Nonlinear Magnetohydrodynamics Simulation Using High-Order Finite Elements*

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A conforming representation composed of two-dimensional finite elements and finite Fourier series is applied to three-dimensional nonlinear non-ideal magnetohydrodynamics using a semi-implicit time-advance. The self-adjoint semi-implicit operator and variational approach to spatial discretization are synergistic and enable simulation in the extremely stiff conditions found in high temperature plasmas without sacrificing the geometric flexibility needed for modeling laboratory experiments. Growth rates for resistive tearing modes with experimentally relevant Lundquist number are computed accurately with moderate resolution when the finite elements have basis functions of polynomial degree (p) two or larger. Time-steps that are large with respect to the global Alfvén time do not hinder accuracy. Error in the magnetic divergence constraint is controlled by error diffusion, which is found to be effective for $p \geq 2$. Anisotropic thermal conduction at realistic ratios of parallel to perpendicular conductivity ($\chi_\parallel/\chi_\perp$) is computed accurately with $p \geq 3$ without mesh alignment. A simulation of tearing-mode evolution in toroidal geometry and shaped tokamak equilibrium demonstrates the effectiveness of the algorithm in nonlinear conditions, and its results are used to verify the accuracy of the numerical anisotropic thermal conduction in three-dimensional magnetic topologies.

KEYWORDS: magnetohydrodynamic simulation, finite element, semi-implicit, anisotropic diffusion

CLASSIFICATIONS: 65M60, 76W05, 76X05
1. INTRODUCTION

High temperature magnetized plasmas are characterized by extremely anisotropic properties relative to the direction of the magnetic field. Perpendicular motions of charged particles are constrained by the Lorentz force, while relatively unrestrained parallel motions lead to rapid transport along magnetic field lines. The orientation and distribution of fluid-like motions of the electrically conducting plasma then determine the degree of restoring force arising from the bending and compression of magnetic flux tubes. When collective motions are able to avoid these restoring forces while releasing available free energy, magnetohydrodynamic (MHD) instability results. As an unstable perturbation grows to finite amplitude, it may induce a nonlinear evolution of the system that includes significant (and sometimes catastrophic) changes in thermal energy and particle confinement. The behavior is often complex, so that analysis must rely on simulation, but the large anisotropies relative to the distorted magnetic field present challenging conditions for numerical methods. For example, numerical truncation errors associated with large parallel thermal conduction produce artificial heat flux in the perpendicular direction, leading to qualitative errors in the simulated energy confinement.

The anisotropies also lead to a wide range of time-scales for different physical effects. For typical conditions in magnetically confined plasmas, parallel thermal conduction is the fastest process in the system. Alfvén-wave propagation occurs on a longer time-scale, followed by sound-wave propagation. Perpendicular thermal conduction and particle diffusion occur on longer time-scales, and global magnetic field diffusion (from nonzero resistivity) is the slowest process. Topology-changing magnetic reconnection occurs on a hybrid time-scale between Alfvénic propagation and global resistive diffusion, so numerical simulation of this behavior must deal with extreme stiffness resulting from relatively fast wave propagation and parallel
thermal conduction. The associated subsonic flows are then nearly incompressible; however, magnetic geometry may preclude exact incompressibility. Simulating the behavior of the system is therefore related to various aspects of the numerical simulation of electromagnetics, incompressible fluid dynamics, convective heat transfer, and linear ideal MHD.

Numerical resolution of magnetohydrodynamic anisotropy leading to singular behavior in ideal conditions has been achieved in linear computations by using specialized low-order discretization methods. These methods rely on using covariant and contravariant components of magnetic-flux coordinate systems as the unknowns, alignment of the numerical mesh with the equilibrium magnetic field, and different finite element basis functions in the parallel and perpendicular directions [1, 2]. For nonlinear simulation, this approach is less compelling. Nonlinear evolution often forms regions with distinct magnetic topology, such as helical islands or regions of magnetic stochasticity embedded in nested flux surfaces. Either occurrence would present formidable challenges for 1) an adaptive meshing algorithm to preserve alignment with the complicated magnetic field and 2) an arrangement of particular basis functions to match the adaptive mesh. Furthermore, a basis function expansion tailored to a particular set of equations may not be suitable for other physical models. For example, discontinuous finite element representations of velocity field components cannot be applied to a system with viscous dissipation without resorting to non-conforming or more complicated mixed approximations. Since closure relations for fluid models remains an active area of research in plasma theory, a specialized discretization will have limited usefulness for a simulation code that is intended to have flexibility in the equations that it solves.

An alternative is to use a numerical representation that has a high rate of spatial convergence. While a number of high-order approximations are possible for simple configurations, the ability
to represent a realistic geometry is important for analyzing laboratory data. High-order finite
difference methods therefore have limited applicability, and the nonlinear character of high-order
finite volume methods [3] (designed for accuracy with discontinuous solutions) is not suited for
conditions where stiff linear behavior and resolution of narrow dissipation layers is important.
The finite element method provides a better approach for nonlinear fusion MHD, where
dissipation terms ensure smoothness with sufficient resolution. The convergence rate realized by
the finite element method is then controlled by the degree (p) of the polynomial basis functions,
relatively independent of geometry and mesh spacing irregularities. In addition, a general finite
element implementation can achieve convergence by increasing p with a fixed mesh [4], which
constitutes a spectral method.

Applying the finite element method to time-dependent systems leads to separate variational
problems for each equation in a marching algorithm if the implicit terms are based on self-
adjoint differential operators. Standard analysis can then be used to estimate convergence rates,
provided that the subspace of piecewise polynomials \( S_h \) of degree p is composed of admissible
functions and that the explicit terms, i.e. the ‘data’ for each variational problem, remain
piecewise continuous functions throughout the evolution. As a very brief summary of the theory,
we first know that the finite element solution \( \bar{u} \) to a variational problem is the function in \( S_h \)
with the least ‘strain energy’ error [5], i.e.

\[
a(u - \bar{u}, u - \bar{u}) \leq a(u - \bar{v}, u - \bar{v}) \quad \text{for all } \bar{v} \in S_h,
\]

(1)
where \( u \) is the best solution among all admissible functions. Then, knowing that the finite element solution is a better approximation in terms of the strain energy than the interpolate function, which is also in \( S_h \), we eventually arrive at relations for convergence rates [5],

\[
|u - \bar{u}|_0 \leq K_0 h^{p+1} |u|_{p+1} \quad \text{and} \\
|u - \bar{u}|_1 \leq K_1 h^p |u|_{p+1},
\]

(2)

(3)

where \( h \) characterizes the possibly irregular mesh spacing, \( |u|_s \) is the norm of the \( s \)-th derivative of \( u \), and \( K_0 \) and \( K_1 \) are independent of \( h \). [The estimates (2-3) are for the relevant special case of second-order spatial derivatives.] For a time-advance that solves for different fields sequentially, there is a unique strain energy for each equation, and a set of minimization problems are carried-out at each time-step. Convergence estimates like (2-3) are then meaningful when the solution remains smooth over the entire simulation.

While the finite element representation allows high-order accuracy without restricting geometry, it introduces other challenges. Besides implementation complications, it is well known from incompressible fluid modeling that continuous finite element representations of vector components cannot reproduce a divergence constraint exactly. Furthermore, ensuring convergence to a divergence-free space requires special attention. For plasma modeling, this issue arises with the zero-magnetic-monopole constraint and with nearly divergence-free velocity distributions associated with many unstable MHD modes. A straightforward approach for the magnetic divergence constraint is to add the diffusive term \( \kappa_{\text{div}} \nabla \nabla \cdot B \) to Faraday’s law [6-8].
This leads to a method that is related to divergence cleaning techniques for finite difference and finite volume methods [9] and to penalty function methods for finite elements [10].

Here, we report on the application of the finite element spatial representation to nonlinear non-ideal MHD, and its implementation in the NIMROD code (Non-Ideal Magnetohydrodynamics with Rotation, Open Discussion) [7]. The objective of the NIMROD project [http://nimrodteam.org] is to achieve accurate and flexible modeling of nonlinear electromagnetic activity in computational domains that are realistic for a variety of laboratory plasmas. Unlike most previous efforts for nonlinear modeling of high temperature plasmas [11-14], we have avoided spatial representations that restrict the geometry in the poloidal domain. The present NIMROD implementation has the parameter p selected at run-time, which is more general than either the finite element implementation reported in Ref. [15] or the earlier NIMROD implementation [7], which used linear and bilinear elements only. This feature has proven useful for exploring the performance of different basis functions in actual applications, and our findings confirm that using p>1 is essential for modeling anisotropies and for satisfying the magnetic divergence constraint. We have restricted our attention to periodic configurations with a two-dimensional boundary, so the finite Fourier series representation with pseudospectral computations of nonlinear terms [16] is applied.

The separation of time-scales in high temperature plasmas is manifest mathematically as stiffness in the non-ideal MHD model, and this is an equally important consideration for numerical simulation. The dominant part of the stiffness can be described through the linear properties of the system at any given time, since propagating shocks do not occur on these slow time-scales. The stiffness is so large that explicit methods are impractical; however, the semi-implicit method [17, 18] is well suited for these conditions. The semi-implicit operator described
here is based on the linear ideal MHD energy integral, as recommended in Ref. [13], but the symmetric part of the solution is incorporated into the “equilibrium” coefficients. In addition, the Laplacian operator used for stabilizing nonlinear pressures has a dynamic coefficient that adjusts to the nonsymmetric part of the solution. This approach makes the algorithm suitable for simulations where the fields evolve significantly from their initial equilibrium configuration, while retaining the accuracy reported in Ref. [13]. Furthermore, each advance in the marching algorithm is self-adjoint, and positive eigenvalues can be ensured, meeting the requirements for the variational approach to spatial discretization. In many cases, there is no implicit dependence among Fourier components, so the resulting algebraic systems have sparse matrices. For equations that have implicit coupling in all three directions, the Fourier representation leads to an algebraic system that is dense in the periodic direction. The preconditioned conjugate gradient method is applied to both systems in the NIMROD implementation, but matrix-free computations are used when Fourier components are coupled.

The NIMROD code has been written for parallel computation on distributed-memory computers with communication routines from the Message Passing Interface (MPI) library. Standard mesh decomposition techniques (with point-to-point communication) work well for the finite element representation of the poloidal plane, where overlap of basis functions is local. Coupling in the periodic direction occurs through Fast Fourier Transforms (FFTs) and algebraic operations on a uniform grid over this coordinate. Here, swapping from Fourier-based decomposition to spatially based decomposition (via collective communication) is used to maintain scalability. A similar approach is applied across the poloidal plane during the preconditioning step of the iterative solves. The preconditioner is a line-Jacobi method, which solves independent one-dimensional linear systems defined by matrix elements that couple
unknowns along grid lines across the entire domain. The global communication required at every iteration for this preconditioner is worth the added computational costs, since the matrices for the semi-implicit temporal advance are ill-conditioned at large time-step.

The organization for the remainder of this article is as follows. Section 2 describes the magnetofluid equations solved by NIMROD, and Section 3 presents the discretization techniques that have been applied. In Section 4, we use a resistive linear MHD benchmark to show convergence properties in stiff conditions and to demonstrate performance with respect to the divergence constraint. We also present NIMROD results on a quantitative test of anisotropic thermal conduction. A sample nonlinear simulation that brings together MHD stiffness and anisotropic energy transport is presented in Section 5. In Section 6, we further discuss divergence control in light of the convergence studies and consider possible refinements. Conclusions are given in Section 7. The Appendix describes our implementation of regularity conditions for simply connected (topologically cylindrical) configurations.

2. EQUATIONS

Resistive MHD is the simplest model capable of reproducing global electromagnetic behavior observed in many laboratory and natural plasmas. For long time-scales, where important nonlinear evolution occurs, it is often necessary to include diffusion and conduction terms, since transport processes act on similar time-scales. The non-ideal model considered in this paper is resistive MHD with anisotropic thermal conduction, kinematic viscous dissipation, particle density diffusion, and the numerical diffusion of magnetic divergence error. Separating terms that represent a steady solution (denoted by the “ss” subscript), this non-ideal MHD model is
\[
\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa_{\text{divb}} \nabla \nabla \cdot \mathbf{B} \tag{4a}
\]

\[
\mathbf{E} = -\mathbf{V} \times \mathbf{B} - \mathbf{V}_{ss} \times \mathbf{B} - \mathbf{V} \times \mathbf{B}_{ss} + \eta \mathbf{J} \tag{4b}
\]

\[
\mu_0 \mathbf{J} = \nabla \times \mathbf{B} \tag{4c}
\]

\[
\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{V} + n_{ss} \mathbf{V} + n \mathbf{V}_{ss}) = \nabla \cdot D \nabla n \tag{4d}
\]

\[
(\rho + \rho_{ss}) \left( \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} + \mathbf{V}_{ss} \cdot \nabla \mathbf{V} + \mathbf{V} \cdot \nabla \mathbf{V}_{ss} \right) + \rho \mathbf{V}_{ss} \cdot \nabla \mathbf{V}_{ss} = \mathbf{J} \times \mathbf{B} + \mathbf{J}_{ss} \times \mathbf{B} + \mathbf{J} \times \mathbf{B}_{ss} - \nabla p + \nabla \cdot (\rho + \rho_{ss}) \nabla \mathbf{V} + \nabla \cdot \nu \rho \nabla \mathbf{V}_{ss} \tag{4e}
\]

\[
\frac{n + n_{ss}}{\gamma - 1} \left( \frac{\partial \mathbf{T}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{T} + \mathbf{V}_{ss} \cdot \nabla \mathbf{T} + \mathbf{V} \cdot \nabla \mathbf{T}_{ss} \right) + \frac{n}{\gamma - 1} \mathbf{V}_{ss} \cdot \nabla \mathbf{T}_{ss} = -p \nabla \cdot \mathbf{V} - p_{ss} \nabla \cdot \mathbf{V} - p \nabla \cdot \mathbf{V}_{ss} - \nabla \cdot \mathbf{q} + \mathbf{Q} \tag{4f}
\]

where \( \mathbf{E} \) is the electric field, \( \mathbf{B} \) is the magnetic induction, \( \mathbf{V} \) is the particle flow velocity, \( \mathbf{q} \) is the heat flux vector, \( \mathbf{Q} \) is a heat source density, and \( \gamma \) is the ratio of specific heats. The units are MKS, except that the Boltzmann constant \( (k) \) has been absorbed into temperature. The particle number density \( n \) and mass density \( \rho \) are related through the mass per ion, and total pressure and temperature follow the ideal gas relation, \( p = 2nT \), assuming quasineutrality \( (n_e \equiv n_i = n) \) and rapid thermal equilibration among ions and electrons. Equations (4a-f) represent the modified
Faraday’s law, the resistive MHD Ohm’s law, the low-frequency limit of Ampere’s law, particle conservation, flow velocity evolution, and temperature evolution, respectively. The particle diffusion term is necessary for simulations over transport time-scales, where physical effects beyond MHD influence the number density profile. However, the implementation is phenomenological, because the particle flux should be consistent with the product of the number density and the flow velocity. Finding a better representation of the particle transport is important, but it is beyond the scope of the present effort.

The steady-state terms make the system of equations suitable for nonlinear computations of deviations from a time-independent solution of the same equations. We note that this is conceptually similar to examining linear stability of an equilibrium solution to the momentum equation; however, for nonlinear non-ideal evolution, consistency requires the steady fields to be time-independent solutions of the complete system. For example, the steady state may have nonzero electric field \( (-\nabla \times B_{ss} + \eta \mathbf{J}_{ss} \neq 0) \), but it is assumed to be curl-free and is not computed with the terms in Eq. (4b) that influence the evolution of the perturbed magnetic field through Eq. (4a). Separating steady-state terms in the equations adds complexity to the coding, but it improves numerical accuracy in simulations where the perturbations are small relative to the steady part of the fields [14]. There are also practical benefits for analyzing MHD activity. Fitting equilibrium MHD solutions to data from laboratory measurements is now common experimental practice. Solving the nonlinear evolution of perturbations about a fitted equilibrium provides a powerful analysis tool without the need for complete information regarding the sources that sustain the equilibrium profiles of current, plasma flow, internal energy density, and particle density. Since NIMROD assumes a domain that is symmetric in the
periodic coordinate, only symmetric steady-state fields are considered. The perturbed fields are fully three-dimensional, however.

Thermal transport in Eq. (4f) can be modeled as local anisotropic diffusion with separate coefficients for the parallel and perpendicular directions [19],

\[
q = -n\left[\chi_{\|}\hat{b}\cdot\nabla T + \chi_{\perp}(1 - \hat{b}\cdot\nabla)\right] \cdot \nabla T
\]  

(5)

where \(\hat{b} \equiv B/|B|\) is the local magnetic direction vector—terms for the separated steady-state fields have been suppressed for clarity. In high temperature plasmas, \(\chi_{\|}\) may be many orders of magnitude larger than \(\chi_{\perp}\), which presents numerically challenging conditions when \(\hat{b}\) is not aligned with the mesh. (Models that represent the non-local effects of rapid particle streaming at arbitrary collisionality are being developed [20]; their implementation in NIMROD also benefits from the high-order discretization described here.) The source term \(Q\) in (4f) represents the sum of Ohmic \(\eta J^2\) and viscous \(\nu \nabla \cdot \nabla \nu^T : \nabla \nu\) heating.

The boundary conditions considered here for Eqs. (4a-f) are Dirichlet conditions for the normal component of \(B\), for \(T\), and for all components of \(V\) along the bounding surface. For the tangential component of \(B\) and for \(n\), fluxes are specified as natural boundary conditions via surface integrals in the variational form of the equations. Here, the respective flux densities are \((\hat{n} \times E)\) and \((D\nabla n)\).

The model represented by Eqs. (4a-f) can be extended to include two-fluid effects and neoclassical [21] and other kinetic effects [20, 22] that are important for the dynamics in many high temperature plasmas. The spatial representation described herein provides a basis for the
numerical development of these advanced models, in addition to its utility for the non-ideal MHD model.

3. NUMERICAL METHODS

3.1. Time-Advance

The numerical approach we have used for Eqs. (4a-f) combines the solution efficiency of a semi-implicit time advance with the geometric flexibility and accuracy of a general finite element method for spatial representation. We arrive at our numerical system of equations by first applying temporal discretization to Eqs. (4a-f). The velocity field values are defined at integer time indices, whereas the remaining fields are defined at half-integer time indices. This creates a leap-frog scheme, and a semi-implicit operator is applied in the velocity advance to eliminate time-step restrictions associated with oscillatory behavior. The stabilizing truncation error in this algorithm is dispersive but not dissipative [23], which is an important consideration for simulating conditions where the physical dissipation terms are small.

Our semi-implicit operator consists of two parts, as in Ref. [13]. The first includes terms that stabilize wave propagation about relatively steady toroidally symmetric fields. The second part is a simpler term that stabilizes propagation about the (usually smaller) nonsymmetric part of the solution. The first part is derived from the method of differential approximation [24] by considering the ideal portion of the system, which describes oscillatory behavior and ideal linear MHD instabilities. After removing the dissipative and heating terms, the temperature and continuity equations are equivalent to the adiabatic pressure relation,

$$\frac{\partial p}{\partial t} = -\mathbf{V} \cdot \nabla p - \gamma p \nabla \cdot \mathbf{V}$$.
Thus, the differential approximation technique is applied to the ideal equations for pressure, magnetic field, and flow velocity.

Applying the approach of Ref. [24] for generic wave equations, the differential approximation of an implicit numerical time-advance for the linear ideal MHD equations is

\[
\rho \frac{\partial \mathbf{V}}{\partial t} - \theta \Delta t \left[ \frac{1}{\mu_0} \left( \nabla \times \frac{\partial \mathbf{B}}{\partial t} \right) \times \mathbf{B}_0 + \mathbf{J}_0 \times \frac{\partial \mathbf{B}}{\partial t} - \nabla \frac{\partial p}{\partial t} \right] = \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B}_0 + \mathbf{J}_0 \times \mathbf{B} - \nabla p \quad (6a)
\]

\[
\frac{\partial \mathbf{B}}{\partial t} - \theta \Delta t \nabla \times \left( \frac{\partial \mathbf{V}}{\partial t} \times \mathbf{B}_0 \right) = \nabla \times (\mathbf{V} \times \mathbf{B}_0) \quad (6b)
\]

\[
\frac{\partial p}{\partial t} + \theta \Delta t \left( \frac{\partial \mathbf{V}}{\partial t} \cdot \nabla p_0 + \gamma \mathbf{V} \cdot \frac{\partial \mathbf{V}}{\partial t} \right) = -\left( \mathbf{V} \cdot \nabla p_0 + \gamma \mathbf{V} \cdot \mathbf{V} \right), \quad (6c)
\]

where \( \theta \) is the centering parameter \( (0 \leq \theta \leq 1) \) and \( \mathbf{V}_0 \equiv 0 \) is assumed so that \( \mathbf{B}_0, \mathbf{J}_0, \) and \( p_0 \) satisfy the static force balance equation, \( \mathbf{J}_0 \times \mathbf{B}_0 = \nabla p_0 \). Differentiating Eq. (6a) with respect to time and eliminating \( \mathbf{B} \) and \( p \) produces the wave equation,

\[
\rho \frac{\partial^2 \mathbf{V}}{\partial t^2} - \theta^2 \Delta t^2 L \left( \frac{\partial^2 \mathbf{V}}{\partial t^2} \right) = (1 + 2\theta \Delta t) L(\mathbf{V}) \quad (7)
\]

where \( L \) is the self-adjoint linear ideal MHD force operator,
\[ L(V) = \frac{1}{\mu_0} [\nabla \times (\nabla \times (V \times B_0))] \times B_0 + J_0 \times \nabla \times (V \times B_0) + \nabla (V \cdot \nabla p_0 + \gamma p_0 \nabla \cdot V) \]  

(8)

The wave equation (7) is then equivalent to the system

\[ \rho \frac{\partial V}{\partial t} - \theta^2 \Delta t^2 L(\partial V / \partial t) = \frac{1}{\mu_0} (\nabla \times B) \times B_0 + J_0 \times B - \nabla p + 2 \theta \Delta t L(V) \]  

(9a)

\[ \frac{\partial B}{\partial t} = \nabla \times (V \times B_0) \]  

(9b)

\[ \frac{\partial p}{\partial t} = -(V \cdot \nabla p_0 + \gamma p_0 \nabla \cdot V) . \]  

(9c)

For oscillatory modes, the eigenvalues of \( L \) are negative, so that the \(- \theta^2 \Delta t^2 L(\partial V / \partial t)\) term on the left side of (9a) effectively adds inertia, while the \(2 \theta \Delta t L(V)\) term on the right side introduces dissipation. For growing modes, the eigenvalues of \( L \) are positive, but there is a finite maximum eigenvalue [25].

As discussed in Ref. [24], we may devise a numerical scheme based on the alternative differential approximation, Eqs. (9a-c). First, we use the freedom to drop the \( \Delta t \) terms on the right side of (9a) before discretizing (the equations remain consistent with ideal linear MHD in the limit of small \( \Delta t \)) to avoid numerical dissipation in stable modes. We then stagger \( B \) and \( p \) in time from \( V \) to obtain a leap-frog scheme that is numerically stabilized by the \(- \Delta t^2 L\) operator, which acts on changes in \( V \). (The numerical equations for the advance are provided with spatial
Applying von Neumann stability analysis with homogeneous equilibria shows that the magnitude of the numerical amplification factor for the stable modes of $L$ is unity as long as the $\theta^2$ coefficient (denoted $C_0$, henceforth) is at least $1/4$ [23]. For unstable physical modes, the scheme correctly reproduces growth, but $\Delta t$ must be less than the inverse of the growth rate of the fastest mode to avoid a singularity in the time-derivative terms.

Two modifications of this operator are applied to improve its effectiveness for nonlinear simulations. First, we relax the definition of $L$ to include the symmetric part of the solution, in addition to the steady-state fields, in $B_0$, $J_0$, and $p_0$, so that the operator will remain accurate for finite distortions that may accumulate over a long time-scale. Though the combined fields may not be in static force balance, in practice they usually represent a state that is near equilibrium, and the operator can be symmetrized explicitly in the weak form described below. The second modification is to include an isotropic Laplacian operator to ensure stability as nonsymmetric pressures develop in nonlinear simulations. The coefficient of this term is computed dynamically from the ‘nonlinear pressure’,

$$ p_{nl}(R,Z) = \max_{\phi} \left| \frac{B^2(R,Z,\phi)}{\mu_0} + \varphi(R,Z,\phi) - \frac{B^2_0(R,Z)}{\mu_0} - \varphi_0(R,Z) \right|, $$

which determines the largest variation in the magnetoacoustic wave speed due to toroidal asymmetries. This semi-implicit approach is closely related to the one discussed in Ref. [13], but the dynamically updated coefficients provide an operator that adapts as fields change in time. Updating coefficients with the evolution implies re-computing matrices and partial factorizations used for preconditioning, but this is done on an as-needed basis rather than at every time-step.
The time advance algorithm must address the numerical aspects of advection in addition to wave propagation. For magnetically confined plasmas, we usually encounter flow speeds that are significantly less than wave speeds, so time-step restriction based on the CFL condition [26] is not prohibitive in many conditions of interest. The semi-implicit algorithm can therefore be combined with predictor/corrector steps to stabilize flow without introducing low-order numerical dissipation associated with wave propagation [27]. The choice of predictor/correct advection over upwind methods simplifies the implementation with the finite element representation.

Advancing the semi-implicit leap-frog scheme with predictor/corrector advection requires the solution of algebraic systems for each equation. In addition to the semi-implicit operator, the dissipation terms are computed implicitly, and the spatial discretization described in Section 3.2 leads to mass matrices. Using implicit dissipation is particularly important for thermal conduction, where parallel transport is typically the fastest behavior in the system. Since wave propagation is also much faster than nonlinear tearing behavior, the advance requires solution of ill-conditioned matrices for the velocity and temperature advances. Furthermore, these linear systems must be solved with sufficient numerical precision to accurately reproduce eigenvectors associated with small eigenvalues, since they represent the slow behavior. In the other equations, implicit dissipation terms typically have small coefficients and introduce no computational penalty, since the mass matrices already necessitate solution of algebraic systems.

3.2. Spatial Representation

A discrete spatial representation is achieved through a basis function expansion and a weak form of the marching equations that is equivalent to a collection of variational problems. The
choice of basis functions and the selection of physical fields to expand are central issues for this approach. Using 2D Lagrange-type finite elements enables representation of arbitrarily shaped regions of the poloidal plane, and it automatically provides the continuity needed for a conforming representation. For the remaining direction, which is periodic, the finite Fourier series is an appropriate expansion. Choosing flow velocity, magnetic field, particle number density and temperature as the fields to expand, the discrete solution space \((S_{h,N,p})\) is the product space composed of all functions \(v \in V_{h,N,p}, \ b \in B_{h,N,p}, \ n \in n_{h,N,p}, \) and \(T \in T_{h,N,p}\) satisfying the essential conditions for the system, i.e. the respective Dirichlet boundary conditions discussed in Section 2. The subscripts denote the measure of the poloidal mesh spacing \(h\), the largest Fourier index \((N)\), and the polynomial degree of the finite element basis functions \((p)\). These parameters identify a particular space \(S_{h,N,p}\) from the family of all such spaces. Members of the \(V_{h,N,p}\) and \(B_{h,N,p}\) spaces have the expansion

\[
A_{h,N,p}(R,Z,\varphi) = \sum_{i,v} a_{iv,v} \alpha_{iv,v} + \sum_{i,v,n} \left( a_{ivn} \alpha_{ivn} + a^{*}_{ivn} \alpha^{*}_{ivn} \right),
\]  

(10a)

while members of \(n_{h,N,p}\) and \(T_{h,N,p}\) have the expansion

\[
F_{h,N,p}(R,Z,\varphi) = \sum_{i} f_{i,n=0} \alpha_{i,n=0} + \sum_{i,n} \left( f_{in} \alpha_{in} + f^{*}_{in} \alpha^{*}_{in} \right).
\]  

(10b)

The vector and scalar basis functions in Eqs. (10a-b) are
\[ \alpha_{\text{inv}} = \hat{e}_i (\phi) \psi_i (\xi_1, \xi_2) \exp(in \phi), \quad \text{and} \]
\[ \alpha_{\text{in}} = \psi_i (\xi_1, \xi_2) \exp(in \phi), \]

where \( \psi_i \) is the \( i \)-th 2D polynomial basis function of degree \( p \) in the element coordinates \( \xi_1 \) and \( \xi_2 \). The Fourier components have indices \( n=0,1,\ldots,N \), and the direction vectors have \( \nu=R,Z,\phi \).

The inverse of the transformation \( R(\xi_1, \xi_2), Z(\xi_1, \xi_2) \) within each finite element is implied in Eqs. (10a-b). For many simulations, we use a topologically polar mesh of quadrilateral elements (for example, see Fig. 1a), where the left side of the logically rectangular mesh is mapped to the \((R,Z)\) coordinates of the magnetic axis of the steady-state fields. In cases with relatively uniform mesh spacing, we define the transformation with bicubic splines of \( R \) and \( Z \) in global mesh coordinates that coincide with the local element coordinates within each quadrilateral element, except for an offset that is unique to each element. For bilinear and biquadratic \( \psi_i \) (\( p=1,2 \), respectively), this mapping is superparametric, i.e. the mapping is of higher order than the representation of the solution fields, and a sufficient condition for convergence is not met [5]. However, for simulations with smoothly varying mesh spacing, we find better accuracy than with lower-order mappings for the same mesh. We also expand the steady-state fields with bicubic splines in these cases. The cubic splines are susceptible to overshoot with strong mesh packing, however, because derivatives with respect to the logical coordinates change abruptly. Where strong mesh packing is applied, we use isoparametric mappings for \( R \) and \( Z \), and the steady-state fields are interpolated with polynomials of the same degree in the element coordinates.
The physical coordinates in Eqs. (10a-b) have been expressed in cylindrical coordinates for toroidal and cylindrical geometry. Taking \( R \to x, Z \to y, \phi \to 2\pi z/L_z \) makes the representation suitable for simulating in Cartesian coordinates where boundary conditions at \( z=0 \) and \( z=L_z \) are periodic. Terms involving derivatives with respect to the periodic coordinate and those resulting from cylindrical curvature have been coded to allow computation with either coordinate system. The implementation of regularity conditions for cylindrical configurations (where the domain includes \( R=0 \)) is discussed in the Appendix.

Using test functions from the same space as the solution fields, \( \{ w^j, e^{j+1/2}, q^{j+1/2}, \Theta^{j+1/2} \} \in S_{h,N,p} \), produces a Galerkin approximation that is equivalent to a variational problem for each step in our time-advance. Starting with flow velocity, the predictor and corrector steps find \( \Delta v_{\text{pre}}, \Delta v_{\text{cor}} \to \Delta v \in V_{h,N,p} \) that satisfy

\[
\int dx \left\{ \rho^{i+1/2} w^* \cdot \Delta v + C_0 \Delta t^2 \left[ \frac{1}{\mu_0} \nabla \times (w^* \times B_0) \cdot \nabla \times (\Delta v \times B_0) + \eta_0 \nabla \cdot (\nabla \times w^*) (\nabla \cdot \Delta v) \right] \\
- \frac{C_0 \Delta t^2}{2} \left[ w^* \cdot J_0 \times \nabla \times (\Delta v \times B_0) + \Delta v \cdot J_0 \times \nabla \times (w^* \times B_0) \right] \\
+ \frac{C_0 \Delta t^2}{2} \left[ (\nabla \cdot w^*) \Delta v \cdot \nabla p_0 + (\nabla \cdot \Delta v) w^* \cdot \nabla p_0 \right] \\
+ C_1 \rho_{nl} \Delta t^2 (\\nabla w^*)^T : (\nabla \Delta v) + \Delta t \rho^{i+1/2} \nu (\\nabla w^* )^T : (\nabla \Delta v) \right\} \\
= \int dx \Delta t \left\{ - \rho^{i+1/2} w^* \cdot (\\nabla \cdot \Delta v) + \frac{1}{\mu_0} w^* \left( \nabla \times b^{i+1/2} \right) \times b^{i+1/2} \\
- w^* \cdot \nabla p^{i+1/2} - \rho^{i+1/2} \nu (\\nabla w^* )^T : (\\nabla v) \right\} 
\]
for all \( w \in V_{h,N,p} \). The new flow velocity is then \( v^{j+1} = v^j + \Delta v_{\text{cor}} \). In (12), the terms with steady-state fields are suppressed, and \( p^{j+1/2} \) is treated as a nodal quantity, i.e. coefficients of \( n^{j+1/2} \) and \( T^{j+1/2} \) are multiplied and \( p^{j+1/2} \) is interpolated from the resulting product coefficients.

In addition, the explicit advection uses \( \nabla = v^j \) for the predictor step and \( \nabla = v^j + f \Delta v_{\text{pre}} \) for the corrector step with the centering coefficient \( f \). For particle number density, we have

\[
\int dx \left\{ q^* \Delta n + D\Delta t (\nabla q^*) \cdot (\nabla \Delta n) \right\} = \int dx \Delta t \left\{ (\nabla q^*) \cdot \overline{n} v^{j+1} - D (\nabla q^*) \cdot (\nabla n^{j+1/2}) \right\}
\]

(13)

for all \( q \in n_{h,N,p} \), where \( \overline{n} = n^{j+1/2} \) for the predictor step and \( \overline{n} = n^{j+1/2} + f \Delta n_{\text{pre}} \) for the corrector step. For the temperature advance, we have

\[
\int dx \left\{ \frac{n}{\gamma - 1} \Theta^* \Delta T + \Delta t (\nabla \Theta^*) \cdot n [\chi_{\parallel} \hat{b} + \chi_{\perp} (I - \hat{b})] \cdot \nabla \Delta T \right\}
\]

\[
= \int dx \Delta t \left\{ -\frac{n}{\gamma - 1} \Theta^* v^{j+1} \cdot \nabla T - n T \Theta^* \nabla \cdot v^{j+1}
\right.

\[
- (\nabla \Theta^*) \cdot n [\chi_{\parallel} \hat{b} + \chi_{\perp} (I - \hat{b})] \nabla T^{j+1/2} + \Theta^* Q \right\}
\]

(14)

for all \( \Theta \in T_{h,N,p} \). Finally, for the magnetic advance, we have
\[
\int dx \left\{ c^* \cdot \Delta b + \Delta t \frac{\eta}{\mu_0} (\nabla \times c^*) \cdot (\nabla \times \Delta b) + \Delta t \kappa_{dibb} (\nabla \cdot c^*) (\nabla \cdot \Delta b) \right\}
\]
\[
= \int dx \Delta t \left\{ (\nabla \times c^*) \cdot (v^{j+1} \times b) - \frac{\eta}{\mu_0} (\nabla \times c^*) \cdot \nabla \times b^{j+1/2} - \kappa_{dibb} (\nabla \cdot c^*) (\nabla \cdot b^{j+1/2}) \right\},
\] (15)

for all \( c \in B_{h,N,p} \), where the surface term represents the influence of an applied electric field.

The semi-implicit operator occupies most of the left side of Eq. (12), including the Laplacian term for stabilizing wave propagation in nonsymmetric states arising from nonlinear dynamics. For conditions of interest, \( p_{nl} \ll B_0^2 / \mu_0 + \gamma p_0 \), and accuracy is not sensitive to the value of \( C_1 \) if it is large enough \( (C_1 \geq 1/4) \) for numerical stability. The terms with coefficient \( C_0 \Delta t^2 / 2 \) result from the ideal MHD operator \( L \) defined in Eq. (8), but they are symmetrized explicitly for conditions where the 0-subscript fields are not in equilibrium, as discussed above. This step ensures that the semi-implicit operator has real eigenvalues, since the finite element method then produces a Hermitian matrix by construction. If \( \Delta t \) does not exceed the inverse of the growth rate of the most unstable mode of the ideal MHD system, the resulting matrix is also positive-definite. This condition needs to be satisfied in initial value problems; thus, it may be acceptable to use discrete formulations of \( L \) that would be unacceptable for calculating eigenvalues of ideal MHD. Even a formulation of \( L \) with ‘spectral pollution,’ the unphysical coupling of modes associated with discrete and continuous eigenvalues [1], may be acceptable as long as the complete marching algorithm with magnetic field, density, and temperature as part of the solution space does not reproduce the unphysical mode coupling as results are converged in time-step.
The linear forces on the right side of Eq. (12) are computed from separate nodal fields for \( \mathbf{B} \) and \( p \), which is analogous to a mixed finite element method and unlike the stabilizing corrections to these forces that appear through the semi-implicit operator. To our knowledge, the disparate representation of implicit and explicit terms does not have negative consequences as long as magnetic divergence error is controlled. We note that early versions of the NIMROD algorithm were based on von Neumann analysis of the differencing equivalent to using bilinear finite elements [7, 28]. We found that the numerical dispersion relation for waves in an infinite uniform equilibrium has the shear and compressional branches decoupled to all orders in \( h \) and \( \Delta t \) when velocity and magnetic field are discretized; this could not be achieved for formulations based on currents and potentials. Thus, the impact of the inconsistent representation of implicit and explicit terms is strongly dependent on how the system is formulated. (In contrast, second-order operators in finite difference and finite volume methods are usually constructed from first-order operators, avoiding inconsistency. However, preserving the symmetry of complicated operators like \( \mathbf{L} \) in general geometry is difficult.)

Nonlinear terms and coefficients that depend on \( \varphi \) require products of Fourier series expansions. We apply the pseudospectral method [16], using the Fast Fourier Transform (FFT) to find data on a uniform grid over the periodic coordinate; however, the Fourier representation is padded with zero coefficients at high wavenumber to prevent aliasing from quadratic nonlinearities [29]. Algebraic operations are performed on the periodic grid to construct the needed terms, followed by a transform of the result to obtain its Fourier decomposition. To allow computations involving spatial derivatives of the expanded fields (like \( \nabla T \)), the transforms and pseudospectral computations are performed at the quadrature points for numerical integration. The appearance of \( \varphi \)-dependent coefficients on the left side of the
equations, like the mass density in the flow velocity advance and the magnetic direction vector in the thermal conduction of the temperature advance, leads to matrices that are dense in the Fourier component index. We solve these systems with a matrix-free iterative method, which uses FFTs in a direct computation of the matrix-vector product instead of computing convolutions explicitly. For magnetic fusion plasmas, the nonsymmetric ($n>0$) Fourier components of $\rho$ are small and do not have a significant effect on the flow velocity evolution equation, (4e). An option to drop the associated small terms expedites computation, since it allows solving $N$ independent 2D linear systems for each velocity update instead of solving one coupled 3D linear system.

The symmetries that exist in the weak form of the temporal advance and the caveat that $\Delta t$ is small enough so that all eigenvalues of the left side of Eq. (12) are positive imply equivalence between Eqs. (12-15) and a set of variational problems. Furthermore, the solution space $S_{h,N,p}$ is admissible, because all terms on the left sides of Eqs. (12-15) are integrable and the essential conditions are enforced. The representation is therefore a conforming approximation, and we can identify the left side of each of Eqs. (12-15) as the respective strain energy. We then expect spatial convergence rates that increase with the polynomial degree of the basis function, $p$, according to Eqs. (2-3). However, the terms on the right sides of Eqs. (12-15) are produced during the course of the temporal advance. If a calculation tends to create fields that cannot be resolved smoothly, assumptions used in deriving the convergence-rate relations are violated, and globally high-order discretization is not effective. Adaptive techniques, such as the $hp$ finite-element method [30], may be better suited for these conditions. For high temperature plasma, numerical accuracy requires resolution of the smallest spatial features (tearing layers), so we restrict attention to conditions where all length-scales can be resolved.
The numerical treatment of the magnetic divergence constraint is another central issue for accurate simulation. Re-expressing Eq. (15) as

$$
\int dx \left\{ c^* \cdot b^{j+3/2} + \Delta t \frac{\eta}{\mu_0} (\nabla \times c^*) \cdot (\nabla \times b^{j+3/2}) + \Delta t \kappa_{\text{div}b} (\nabla \cdot c^*) (\nabla \cdot b^{j+3/2}) \right\}
$$

$$
= \Delta t \int dx (\nabla \times c^*) \cdot (v^{j+1} \times b) - \Delta t \int ds \cdot E^* c^*
$$

(16)

for all $c \in B_{h,N,p}$, shows that $\Delta t \kappa_{\text{div}b}$ has the role of a Lagrange multiplier for the constraint

$$
(\nabla \cdot b^{j+3/2})^2 = 0
$$

in the variational problem for $b^{j+3/2}$. If it were necessary to use arbitrarily large values of the product $\Delta t \kappa_{\text{div}b}$, our continuous solution space $B_{h,N,p}$ would not approach a divergence-free representation in the limit of $h \to 0$, because the formulation does not satisfy divergence-stability (see [31] and references therein). As described below in Section 6, the lack of divergence-stability in this case results from imposing too many constraints through the numerical calculation of $\left( \nabla \cdot b^{j+3/2} \right)^2$ for the finite number of degrees of freedom in the space $[32]$. Alternatively, if the value of $\Delta t \kappa_{\text{div}b}$ is too small, the constraint is not imposed, and the results may contain magnetic monopoles. In either case, the ‘strain energy’ represented by the left side of Eq. (16) is a poor norm for choosing the best available solution. For time-dependent problems like the ones considered here, arbitrarily large values of $\Delta t \kappa_{\text{div}b}$ are not required, provided that the generation of error per time-step is controlled. Convergence studies presented in Section 4 show that acceptable results are achieved routinely for basis function with $p \geq 2$. The appearance of terms that act like constraints in the strain energy for the flow velocity advance is discussed in Section 6.
Regarding practical considerations, the poloidal mesh is divided into structured blocks of quadrilateral elements and unstructured blocks of triangular elements (see Fig. 1b). This organization facilitates domain decomposition for parallel computation and adds geometric flexibility. At this time, the implementation of triangular elements in NIMROD is incomplete (the $\psi_l$ in triangular elements are restricted to linear basis functions), so the results described below consider computations with quadrilateral elements only.

4. BENCHMARKS AND CONVERGENCE RATES

The performance of a numerical algorithm for magnetic fusion application should be examined in conditions that are sufficiently stiff and anisotropic to represent laboratory plasmas. Since stiffness associated with the rapid propagation of MHD waves arises primarily from linear terms, the linear resistive tearing mode described below is an important benchmark for large time-step performance. The highly localized nature of the eigenfunction also exercises the treatment of magnetic field divergence error and nonuniform meshing. The second test problem, presented in Section 4.2, provides a quantitative benchmark of anisotropic thermal conduction.

4.1 Linear Tearing Mode

The domain for our resistive MHD benchmark is a straight cylinder with periodic ends. For a selected helical perturbation ($\sim e^{im\theta+i2\pi n z/L_z}$, where $m$ and $n$ are fixed integers, and $L_z$ is the cylinder length), there exists a concentric cylindrical surface within the domain where the perturbation has constant phase along the equilibrium magnetic field lines, which lie within the surface. The linear MHD response to the perturbation is a resonance (due to anisotropy) such that flows will be local to this surface. However, resistivity, inertia, and viscosity prevent
singular behavior by smoothing spatial scales that are small relative to global length-scales. We
have chosen cylindrical geometry for the test to allow comparison of numerical results with an
analytic dispersion relation that is valid in the limit of vanishing resistivity. For comparison, we
determine the analytic eigenvalue, the matching parameter $\Delta'$ resulting from singular
perturbation [33, 34], by integrating the Euler-Lagrange equations for the helical perturbation
[35] in the regions outside the tearing layer. In the pressureless limit, the growth rate for
asymptotically small resistivity is then computed from the dispersion relation [34]

$$\gamma = \left(\frac{2\Gamma(5/4)}{\pi \Gamma(3/4)} \Delta'\right)^{4/5} \left[ \frac{m^2}{R^2 q^4} \left( \frac{dq}{dr} \right)^2 \right]^{1/5} \left( \frac{B_z}{\sqrt{\mu_0 \rho}} \right)^{2/5} \left( \frac{\eta}{\mu_0} \right)^{3/5} ,$$

(17)

where $q$ is the ‘safety factor’ or magnetic winding number ($2\pi B_z / L_z B_{z\theta}$ in a periodic cylinder)
using equilibrium values at the resonant surface radius ($r_s$, where $q(r_s)=-m/n$). The equilibrium
we consider is the pressureless paramagnetic pinch [36] with normalized on-axis current density
($\mu_0 a J / B$, where $a$ is the cylinder radius) set to 3. The $q$ profile varies from 1.2 on axis to 0.19
at $r=a$ for an aspect ratio $L_z/2\pi a=5/9$, and resonance for the $m=1$, $n=-1$ perturbation occurs at
$r=0.3859a$ (see Fig. 2). Solving the Euler-Lagrange equations for this equilibrium and resonant
surface yields $\Delta'=6.679$. This value is verified with Fig. 3 of Ref. [37] after changing
normalization (Ref. [37] has $J$ normalized to unity on axis, and $a$ is varied).

The NIMROD computations use the finite element mesh to represent the $r-\theta$ plane of the
cylinder with Fourier representation for the axial direction. The meshes are circular-polar with
grid lines running along constant $\theta$-values with uniform spacing and along constant $r$-values with
nonuniform spacing to allow packing near the resonant surface. An example is the 16x16 mesh of bicubic elements with isoparametric mapping shown in Fig. 1a. The radial mesh spacing as a function of radial cell index is based on the local $q$-value by defining a discrete cumulative distribution,

$$f_i = \sum_{j=1}^{i} 1 + A_p \exp\left\{-\frac{[q(r_j) - q(r_i)]^2}{W_p^2[q(0) - q(a)]^2}\right\} \quad \text{for } i = 1, 2, \ldots N_\xi,$$

where $A_p$ and $W_p$ are dimensionless parameters that control the magnitude and extent of packing, and $r_j$, $j = 1, 2, \ldots N_\xi$ are cell-center locations of a preliminary uniform mesh. Partitioning the cumulative distribution function uniformly then determines the desired mesh locations by linear interpolation of the associated $r_j$-locations. Results for the tearing mode have been computed with $W_p = 0.075$, $5 \leq A_p \leq 12$, and meshes ranging from $8 \times 8$ (with bicubic elements) to $256 \times 256$ (with bilinear elements). The resulting mesh spacing changes too abruptly to avoid overshoot with cubic splines, so the mapping and equilibrium field data are interpolated with the same basis functions used for the solution space. For numerical integration, the tests have been completed with 9 Gaussian quadrature points per element for bilinear elements, 16 for biquadratic, and 25 for bicubic, which is an additional point per direction relative to what is normally used.

The calculations are run as initial value problems, but only linear terms are included in the time-advance, so that the behavior is independent of the perturbation amplitude. The initial flow velocity perturbation is chosen to be smooth and to have nonzero curl to excite the tearing instability, but otherwise, it is arbitrary. The value of kinematic viscosity is chosen to be
sufficiently small as to have no significant effect on the computed growth; through experimentation this condition is found to be \( Pm \equiv \frac{\nu_0/\eta}{10^{-3}} \) for this mode. We fix the mass density and equilibrium magnetic field to set the Alfvén speed \( (v_A \equiv B/\sqrt{\mu_0 \rho}) \) to 1 m/s on axis, so with \( a=1 \) m, the Lundquist number \( (S \equiv \mu_0 a v_A/\eta) \) is numerically equivalent to the inverse of the electrical diffusivity.

The essential features of the mode are 1) adherence to the asymptotic analytic scaling \( S^{-3/5} \) evident in Eq. (17) and 2) near-singular behavior of the eigenfunction in the vicinity of the resonant surface. Figure 3 displays computed growth rates on a logarithmic scale to show the asymptotic behavior at large \( S \)-values. At the smaller \( S \)-values, the tearing layer extends over non-negligible variations in the equilibrium, and the behavior is more diffusive than what is assumed in the asymptotic analytic calculations of Refs. [33, 34]. The NIMROD results for \( S=10^5-10^6 \) have been computed with a \( 32 \times 32 \) mesh of bicubic elements with \( A_p=5 \). At \( S=10^7 \), a \( 48 \times 48 \) mesh of bicubic elements with \( A_p=8 \) resolves the more localized eigenfunction. The computation at \( S=10^8 \) proved challenging for our iterative solution method due to the large condition number of the matrix for advancing velocity with sufficient spatial resolution and adequate time-step. Here, a larger mesh of biquadratic elements proved more effective, and resolution to within 5% of the analytic growth rate is achieved with a \( 144 \times 144 \) mesh with \( A_p=12 \).

Flow velocity components of the eigenfunction for \( S=10^6 \) computed with the \( 32 \times 32 \) mesh of bicubic elements show the localized response associated with the resonant surface (see Fig. 4). Although the growth rate is converged with respect to spatial resolution and at \( \Delta t=100 \tau_\ell \) is accurate to within 2% of the temporally converged value, there are azimuthal variations in the
axial velocity projection evident at the scale of the mesh (Fig. 4c). These variations are reduced when the computation is performed with a larger number of bicubic finite elements. However, a similar computation with a 48×48 mesh of biquadratic elements, i.e. with the same amount of data as the 32×32 bicubic mesh, also performs better in this regard (Fig. 4d), and at $\Delta t=100\tau_t$, there is only 0.3% difference in the computed growth rate with respect to the 32×32 bicubic calculation. The source of the variations in the bicubic calculation is not well understood at present.

Spatial convergence properties with respect to the mode growth rate at $S=10^6$ for biquadratic and bicubic elements are shown in Fig. 5. For each calculation, the numbers of elements in the radial and azimuthal directions are identical, and the mesh-packing parameters $A_p$ and $W_p$ are kept fixed as the number of elements is varied. Clearly, convergence to within 1-2% is quite rapid with $p\geq2$ basis functions. In comparison, the growth rate for a 256×256 bilinear mesh with $A_p=10$ and otherwise similar parameters is in error by more than 25%. Since the matching parameter in the growth rate dispersion relation is the change in the slope of $b_r$ across the resonant surface, one might expect convergence rates equivalent to the polynomial degree of the basis functions ($p$), according to Eq. (3). The results for biquadratic and bicubic elements indicate faster convergence. For example, the behavior of the biquadratic series for 48, 96, and 192 elements per direction is $\gamma(h) - \gamma(0) \sim h^{3.2}$, which is consistent with convergence of order $p+1$. Further spatial resolution for $p=2$ and $p=3$ becomes prohibitive at the chosen time-step, since the velocity-advance matrix becomes extremely ill-conditioned. (The largest eigenvalue of the matrix can be estimated as $\omega_{\text{max}}^2\Delta t^2$, where $\omega_{\text{max}}$ is the largest wave frequency supported by the spatial discretization, and the smallest eigenvalue is approximately unity. For the bicubic
calculation with 64 elements per direction and $\Delta t=100$, the condition number estimate exceeds $10^{11}$. Since $\omega_{\max}$ increases with spatial resolution, achieving accuracy to an increasing number of significant figures becomes difficult.)

Performance with respect to the magnetic divergence constraint is more easily related to finite element analysis. In Fig. 6, we plot the 2-norm of the error vs. $h$ on a log-log scale for the bicubic calculations represented in Fig. 5 and for three bilinear computations. As $h$ is decreased, the convergence rate for each basis approaches the value of $p$, consistent with Eq. (3). In all of these cases, $\Delta t=100$ and $\kappa_{\text{div}}=0.1$, where the value of $\kappa_{\text{div}}$ has been chosen to achieve an acceptable error level for the computation with the coarsest mesh, the $8\times 8$ mesh of bicubic elements.

Since the diffusivity $\kappa_{\text{div}}$ is numerical, a result is not converged unless it is insensitive to the $\kappa_{\text{div}}$-value. Therefore, achieving this independence readily as $h$ is reduced is a desirable property for the algorithm. To determine the sensitivity in the tearing-mode calculations, we have varied $\kappa_{\text{div}}$ in computations with different basis functions. The resulting growth rate and magnetic divergence error for a $128\times 128$ bilinear mesh, a $48\times 48$ biquadratic mesh, and a $32\times 32$ bicubic mesh are plotted in Fig. 7. The broad range of $\kappa_{\text{div}}$-values producing the same growth rate for the biquadratic and bicubic cases provides confidence that the error diffusion approach leads to a good strain energy norm for the magnetic advance when $p\geq 2$. In contrast, the sensitivity of the bilinear result to the $\kappa_{\text{div}}$-value implies proximity between conditions where the error diffusion term is insufficient to control the error and conditions where the term imposes too many constraints. However, we note that while the performance of bilinear elements is poor
in this test, they have been used effectively in simulations with larger levels of physical dissipation.

The temporal convergence rate for the semi-implicit advance is predicted to be second-order accurate, and this is achieved in this test problem. Computed growth rates as a function of $\gamma_0 \Delta t$, where $\gamma_0$ is the converged growth rate, are plotted in Fig. 8, for computations at $S=10^6$ with both forward- and centered-time-differencing of the resistive, viscous, and divergence-error dissipation terms. The cubic fits in Fig. 8 show that the error with centered-differencing is dominated by the quadratic terms over the time-step values used—the linear term in the fit is comparable to the quadratic term at a time-step that is just slightly above the lowest data point. With forward-centering, the linear error term dominates the fit up to $\gamma_0 \Delta t=0.029$, and the behavior over the rest of the computed range is dominated by quadratic error. The transition to quadratic behavior for the forward-centering result occurs where the computed growth rate is still quite accurate, and the coefficient of the quadratic error term is within 20% of that from centered-differencing. Thus, the centering of the dissipation terms has only a small effect on the accuracy in this representative calculation, which results from the physical conditions being nearly dissipation-free. Temporal convergence is then primarily determined by the approach used for the large ideal terms, and the semi-implicit advance is second-order accurate. Forward-differencing of dissipation terms is routinely used in nonlinear NIMROD simulations to provide damping for all wavenumbers that are represented, unlike centered dissipation.

4.2 Anisotropic Thermal Conduction

A meaningful test of anisotropic diffusion requires variation in the direction of anisotropy across a mesh in addition to large diffusivity coefficient ratios. Since the most common result
from numerical truncation error is artificial perpendicular heat flow, we consider a problem that quantitatively measures effective perpendicular diffusivity. The domain is the unit square, \(-0.5 \leq x \leq 0.5, -0.5 \leq y \leq 0.5\), and homogeneous Dirichlet boundary conditions are imposed on \(T\) along the entire boundary. The source \(Q = 2\pi^2 \cos(\pi x)\cos(\pi y)\) is used in the temperature evolution equation to drive the lowest eigenmode of the configuration, and a perpendicular current density is induced by an imposed electric field having the same spatial dependence as the heat source. An extremely large mass density prevents MHD motions, so that diffusive behavior dominates. Analytically, the resulting magnetic field is everywhere tangent to the contours of constant temperature in the solution for isotropic thermal conduction, \(T(x, y) = \chi^{-1} \cos(\pi x)\cos(\pi y)\). Introducing anisotropy, \(\chi \rightarrow \chi_{\perp}\) and \(\chi_{\parallel} \gg \chi_{\perp}\), then leaves the analytical result unaltered. This simple problem provides a revealing test for numerical computation if the mesh is nonuniformly misaligned with the magnetic flux surfaces. A simple rectangular mesh meets this requirement. With \(\chi_{\perp} = 1\), the computed steady state value of \(T^{-1}(0,0)\) is then a measure of the resulting effective \(\chi_{\perp}\) including truncation error. As a guide, errors of order \(10^{-2}\) would normally be considered acceptable for nonlinear simulations.

To study convergence properties, the conduction problem is run to steady state with \(\chi_{\parallel}/\chi_{\perp}\) - ratios of \(10^3, 10^6, \) and \(10^9\) with a range of mesh sizes and basis function \(p\)-values. Numerical integration for the finite elements is performed with the standard number of Gaussian quadrature points for a given basis (4 for \(p=1\), 9 for \(p=2\), etc.). The resulting error in perpendicular diffusivity, \(|T^{-1}(0,0) - 1|\), is plotted in Fig. 9. Clearly, the accuracy and convergence rate improve substantially with \(p\) for this problem where the solution is a smooth function of position.
Convergence rates approach the values predicted by Eq. (2) for \( \chi_{||}/\chi_{\perp} \)-ratios of 10\(^3\) and 10\(^6\).

For \( \chi_{||}/\chi_{\perp} = 10^9 \), the obtained convergence rates are slightly less than the predictions. Nonetheless, we find that elements with \( p \geq 3 \) can meet a sufficient level of accuracy in these extreme but laboratory-plasma-relevant conditions, whereas bilinear elements struggle at \( \chi_{||}/\chi_{\perp} = 10^3 \) and are entirely inadequate at \( \chi_{||}/\chi_{\perp} = 10^6 \). A realistic application including three-dimensional magnetic topology is considered in the following section and confirms the effectiveness of our spatial representation in challenging conditions.

### 5. NONLINEAR TEARING EVOLUTION

As an example of a nonlinear simulation in stiff conditions with large anisotropy, we consider a resistive tearing mode in a toroidal MHD equilibrium with noncircular cross-section, tokamak safety-factor profile, and aspect ratio \( R/a = 3 \) (see Fig. 10). A vanishingly small value of plasma-beta (\( \beta \equiv 2 \mu_0 P/B^2 \)) has been chosen to prevent stabilization of the current-driven mode [38]. In these conditions, the internal energy evolution serves as a measure of confinement properties, but it does not play a role in the MHD activity. The mode, while in its linear stage, is then similar to the cylinder mode described in Section 4.1. The primary distinguishing feature is coupling among poloidal harmonics due to toroidal geometry and the shaped cross-section. Responses that are resonant at surfaces with different rational \( q \)-values are coupled if they have the same toroidal Fourier index, \( n \). Other parameters for the simulation are: \( n_{ss} = 10^{20} \text{ m}^{-3}, \tau_A = 1 \mu s, S = 10^6, P_m = 0.1, \chi_{\perp} = 42 \text{ m}^2 \text{s}^{-1} = 100 \eta/\mu_0, \) and \( \chi_{||} = 4.2 \times 10^7 \text{ m}^2 \text{s}^{-1} \). Here, the Alfvén time is defined as \( \tau_A \equiv q(0)R\sqrt{\mu_0 \rho}/B_{\phi_{\text{vac}}} \), where the denominator is the value of the corresponding
vacuum toroidal magnetic field at the geometric center of the cross section. The numerical particle diffusivity is set to the same value as the perpendicular thermal diffusivity, $D = \chi_\perp$, and for controlling divergence error, $\kappa_{\text{divb}} = 100 \text{ m}^2\text{s}^{-1}$.

Since the tearing mode is the only MHD instability of the equilibrium, we first run a linear computation for the $n=1$ toroidal Fourier harmonic. The resulting eigenmode, plotted in Fig. 11, shows coupling from the dominant $m=2$ poloidal harmonic to the $m=3$ and $m=4$ harmonics, and the computed growth rate is $1.41 \times 10^7 \text{s}^{-1}$. The nonlinear simulation has toroidal resolution $0 \leq n \leq 2$, and the $n=1$ eigenmode from the linear computation is used as the initial condition with its amplitude adjusted to create a small but finite-sized magnetic island. Both computations (linear and nonlinear) use a $32 \times 32$ mesh of biquartic elements ($p=4$) with moderate packing at the $q=2$ and $q=3$ surfaces (see Fig. 10a). The time-step in the linear computation is $\Delta t = 2\tau_A$, and in the nonlinear simulation its value is allowed to increase by a factor of two during the simulation. (Here, the performance of the iterative linear-system solver places a more severe time-step restriction than accuracy considerations.) The boundary conditions described in Section 2 imply that the MHD dynamics reproduce fixed-boundary behavior in this configuration where there is no vacuum region surrounding the conducting plasma.

In the nonlinear simulation, the growth of the mode is immediately slowed from the exponential time-dependence that characterizes linear behavior. This is observed from Fig. 12a through the non-constant slope of magnetic perturbation energy evolution plotted on a semi-log scale. The result is consistent with analytic theory in that the island width (proportional to the fourth root of perturbation energy) is predicted to have linear-in-time growth starting when the helical island chain extends beyond the resistive tearing layer [39]. Here, the linear time-dependence of the island width occurs for $t < 12 \text{ ms}$, as shown in Fig. 12b, and the slope is within
33% of an estimate for the analytical relation \( \frac{dw}{dt} = 1.22 \Delta' \frac{\eta}{\mu_0} [40] \); for convenience, the matching parameter \( \Delta' \) is estimated from the cylindrical dispersion relation, Eq. (17), using a growth rate that has been calculated with the same toroidal equilibrium but with reduced viscosity. Over a time-scale that is long relative to the energy transport time-scale, \( a^2/\chi_{\perp} \), the free energy in the equilibrium current density profile is expended, and a three-dimensional steady state is achieved. The simulation also shows that the coupling of harmonics illustrated in Fig. 11b leads to a secondary magnetic island chain at the \( q=3 \) surface. Thus, the final state shown in Fig. 12c has two sets of helical magnetic surfaces that are embedded in nested toroidal surfaces.

Changes in temperature profile due to the presence of a magnetic island can lead to nonlinear neoclassical effects in tokamaks [41, 42], so accurate modeling of island thermodynamics is also important for tokamak simulation studies. Whether anisotropic heat conduction affects the temperature profile in the presence of the island depends on the balance of diffusion in the parallel and perpendicular directions [43]. The parallel length-scale approaches infinity at the island separatrix and at its magnetic axis, where the winding numbers retain their unperturbed rational-number value. However, flattening of the temperature profile occurs within the island if magnetic reconnection decreases the parallel length-scale enough so that parallel conduction occurs at a rate that is competitive with perpendicular conduction, i.e. \( \chi_{\parallel}/L_{\parallel}^2 \sim \chi_{\perp}/L_{\perp}^2 \). Since the parallel length-scale within the island is inversely proportional to the island width (for island widths that are small in comparison to the length-scale of the equilibrium magnetic shear), and the perpendicular length-scale is proportional to the island width, the critical island width required to affect the temperature is expected to follow \( W_c \sim \left( \frac{\chi_{\parallel}}{\chi_{\perp}} \right)^{1/4} [43] \).
To test whether the NIMROD algorithm reproduces the theoretical dependence, we use the magnetic field configuration from five different times in the nonlinear simulation and run thermal-conduction-only computations with gradually increasing $\chi_\parallel$ in each configuration. Recording the $\chi_\parallel/\chi_\perp$-ratio required to produce an inflection of the temperature profile at the resonant surface as a function of island width then permits comparison. (The alternative of running a series of nonlinear MHD simulations with different $\chi_\parallel/\chi_\perp$-ratios would require far more computation.) The simulation result for the island-width scaling, $w \sim \left(\chi_\parallel/\chi_\perp\right)^{0.24}$, is in good agreement with the analytic scaling of Ref. [43], and even the numerical coefficients are not too different, as illustrated in Fig. 13. The discrepancy reflects the fact that the numerically observed $w$ and $W_c$ are different quantities. The analytic relation has been derived as a scaling argument to distinguish small- and large-island-width behavior by identifying when the parallel and perpendicular diffusion times match. It is not a precise relation for the condition recorded from the simulations, the inflection of the $T$-profile. The analytic relation has also been derived for cylindrical geometry and does not account for any toroidal effects that influence the island geometry. In fact, the simulation results provide empirical evidence supporting the application of the analytic scaling to toroidal configurations.

6. DISCUSSION

Comparing the error diffusion scheme for controlling magnetic field divergence with methods that have been applied in computations of incompressible fluid flow helps explain the numerical properties observed in the cylindrical tearing-mode test of Section 4.1 and in other simulations.
Consider introducing an auxiliary scalar variable in the magnetic field advance to create a *mixed method* [44]. In this approach, the weak form finds \( b^{j+3/2} \) and \( X \) that satisfy

\[
\int dx \left\{ \mathbf{c} \cdot b^{j+3/2} + \Delta t \frac{\eta}{\mu_0} (\nabla \times \mathbf{c}) \cdot (\nabla \times b^{j+3/2}) - (\nabla \cdot \mathbf{c}) X \right\} = \int dx \Delta t (\nabla \times \mathbf{c}) \cdot (\mathbf{v}^{j+1} \times \mathbf{b}) - \Delta t \int ds \mathbf{E} \cdot \mathbf{c} \tag{18a}
\]

\[
\int dx \left\{ \frac{\Xi X}{\lambda} + \Xi \nabla \cdot b^{j+3/2} \right\} = 0 \tag{18b}
\]

for all \( \mathbf{c} \in \mathbf{B}_{h, N, p} \) and for all \( \Xi \in X_{h, N, p'} \), where \( X_{h, N, p'} \) is a discrete space for the additional scalar \( X \). Note that there is no differentiation of the auxiliary scalar, so its representation only needs to be piecewise continuous to satisfy the requirements for a conforming approximation. This method is related to the projection method of Brackbill and Barnes [9], but solving Eqs. (18a-b) simultaneously with a large value of \( \lambda \) prevents the formation of monopoles, whereas projection removes them through a separate step. Numerical analysis of finite elements for steady incompressible fluid applications proves that it is possible to choose a subspace \( X_{h, p'} \) for some continuous representations of \( b^{j+3/2} \) such that the product space of \( \{ \mathbf{B}_{h, N, p}, X_{h, N, p'} \} \) satisfies divergence-stability [31, 45]. Convergence to a divergence-free vector field is then assured even in the limit of \( \lambda \to \infty \), which is comparable to taking the limit \( \Delta t \kappa_{\text{divb}} \to \infty \).

If one were to replace (18b) with the local relation \( X = -\lambda \nabla \cdot b^{j+3/2} \), substituting \( X \) into (18a) recovers Eq. (16) with \( \Delta t \kappa_{\text{divb}} \to \lambda \), but this changes the numerical character of the finite element solution. The space represented by \( \{ (\nabla \cdot b) | b \in \mathbf{B}_{h, N, p} \} \) is not among the \( X_{h, N, p'} \).
spaces that satisfy divergence-stability in combination with continuous representations of $B_{h,N,p}$. It imposes too many constraints [32], and in the worst case, the matrix resulting from
\[ \int d\mathbf{x} \lambda (\nabla \cdot e^*) (\nabla \cdot \mathbf{b}^{1/3}) \] is invertible. Here, large values of $\lambda$ imply that the physical terms in (18a) have no effect on the solution. The penalty method described in Ref. [10] uses this form of the constraint relation, but selective reduced numerical integration, i.e. intentionally inaccurate numerical integration, of the constraint terms ensures that the matrix resulting from
\[ \int d\mathbf{x} \lambda (\nabla \cdot e^*) (\nabla \cdot \mathbf{b}^{1/3}) \] is singular. Moreover, Malkus has shown that in some cases, reduced numerical integration is identical to using a mixed method that satisfies divergence-stability [46].

Without selective reduced integration, poor performance of the error diffusion technique results when the value of $\Delta t \kappa_{\text{div} b}$ is chosen to be too large for a given continuous representation of magnetic field. The increasing range of acceptable $\Delta t \kappa_{\text{div} b}$-values with polynomial degree (p), illustrated by the results shown in Fig. 7a, reflects better separation of the longitudinal and solenoidal parts of the expanded vector field as the number of degrees of freedom in each element are increased. This increasing separation implies that the matrix from
\[ \int d\mathbf{x} \lambda (\nabla \cdot e^*) (\nabla \cdot \mathbf{b}^{1/3}) \] tends to singularity as p is increased and therefore does not dominate the physical terms when $\Delta t \kappa_{\text{div} b}$ is finite. As described in Section 4, we routinely achieve good performance for $p \geq 2$, and choosing $\Delta t \kappa_{\text{div} b} / h^2 \sim O(1)$ or $O(10)$ sufficiently enforces the constraint for most of our applications without the risk of dominating the physical terms. (The 8×8 mesh applied to the high-S cylindrical tearing mode in Section 4.1 is an extreme example).

The preceding discussion has not considered variation in the periodic direction, which is also involved in satisfying the divergence constraint. Since the divergence operator is linear, the
constraint needs to be satisfied separately for each Fourier component. The n=0 component is identical to 2D finite element computations, and the divergence-stability condition applies without modification. For all other Fourier components, the number of additional degrees of freedom due to the third dimension is equivalent to the number of nodes in the representation of $b_\phi$. The number of test functions, and hence the number of constraints, represented in $(\nabla \cdot \mathbf{c}^*)$ increases by the same number, since $c_\phi$ enters the divergence calculation algebraically through $-inc_\phi / R$. Using the same continuous representation for all vector components then implies that the ratio of equations to constraints is closer to unity for each n≠0 calculation relative to the n=0 calculation. Since the optimal constraint ratio is two in 2D computations [32], and the n=0 problem is already over-constrained in the limit $\Delta t \kappa_{d\text{ivb}} \to \infty$, the difficulties are heightened by the nonsymmetric components. However, our experience is that error diffusion with finite $\Delta t \kappa_{d\text{ivb}}$ and $p \geq 2$ is effective regardless of the Fourier index.

The representation of divergence also affects the flow velocity advance. Although the equations we solve are compressible, the anisotropies of the MHD system lead to very different responses between shearing and compression with sensitivity to the magnetic field direction and its variation in space. Flows that should be nearly incompressible may numerically excite compressive responses in an unphysical manner. The numerical operator $\mathbf{L}$ appearing on the left side of Eq. (12) contains the terms

$$C_0 \Delta t^2 \left[ \frac{B_0^2}{\mu_0} (\nabla \cdot \mathbf{w}_\perp^*) (\nabla \cdot \Delta \mathbf{v}_\perp) + \gamma \rho_0 (\nabla \cdot \mathbf{w}^*) (\nabla \cdot \Delta \mathbf{v}) \right], \quad (19)$$
where the first term arises from motion perpendicular to $B_0$. Since the coefficients can be very large compared to others in the equation—the ratio $\Delta t^2 (\gamma \rho_0 + b_0^2 / \mu_0) / \rho_0$ is the square of the distance traveled by the fastest wave in the MHD system in a time-step—it enforces near-incompressibility. However, we know that our basis functions cannot represent arbitrarily small levels of compressibility at finite $h$, so comparing (19) with (15) or (16) indicates the possibility of similar over-constraint issues that arise when computing $b^{i+3/2}$ with a large value of $\Delta t \kappa_{\text{div} b}$. This numerical effect may underlie the azimuthal variations in the bicubic result for the linear tearing mode shown in Fig. 4c, for example. For incompressible fluid computations, pressure is the natural choice for the piecewise continuous scalar field in the mixed method. For non-ideal MHD, however, a high-order representation of $T$ is important for accurate anisotropic thermal conduction, so an appropriate relation between temperature and pressure in a mixed formulation is not apparent. Furthermore, the magnetic field is often more important for enforcing perpendicular incompressibility, and a lower-order representation of magnetic field conflicts with the need to satisfy the magnetic divergence constraint. The results reported in this article indicate that any numerical effects arising from these terms are not too restrictive, but further development—possibly an application of selective integration—may improve performance.

7. CONCLUSIONS

We have described an algorithm that combines a variational spatial representation with a semi-implicit time-advance to achieve flexibility and accuracy for application to non-ideal MHD. The marching algorithm is considered a set of variational problems, and the hyperbolic character of the nonlinear PDE system is brought out in a sequence of complete advances. The temporal and spatial techniques benefit from each other through their symmetry characteristics. The time-
advance stabilizes the propagation of waves at large time-step by introducing an implicit self-
adjoint differential operator, and the finite element approach ensures that the matrices resulting
in the fully discretized system are Hermitian. Conversely, the variational approach to spatial
discretization provides the required accuracy, and the self-adjoint semi-implicit operator allows
us to create a variational form of the velocity-advance equation. A more general Galerkin
approach may be useful for treating either ion or electron flows implicitly, however.

The benchmark cases presented in Section 4 and the nonlinear simulation presented in Section
5 demonstrate the effectiveness of the algorithm. The resistive tearing calculations show that a
modest number of finite elements with $p > 1$, sufficient mesh packing, and a large time-step can
reproduce the subtle force balances associated with MHD anisotropy. For example, even the
computation with a $16 \times 16$ mesh of bicubic elements and $\Delta t = 100 \tau_A$, which is nearly $10^5$ times
greater than the limit for an explicit computation with the same spatial representation, finds a
growth rate that is within 12% of the converged result for $S = 10^6$ and $P_m = 10^{-3}$. The anisotropic
thermal conduction test in simple geometry shows that sufficient accuracy can be achieved to
resolve parallel and perpendicular transport properties in realistic conditions without aligning the
grid to the magnetic field; any additional effort to align the grid will further increase accuracy.
The simulation discussed in Section 5 demonstrates performance with respect to slowly growing
nonlinear MHD activity, and the comparison between numerical and analytic results on the
magnetic island width required for temperature profile modification verifies anisotropic diffusion
accuracy in three-dimensional magnetic topologies.

The geometric flexibility of the algorithm makes it suitable for many applications in magnetic
confinement fusion. The nonlinear tearing evolution illustrates conditions encountered while
using NIMROD to simulate neoclassical tearing modes and high-beta disruptions in tokamaks
[21, 47], where accuracy of anisotropic diffusion is critical. In combination with a temperature-dependent resistivity, the accurate modeling of anisotropic diffusion permits us to address nonlinear free-boundary tokamak computations, where Ohmic heating leads to large electrical conductivity in the region of closed magnetic flux surfaces only [48]. NIMROD is also being used to simulate nonlinear magnetic relaxation in alternate configurations, such as spheromaks [49-51] and reversed-field pinches [48, 52], where separation of time-scales tends to be less extreme than in tokamak plasmas, but the behavior often includes evolution to MHD turbulence. Although numerical issues associated with relaxation simulations have not been discussed in this paper, the flexibility to address many different topics with one code has been a goal since the inception of NIMROD development. Additional geometric flexibility will be achieved with further development of triangular elements. (For simulating experimental configurations without toroidal symmetry, the numerical algorithm can be implemented with finite elements in all three directions.)

Development of the algorithm is proceeding along two general paths. First, we continue to make numerical refinements for the non-ideal MHD model described here. The most important computational issue is the performance of the parallel iterative solver for ill-conditioned matrices resulting from the implicit terms in application to stiff conditions. We also expect to improve the existing predictor/corrector treatment of flow with regard to accuracy and efficiency in extreme (but not shocked) conditions. Using selective integration for improving the accuracy of the semi-implicit operator at large time-step will also be considered. The second path of development concerns expanding the algorithm to solve more realistic models for high temperature plasmas. The NIMROD implementation is designed to have flexibility in the equations that it solves, and the modularity facilitates efforts to improve numerical methods for
more realistic plasma models. Some development has already been completed in the area of two-fluid effects [7], and we are presently working to improve accuracy at the large time-steps needed for nonlinear fusion studies. We are also adding kinetic effects [20-22] that have a strong influence on the MHD-like behavior of nearly collisionless plasmas.

APPENDIX

Several applications require simply connected, topologically cylindrical domains. For these cases, we use the finite element representation for the R-Z plane, and one side of the mesh lies along the Z-axis. Physical fields and their partial derivatives must have unique values at the axis, which leads to a set of regularity conditions for the Fourier components in the limit of $R \to 0$. The conditions are derived with a 2D Taylor series expansion of an arbitrary function of Cartesian $x$ and $y$ coordinates with origin at $R=0$ in a constant-Z plane. Substituting $R(e^{i\varphi} + e^{-i\varphi})/2$ and $R(e^{i\varphi} - e^{-i\varphi})/2i$ for the Cartesian $x$ and $y$, respectively, while leaving the expansion coefficients in terms of Cartesian derivatives, determines the appropriate functional form for each Fourier component in the limit of $R \to 0$. For scalars we have

$$\lim_{R \to 0} F(R, \varphi) = f_0(R^2) + \sum_{n=1}^{N} R^n \left[ f_n(R^2) + f_n^*(R^2) \right]$$  \hspace{1cm} (A.1)$$

for the finite Fourier series, where $f_n$, $n=0,1,..N$ are polynomial functions of their argument. For vectors, we have
\[ \lim_{R \to 0} A(R, \varphi) = RaR_0,\varphi_0 (R^2) + \sum_{n=1}^{N} R^{n-1} \left[ a_{R_n,\varphi_n} (R^2) + a_{R_n,\varphi_n}^* (R^2) \right] \]  

where \( a_{R_n} \) and \( a_{\varphi_n} \) are polynomial functions. The limiting behavior of \( A_z(R,Z) \) is the same as for scalars. The radial and azimuthal expansions must also satisfy

\[ a_{\varphi_1} (0) = i a_{R_1} (0) , \quad (A.3) \]

so that the vector has a unique direction at \( R=0 \).

Since conditions (A.1-A.3) apply in the limit of \( R \to 0 \), discrete representations in \( R \) need only consider the leading behavior for each Fourier component index. Conditions where the polynomial expansion goes to zero at \( R=0 \) are applied as essential conditions on the solution space, like Dirichlet boundary conditions. Satisfying condition (A.3) for \( n=1 \) vector components is more complicated, since the \( R \) and \( \varphi \) components of a vector are computed simultaneously according to the algebraic system resulting from the weak form of the implicit terms in a given equation. Our approach is to first compute the matrix elements for the coefficients of the spatial representation (denoted by \( \hat{a} \)) in the usual manner without considering (A.3). Then for each node located on the \( Z \)-axis, we change to sum and difference coefficients,

\[ \hat{a}_+ = \frac{\hat{a}_{R_1} + i \hat{a}_{\varphi_1}}{2} \]
\[ \hat{a}_- = \frac{\hat{a}_{R_1} - i \hat{a}_{\varphi_1}}{2} , \]
in the algebraic system. If \( \left( \overline{M} \right)_c \) denotes the two columns of the matrix corresponding to the \( a_{R_1} \) and \( a_{\varphi_1} \) elements in the algebraic vector of unknown coefficients, the variable change modifies these columns to

\[
\left( \overline{M} \right)_c \Rightarrow \left( \overline{M} \right)_c \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}.
\]

The number of rows of the linear system is then reduced by taking a linear combination of the two rows \((r)\) corresponding to \( \hat{a}_+ \) and \( \hat{a}_- \),

\[
\left( \overline{M} \right)_r \Rightarrow \begin{pmatrix} 1 \\ -i \end{pmatrix} \left( \overline{M} \right)_r \quad \text{and} \quad (b)_r \Rightarrow \begin{pmatrix} 1 \\ -i \end{pmatrix} (b)_r,
\]

and the regularity condition (A.3) is enforced at the given node by setting an essential condition on the sum coefficient, \( \hat{a}_+ = 0 \). The operations are repeated for each node along the axis, and the resulting matrix retains the Hermitian property of the original.

For the \( n=0 \) component of scalars, the \( n=0 \) \( Z \)-component of vectors, and the \( n=1 \) \( R \)- and \( \varphi \)-components of vectors, the leading behavior of the polynomial expansion in \( R \) is that the slope vanishes in the limit \( R \to 0 \). For each equation in the time advance, this behavior is enforced by the respective strain energy without any modification to the spatial representation or the resulting linear system. For example if the \( n=0 \) Fourier component in the expansion of \( B_z \) has a nonzero radial derivative at small \( R \), computations of the \( n=0 \) part of the local \( J_\varphi \) will be nonzero, leading to resistive diffusion or radial forces that generate flows to reduce the derivative. The weak form
used in the finite element approach avoids singular terms at \( R=0 \) that need special treatment in a finite difference or finite volume scheme, where the conditions are explicitly applied to the differences [29]. As another example of the finite element implementation, consider radial derivatives in the \( n=1 \) \( R \)-component of magnetic field near \( R=0 \). Since the axial \( n=1 \) component is set to 0 on axis, and condition (A.3) is satisfied, the \( n=1 \) part of magnetic divergence reduces to \( \partial b_r / \partial r \), and the error diffusion term in the strain energy for the magnetic advance will tend to eliminate any nonzero derivative. The conditions are realized as natural conditions, although there is no corresponding surface integral.

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FIGURE CAPTIONS

FIG. 1. Finite element meshes illustrating (a) radial packing with piecewise bicubic mapping from a logically rectangular mesh of quadrilateral elements to a topologically polar arrangement of nodes and (b) combining regions of triangular and quadrilateral elements, using linear mappings, to align with equilibrium magnetic flux surfaces in a tokamak interior while matching to a realistic experimental cross-section at the boundary.

FIG. 2. Profiles of equilibrium safety factor or magnetic winding number \( q = 2\pi B_z / L_z B_\theta \) for the cylinder with periodic length \( L_z \) (a) and normalized parallel current density (b) for the tearing-mode benchmark.

FIG. 3. Comparison of a NIMROD-computed growth-rate scaling for the cylindrical tearing mode with the asymptotic analytic dispersion relation, Eq. (17).

FIG. 4. Eigenfunctions for the cylindrical tearing-mode computed with \( \Delta t = 100\tau_A \). Profiles are plotted in the radial coordinate \( \sqrt{\Psi} \) in (a-b), where \( \Psi \) is the normalized poloidal flux function for the equilibrium, and in the azimuthal angle at a fixed radial coordinate just outside the resonance in (c-d). Frames (a-c) show the eigenfunction resulting from a \( 32 \times 32 \) mesh of bicubic elements, whereas (d) shows the result from a \( 48 \times 48 \) mesh of biquadratic elements. Boxes indicate the locations of element-boundary nodes.

FIG. 5. Convergence of the computed cylindrical tearing-mode growth rate with mesh spacing for biquadratic and bicubic finite elements with \( S=10^6 \), and \( \Delta t = 100\tau_A \). The parameter \( h \) is the
inverse of the number of quadrilateral finite elements in each of the radial and azimuthal
directions.

**Fig. 6.** Logarithm of the normalized magnetic divergence error, \( a \sqrt{\int d\mathbf{x} (\nabla \cdot \mathbf{b})^2 / \int d\mathbf{x} b^2} \), in the computed cylindrical tearing-mode eigenfunctions at \( S=10^6 \) and \( \Delta t = 100 \tau_A \), plotted with respect to mesh spacing for bilinear, biquadratic, and bicubic finite elements.

**Fig. 7.** Growth rate (a) and normalized magnetic divergence error (b) in the computed cylindrical tearing-mode eigenfunctions at \( S=10^6 \) and \( \Delta t = 100 \tau_A \), plotted with respect to the error diffusivity parameter, \( \kappa_{divb} \), for \( 128 \times 128 \) bilinear, \( 48 \times 48 \) biquadratic, and \( 32 \times 32 \) bicubic finite element meshes.

**Fig. 8.** Convergence of the computed cylindrical tearing-mode growth rate with time-step for forward- and centered-differencing of the dissipation terms as indicated. The spatial representation is a \( 32 \times 32 \) mesh of bicubic finite elements, and the \( S \)-value is \( 10^6 \). The horizontal axis is normalized with the converged growth rate, \( \gamma_0 \). The cubic polynomial fits \( 6.441 \times 10^{-4} + 1.767 \times 10^{-4} (\gamma_0 \Delta t) - 5.991 \times 10^{-3} (\gamma_0 \Delta t)^2 + 1.126 \times 10^{-2} (\gamma_0 \Delta t)^3 \) and \( 6.442 \times 10^{-4} - 2.578 \times 10^{-5} (\gamma_0 \Delta t) - 5.112 \times 10^{-3} (\gamma_0 \Delta t)^2 + 5.646 \times 10^{-3} (\gamma_0 \Delta t)^3 \), for forward- and centered-differencing, respectively, are also shown.
FIG. 9. Error in the effective perpendicular diffusivity resulting in the anisotropic thermal conduction test for the indicated values of parallel diffusivity. Results are plotted with respect to the (uniform) mesh spacing for bilinear through biquintic finite elements, as labeled.

FIG. 10. Steady-state distributions used in the nonlinear simulation. The safety factor profile \(q = \frac{d\Phi}{d\Psi}\), where \(\Phi\) is the toroidal magnetic flux function, is shown in (a) with boxes indicating element boundary locations in the topologically polar mesh. The distribution of \(\sqrt{\Psi}\) in the poloidal plane is plotted in (b) with the heavy lines indicating the locations of the \(q=2\) and \(q=3\) surfaces.

FIG. 11. Computed eigenfunction of the \(S=10^6\) Pm=0.1 linear tearing mode that is unstable in the equilibrium shown in Fig. 10. The poloidal projection of \(\mathbf{b}\) is shown in (a), and the toroidal component of the perturbed ideal electric field \(\hat{\mathbf{\phi}} \cdot \mathbf{v} \times \mathbf{B}^{ss}\) is shown in (b).

FIG. 12. Simulated nonlinear evolution of the toroidal tearing mode. Magnetic energy for each toroidal Fourier component is shown in (a), where
\[
E_n = \int \left( (\mathbf{B}^{ss} + \mathbf{b}_n)^2 \right) / 2\mu_0 \quad \text{for} \quad n=0
\]
\[
E_n = \int \left( \mathbf{b}_n^* \cdot \mathbf{b}_n / \mu_0 \right) \quad \text{for} \quad n=1,2.
\]
The island-width evolution is shown in (b) with bars indicating the estimated error in measuring the separatrix from Poincaré surfaces of section. The analytic small-island evolution from Refs. [39, 40] with an estimated \(\Delta'\) is also plotted in (b). The Poincaré surface of section for the final magnetic configuration is shown in (c).
FIG. 13. Magnetic island width on the outboard side of the $q=2$ surface that produces an inflection in the temperature profile, plotted vs. the ratio of thermal diffusivity coefficients. The solid line is the power-law fit of the simulation results, $w = 433(\chi_\parallel/\chi_\perp)^{-0.237}$ cm, and the dashed line is the analytic scaling of the critical width $W_c \equiv (\chi_\parallel/\chi_\perp)^{-1/4}(8R_0q/nq')^{1/2}$, where the parallel and perpendicular diffusion times match in cylindrical geometry [43]. The latter is evaluated as an approximate for the toroidal configuration by averaging $q' = dq/dr$ from the inboard and outboard sides of the equilibrium; this yields $W_c = 295(\chi_\parallel/\chi_\perp)^{-1/4}$ cm.
Sovinec, et al. Figure 1
Sovinec, et al.  Figure 2
Sovinec, et al. Figure 3.
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Sovinec, et al. Figure 8
Sovinec, et al.    Figure 9
Sovinec, et al.   Figure 10
Sovinec, et al. Figure 11
Soinec, et al.  Figure 12
Sovinec et al. Figure 13