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Global Gyrokinetic Simulation of Tokamak Transport

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Abstract

A kinetic simulation code based on the gyrokinetic ion dynamics in global general metric (including a tokamak with circular or noncircular cross-section) has been developed. This gyrokinetic simulation is capable of examining the global and semi-global driftwave structures and their associated transport in a tokamak plasma. We investigate the property of the ion temperature gradient (ITG) or η_i ($\eta_i \equiv \partial \ln T_i / \partial \ln n_i$) driven drift waves in a tokamak plasma. The emergent semi-global drift wave modes give rise to thermal transport characterized by the Bohm scaling.

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1 Introduction

The tokamak heat transport is a central question in the contemporary fusion research as well as a fundamental physics question in complex dissipative systems. This anomaly is long recognized as an outstanding theoretical mystery and a steady effort and progress have been maintained over the past decades. In recent years of research on this gargantuan scientific undertaking the computational effort has taken an increasingly important role. (The increased recognition of the tokamak transport problem as a complex dynamical system with similarities to the geophysical problems of weather and space weather is partly responsible for expanded computational efforts.) These expanded computational approaches include both magnetohydrodynamic (or hydrodynamic) models and kinetic models. Many authors have suspected [1] that the chief culprit for the anomalous transport includes a high level of plasma fluctuations or turbulence which lead to wave-enhanced transport.

Starting with the pioneering efforts by Okuda and Dawson [2], Cheng and Okuda [3], and Lee and Okuda [4], a kinetic model (PIC or the Particle-in-Cell model) with guiding-center electrons (the concept of guiding center was first introduced by Alfvén) has been introduced and the first (perhaps crude by the present-day standards) simulations of fluctuation driven transport in a magnetized tokamak-like plasma has been carried out. The guiding-center model has greatly accelerated the voluminous computations in the PIC model. This model [5] successfully reproduced the correct eigenmode [6, 7] of electron drift waves in a shear magnetic field. Because of the limitation of algorithm and computational resources, these early models were by necessity a slab plasma model. Only since Cheng *et al.* [8] pointed out that the inclusion of toroidal geometry and trapped particle effects leads to absolute instability of the toroidicity-induced branch, the importance of a toroidal model is well recognized. In the subsequent decade a large number of theoretical as well as experimental investigations have been carried out. In particular, in addition to electron drift

waves, ion drift waves have become an important topic of research, in part due to the experimentally realized high ion temperature plasma and observed associated anomalous ion heat conductivity. A collection of such efforts may be found in the conference proceedings such as Ref. [9]-[20] and the references therein. For example, a historical overview of the ion thermal transport experimental studies is given by Scott in Ref. [10]. The previous paper [11] is an example for such an effort. In the above-mentioned models [3, 5, 11] ions have been treated with the full dynamics. In order to further accelerate the calculation, Lee [12] introduced the gyrokinetic PIC algorithm, followed by a number of authors such as Ref. [13]. In the present investigation it is our main objective to incorporate the gyrokinetic algorithm in general metric (specifically the toroidal geometric of a tokamak), building upon the earlier toroidal particle code (TPC) [17].

In the so-called L-mode (low confinement mode), or the standard operation of a tokamak with high-powered neutral beams giving a direct ion energy injection in the core plasma, it has been observed that (i) there is a significant ion energy loss (anomalous ion thermal transport) from the core plasma; (ii) this anomalous transport is accompanied by the development of the so-called ITG mode (the ion temperature gradient drift wave mode) or the η_i -mode ($\eta_i \equiv \partial \ln T_i / \partial \ln n_i$) which exhibits a (relatively) large radial electric potential structure [19]. In these discharges the transport is often characterized by the Bohm scaling [20, 21]. Meanwhile, it has been theoretically pointed out [21, 22] that the toroidal drift wave exhibit an eigenmode structure that is radially extended much beyond the local eigenmode structure obtained in a sheared slab plasma. This is because the toroidal coupling of adjacent poloidal modes (m 's) (with a fixed toroidal mode number n) allows the adjacent modes to form a radially connected global (or more accurately, semi-global) mode. This is based on linear theory. However, even in the fully nonlinear global kinetic simulation [17] a similar radially extended eigenmode structure is found to persist and to play an important role in characterizing the transport. The global (or semi-global) radial electric potential

structure is not so far deviating from that of the linear eigenmode analysis of Ref. [24]. The mode activity is regulated by the temperature gradient that sustains the ITG instability but not virulently unstable and thus not in a highly nonlinear state. Perhaps this is the reason why the semi-global mode structure plays a rather important role. It is, therefore, essential to incorporate the gyrokinetic model of Refs. [12] and [13] in toroidal geometry to have the global toroidal features of the transport problem. This goal of the present investigation is thus to develop a *global* gyrokinetic (PIC) model in toroidal geometry.

In the following we develop the toroidal gyrokinetic algorithm that does not rely on the local assumption, allowing the physical quantities such as temperature, magnetic fields, the safety factor, etc. to globally vary over the full extent of the radius of a tokamak plasma. We first examine the algorithm in Sec. 2 and then computational and software considerations in Sec. 3. The resultant computer simulation code is the Generalized Tokamak Simulator (GTS). In Sec. 4 we present the survey and individual cases of our simulation runs based on this code. We analyze these results in Sec. 5. A summary is given in Sec. 6.

2 Algorithm in General Metric

In order to carry out global gyrokinetic PIC calculations in the toroidal coordinates, we need to develop the algorithm appropriate for this task. The theory of gyrokinetic particle simulation has been developed adequately by Lee [12] and by Dubin *et al.* [13]. Application of gyrokinetic particle simulation to drift wave studies in tokamak-like regimes has been addressed by Parker *et al.* [14]. Consequently, the discussion here is limited to a brief overview of the algorithm of the physical model.

The gyrokinetic approach involves a gyroaveraging of the Vlasov equation and the field equations for a magnetized plasma. In the reduction of the full Vlasov equation to the

gyrokinetic equation the gyrokinetic ordering is employed:

$$\frac{e\phi}{T} = \mathcal{O}(\epsilon) \quad (1)$$

$$\frac{\rho_i}{L_{eq}} = \mathcal{O}(\epsilon) \quad (2)$$

$$k_{\parallel}\rho_i = \mathcal{O}(\epsilon) \quad (3)$$

$$\frac{\omega}{\Omega} = \mathcal{O}(\epsilon), \quad (4)$$

where L_{eq} is a characteristic scale length of the profiles, ρ_i is the ion Larmor radius, Ω is the ion cyclotron frequency, and ϵ is a smallness parameter. Provided that the simulation parameters represent this ordering, the gyrokinetic technique provides an efficient and accurate approach to simulation of low frequency plasma behavior such as drift waves in a tokamak plasma.

2.1 Gyrokinetic algorithm

The gyrokinetic equations consist of the gyroaveraged Vlasov equation to the order of ϵ^2 and the gyroaveraged Poisson equation to the order of ϵ for electrostatic problems:

$$\frac{\partial F_i}{\partial t} + \left(\bar{v}_{\parallel} \hat{b} - \epsilon \frac{e_i}{m_i \Omega_i} \bar{\nabla} \psi \times \hat{b} \right) \cdot \bar{\nabla} F_i - \epsilon \frac{e_i}{m_i} \hat{b} \cdot \bar{\nabla} \psi \frac{\partial F_i}{\partial \bar{v}_{\parallel}} = \mathcal{O}(\epsilon^3), \quad (5)$$

with

$$\psi = \bar{\Phi} - \epsilon \frac{e}{2m_i \Omega_i} \left(\frac{\partial}{\partial \bar{\mu}} \langle \bar{\Phi}^2 \rangle + \left\langle \bar{\nabla} \bar{\Phi} \cdot \frac{\hat{b} \times \bar{\nabla} \bar{\Phi}}{\Omega_i} \right\rangle \right) \quad (6)$$

and

$$\nabla^2 \Phi(\mathbf{x}, t) = -4\pi e \left\{ -n_e + \int \left[F_i + \epsilon \frac{e}{m_i \Omega_i} \left(\bar{\Phi} \frac{\partial F_i}{\partial \bar{\mu}} + \frac{\bar{\nabla} \bar{\Phi}}{\Omega_i} \cdot \hat{b} \times \bar{\nabla} F_i \right) \delta(\bar{\mathbf{X}} + \bar{\boldsymbol{\rho}} - \mathbf{x}) d\bar{\mathbf{Z}} \right] \right\}. \quad (7)$$

Here the notations of Dubin *et al.* [13] are followed. For example

$$\bar{\Phi}(\bar{\mathbf{X}}, \bar{\mu}, \bar{T}) \equiv \langle \Phi(\bar{\mathbf{X}} + \bar{\boldsymbol{\rho}}, \bar{T}) \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\bar{\theta} \Phi(\bar{\mathbf{X}} + \bar{\boldsymbol{\rho}}, \bar{T})$$

$$= \int \frac{d^3k}{(2\pi)^3} \Phi_k J_0(k_\perp \bar{\rho}) \exp(i\mathbf{k} \cdot \bar{\mathbf{X}}), \quad (8)$$

$$\bar{\Phi}(\bar{\mathbf{X}}, \bar{\mu}, \bar{\theta}, \bar{T}) = \Phi(\bar{\mathbf{X}} + \bar{\rho}, \bar{T}) - \bar{\Phi}, \quad (9)$$

$$\tilde{\Phi}(\bar{\mathbf{X}}, \bar{\mu}, \bar{\theta}, \bar{T}) = \int_0^{\bar{\theta}} \bar{\Phi} d\bar{\theta}, \quad (10)$$

where

$$\bar{\rho} = \left(\frac{2\bar{\mu}}{\Omega} \right)^{1/2} \hat{a}(\bar{\theta}), \quad (11)$$

and the volume element transforms as

$$d^6\bar{\mathbf{Z}} = \left\| \frac{\partial \mathbf{z}}{\partial \bar{\mathbf{Z}}} \right\| d\bar{\mathbf{X}} d\bar{\mu} d\bar{v}_\parallel d\bar{\theta}, \quad (12)$$

and θ is the gyrophase angle and $\mathbf{X}$ is the guiding center position. The bracket $\langle \rangle$ indicates the gyroaverage. This procedure is discussed in more detail later. We use the notations for the ion and electron Debye wavenumber as $k_i = k_{Di}$, $k_e = k_{De}$. The bar means that the quantity is the gyroaveraging Lie transformed quantity [13].

We discuss the Vlasov and Poisson equations in a form more appropriate to particle simulation. For illustration, let us consider the case where there is only density gradient in the plasma. The first two terms on the right-hand side of Eq. (7) are

$$I_1 = 4\pi e \left(\int F_i \delta(\bar{\mathbf{X}} + \bar{\rho} - \mathbf{X}) d^6\bar{\mathbf{Z}} - n_e \right). \quad (13)$$

The next terms in Eq. (7) are

$$I_2 = -\frac{4\pi e^2}{m_i \Omega_i} \int \tilde{\Phi} \frac{\partial F_i}{\partial \bar{\mu}} \delta(\bar{\mathbf{X}} + \bar{\rho} - \mathbf{X}) d^3z \quad (14)$$

and

$$I_3 = \frac{4\pi e^2}{m_i \Omega_i} \int \frac{1}{\Omega} \nabla \tilde{\Phi} \cdot \hat{\mathbf{b}} \times \nabla F_i \delta(\bar{\mathbf{X}} + \bar{\rho} - \mathbf{x}) d^6\bar{\mathbf{Z}}. \quad (15)$$

Using the locally Maxwell distribution (and $T_\parallel = T_\perp$, $\mu = \frac{1}{2} v_\perp^2 / \Omega$),

$$F_i \cong \left(\frac{M}{2\pi T} \right)^{3/2} n_i(\mathbf{x}) e^{-\bar{\mu} \Omega_i / (T/m)}$$

and

$$\frac{\partial F_i}{\partial \mu} = -\frac{\Omega_i}{(T/m)} \left(\frac{m}{2\pi T}\right)^{3/2} n_i(\mathbf{x}) \theta^{-\bar{\mu}\Omega_i/(T/m)} e^{-\bar{v}_{\parallel}^2/2(T/m)}.$$

Then Eq. (14) can be written as

$$I_1 = \frac{4\pi e^2}{T} n_i(x) [\Phi(\mathbf{x}) - \tilde{\Phi}(\mathbf{x})], \quad (16)$$

where

$$\tilde{\Phi}(\mathbf{x}) = \sum_{\mathbf{k}} \Phi(\mathbf{k}) \Gamma_0(k_{\perp}^2 \rho_i^2) e^{i\mathbf{k} \cdot \mathbf{x}} \quad (17)$$

and $\Gamma_0(b) \equiv I_0(b)e^{-b}$, or Eq. (16) is cast in a form

$$I_1 = k_i^2 \frac{n_i(x)}{n_0} (\Phi - \tilde{\Phi}), \quad (18)$$

which is what Lee obtained [12].

With these considerations the Poisson equation takes the form

$$\nabla^2 \Phi - k_i^2 \frac{n_i}{n_0} (\Phi - \tilde{\Phi}) + \frac{k_i^2 \rho_i^2}{n_0} \nabla_{\perp} (n_i \cdot \nabla_{\perp} \Phi) = S, \quad (19)$$

where S is a source term. We have dropped the upper bar on the gyroaveraged quantities in Eqs. (16)–(19) and here on. The first term on the left-hand side of Eq. (19) is the usual space charge Laplacian, the second is the dominant gyrokinetic term in the Poisson equation, the third term was first added by Dubin *et al.* [13]. In addition there can be terms like $\nabla_{\perp} n \cdot \nabla_{\perp} \Phi$, $\nabla_{\perp} I \cdot \nabla_{\perp} \Phi$, and $\nabla_{\perp} n \cdot \nabla_{\perp} T$ (some of which appear only when the temperature gradient is present **and are considered later**), which have been seldom incorporated in the literature or codes. The second term in Eq. (19) in k -space may be conveniently approximated by using the first Padé approximant as

$$\Phi - \tilde{\Phi} = [1 - \Gamma_0(b)]\Phi(k) \approx \left(1 - \frac{1}{1+b}\right)\Phi = \frac{b}{1+b}\Phi. \quad (20)$$

This gives rise to a new Poisson equation in real space

$$k_i^2 \rho_i^2 \nabla_{\perp}^2 \Phi = (1 - \rho_i^2 \nabla_{\perp}^2) \left[\frac{T}{n_i} (S - \nabla^2 \Phi) \right]. \quad (21)$$

If, for example, electrons can be treated adiabatically, $n_e = n_{i0} \exp(e\phi/T_e) \approx n_{i0}(1 + e\Phi/T_e)$ and then

$$S = 4\pi e(\langle n_i \rangle - n_{i0}). \quad (22)$$

By writing the left-hand side of Eq. (21) as LHS, Eq. (21) can be cast in a form

$$\text{LHS} = \text{LHS} - (k_i \rho_i)^2 \nabla_{\perp}^2 \Phi + [1 - \rho_i^2(x) \nabla_{\perp}^2] \left[\frac{1}{n_i(x)} (S + k_e^2 \Phi - \nabla^2 \Phi) \right], \quad (23)$$

where we note that assuming $\rho_i = \rho_i(x)$, the combined factor in $(k_i \rho_i)$ terms is constant in x and $\rho_i(x)$ dependence appears only in the Padé terms. Equation (23) implies that the second and third terms on the right-hand side of Eq. (21) add up to zero. We now wish to derive a good approximation for the left-hand side appropriate for our purpose. By operating $\langle \quad \rangle$ on the right-hand side of Eq. (21) and manipulating a few steps, we obtain

$$\begin{aligned} \text{LHS} = & \left[(k_i \rho_i)^2 + \left\langle \frac{1}{n_i} \right\rangle k_e^2 \rho_i^2(x) - \left\langle \frac{1}{n_i} \right\rangle \right] \langle \nabla^2 \rangle \Phi \\ & - \left[(k_i \rho_i)^2 + \left\langle \frac{1}{n_i} \right\rangle k_e^2 \rho_i^2(k) \right] \langle \nabla_{\parallel}^2 \rangle \Phi + \left[\rho_i^2(x) \left\langle \nabla_{\perp}^2 \left(\frac{k_e^2}{n_i} \right) \right\rangle k_e^2 \left\langle \frac{1}{n_i} \right\rangle \right] \Phi. \end{aligned} \quad (24)$$

In Eq. (24) the operator $\nabla_{\perp}^2$ is not trivial in general metric and in particular in toroidal metric. The parallel operator is $\nabla_{\parallel} = \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla)$, where $\hat{\mathbf{b}} = \frac{\mathbf{B}}{B}$. The perpendicular Laplacian is

$$\nabla_{\perp}^2 = [\nabla - \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla)] \cdot [\nabla - \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla)], \quad (25)$$

which gives rise to

$$\nabla_{\perp}^2 = \nabla^2 - \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla) \cdot \nabla - \nabla \cdot \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla) + \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla) \cdot \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla). \quad (26)$$

Using relations such as $\partial \hat{q}_1 / \partial q_2 = \hat{q}_2 (\partial h_2 / \partial h_1) / h_1$, we obtain

$$\nabla_{\perp}^2 = \nabla^2 - \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \nabla) \cdot \nabla - (\nabla \cdot \hat{\mathbf{b}}) \hat{\mathbf{b}} \cdot \nabla. \quad (27)$$

In general geometry we need to compute the following quantities:

$$\hat{\mathbf{b}} \cdot \nabla = \frac{b_x}{h_x} \frac{\partial}{\partial x} + \frac{b_y}{h_y} \frac{\partial}{\partial y} + \frac{b_z}{h_z} \frac{\partial}{\partial z}, \quad (28)$$

$$\nabla^2 = \frac{1}{h_x h_y h_z} \left[\frac{\partial}{\partial x} \left(\frac{h_y h_z}{h_x} \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{h_z h_x}{h_y} \frac{\partial}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{h_x h_y}{h_z} \frac{\partial}{\partial z} \right) \right], \quad (29)$$

where the local general metric coordinates are defined by $b_x = \frac{\mathbf{B} \cdot \hat{\mathbf{x}}}{B}$, $b_y = \frac{\mathbf{B} \cdot \hat{\mathbf{y}}}{B}$, $b_z = \frac{\mathbf{B} \cdot \hat{\mathbf{z}}}{B}$. The $\nabla_{\perp}^2$ operator (27) is derived in Appendix A in detail. For example, for general orthogonal axisymmetric toroidal coordinates (ψ, η, ζ) where ψ is the flux coordinate, ζ is the negative of the toroidal angle, and $\hat{\eta}$ is perpendicular to $\hat{\psi}$ and $\hat{\zeta}$, we have

$$\hat{\psi} = \hat{R} \cos \theta + \hat{y} \sin \theta,$$

$$\hat{\eta} = \hat{R} \sin \theta + \hat{y} \cos \theta,$$

$$\frac{\partial \hat{\psi}}{\partial \eta} = \hat{\eta} \frac{\partial \theta}{\partial \eta}, \quad \frac{\partial \hat{\eta}}{\partial \eta} = -\hat{\psi} \frac{\partial \theta}{\partial \eta}, \quad \frac{\partial \hat{\zeta}}{\partial \eta} = 0,$$

$$\frac{\partial \hat{\psi}}{\partial \zeta} = \hat{\zeta} \cos \theta, \quad \frac{\partial \hat{\eta}}{\partial \zeta} = -\hat{\zeta} \sin \theta, \quad \frac{\partial \hat{\zeta}}{\partial \zeta} = -\hat{R} \quad \text{etc.}$$

where R and θ are the major radius and θ the poloidal angle. For example, we need to calculate $(\hat{\mathbf{b}} \times \nabla) \cdot (\hat{\mathbf{b}} \times \nabla)(\nabla_{\perp}^2 \text{ operator})$, which reads

$$\begin{aligned} (\hat{\mathbf{b}} \times \nabla) \cdot (\hat{\mathbf{b}} \times \nabla) &= \frac{1}{k_{\psi}^2} \frac{\partial^2}{\partial \psi^2} - h_{\psi}^3 \frac{\partial h_{\psi}}{\partial \psi} \frac{\partial}{\partial \psi} + \frac{1}{h_{\psi}^2} \left(b_{\eta} \frac{\partial b_{\psi}}{\partial \psi} + b_{\zeta} \frac{\partial b_{\zeta}}{\partial \psi} \right) \frac{\partial}{\partial \psi} \\ &+ \frac{b_{\zeta}}{h_{\eta}} \frac{\partial}{\partial \eta} \left(\frac{b_{\zeta}}{b_{\eta}^2} h_{\zeta}^2 \frac{\partial}{\partial \eta} \right) + \frac{b_{\eta}^2}{h_{\zeta}^2} \frac{\partial^2}{\partial \zeta^2} - 2 \frac{b_{\eta} b_{\zeta}}{h_{\eta} h_{\zeta}} \frac{\partial^2}{\partial \eta \partial \zeta} - \frac{b_{\zeta}}{h_{\eta}} \frac{\partial}{\partial \eta} \left(\frac{b_{\eta}}{h_{\zeta}} \frac{\partial}{\partial \zeta} \right) + \frac{b_{\zeta}^2}{h_{\zeta} h_{\eta}} \frac{\partial \theta}{\partial \eta} \frac{\partial}{\partial \psi} \\ &+ \frac{b_{\eta}^2}{h_{\psi} h_{\zeta}} \cos \theta \frac{\partial}{\partial \psi} + \frac{b_{\zeta}}{h_{\psi}} \frac{\partial \theta}{\partial \psi} \left(\frac{b_{\eta}}{h_{\zeta}} \frac{\partial}{\partial \zeta} - \frac{b_{\zeta}}{h_{\eta}} \frac{\partial}{\partial \eta} \right). \end{aligned} \quad (30)$$

In particular in (r, θ, ϕ) toroidal coordinates, $h_r = 1$, $h_{\theta} = r$, and $h_{\phi} = R$.

Since it is important to retain the global profile of the ion temperature T_i in the present investigation, we now scrutinize the global gyrokinetic equations with the global variations

in $T_i(\mathbf{x})$. Let

$$F_i = \left(\frac{m}{2\pi T_\perp} \right) \left(\frac{m}{2\pi T_\parallel} \right)^{1/2} n_i(\mathbf{x}) e^{-\mu\Omega_i/[T_i(\mathbf{x})/m]} e^{-v_\parallel^2/2[T_\parallel(\mathbf{x})/m]}. \quad (31)$$

The term Eq. (14) after immediate integrations over $v_\parallel$ and $\mathbf{x}$ gives rise to

$$I_2 = -\frac{4\pi e^2}{m_i} \int dv_\perp v_\perp \left(\int_0^{2\pi} \frac{d\theta}{2\pi} e^{-\mu\Omega_i/T_\perp/m} \left(\frac{m}{T_\perp} \right)^2 \bar{\phi}(\mathbf{x} - \boldsymbol{\rho}) n(\mathbf{x} - \boldsymbol{\rho}) \right) \quad (32)$$

where $T_\perp \equiv T_\perp(\mathbf{x} - \boldsymbol{\rho})$. We expand quantities in powers of $\boldsymbol{\rho}$ as (only up to the first order is retained)

$$\begin{aligned} T_\perp(\mathbf{x} - \boldsymbol{\rho}) &= T_\perp(\mathbf{x}) - \boldsymbol{\rho} \cdot \nabla T_\perp \\ \Phi(\mathbf{x} - \boldsymbol{\rho}) &= \Phi(\mathbf{x}) - \boldsymbol{\rho} \cdot \nabla \Phi, \\ n(\mathbf{x} - \boldsymbol{\rho}) &= n(\mathbf{x}) - \boldsymbol{\rho} \cdot \nabla n. \end{aligned} \quad (33)$$

Substitution of Eq. (33) into Eq. (32) after integrals over θ and $v_\perp$ yields

$$I_2 = 4(k_i^2 \rho_i^2) \left[\left| \frac{\nabla_\perp T_\perp}{T_\perp} \right|^2 \Phi n + \left(\frac{\nabla_\perp T_\perp}{T_\perp} \right) \cdot \nabla (n\Phi) \right]. \quad (34)$$

Now let us discuss the phase angle average (or gyroaverages). In our computation we would like to approximate the integral over θ in Eq. (8) by a finite sum, which means

$$e^{ik \cdot \boldsymbol{\rho}} = \sum_{m=-\infty}^{\infty} i^m J_m(k_\perp \rho) e^{im\theta} \approx \frac{1}{N} \sum_i^N e^{k_\perp \rho \cos 2\pi n/N} = \sum_{m=-\infty}^{\infty} i^m J_m(k_\perp \rho) \frac{1}{N} \sum_{n=1}^N e^{im(n\Delta\theta - \phi)}, \quad (35)$$

where $\Delta\theta = 2\pi n/N$. Thus this approximation means that $J_0(k_\perp \rho)$ in Eq. (35) is replaced by

$$J_0(k_\perp \rho) + 2\beta J_4 + \dots \quad (36)$$

In case of $N = 4$, $J_0(k_\perp \rho) = \frac{1}{2}(\cos \alpha + \cos \alpha\beta)$, with $\alpha = k_\perp \rho$, $\beta = k_y/k_x$. We typically take $N = 4$.

2.2 Particle pushing

Gyrokinetic particles are implemented as standard drift particles, except that force interpolation and charge accumulation must be gyroaveraged. The guiding-center dynamics of drift particles [3] are specified by

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}_d + v_{\parallel} \mathbf{b} \quad (37)$$

$$\mathbf{v}_d = \mathbf{u}_E + \frac{\mathbf{b}}{\Omega_i} \times \left\{ \left(\frac{\mu}{m} \right) \nabla B + v_{\parallel}^2 (\mathbf{b} \cdot \nabla \mathbf{b}) \right\} \quad (38)$$

$$\frac{dv_{\parallel}}{dt} = \frac{q}{m} E_{\parallel} - \frac{\mu}{m} \mathbf{b} \cdot \nabla B \quad (39)$$

where q is the ion species charge, $\mathbf{u}_E = c\mathbf{E} \times \mathbf{b}/B$, $\mathbf{b} = \mathbf{B}/B$, $\mu = \frac{1}{2}mv_{\perp}^2/B$, and $\Omega_i = eB/mc$. Equations (37)–(39) are advanced in time via a predictor–corrector algorithm [4].

The gyroaveraging of the charge accumulation and force interpolation is done using the four-point averaging [12], as $N = 4$ in Eq. (35). The procedure is to take the sampled quantity at four points equally spaced around the cyclotron orbit, at one quarter weight each. (Note, however, that mathematically rigorous vector transformations in a stretched coordinate system are quite expensive. Specifically, a transformation to slab coordinates, followed by the vector addition, followed by a transformation back to the stretched system, is required. For gyrokinetic particles with four-point weighting, this results in a total cost of 32 vector transformations per particle per timestep.) This is optimized in GTS by taking advantage of the locally orthogonal computational grid. The gyroweight handling is performed by simply performing the vector additions directly in the stretched coordinate system, thus avoiding the cost of the transformations to and from slab coordinates. Since the gyrokinetic ordering implies a not large ρ_i , this is a fast and reasonable mathematical approximation for the parameter regime under consideration.

3 Numerical Method for Global Nonuniform Systems

3.1 Field solver considerations

We consider the field solving. Field quantities are represented as mode expansions so that for example, we have

$$\rho(x, y, z) = \sum \rho_n(x, y) e^{ik_z z}, \quad (40)$$

$$\phi(x, y, z) = \sum \phi_n(x, y) e^{ik_z z}, \quad (41)$$

$$E(x, y, z) = \sum E_n(x, y) e^{ik_z z}, \quad (42)$$

and $k_z = 2\pi n/L_z$. Since we have an axisymmetric system, we can compute each toroidal mode component independently and then sum them during interpolation. Note that this holds even for a 3-d grid, since we transform to k -space in z . As discussed elsewhere, the actual solution is achieved by transforming to mode space in the poloidal coordinate, and using finite differencing in the radial coordinate, which leads to a tridiagonal equation for each m mode.

When the cross-section of the torus is noncircular such as D -shaped, it can be generated via a Fourier series [25]. Specifically, we choose the representation

$$R(r, \theta) = \sum_{n=0}^3 R_n \left(\frac{r}{a}\right)^n \cos(n\theta), \quad (43)$$

$$Z(r, \theta) = \sum_{n=1}^3 Z_n \left(\frac{r}{a}\right)^n \sin(n\theta). \quad (44)$$

Here R is the major radius, and Z is the height referred to the midplane. R_0 is the distance from the center of the torus to the magnetic axis, which is usually near the center of the cross-section. a is taken to be the distance from the magnetic axis to the outer edge in the midplane, Z_0 is taken to be zero. We typically retain only three terms in the power series.

The actual two-dimensional grid is then generated by regarding r and θ in the above equations as discrete variables. Typically, we take the θ points to be equally spaced, and use a one-dimensional stretched grid in the radial direction for production of the discrete r points. The properties of this radially stretched grid have been described in [26].

There are several different coordinate systems employed in GTS for various distinct purposes. The grid coordinates we refer to as u and v , and represent the radial, poloidal, and toroidal directions respectively. For example, u increases by one as we move one grid spacing in the outward radial direction, and v increases by one as you move on grid spacing in the counterclockwise poloidal direction. Δu , Δv , and Δw the common notation for one grid spacing in each coordinate, are thus both identically one. In the discussion which follows, the location of each grid vertex in the Cartesian plane is identified by (x, y) , where x is essentially the same as $R - R_0$, and y is essentially the same as Z in Eqs. (43) and (44) above. This conceptual Cartesian system is used just for the calculation of the grid properties such as the metric, and those derivatives of the metric which are required by the field solver. The following choice is made: there are no grid vertices at the magnetic axis, since the Jacobian at $r = 0$ vanishes in a polar system. Rather the innermost grid vertices are displaced from the origin by one-half of a grid spacing. This further implies that the outermost grid vertices will be half a grid spacing inside the outer boundary. [u is conventionally indexed by i and v by j . Consequently, “ i -lines” are lines of constant v (concentric shells) and “ j -lines” are lines of constant u . Figure 1 shows an example grid generated by this procedure. For this case we have chosen $R_1 = 60$, $R_2 = 4$, $Z_1 = 90$, and $z_2 = -10$. We have also employed a stretched radial grid, typical of those used in our simulations discussed in Sec. 4. This formulation is general enough to model the cross-sections of current and envisioned tokamaks. Increasing Z_1/R_1 increases the vertical elongation, for example. Even “bean-shaped” cross-sections can be generated (not shown here). It is worth noting that the conventional simple toroidal grid employed in [26] is easily recovered in this formulation by setting $R_1 = Z_1 = a$ and

$$R_2 = R_3 = Z_2 = Z_3 = 0 \text{ [27].}$$

As noted previously, the field solvers and particle pushers currently employed require an orthogonal grid. The nonorthogonal grid generated by the prescription above is orthogonalized by the procedure suggested by Davies [28]. (The nonorthogonal grid system for PIC has been considered by Umegaki and Tajima). This technique works by keeping the i -lines fixed, and moving the j -lines in such a way as to produce an orthogonal system. (Actually, Davies [28] discusses moving the i -lines and holding the j -lines fixed, but this differs only by a transpose, so we describe the technique in the natural language of GTS.)

The expression of differential operators in the coordinate system is defined by the grid, and we must be able to provide the metric coefficients h_1, h_2 , and h_3 , along with various derivatives of these. We have in general (see for example, [29]) the symmetric metric

$$h_{ij}^2 = \frac{\partial x}{\partial q_i} \frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i} \frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i} \frac{\partial z}{\partial q_j}, \quad (45)$$

which reduces for orthogonal to $b_{ij}^2 = b_i^2 \delta_{ij}$. In this case we take q_i to range over the grid coordinates u, v, w to find

$$h_u = \sqrt{\left(\frac{\partial x}{\partial u}\right)^2 + \left(\frac{\partial y}{\partial u}\right)^2} \quad (46)$$

$$h_v = \sqrt{\left(\frac{\partial x}{\partial v}\right)^2 + \left(\frac{\partial y}{\partial v}\right)^2} \quad (47)$$

$$\begin{aligned} h_w &= \sqrt{\left(\frac{\partial x}{\partial w}\right)^2 + \left(\frac{\partial y}{\partial w}\right)^2} \\ &= \frac{2\pi x}{L_w}. \end{aligned} \quad (48)$$

These quantities are enough to allow pushing particles in this coordinate system. However, in order to support the differential operators needed for solution of the Poisson or gyrokinetic

Poisson equation, we also need

$$\frac{\partial h_u}{\partial u} = \frac{1}{h_u} \left(\frac{\partial x}{\partial u} \frac{\partial^2 x}{\partial u^2} + \frac{\partial y}{\partial u} \frac{\partial^2 y}{\partial u^2} \right) \quad (49)$$

$$\frac{\partial h_u}{\partial v} = \frac{1}{h_u} \left(\frac{\partial x}{\partial u} \frac{\partial^2 x}{\partial u \partial v} + \frac{\partial y}{\partial u} \frac{\partial^2 y}{\partial u \partial v} \right) \quad (50)$$

$$\frac{\partial h_v}{\partial u} = \frac{1}{h_v} \left(\frac{\partial x}{\partial v} \frac{\partial^2 x}{\partial u \partial v} + \frac{\partial y}{\partial v} \frac{\partial^2 y}{\partial u \partial v} \right) \quad (51)$$

$$\frac{\partial h_v}{\partial v} = \frac{1}{h_v} \left(\frac{\partial x}{\partial v} \frac{\partial^2 x}{\partial v^2} + \frac{\partial y}{\partial v} \frac{\partial^2 y}{\partial v^2} \right) \quad (52)$$

$$\frac{\partial h_w}{\partial u} = \frac{2\pi}{L_w} \frac{\partial x}{\partial u} \quad (53)$$

$$\frac{\partial h_w}{\partial v} = \frac{2\pi}{L_w} \frac{\partial x}{\partial v} \quad (54)$$

Derivatives with respect to w are zero because of axisymmetry.

The individual terms evident in the above equations must be determined by numerical differentiations on the grid. Although the grid has been orthogonalized, this only means that the grid is locally orthogonal. That is, the coordinates are orthogonal at each vertex. A quick glance at one of the orthogonal grids (such as in Fig. 1), however, makes it clear that distances of even a couple of cells will introduce obvious departures from orthogonality for much of the spatial domain. In order to calculate the required partial derivatives at the grid vertices in an accurate fashion, we thus introduce a new "virtual grid," used only at initialization, which contains vertices at all the same places as our computational grid (we will call these the primary vertices), but which also contains secondary vertices on each side of the primary vertices, located a small distance away. For a primary vertex indexed by (i, j) , we can employ the standard spatially centered finite difference (see for example, [30]).

Representation of the magnetic field in the case of a stretched cross-section is handled by using the conventional formulas for a tokamak magnetic field $\mathbf{B}$ (where elements 1, 2, 3 correspond to r, θ, ϕ directions, and adding a factor α to B_2 to account for the stretched

metric. Specifically,

$$B_1 = 0 \quad (55)$$

$$B_3 = B_0 \frac{R_0}{R} \quad (56)$$

$$B_2 = \frac{r}{R_0 q(r)} B_3 \alpha \quad (57)$$

where the stretch factor $\alpha = \alpha(r, \theta)$ is to be determined. Recalling the expression for the divergence of a vector $\mathbf{V}$ in general coordinates,

$$\nabla \cdot \mathbf{V} = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial(V_1 h_2 h_3)}{\partial q_1} + \frac{\partial(V_2 h_1 h_3)}{\partial q_2} + \frac{\partial(V_3 h_1 h_2)}{\partial q_3} \right) \quad (58)$$

we note that the first term drops out immediately since $B_1 = 0$, and the third term drops out because of axisymmetry. Plugging in the expressions for B_2 , we find the requirement

$$\frac{\partial(\alpha h_1)}{\partial \theta} = 0, \quad (59)$$

which we achieve by choosing

$$\alpha = \frac{\langle h_1 \rangle_\theta}{h_1}. \quad (60)$$

As a test, we examine the motion of guiding center particles in the presence of a tokamak field. The orbits of a representative sample of particles, exhibiting both the circulating orbits of transiting particles and the banana orbits of trapped particles (not shown here), have been examined. We have in fact observed that all the orbits are closed, and symmetric about the midplane.

3.2 Discussion of timestep and spatial resolution

The timestep for PIC simulation is determined by the physics (and its model) and by the computational constraints to avoid numerical instabilities [32]. The present model employs the gyrokinetic ion dynamics [12], drift kinetic electron dynamics [4], and the gyrokinetic

Poisson equation [12] in toroidal geometry whose metric and coordinates are “natural” [17]. While the gyrokinetic algorithm removes the timescale of ion cyclotron period Ω_i^{-1} , the natural toroidal coordinate facilitates to avoid short timescales associated with particle traversed times along magnetic field lines [17]. However, there are other modes that are represented in the model which also restrict the allowed timestep. We need to elaborate on this.

The main mode that we wish to represent and in fact that are represented in the gyrokinetic PIC simulation is the drift wave mode. The frequency of the drift frequency ω_* may be written in terms of the electron bounce frequency as

$$\begin{aligned}\frac{\omega_*}{\omega_{et}} &= \frac{\Omega_i k \rho_s k_\theta \rho_s}{k_\parallel v_e} = \left(\frac{\omega_*}{k_\parallel v_i} \right) \left(\frac{m_e}{m_i} \right)^{1/2} \left(\frac{T_i}{T_e} \right)^{1/2} \\ &\lesssim \left(\frac{m_e}{m_i} \right)^{1/2} \left(\frac{T_i}{T_e} \right)^{1/2}.\end{aligned}\quad (61)$$

Since we need to demand the timestep Δt to satisfy

$$\omega_{et} \Delta t \lesssim 1, \quad (62)$$

we have

$$\omega_* \Delta t \lesssim \left(\frac{m_e}{m_i} \right)^{1/2} \left(\frac{T_i}{T_e} \right)^{1/2}. \quad (63)$$

Writing $\omega_* \equiv 2\pi/T_*$, for a hydrogen plasma

$$\frac{\Delta t}{T_*} \lesssim 4 \times 10^{-3}. \quad (64)$$

We also need to satisfy $k_\parallel v_e \Delta t < 1$. For ion resonant being fulfilled, $k_\parallel(r=0, \text{ as well as } r=a)v_i z \omega_*$. Thus

$$\begin{aligned}\omega_* \Delta t &\lesssim k_\parallel v_i \Delta t = k_\parallel v_e \Delta t \left(\frac{T_i}{T_e} \right)^{1/2} \left(\frac{m_e}{m_i} \right)^{1/2} \\ &\sim \left(\frac{T_i}{T_e} \right)^{1/2} \left(\frac{m_e}{m_i} \right)^{1/2}.\end{aligned}\quad (65)$$

The gyrokinetic algorithm may gain timesteps over drift kinetics when the available highest frequency is the lower hybrid frequency $\omega_{\text{LH}} = \left(\frac{m_e}{m_i} \right)^{1/2} \omega_{pe} \sqrt{1 + \frac{m_e}{m_i} \frac{\Omega_i^2}{\Omega_e^2}}$. The above ion

resonance condition also yields

$$\Delta t \Omega_i k \rho_s \tau^{1/2} \left(\frac{m_i}{m_e} \right)^{1/2} \lesssim 1, \quad (66)$$

where $\tau = (T_e/T_i)$. If we examine the amount of numerical diffusion in the “square torus” configuration (unlike our natural coordinate torus) due to the poloidal field, we find that the deviation per time step from the flux surface will be on the order of

$$\delta \sim \left(v_{\parallel} \delta t \frac{B_x}{B} \right)^2 \quad (67)$$

Although this is second order in δt , the product $v_{\parallel} \delta t$ for electrons may be appreciable for typical simulation parameters, creating a definite concern about numerical diffusion in this system. The last modification necessary in the presence of the $r = 0$ point concerns the particle dynamics. No modification of the ion push is required, since the ions are being pushed in a cartesian coordinate system, but the $1/r$ terms in the electron guiding-center pusher require some special handling. Although the number of electrons near the origin will typically be small, eventually an electron will pass close enough to $r = 0$ to cause very inaccurate integration of the equations of motion (possibly a floating-point overflow as well). This problem is resolved by letting electrons undergo a collision when passing too close to the origin. We can imagine a small, hard cylinder (or torus) centered at $r = 0$; the continuity condition demands that an electron passing within the critical radius will exit with its θ coordinate shifted by 180° (i.e. $r \rightarrow -r$). Since the electron orbits in the (r, θ) plane are drift-dominated at the origin, and the dominant magnetic drifts vertical, this treatment is reasonable. The location of this critical radius can be estimated given the maximum tolerable theta increment in a given time-step for a thermal particle, and assuming the drift is dominated by the gradient- B term. The critical radius is then given approximately by

$$\frac{r_{\min}}{\Delta} \sim \frac{4\epsilon_z(\omega_e/\Omega_e)v_e^2}{N(\Delta\theta)_{\max}}$$

where $\bar{\Delta}$ is the average grid spacing, N is the number of radial grid-points, ω_e and Ω_e are the electron plasma and cyclotron frequencies, and v_e is the electron thermal velocity, normalized to $\bar{\Delta}\omega_e$. The maximum tolerable theta increment is of order one, where the distortion of the "true" particle motion due to the finite integration step rivals that from a collision with the artificial boundary near $r = 0$. Using typical simulation parameters, we obtain

$$\frac{r_{\min}}{\bar{\Delta}} \sim 10^{-2}-10^{-3}.$$

The smallness of this value indicates that a collision is not likely to influence the calculated fields significantly. Depending on the plasma profile and other simulation parameters, actual runs of approximately 50,000 particles suffer at most only a few collisions per time-step at the origin; often no collisions occur.

We now turn to the discussion of spatially nonuniform grid. In any numerical calculation, the motivation for using a nonuniform mesh is to more closely match the sampling method (i.e. grid) with the behavior of the solution. In our global gyrokinetic toroidal code, we are interested in drift modes that tend to localize at a certain rational surface (at a certain radial position). As discussed, these modes radially couple with each other due to the toroidal geometry, forming a semi-global drift mode structure. Thus where we are interested is where these modes reside.

Clearly, the finite-difference approximation does well for long wavelength modes, but becomes very inaccurate for $k\Delta \gtrsim \pi/2$. For $k\Delta = \pi/4$, the first derivative approximation is accurate to within about 10 percent; this is reduced to about 5 percent for the second derivative approximation. This is an important observation, because most particle codes do not resolve mode numbers much higher than this range ($k\Delta \sim \pi/4-\pi/2$). Particle codes usually employ k -space filters to eliminate the high mode numbers (discussed in Appendix B); the weakening effect due to such a filter will often far exceed that of the finite-difference operator. For example, a gaussian filter, for a particle the size of the grid spacing, halves

the signal strength at $k\Delta = \pi/4$. This leads us to conclude that the second-order finite difference expressions will usually be sufficiently accurate for use in a particle code.

We consider a radial, nonuniform (stretched) grid. The finite-difference approximation to the first derivative generalizes easily:

$$\frac{df}{dx} \simeq \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}}. \quad (68)$$

However, the expressions for the second derivative approximation and the truncation errors are somewhat cumbersome. It is helpful to adopt the notation

$$\begin{aligned} \bar{\Delta}_i &\equiv (\Delta_{i+1/2} + \Delta_{i-1/2})/2 \\ \delta_i &\equiv (\Delta_{i+1/2} - \Delta_{i-1/2}) \\ \gamma_i &\equiv \delta_i/(2\bar{\Delta}_i) \end{aligned} \quad (69)$$

where $\bar{\Delta}_i$ is the mean cell size and δ_i is the change in grid spacing at the i th grid point. The quantity γ_i is approximately 1/2 the rate of change of the grid spacing, a useful measure of the nonuniformity of the grid. With these definitions, the finite difference approximation for the first derivative is

$$\frac{f_{i+1} - f_{i-1}}{2\bar{\Delta}_i} = f'_i + \gamma_i \bar{\Delta}_i f''_i + (1 + 3\gamma_i^2) \frac{\bar{\Delta}_i^2}{6} f'''_i + \dots \quad (70)$$

and for the second derivative is

$$\frac{(1 - \gamma_i) f_{i+1} - 2f_i + (1 + \gamma_i) f_{i-1}}{\bar{\Delta}_i^2 (1 - \gamma_i^2)} = f''_i + \gamma_i \frac{2\bar{\Delta}_i}{3} f'''_i + (1 + 3\gamma_i^2) \frac{\bar{\Delta}_i^2}{12} f^{IV}_i + \dots \quad (71)$$

which, aside from notation, match the expressions given by de Rivas [31]. These expressions show clearly the effect of the stretched variable, and are different from their uniform grid counterparts in an important qualitative way—these approximations are no longer formally second-order accurate in the grid spacing. The reason for this loss of formal accuracy is that

for a nonuniform grid, these approximations to the first and second derivatives are no longer perfectly centered, resulting in the first-order Δ_i term in the truncation error. For extremely rapidly varying grid size, γ_i can become of order unity, which will cause the approximation to be first order accurate only (in this case, the finite-difference approximations have become essentially one-sided). It is clear that by changing the grid spacing sufficiently slowly, γ_i can be neglected and formal second order accuracy will be retained. This is the idea behind the condition given by Blottner and Roache [33], which in this notation takes on the form

$$\gamma_i \sim \bar{\Delta}_i \quad (72)$$

recovering the formal second order accuracy. (This condition assumes the above equations to be in dimensionless form, since the quantity γ_i is itself dimensionless.)

It is usually much simpler to express derivatives in terms of a transformed variable. We define the transformed coordinate

$$\xi = \xi(x)$$

where the $\xi(x)$ is our stretching-function, and grid-points occur in ξ -space at intervals of constant $\Delta\xi$ (arbitrarily set to 1). Then expressing the derivatives of f in terms of ξ , we have

$$\frac{\partial f}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial f}{\partial \xi} \quad (73)$$

$$\frac{\partial^2 f}{\partial x^2} = \left(\frac{\partial \xi}{\partial x} \right)^2 \frac{\partial^2 f}{\partial \xi^2} + \frac{\partial^2 \xi}{\partial x^2} \frac{\partial f}{\partial \xi}. \quad (74)$$

Since the partial derivatives of $\xi(x)$ are assumed to be known, all that remains is to replace $\partial f / \partial \xi$ and $\partial^2 f / \partial \xi^2$ by their corresponding uniform grid finite difference representations. This method is guaranteed to be second order in $\Delta\xi$, which might seem to be an improvement over Eqs. (70)–(71). This is an erroneous conclusion (although seen in some of the literature, e.g. [33]); either representation can be shown to have exactly the same truncation error. This

was probably first indicated in the work by de Rivas [31], where it was shown that Eqs. (70)–(71) could be transformed via a stretched coordinate, yielding second order equations. This was also discussed by Hoffman [34], who noted that the $\mathcal{O}(\Delta\xi^2)$ dependence of the truncation error implies that these equations behave in a second order way if the grid points are chosen appropriately.

The question as to the formal order of these methods, while being a concern, still leaves us without a clear estimate of the total error. To obtain a more meaningful measure of accuracy, we again adopt an oscillatory form for the arbitrary function f . Upon Fourier-analysis, the finite-difference approximation to the first derivative becomes

$$f'(x) \approx (f_{i+1} - f_{i-1}) / (2\bar{\Delta}_i) \quad (75)$$

$$= \sum f_k e^{ikx} (e^{ik\Delta_{i+1/2}} - e^{-ik\Delta_{i-1/2}}) / (2\bar{\Delta}_i) \quad (76)$$

$$= \sum f_k e^{ikx} i e^{ik\delta_i/2} (\sin k\bar{\Delta}_i) / \bar{\Delta}_i. \quad (77)$$

This is virtually equivalent to the uniform grid result, the main difference being the presence of a phase factor $e^{ik\delta_i/2}$. We obtain an accuracy condition on the nonuniformity of the grid, relevant to particle simulation, by requiring the argument of this phase factor to be small at the cut-off value $k\bar{\Delta}_i \sim \pi/2$. Given $k\delta_i/2 \ll \pi/2$, we then have

$$\gamma_i \ll 1 \quad (78)$$

for our nonuniform grid condition.

We now wish to construct a stretching function according to some prescribed grid spacing. Denoting the grid spacing by $\Delta(x)$, we have the relation

$$\Delta(x) \equiv \frac{\Delta x}{\Delta \xi}(x) \simeq \frac{1}{\partial \xi / \partial x} \quad (79)$$

which gives the expression for the stretching function

$$\xi(x) = \int \frac{dx}{\Delta(x)} \quad (80)$$

This specification of $\xi(x)$ is taken to be exact; the resulting grid spacing will not precisely match the function $\Delta(x)$ because of discreteness effects, but will usually be close. The first restriction on $\Delta(x)$ is that it yield a $\xi(x)$ with continuous first and second partial derivatives (this will be true if $\Delta(x)$ and $\Delta'(x)$ are continuous and nonzero). These derivatives are required to solve the Poisson equation. In general, this condition is not difficult to satisfy.

The second restriction we will make on the generation of the stretching function is that $\xi(x)$ be simple, that is, $\xi(x)$ should be analytically expressible with a minimum of special function evaluations. This is done to simplify the transformation of the particle positions x_i to the transformed coordinate, which is necessary in both the charge accumulation and the field interpolation phases.

We now consider the noise properties of the nonuniform number weighting scheme for two simplified cases. The first concerns a uniform grid and an exponential density profile. An appealing weighting scheme in this case would be to weight the particles so that the density profile is maintained, with an equal number of particles per cell. However, this would cause the physics to be dominated by discreteness effects caused by the particles with high weights. This fact has indeed been observed in short time scale simulations of this situation.

The second case involves starting with a uniform grid and the particles loaded to some prescribed density profile. The grid is then stretched to the desired configuration, keeping the number of particles per cell constant. The number weights of the particles are changed in conjunction with grid spacing, to maintain the necessary density profile. In this case, the charge density fluctuations can be written in terms of an averaging operator $\langle \dots \rangle$ as

$$\langle \rho(x) \rangle = \left\langle q(\xi) \frac{\partial \xi}{\partial x} \right\rangle \quad (81)$$

$$= \langle q(\xi) \rangle \frac{\partial \xi}{\partial x} \quad (82)$$

where $q(\xi)$ is the particle charge times the number weight in the transformed coordinate system, and $\partial \xi / \partial x$ is the transformation weight (see Appendix B or section for discussion of

metric effects in the charge accumulation). If we now assume no transverse diffusion, then we can approximate

$$\langle q(\xi) \rangle \sim q_0 \langle N(\xi) \rangle d(x) \frac{\partial \xi}{\partial x} \quad (83)$$

where q_0 is the average charge and $d(x)$ is initial number weighting function. Thus, we choose

$$d(x) \sim \frac{1}{\Delta_0 \partial \xi / \partial x} \quad (\approx \Delta(x) / \Delta_0) \quad (84)$$

for the weighting function, where Δ_0 is the average grid spacing. We then have

$$\langle \rho(x) \rangle = \frac{1}{\Delta_0} \langle N(\xi) \rangle \quad (85)$$

This shows that as the grid spacing changes, the fluctuation level of the charge density due to discreteness effects alone remains approximately constant, since the number of particles per cell does not change.

4 Global Simulation of Toroidal Drift Waves

We now present the results of runs of computer simulation of the drift wave plasma dynamics and its associated transport of a tokamak plasma. The runs presented here concentrate on the case $\eta_i = 4$, and sweep in a/ρ_i , providing a picture of the η_i mode over the range $70 \leq a/\rho_i \leq 540$. Gyrokinetic ions are employed, and the gyrokinetic modifications to the Poisson equation are included. Electrons are taken as adiabatic. (This allows a realistic hydrogen ion mass to be employed, $m_i/m_e = 1836$). The range of admitted poloidal modes is chosen to ensure that there are mode rational surfaces available throughout the simulation domain [26]. The q profile for these runs is shown in Fig. 2. Setting up the parameters for each run requires ensuring that the included modes and the specified temperature admit a reasonable value of $k_\theta \rho_i$. For η_i modes, we usually find the linearly most unstable mode at $k_\theta \rho_i \sim 0.22$. Once the parameters have been set up suitably for a run at one value of ρ_i , we accommodate other values of ρ_i by raising k_θ by the same factor by which we lower ρ_i .

Recall that $k_\theta = m/r$, and $q = m/n$ (at a mode rational surface). When we lower ρ_i/a we normally want to try to hold the mode in roughly the same radial location, in order to avoid changing the **background equilibrium parameters** at the same time. In the runs presented here, the number of particles is also increased when increasing n in order to retain the same statistical weight from particles per given mode resolution. The choice of the grid size and the number of particles as well as the time step has been carefully studied as discussed in Sec. 3.2 and in [26, 27] and is based on a set of constraints to ensure the legitimate physics of drift waves to emerge in simulations.

4.1 Case: $a/\rho_i = 70$ and Case: $a/\rho_i = 90$

The first run considers the case $a/\rho_i = 70$. This run employs 800,000 ions, and uses the modes $m/n \in 6 - 16/7$. The electric potential for this case is depicted in Fig. 3, which showed saturation at about $t = 2 \times 10^4 \Omega_i^{-1}$.

The run with $a/\rho_i = 90$ is our baseline run for the ρ_i scaling series. The basic parameters were chosen to be similar to the $\eta_i = 4$ run presented in [17], but there are important differences. For this case, 800,000 ions and 10,000 transport particles were used. The modes included in the system were $m/n \in 8 - 20/9$. Figure 4 shows the electric potential at three different points in time. The first frame is taken at the end of the linear growth phase. As expected, there is clear evidence of a robust mode with very elongated radial structures [17, 22]. The second frame, taken in the saturated state, shows activity in an even wider radial range, with possible suggestion of independent radial bands. The third frame, taken even later in the saturated state makes this much clearer. There are evidently two radial regions of mode activity, each of fairly significant radial extent. The inner one is stronger in the sense that the amplitude is higher, and the outer one is arguably wider, and more concentrated in the bad curvature region toward the outside edge of the torus.

Figure 5 shows the spectral density as well as the ion thermal diffusivity for this case.

We see again that there is clear spectral evidence for a radially elongated global mode, again falling just under the magnetic drift frequency ω_d line. Of special note is the spectral activity evident at decreases radius and increase frequency, which is caused by the breakup of the mode which is just becoming evident in the final frame of Fig. 4. Specifically, the inner band evident in the third frame occurs at roughly $r/a = 0.43$, which coincides with the spectral activity in Fig. 5.

In summary, this is seen to be a robust mode, possessing much of the character of the mode observed in or consistent with [35, 36]. It is seen again to be a radially extended “global” mode, with mode coupling between adjacent mode rational surfaces resulting in a nearly constant frequency for the mode across several surfaces. Moreover, the transport is seen to be characterized by a radially increasing functional form crossing more than an order of magnitude, much as is observed in experiments.

4.2 Case: $a/\rho_i = 180$

With this case of $a/\rho_i = 180$, we recall that as we decrease ρ_i we must increase k_θ . Since this run has halved ρ_i compared to the prior case, we double n and the range of m 's. The modes included in this run are $m/n \in 15 - 40/18$. Also, as previously noted, in order to ensure that this higher n is well resolved, we boost the particle count to 1,600,000. The number of transport particles was also increased to 20,000.

The instantaneous electric potential near the end of the linear growth phase, and again late in the saturated state in ion simulation exhibits (not shown) the effect of banding in the potential time history as the run evolves. In the spectral density for this run (not shown), once again, there is clear evidence for a strong global mode spanning many mode rational surfaces. And also, the ion thermal transport is seen to be an increasing function of radius.

4.3 Case: $a/\rho_i = 270$

This run employs modes $m/n \in 24-60/27$, which requires that the grid size in θ be increased to 256 in order to adequately resolve the higher poloidal mode numbers. Due to the increased n , the number of particles is increased to 2,400,000. The number of diagnostic transport particles was increased to 30,000.

Snapshots of the electric potential are shown in Fig. 6. The first, at $t = 1.5 \times 10^4 \Omega_i^{-1}$ is near the end of the linear growth phase. The second, at $t = 3.98 \times 10^4 \Omega_i^{-1}$ is late in the run. We see clear evidence of extended radial structures in the potential data, with evidence of banding in the radial coordinate as the simulation progresses into the saturated state. The spectral density and ion heat transport χ_i are shown in Fig. 7.

4.4 Case: $a/\rho_i = 360$

For this case we use $m/n \in 32-80/36$, and require 512 grid cells in the θ direction in order to support these poloidal mode numbers. 3,200,000 particles are employed in order to handle the high n , and 50,000 diagnostic transport particles are used. The electric field energy history for this run is depicted in Fig. 8. The linear growth phase extends up to roughly $t = 1 \times 10^4 \Omega_i^{-1}$. The time history of the previous case is about the same as in Fig. 8 and thus has not been presented.

Snapshots of the electric potential are shown in Fig. 9 at $t = 1 \times 10^4 \Omega_i^{-1}$ (end of the linear growth phase), $t = 2 \times 10^4 \Omega_i^{-1}$ (after the first major drop in field amplitude), and $t = 3 \times 10^4 \Omega_i^{-1}$ (after allowing the system to evolve in the saturated state for a while). This time span is evidently long enough to support significant variations in the radial banding structure. By the third frame, there are apparently at least 4 different radial bands of activity.

The spectral density shown in Fig. 10 appears to indicate a shifting to lower frequency and lower radius of the mode activity over time. An improved diagnostic tool would be

needed to investigate this more thoroughly. The ion thermal diffusivity continues to show the same functional form of steady increase with minor radius familiar from other runs.

4.5 Case: $a/\rho_i = 540$

This final case in the ρ_i scaling series considers a case well into the regime of large operational and/or future tokamaks.

The run employs $m/n \in 45 - 120/54$, and retains the grid size in θ of 512 used in the previous case. 4,800,000 ions are used in order to resolve the elevated n mode number, and 50,000 diagnostic transport particles are employed. The electric field energy history is presented in Fig. 11, showing initial saturation of the linear growth at roughly $t = 2.8 \times 10^4 \Omega_i^{-1}$.

Snapshots of the electric potential are provided in Fig. 12, showing the state of the system at the end of the linear growth phase at $t = 2.2 \times 10^4 \Omega_i^{-1}$ and again at $t = 4.98 \times 10^4 \Omega_i^{-1}$ after the first "crash" in the field energy. The banding is even more pronounced than the cases with smaller a/ρ_i , and in particular, it is becoming clear that the different bands balloon in somewhat different positions. By way of crude characterization, we can say that the outer most bands tend to balloon strongly toward the bad curvature region, whereas the inner most bands exhibit less preference for the outward direction.

The spectral density shown in Fig. 13 is perhaps the most difficult to interpret of any seen so far. The radial width of the spectral density island is quite small with respect to a , perhaps linking of only a couple of mode rational surfaces, though it is large with respect to ρ_i . This observation will be expanded on below in the discussion of transport analysis. The χ_i plot once again shows the same basic functional form which has become so familiar.

The radial profile of χ_i as a function of r at a typical time is shown in Fig. 14. In this figure the case of $a/\rho_i = 270$ is also shown. In both cases an approximate tendency of χ_i as an increasing function of r is observed (this is the case in all of our cases of a/ρ_i runs).

4.6 Cylindrical limit

We have mentioned that toroidicity is found to have a profound effect on the mode structure of the η_i simulation. Specifically, although the coupling of toroidal modes is weak or nonexisting, the introduction of finite toroidicity introduces strong coupling of poloidal modes. The mode structure in the cylindrical limit is characterized by independent poloidal modes localized to individual mode rational surfaces, with no coupling between them, and the level of transport is greatly reduced. These observations are the same as we found in [17].

4.7 Cross-sectional shaping

We explore the effects of cross-sectional shaping with some triangularity. In each of these runs we use parameters which are otherwise similar to the case $a/\rho_i = 70$ with circular cross-section described in Sec. 4.1.

Figure 15 presents a run performed in a modestly “D shaped” cross-section. The grid method is explained in Sec. 3. In addition to exhibiting both vertical elongation and triangularity, this grid also has the magnetic axis pushed toward the outside of the torus, as would occur in a finite β tokamak.

With this run we are able to see evidence of changes in the mode structure due to the more realistic system geometry. Specifically, ballooning in the mode structure is now evident on the inside of the magnetic axis, which is a noteworthy change from the case with circular cross-section presented in Fig. 3.

5 Mode and Transport Analysis of Tokamak Plasma

In order to analyze the mode structure and its associated transport properties from the runs presented, we consider each viewpoint and look for compatible features.

Using the instantaneous electric potential plots, we are able to directly measure the radial extent Δr of the extended radial structure of the drift wave potential for each run. This

allows comparisons of the scaling of the critical ratios $\Delta r/\rho_i$ and $\Delta r/a$. Results of these measurements are presented in Figs. 16 and 17. We note the clear increasing tendency of $\Delta r/\rho_i$ over the entire a/ρ_i range. This is an indication of Bohm-like transport. This is similar to the finding in [37]. Had $\Delta r/\rho_i$ been constant over the range of a/ρ_i , it would have been an indication of gyroBohm transport scaling [38, 39]. The plot of $\Delta r/a$ as a function of a/ρ_i does show some fall-off, which is a possible sign of gyroBohm behavior, but the trend is not convincing as the data is actually arguably fairly flat for large a/ρ_i , which is the more realistic end of the spectrum. On balance, the instantaneous electric potential snapshots seem to indicate a Bohm-like scaling. The linear theoretical analysis of toroidal drift wave, in contrast to the local ballooning treatment, takes into account the global variation of the equilibrium quantities such as the background temperature and density. Connor *et al.* [18] formulated this problem, implying the extent of the radial eigenmode extending beyond the local mode size ($\sim \rho_i$), but being broken in radial translational symmetry. This results in a semilocal radial mode size of

$$\Delta r \sim \left(\frac{\rho_i L_T}{\hat{s}} \right)^{1/2}, \quad (86)$$

where $\hat{s}$ is the magnetic shear parameter. A more detailed analysis yields the linear eigenmode size of drift waves (η_i or ITG mode) in toroidal geometry as

$$\Delta r = \left(\frac{2\gamma_0 \sin \theta_0}{k_\theta \hat{s} \partial \omega_r / \partial r} \right)^{1/2}, \quad (87)$$

where γ_0 is the linear growth rate, ω_d is the drift frequency, θ_0 the ballooning angle [23], and ω_r the real part of the eigenmode frequency. Ordinarily ($k_\theta \rho_i$) for the maximally growing linear mode is approximately equal to 0.2–0.3. The ratio of the growth rate to the bounce frequency γ_0/ω_d is approximately unity

$$\frac{\gamma_0}{\omega_d} = \mathcal{O}(1) \quad (88)$$

for robust mode in the hydrodynamic regime [38, 40] while for a near marginal (“critical

gradient") regime

$$\frac{\gamma_0}{\omega_d} \approx \frac{1}{k_\theta \rho_i} \left(\frac{R}{L_T} \right)^{1/2} (\eta - \eta_c)^{1/2}, \quad (89)$$

where $\eta \equiv R/L_T$, η_c the critical value for R/L_T ($\eta - \eta_c \ll \eta_c$). In the hydrodynamic regime the radial mode width Eq. (87) roughly coincides with Eq. (86), while in the near marginal regime the radial mode width scaling may be slightly different from Eq. (87). However, in either case the radial size Δr is a mixture of the ion Larmor radius and the global length L_T , i.e. $\Delta r = \rho_i^{1-\alpha} L_T^\alpha$ (with $\alpha \lesssim 1/2$). Our own simulations, though we see both linear (robustly unstable or near marginal cases and nonlinear phases, indicates a clear tendency of the radial mode size greater than the gyroradius, agreeing with the analytic results of semiglobal scale.

6 Conclusion

We have developed a global gyrokinetic PIC simulation code for shaped cross-section tokamak plasmas. Since the drift wave modes in toroidal geometry are coupled radially and form a semi-global extended mode structure which is a sensitive function of the global parameters such as the equilibrium plasma temperature profile, it is imperative to include the global profiles in the calculation. In non-circular (i.e. shaped) cross-section plasmas this incorporation of global profiles is even more acute. A series of numerical and mathematical developments dedicated for this purpose over the years [26, 27, 32] have been implemented in the code, Generalized Tokamak Simulator. The code has been thoroughly tested in various controlled runs as well as in standard runs of drift wave simulation. The code has been applied to examine the fundamental problem of the scaling of the radial mode structure and associated heat transport arising from the drift wave excitation.

The series of runs presented in Sec. 4 show evidence that in these cases the plasma and its excited modes settle toward the self-organized critical state [23], not so far different from linear or weak turbulence theory would describe as far as the mode structure is concerned.

The detailed study presented herein has concentrated on the case $\eta_i = 4$ and has employed the gyrokinetic model to cover the range $70 \leq a/\rho_i \leq 540$. This includes simulations at values of $a/\rho_i \sim 90$ similar to previous full ion dynamic global simulations [17], and extending all the way to simulations with $a/\rho_i = 360$ and $a/\rho_i = 540$ which are into the operation regime of current and future tokamaks. The mode structure is strongly influenced by the global temperature profile such as the temperature scale length L_T . Analysis of transport in these runs has yielded a Bohm-like transport for the above tokamak parameter regime. Moreover, these simulations have uncovered new structure in the potential eigenmodes. Specifically, the potential is seen to possess a banded structure at high values of a/ρ_i , which were inaccessible to previous simulations.

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Appendix A: Transverse Laplacian

The operator $\nabla_{\perp}^2$ is explicitly derived as follows:

$$\begin{aligned}
 \nabla_{\perp}^2 &= \frac{(1-b_x^2)}{h_x^2} \frac{\partial^2}{\partial x^2} + \frac{(1-b_y^2)}{h_y^2} \frac{\partial^2}{\partial y^2} + \frac{(1-b_z^2)}{h_z^2} \frac{\partial^2}{\partial z^2} \\
 &\quad - \frac{2b_x b_y}{h_x h_y} \frac{\partial^2}{\partial x \partial y} - 2 \frac{b_x b_z}{h_x h_z} \frac{\partial^2}{\partial x \partial z} - 2 \frac{b_y b_z}{h_y h_z} \frac{\partial^2}{\partial y \partial z} \\
 &\quad + \frac{1}{h_x^2} \left[-\frac{(1-b_x^2)}{h_x} \frac{\partial h_x}{\partial x} + \frac{(1-b_y^2)}{h_y} \frac{\partial h_y}{\partial x} + \frac{(1-b_z^2)}{h_z} \frac{\partial h_z}{\partial x} + \frac{b_x b_y}{h_y} \frac{\partial h_x}{\partial y} + \frac{b_x b_z}{h_z} \frac{\partial h_x}{\partial z} \right] \frac{\partial}{\partial x} \\
 &\quad + \frac{1}{h_y^2} \left[+\frac{(1-b_x^2)}{h_x} \frac{\partial h_x}{\partial y} - \frac{(1-b_y^2)}{h_y} \frac{\partial h_y}{\partial y} + \frac{(1-b_z^2)}{h_z} \frac{\partial h_z}{\partial y} + \frac{b_x b_y}{h_x} \frac{\partial h_y}{\partial x} + \frac{b_y b_z}{h_z} \frac{\partial h_y}{\partial z} \right] \frac{\partial}{\partial y} \\
 &\quad + \frac{1}{h_z^2} \left[+\frac{(1-b_x^2)}{h_x} \frac{\partial h_x}{\partial z} + \frac{(1-b_y^2)}{h_y} \frac{\partial h_y}{\partial z} - \frac{(1-b_z^2)}{h_z} \frac{\partial h_z}{\partial z} + \frac{b_x b_z}{h_x} \frac{\partial h_z}{\partial x} + \frac{b_y b_z}{h_y} \frac{\partial h_z}{\partial y} \right] \frac{\partial}{\partial z} \\
 &\quad - (\nabla \cdot \hat{\mathbf{b}}) \frac{b_x}{h_x} \frac{\partial}{\partial x} - (\nabla \cdot \hat{\mathbf{b}}) \frac{b_y}{h_y} \frac{\partial}{\partial y} - (\nabla \cdot \hat{\mathbf{b}}) \frac{b_z}{h_z} \frac{\partial}{\partial z}
 \end{aligned}$$

Appendix B: Nonuniform Grid and Weighting

Linear weighting is second-order accurate in the grid spacing and the interpolated function is continuous as the particle crosses a cell boundary. Quadratic weighting is also second-order accurate, but both the interpolated function and its first derivative are continuous as the particle crosses a cell boundary. The additional smoothness of quadratic weighting results in less error due to undersampling—the aliased wavenumber contributions are much smaller than in linear weighting [41]. The simulation will thus be better able to tolerate small values of λ_D/Δ without numerical heating, as well as needing less k -space filtering. This is important mainly along the direction of the magnetic field (long dimension). Therefore, we typically use quadratic weighting in the ζ coordinate for the usual 3-d grid configuration; linear weighting is used in the cross-field variables ξ and χ . Both weighting methods cause an order $(k\Delta)^2$ flattening of the spectrum at low wavenumbers. This flattening can be corrected to order $(k\Delta)^4$ by using a k -space compensating factor [41] (this type of post-sampling correction is also known as deconvolution [42]). Finally, note that the flat-metric type of interpolation allows straightforward substitution of higher-order methods.

The next step in obtaining the charge density for the Poisson solver is to include the effects due to the metric. The actual charge density is determined from the differential relation

$$\rho = \frac{\partial V'}{\partial V} \rho' = \frac{1}{J} \rho' \quad (\text{B1})$$

where J is given by $J = h_r h_\chi h_\zeta$ and represents the transformation Jacobian for the toroidal coordinate system (h_r includes the effect of the nonuniform grid). This becomes

$$\rho = \frac{\partial \xi / \partial r}{h_\chi h_\zeta} \rho' \quad (\text{B2})$$

which must be performed in (r, χ) space, due to the θ -dependence in h_ζ . The main problem with this approach is when the Jacobian vanishes at some point within the simulation region, as it does in the toroidal system at $r = 0$. This problem can be avoided by placing the

boundaries between gridpoints; there will be no grid point at $r = 0$ and thus no singularity. The given method of charge accumulation, together with the filter techniques discussed below, allow the adoption of a wide variety of coordinate metrics, in principle. A similar approach to handling the metric was used in [43] for two-dimensional particle-in-cell fluid simulations with an adaptive grid.

Finally, the filtering (or finite-size-particle shaping) must be considered. A commonly-used filter in particle simulations is the convolution of the accumulated charge density with a shape-factor, often a Gaussian, which is performed in k -space:

$$\rho(\mathbf{k}) \rightarrow \rho(\mathbf{k}) \exp(-[\mathbf{k} \cdot \mathbf{a}]^2/2)$$

where $\mathbf{k}$ is the wavevector and $\mathbf{a}$ is a measure of the particle size. This type of global filtering operator has the advantages of flexibility and ease of implementation, and can be used to partially compensate for errors introduced in the Poisson solver or the sampling method [41]. At present, a simple Gaussian shape-factor in the χ and ζ variables is used.

The use of a global filtering operator for a highly nonuniform or non-cartesian coordinate is questionable, however. For the radial variable in a cylindrical system, a non-standard (Bessel) representation must be used in order to have a rigorously convergent eigenfunction expansion. This problem can be avoided by considering a region far from the origin, as in the work of Cheng and Okuda [3]. In the case of a nonuniform grid, the non-locality of the above operator is somewhat inappropriate, although a transform in the stretched variable ξ is reasonable if a rigorously convergent transform can be found.

A better alternative exists for such situations, known as digital filtering, and is described by Birdsall and Langdon [41]. (Although the term digital filtering may refer to any discrete filtering process, we follow the convention of Birdsall and Langdon [41] in applying it only to filtering in the natural coordinate, i.e. without resorting to a transform of some sort.) The digital filter employed here is written as $\hat{S}_D^N$, denoting the N -fold application of the simple

filter

$$\hat{S}_D(\rho_i) = \frac{\rho_{i-1} + 2\rho_i + \rho_{i+1}}{4} \quad (\text{B3})$$

where i stands for the ξ -coordinate. This is known as a binomial filter, and is equivalent to a gaussian shape factor in the limit of $N \rightarrow \infty$. To see this, we write this filter in terms of its k -space representation in a uniform grid system [41] and then expand, assuming small $k\Delta$:

$$\hat{S}_D^N(k) = \left(\cos \frac{k\Delta}{2} \right)^{2N} \quad (\text{B4})$$

$$\approx \left[1 - \left(\frac{k\Delta}{2} \right)^2 \right]^N \quad (\text{B5})$$

When using this filter, the effective particle size will increase as N increases. Anticipating the result, we let

$$a_* = \sqrt{\frac{N}{2}} \Delta \quad (\text{B6})$$

whereupon the $N \rightarrow \infty$ limit of the filter becomes

$$\lim_{N \rightarrow \infty} \hat{S}_D^N(k) = \lim_{N \rightarrow \infty} \left[1 - \frac{k^2 a_*^2}{N} \right]^N \quad (\text{B7})$$

$$\equiv \exp \left(-\frac{k^2 a_*^2}{2} \right). \quad (\text{B8})$$

Although this only holds exactly in the large N , small $k\Delta$ limit, it nevertheless gives some feel for the particle "size" associated with the application of the filter. The total filtering operator can thus be written as

$$\rho(\xi, k_\chi, k_\zeta) \rightarrow \hat{S}_D^N(\rho) \hat{S}(k) \quad (\text{B9})$$

where $\hat{S}(k)$ is given by

$$\hat{S}(k) = \exp \left[-(k_\chi^2 a_\chi^2 + k_\zeta^2 a_\zeta^2)/2 \right] \quad (\text{B10})$$

Next we consider the filtering of the electric fields and their interpolation onto the particle positions. This is handled in the same way as the charge accumulation and filtering, except that no transformation weighting is required. It is important here to determine the conditions under which there is no numerical self-force term. The early research in particle simulation showed that for this type of code, a self-force was avoided by using the same interpolation scheme in the field interpolation as in the charge accumulation, and by adopting a filter that was symmetric in its argument. These conditions are relevant in the toroidal system as well. One problem with the early proof is its assumption of periodicity, which is inapplicable in our radial coordinate. In the presence of non-periodic boundaries, there will in general be a self-force—from an induced image charge. However, this boundary term can be included in the theory, and we refer to a numerical self-force more accurately as a failure to conserve momentum by the algorithm.

To examine the approximations that have been made in our model and determine whether it is momentum-conserving we must express formally the interpolation steps that have been given. The interpolation (accumulation) and filtering are two distinct processes, but we shall initially express these in terms of some general operator $\mathcal{L}$. The interpolation and filtering operations on the charge density can then be written in terms of a continuous variable as

$$\mathcal{L} \circ \rho(\mathbf{x}) = \int \rho(\mathbf{x}') \mathcal{L}(\mathbf{x}'; \mathbf{x}) J(\mathbf{x}') d\mathbf{x}' \quad (\text{B11})$$

where $\rho(\mathbf{x}')$ is the charge distribution, $\mathcal{L}(\mathbf{x}'; \mathbf{x})$ is the interpolation or filter distribution, and $J(\mathbf{x}') d\mathbf{x}' = J(\mathbf{x}') dx'_1, \dots, dx'_n$, is the volume element, for dimensionality n . In this operation we are simply summing the weights given to the point at $\mathbf{x}$ from every point in space ($\mathbf{x}'$); this will naturally depend on the geometry at $\mathbf{x}'$. Therefore we generally will have $\mathcal{L}(\mathbf{x}'; \mathbf{x}) \neq \mathcal{L}(\mathbf{x}; \mathbf{x}')$, where the coordinate in the second position denotes the fixed point. Furthermore, we require that $\mathcal{L}$ be linear, so the distribution satisfies

$$\int \mathcal{L}(\mathbf{x}'; \mathbf{x}) J(\mathbf{x}') d\mathbf{x}' = 1 \quad (\text{B12})$$

The interpolation and filter distributions will be simply the transformed flat-metric distributions :

$$\mathcal{L}(\mathbf{x}'; \mathbf{x}) = \frac{1}{J(\mathbf{x}')} \prod_{i=1}^n L_i(x'_i - x_i) \quad (\text{B13})$$

where $L_i(x'_i - x_i)$ is the flat-metric distribution of the i th coordinate. Note that $L_i(x'_i - x_i) = L_i(x_i - x'_i)$. The interpolation distribution is now written as

$$\mathcal{W}(\mathbf{x}'; \mathbf{x}) = \frac{1}{J(\mathbf{x}')} \prod_{i=1}^n W_i(x'_i - x_i) \quad (\text{B14})$$

$$\equiv \frac{1}{J(\mathbf{x}')} W(\mathbf{x}' - \mathbf{x}) \quad (\text{B15})$$

and the filtering distribution as

$$\mathcal{S}(\mathbf{x}'; \mathbf{x}) = \frac{1}{J(\mathbf{x}')} \prod_{i=1}^n S_i(x'_i - x_i) \quad (\text{B16})$$

$$\equiv \frac{1}{J(\mathbf{x}')} S(\mathbf{x}' - \mathbf{x}) \quad (\text{B17})$$

Here we have employed the symbols $W(\mathbf{x}' - \mathbf{x})$ and $S(\mathbf{x}' - \mathbf{x})$ to denote the total flat-metric distribution (i.e. the product of the individual coordinate distributions). The metric-dependent distributions $\mathcal{W}$ and $\mathcal{S}$ are analogous to the general distribution $\mathcal{L}$.

We now take the general charge density distribution $\rho(\mathbf{x}')$ to be the charge density due to an individual point source at $\mathbf{x}_j$:

$$\rho_j(\mathbf{x}') = q_j \delta(\mathbf{x}' - \mathbf{x}_j) \quad (\text{B18})$$

$$\equiv \frac{q_j}{J(\mathbf{x}')} \prod_{i=1}^n \delta(x'_i - x_{j,i}) \quad (\text{B19})$$

Using this value in the interpolation equation (B11), the charge density becomes

$$\rho_j(\mathbf{x}) = q_j \mathcal{W}(\mathbf{x}_j; \mathbf{x}) = \frac{q_j}{J(\mathbf{x}_j)} W(\mathbf{x}_j - \mathbf{x}) \quad (\text{B20})$$

Although Eq. (B20) can be used as a basis for a charge accumulation scheme (as in Ref. [3]), there are several problems with this approach. First, conservation of charge requires that

$$q_j = \int \rho_j(\mathbf{x}) J(\mathbf{x}) d\mathbf{x} \quad (\text{B21})$$

$$= q_j \int d\mathbf{x} \frac{J(\mathbf{x})}{J(\mathbf{x}_j)} W(\mathbf{x}_j - \mathbf{x}) \quad (\text{B22})$$

which cannot in general be satisfied simultaneously with condition (B12). Further, one must decide how to handle the $1/J(\mathbf{x}_j)$ term for particles that pass too close to a point where the metric vanishes (as for $r = 0$ in a cylindrical or toroidal system).

These problems may be avoided, while retaining our differential approach, by approximating the charge density equation Eq. (B20) by

$$\rho_j(\mathbf{x}) \approx \frac{q_j}{J(\mathbf{x})} W(\mathbf{x}_j - \mathbf{x}) = \frac{q_j}{J(\mathbf{x})} W(\mathbf{x} - \mathbf{x}_j) \equiv q_j \mathcal{W}(\mathbf{x}; \mathbf{x}_j). \quad (\text{B23})$$

This is reasonable since the interpolation distribution is strongly peaked about zero. The conservation of charge equation (B22) is now automatically satisfied when using the transformed slab-like interpolation and filtering distributions, regardless of the metric. Further, since the particle coordinates are virtually continuous and the grid is discrete, the vanishing of the metric at a point in the simulation region is no longer a problem—we simply avoid placing a grid-point at that location. In this case, the first grid-point is a half-cell away from the $r = 0$ point (farther when grid stretching is employed).

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FIGURE CAPTIONS

- FIG. 1. The grid system: (a) Example of orthogonal grid. Orthogonalization proceeding both inward and outward, from the 25th ring; (b) Example of nonorthogonal grid.
- FIG. 2. The tokamak safety factor (q) profile used for the ρ_i scaling runs.
- FIG. 3. Global gyrokinetic simulation results on electric potential for the case $a/\rho_i = 70$.
- FIG. 4. Electric potential for the simulation case $a/\rho_i = 90$.
- FIG. 5. Spectral density and ion thermal diffusivity for the simulation case $a/\rho_i = 90$.
- FIG. 6. Electric potential for the case $a/\rho_i = 270$.
- FIG. 7. Spectral density and ion thermal diffusivity for the case $a/\rho_i = 270$.
- FIG. 8. Time history of electric field energy (in a normalized unit) for the case $a/\rho_i = 360$.
- FIG. 9. Electric potential for the case $a/\rho_i = 360$.
- FIG. 10. Spectral density and ion thermal diffusivity for the case $a/\rho_i = 360$.
- FIG. 11. Time history of electric field energy for the case $a/\rho_i = 540$.
- FIG. 12. Electric potential for the case $a/\rho_i = 540$.
- FIG. 13. Spectral density and ion thermal diffusivity for the case $a/\rho_i = 540$.
- FIG. 14. Radial profile of ion thermal diffusivity as a function of r for the cases of $a/\rho_i = 270$ and $a/\rho_i = 540$.
- FIG. 15. Electric potential for the case $a/\rho_i = 70$, with modest D shaping of tokamak poloidal profile.
- FIG. 16. Transport coefficient: (a) Scaling of $\Delta r/\rho_i$ with a/ρ_i ; (b) Scaling of $\Delta r/a$ with a/ρ_i .

FIG. 17. Comparison of maximum transport for each run, expressed in Bohm-like normalization (in the lower panel we show the transport coefficient in the gyroBohm normalization).

(a)

(b)

FIG. 2

FIG. 3

FIG. 4

FIG. 5

FIG. 6

FIG. 7

FIG. 8

FIG. 9

FIG. 10

FIG. 11

FIG. 12

FIG. 13

FIG. 14

($\times 10^{-5}$)

Electric Potential

GK $a/\rho_i = 70$ $n=7$ D shaping, magnetic axis translation $810.0 \Omega_i^{-1}$

FIG. 15

FIG. 16

FIG. 17

Figure 2.1: Schematic layout of optics for 3.5 cm beam. The cylindrical mirrors L1 and L2 are used to transform the circular cross-section beam out of the laser to an elliptical cross-section beam to fit the tokamak ports.

This 'object' beam was produced using two mutually perpendicular cylindrical mirrors (L1 and L2 in Fig. 2.1) that transformed the output of the laser to the required sizes of the 'object.' Since the position of the parabolic mirror was fixed with respect to the plasma equatorial plane and the laser was to be mounted at a fixed location on the breadboard, the transformation distance for the cylindrical mirrors was then fixed (299 cm). Changing the focal length of one of the cylindrical optics (L2) and its placement then changed the beam size in the plasma in the major radial direction, independent of the beam size and placement in the toroidal direction (determined by L1). Appendix A contains the procedure used to determine the focal lengths and distances.

Implementation

We implemented a modular design with most of the optics in Delrin boxes to minimize the effect of air currents that were noticed to produce adverse effects on the wavefront in sidelab tests. The apertures for all the modules were made

Figure 2.2: **Sections of parabolic mirror.** Two matching sections were used out of a single parabolic telescope mirror.

larger than thrice the beam radius, such that the beam was diffraction limited at the vacuum windows. The expansion optics were all assembled in two modules (M1 and M2) as shown in Fig. 2.3. The first module (M1), consisting of an off center section of a parabolic mirror and two turning mirrors were used to shorten the effective distance from the parabolic mirror to its focal point.

The location of the focal point with respect to this module was experimentally determined by using a fiber optic as a point source and measuring the beam sizes in the far field. The emergent beam was collimated when the fiber optic was at the focal point. The experimental precision of this method was better than 0.25 cm. The practical advantage of this method over more precise methods (e.g. knife edge) is that once the focal point on the expansion side is located, the fiber optic point source is at a conjugate point of the loca-

Figure 2.3: **The PCI system on TEXT-U.** The expansion modules M1 and M2 were on the bottom breadboard and the receiver module M3 was mounted on the top breadboard.

tion of the phase plate and its point image on the receiver side can be used to determine the location of the phase plate.

The module M1, in Fig. 2.3, held the parabolic mirror and two flat turning mirrors. The other module (M2) of the expansion set consisted of the cylindrical mirrors (L1 and L2) and some turning mirrors mounted on rails. The modules were aligned and the expansion set was tuned in the side lab, so that the installation and alignment on the tokamak was simple.

The expansion set modules were mounted on a breadboard below the tokamak along with the laser, as shown in Fig. 2.3. The expanded beam emerged from the top of the module M1, toroidally offset by 5 cm from the

center of the port. A periscope was used to translate the axis of the beam so that it was aligned with the port and also to adjust the angle of the beam in the toroidal and radial directions. The beam was received by the receiver module (M3) that was mounted on the top breadboard.

The receiver set of the optics consisted of a section of the parabolic mirror, similar to the one used for the expansion set, that focused the beam on to the phase plate and a single ZnSe lens that formed an image of the phase plate at the detector location, as shown in Fig. 2.4. The receiver set design was done with each optic at a focal length from the object and image planes. This afocal design allowed the receiver set to be treated as a set of Fourier optics for which Fraunhofer diffraction is valid. This was consistent with the treatment of the theory of the PCI diagnostic in which the image at the focal plane of the first optic after the plasma is assumed to be the Fourier transform of the image in the plasma. Also, the magnification of the receiver set was then just the ratio of the focal lengths of the elements. To avoid buying multiple expensive ZnSe cylindrical lenses, we used a single spherical ZnSe lens (L3 in Fig. 2.4) that imaged the 3.88 cm beam onto 14 consecutive elements of the detector array in the x (radial) direction ($3.88 \times (7.5/203) = 0.143$ cm) and matched the detector width very closely in the y (toroidal) direction ($0.32 \times (7.5/203) = 120 \times 10^{-4}$ cm) . For larger beams we planned to use more detector elements, spaced appropriately.