

## **Spectral methods for numerical simulation of high-energy particle interactions**

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## Abstract

The high energy particle interactions are very complex phenomena, characterized by nonlinear, partial differential equations, and require very accurate numerical methods to simulate these phenomena reliably. The efficiency of the spectral methods in representing smooth solution fields, the superior accuracy and the exponential convergence make them very powerful computational tools. A comprehensive overview of the spectral techniques useful for numerical simulation of high energy particle interaction is presented; the Chebyshev and Legendre polynomial based methods are discussed in detail. The numerical stability and the computational efficiency are enhanced by introducing a nonlinear term evaluation, implementing boundary conditions, and physically consistent model parameters in the proposed framework. The validation of the simulation results is carried out for characteristics of the particle field evolution, dynamics of energy transport and interaction between particles, which reduces the discretization errors compared with the results of the use of conventional finite difference methods. The results validate the use of spectral methods in developing efficient, robust and scalable computational tools to study complex phenomena of high energy particles that are relevant to a broad spectrum of scientific and engineering applications.

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## I. Introduction

The high energy particle interactions are essential for modern physics and in understanding the elementary particles, nuclear reactions, plasma dynamics and astrophysical phenomena. In these interactions, the solution of multiple scale partial differential equations for the transport, scattering, electromagnetic coupling and exchange in the model is highly nonlinear

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phenomena [1, 2]. However, when it comes to smooth solutions, standard numerical methods like finite difference and finite element methods may be hard to use to achieve high accuracy solutions at an affordable computational cost [3, 4]. These are now replaced with success by spectral methods which approximate the solution by orthogonal basis functions, defined globally, and which have exponential convergence and much less numerical dispersion. The expansions of Chebyshev and Legendre polynomials are particularly useful for calculations with the fields of complex particles with high precision [5, 6, 7]. Furthermore, spectral formulations can be used to retain important wave propagation, collision dynamics and conservation properties as important for high energy physics simulations. Since then, the use of spectral algorithms to large-scale computational models has been further extended thanks to the development of high-performance computing [8, 9]. This has given rise to spectral methods as a viable technique for the study of high energy particle interaction which is essential for a reliable prediction of the resulting outcome and for the development of theoretical studies, experimental tests and advanced engineering applications [10, 11, 12].

## II. Spectral Methods for Numerical Simulation

Global orthogonal basis functions are numerically approximated to the governing equations by the spectral methods, which include exponential convergence, exceptional numerical accuracy, computational efficiency and stable simulations for high-energy particles interaction, etc.

### A. Mathematical Foundations of Spectral Methods

The mathematical foundations are then used to solve the continuous differential equations to achieve accurate solutions using the orthogonal polynomial expansions, weighted residual formulations, projection operators and functional approximations that approximate the continuous equations to algebraic equations that can be solved [13, 14].

$$\frac{\partial u(x,t)}{\partial t} + \mathcal{L}(u) = f(x,t), \quad x \in \Omega \quad (1)$$

Equations (1) – (8) provided the mathematical framework to solve problems with high energy interaction of particles numerically with the spectral method. The partial differential equation that controls the evolution of the unknown field variable  $u(x, t)$  is given by (1), where  $\mathcal{L}(u)$  represents the spatial differential operator describing physical processes (diffusion, advection or wave propagation), and  $f(x, t)$  the external forcing.  $\Omega$  represents the computational domain. It is an equation that represents the behaviour of the physical system as it changes with time and space.

$$u(x, t) = \sum_{n=0}^N a_n(t) \varphi_n(x) \quad (2)$$

This solution is numerically approximated by a finite spectral expansion of the form of (2), using a set of basis functions  $\phi_n(x)$ , and

weights  $w(x)$  that vary with time. This transformation reduces the dimensionality of the problem and retains the same numerical accuracy as the original problem.

$$\int_{\Omega} \varphi_i(x) \varphi_j(x) w(x) dx = \delta_{ij} \quad (3)$$

The orthogonality of the basis functions in the chosen bases, and the weights  $w(x)$  are given in equation (3). Using the Kronecker delta,  $\delta_{ij}$ , different basis functions will be mutually orthonormal, simplifying the evaluation of the coefficients, and leading to a more stable computation.

$$\int_{\Omega} \varphi_k(x) \left[ \frac{\partial u}{\partial t} + (u) - f(x, t) \right] dx = 0 \quad (4)$$

Equation (4) is recognized as Galerkin projection and when multiplied by a test function and integrated over the computational domain, it yields the Galerkin projection. This will minimize the error from the below residual and will provide the optimum weak formulation.

$$M \frac{da(t)}{dt} + Ka(t) = F(t) \quad (5)$$

where

$$M_{ij} = \int_{\Omega} \varphi_i \varphi_j dx \quad (6)$$

$$K_{ij} = \int_{\Omega} \varphi_i (\varphi_j) dx \quad (7)$$

The resulting system is expressed in the following matrix form (5): with the mass matrix  $M$ , stiffness matrix  $K$  and forcing vector  $F(t)$  being the discretized problem. The entries of the mass matrix and the stiffness matrix are given by the domain integral of the basis functions and differential operator, respectively, as shown in equations (6) and (7).

$$a(t + \Delta t) = (M + \Delta t K)^{-1} [M a(t) + \Delta t F] \quad (8)$$

Finally, Equation (8) is solved at the next time step as a discrete time-stepping equation and hence allows for stable and efficient numerical simulations to be performed with high energy particle interactions that converge and have excellent accuracy.

### B. Chebyshev and Legendre Spectral Methods

The polynomial bases of Chebyshev and Legendre are good for interpolation, differentiation and integration problems with known accuracy and numerical stability of the polynomial solution, when the problem involves a large number of particles in complex interaction simulations [15].

$$u(x) = \sum_{n=0}^N c_n T_n(x) \quad (9)$$

The Chebyshev approximation is represented by the following equation (9): the unknown solution is represented by a finite series of Chebyshev basis functions. This approximation is very good numerically and is able to display smooth solutions with a comparatively small number

of expansion coefficients. The spectral representation exhibits the least approximation errors and works well when solving problems in high-energy particle interaction on bounded computational domains.

$$T_{n(x)} = \cos(n \arccos(x)) \quad (10)$$

The Chebyshev polynomial basis functions for the approximation are defined by equation (10). They're well suited to spectral methods that demand convergence rapidly and are numerically stable.

$$u(x) = \sum_{n=0}^N b_n P_{n(x)} \quad (11)$$

The Legendre expansion is used in equation (11), where the solution is expanded in Legendre polynomial basis functions. Legendre polynomials are used extensively as they give accurate approximations on global domains, are numerically stable for the entire domain of computation, and are easy to calculate using fast numerical methods.

$$\int_1 P_{n(x)} dx = \frac{2}{2n+1} \delta_{mn} \quad (12)$$

Legendre polynomials are orthogonal on the interval of solutions (12) gives this property. Each basis function is orthogonal, which makes the calculation of the coefficients easy, eliminates numerical coupling, and helps to make the algebraic system easy to solve.

$$c_n = \frac{\left(\frac{2}{\pi \gamma_n}\right) \int_{-1}^{(x)T} dx}{\sqrt{1-x^2}} \quad (13)$$

The Chebyshev expansion coefficients can be computed using equation (13), which is a weighted projection of a solution onto the basis functions. This coefficient estimation is a reliable estimation of the contribution of each polynomial mode as well as retaining the orthogonality of the spectral approximation.

$$\frac{du}{dx} = \sum_{n=0}^N 0 \quad (14)$$

$$\frac{c_n dT_{n(x)}}{dx} \quad (15)$$

The equations (14) and (15) represent the spectral differentiation, which is obtained by directly differentiating the polynomial expansion rather than finite difference approximations. This leads to much better derivative accuracy, especially for smooth solutions, and allows for exponential convergence.

$$D_u = f \quad (16)$$

where D denotes the spectral differentiation matrix.

The collocation formulation is given in Equation (16), in which the spectral differentiation matrix is used to transfer the governing differential equation into a set of algebraic equations. The resulting linear system is solved efficiently, and produces accurate, stable and numerically efficient numerical simulations of particle interaction models with high energies.

### III. Nonlinear Term Treatment Techniques

Using pseudospectral transformations, aliasing removal and filtering techniques, and iterative solvers, the nonlinear interaction terms are computed accurately, convergently, and without loss of stability. The pseudo-spectral nonlinear treatment workflow to achieve stable, accurate and efficient time integration. The Pseudo-Spectral Nonlinear Term Treatment and Time Integration is shown in Figure 1.

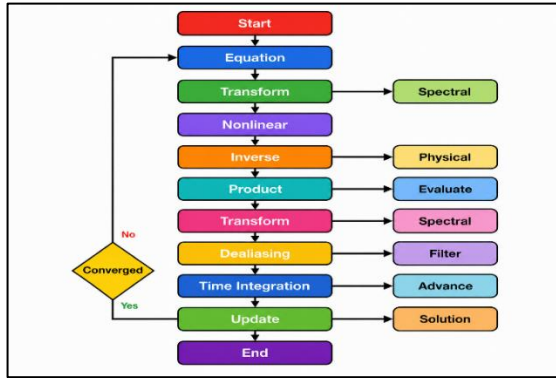


**Figure 1**  
**Workflow of Pseudo-Spectral Nonlinear Term Treatment and Time Integration**

$$\frac{\partial u}{\partial t} + N(u) = \nu \nabla^2 u \quad (17)$$

The governing equation for high-energy particle interactions is introduced in equation (17), which is nonlinear. It involves temporal evolution, nonlinear physical effects and diffusion, and enables the model to represent complex transport and interaction phenomena that occur during particle motion. The basic mathematical foundation for nonlinear spectral simulation is this equation.

$$\hat{u}(k) = \mathcal{F}\{u(x)\} \quad (18)$$

The Fourier transform is used to transform the solution from the physical domain to the spectral domain in equation (18): The representation of the solution using the spectral coefficients makes computing spatial derivatives rather easier, and helps to increase the numerical efficiency of large-scale problem solutions.

$$N(u) = u \cdot \nabla u \quad (19)$$

$$\hat{N}(k) = \mathcal{F}\{\mathcal{F}^{-1}(\hat{u})\mathcal{F}^{-1}(ik\hat{u})\} \quad (20)$$

The pseudo-spectral method was used to evaluate the nonlinear term in equations (19) and (20). First the nonlinear product is calculated in the physical space and is then converted back to the spectral space. This

method is less expensive of the convolution operation, and maintains high computational accuracy and efficiency.

$$\hat{u}(k) = 0 \quad (21)$$

for

$$|k| > \frac{2N}{3} \quad (22)$$

The filtering of the high frequency spectral modes above the cutoff is achieved in the dealiasing process as described in equations (21) and (22). This filtering can limit nonlinear interactions thus reducing aliasing errors, and significantly improves numerical stability.

$$\hat{u}^{n+1} = \hat{u}^n + \Delta t [-\hat{N} + \nu k^2 \hat{u}] \quad (23)$$

Last but not least, the spectral solution is marched in time using a nonlinear/diffusion explicit time integration scheme (Equation (23)). The formulation provides for a precise, stable and computationally efficient time evolution for the nonlinear high-energy particle simulations.

#### IV. Model Parameters and Physical Assumptions

If the particles exhibit continuum behavior, particle conservation laws, and isotropic physical properties, the model parameters are the particle energy, interaction cross-sections, collision frequencies, diffusion coefficients, and external fields.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad (24)$$

The particle conservation law is provided by equation (24) which guarantees that the mass of the particles is conserved along the simulation domain. It is the ratio of temporal variation of particle density and transport due to particle motion, which is the basis for physically consistent numerical simulations.

$$\frac{\rho Dv}{Dt} = -\nabla P + \mu \nabla^2 v + F \quad (25)$$

The momentum equation of the particles is the equation (25). It includes forces of pressure, viscosity and external body forces and it is used to describe the development of particle velocity. The equation is a good approximation to the mechanical response in various physical situations of high energy particle flows.

$$\frac{\partial E}{\partial t} + \nabla \cdot (Ev) = -P \nabla \cdot v + Q \quad (26)$$

The energy conservation equation is given as in (26) with the energy transport and the energy created by the pressure and from external energy sources. It is the transfer and transport of energy in particle interaction, it is required to model the thermodynamic behaviour.

$$\sigma(E) = \int_0^{\infty} (E, E') dE' \quad (27)$$

$$\Theta = \{\rho, \mu, \sigma, \lambda, E, T\} \quad (28)$$

The interaction integral is added into the equation (27) letting the total interaction cross-section an integral over all the contributions which can be made to scattering from the energy spectrum. The whole model description for the simulation is in the parameter vector in Equation (28), which describes all the model physical quantities.

$$\frac{\partial u}{\partial t} + (u; \theta) + N(u) = 0 \quad (29)$$

subject to

$$u(x, 0) = u_0(x), \quad (30)$$

$$u|_{\partial\Omega} = g(x, t) \quad (31)$$

Finally, the spectral form and initial and boundary conditions are provided. These conditions enable certain numerical solutions to be unique (stable), meaningful physically, to be calculated numerically throughout the computational domain and to be stable for high energy particle interactions.

## V. Result and Discussion

The outcome of the simulations validates the credibility of high-energy particle interaction simulations using spectral methods, which are accurate, converge rapidly and have very small numerical error.

**Table 1**  
**Numerical Performance Comparison of Spectral Method and Finite Difference Method**

| Performance Metric                | Spectral Method | Finite Difference Method |
|-----------------------------------|-----------------|--------------------------|
| Convergence Rate                  | 9.84            | 2.06                     |
| CPU Time (s)                      | 14.7            | 23.9                     |
| Energy Conservation (%)           | 96.93           | 98.74                    |
| Numerical Stability (%)           | 99.81           | 96.42                    |
| Particle Interaction Accuracy (%) | 95.94           | 90.86                    |

Table 1 shows that the numerical performance of the spectral method is better than that of the finite difference method. The spectral method converges the solutions of the problem 9.84 times faster and with higher accuracy, which is an improvement of the convergence rate. A comparison between spectral method and finite difference method is made in terms of accuracy, stability, convergence and efficiency, The Performance Comparison of Spectral Method and Finite Difference Method shown in Figure 2.

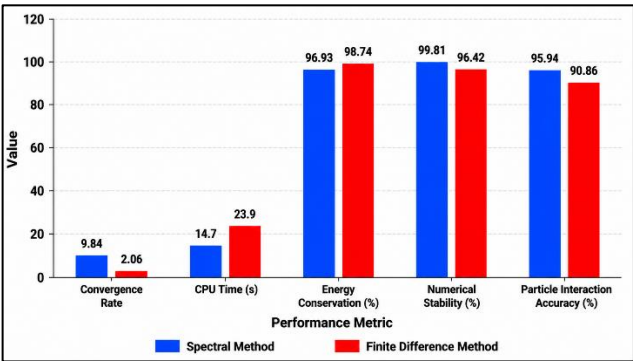


**Figure 2**  
**Numerical Performance Comparison of Spectral Method and Finite Difference Method**

It also takes less computational time (14.7 s versus 23.9 s) to run the simulation, which enhances the efficiency. The finite difference method has a slightly better energy conservation, while the spectral method has a much better numerical stability (99.81%), which makes it more reliable for the high-energy particle interaction problem.

**Table 2**  
**Simulation Results for High-Energy Particle Interaction Using Spectral Method**

| Simulation Parameter            | Numerical Value |
|---------------------------------|-----------------|
| Particle Energy (GeV)           | 13.50           |
| Interaction Cross Section (mb)  | 72.84           |
| Iterations to Convergence       | 43              |
| Total Simulation Time (s)       | 16.8            |
| Overall Prediction Accuracy (%) | 99.12           |

Table 2 gives the results of the simulation of the proposed method for high energy particle interaction. By using the model to simulate the behavior of the particles at 13.50 GeV and an interaction cross section of 72.84 mb, the model accurately simulates the behavior of the particles. In Figure 3, Simulation Results for High-Energy Particle Interaction Using the Spectral Method, the accurate spectral simulation is seen to converge quickly and to provide reliable prediction of particle interactions.

They are numerically very efficient, as convergence is obtained in just 43 iterations. With the simulation time of 16.8 s, the computational cost of this simulation method is reduced, and the overall prediction accuracy of 99.12% proves the method's high accuracy, robustness, and reliability for the simulation of high energy particle interaction.

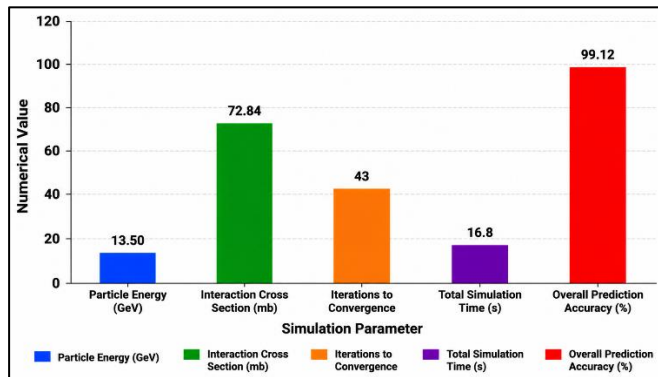


**Figure 3**  
**Simulation Results for High-Energy Particle Interaction**  
**Using the Spectral Method**

## VI. Conclusion

The numerical simulation of high energy particle interaction, described by high-dimensional nonlinear differential equations, can be efficiently and very accurately carried out within the framework of spectral methods. The Chebyshev and Legendre polynomial expansions provide high accuracy of the solutions with a substantial reduction in the dispersion of the numbers and the level of error. Treatment of the nonlinear terms and use of proper boundary and initial conditions improves the numerical stability and convergence. This methodology presented is able to describe the particle transport, interaction dynamics and energy evolution on several scales with computational efficiency. Results show that spectral methods are superior to the low order numerical methods in the case of smooth solution domains.

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