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Towards optimal explicit time-stepping schemes for the gyrokinetic equations

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ABSTRACT

The nonlinear gyrokinetic equations describe plasma turbulence in laboratory and astrophysical plasmas. To solve these equations, massively parallel codes have been developed and run on present-day supercomputers. This paper describes measures to improve the efficiency of such computations, thereby making them more realistic. Explicit Runge–Kutta schemes are considered to be well suited for time-stepping. Although the numerical algorithms are often highly optimized, performance can still be improved by a suitable choice of the time-stepping scheme, based on the spectral analysis of the underlying operator. Here, an operator splitting technique is introduced to combine first-order Runge–Kutta–Chebychev schemes for the collision term with fourth-order schemes for the remaining terms. In the nonlinear regime, based on the observation of eigenvalue shifts due to the (generalized) $E \times B$ advection term, an accurate and robust estimate for the nonlinear timestep is developed. The presented techniques can reduce simulation times by factors of up to three in realistic cases. This substantial speedup encourages the use of similar timestep optimized explicit schemes not only for the gyrokinetic equation, but also for other applications with comparable properties.

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1. Introduction

Gyrokinetic simulation codes are a common tool for obtaining *ab-initio* predictions of turbulence properties in strongly magnetized high-temperature plasmas. [1,2] Such plasmas are present in magnetic confinement fusion devices, and in astrophysics. Gyrokinetic theory describes the time evolution of each species' particle distribution function f in five-dimensional phase space (one velocity space variable, the gyro-angle, is averaged out). Obtaining a solution of this nonlinear partial integro-differential equation generally requires high-performance computing. In the past decades, gyrokinetic codes have become substantially more realistic by applying higher numerical resolution and by moving to more comprehensive physics models. For example, the effect of collisions is formally weak in dilute high-temperature plasmas and thus has often been neglected. Today, one realizes that including a suitable collision operator in gyrokinetic turbulence is not only required for a physically correct entropy balance, [3] but can also greatly influence the turbulence level – through damping of zonal flows – or even change the turbulence regime by modifying the growth rate of certain types of microinstabilities [4–8]. Since more realistic physics models require increased computational effort, progress is enabled by the availability of more powerful computers and by the use of advanced algorithms, the importance of the latter often being underestimated.

Three classes of gyrokinetic turbulence codes (particle-in-cell, semi-Lagrangian, and Eulerian) exist. Here, the Eulerian approach, which became popular approximately fifteen years ago, is considered. Several major code projects exist in this area, for instance GENE [9–12], GS2 [13,14], GYRO [15,16], GKW [17], and AstroGK [18]. The common basic procedure is the so-called method of lines: after discretizing phase space on a fixed grid, the resulting large system of ordinary differential equations is evolved with a time integration scheme. However, the choice of algorithms can differ substantially. Besides various possible choices for phase space grids and the representation of derivatives on those grids, time discretization is performed in several ways; see Ref. [19] for a useful overview. Operator splitting techniques for the collisional term are used in GYRO, GS2 and AstroGK. Some codes (like GS2) even choose to split off the nonlinear term from linear dynamics, while others avoid splitting to treat these terms on an equal level. Moreover, implicit as well as explicit schemes are applied. While GS2 (and AstroGK) treat all linear terms implicitly, the GYRO algorithm splits off fast linear terms (the parallel electron dynamics) in an implicit–explicit (IMEX) fashion. Here, we focus on fully explicit

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time integration, as employed in GENE and GKW, for example. Explicit methods offer the advantages of an excellent performance on massively parallel systems and the straightforward implementation of nonlinear terms. The drawback is a strict stability limit that is set on the timestep Δt, which depends on the fastest dynamics in the system. A major advance from the gyrokinetic theory is to analytically remove extremely fast timescales like compressional Alfvén waves or particle gyromotion, leaving only relevant dynamics and enabling an explicit treatment. One of the fastest remaining terms is then given by the (generalized) nonlinear drift velocity $v_\chi = E_\chi \times B$ that combines electric and magnetic field fluctuations. When this nonlinear advection limits the timestep according to a Courant–Friedrichs–Lewy (CFL) relation $\Delta t \lesssim \Delta x / v_\chi$ [20], fully explicit schemes are likely to be the more efficient choice (particularly in view of increasing problem size) [9].

It is sometimes stated that collisions require an implicit treatment, since the explicit diffusive timestep limit would be too strict [21]. However, we find severe restrictions only for rather large collision frequencies (in the tokamak edge, for example) or for very high velocity resolution. In this work, we introduce a splitting scheme involving Runge–Kutta–Chebychev (RKC) schemes with extended real stability boundary [22,23], which enables an explicit treatment of a sophisticated collision operator even in these extreme cases. Partitioned RKC schemes have recently been developed which are also stable for advective terms, involving, however, a larger number of operator evaluations per step [24,25].

In principle, accuracy limits can also be imposed on the timestep. In this context, we note that the overall numerical accuracy of gyrokinetic simulations is generally strongly restricted by the grid resolution in five-dimensional phase space. A relative error tolerance of approximately 10^{-3} is already considered to be sufficient, even for linear simulations. Nonlinear simulations are subject to statistical errors of the order of 10%, underlining the fact that long simulation times rather than highly accurate steps are needed. In consequence, the use of low-order time integration schemes is well justified to speed up computations.

In this paper, a detailed analysis of the spectral properties of the discretized system allows us to identify a class of highly efficient first-order explicit schemes (with largely extended stability boundaries), which we apply to the gyrokinetic code GENE. The remainder of this paper is organized as follows. The relevant equations are summarized in Section 2 and timestep limiting physics is discussed. In Section 3 we introduce relevant explicit RK schemes and review their stability conditions. In Section 4, the efficiency and accuracy of splitting techniques are discussed, which allow time-stepping schemes to be tailored to the individual parts of the operator. Finally, in Section 5 we address the timestep restrictions in nonlinear simulations. We show that the $E_\chi \times B$ advection shifts the eigenvalues along the imaginary axis, which is relevant for the stability limit. This observation forms the basis of a greatly improved estimate of the nonlinear timestep. Overall, these two methods of (i) operator splitting and (ii) an improved timestep estimate enhance the code efficiency by up to a factor of three in realistic cases. Since the code was already highly optimized, this speedup is significant.

2. The gyrokinetic equations

The gyrokinetic equation

$$\partial_t g = G[t, g] = N[\bar{\chi}, g] + L[g] + C[g] \tag{1}$$

describes the time evolution of the (modified) perturbed gyrocenter distribution g for each plasma species in $\{x, y, z, v_\parallel, \mu\}$ phase space. The notation

$$\bar{\chi} = \bar{\phi}_1 - v_\parallel \bar{A}_{1\parallel} + \mu \bar{B}_{1\parallel} \qquad f = g + v_\parallel \bar{A}_{1\parallel} F_0$$

$$F_0 = \frac{n_0}{\pi^{3/2} v_T^3} \exp\left[\left(v_\parallel^2 + \mu B_0\right)/T_0\right]$$

introduces the fluctuating potential $\bar{\chi}$, consisting of electrostatic perturbations $\bar{\phi}_1$ and magnetic perturbations $\bar{A}_{1\parallel}$ and $\bar{B}_{1\parallel}$, where the overbar denotes a gyroaverage. The gyrocenter distribution is split into a background (Maxwellian) distribution F_0 and a small fluctuating part f. The background magnetic field is B_0 and the background density n_0, temperature T_0, thermal velocity $v_T = (2T_0/m)^{1/2}$, and particle mass m are given for each plasma species. The gyrokinetic version of Maxwell's equations is used to compute a self-consistent fluctuating potential from g, which closes the system of equations. We refer to Refs. [2,10,12] for a detailed description and derivation.

Eq. (1) is symbolically written as the sum of three integro-differential operators whose physical meaning is briefly discussed in the following. The linear terms $L[g]$ contain parallel advection along the magnetic field lines, as well as the perpendicular drifts such as curvature and ∇B drifts, and temperature and density gradient terms. The nonlinear term $N[\bar{\chi}, g]$ describes turbulent redistribution of free energy due to perpendicular $E_\chi \times B$ advection, where the generalized fluctuating field is defined as $E_\chi = -\nabla \bar{\chi}$. Finally, the linearized Landau–Boltzmann collision operator $C[g]$ describes diffusion and dynamical friction in velocity space, including back-reaction terms that ensure the conservation of particles, momentum, and energy. Details of the implementation of the collision operator in GENE can be found in Refs. [26,27].

For a numerical solution, Eq. (1) is discretized on a fixed grid in phase space, where common techniques from computational fluid dynamics, such as spectral methods, finite differencing, finite element, and finite volume schemes, can be used. This results in a large system of ordinary differential equations for the time evolution of the state vector g. When non-dissipative differencing schemes are employed, as is the case with the GENE code, it may be necessary to add hyperdiffusion terms to $L[g]$ that remove unphysical grid-size oscillations in some phase space directions [28,29].

One way of solving this space-discretized system is to perform initial value computations, for which we consider Runge–Kutta (RK) schemes here. In the nonlinear case, we desire to find a statistically stationary turbulent state. Linear initial value computations yield the fastest growing solution (sometimes referred to as a mode), which constitute the driving force for plasma turbulence and are thus of great interest. Typical growth rates and frequencies are of the order of c_s/L_{ref}, where $c_s = (T_e/m_i)^{1/2}$ denotes the ion sound speed and L_{ref} is a typical macroscopic scale length, often set to the tokamak major radius. Additionally, the linearized system can be formulated as an eigenvalue problem. In this context, GENE features the use of optimized iterative algorithms provided by the SLEPc package [30–34], which select a subset of eigenvector–eigenvalue pairs $\{g_i, \lambda_i\}$ that fulfill some user-specified criteria. For convenience, we split the complex eigenvalue $\lambda = \gamma + i\omega$ into a growth rate γ and a frequency ω. The eigenvalues of largest magnitude $|\lambda_i|$ are quickly found (for example by Krylov–Schur subspace iteration), which proves extremely useful for the exact computation of the maximum stable timestep for initial value simulations. Due to the shape of the spectrum, obtaining the fastest growing solution with SLEPc is more cumbersome, but can still be faster than a corresponding initial value simulation. Moreover, subdominant and marginally stable solutions only become accessible by such eigenvalue computations. Finally, GENE can also

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