

Automatic Generation of Finite Difference Field Solvers for Toroidally Confined Plasmas

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Abstract. Flux coordinates and field-line coordinates are ubiquitous in magnetically confined plasma research. Most of these coordinates are essentially non-orthogonal curvilinear coordinates, in which the differential operators are rather complicated. This article reports an automatic tool, *OpGen*, for generating a finite difference coefficient matrix for field solvers by using a computer symbolic computation system. This tool is suitable for, but is not limited to, code development for toroidally confined plasmas.

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1 Introduction

In magnetically confined fusion research, toroidal flux coordinates and field-line following coordinates have long been extensively used in theoretical analysis and computations. Field perturbations and particle motions can be well separated in these coordinate systems into multiple spatial and temporal scales. For example, in the particle simulation

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code GTC [1], the field-line coordinates greatly ease the requirement for the toroidal grid number and dramatically improve the computing accuracy of parallel derivatives. In addition, the field-line coordinates well separate the directions parallel and perpendicular to the equilibrium magnetic field and greatly reduce the computational cost by reducing a 3-dimensional problem to a quasi-2-dimensional problem in the long wavelength limit $k_{\perp} \gg k_{\parallel}$ such that $\nabla \simeq \nabla_{\perp}$. The scalability of this parallel code also benefits from this feature. However, owing to the complex geometry of fusion devices, these coordinates are either weakly or highly non-orthogonal curvilinear coordinates, which makes the differential operator expression very complex. Many terms in the differential operators that vanish in Cartesian coordinates will emerge in these curvilinear coordinates. In addition, numerical simulation codes tend to use a complex discrete scheme to calculate the finite differences more accurately. These facts make the derivation of these discrete differential operators tedious and mistake-prone.

In this work, a symbolic package, *OpGen*, is introduced to automate this expansion and substitution process, making the creation and implementation of a new finite difference solver faster, easier and typo-free. There have already been some applications of computer algebra systems in plasma physics. These include the derivation of vector formulas [2], derivation of the dielectric tensor [3] and simplification of complex vector expressions induced by the gyrokinetic expansion [4,5]. These works, together with many other famous symbolic packages developed in general relativity research, mainly focus on assisting the derivation process in the theoretical domain. Many of these packages strive to be as general as possible to be suitable for use in various theoretical scenarios. By contrast, the code presented here, *OpGen*, will focus on bridging the analytical expressions and the simulation codes.

The finite difference field solver in toroidal geometry is rather complicated even in symmetric toroidal geometry [6], for which significant efforts were required for its manual derivation and implementation. An asymmetric version [7] makes this situation even more problematic. The powerful *OpGen* tool was applied to newly developed toroidal particle-in-cell (PIC) code with fully kinetic ions and gyrokinetic electrons for radio frequency wave simulations [8], where it is utilized to automatically generate a much more complex vector Laplacian solver in the field-line coordinate system with the 11-point discretization scheme. The generated field solver was then benchmarked in cylindrical geometry using the method of manufactured solutions [9]. The numerical results are in accord with the analytical results, which verifies the excellent fidelity of the automatically generated field solver.

This paper is organized as follows: In Section 2, the differential operator is derived in general curvilinear coordinates. In Section 3, an overview of the symbolic program and its typical application routine are provided. Section 4 includes the application of this symbolic expansion package in the development of toroidal fusion simulation code. A new integrated field solver for vector potentials is generated utilizing the 11-point scheme. The benchmark is reported in Section 5. Section 6 provides the summary of this work.