Nonlocal closures for plasma fluid simulations^{a)}

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The application of fluid models in studies of transport and macroscopic stability of magnetized, nearly collisionless plasmas requires closure relations that are inherently nonlocal. Such closures address the fact that particles are capable of carrying information over macroscopic parallel scale lengths. In this work, generalized closures that embody Landau, collisional and particle-trapping physics are derived and discussed. A gyro/bounce-averaged drift kinetic equation is solved via an expansion in eigenfunctions of the pitch-angle scattering operator and the resulting system of algebraic equations is solved by integrating along characteristics. The desired closure moments take the form of integral equations involving perturbations in the flow and temperature along magnetic field lines. Implementation of the closures in massively parallel plasma fluid simulation codes is also discussed. This implementation includes the use of a semi-implicit time advance of the fluid equations to stabilize the dominant closure terms which are introduced explicitly. Application of the nonlocal, parallel heat flow closure, $\mathbf{q}_{\parallel}$, in studies of temperature flattening across helical magnetic islands in toroidal geometry reveal a scaling of temperature versus critical island width for flattening of $T \sim w_d^{-1.5}$. This result predicts more robust flattening at small island widths when compared to the diffusive scaling, $T \sim w_d^{-1.7}$, which assumes a Braginskii-type parallel heat conductivity. Preliminary application of $\mathbf{q}_{\parallel}$ to tokamak disruption simulations shows qualitative agreement of wall heat loads with experimental observations, smooth distribution in toroidal angle, and striation in the poloidal direction along the wall. © 2004 American Institute of Physics.

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I. INTRODUCTION

Theoretical tools applied to long-collision-length terrestrial and astrophysical plasmas tend toward two extremes: kinetic models rife with physics but operating for short times, and fluid models employing simplified closure relations to capture kinetic physics but operating for long times. Until computers are fast enough to calculate full kinetic physics over resistive and transport time scales, efforts to extend fluid models to handle a wider range of physics are critical to improving our predictive capability of nearly collisionless plasmas such as those in next-step fusion experiments. In this work we describe one such effort which advances the realism of fluid models by generalizing the program of fluid closure to capture kinetic effects in nonlocal, integral forms for higher-order fluid moments. The term *nonlocal closure* implies integrating fluid and closure variables along lowest-order characteristics of the distribution function, F . For the five moment model, these integrals in-

volve perturbations in flow ($\mathbf{u}$), and temperature (T), and in general, the viscous stress (Π) and conductive heat flow ($\mathbf{q}$) closures.

For magnetized plasmas confined by slowly evolving magnetic fields, the lowest-order characteristics are simply magnetic field lines and the dominant parallel closure components, $\Pi_{\parallel}$ and $\mathbf{q}_{\parallel}$, have a general, nonlocal dependence on thermodynamic drives.¹⁻³ This is in contrast to collisional transport theory which writes closures in terms of local gradients of fluid quantities.⁴ In general, local forms for the closures are the result of collisions spatially localizing the generalized, integral expressions. Although this work focuses on closures that are spatially nonlocal, such integral forms may also occur in time. For example, when investigating the damping of poloidal flows in axisymmetric toroidal geometry, the parallel viscous stress closure couples time integrals of $\mathbf{u}$, $\Pi_{\parallel}$ and a momentum restoring term. Instances of nonlocality describe situations in which particles are capable of carrying information over macroscopic parallel scale lengths or long time scales. It is important to note that previous efforts in closure theory have arrived at ostensibly nonlocal forms for closures.⁵⁻⁸ However, the construction of generalized integral closures that emphasize the continuous mapping

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from the collisional to the nearly collisionless regimes and allow for more complicated magnetic geometry² and integral forms for collision operators³ is more recent.

Specifically, this work describes the derivation of nonlocal closures that embody Landau, collisional, and particle-trapping physics using a Chapman–Enskog-like procedure to derive and solve a reduced kinetic equation. In Sec. II we derive an equation that ignores finite-gyroradius effects and uses the dominant parallel component of the guiding center velocity in the advective derivative acting on F . In Sec. III we discuss the solution of this kinetic equation which requires inverting an operator that includes collisional and either spatial or time-dependent effects. We begin by expanding in eigenfunctions of the bounce-averaged Lorentz, pitch-angle scattering operator. Next, the characteristics of F are identified by diagonalizing the resultant system of ordinary differential equations. Finally, the desired closure moments of F are calculated. Specifically, it is shown that the nonlocal, integral $\mathbf{q}_{\parallel}$ moment maps continuously from the collisional to nearly collisionless regimes. In addition to significantly advancing the realism of previous fluid closures, integration along comparatively few characteristics represents a significant reduction in work compared to a statistically-relevant kinetic treatment that follows millions of particles. In essence, these characteristics uncover the essential velocity–space dependence of F and hence render this closure scheme suitable for simulation of long timescale, macroscopic behavior. A massively parallel implementation of these closures is discussed in Sec. IV, including the application of a semi-implicit operator to stabilize the advance of the temperature evolution equation. We conclude in Sec. V by discussing the application of the nonlocal $\mathbf{q}_{\parallel}$ closure to studies of heat flow dynamics in high-performance, toroidal fusion experiments.

II. CHAPMAN–ENSKOG-LIKE DRIFT KINETIC EQUATION

Before deriving nonlocal forms for closures, we consider first the moment evolution equations of the five moment model. The macroscopic fluid quantities of density, n , flow, $\mathbf{u}$, and temperature, T , for each species evolve according to the following set of unclosed equations:

$$\begin{aligned}\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{u} &= 0, \\ mn \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) &= en \left(\mathbf{E} + \frac{1}{c} \mathbf{u} \times \mathbf{B} \right) - \nabla p - \nabla \cdot \underline{\underline{\Pi}} + \mathbf{R}, \\ \frac{3}{2} n \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) &= -p \nabla \cdot \mathbf{u} - \underline{\underline{\Pi}} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q} + Q, \quad (1)\end{aligned}$$

where underlined terms contain the unspecified closure moments. The right-hand side of the $\mathbf{u}$ equation contains the Lorentz, $en(\mathbf{E} + (1/c)\mathbf{u} \times \mathbf{B})$, pressure-gradient, $-\nabla p$, collisional friction, $\mathbf{R}$, and viscous stress, $-\nabla \cdot \underline{\underline{\Pi}}$, forces. The right-hand side of the T equation includes compressional, $-p \nabla \cdot \mathbf{u}$, viscous, $-\underline{\underline{\Pi}} : \nabla \mathbf{u}$, and collisional, Q , heating terms, as well as the conductive heat flow, $\mathbf{q}$. The program of fluid closure attempts to close these equations by specifying

forms for $\underline{\underline{\Pi}}$ and $\mathbf{q}$. The simplest form of closure is brute truncation, $\underline{\underline{\Pi}} = \mathbf{0}$ and $\mathbf{q} = \mathbf{0}$. A less drastic approach that allows for long-collision-length physics entails solving an appropriate kinetic equation for the distribution function, f , and then taking the closure moments defined as

$$\mathbf{q} \equiv \int d^3v \, \frac{1}{2} m v'^2 \mathbf{v}' f,$$

and

$$\underline{\underline{\Pi}} \equiv \int d^3v \, m \left[\mathbf{v}' \mathbf{v}' - \frac{v'^2}{3} \mathbf{I} \right] f, \quad (2)$$

where $\mathbf{v}' \equiv \mathbf{v} - \mathbf{u}$ is the random particle velocity and $\mathbf{I}$ is the unit dyad.

In the interest of keeping the fluid and kinetic physics separate, we advocate a Chapman–Enskog-like (CEL) approach which posits that the distribution function, f , is the sum of a dynamic Maxwellian, f_M , plus a kinetic distortion, F :

$$f = f_M + F = n \left(\frac{m}{2\pi T} \right)^{3/2} \exp \left(-\frac{mv'^2}{2T} \right) + F, \quad (3)$$

where the n , $\mathbf{u}$, and T moments of f_M satisfy Eq. (1). Using this ansatz along with the moment equations, one can recast the full kinetic equation, $df/dt = C(f)$, in the following form:⁶

$$\begin{aligned}\frac{\partial F}{\partial t} + \mathbf{v} \cdot \nabla F + \mathbf{a} \cdot \nabla_{\mathbf{v}} F - C(f) &= \frac{m}{T} \left(\mathbf{v}' \mathbf{v}' - \frac{v'^2}{3} \mathbf{I} \right) : \nabla \mathbf{u} f_M + \mathbf{v}' \cdot (\nabla \cdot \underline{\underline{\Pi}} - \mathbf{R}) \frac{f_M}{p} \\ &+ \left(\frac{mv'^2}{3T} - 1 \right) (\underline{\underline{\Pi}} : \nabla \mathbf{u} + \nabla \cdot \mathbf{q} - Q) \frac{f_M}{p} \\ &- \left(\frac{mv'^2}{2T} - \frac{5}{2} \right) \mathbf{v}' \cdot \nabla T \frac{f_M}{T}.\end{aligned} \quad (4)$$

As in the traditional, collisional Chapman–Enskog approach,⁹ F satisfies $\int d^3v \{ \mathbf{v}'^0, \mathbf{v}'^1, \mathbf{v}'^2 \} F = 0$ for the first three velocity moments. On the left-hand side, $\mathbf{a} = (e/m)(\mathbf{E} + (1/c)\mathbf{v} \times \mathbf{B})$ is the acceleration and $C(f)$ is the collision operator which represents binary, collisional scattering events. Note that along with the traditional gradient drives, $\nabla \mathbf{u}$ and ∇T , the closures needed for the five moment model, namely, $\underline{\underline{\Pi}}$ and $\mathbf{q}$, appear on the right-hand side. This is the result of using the moment equations to simplify df_M/dt . Although Eq. (4) contains all of the information of the full kinetic equation, it is neither possible nor desirable to solve in its present form. We are interested in extracting the essential kinetic physics that plays a role in the macroscopic evolution of plasmas confined by resistively evolving magnetic fields.

The reduction of Eq. (4) to a form amenable to an analytical/numerical solution begins by making a small gyroradius assumption and applying the gyroaveraging opera-

FIG. 1. Poincaré plot showing saturated 2/1 and 3/1 magnetic islands resulting from resistive tearing mode evolution. The **X** marks the starting location of the field line integration in Fig. 2.

tor, $\oint d\gamma/2\pi$. Approximating F to lowest-order as independent of gyrophase, γ , yields the following equation that emphasizes the dominant kinetic physics of motion along magnetic field lines:

$$\begin{aligned} \frac{\partial F}{\partial t} + \mathbf{v}_{\parallel} \cdot \nabla F - C(f) \\ = -\frac{m}{T} \left(v_{\parallel}^2 - \frac{v_{\perp}^2}{2} \right) \left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \frac{\mathbf{I}}{3} \right) : \nabla \mathbf{u} f_M + \mathbf{v}_{\parallel} \cdot (\nabla \cdot \Pi_{\parallel} - \mathbf{R}) \frac{f_M}{p} \\ + L_1^{1/2} \left(\frac{d \ln T}{dt} + \nabla \cdot \mathbf{u} \right) f_M - L_1^{3/2} \mathbf{v}_{\parallel} \cdot \nabla T \frac{f_M}{T}. \end{aligned} \quad (5)$$

Here $L_1^{1/2}(v)$ and $L_1^{3/2}(v)$ are Laguerre polynomials and $\hat{\mathbf{b}}$ is a unit vector parallel to the magnetic field. Note that the cross and perpendicular components of Π , which may be derived from a fluid analysis,¹⁰ have been ordered small compared to $\Pi_{\parallel}$.^{6,11} Here we have used the temperature evolution equation to rewrite the term involving $\nabla \cdot \mathbf{q}$. It is important to note as well that although the left-hand side of Eq. (5) does not contain the particle drift velocity, the right-hand side has drive terms related to drift effects.¹¹

A further reduction of the drift kinetic equation is possible by averaging over a particle's bounce orbit in magnetic wells. In order to justify this average we consider a NIMROD (Ref. 12) simulation of classical, resistive tearing modes in shaped toroidal geometry.¹² Figure 1 shows a Poincaré plot of saturated 2/1 and 3/1 magnetic islands resulting from this simulation. While traveling along magnetic field lines in this geometry, particles experience Coulomb collisional effects while seeing varying fluid quantities and magnetic field modulus, B . Figure 2 shows the variations in B and T when integrating along a magnetic field line just inside the 2/1 island O-point. The starting point of this integration is marked by the **X** in Fig. 1. It is clear from the plot that variations in B occur over a shorter scale length, l , than

FIG. 2. Plot shows variation in B and T inside the 2/1 island in Fig. 1 when integrating along the magnetic field. Note that the temperature gradient scale length, L_T , the collision length, L_ν , and the length of variations in B , l , satisfy $L_T \sim L_\nu \sim 100 \text{ m} \gg l$.

those of T which are comparable to the collision length, $L_T \sim L_\nu \approx 100 \text{ m}$, for $T = 1 \text{ keV}$, and $n = 10^{20} \text{ m}^{-3}$.

Calculating spatially nonlocal, parallel closures in the vicinity of helical magnetic islands requires a solution of Eq. (5) that accounts for particle trapping in short magnetic wells and puts collisional ($C(f)$) and parallel free-streaming ($\mathbf{v}_{\parallel} \cdot \nabla$) effects on an equal footing. Expanding the operator $\mathbf{v}_{\parallel} \cdot \nabla = \mathbf{v}_{\parallel} \cdot (\nabla_{\perp} + \nabla_{\parallel})$ in Eq. (5) permits writing the lowest order in $\delta \equiv (\mathbf{v}_{\parallel} \cdot \nabla_{\perp} / \mathbf{v}_{\parallel} \cdot \nabla_{\parallel}) \ll 1$ equation as

$$\mathbf{v}_{\parallel} \cdot \nabla_{\parallel} F^0 = -\frac{m}{T^0} \left(v_{\parallel}^2 - \frac{v_{\perp}^2}{2} \right) \left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \frac{\mathbf{I}}{3} \right) : \nabla \mathbf{u}^0 f_M^0, \quad (6)$$

which has the solution

$$F^0 = g(L, \psi, \mathbf{v}, t) + \frac{mv_{\parallel}}{T^0} u_{\parallel}^0 f_M^0. \quad (7)$$

Here it has been assumed that the lowest-order, divergence-free flow can be written $\mathbf{u}^0 = \mathbf{B} \times \nabla \phi / B^2$, where $\phi = \phi(\psi)$ is a function of the equilibrium flux surfaces labeled by ψ . Also, we have assumed that $T^0 = T^0(\psi)$ and the remaining drive terms are first order. Applying the bounce-average operator, $\langle \rangle \equiv \oint dL B / (B_0 v_{\parallel})$, to the first order equation eliminates the $\mathbf{v}_{\parallel} \cdot \nabla_{\perp} F^1$ term with the result

$$\begin{aligned} \left\langle \left(\frac{\partial}{\partial t} + \sigma \mathbf{v}_{\parallel} \cdot \nabla_{\parallel} \right) F^0 \right\rangle - \langle C(F^0 + f_M^0) \rangle \\ = - \left\langle \frac{m}{T} \left(v_{\parallel}^2 - \frac{v_{\perp}^2}{2} \right) \left(\hat{\mathbf{b}}\hat{\mathbf{b}} - \frac{\mathbf{I}}{3} \right) : (\nabla_{\perp} \mathbf{u}^1 + \nabla_{\parallel} \mathbf{u}^0) f_M^0 \right\rangle \\ + \left\langle \mathbf{v}_{\parallel} \cdot (\nabla_{\perp} \cdot \Pi_{\parallel} - \mathbf{R}^1) \frac{f_M^0}{p^0} \right\rangle - \sigma \left\langle L_1^{3/2} \mathbf{v}_{\parallel} \cdot \nabla_{\perp} T^0 \frac{f_M^0}{T^0} \right\rangle. \end{aligned} \quad (8)$$

Here $\sigma = 0$ for trapped particles and 1 for passing particles. Also, we have ignored the $d \ln T / dt + \nabla \cdot \mathbf{u}$ term for simplicity which is appropriate when deriving closures driven by slow magnetic evolution. In such cases, the temperature evolution

equation is well approximated by $\nabla \cdot \mathbf{q} = 0$. Equation (8) is a CEL version of the gyro/bounce averaged kinetic equation and is appropriate for deriving $\mathbf{q}_{\parallel}$ and $\Pi_{\parallel}$ in order to close the five moment model fluid equations. The construction of non-local closures from this equation is discussed in the next section.

III. CONSTRUCTION OF NONLOCAL CLOSURES

Constructing nonlocal closures from Eq. (8) requires a maximal ordering between two of the terms on the left-hand side of the equation. Addressing collisional and free-streaming physics and ordering $\partial/\partial t$ small results in nonlocal equations in space. Addressing collisional and time-dependent physics in axisymmetric toroidal geometry results in integral closures in time. Before discussing solutions of Eq. (8), however, we first state the form of the collision operator which will be inverted via an expansion in orthogonal eigenfunctions.

Parallel flow and heat flow play a fundamental role in the dynamics of magnetized plasmas. A simplified collision operator should therefore account for the scattering of a particle's parallel directed velocity in pitch-angle. Inverting the collision operator along with either the free-streaming operator or time-derivative is most easily accomplished by expanding F^0 in orthogonal, pitch-angle eigenfunctions. A linear form for the bounce-averaged scattering in pitch angle of a test species, F^0 , colliding with multiple background Maxwellian species is

$$\langle C(F^0) \rangle = \sum_s \langle L_s(F^0) \rangle = \sum_s \frac{v_{\perp s}}{2v\xi} \frac{\partial}{\partial \xi} \frac{(1-\xi^2)}{\xi} \left(\oint dl \frac{v_{\parallel}}{v} \right) \frac{\partial F^0}{\partial \xi}, \quad (9)$$

where the pitch-angle type variable $\xi = \pm \sqrt{1 - (v_{\perp}^2 B/v^2)}$. For electrons and ions, $\sum_s v_{\perp s} = v_{\perp ee} + \sum_{\text{ions}} v_{\perp s}$ and $\sum_s v_{\perp s} \approx \sum_{\text{ions}} v_{\perp s}$, respectively. For simplicity, we write $\sum_s v_{\perp s} = v_{\perp}$. The self-adjointness of the operator $\langle L_s \rangle$ permits the solution of separated eigenvalue equations,

$$\frac{\partial}{\partial \xi} \frac{(1-\xi^2)}{\xi} \left(\oint dl \frac{v_{\parallel}}{v} \right) \frac{\partial C_n}{\partial \xi} + \lambda_n J C_n = 0, \quad (10)$$

and an expansion of the distribution function in the orthogonal basis, $F^0 = \sum_n F_n C_n(\xi)$. Here the averaged Jacobian is $J \equiv v^2 \oint dl (v \xi B/B_0 v_{\parallel})$ for the guiding center variables γ, v , and ξ .

In toroidal geometry, the bounce averages needed for the pitch-angle eigenfunction equation may be calculated based on an axisymmetric equilibrium. Figure 3 shows eigenfunctions satisfying Eq. (10) for sinusoidal B wells of the form, $B = B_0(1 + \epsilon)/(1 + \epsilon \cos(2\pi l/l_0))$ with $\epsilon = 0.2$. The solution of Eq. (10) has been discussed in previous work.^{2,13} Inserting the expansion for F^0 into Eq. (8) and integrating over pitch angle yields the following system of algebraic equations for the passing particles:

FIG. 3. Eigenfunctions for sinusoidal B wells of the form $B = B_0(1 + \epsilon)/(1 + \epsilon \cos(2\pi l/l_0))$ with $\epsilon = 0.20$ and the trapped/passing boundary at $\xi = \pm 0.58$.

$$\left(\mathbf{I} \frac{\partial}{\partial t} + \mathbf{L} \right) \mathbf{F} + \mathbf{A} v \frac{\partial \mathbf{F}}{\partial L} = \mathbf{g}, \quad (11)$$

where $\mathbf{F}$ is a vector of the coefficients F_n , $\partial/\partial L \equiv \hat{\mathbf{b}} \cdot \nabla_L$, and $\mathbf{g}$ is the projection of the drives onto the pitch-angle basis. In general $\mathbf{g}$ contains moments of F^0 . Note that the diagonal operator $\mathbf{I} \partial/\partial t + \mathbf{L}$, which looks like $\partial/\partial t + \lambda_n(v_{\perp}(v)/2)$ in the n th equation, retains speed dependence in the collision term. The free-streaming operator, $\mathbf{A}$, couples the odd and even coefficient equations making the inversion of the operator on the left-hand side of Eq. (11) nontrivial.

For the purpose of this paper, we solve Eq. (11) by ignoring the $\partial/\partial t$ on the diagonal. This solution addresses low frequency physics which is appropriate when deriving closures that are the result of slow, resistive phenomena such as tearing modes. In such cases, the emphasis is on accurately assessing the effect of slowly changing magnetic geometry. Inverting the collision and free-streaming operators, $(\mathbf{L} + \mathbf{A} v \partial/\partial L)$, is accomplished by expanding $\mathbf{F}$ as a linear sum of the eigenvectors of the matrix $\mathbf{A}$, $\mathbf{F} = \mathbf{W} \mathbf{h}$, where $\mathbf{A}$ has the elements, $\mathbf{A}_{n,m} = A_{n,m}/\lambda_n$ for $m = 1$ to N . The resulting ordinary differential equations for the coefficients, h_i , are

$$\frac{\partial h_i}{\partial L} + \frac{v_{\perp}}{2v\gamma_i} h_i = \frac{g_i}{v\gamma_i}, \quad (12)$$

where g_i are the elements of $\mathbf{W}^{-1} \mathbf{g}$ and the γ_i 's are the eigenvalues of the matrix $\mathbf{A}$. The bounded solutions are

$$h_i = \int^L dL' \frac{g_i}{v\gamma_i} e^{-\mathbf{k}_i(L-L')}, \quad (13)$$

where the effective inverse collision lengths, $\mathbf{k}_i \equiv v_{\perp}/2v\gamma_i$. At this point, we define the parallel heat flow closure moment as

$$\mathbf{q}_{\parallel} \equiv -T^0 \int \langle d^3v \rangle L_1^{3/2} v C_1(\xi) F^0, \quad (14)$$

where the parallel velocity weighting, $v C_1(\xi)$, which replaces $v_{\parallel}$, is consistent with the expansion of F^0 in the pitch-

angle basis. As a specific example of a spatially nonlocal form for $q_{\parallel}$, we ignore all but the temperature gradient drive in Eq. (8) and restate the result that appeared in Ref. 2:

$$q_{\parallel}(L') = \frac{n^e q v_{th}}{\pi^{3/2}} \int_{L'}^{\infty} dL [T(-L) - T(+L)] K(L', L), \quad (15)$$

where the kernel $K(L', L)$ is given as

$$K(L', L) = \frac{1}{v_{th}^3} \int \langle d^3 v \rangle (L_1^{(3/2)})^2 e^{-v^2/v_{th}^2} C_1^2(\xi) \times \sum_{i=1}^{N/2} a_i e^{-|\mathbf{k}_i|(L-L')}. \quad (16)$$

Here $a_i = |W_{1i} \mathbf{g}_i \mathbf{k}_i / \gamma_i|$ and $K(L', L)$ contains the collisional and trapping information of a distribution of electrons as they scatter in pitch angle off a background Maxwellian plasma. The similarities between this generalized $q_{\parallel}$ and previous collisionless expressions^{5,7,8} were emphasized in Ref. 1. It was also shown there that Eq. (15) reduces to the familiar form, $q_{\parallel} = -\kappa_{\parallel} \nabla_{\parallel} T$, in the collisional limit.⁴ It is important to note, however, that here the parallel conductivity, $\kappa_{\parallel}$, is reduced by particle trapping and collisions near the trapped/passing boundary. Furthermore, the nearly collisionless limit of Eq. (15) contains important corrections due to particle trapping that were absent in previous collisionless expressions for the parallel heat flow. These results are summarized in Fig. 4 where the heat flow is plotted versus the ratio of collision length, $L_{\nu} \equiv v_{th}/\nu_0$, to gradient scale length, L_T , for sinusoidal temperature perturbations. The application of this nonlocal parallel heat flow closure is discussed in the following sections.

Although we have focused on deriving a spatially nonlocal form for $q_{\parallel}$, we will comment briefly on the derivation of an integral expression for $\Pi_{\parallel}$ in axisymmetric geometry. This requires adding a momentum conserving term, $\langle v_{\parallel} N_{\parallel} f_M^0 \rangle$, to the collision operator in Eq. (9), as was done in Ref. 3. This term represents the distortion of the background due to collisions with test particles and is responsible for restoring momentum to the Maxwellian species. In axisymmetric geometry, the bounce average eliminates the free streaming terms in Eq. (11) leaving the leading diagonal operator only, $\mathbf{I} \partial / \partial t + \mathbf{L}$. In this case the coefficients, F_n , satisfy

$$F_n = b_n e^{-\lambda_n v_{\perp}(v)/t/2} + \int_0^t dt' g_n e^{-\lambda_n v_{\perp}(v)(t-t')/2}. \quad (17)$$

Taking the viscous stress tensor moment and enforcing the requirement that the flow moment of F^0 must vanish couples $\Pi_{\parallel}$ to the momentum restoring term in the collision operator. The form of the closure is a set of coupled Volterra equations, an expression for $\Pi_{\parallel}$ that is nonlocal in time. An analogous form for $\Pi_{\parallel}$ that is nonlocal in space has been the subject of previous research³ which may be adapted to this case of a time-dependent viscous stress closure in axisymmetric, toroidal geometry.

FIG. 4. Heat flow response to sinusoidal temperature perturbations of the form $T(L) = T^{eq} + \tilde{T} \sin(2\pi L/L_T)$ for sinusoidal B wells of the form $B = B_0(1 + \epsilon)/(1 + \epsilon \cos(2\pi l/l_0))$ with $\epsilon = 0.0, 0.20$, and 0.40 . The flow is reduced by trapped particle effects in both the collisional and nearly collisionless regimes.

IV. NUMERICAL IMPLEMENTATION OF NONLOCAL CLOSURES

As an example of the numerical implementation of nonlocal closures, we consider incorporating the parallel heat flow closure in Eq. (15) in plasma fluid studies using the NIMROD code.¹² Two major issues arise in such an implementation. The first involves the formal calculation of the nonlocal closure throughout the domain. This requires a massively parallel computational approach. The second deals with the implementation of the temperature evolution equation with the large $q_{\parallel}$ closure appearing explicitly on the right-hand side.

The first step in calculating $q_{\parallel}$ entails solving for the kernel, $K(L, L')$, that appears in Eq. (15) so that it may be interpolated in L when integrating along magnetic field lines. The eigenfunctions, $C_n(\xi)$, are calculated based on the equilibrium toroidal magnetic geometry. It is important to note that the shape and depth of the magnetic wells depend on the equilibrium flux surface. For this reason, NIMROD uses multiple processors to generate pitch-angle bases at different radii. Individual processors then solve the system of equations given in Eq. (11) to determine the coefficients, a_i , and effective inverse collision lengths, $\mathbf{k}_i$, needed in Eq. (15). Finally, the processors calculate the kernel, $K(L, L')$, as a function of L and the results are shared and interpolated so that all processors can calculate $q_{\parallel}$ anywhere in the domain.

For toroidal calculations, NIMROD uses two-dimensional finite elements in the poloidal plane and Fourier decomposition in toroidal angle. A representative finite-element grid in the poloidal plane is shown in Fig. 5. For higher-order finite elements, the closure must be calculated at interior and side nodes in addition to the grid vertices. For

FIG. 5. Finite-element grid used by NIMROD for tearing mode calculation shown in Fig. 1. Closures are calculated at grid vertices as well as side and interior nodes for higher-order finite elements.

bi-quadratic, bi-cubic, and bi-quartic finite elements, a single cell has 9, 16, and 25 nodes, respectively. For the 32×32 grid in Fig. 5 with bi-quartic elements, the total number of unique nodes in the poloidal plane is approximately 10^4 . Furthermore, resolving a toroidal spectrum of N modes requires evaluation at 2^N poloidal planes. For modest simulations, this adds a factor of ten bringing the number of closure calculations to $\approx 10^5$. The distance integrated to convergence depends on L_ν and L_T , but ranges from meters to kilometers. Presently, the parallel implementation in NIMROD is capable of calculating $q_\parallel$ for $T \leq 5$ keV and $n \geq 10^{19} \text{ m}^{-3}$ in reasonable wall clock time when using hundreds of processors.

Once $q_\parallel$ has been calculated throughout the computational domain, it is mapped to Gaussian quadrature points for finite-element integrations on the right side of the temperature evolution equation. In high-temperature plasmas, $\nabla \cdot \mathbf{q}_\parallel$ is large and often dominates temperature evolution. Since a purely explicit treatment would be unreasonably stiff, a semi-implicit time advance is used. Recall that the general, nonlocal heat flow closure reduces to the diffusive form, $q_\parallel \sim \nabla_\parallel T$, in the collisional limit. For this reason, we use the relatively easily inverted anisotropic heat diffusion operator on the left-hand side of the time-discretized temperature evolution equation in the following manner:¹²

$$[n\mathbf{I} - \Delta t f(\kappa_\perp \nabla^2 + \nabla \cdot (\kappa_\parallel - \kappa_\perp) \hat{\mathbf{b}} \hat{\mathbf{b}} \cdot \nabla)] \Delta T = \Delta t [\kappa_\perp \nabla^2 T - \nabla \cdot \kappa_\perp \hat{\mathbf{b}} \hat{\mathbf{b}} \cdot \nabla T + \nabla \cdot \mathbf{q}_\parallel]. \quad (18)$$

Here $\kappa_\parallel$ and $\kappa_\perp$ are the parallel and perpendicular diffusive thermal conductivities, respectively. It is possible to show that there exists a minimum value of the centering parameter, f , such that Eq. (18) is numerically stable for any time step, Δt . It is important to note, however, that the semi-implicit implementation introduces errors that are proportional to Δt . In order to demonstrate the numerics of Eq. (18), simulations of heat transport across a magnetic island in slab geometry have been conducted. Figure 6 shows the temperature at one

FIG. 6. Plot shows convergence of temperature evolution in slab magnetic island geometry for time steps $\Delta t = 10$, 1.0, and 0.1 ms. In steady state, the effect of the semi-implicit operator vanishes as shown by the agreement at $t = 30$ ms for $\Delta t = 1.0$ and 0.1 ms.

point in the domain for simulation time steps of $\Delta t = 10$, 1.0, and 0.1 ms. As the time step is reduced, the evolution becomes more accurate. Note also that because the semi-implicit operator acts on the change in T , its effect vanishes in steady-state. This is shown by the agreement in the $\Delta t = 1.0$ and 0.1 ms simulations at $t = 30$ ms. Because we are interested in studying heat flow dynamics in plasmas confined by slowly evolving magnetic fields, the advantage of taking large, stable time steps with the semi-implicit operator outweighs the small errors that are introduced.

V. APPLICATION OF NONLOCAL CLOSURES IN TOKAMAKS

In this section we explore two applications of the nonlocal parallel heat flow closure in DIII-D tokamak geometry using the NIMROD code. The first looks at temperature evolution in the vicinity of helical magnetic islands and estimates the critical island width at which temperature begins to flatten across the island O-point. The second explores the local heat load on the wall that results when the plasma disrupts and chaotic magnetic field lines allow heat to flow rapidly out from the core. The results are compared with those of the diffusive heat flow closure.

The flattening of temperature across magnetic seed islands leads to bootstrap current perturbations which drive island growth in regions of positive magnetic shear. This nonlinear instability, referred to as neoclassical tearing modes (NTMs),^{14–16} is predicted to limit advanced tokamak performance. Previous theoretical models¹⁷ used a diffusive, Braginskii form for the heat flow closure in cylindrical geometry to predict that the critical island width for temperature flattening, $\kappa_\parallel / \kappa_\perp \sim w_d^{-4}$. This result has been confirmed numerically in toroidal NIMROD simulations using the diffusive closure¹⁸ which reveal a scaling, $\kappa_\parallel / \kappa_\perp \sim w_d^{-4.2}$.

FIG. 7. Scaling of temperature, T , versus critical island width, w_d , at which temperature flattens across the island O-point, $T \sim w_d^{-1.5}$, for nonlocal $q_{||}$. The scaling for the diffusive $q_{||}$ is $T \sim w_d^{-1.7}$.

In this work, we apply the parallel heat flow closure in Eq. (15) to predict the scaling of w_d as a function of temperature. The magnetic geometry is the result of the NIMROD simulation used to motivate the orderings in Sec. II (see Fig. 1). The magnetic field is frozen at specific island widths, $w_d = 1.2, 3.2$, and 6.7 cm, and the temperature is evolved to steady state. For simplicity, a uniform plasma density, $n = 10^{20} \text{ m}^{-3}$, is assumed and the temperature characterizing the effective inverse collision lengths in Eq. (15) is increased until the temperature difference across the island

FIG. 8. Plot shows magnetic field line chaos resulting from high-beta disruption simulation of DIII-D discharge 87009 using NIMROD.

O-point at half the island width is reduced by 25%. The result of this exercise is shown in Fig. 7 which predicts the scaling, $T \sim w_d^{-1.5}$. Given that $\kappa_{||} \sim T^{5/2}$, the previous, diffusive NIMROD result yields $T \sim w_d^{-1.7}$. Figure 7 shows fair agreement between the diffusive and generalized heat flow models with the nonlocal $q_{||}$ predicting more robust flattening at smaller island widths. It is important to point out, however, that temperature flattening does not solely determine the onset of NTMs. The polarization current also plays a role, possibly stabilizing NTMs even when there is temperature flattening inside the island.¹⁹ Understanding the role of

FIG. 9. Plot compares the normal heat load on the wall for nonlocal and diffusive $q_{||}$ as a function of distance along the wall and toroidal angle, ϕ . Dotted lines correspond to points A–E shown in the plot of temperature contours. The smooth distribution in toroidal angle and striation in poloidal angle predicted by the nonlocal $q_{||}$ are consistent with experimental observations.

competing stabilizing and destabilizing effects for seed islands will be the subject of future research.

For our second example of heat flow dynamics in tokamaks, we explore the localized wall heat load that results in a NIMROD simulation of DIII-D discharge 87009.²⁰ The Poincaré plot in Fig. 8 shows the magnetic field line chaos that results from an ideal MHD plasma instability. In such discharges, heat flows rapidly along field lines from the core out to the wall. Ideally, the local heat load should be concentrated near the divertor in order to mitigate damage to the wall. Simulations of heat transport have been performed using the diffusive and nonlocal $q_{\parallel}$ closures. In the diffusive case, $\kappa_{\parallel}/\kappa_{\perp}=10^8$ throughout the plasma. Analogously, the temperature used to determine the collision length, L_{ν} , for the nonlocal $q_{\parallel}$ is set to the constant value, $T=500$ eV. Figure 9 compares the normal heat load on wall for the nonlocal and diffusive $q_{\parallel}$ as a function of distance along wall and toroidal angle, ϕ . The dotted lines in the heat flux plots correspond to points A–E shown in the temperature contour plot. Note that although there is rough agreement in the predictions made by the closures on the outboard side of the torus (points B and C), the nonlocal closure predicts that the heat load is roughly constant in the toroidal direction. A possible explanation for this involves the smoothing process in the calculation of the nonlocal $q_{\parallel}$, which integrates temperature perturbations along field lines. Also, the nonlocal $q_{\parallel}$ predicts that the magnitude of the heat load is larger than that of the diffusive case. Finally, it is important to note that both closures predict substantial heat load near the divertor separatrix (points D and E), a desirable result for mitigating wall damage. Future work on this problem requires improving the $q_{\parallel}$ calculations in both cases. Improvements include evolving separate ion and electron temperature equations and adding a continuity equation for plasma density. Also writing $L_{\nu}=L_{\nu}(n,T)$ for the nonlocal $q_{\parallel}$ and $\kappa_{\parallel}=\kappa_{\parallel}(T)$ in the diffusive case would improve the simulations and allow for predictions of the absolute magnitude of the wall heat load. Such improvements will be the subject of further research.

In this work, the derivation and application of nonlocal closures in plasma fluid simulations of nearly collisionless, magnetized plasmas have been discussed. Specifically, the nonlocal form for $q_{\parallel}$ appearing in Eq. (15) was shown to map continuously from the collisional to nearly collisionless regimes and included important corrections due to trapped particle effects. This generalized $q_{\parallel}$ incorporates Landau, collisional and particle-trapping physics in an integral relation that depends nonlocally on temperature perturbations along magnetic field lines. In addition, a massively parallel, semi-implicit implementation of nonlocal closures in the NIMROD code was shown to be numerically feasible. The com-

bination of generalized closure theory and massively parallel numerics permits simulation of parallel particle dynamics on fluid time scales. The application of the nonlocal $q_{\parallel}$ to the problem of temperature flattening inside islands reveals a scaling of temperature versus critical island width for flattening of $T\sim w_d^{-1.5}$. This result predicts more robust flattening at small island widths when compared to the diffusive scaling, $T\sim w_d^{-1.7}$, which assumes a Braginskii-type parallel heat conductivity. Preliminary application of $q_{\parallel}$ to tokamak disruption simulations shows qualitative agreement of wall heat loads with experimental observations, smooth distribution in toroidal angle and striation in the poloidal direction along the wall. Both applications show promise for future quantitative calculations involving nonlocal closures applied to present-day and next-step tokamak fusion experiments.

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