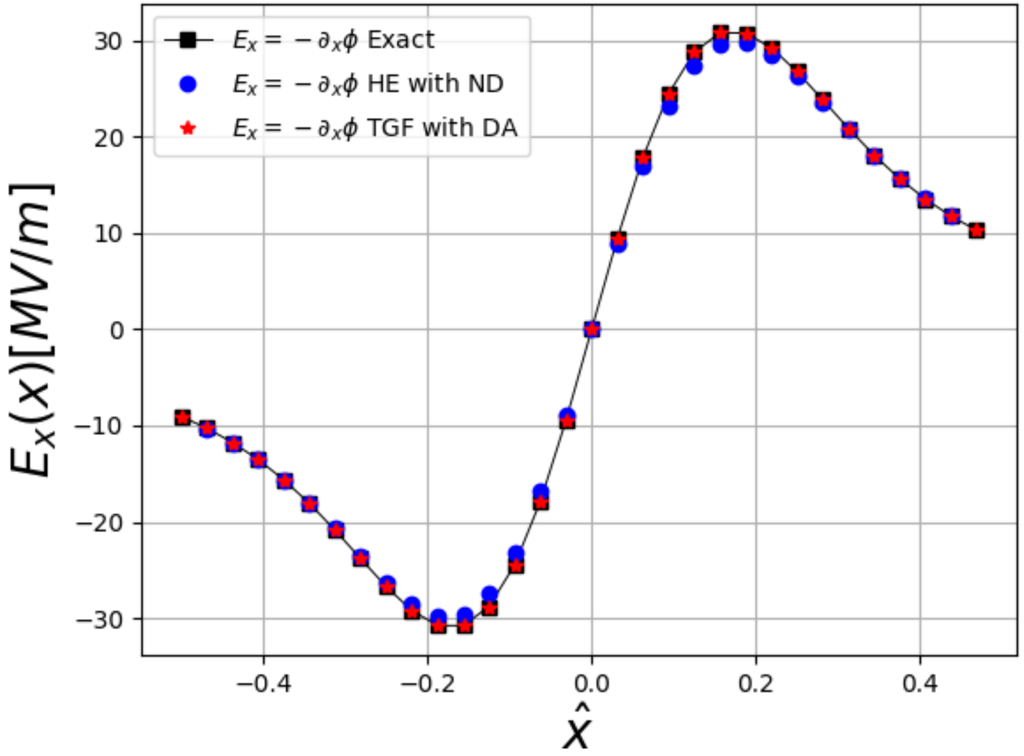
- **PIC Method for Space Charge Field Computation and Its Numerical Errors**
  - Particle-in-Cell (PIC) method is widely used in accelerator simulations but introduces computational errors due to its numerical nature.
  - Numerical computation of field derivatives is also susceptible to errors.
- **The Convolutional Approach**
  - An alternative approach involves direct field computation using a convolutional method with the truncated Green function.
  - This method helps mitigate computational errors inherent in PIC simulations.
- **Direct Electric Field Calculation**
  - With the truncated Green's function, electric fields can be directly calculated.

$$\vec{E}(\vec{r}) = -\vec{\nabla}\phi = \frac{1}{\varepsilon_0}\frac{1}{(2\pi)^3}\int i\vec{k}e^{i\vec{k}\cdot\vec{r}'}2\left[\frac{\sin\left(\frac{L|\vec{k}|}{2}\right)}{|\vec{k}|}\right]^2 \mathcal{F}\{\rho\}(\vec{k})d^3\vec{k}$$

- **Advantages of TPSA Techniques**
  - Truncated Power Series Algebra (TPSA) techniques facilitate the automatic calculation of higher-order derivatives.
  - Provide a systematic and efficient approach to handle these derivatives.
  - Enable precise and reliable computations of space charge field properties concerning beam properties.

Advancing Space Charge Potential Analysis with DA

- **Leveraging Differential Algebra (DA)**
  - Utilizing a DA vector and DA operations for higher-order derivative calculations.
  - Accurate and efficient assessment of space charge potential properties using the truncated Green's function.
- **DA Vector for Systematic Differentiation**
  - The DA vector represents the potential function.
  - Systematic differentiation with respect to variables of interest becomes feasible.
- **Comprehensive Understanding of Space Charge Potential**
  - These operations enable the calculation of derivatives of arbitrary order.
  - Providing a comprehensive understanding of space charge potential and its associated properties.



Summary

- **Accelerator Modeling Simulations**
  - Traditional modeling demands extensive simulations to assess machine parameter influences on beam properties.
  - Differentiable simulations allow for efficient gradient calculation with respect to inputs, crucial for machine learning and optimization
- **Improvement in Space Charge Field Calculations**
  - Comparative analysis highlights the strengths and limitations of space charge solvers
  - Noting that the Truncated Green’s Function method's efficiency in handling long-range integrations and singularities.
- **Differentiable Simulations in Beam Dynamics**
  - Differentiable simulation techniques are integrated within accelerator design to optimize the beam properties, employing advanced tools like TensorFlow and PyTorch.
  - The use of DA and TPSA in accelerator physics ensures precision in the simulation and optimization processes, paving the way for more accurate models with space charge field calculations

Thank You for Your Attention!