Princeton Plasma Physics Laboratory

PPPL-4040 PPPL-4040

Introduction to Gyrokinetic Theory with Applications in Magnetic Confinement Research in Plasma Physics

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January 2005

Prepared for the U.S. Department of Energy under Contract DE-AC02-76CH03073.

INTRODUCTION TO GYROKINETIC THEORY WITH APPLICATIONS IN MAGNETIC CONFINEMENT RESEARCH IN PLASMA PHYSICS

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Abstract
The present lecture provides an introduction to the subject of gyrokinetic theory with applications in the area of magnetic confinement research in plasma physics – the research arena from which this formalism was originally developed. It was presented as a component of the "Short Course in Kinetic Theory within the Thematic Program in Partial Differential Equations" held at the Fields Institute for Research in Mathematical Science (24 March 2004). This lecture also discusses the connection between the gyrokinetic formalism and powerful modern numerical simulations. Indeed, simulation, which provides a natural bridge between theory and experiment, is an essential modern tool for understanding complex plasma behavior. Progress has been stimulated in particular by the exponential growth of computer speed along with significant improvements in computer technology. The advances in both particle and fluid simulations of fine-scale turbulence and large-scale dynamics have produced increasingly good agreement between experimental observations and computational modeling. This was enabled by two key factors: (i) innovative advances in analytic and computational methods for developing reduced descriptions of physics phenomena spanning widely disparate temporal and spatial scales; and (ii) access to powerful new computational resources. Excellent progress has been made in developing codes for which computer run-time and problem size scale well with the number of processors on massively parallel processors (MPP's). Examples include the effective usage of the full power of multi-teraflop (multi-trillion floating point computations per second) supercomputers to produce three-dimensional, general geometry, nonlinear particle simulations which have accelerated advances in understanding the nature of turbulence self-regulation by zonal flows. These calculations, which typically utilized billions of particles for thousands of time-steps, would not have been possible without access to powerful present generation MPP computers and the associated diagnostic and visualization capabilities. In looking towards the future, the current results from advanced simulations provide great encouragement for being able to include increasingly realistic dynamics to enable deeper physics insights into plasmas in both natural and laboratory environments. However, it should be kept in mind that even with access to greatly improved

computational hardware and software advances, there will remain limitations to what can be practically achieved. For example, some of the most complex plasma phenomena involving highly transient nonlinear behavior may defy mathematical formulation and be beyond the reach of computational physics.

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1. Introduction

Plasmas are ionized gases which are often referred to as "the fourth state of matter" and comprise over 99% of the visible universe. They are rich in complex, collective phenomena and encompass major areas of research including plasma astrophysics and fusion energy science. Fusion is the power source of the sun and other stars, which occurs when forms of the lightest atom, hydrogen, combine to make helium in a very hot (100 million degrees centigrade) plasma. The development of fusion as a secure and reliable energy system that is environmentally and economically sustainable is a truly formidable scientific and technological challenge facing the world in the twenty-first century. As such, progress toward this goal requires the acquisition of the basic scientific understanding to enable the innovations that are still needed for making fusion energy a practical realization. In this as well as other areas facing major scientific challenges, it is well recognized that research in plasma science requires the accelerated development of computational tools and techniques that aid the acquisition of the scientific understanding needed to develop predictive models which can prove superior to empirical scaling. This is made possible by the rapid advances in high performance computing technology which will allow simulations of increasingly complex phenomena with greater physics fidelity. Accordingly, advanced computational codes, properly benchmarked with theory and experiment, are now generally recognized to be a powerful new tool for scientific discovery. In the key area of turbulent transport of the plasma, the development of the gyrokinetic formalism and its subsequent implementation in advanced simulations have enabled major progress

In a magnetically-confined plasma, the interplay between the complex trajectories of individual charged particles and the collective effects arising from the long-range nature of electromagnetic forces leads to a wide range of waves, oscillations, and instabilities characterizing the medium. As a result, there is an enormous range of temporal and spatial scales involved in plasmas of interest. As illustrated in Figure 1, the relevant physics can span over ten decades in time and space. Associated processes include the turbulence-driven ("anomalous") transport of energy and particles across a confining magnetic field, the abrupt rearrangements (disruptions) of the plasma caused by large-scale instabilities, and the interactions involving the plasma particles with electromagnetic waves and also with neutral atoms. Many of the these phenomena involve short length and time scales (nanoseconds and microns) while others occur on long time scales (seconds and minutes) and length scales on the order of the device size (meters). Although the fundamental laws that determine the behavior of plasmas, such as Maxwell's equations and those of classical statistical mechanics, are well known, obtaining their solution under realistic conditions is a scientific problem of extraordinary complexity. Effective prediction of the properties of energy-producing fusion plasma systems depends on the successful integration of many complex phenomena spanning vast ranges. This is a formidable challenge that can only be met with advanced scientific computation properly cross-validated against experiment and analytic theory.

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Figure 1. Huge ranges in spatial and temporal scales present major challenges to plasma theory and simulation.

In magnetic confinement fusion experiments, the plasma interacts directly with the "confining" electromagnetic fields, which can come from an external source and/or from currents produced within the plasma. This can lead to unstable behavior, where the plasma rapidly rearranges itself and relaxes to a lower energy state. The resultant thermodynamically favored state is incompatible with the conditions needed for fusion systems, which require that more power output be generated than it takes to keep the hot plasma well confined. However, the hot plasma state is naturally subject to both large and small-scale disturbances ("instabilities") which provide the mechanisms for lowering its energy state. It is therefore necessary to first gain an understanding of these complex, collective phenomena, and then to devise the means to control them. The larger-scale ("macro") instabilities can produce rapid topological changes in the confining magnetic field resulting in a catastrophic loss of fusion power density. Even if these instabilities can be controlled and/or prevented, there can remain smaller-scale ("micro") instabilities which prevent efficient hot plasma confinement by causing the turbulent transport of energy and particles. In order to make progress on these issues, researchers in this field have effectively developed the requisite mathematical formalism embodied by gyrokinetic theory to deal with the complexity of the kinetic electromagnetic behavior of magnetically-confined plasmas.

2. Basic Ordering

The general ordering appropriate for dealing with particle motion in strongly magnetized plasmas involves the assumption that the Larmor radius (or gyro-radius), ρ, of the particles is small compared to the spatial variation of the electromagnetic fields (L_B); i.e., $L_B \equiv | B/\nabla B |$, with $\varepsilon_B \equiv | \rho / L_B | << 1$, where $\rho = v/\Omega$, v = thermal velocity, and Ω = gyrofrequency. In addition, when addressing low frequency, long parallel wavelength phenomena, the following ordering is usually adopted: $\omega < \Omega$, $k_\perp \rho \leq 1$, $k_\parallel < k_\perp$, with **k** being the wave number and δ designating the smallness ordering parameter. This leads to a more tractable or simplified version of the Boltzmann-Maxwell system of kinetic equations in which the key components of the particle motion are the fast gyro-motion plus the slow guiding center motion.

In particular, the ordering of the terms in the Boltzmann Equation can be represented as follows:

$$\frac{\partial \hat{F}}{\partial t} + \mathrm{v} \cdot \nabla \hat{F} + \frac{Ze}{m}(\vec{\varepsilon} + \frac{1}{c}\vec{\mathrm{v}} \times \vec{\mathrm{B}})\nabla_{\mathrm{v}} \hat{F} = C(\hat{F}, \hat{F}) \tag{1}$$

	δ	δ	1	δ	(F)
δ	1	1	1	δ	(f)

where $\hat{F} = F + f$, and $\vec{\varepsilon} = -\nabla(\Phi_0 + \Phi)$, with F and f being respectively the equilibrium and perturbed distributions and Φ_0 and Φ being respectively the equilibrium and perturbed potentials governing the electric field, and $C(\hat{F},\hat{F})$ being the collision operator.

Accordingly, the gyrokinetic equation governing the equilibrium is

$$\mathrm{v}\cdot\nabla F^{(0)} - \vec{\mathrm{v}}\cdot(\mu\nabla \mathrm{B} + \mathrm{v}_{\parallel}\nabla\hat{n}\cdot\vec{\mathrm{v}}_{\perp})\frac{1}{B}\frac{\partial}{\partial\mu}F^{(0)}$$
$$-\frac{Ze}{m}\nabla\Phi_0\cdot\vec{\mathrm{v}}_{\perp}\frac{1}{B}\frac{\partial}{\partial\mu}F^{(0)} - \Omega\frac{\partial}{\partial\phi}F^{(1)} = C[F^{(0)},F^{(0)}] \tag{2}$$

and averaging over the gyrophase φ gives

$$\mathrm{v}_{\parallel}\hat{n}\cdot\nabla F^{(0)} = C[F^{(0)},F^{(0)}] \tag{3}$$

which implies that $F^{(0)}$ is a Maxwellian.

The equation governing the perturbed distribution function is:

$$(\vec{\mathrm{v}}_{\perp}\cdot\nabla - \Omega\frac{\partial}{\partial\phi})h = 0, \tag{4}$$

where $h = f^{(0)} + F_M e\Phi/T$. The "guiding-center" coordinate system is given by

$$\psi' = \psi - \frac{1}{\Omega}\hat{n}\times\vec{\mathrm{v}}_{\perp}\cdot\nabla\psi \tag{5}$$

$$\chi' = \chi - \frac{1}{\Omega}\hat{n}\times\vec{\mathrm{v}}_{\perp}\cdot\nabla\chi \tag{6}$$

$$\phi' = \phi \tag{7}$$

where $\vec{B} = B\hat{n} = B_p\hat{\chi} + B_t\hat{\zeta}$, with $B_p\hat{\chi} = \nabla\chi = \nabla\zeta\times\nabla\psi$. This coordinate transformation changes the gyrokinetic equation to $\partial h/\partial\phi' = 0$. Note that this transformation is sufficient for magnetostatics, but a somewhat different "gyro-center" coordinate transformation is needed for electromagnetic perturbations. This topic is addressed in H. Qin's lecture on "A Short Introduction to General Geometric Gyrokinetic Theory" within this set of Fields Institute Communications.

The gyro-average of the next-order equation leads to:

$$[\frac{\partial}{\partial t} + \mathrm{v}_{\parallel}\hat{n}\cdot\nabla s\frac{\partial}{\partial s} + \vec{\mathrm{v}}_{\mathrm{D}}\cdot(\nabla\psi\frac{\partial}{\partial\psi} + \nabla\chi\frac{\partial}{\partial\chi})]h$$
$$= \frac{Ze}{T}F_M\frac{\partial}{\partial t}<\Phi>_{\phi'} + \frac{Ze}{m}\frac{1}{\Omega}B(\frac{\partial}{\partial\psi}F_M)(\frac{\partial}{\partial\chi}<\Phi>_{\phi'}) \tag{8}$$
$$+ <C(F_M,h)>_{\phi'}$$

where

$$<A>_{\phi'} \equiv (1/2\pi)\int_0^{2\pi} d\phi' A(\phi') \tag{9}$$

The Poisson equation is

$$\nabla^2\Phi = -4\pi\sum_j Z_j e\int d^3\mathrm{v}\mathrm{f}_{\mathrm{j}}^{(0)} \tag{10}$$

which reduces here to the quasi-neutrality condition

$$\sum_j Z_j e\int d^3\mathrm{v}\mathrm{f}_{\mathrm{j}}^{(0)} = 0$$

when $k^2\lambda_{De}^{\ 2} << 1$,with λ_{De} being the Debye length.

The preceding equations are valid in the electrostatic limit. For the electromagnetic generalization of this formalism, the magnetic vector potential must be taken into account along with Ampere's Law from Maxwell's Equations. The governing gyro-kinetic equation for perturbations then becomes:

$$\begin{aligned}
&[\frac{\partial}{\partial t} + \mathrm{v}_{\|}\hat{n}\cdot\nabla s\frac{\partial}{\partial s} + \vec{\mathrm{v}}_{\mathrm{D}}\cdot(\nabla\psi\frac{\partial}{\partial\psi} + \nabla\chi\frac{\partial}{\partial\chi})]h \\
&= \frac{Ze}{T}F_M\frac{\partial}{\partial t} < \Psi >_{\phi'} + \frac{Ze}{m}\frac{1}{\Omega}B(\frac{\partial}{\partial\psi}F_M)(\frac{\partial}{\partial\chi} < \Psi >_{\phi'}) \\
&+ < C(F_M, h) >_{\phi'}
\end{aligned} \tag{11}$$

where

$$\Psi = J_0\left(\tfrac{k_\perp \mathrm{v}_\perp}{\Omega}\right)\left(\Phi - \frac{\mathrm{v}_{\|}}{c}A_{\|}\right) + \frac{J_1\left(\frac{k_\perp \mathrm{v}_\perp}{\Omega}\right)}{\frac{k_\perp \mathrm{v}_\perp}{\Omega}}\frac{m\mathrm{v}_\perp^2}{Ze}\frac{\delta B_{\|}}{B} \tag{12}$$

Ampere's Law can be expressed as:

$$\nabla_\perp^2 A_{\|} = -\frac{4\pi}{c}\sum_j\int d^2\mathrm{v}\ \ Z_j e\mathrm{v}_{\|}J_0\left(\tfrac{k_\perp \mathrm{v}_\perp}{\Omega_j}\right)h_j \tag{13}$$

and

$$\frac{\delta B_{\|}}{B} = -\frac{4\pi}{B^2}\sum_j\int d^2\mathrm{v}\ \ m_j\mathrm{v}_\perp^2\,\frac{J_1\left(\frac{k_\perp \mathrm{v}_\perp}{\Omega_j}\right)}{\frac{k_\perp \mathrm{v}_\perp}{\Omega_j}}h_j \tag{14}$$

where $A_{\|}$ is the perturbed parallel magnetic vector potential and $\delta B_{\|}$ is the perturbed parallel magnetic field, with J_0 and J_1 being the familiar Bessel functions. The nonlinear generalizations of these linearized equations are discussed in H. Qin's lecture on “A Short Introduction to General Geometric Gyrokinetic Theory” within this set of Fields Institute Communications.

3. Numerical Simulations: Particle-in-Cell (PIC) Approach

The scientific challenges related to magnetically-confined plasmas can be categorized into four areas: macroscopic stability, wave-particle interactions, microturbulence and transport, and plasma-material interactions. In addition, the integrated modeling of the physical processes from all of these areas is needed to effectively (i) harvest the physics knowledge from existing experiments and (ii) design future devices. Because charged particles, momentum, and heat move more rapidly along the magnetic field than across it, magnetic fusion research has focused on magnetic traps in which the magnetic field lines wrap back on themselves to cover a set of nested toroidal surfaces called magnetic flux surfaces (because each surface encloses a constant magnetic flux). Macroscopic stability is concerned with large-scale spontaneous deformations of magnetic flux surfaces. These major displacements or macroinstabilities are driven by the large electrical currents flowing in the plasma and by the plasma pressure. Wave-particle interactions deal with how particles and plasma waves interact. Detailed calculations of particle motions in background electromagnetic fields are needed to assess the application of waves to heat the plasma as well as address the dynamics of energetic particles resulting from intense auxiliary heating and/or alpha particles from the fusion reactions. Microturbulence and the associated transport come from fine-scale turbulence, driven by inhomogeneities in the plasma density and temperature, which can cause particles, momentum, and heat to leak across the flux surfaces from the hot interior to be lost at the plasma edge. Plasma-material interactions determine how high-temperature plasmas and material surfaces can co-exist. Progress in the scientific understanding in all of these areas contributes in an integrated sense to the interpretation and future planning of fusion systems. This demands significant advances in physics-based modeling capabilities – a formidable challenge which highlights the fact that advanced scientific codes are a realistic measure of the state of understanding of all natural and engineered systems.

As illustrated schematically in Figure 2, the path for developing modern high performance computational codes as validated tools for scientific discovery involves a multi-disciplinary collaborative process. This begins with basic theoretical research laying the foundations for the mathematical formulation of the physical phenomena of interest observed in experiments. Computational scientists produce the codes which solve these equations. In order to implement the best possible algorithms which efficiently utilize modern high-performance computers, the optimal approach is to do so in partnership with applied mathematicians who provide the basic mathematical algorithms and the computer scientists who provide the requisite computer systems software. The next step is the critical scientific code validation phase where the newly computed results are compared against experimental/observational data. This is a major challenge involving a hierarchy of benchmarking criteria which begin with cross-checks against analytic theory, empirical trends, and suggestive "pictorial" levels of agreement. It then graduates to sensitivity studies, where agreement is sought when key physical parameters are simultaneously varied in the simulation and experiment/observation. At the next level, richer physics validation is dependent on the availability of advanced experimental diagnostics which can produce integrated measurements of key physical quantities such as spectra, correlation functions, heating rates, and other variables of interest. If the simulation/experimental data comparisons are unsatisfactory at any of these validation levels, the work flow moves back to: [i] the theorists (in consultation with experimentalists) if the problem looks to be with the mathematical model; and [ii] computational scientists (in consultation with applied mathematicians and computer scientists) if the problem appears to be with the computational method. Even when the theory/experiment comparisons prove satisfactory, code performance criteria for speed and efficiency could dictate another round in the computational science box. If all criteria are met, then the new "tool for scientific discovery" can be effectively utilized for interpreting experimental data, designing new experiments, and even predicting new phenomena of interest. This cycle of development will of course be repeated as new discoveries with associated modeling challenges are encountered. In addition, it should be kept in mind that the continuous development of a robust computational infrastructure (including hardware, software, and networking) is needed to enable capabilities which minimize time-to-solution for the most challenging scientific problems. Of course, even with the successful application of the most advanced hardware and software, there will remain complex problems that defy numerical solution.

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Figure 2. Development path for high performance codes as validated tools for scientific discovery.

It is clear that since any given plasma simulation can only address a finite range of space and time scales, the associated domains have both minimum and maximum limits on spatial and temporal resolution. Accordingly, simulation models are commonly developed from simplified sets of equations, or "reduced equations," which are valid for only limited ranges of time and space scales. Examples include "gyrokinetic equations" [4] for dealing with turbulent transport problems and the "MHD equations" [5] for addressing the large-scale stability issues. While the reduced equations have enabled progress in the past, fundamental restrictions on their regions of validity have motivated the drive for improvements. In actual laboratory or natural plasmas, phenomena occurring on different time and space scales interact and influence one another. Simulations with greater physics fidelity thus demand increased simulation domains, which can only result from the derivation and application of more general equations that are valid on a wider range of space and time scales.

The most fundamental theoretical description of a plasma comes from kinetic equations for the distribution function within a six-dimensional phase-space of each particle species (plus time). They are coupled to each other through self-consistent electric and magnetic fields. Velocity moments of these kinetic equations produce a hierarchy of fluid equations amenable to modeling. In general, the simulation techniques used in plasma physics fall into two broad categories: kinetic models and fluid models. The most mature kinetic approach is the particle-in-cell method, pioneered by John Dawson and others [6]. This method involves integrating a (possibly reduced) kinetic equation in time by advancing marker-particles along a representative set of characteristics within the (possibly reduced) phase space. It basically involves a Lagrangian formulation in which the dynamics of an ensemble of gyro-averaged particles are tracked. Simulation techniques such as "finite sized particles" [7] (to reduce the "noise" due to discrete marker particles), "gyro-kinetics" [8] (a reduction of the full kinetic equation to a five-dimensional phase space which removes high-frequency motion not important to turbulent transport), and "delta-f" [9] (a prescription for further reducing the discrete particle noise by separating the perturbed from the equilibrium part of the distribution function before integrating the gyrokinetic equation along the appropriate characteristics) have been developed over the last 20 years. These advances have served to reduce the requirements on the number of "particles" necessary to faithfully represent the physics and contributed to dramatically increasing the accuracy and realism of the particle-in-cell simulation technique. An alternative approach in kinetic simulations is the Vlasov or "Continuum" method [10], which involve the direct solution of the kinetic equation governing the distribution function (examples include the Boltzmann and Gyrokinetic equations) on a fixed Eulerian grid in both coordinate and velocity space. Progress in the development of associated codes in recent years has also had a significant impact on the ability to realistically simulate microturbulent transport phenomena.

In order to carry out particle-in-cell simulations, the starting point is the Boltzmann equation from by Eq (1) – a nonlinear partial differential equation in Lagrangian coordinates. For particle simulations, an equivalent form is given by

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \left(\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) \cdot \frac{\partial F}{\partial \mathbf{v}} = C(F). \tag{15}$$

where the distribution F is specified by the Klimontovich-Dupree representation:

$$F = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\delta(\mathbf{v} - \mathbf{v}_j), \tag{16}$$

with x_j and v_j being the phase-space positions of the j-th particle and N being the total number of particles in the system.

Equation (1) can be recovered from Eq (15) by ensemble averaging F via the introduction of finite-size particles in the simulations [6]. In particular, when dealing with plasmas, it is clear (as shown in Figure 3) that the Coulomb potential for finite-sized particles is modified by Debye shielding [see Ref. (7) and references cited therein]. Short range interactions are accordingly reduced dramatically because there are equal numbers of electrons and ions within a Debye sphere.

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Figure 3. Debye-shielding modification of the Coulomb potential for a finite-sized particle.

This leads to a great simplification of the expression for the short-range force on the i-th particle due to the electric-field generated by all of the other particles, which is generally given by:

$$\mathbf{F}_i = q_i \mathbf{E}(\mathbf{x}_i) = \sum_{j \neq i} q_i q_j (\mathbf{x}_i - \mathbf{x}_j) / |\mathbf{x}_i - \mathbf{x}_j|^3 \tag{17}$$

Now, for short ranges where $|\mathbf{x}_i - \mathbf{x}_j| \leq 1$, the denominator, $|\mathbf{x}_i - \mathbf{x}_j|^3$, in Eq. (17) is simply replaced by λ_D^3; i.e.,

$$\mathbf{F}_i = q_i \mathbf{E}(\mathbf{x}_i) = \sum_{j \neq i} q_i q_j (\mathbf{x}_i - \mathbf{x}_j) / \lambda_D^3 \tag{18}$$

The point particles here are now effectively uniformly charged spheres of Debye-length radius. Although collisional dynamics are eliminated by this approximation, they can be recovered as "subgrid" phenomena via Monte Carlo methods with collision operators that can account for the scattering and diffusion of particles in velocity space [see Ref. (6) and references cited therein].

Equation (15) can be solved by tracking the temporal change of the phase space positions of the particles. The associated basic equations of motion for the particles are specified by the ordinary differential equations:

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j, \tag{19}$$

and

$$\frac{d\mathbf{v}_j}{dt} = \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}_j \times \mathbf{B}\right)_{\mathbf{x}_j}. \tag{20}$$

Since the number density of species alpha is given by

$$n_\alpha(\mathbf{x}) = \int F_\alpha d\mathbf{v} = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \tag{21}$$

the electrostatic potential ϕ, as noted earlier in Eq (10) is governed by Poisson's Equation with $E = -\nabla\phi$.

$$\nabla^2\phi = -4\pi \sum_\alpha q_\alpha \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \tag{22}$$

Note that this linear partial differential equation is in Eulerian coordinates (lab frame). So, unlike the "particle pushing" following Eqs (16) and (17) in the x and v phase space, the field calculation is carried out in the lab frame. As described in Ref. (11), the electromagnetic generalization of this formalism requires inclusion of the gyrokinetic form of Ampere's Law.

Major progress in the simulation of the gyrophase-averaged Vlasov-Maxwell system of equations governing low frequency microinstabilities followed the introduction of the gyro-kinetic methodology by W. Lee [8]. This involved incorporating the ion polarization density into Poisson's Equation, and, as illustrated in Fig. 4, the effective separation of the particle gyro-motion from its gyro-center motion. Basically, the actual spiral motion of a charged particle in a magnetic field is modified into that of a rotating charged ring subject to guiding center electric and magnetic drift motion together with parallel acceleration.

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Figure 4. Spiral motion of a charged particle in a magnetic field (B) is modified by gyrokinetic approximation into that of a rotating charged ring subject to guiding center electric and magnetic drift motion together with parallel acceleration.

As observed from computational results [8] and supported by analytic studies [12], the noise level from the gyro-kinetic PIC simulations was found to be dramatically reduced. One interpretation of this property is that the Debye shielding depicted in Fig. 3 is effectively replaced by the "gyro-radius shielding" introduced by the presence of the ion polarization density in the gyro-kinetic Poisson's Equation [11]. Along with the "delta-f" prescription for further reducing the discrete particle noise via separation of the perturbed from the equilibrium part of the distribution function [9], modern gyro-kinetic methods have effectively speeded up computations by 3 to 6 orders of magnitude in time steps and 2 to 3 orders of magnitude in spatial resolution. The accuracy and realism of the associated simulations have accordingly benefited from such advances.

4.0 Some Results from Advanced Simulations

Even if the larger scale macroscopic disturbances in a magnetically confined plasma could be avoided, the inherent free energy (such as the expansion free energy in the temperature and density gradients) can still drive turbulent cross-field losses of heat, particles, and momentum. In fact, such increased ("anomalously large") transport is experimentally observed to be significantly greater than levels expected from the collisional relaxation of toroidally-confined plasmas ("neoclassical theory"). This is particularly important for fusion because the effective size (and therefore cost) of an ignition experiment will be determined largely by the balance between fusion self-heating and turbulent transport losses. The growth and saturation of the associated drift-type microinstabilities [13] have been extensively studied over the years because understanding this turbulent plasma transport process is not only an important practical problem but is generally recognized as a true scientific grand challenge. With the advent of increasingly powerful supercomputers, it is generally agreed that this problem is particularly well-suited to be addressed by modern terascale MPP computational resources.

Building on the continuous progress in this area, significantly improved models with efficient grids aligned with the magnetic field have now been developed to address realistic 3D (toroidal) geometry with both global and local approaches [14]. As noted earlier, solution approaches include the particle-in-cell method, which follows the gyro-averaged orbits of an ensemble of discrete particles in a Lagrangian formulation, and the continuum (Vlasov) method, which directly solves the gyrokinetic equation on a fixed Eulerian grid in both coordinate and velocity space. With regard to the geometry of the problems addressed, the "flux tube" codes can concentrate on the fine-scale dynamical processes localized to an annular region depicted in Figure 5. The associated coordinates can be described as being extended along equilibrium magnetic field lines, while being localized in the perpendicular directions. Global codes have the more imposing multi-scale challenge of capturing the physics both on the small scale of the fluctuations (microinstabilities) and the large scale of the equilibrium profile variations. Improved implementation of gyrokinetic particle-in-cell algorithms as well as gyrokinetic continuum (Vlasov) approaches have been productively advanced [15].

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Figure 5. Flux-tube simulation results of turbulence localized to an annular region of a 3D toroidal plasma.

If reliably implemented, high resolution simulations of the fundamental equations governing turbulent transport can provide a cost-effective means to address key phenomena that would otherwise require expensive empirical exploration of a huge parameter space. The progress in capturing the ion dynamics has been impressive. For example, studies of electrostatic turbulence suppression produced by self-generated zonal flows within the plasma show that the suppression of turbulence caused by prominent instabilities driven by ion temperature gradients (ITGs) is produced by a shearing action which destroys the finger-like density contours which promote increased thermal transport in a 3D toroidal system. [16]. This dynamical process is depicted by the sequences shown in Figure 6. The lower panels, which show the nonlinear evolution of the turbulence in the absence of flow, can be compared against the upper panel sequence which illustrates the turbulence decorrelation caused by the self-generated **ExB** flow. This is also a good example of the effective use of powerful supercomputers (*e.g.,* the 5 teraflop IBM-SP). Typical global particle-in-cell simulations [17, 18] of this type have used one billion particles with 125 million grid-points over 7000 time-steps to produce significant physics results. In particular, large-scale simulations have been carried out to explore some of the key consequences of scaling up from present-day experimental devices (around 3 meters radius for the largest existing machines) to those of reactor dimensions (about 6 meters). As shown in Figure 7, transport driven by electrostatic ITG turbulence in present scale devices can change character in larger systems. This transition from Bohm-like scaling to Larmor-orbit-dependent "Gyro-Bohm" scaling is a positive trend, because simple empirical extrapolation of the smaller system findings would be more pessimistic. Some experimental observations in a number of representative present-day experiments indicate that the relative level of turbulent heat loss increases with plasma size while the size of these eddies remains the same [19]. However, exceptions to this trend, where Gyro-Bohm-like scaling sensitive to plasma rotation was observed, have also been reported in certain high-confinement ("H-mode") cases [20]. Such experiments on confinement scaling properties remain a challenging area of investigation. Nevertheless, for the larger sized reactor-scale plasmas of the future, the present simulations would suggest that the relative level of turbulent heat loss from electrostatic turbulence does not increase with size. The underlying causes for why such a transition might occur around the 400 gyroradii range indicated by the simulations have been explored and theoretical models based on the spreading of turbulence have been proposed [21] . Although this predicted trend is a very favorable one, the fidelity of the analysis needs to be further examined by investigating additional physics effects which might alter the present predictions. The analysis of associated scientific issues will naturally demand more comprehensive physics models within microturbulence codes. In addition to addressing experimental validation challenges, the interplay between analytic theory and advanced simulations will be increasingly important. For example, in addition to the turbulence spreading theory noted, progress in physics understanding of the nonlinear processes associated with zonal flow dynamics has resulted both from directions provided by analytic theory as well as by simulation results which have inspired new analytic models [22, 23, 24, 25].

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Figure 6. Turbulence reduction via sheared plasma flow compared to case with flow suppressed.

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Figure 7. Full torus particle-in-cell gyrokinetic simulations (GTC) of turbulent transport scaling.

An important multi-scale challenge for particle-in-cell kinetic simulations involves dealing with the realistic implementation of complete electron ("non-adiabatic") physics (including important kinetic effects, such as trapping in equilibrium magnetic wells, drift motions, and wave-particle resonances) and electromagnetic dynamics. These effects have largely been incorporated into gyrokinetic flux tube (local) codes [25], and present capabilities in gyrokinetic global codes for dealing with electrostatic perturbations have been successfully extended to include non-adiabatic electrons [26]. Much more challenging for the global simulations are the electromagnetic perturbations, which can alter the stability properties of the electrostatic modes and also generate separate instabilities associated with deformations of magnetic surfaces. In fact, answering the long standing question about what causes the ubiquitously-observed anomalously large electron thermal transport is likely linked to the ability to deal with magnetic perturbations. They can potentially cause a great increase in electron heat flux either through transient deformations of the magnetic field ("magnetic flutter") or, more plausibly, by producing an ergodic region in which the magnetic field lines no longer rest on nested flux surfaces but wander instead through a finite volume "breaking" the flux surfaces.

In general, significant challenges for gyrokinetic simulations remain in extending present capabilities for dealing with electrostatic perturbations to include magnetic perturbations in cases where they are sufficiently large to alter the actual geometric properties of the self-consistent magnetic field. In such circumstances, microinstabilities can drive currents parallel to the equilibrium magnetic field, which in turn produce magnetic perturbations in the perpendicular direction. These kinetic electromagnetic waves can modify the stability properties of the electrostatic modes or act as separate instabilities, such as kinetic ballooning modes [27], which can alter the magnetic topology.

In order to effectively deal with the challenging scientific issues highlighted here, the plasma science community must address advanced code development tasks which are important for most areas of research. The basic goal of enhancing the physics fidelity of the codes and developing the significantly improved software to deal with highly complex problems involves addressing: (i) multi-scale physics such as kinetic electromagnetic dynamics which have been discussed in earlier sections of this review; (ii) more efficient algorithms compatible with evolving computational architectures; and (iii) scalability of codes necessary for utilizing terascale platforms. As the computational hardware advances to meet the demands from the largest, most difficult problems, it is essential to also meet the continuing challenge of improving the scientific applications software and the associated algorithms. Innovative approaches, such as adaptive mesh refinement for dealing with higher dimensionality phase-space challenges, are expected to be actively explored.

With regard to efficiently implementing present-generation codes on the most powerful MPP computers, it is encouraging that the plasma science community has had success in developing codes for which computer run-time and problem size scale well with the number of processors. A good example of this trend is illustrated in Figure 8, where the global microturbulence PIC code, GTC, has demonstrated excellent scalability for more than 2000 processors on the IBM-SP computer at the National Energy Research Supercomputer Center (NERSC). This code is the representative from the Fusion Energy Science area within the NERSC suite of demonstration/benchmark codes to evaluate realistic performance on new advanced computational platforms. Active collaboration on the world's most powerful supercomputer, the Earth Simulator Computer (ESC) in Japan, has just commenced and involved the recent porting of this code to the ESC site. The goal of this on-going project is to evaluate the importance of the ESC's vector-parallel architecture compared to the much more widespread super-scalar MPP architecture. An active collaboration has also been initiated with a complementary global particle simulation effort in Japan [28]. Results from these early benchmark runs were quite impressive. Specifically, utilization of 64 ESC processors yielded results which were not only more efficient (by about a factor of two) but were more than 20% faster than 1024 processors on the IBM-SP supercomputer at NERSC. Efficiency in this context refers to measured ability of a given code to achieve the theoretically-rated performance level of the computer processors. In addition to the ESC, the new X1 vector supercomputer at the Oak Ridge National Laboratory has commenced bench-marking activities involving the particle-in-cell code, GTC [29]. Overall, the practical goal here is to effectively utilize the tools, technologies, and advanced hardware systems that will help minimize the time-to-solution for the most challenging computational plasma physics problems.

INSERT Figure 8 from end of this document

Figure 8. 3D gyrokinetic global particle-in-cell codes have demonstrated excellent scaling as the number of processors is increased.

It should be emphasized that a natural consequence of the effective utilization of supercomputers is the tremendous amount of data generated, as illustrated in Figure 9. Terabytes of data are even now generated at remote locations (e.g., where supercomputing centers are located), presenting data management and data grid technology challenges [30]. The data must be efficiently analyzed to compute derived quantities. New advanced visualization techniques are needed to help identify key features in the data. There are also significant programming and algorithmic challenges, which must be met in order to enable computational capabilities for addressing more complex scientific problems. These include multi-dimensional domain decomposition in toroidal geometry and mixed distributed/shared memory programming. Other problems include load balancing on computers with large numbers of processors, optimization of fundamental gather-scatter operation in particle-in-cell codes, and scalable parallel input/output (I/O) operations for the petascale range of data sets.

INSERT Figure 9 from end of this document

Figure 9. Terabytes of data are now generated at remote locations, as for example the heat potential shown here on 121 million grid points from a particle-in-cell turbulence simulation.

As noted earlier, it should be kept in mind that even with access to greatly improved computational hardware and software advances, there will remain limitations to what can be practically achieved [31]. Indeed, some of the most complex plasma phenomena involving highly transient nonlinear behavior may defy mathematical formulation and be beyond the reach of computational physics.

5.0 Future Challenges and Directions

The "computational grand challenge" nature of plasma physics in general and fusion research in particular is a consequence of the fact that in addition to dealing with vast ranges in space and time scales which can span over ten decades, the relevant problems involve extreme anisotropy, the interaction between large-scale fluid-like (macroscopic) physics and fine-scale kinetic (microscopic) physics, and the need to account for geometric detail. Moreover, the requirement of causality (inability to parallelize over time) makes this problem among the most challenging in computational physics. There has been excellent progress during the past decade in fundamental understanding of key individual phenomena in high temperature plasmas. Modern magnetic fusion experiments are typically not quiescent, but exhibit macroscopic motions that can affect their performance, and in some cases can lead to catastrophic termination of the discharge. Major advances have been achieved in the modeling of such dynamics, which require an integration of fluid and kinetic physics in complex magnetic geometry. Significant progress has also been made in addressing the dynamics governing the breaking and reconnection of magnetic field lines, which is a central scientific issue for fusion energy as well as allied fields such as astrophysics and space and solar physics. Another key topic, where there have been exciting advances in understanding, is the degradation of confinement of energy and particles in fusion plasmas caused by turbulence associated with small spatial-scale plasma instabilities driven by gradients in the plasma pressure. While progress has been impressive, the detailed physics of the growth and saturation of these instabilities, their impact on plasma confinement, and the knowledge of how such turbulence might be controlled remain major scientific challenges. Finally, the understanding of overall plasma performance requires integrating all of these issues in a simulation that includes interactions between phenomena which were previously studied as essentially separate disciplines. To achieve the ultimate goal of such integration, it becomes necessary to follow the evolution of the global profiles of plasma temperature, density, current and magnetic field on the energy-confinement time scale with the inclusion of relevant physics on all important time scales. While this is a formidable long term goal, research efforts are beginning to address such cross-disciplinary studies and to increase the physics content of existing integrated codes. This will necessitate the development of an architecture for bringing together the disparate physics models, combined with the algorithms and computational infrastructure that enables the models to work together. The associated integration of code modules, many of which are individually at the limits of computational resources, will clearly require substantial increases in computer power. With the rapid advances in high-end computing power, researchers in plasma physics as well as other fields can expect to be able to model such systems in far greater detail and complexity, leading eventually to the ability to couple individual models into an integrated capability which can enable significantly improved understanding of an entire system.

Overall, significant advances in the development of mathematical methodology, such as gyro-kinetic theory, together with the rapid progress in scientific computing capabilities have enabled key contributions to all areas of plasma science. While formidable challenges remain, the achievements and approaches highlighted in this article hold great promise for improving scientific understanding of experimental data, for stimulating new theoretical ideas, and for helping produce innovations leading to the most attractive and viable designs for future experimental facilities. This has helped transform traditional research approaches and has provided a natural bridge for fruitful collaborations between scientific disciplines leading to mutual benefit to all areas. As a natural consequence, a stimulating path forward is provided to address the challenge of attracting, educating, and retaining the bright young talent essential for the future health of the field.

Acknowledgements

The authors is grateful to Dr. Wei-li Lee for his clear description of the basic schemes for particle-in-cell simulations and to Dr. Greg Rewoldt for his invaluable assistance in assembling the final version of this document.

Supported by U. S. Department of Energy contract DE-ACO2-76CH03073.

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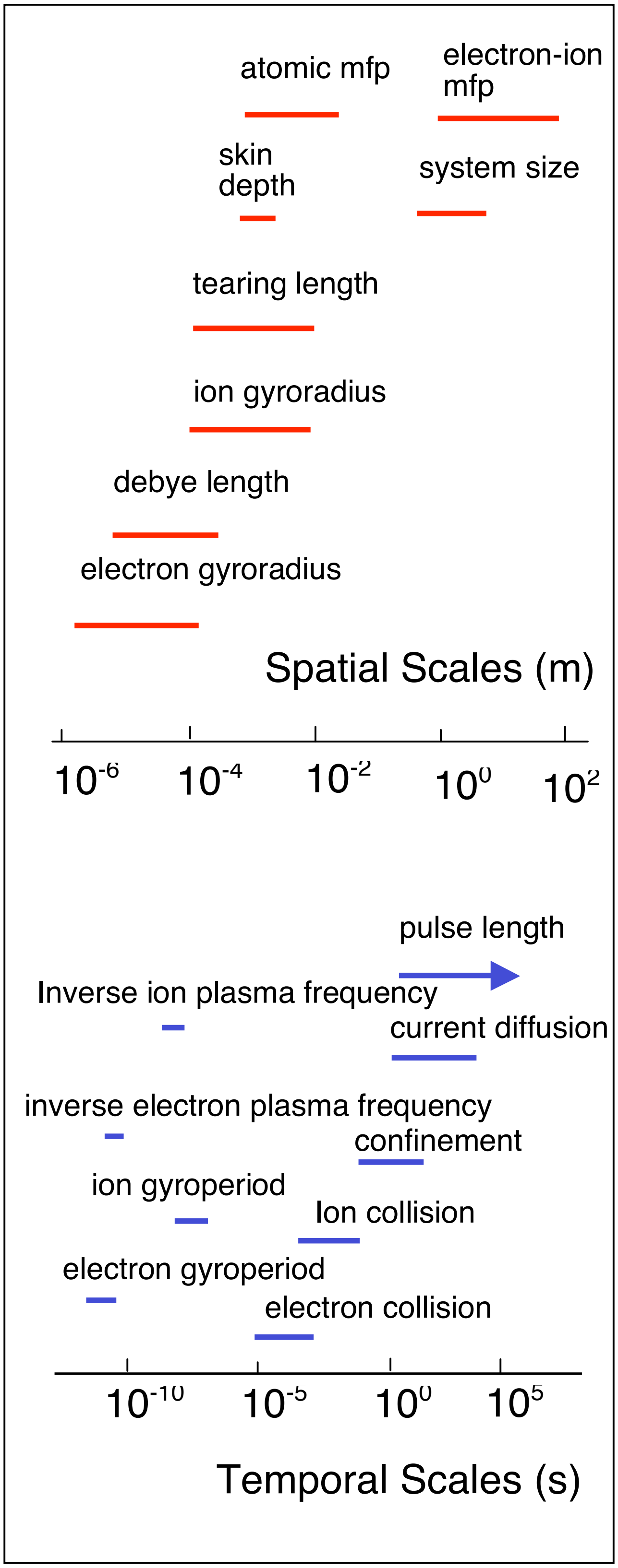


Figure 1. Huge ranges in spatial and temporal scales present major challenges to plasma theory and simulation.

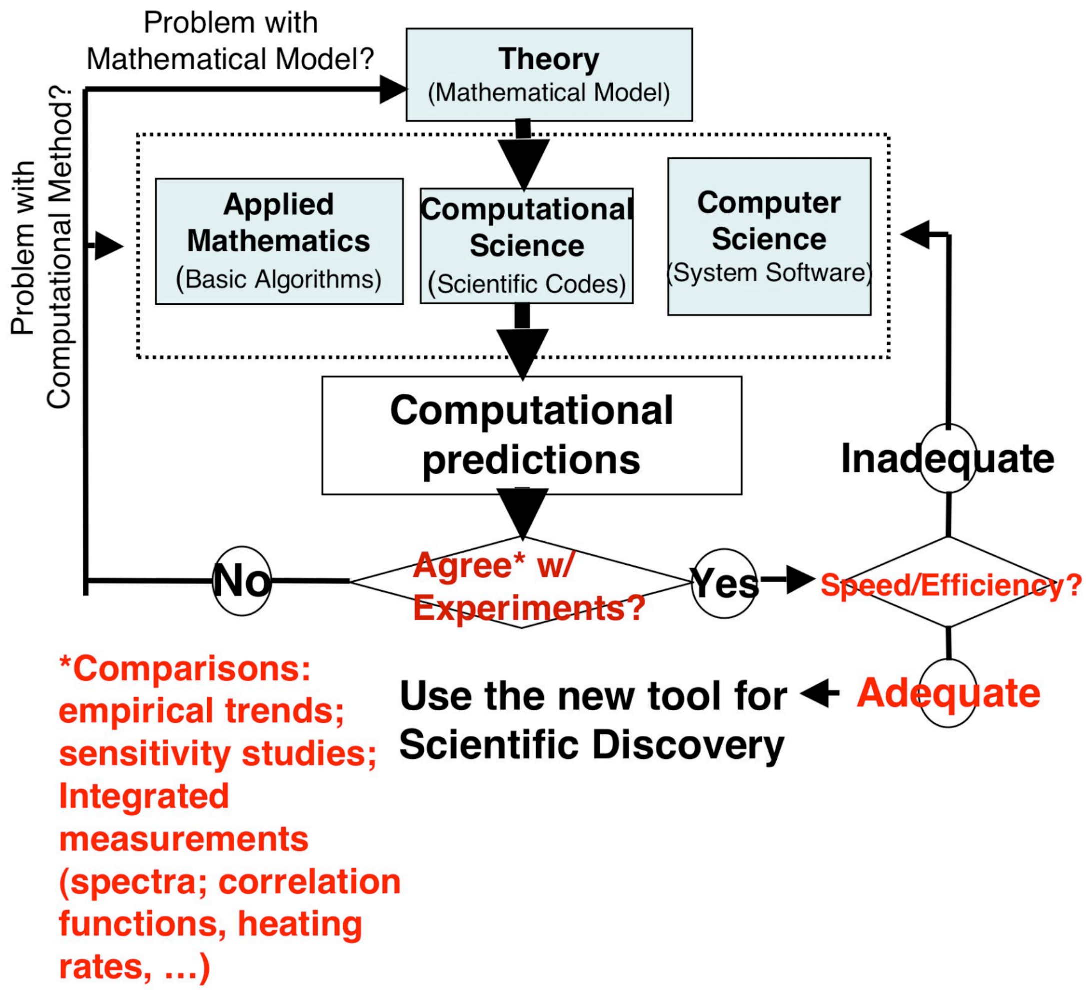


Figure 2. Development path for high performance codes as validated tools for scientific discovery.

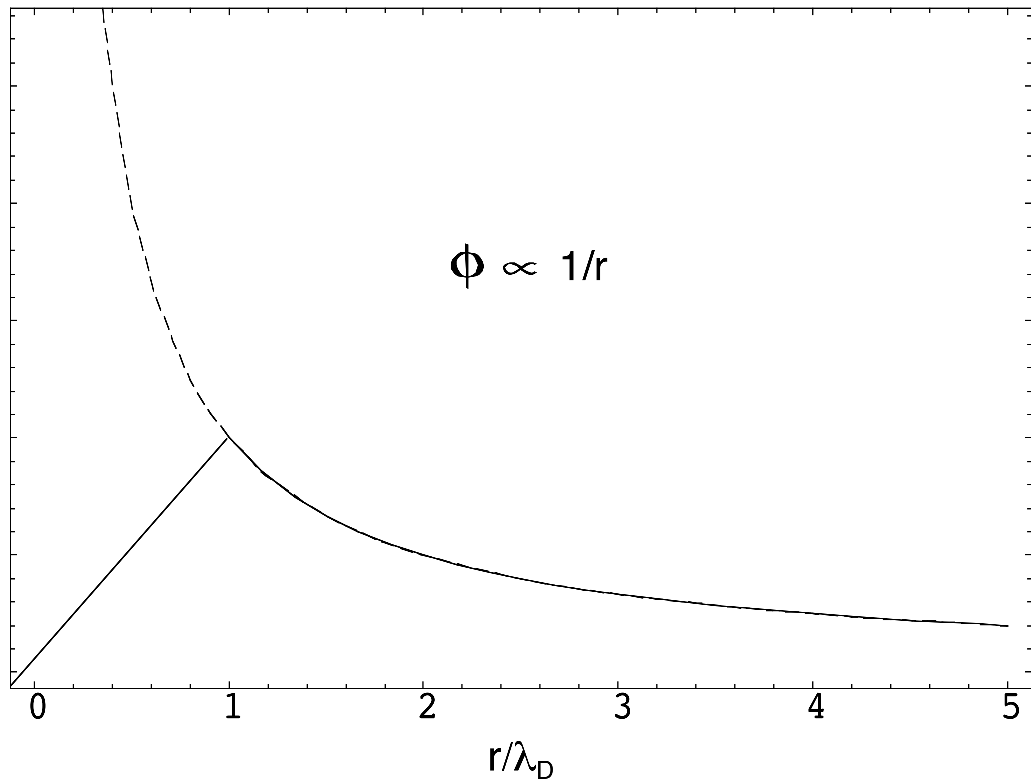


Figure 3. Debye-shielding modification of the Coulomb potential for a finite-sized particle.

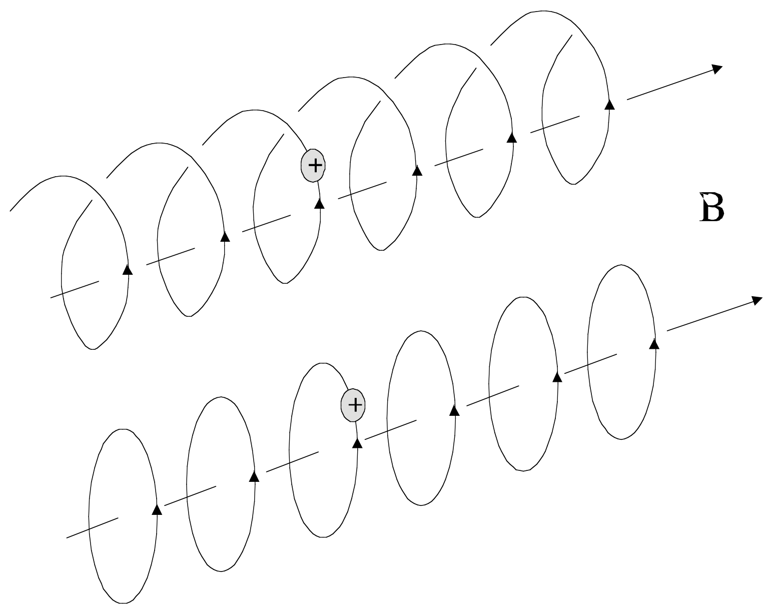


Figure 4. Spiral motion of a charged particle in a magnetic field (B) is modified by gyrokinetic approximation into that of a rotating charged ring subject to guiding center electric and magnetic drift motion together with parallel acceleration.

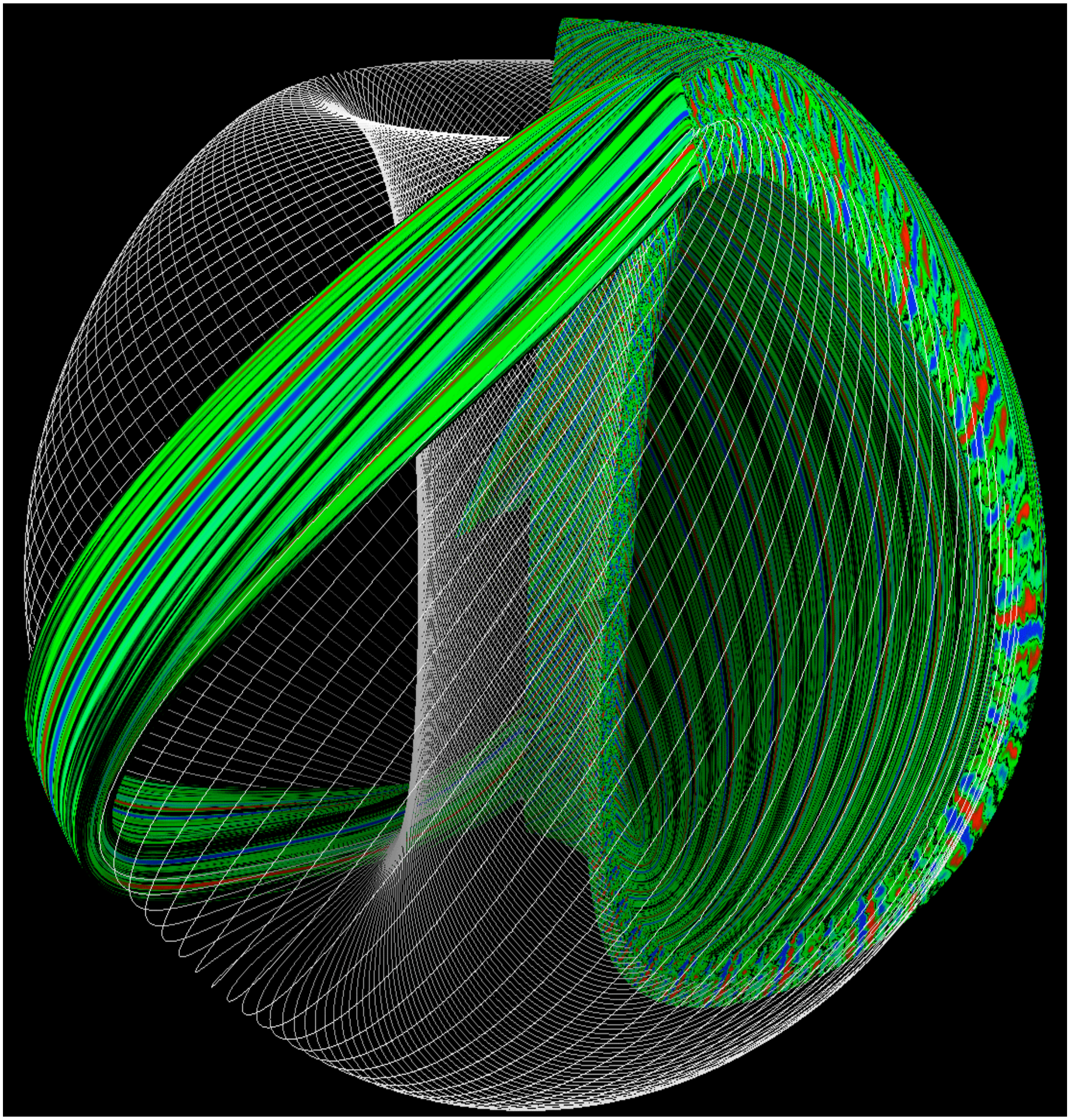


Figure 5. Flux-tube simulation results of turbulence localized to an annular region of a 3D toroidal plasma.

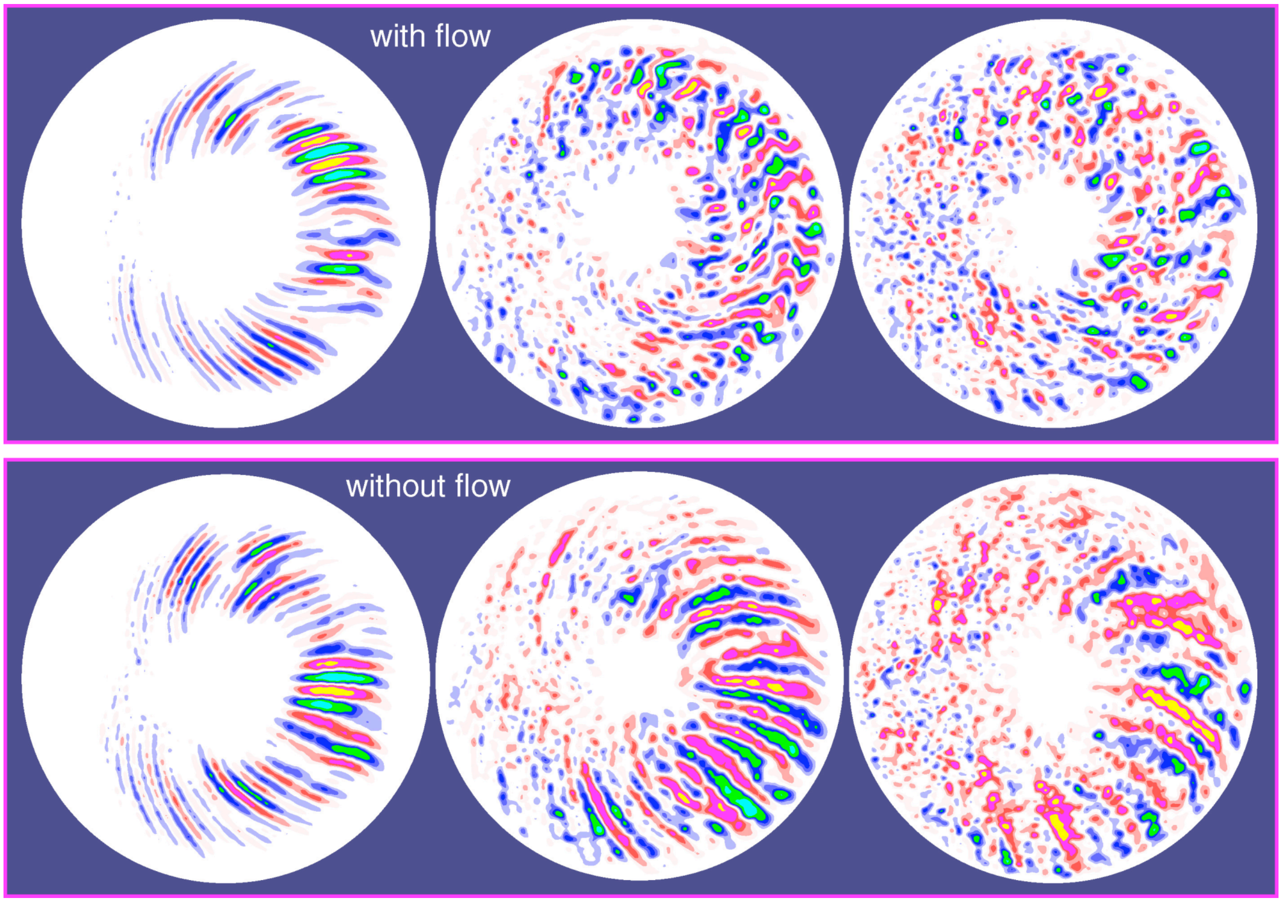


Figure 6. Turbulence reduction via sheared plasma flow compared to case with flow suppressed.

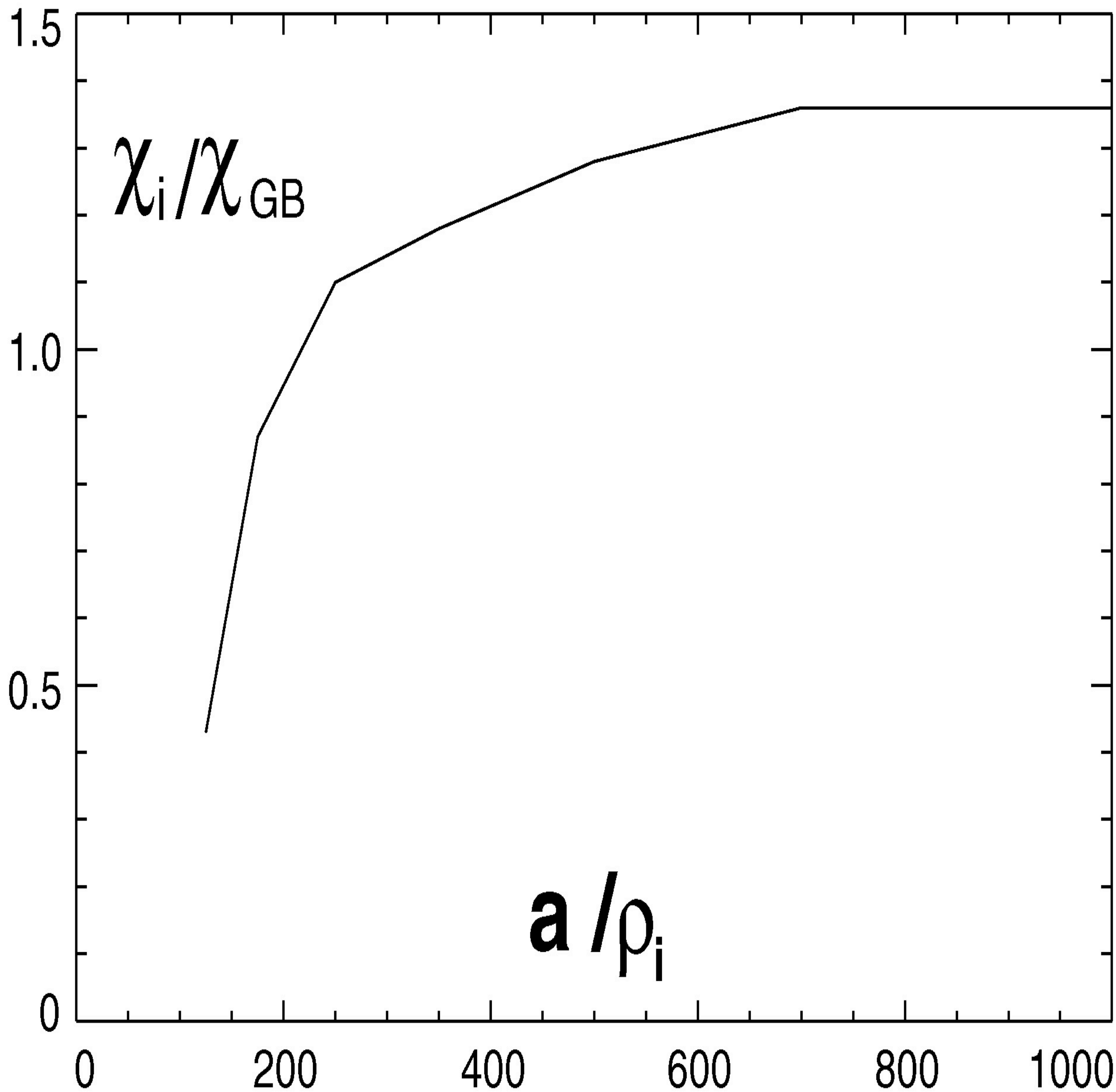
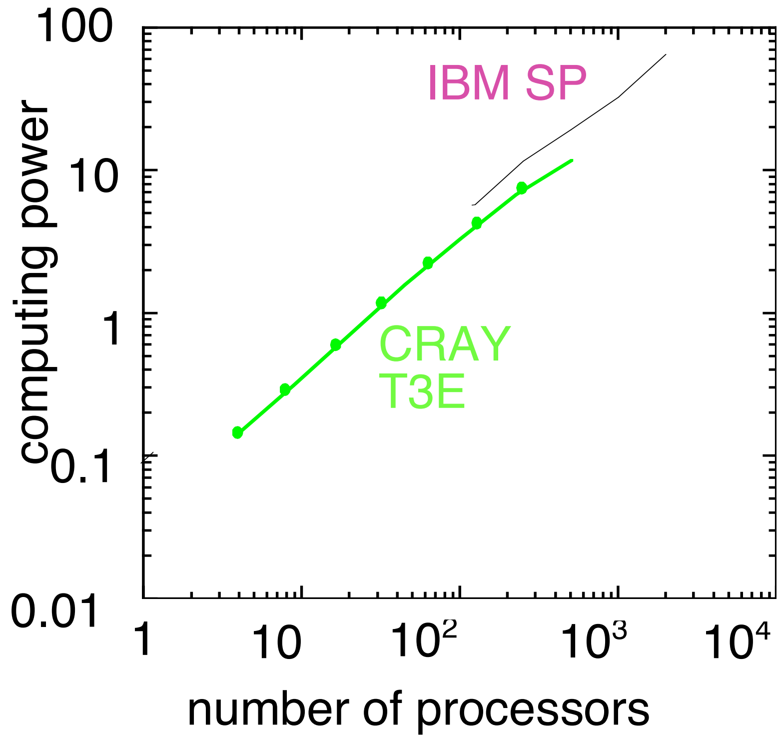


Figure 7. Full torus particle-in-cell gyrokinetic simulations (GTC) of turbulent transport scaling.



Y-axis: number of particles (in millions)
which move one step in one second

Figure 8. 3D gyrokinetic global particle-in-cell codes have demonstrated excellent scaling as the number of processors is increased.

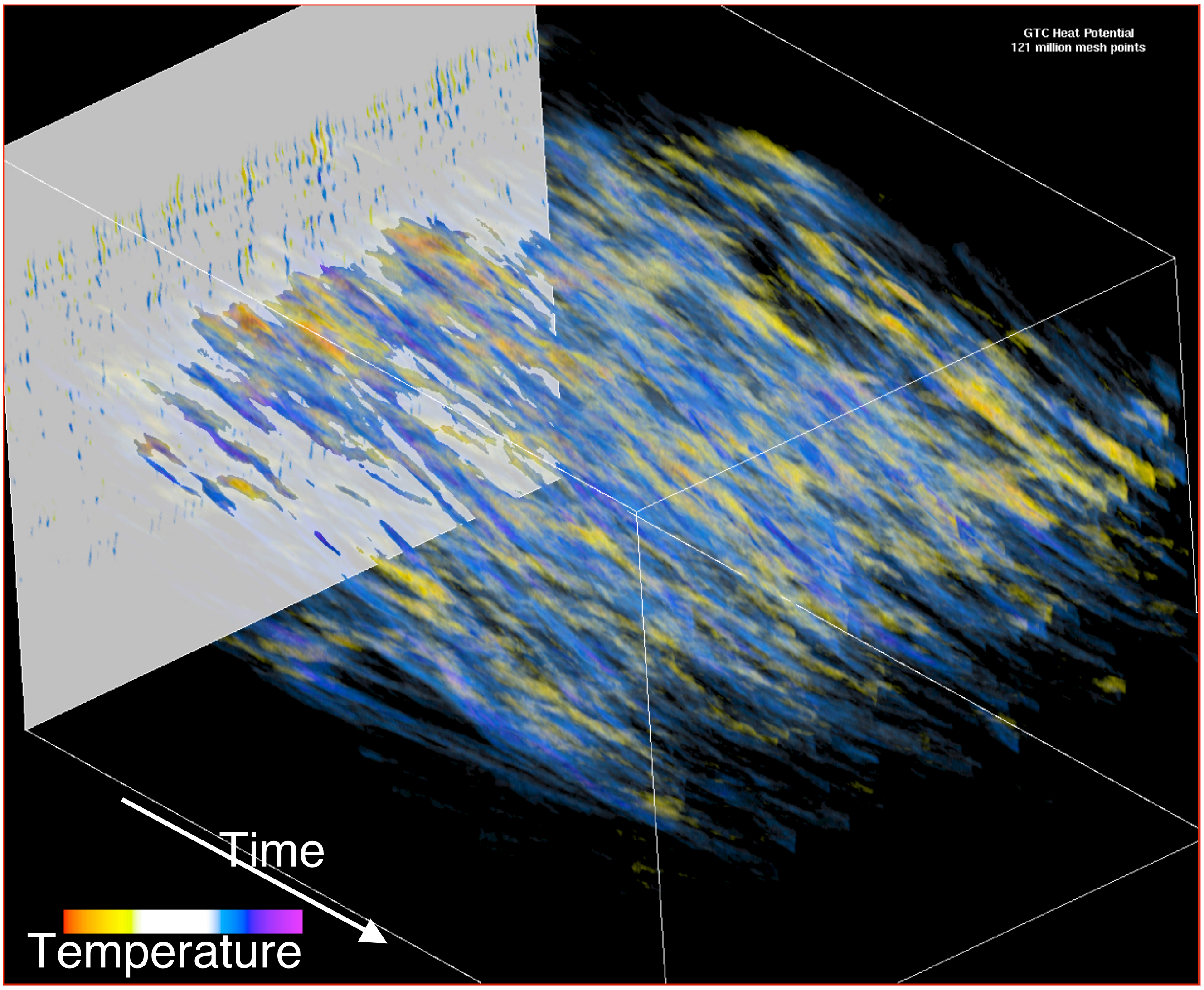


Figure 9. Terabytes of data are now generated at remote locations, as for example the heat potential shown here on 121 million grid points from a particle-in-cell turbulence simulation.

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