A comment on the iterative approach for computing MHD equilibria with pressure-gradients in chaotic fields, and a proposed regularized approach

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This comment raises questions regarding the iterative approach for approximating MHD equilibria with pressure-gradients across the irregular, chaotic regions of non-integrable magnetic fields suggested by Reiman et al. [1], where a non-zero, parallel pressure-gradient is supported by unspecified forces. This approach, as it stands, allows for arbitrarily large pressure gradients parallel to the magnetic field and violates quasineutrality, $\nabla \cdot \mathbf{j} \neq 0$, and so $\nabla \times \mathbf{B} = \mathbf{j}$ becomes meaningless.

A regularized, alternative algorithm is suggested, which guarantees that the non-ideal forces will be small by including an anisotropic-diffusion equation for the pressure, and places the algorithm on a reliable computational foundation: no assumptions are made regarding the structure of the field, a source-correction term is included to ensure that the solvability conditions required to invert magnetic differential equations are satisfied, and the inversion of singular, linear operators is avoided.

I. MHD EQUILIBRIA WITH CHAOTIC FIELDS

Increasingly it is recognized that a more detailed understanding of MHD equilibria with chaotic fields is required for both stellarators and tokamaks with applied non-axisymmetric fields. Toroidal magnetic fields are analogous to $1\frac{1}{2}$ dimensional Hamiltonian systems [2], so configurations without a continuous symmetry will generally be non-integrable. How does a field without a continuously-nested family of flux-surfaces support a non-trivial pressure?

Chaotic magnetic fields are a mix of invariant, irrational surfaces that are guaranteed to survive small perturbations by virtue of the KAM theorem; chains of magnetic islands; and, where the magnetic islands overlap, "irregular" fieldlines that wander about in a complicated fashion and, under *some* conditions, seemingly diffusively over an irregular, chaotic volume [3]. Interspersed within the chaotic volumes are cantori, which are sets invariant under the field-line flow that remain after the irrational surfaces disintegrate. Because the radial fieldline flux across cantori can be extremely small, they can present effective partial barriers [4] and severely inhibit the "diffusion" of field-lines even within the irregular volumes.

If the ideal equilibrium equation, $\nabla p = \mathbf{j} \times \mathbf{B}$, is employed, then $\mathbf{B} \cdot \nabla p = 0$ and the irregular regions cannot support pressure-gradients. To allow for pressure-gradients across a chaotic region, additional non-ideal forces must be included in order to balance a non-zero, but small, parallel pressure-gradient.

One approach for constructing nearly-ideal equilibria with non-trivial pressure is the relaxation algorithm: the equations of weakly-resistive MHD are integrated in time until a resistive steady-state is obtained [5]. This approach forms the basis of the HINT code [6, 7], M3D & M3D-C1 [8, 9], and NIMROD [10], which recently has been used [11, 12] to construct nearly-ideal equilibria in stellarator geometry.

There is also the iterative approach [13, 14] that, rather than attempting to follow the dynamics on the resistive timescale, seeks to solve for the equilibrium state directly. This is the basis of the PIES code [15]. In the original iterative scheme, the pressure was adjusted during the iterations to satisfy $\mathbf{B} \cdot \nabla p = 0$.

A "modified" iterative method has been suggested by Reiman et al. [1] that is claimed to compute nearly-ideal equilibria with pressure-gradients across chaotic regions, where the parallel pressure gradient is supported by implied, non-ideal forces. This modified iterative approach is the primary topic of this article.

II. ITERATIVE ALGORITHM

Consider the following modified, iterative algorithm [1]

$$\mathbf{j}_\perp = \mathbf{B}_n \times \nabla p / B_n^2 \tag{1}$$

$$\mathbf{B}_n \cdot \nabla \sigma = -\nabla \cdot \mathbf{j}_\perp \tag{2}$$

$$\nabla \times \mathbf{B}_{n+1} = \mathbf{j}, \tag{3}$$

where the subscript n denotes iteration. The first equation is a statement of ideal, perpendicular force-balance. The second equation results from quasineutrality, $\nabla \cdot \mathbf{j} = 0$, by writing $\mathbf{j} = \sigma \mathbf{B} + \mathbf{j}_\perp$.

The first two equations determine $\mathbf{j}$ given $\mathbf{B}$ and ∇p. Ampere's Law is used to determine $\mathbf{B}$ given $\mathbf{j}$, i.e. $\mathbf{B} = (\nabla\times)^{-1}\mathbf{j}$, where $(\nabla\times)^{-1}$ represents the inverse curl operator. If quasineutrality is *not* satisfied, i.e. if Eq.(2) is not, or cannot be, solved accurately, then Ampere's Law becomes nonsense.

The pressure profile is to be provided. It is assumed that the given pressure is consistent with an experimentally measured profile, or perhaps an equilibrium reconstruction calculation. In the iterations Eq.(1-3), the pressure-gradient, ∇p, is taken as a given, smooth function, and *is not changed during the iterations.*

The magnetic field is initialized using a VMEC [16] calculation, which solves $\nabla p = \mathbf{j} \times \mathbf{B}$ under the constraint that the magnetic field has a perfect family of flux-surfaces. The assumption of nested flux-surfaces, however, generally results in $1/x$ and δ-function singular parallel currents at the rational flux-surfaces – see Eq.(5) below – which the assumption-of-continuity and the finite-difference method, as is used in VMEC, cannot accurately resolve. Nevertheless, VMEC is widely recognized

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as providing a good, *global* approximation to ideal force balance.

The VMEC solution satisfies $\mathbf{B}\cdot\nabla p = 0$, and the current is defined by $\mathbf{j} = \nabla\times\mathbf{B}$, so that $\nabla\cdot\mathbf{j} = 0$ by construction. The energy minimization algorithm employed by VMEC ensures that the field satisfies $\nabla p = \mathbf{j}\times\mathbf{B} + \epsilon\mathbf{f}_\perp$, where $\epsilon\mathbf{f}_\perp$ is a small error that may be identified as an unspecified, non-ideal force. If the goal is to construct a field that almost satisfies ideal force balance consistent with a given pressure profile, then the VMEC field will presumably suffice.

The modified, iterative algorithm, Eq.(1-3), relaxes the constraints on the topology of the field: islands will open where the rotational-transform is rational and, where the islands overlap, volumes covered by irregular fieldlines will emerge [17]; elsewhere, irrational flux surfaces may survive intact. It is claimed that this algorithm leads to solutions that satisfy $\nabla p = \mathbf{j}\times\mathbf{B} + \epsilon\mathbf{f}$, where $\epsilon\mathbf{f}$ is a small, non-ideal force that allows for non-zero, parallel pressure-gradients, which in turn allows for finite pressure-gradients to be supported across the irregular, chaotic regions. While this non-ideal force is itself left unspecified, we may understand that the additional force is derived from any number of implied non-ideal effects, a small plasma flow for example.

III. FORCE-BALANCE

Generally we may write

$$\mathbf{j}\times\mathbf{B} = \nabla p + \lambda\mathbf{B} + \mathbf{u}_\perp\times\mathbf{B}, \tag{4}$$

where to qualify as a physically meaningful, nearly-ideal equilibrium it is required to show that $|\lambda|$ and $|\mathbf{u}_\perp|$ are small. The algorithm Eq.(1-3) guarantees that ideal, perpendicular force-balance is exactly satisfied by virtue of Eq.(1), and we see immediately that $\mathbf{u}_\perp = 0$.

However, parallel force-balance is unconstrained: there is no reason to expect that the iterative scheme, Eq.(1-3), will result in a state where $|\lambda|$ is small. Unless there is some equation that constrains parallel force-balance, e.g. adjusting the pressure according to $\mathbf{B}\cdot\nabla p = 0$ as in the original iterative scheme [13–15], or more realistically solving an anisotropic-diffusion equation for the pressure as suggested in Sec.V, then the above algorithm generally leads to the implausible result that the magnetic field can be *arbitrarily chaotic without any impact on the pressure-gradient*. The algorithm Eq.(1-3) does not lead to a magnetic field that is consistent with the given pressure profile and allows for the counter-intuitive result that islands and chaotic regions are as equally capable of supporting pressure-gradients as regions dominantly filled with flux-surfaces.

In order to satisfy parallel force balance, either (i) the pressure must be adapted to the magnetic field, i.e. the parallel-transport problem must be addressed; or (ii) the magnetic field must constrained in order to satisfy $\mathbf{B}\cdot\nabla p \approx 0$. In the algorithm Eq.(1-3) neither of these steps is taken: the algorithm Eq.(1-3) is incomplete.

IV. MAGNETIC DIFFERENTIAL EQUATIONS

Mathematically, the most problematical aspect of the above algorithm is Eq.(2), the magnetic differential equation for the parallel current. This may be recognized, and solved, as a linear equation.

A. a linear equation

In toroidal coordinates, (ψ,θ,ζ), the parallel current may be represented as a sum of Fourier harmonics, $\sigma = \sum \sigma_{m,n}(\psi)\exp(im\theta - in\zeta)$, where $\sigma_{m,n}(\psi)$ may be discretized using finite-differences, finite-elements, or Chebyshev polynomials. By writing an arbitrary, chaotic magnetic field in the general, canonical form $\mathbf{B} = \nabla\times(\psi\nabla\theta - \chi\nabla\zeta)$, where $\chi = \sum\chi_{m,n}(\psi)\exp(im\theta - in\zeta)$, the equation $\mathbf{B}\cdot\nabla\sigma = -\nabla\cdot\mathbf{j}_\perp$ may be transformed, by applications of the double-angle formulae and equating Fourier coefficients, to a matrix equation, $\mathcal{L}\cdot\mathbf{x} = \mathbf{c}$, where the matrix $\mathcal{L}\equiv\mathbf{B}\cdot\nabla$ depends entirely on the magnetic field, the vector $\mathbf{x}$ is the solution $\sigma_{m,n}$, and $\mathbf{c}$ depends entirely on the "source" term, $-\nabla\cdot\mathbf{j}_\perp$.

If the matrix $\mathcal{L}$ were non-singular, then the equation $\mathcal{L}\cdot\mathbf{x} = \mathbf{c}$ could be inverted and the solution for the parallel current would be provided with an error that reliably diminishes as the numerical resolution increases. The solution is arbitrary up to a function that lies in the null-space, $\mathcal{L}\cdot\bar{\mathbf{x}} = 0$.

Some thought should be given to ensure that the most accurate and efficient discretization is employed. If the field magnetic field is integrable, straight-field-line coordinates can be constructed and the magnetic field can be written $\mathbf{B} = \nabla\psi\times\nabla\theta + \iota\!\!\!{}^-(\psi)\nabla\zeta\times\nabla\psi$, where $\iota\!\!\!{}^-$ is the rotational-transform. The directional derivative then becomes $\mathbf{B}\cdot\nabla \equiv \sqrt{g}^{-1}(\partial_\zeta + \iota\!\!\!{}^-\partial_\theta)$. The matrix $\mathcal{L}$ is diagonalized and the linear equation for the parallel current reduces to

$$(m\,\iota\!\!\!{}^- - n)\,\sigma_{m,n} = i(\sqrt{g}\nabla\cdot\mathbf{j}_\perp)_{m,n}. \tag{5}$$

The null-space is easily identified: this equation leaves $\sigma_{0,0}$ undetermined, which must be provided as an integration constant [1]. Unfortunately, straight field-line coordinates, by definition, cannot be constructed in the irregular, chaotic regions.

B. field line integration

Another method that allows the magnetic differential equation to be solved to arbitrary precision is to integrate along a field-line: given σ at any point on a field-line, σ at every point along the field-line may be constructed by field-line integration. If the field-line ergodically traces out a flux-surface, then σ on that surface may be constructed. Reiman et al. [1, 18] claim that, for chaotic fieldlines, this approach will not yield accurate solutions because of the difficulty of following irregular fieldlines due to the exponential increase of small numerical errors.

However, it is easy to follow irregular lines a short distance with arbitrary accuracy: it is only after a sufficiently long distance that the exponential magnification of error will cause problems. Consider the following algorithm for solving for the parallel current by directly integrating Eq.(2). Let an initial guess for σ be given on a Poincaré section. Then, throughout the computational domain, σ could be determined by field-line integration through one toroidal period. If the solvability conditions, see Eq.(6) below, on the magnetic differential equation were satisfied, one could then iterate on σ on the Poincaré section to obtain a single-valued solution for the parallel current. At no point is it needed to follow along the fieldlines a distance greater than one toroidal period, and this may be performed to arbitrary accuracy. For a given magnetic field, the field-line integrations need only be performed once.

The problems with directly solving the magnetic differential equation by field-line integration are *not* due to the fact that the field may or may not be chaotic; the problem is that the magnetic differential equation is singular – in fact, it is densely singular – and excruciating solvability conditions [19] must be satisfied for a single-valued solution to exist.

C. solvability conditions on periodic orbits

The magnetic differential equation, Eq.(2), describes how σ varies along a field-line. If this equation is integrated along a closed magnetic field-line, i.e. a periodic orbit, $\mathcal{C}$, then for the parallel current to be single-valued the perpendicular current must satisfy

$$\oint_{\mathcal{C}} \nabla \cdot \mathbf{j}_\perp dl/B = 0. \tag{6}$$

This solvability condition must be satisfied on every periodic orbit.

For integrable fields, for every rational, $\iota\!\!\!- = n/m$, there is a family of periodic orbits that together comprise a rational flux-surface. In this case, the singularity in $\sigma_{m,n}$ is evident in Eq.(5), where we see that the condition for $\sigma_{m,n}$ to remain finite at $\iota\!\!\!- = n/m$ is that $(\sqrt{g}\nabla \cdot \mathbf{j}_\perp)_{m,n}$ must go to zero at least as fast as $m\iota\!\!\!- - n$.

The rational flux-surfaces are generally destroyed by even an infinitesimal perturbation [20] and are replaced by island chains. The Poincaré-Birkhoff theorem [21] guarantees that, for systems with shear, for every rational, $\iota\!\!\!- = n/m$, two periodic orbits will survive, namely the minimax (stable) and minimum (unstable) orbits. Additional periodic orbits will result from period-doubling bifurcation phenomena. From a practical perspective, where for example a finite set of Fourier harmonics is included in the calculation, the number of singularities in the solution is $\mathcal{O}(MN)$, where M and N are the poloidal and toroidal Fourier resolution. Neither the location of the periodic orbits, i.e. the location of the singularities, nor the null-space of the linear operator can be determined without some painstaking computational effort.

In the original iterative method [13–15], the pressure is adjusted iteratively in order to satisfy $\mathbf{B} \cdot \nabla p = 0$. This ensures that the solvability conditions *are* satisfied, as generally we may expect that, in a neighborhood of the periodic orbits, that islands [22] and irregular, chaotic volumes will be present, and $\mathbf{B} \cdot \nabla p = 0$ ensures that ∇p and $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2$ will be zero.

In the iterations described by Eq.(1-3), however, there is no reduction of the pressure-gradient across the islands and chaotic regions. There is no reason to expect, for an arbitrary $\mathbf{B}$ and ∇p, that the vector $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2$ satisfies the solvability conditions. If $\mathbf{j}_\perp$ does not satisfy the solvability conditions at the periodic orbits, then a single-valued parallel-current that satisfies $\nabla \cdot \mathbf{j} = 0$ *cannot be constructed*, and consequently Ampere's Law cannot be satisfied. The algorithm Eq.(1-3) breaks down.

D. resonance broadening approximation

Reiman et al. approximate the solution for the parallel current by exploiting a similarity between the magnetic differential equation with a chaotic field, and the non-linear equations governing the evolution of turbulent plasmas, such as the collisionless Vlasov equation, and apply the mathematical methods of turbulence theory. Their argument begins by realizing that any magnetic field can be written $\mathbf{B} = \mathbf{B}_0 + \delta\mathbf{B}$, where $\mathbf{B}_0$ is an integrable field and $\delta\mathbf{B}$ is a chaos-inducing perturbation.

There is, however, some ambiguity in this decomposition. To construct the integrable field that is "nearest" to $\mathbf{B}$, it is required to minimize $|\delta\mathbf{B}|^2$ in some sense, and this leads to the theory of quadratic-flux minimizing surfaces [23] and the closely-related ghost-surfaces [24]. Reiman et al. suggest by following along the irregular fieldlines of a chaotic field that straight field-line coordinates for the appropriate, nearby integrable field can be constructed. Reiman et al. [1] state: *"The field lines in the stochastic region are calculated to behave as if the flux surfaces are broken only locally near the outer midplane and are preserved elsewhere."*, which is flagrantly inconsistent with what is known about the break up of invariant surfaces in Hamiltonian dynamical systems. The irregular fieldlines are associated with the unstable manifolds of the unstable periodic orbits, and the unstable manifolds have a fantastically complex structure.

Reiman et al. argue that statistical averaging methods can be used to solve the linear, magnetic differential equation. Their "solution" for the parallel current is

$$\sigma_{m,n} = \frac{(m\iota\!\!\!- - n) i (\sqrt{g}\nabla \cdot \mathbf{j}_\perp)_{m,n}}{(m\iota\!\!\!- - n)^2 + \eta^2}, \tag{7}$$

where η is related to the magnetic field-line diffusion coefficient.

There is a rather simple derivation of Eq.(7) that allows the approximations involved to be identified [25]. For a magnetic field $\mathbf{B} = \mathbf{B}_0 + \delta\mathbf{B}$, the outstanding effect of the perturbation is to introduce a radial derivative so that $\mathbf{B} \cdot \nabla \approx \mathbf{B}_0 \cdot \nabla + \delta B^\psi \partial_\psi$, where the terms $\delta B^\theta / B_0^\theta$ and $\delta B^\zeta / B_0^\zeta$ are ignored. Consider applying this operator once more to the magnetic differential equation, $\mathbf{B} \cdot \nabla f = s$, to obtain

$$(\mathbf{B} \cdot \nabla)(\mathbf{B} \cdot \nabla f) = \mathbf{B} \cdot \nabla s. \tag{8}$$

Realizing that for $\delta\mathbf{B} = 0$ the solution is singular at every rational surface, and so the highest order radial derivative of f will dominate, and by discarding small terms, this may be approximated by

$$(\mathbf{B}_0 \cdot \nabla)(\mathbf{B}_0 \cdot \nabla) f + (\delta B^\psi)^2 \partial^2_{\psi\psi} f = \mathbf{B}_0 \cdot \nabla s, \qquad (9)$$

which, after a suitable averaging operation, is similar to an anisotropic-diffusion equation, and is non-singular. While this is not a rigorous proof, it suggests that the effect of a small radial field is to induce a small diffusion of f across the flux-surfaces of $\mathbf{B}_0$. This is where the choice of $\mathbf{B}_0$ in the decomposition $\mathbf{B} = \mathbf{B}_0 + \delta\mathbf{B}$ is important.

If one, conveniently, replaces the radial diffusion term, $(\delta B^\psi)^2 \partial^2_{\psi\psi} f$, with $\eta^2 f$, where η is a constant, then the usual resonance broadening heuristic, Eq.(7), is obtained. This approximation may be compared to approximating the singular function $1/x$, at $x = 0$, by $x/(x^2+\eta^2)$, where η is some small, non-zero constant. This approximation, $(\delta B^\psi)^2 \partial^2_{\psi\psi} f \approx \eta^2 f$, cannot be derived rigorously, is not quantitatively accurate, and cannot be justified other than an expedient simplification.

In other contexts this approximation may be useful; in this context, perhaps not. Recall that the three steps of the modified iterative algorithm are derived from ideal perpendicular force-balance, quasi-neutrality, and Ampere's law. The resonance broadening approximation violates quasi-neutrality and, therefore, it also violates Ampere's law.

Including a perturbed radial field *appears* to have eliminated the singularity; however, Eq.(8) is no less, and no more, singular than the original magnetic differential equation. The singularities in the $\mathbf{B} \cdot \nabla$ operator are *not* been removed by the introduction of perturbed radial or chaotic fields. The singularities are associated with the existence of periodic orbits, and periodic orbits are guaranteed to survive perturbation, for any system with shear, by the Poincaré -Birkhoff theorem [21]. Magnetic differential equations are *guaranteed to be densely singular*, regardless of the degree of chaos. The resonance broadening theory of Reiman et al. has the fatal flaw of ignoring the resonances.

E. concerns

In addition to the fact that the algorithm suggested by Reiman et al. does not even attempt to satisfy parallel force balance, and so cannot construct equilibria of physical relevance, there are the following concerns:

1. The introduction of chaotic fields does not in itself regularize the magnetic differential equation. This equation is singular because of the existence of periodic orbits, which are guaranteed to be densely scattered in space, even for chaotic fields. If the solvability conditions are not satisfied, then there is no single valued solution for the parallel current.

2. Regardless of the numerical method used to solve for the parallel current, the extent to which quasineutrality is violated is determined by the extent to which the solvability conditions, Eq.(6), on $\mathbf{j}_\perp$ are violated. With $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2$, the greater the pressure gradient across the periodic orbits, the greater that quasineutrality is violated.

3. To obtain Eq.(7) it is assumed that the fieldlines are weakly-diffusing, but the approximation that fieldlines weakly diffuse is only reliable for magnetic fields that are well beyond the stochastic threshold, as indicated by the Chirikov island-overlap criterion [17], for example. It is ridiculous that the algorithm allows the magnetic field to become so chaotic without any reduction of the pressure-gradient.

4. The assumption that the magnetic islands are strongly overlapping and the fieldlines are weakly-diffusing is not necessarily incorrect, but it obviously not general. Because of the "rich diversity" [26] of Hamiltonian chaotic dynamics, no simple assumption is reliable for arbitrarily perturbed fields. One cannot simply choose to consider only the strongly-chaotic fieldlines that seem to diffuse, and ignore the fieldlines that may be periodic orbits, or lie inside magnetic islands; KAM surfaces or cantori; Levy flights, i.e. fieldlines that display large radial excursions; or fieldlines that have long-time correlations due to the "stickiness" of cantori [27]. Given that the singularities are associated with periodic orbits, the periodic orbits should certainly *not* be ignored. The assumption that the fieldlines are weakly-diffusing is not consistent with the numerical approach, where the magnetic field is provided by inverting Ampere's Law, Eq.(3), where no constraints are placed on the structure of the field.

5. Eq.(7) is not an exact solution to the magnetic differential equation. Even if, by chance, the solvability conditions were satisfied, the solution provided by Eq.(7) would still violate quasineutrality.

6. Ampere's Law *cannot* be satisfied if quasineutrality is not satisfied, because $\nabla \times \mathbf{B} = \mathbf{j}$ becomes nonsense if $\nabla \cdot \mathbf{j} \neq 0$.

7. A reliable numerical scheme must quantify the error and show that the error decreases as the numerical resolution increases; but no error estimate on the accuracy of the solution provided by Eq.(7) for the parallel current has been provided. It is implausible, and no supporting evidence has been presented, that the statistical methods of turbulence theory will reliably yield a more accurate solution of the magnetic differential equation than a direct numerical solution, such as the methods suggested in Sec.IV A or Sec.IV B.

V. REGULARIZED ALGORITHM

The "regularized" iterative approach [25] described in this section recognizes that the magnetic differential equation is a linear equation, and that the problems arise because this equation is singular and the solvability conditions on the source, $-\nabla \cdot \mathbf{j}_\perp$, are generally violated. By

explicitly including small, non-ideal effects into the numerical algorithm, the equations are regularized so that the matrix to be inverted has a well defined inverse and a source correction term is explicitly calculated. An equation that constrains parallel force-balance is included.

Given that the parallel transport of pressure is large but not infinite, and that collisions and other non-ideal effects will induce a small perpendicular transport of pressure, it is reasonable to assume that parallel force balance will governed by the anisotropic-diffusion equation,

$$\nabla \cdot \left(\kappa_\parallel \nabla_\parallel p + \kappa_\perp \nabla_\perp p \right) = S, \tag{10}$$

where the parallel derivative is $\nabla_\parallel p \equiv \mathbf{b}\,\mathbf{b} \cdot \nabla p$ and the perpendicular derivative is $\nabla_\perp p \equiv \nabla p - \nabla_\parallel p$. The source, S, which may be a function of position, may be adjusted as desired to drive non-trivial solutions. The parallel diffusion is assumed to strongly dominate the perpendicular diffusion, $\kappa_\parallel >> \kappa_\perp$. A similar suggestion has been made by Schlutt & Hegna [28].

Solving this equation for the pressure, given the field, will ensure that $|\lambda|$ in Eq.(4) is small. The pressure-gradient will be reduced [29] across islands larger than a critical width, $\Delta w \sim \mathcal{O}(\kappa_\perp/\kappa_\parallel)^{1/4}$. In chaotic regions, the pressure will deform and adapt to the invariant structures of the magnetic field, such as the KAM surfaces and cantori [30]. These invariant sets impede the radial transport of the fieldlines and so also impede the radial transport of pressure.

As $\kappa_\perp/\kappa_\parallel$ decreases, the critical island width decreases and the pressure will adapt to structures of the chaotic field with smaller scale length; and the numerical resolution required to resolve the solution increases. In limit $\kappa_\perp/\kappa_\parallel \to 0$, the anisotropic-diffusion equation reduces to $\mathbf{B} \cdot \nabla p = 0$, which is pathological because there is no minimum length scale to chaos: the solution has infinite structure and infinite numerical resolution is required.

As part of earlier work on this topic [30] [31], a fourth-order-accurate discretization of the anisotropic-diffusion equation has been implemented, where Eq.(10) is cast as a sparse matrix and is efficiently solved using iterative Krylov methods without making any assumptions regarding the structure of the field.

The two problems associated with the magnetic differential equation for the parallel current are (i) that the solvability conditions must be satisfied for a single valued solution to exist; and (ii) the numerical problem of inverting a singular operator. These two problems can be addressed simultaneously.

Using the general equation for force-balance given in Eq.(4), the equation for the parallel current becomes

$$\mathbf{B} \cdot \nabla \sigma \;=\; -\nabla \cdot \left(\mathbf{B} \times \nabla p / B^2 \right) - \nabla \cdot \mathbf{u}_\perp. \tag{11}$$

The solvability conditions may be satisfied by suitably choosing $\mathbf{u}_\perp$. We take the approach that provided $\mathbf{u}_\perp$ is *small* and *localized* to regions near the resonances, i.e. where the solvability conditions are violated, then the precise form of $\mathbf{u}_\perp$ is inconsequential: if $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B_n^2$ is inconsistent with quasineutrality, as it generally will be, then there must be some additional, non-ideal force that allows the solvability conditions to be satisfied and thus allows for a finite, single-valued parallel current.

For simplicity, let $\mathbf{u}_\perp = D \nabla_\perp \sigma$, where D is a small constant. The equation for the parallel current becomes the advection-diffusion equation,

$$\mathbf{B} \cdot \nabla \sigma + D \nabla \cdot \nabla_\perp \sigma \;=\; -\nabla \cdot \left(\mathbf{B} \times \nabla p / B^2 \right). \tag{12}$$

The $D \nabla \cdot \nabla_\perp \sigma$ constitutes a "source-correction" term, and the linear operator, $\mathcal{L} \equiv \mathbf{B} \cdot \nabla + D \nabla \cdot \nabla_\perp$, to be inverted is non-singular. By taking $D \to 0$, the source correction term can be made arbitrarily small *except* where the solvability conditions are violated, as in these regions we have $|\nabla_\perp \sigma| \to \infty$ and $|D \nabla_\perp \sigma|$ remains finite even as $D \to 0$. Numerically, the advection-diffusion equation is similar to the anisotropic-diffusion equation. The advection-diffusion equation with a chaotic magnetic field was studied in [32]. The expression for the perpendicular current, which is consistent with quasineutrality *by construction*, is

$$\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2 + D \nabla_\perp \sigma. \tag{13}$$

VI. CONCLUSIONS

The regularized iterative scheme is thus: (i) given $\mathbf{B}$, the anisotropic-diffusion equation, Eq.(10), is solved for the pressure; (ii) given $\mathbf{B}$ and p, the advection-diffusion equation, Eq.(12), is solved for the parallel current; and (iii) the magnetic field is updated by inverting Ampere's law, $\nabla \times \mathbf{B}_{n+1} = \sigma \mathbf{B}_n + \mathbf{j}_\perp$, where $\mathbf{j}_\perp$ is given by Eq.(13).

From a numerical perspective, this algorithm has the advantage that none of the linear operators to be inverted is singular – of course, this is essential for a stable, accurate algorithm! The numerical techniques for solving the anisotropic-diffusion and the advection-diffusion equation have already been developed and could, with moderate effort, be implemented into the PIES algorithm.

The construction of the source correction term recognizes that some additional perpendicular force must drive an additional perpendicular current, $\mathbf{u}_\perp$, if the pressure-gradient is not zero across the resonances. This is to ensure that the solvability conditions are satisfied. To obtain a closed system of equations, it was assumed that $\mathbf{u}_\perp$ is related to the parallel current, $\mathbf{u}_\perp = D \nabla_\perp \sigma$. This choice is somewhat arbitrary, and it would be interesting to investigate whether $\mathbf{u}_\perp$ could be related to the parallel current using more precise physical arguments.

The magnitude of $\kappa_\perp/\kappa_\parallel$ determines the magnitude of the non-ideal parallel force, which determines the extent to which the chaotic volumes can support pressure-gradients. As $\kappa_\perp/\kappa_\parallel \to 0$, the pressure-gradient goes to zero across the islands and chaotic volumes, and in this case $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2$ automatically satisfies the solvability conditions and so the perpendicular current source-correction term is not required. However, to ensure that the pressure is differentiable and to avoid the pathologies associated with densely singular magnetic differential equations, e.g. $\mathbf{B} \cdot \nabla p = 0$ it is essential that $\kappa_\perp/\kappa_\parallel$ be non-zero.

For small-but-finite $\kappa_\perp/\kappa_\parallel$, small pressure gradients can be supported across the chaotic volumes and the surfaces of constant pressure will deform and adapt to the structure of the cantori. As $\kappa_\perp/\kappa_\parallel$ is increased, the pressure gradient supported across the chaotic volumes and periodic orbits increases and the solvability conditions on the magnetic differential equation for the parallel current will generally be violated to a greater extent, and thus the source correction term becomes more important. The magnitude of the term D ultimately controls the degree of localization of the source-correction term about the resonances.

The regularized algorithm is consistent with the spirit of the approach adopted by Reiman et al., that there will be small, non-ideal forces that balance parallel pressure-gradients and that the precise form of these non-ideal forces is largely inconsequential. Given that the goal is to construct nearly-ideal MHD equilibria with pressure-gradients across arbitrarily chaotic magnetic fields, the regularized algorithm has the following advantages: (i) it guarantees that the non-ideal forces will indeed be small; (ii) it guarantees that the structure of the pressure and the magnetic field are consistent; (iii) it does not make any assumptions regarding the chaotic structure of the magnetic field; and (iv) the singularities in the parallel current are removed and quasineutrality is satisfied.

Whether or not this regularized iterative algorithm has advantates over the relaxation algorithm remains to be determined.

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