Differential Algebra for Accelerator Optimization with Truncated Green's Function

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Chong Shik Park

Department of Accelerator Science / Accelerator Research Center

Korea University, Sejong Campus

KOREA UNIVERSITY

Outline

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Introduction

- **Challenges in Space Charge Field Computation**
  - **Analytical Complexity:** Analytical solutions for EM and ES space charge fields are intrinsically complex.
  - **Particle-in-Cell (PIC) Methods:** Numerous solvers rely on PIC methods with open boundary conditions.
- **Accelerator Optimization**
  - Due to limited derivative information of beam properties, gradient-free algorithms are commonly used in accelerator optimization simulations.
- **Techniques to Address Derivative Constraints**
  - Differential Algebra (DA) and Truncated Power Series Algebra (TPSA)
  - DA and TPSA are effective for calculating nonlinear maps, widely adopted in accelerator codes
- **Differentiable Space Charge Model**
  - Differentiable self-consistent space charge model based on Truncated Green's function solvers
- **Advantages:**
  - Enhances computational efficiency for beam dynamics simulations and enables effective management of differentiable space charge effects.

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.

Hockney-Eastwood Algorithm

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

$$\phi(p,q) = \frac{h_x h_y h_z}{4\pi\varepsilon_0} \sum G(p,q;p',q')\rho(p',q')$$

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

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

- **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 Method

Vico-Greengard-Ferrando Poisson Solver

- **Limitation of HE FFT Method**
  - Utilizes Green's function with long-range definition and singularities at $\vec{r} = \vec{r}'$
- **Introducing Truncated Spectral Kernel**
  - Transforming the Green's function:

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

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

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

- **Analytical Green's Function**
  - The Fourier transform of the Green's function is solvable analytically.
- **Fourier Transform of G^L**

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

- **The potential:**

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

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

Implementation of Algorithms and Benchmarking

Benchmarking

- **Gaussian Charge Distribution:**

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

- **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**

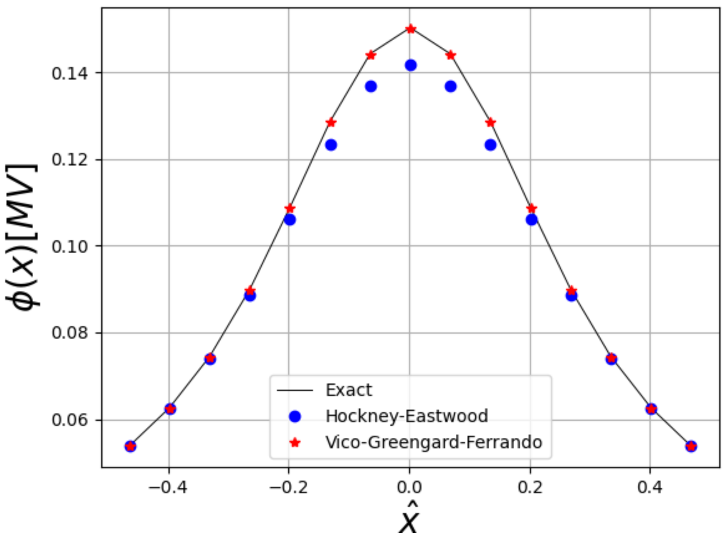
$$\phi(\vec{r}) = \frac{2}{(2\pi)^3\varepsilon_0}\int e^{i\vec{k}\cdot\vec{r}}\left[\frac{\sin\left(\frac{L|\vec{k}|}{2}\right)}{|\vec{k}|}\right]^2 \mathcal{F}\{\rho\}(\vec{k})d^3\vec{k}$$

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

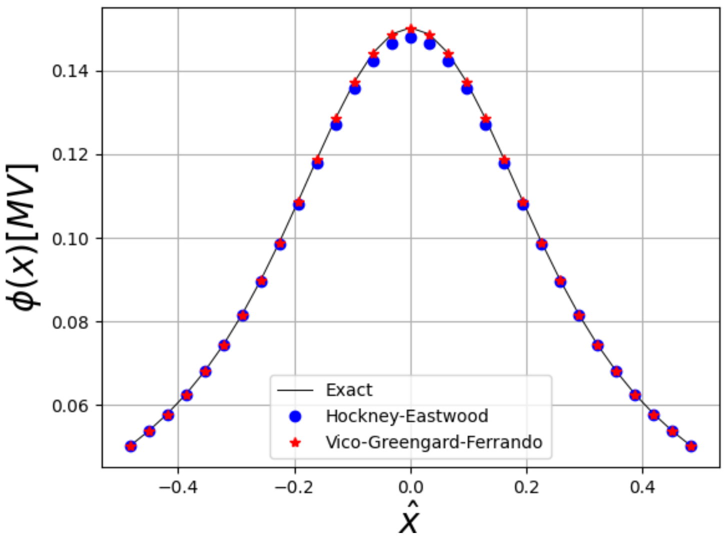
- **Grid Domain for Efficient Computation**
  - (4N) grid domains are needed in each direction.
  - *cf. (2N) number of grid domains is needed for HE*

Comparison of Space Charge Solvers

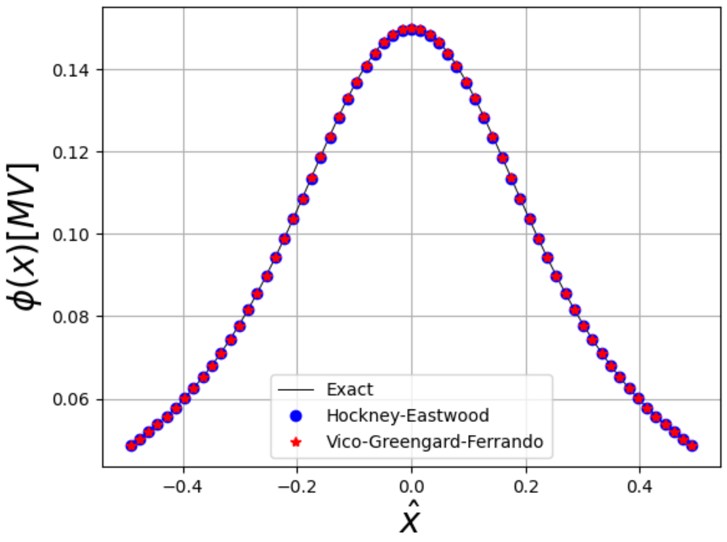
Potentials along the x-axis for a different number of grids



N = 16



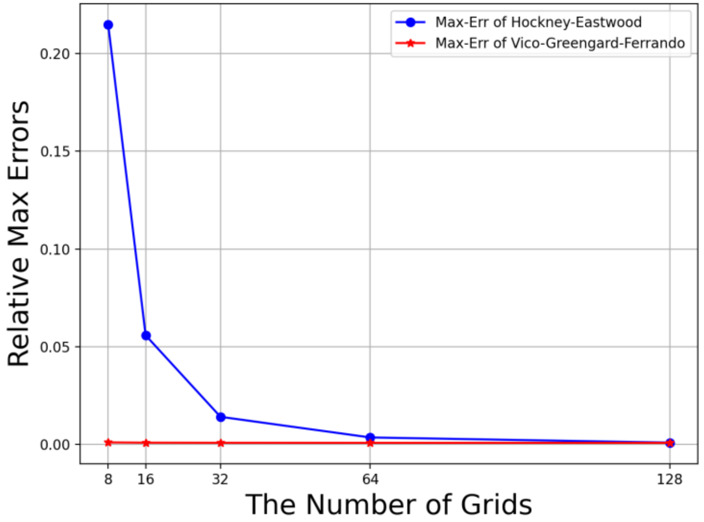
N = 32

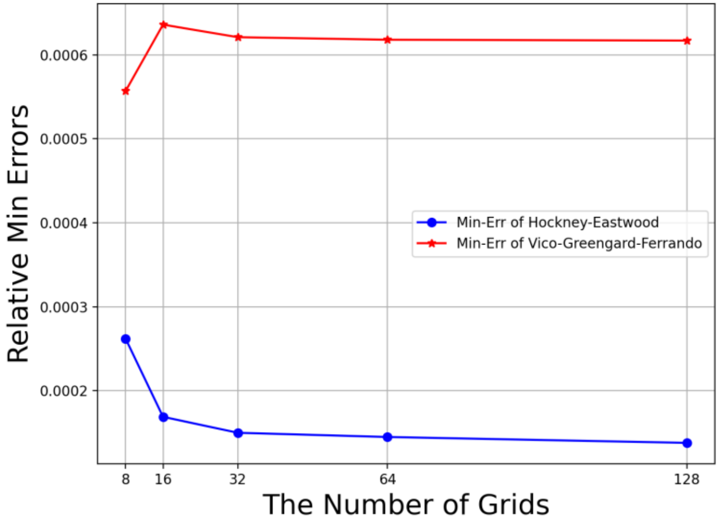


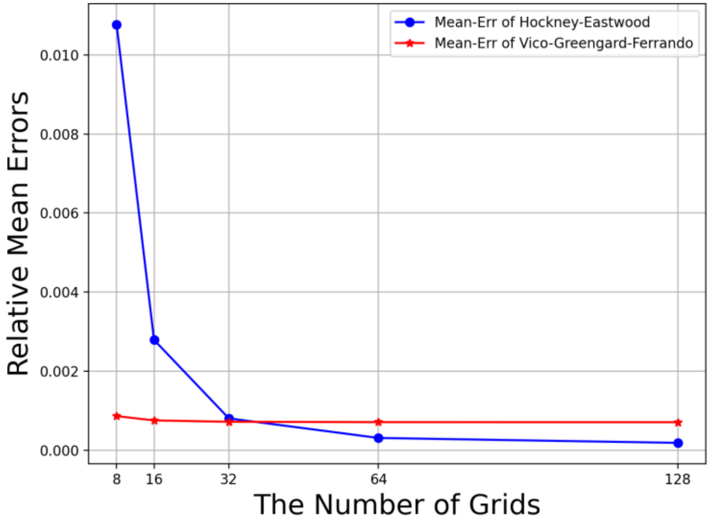
N = 64

- 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.

VGF vs. HE: Relative Errors



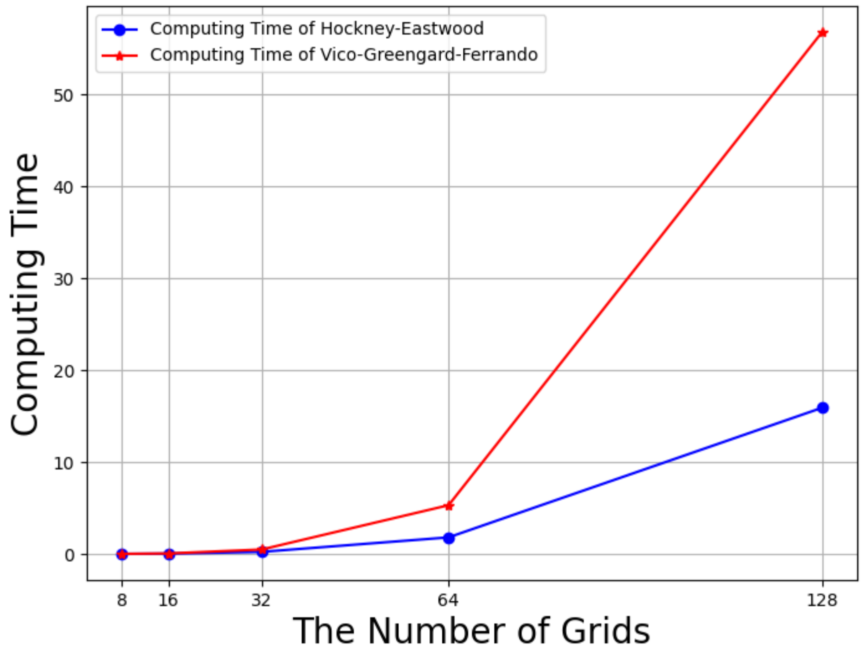


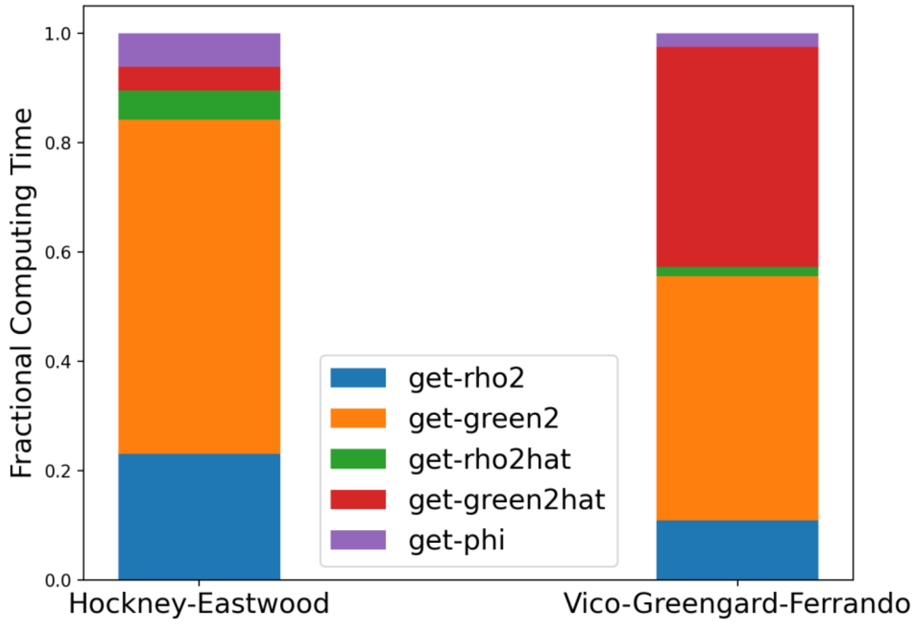


- **VGF Algorithm:**
  - Smaller maximum and mean errors observed for small grid sizes.
  - Larger minimum errors across all grid sizes.
  - Maximum relative error at the grid edge.
- **HE Algorithm:**
  - Maximum relative error occurs at the grid center.
  - Opposite behavior observed for minimum relative error.

- **Impact on Algorithm Accuracy**
  - Unlike HE, the accuracy of the VGF algorithm is not significantly influenced by the number of grid sizes.
  - Highlighting the robustness and consistent performance of the VGF algorithm across different scenarios.

Computing Time





- **Challenges with Increasing Grid Count**
  - In the Vico-Greengard-Ferrando (VGF) algorithm, computation time shows a noticeable increase as the number of grids rises.
- **Efficiency of VGF Algorithm**
  - Despite increased computation time with more grids, the VGF algorithm shines in its ability to achieve fast convergence with a relatively smaller number of grids.

Differential Algebra and TPSA

- **Differential Algebra (DA) and Truncated Power Series Algebra (TPSA)**
  - 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.

Differential Algebra and TPSA (Cont'd)

- **Expanding the Toolbox with TPSA Libraries**
  - In the realm of Differential Algebra (DA), several Truncated Power Series Algebra (TPSA) libraries have emerged independently.
- **Utilizing TPSA Libraries for Space Charge Field Calculations**
  - We harnessed these TPSA libraries to implement the DA method for space charge field calculations.
- **The Advantage of TPSA Libraries**
  - These libraries offer a remarkable advantage: they are adaptable to any aspect of accelerator simulation optimization.
  - Their versatility and wide applicability enhance the capabilities of DA techniques.
- **Notable TPSA Libraries**
  - TPSA-python by H. Zhang (https://github.com/zhanghe9704/tpsa)
  - PyTPSA by Y. Hao (https://github.com/YueHao/PyTPSA.git)

Basics of Truncated Power Series Algebra

Basic Operations in DA, ${}_1D_1$

- $(a_0, a_1) + (b_0, b_1) = (a_0 + b_0, a_1 + b_1)$
- $c(a_0, a_1) = (ca_0, vca_1)$
- $(a_0, a_1) \cdot (b_0, b_1) = (a_0 b_0, a_0 b_1 + a_1 b_0)$
- $(a_0, a_1)^{-1} = \left(\frac{1}{a_0}, -\frac{a_1}{a_0{}^2}\right)$
- 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)
  - Zhang and colleagues 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.
  - Reference: Nucl. Inst. Meth. A 645 (2011) 338-344
- **B. Erdelyi et al: Duffy Transformation (**Comm. Comp. Phys. 17 (2015), pp 47-78)
  - Erdelyi and team 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))
  - J. Qiang's research focuses on using Truncated Power Series Algebra (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 and 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.

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

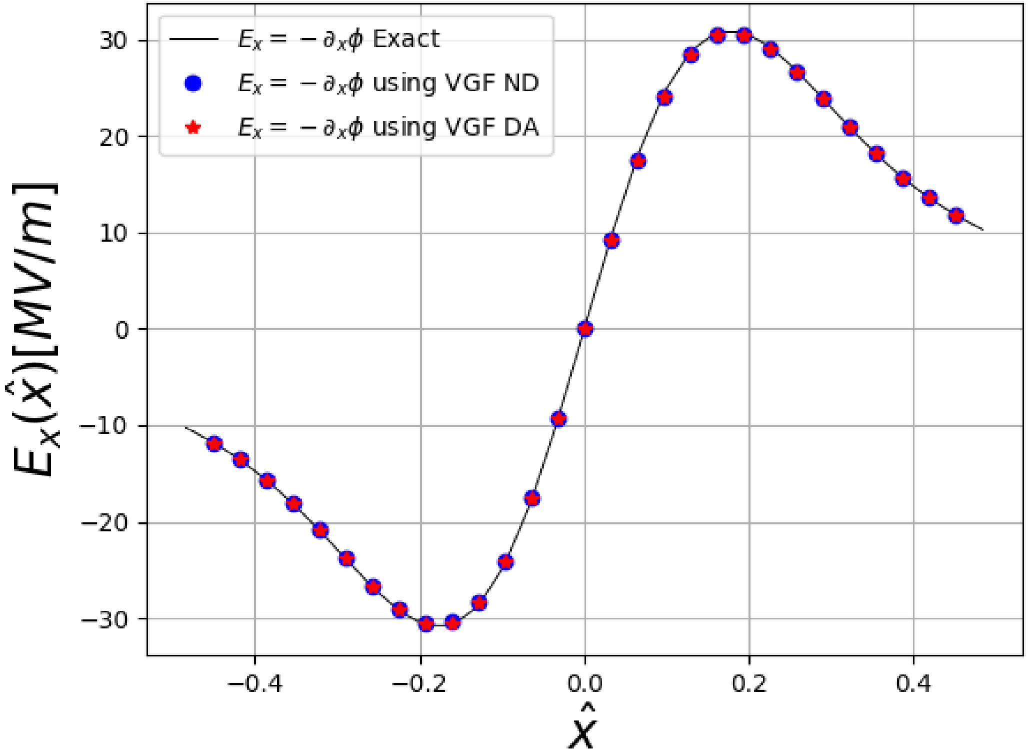
- **Advantages of TPSA Techniques**
  - Truncated Power Series Algebra (TPSA) techniques facilitate the automatic calculation of higher-order derivatives.
  - Provide a systematic and efficient approach to handle these derivatives.
  - Enable precise and reliable computations of space charge field properties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

Advancing Space Charge Potential Analysis with DA

- **Space Charge Potential Expansion**

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

- **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

- **Challenges in Space Charge Field Computations**
  - Accelerator simulations pose complex challenges in space charge field computations.
  - Hockney and Eastwood's algorithm offers efficient solutions for Poisson equations with open boundaries.
- **The Vico-Greengard-Ferrando (VGF) Poisson Solver**
  - Implementation of VGF with a truncated Green's function method.
  - Enhanced performance and accuracy in space charge field computations.
- **Automatic Higher-Order Derivatives with DA**
  - Differential Algebra (DA) enables automatic computation of higher-order derivatives.
  - Systematic and efficient analysis and optimization of accelerator systems.
- **Differentiable Space Charge Model Integration**
  - Integration of the truncated Green's function-based model into beam dynamics optimization simulations.
  - Expectations: Improved accuracy and efficiency in the optimization process.
  - Optimization with Gradient: Leveraging gradient-based optimization techniques for enhanced precision.

Thank You for Your Attention!