DOE/ER/54975

Center for Extended Magnetohydrodynamic Modeling (CEMM)
Grant Recipient: Board of Regents University of Wisconsin System

Final Scientific Report
February 15, 2008 – February 14, 2018

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May 15, 2018

THE U.S. DEPARTMENT OF ENERGY
OFFICE OF FUSION ENERGY SCIENCES
AWARD NO. DE-FC02-08ER54975

1. Public Abstract

The Center for Extended Magnetohydrodynamic Modeling (CEMM) focused on the further development, verification, validation, and application of two scientific computation programs, the NIMROD and M3D-C1 codes, for modeling macroscopic dynamics in magnetized plasma. Both NIMROD and M3D-C1 solve the mathematical equations that model two-fluid 3D magnetohydrodynamic (MHD). They are designed and optimized to be efficient and accurate for toroidal confinement physics calculations. The effort improved the fidelity of the physics models, the realism of the treatment of the surrounding vessel, coils, and other structures, the accuracy and efficiency of the algorithms, and the ability to scale calculations to thousands of processors in order to take advantage of leading-edge computers. The primary application areas of Resonant Magnetic Perturbations (RMP), Edge Harmonic Oscillations (EHO), Edge Localized Modes (ELMs), Disruption Studies, Sawteeth and Stationary States, and Kinetic MHD and Neoclassical Tearing Modes (NTM) are of concern for the international ITER experiment, which is under construction in France.

The effort by the UW-Madison Engineering Physics component of CEMM improved the numerical methods in the NIMROD code with respect to modeling MHD interchange and two-fluid effects. It also improved the algorithm for solving large algebraic systems to enhance NIMROD's computational performance when running the code in parallel on increasing numbers of processor cores. The modeling efforts included a study of the nonlinear evolution of ballooning, and the findings were supported by analytical theory and computation. Numerical MHD modeling also examined the influences of two-fluid effects on ELMs and RMPs, where "two-fluid" refers to separation of electron dynamics from ion dynamics. Another related aspect considered the effects of a localized layer of electrical current density near the edge of the plasma confinement region. Two-fluid effects on resonant reconnecting instabilities were verified and applied to computations of sawtooth and drift-tearing dynamics.

2. Project Summary

2.0. Introduction

The overarching objectives for the UW-Madison Engineering Physics component of CEMM were to improve the accuracy and efficiency of the NIMROD simulation code [1] and to apply it to important questions of macroscopic stability in tokamak experiments. The code had previously been applied to problems of linear and nonlinear macroscopic plasma dynamics in reversed-field pinches, spheromaks, field-reversed configurations, the earth's magnetosphere, and in basic plasma experiments, in addition to tearing, internal kink, ELMs, and high-beta disruption in tokamaks. The further development, testing, and application supported by the FC02-08ER54975 CEMM grant extended the code's capabilities to obtain new physics results. Improvements to the computational methods in the NIMROD code made it more robust and efficient when applied to tokamak macroscopic dynamics. The modeling applications addressed questions on the linear and nonlinear evolution of edge modes in tokamaks and on dynamics that involve magnetic reconnection. These contributions are summarized in the following subsections. As an aside, there was an educational component of the project in that it helped support Eric Howell, Jacob King, Zz Riford, Kyle Bunkers, and Brian Cornille during parts of their graduate careers at UW-Madison. Also, Prof. Ping Zhu was partly supported as a scientist/Co-Investigator.

2.1. Improve NIMROD's spatial representation of MHD dynamics

The NIMROD spatial representation uses spectral-element/Fourier basis functions in a C0 expansion for all fields. While it allows high-order accuracy for the anisotropies of evolving macroscopic dynamics [1], it exhibited convergence on MHD interchange from the unstable side, meaning that unresolved modes grow too fast, and numerical interchange can be unstable in physically stable conditions. Many approaches to changing this numerical behavior were investigated as part of the CEMM project. Each of those that were based on existing methods in computational MHD and fluid dynamics had at least one significant shortcoming. In the end, a novel approach that combined ideas from penalty methods for MHD eigenvalue solvers [2] and from spectral-element stabilization schemes [3] was developed and found to be both effective and practical [3.JP.8[1]]. The numerical investigations were facilitated by the development of the CYL_SPEC and NIMEIG codes [3.CP.12]. In addition to the development of the novel projections for stabilizing flow-divergence and parallel vorticity, the effort produced an alternative method for suppressing numerical divergence errors in the magnetic-field expansion. The developments for interchange stabilization and magnetic divergence have been incorporated in the main repository for the code.

While the interchange stabilization scheme works well for MHD computations, by itself, it does not ensure reliable computation with the two-fluid advance of magnetic field. This finding and numerical results in conditions with strong flow prompted investigation of first-order system least squares (FOSLS) formulations [4]. Initial results, achieved during this grant period, show that selected use of FOSLS helps avoid accumulation of numerical noise in the number density and temperature fields [3.CP.21]. Investigation for the two-fluid advance of **B** is continuing past the grant period.

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[1]Citations that start with 3.JP and 3.CP refer, respectively, to entries in Section 3 under Journal Publications and Conference Presentations.

2.2. Investigate possible improvements of NIMROD's time-advance

An implicit leapfrog time-advance for two-fluid models was developed under the previous CEMM grant. During the grant period, numerical analysis based on differential approximation was derived for this algorithm, and it was published with results from verification tests on linear two-fluid tearing [3.JP.3]. Possible improvements have also been researched. A linear version of NIMROD without temporal staggering was developed for comparing the Crank-Nicolson method (time-centered) with the implicit leapfrog. Tests on slab-geometry two-fluid tearing demonstrated the accuracy advantage of the Crank-Nicolson method at large time-step values (Fig. 1), but also pointed to the additional computational cost associated with its larger algebraic system. A separate development for the nonlinear contributions to the Hall electric field, $(1/ne)\mathbf{J}\times\mathbf{B}$, and the momentum advection term, $\rho\mathbf{V}\cdot\nabla\mathbf{V}$, applies Newton iteration to center each of these terms within the context of the implicit leapfrog. This work is described in Ref. [5] and has been incorporated in the code repository. Also, the accuracy of the operator that stabilizes MHD waves at large time-step, i.e. the "semi-implicit" operator, has been improved by having it represent the toroidal variation of the magnetic field and plasma pressure [6]. This is particularly important for maintaining accuracy at large time-step values for strongly shaped configurations [3.JP.9].

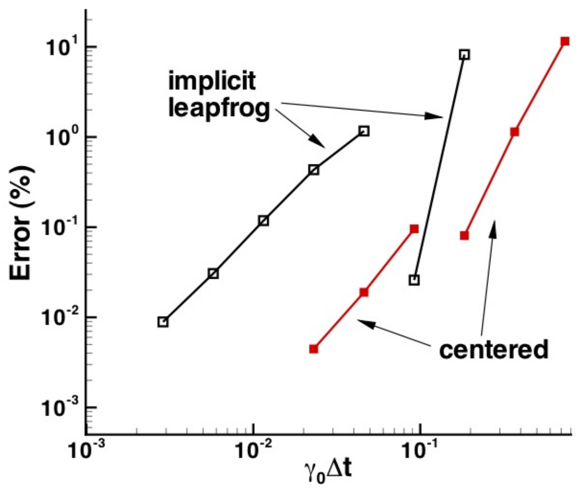

Figure 1. Comparison of convergence properties for NIMROD’s implicit leapfrog algorithm (black) and the time-centered Crank-Nicolson method (red) for a linear two-fluid tearing mode in slab geometry. The truncation error changes sign for both algorithms, hence the break in both curves. [See Ref. 7 for details.]

2.3. Increase parallel scaling performance

The ability to use large numbers of processor cores, efficiently, is important for modern scientific computing. Accuracy for some nonlinear NIMROD computations can require more than 100 toroidal Fourier harmonics, and the performance of the "preconditioner" that accelerates solution of algebraic systems can be a bottleneck for scaling to large numbers of cores. Among the different methods considered, one that helps NIMROD scale as toroidal resolution is increased is a limited block-Gauss-Seidel operation over selected couplings among the Fourier components. A discussion of parallel scaling with this approach is posted on the NIMROD website as Ref. 8. Another approach for cases with diffusion coefficients that vary strongly over the toroidal coordinate, is to use two different block-Jacobi solves, one by Fourier component and one by toroidal angle [3.CP.22], alternating between the two on consecutive steps of the flexible generalized minimum residual (FGMRES) solver [9]. We found that other approaches, such as the polynomial method [9] and using incomplete factorization in the block solves instead of full factorization, detracted from performance.

2.4. Model ELMs and the effects of RMP on tokamaks

Dr. Ping Zhu analyzed the nonlinear development of line-tied interchange and MHD ballooning. Analytically, he derived the evolution of the mode in the intermediate regime, where the amplitude of the displacement is comparable to the mode width in the flux-normal direction. He found that the nonlinear mode continues to grow exponentially at the rate of the corresponding linear mode [3.JP.1, 3.JP.2] in contrast to the prevailing theory that predicted explosive nonlinear growth [10]. Zhu's study included numerical computations with the BIC and NIMROD codes for slab and toroidal computations, respectively, which confirm the behavior predicted for the intermediate regime. Two-fluid effects on the linear stability of interchange in simplified configurations [3.CP.8] and in toroidal configurations without a separatrix [11] were also investigated. In addition, earlier work on profile effects on interchange in slab configurations subject to gyroviscous stress [12] was extended to include both gyroviscous stress and the Hall effect [3.JP.10].[1] The more recent study found a second instability resulting from the interaction of an ion drift wave with the interchange mode, and the diamagnetic heat-flux density has an important role in the mode's stability.

Other aspects of the ELM study include the behavior of the modes when the equilibrium configuration has a magnetic separatrix [3.CP.6]. Zhu found that in low-dissipation conditions, the mode structure is more concentrated near the X-point of the separatrix. Another study found that the growth rate of long-wavelength edge modes has a non-monotonic dependence on edge current density. While increasing current density is destabilizing when positive magnetic shear is maintained, it becomes stabilizing when the current density is large enough to reverse the magnetic shear [3.JP.5]. A related study that was also supported by this grant found the nonlinear formation of blobs from MHD interchange in configurations without magnetic shear [3.JP.7].

2.5. Model two-fluid effects on reconnecting instabilities

Computations of reconnecting instabilities with two-fluid effects included nonlinear internal kink in tokamaks, linear and nonlinear drift-tearing in cylindrical pinch configurations, and linear computations of drift-tearing in slab configurations. The internal kink computations were the first toroidal two-fluid computations [3.JP.3] to show an increasing kinetic-energy growth rate during the nonlinear phase that transitions reconnection geometry from a current sheet to a helical X-point [13]. Efforts to examine drift effects on the internal kink were challenged by a faster-growing mode at large Hall parameter (the ratio of ion skin-depth and minor radius) when using the Hall electric field in conditions with a pressure gradient [3.CP.19, 14]. The faster-growing mode may be related to the second instability found in two-fluid interchange computations, described in Section 2.4.

[1]This work was also supported by grant DE-FG02-06ER54850.

Analytical theory and numerical computations in cylindrical pinch configurations, including the Hall effect and ion gyroviscous stress, found drift effects that reduce the growth-rate of tearing in the absence of a pressure gradient [3.JP.4, 3.JP.6]. In pinch configurations (safety factor values below unity), poloidal magnetic curvature dominates toroidal effects, and flux-surface-averaged drifts from ∇B and magnetic curvature are significant.[1] Slab drift-tearing computations with a pressure gradient and with real frequencies significantly larger than growth rates proved to be problematic, prompting some of the new numerical work described at the end of Section 2.1.

2.6. Tasks not completed during the grant period

Some of the research tasks that were listed in the proposed scope of work were not completed. They are:

- The nonlinear version of the fluid-model electron parallel stress was not implemented. It may provide a practical alternative to the full kinetic computation, but NIMROD and CEMM collaborators have made significant progress on the more accurate kinetic model. Moreover, improving the behavior of NIMROD two-fluid computations with a pressure gradient was given priority.
- Despite the early success with the two-fluid internal kink, the behavior of the numerical model hampered nonlinear studies with a pressure gradient.
- Linear two-fluid benchmarking of ELMs between NIMROD and M3D-C1 was successful, but nonlinear benchmarking and nonlinear two-fluid ELM modeling was not completed, due to a shift in priority to disruption modeling.

2.7. Conclusions

Although some of the specific proposed tasks were not completed, the primary objectives of the project were met. The work on nonlinear ballooning clarified limitations on the possibility for explosive growth and set the stage for studies of ELM dynamics. The work on two-fluid reconnection in pinch and tokamak configurations identified curvature and ∇B driven drift effects. Extensions to that work also pointed to a shortcoming in NIMROD's capabilities, and it is now a focus of algorithm development. The novel projection method for stabilizing numerical interchange has proven successful and is used routinely in NIMROD MHD computations. Finally, efforts to improve preconditioning of the algebraic solves resulted in favorable scaling over thousands of processor cores, surpassing the 10,000-core level early in the course of this project.

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3. Products

The work supported by this grant appears in the following peer-reviewed journal articles and contributed conference presentations.

Journal Publications

1. P. Zhu, C. C. Hegna, and C. R. Sovinec, "Exponential Growth of Nonlinear Ballooning Instability," Physical Review Letters **102**, 235003 (2009). DOI 10.1103/PhysRevLett.102.235003
2. P. Zhu, C. C. Hegna, C. R. Sovinec, A. Bhattacharjee, and K. Germashewski, "Intermediate Nonlinear Regimes of Line-tied *g* mode and Ballooning Instability," Nuclear Fusion **49**, 095009 (2009). DOI 10.1088/0029-5515/49/9/095009
3. C. R. Sovinec, J. R. King, and the NIMROD Team, "Analysis of a Mixed Semi-Implicit/Implicit Algorithm for Low-Frequency Two-Fluid Plasma Modeling," Journal of Computational Physics **229**, 5803 (2010). DOI 10.1016/j.jcp.2010.04.022

4. J. R. King, C. R. Sovinec, and V. V. Mirnov, "First-Order Finite-Larmor-Radius Effects on Magnetic Tearing in Pinch Configurations," Physics of Plasmas **18**, 042303 (2011). DOI 10.1063/1.3571599
5. P. Zhu, C. C. Hegna, and C. R. Sovinec, "Stabilizing Effects of Edge Current Density on Pedestal Instabilities," Physics of Plasmas **19**, 032503 (2012). DOI 10.1063/1.3692089
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8. C. R. Sovinec, "Stabilization of numerical interchange in spectral-element magnetohydrodynamics," Journal of Computational Physics **319**, 61 (2016). DOI 10.1016/j.jcp.2016.04.063
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10. E. C. Howell and C. R. Sovinec, "Parameter-space survey of linear g-mode and interchange in extended magnetohydrodynamics," Physics of Plasmas **24**, 102117 (2017). DOI 10.1063/1.4993440

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2. C. R. Sovinec and E. D. Held, "Preconditioning for Three-Dimensional Two-Fluid NIMROD Applications," presentation BAPS.2008.DPP.BP6.42, Bull. Am. Phys. Soc. **53**, No. 14 (2008).
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4. C. R. Sovinec, E. C. Howell, and P. Zhu, "Three-Dimensional Computation of Toroidal Two-Fluid Internal Kink," presentation BAPS.2009.APR.S1.15, Bull. Am. Phys. Soc. **54**, No. 4 (2009).
5. P. Zhu, C. C. Hegna, and C. R. Sovinec, "Exponential Growth and Filamentary Structure of Nonlinear Ballooning Instability," presentation BAPS.2009.APR.W15.3, Bull. Am. Phys. Soc. **54**, No. 4 (2009).
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11. C. R. Sovinec, "Interchange Convergence with Spectral-Element Extended MHD," International Sherwood Fusion Theory Conference, Austin, TX, May 2-4 (2011).

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18. E. C. Howell and C. R. Sovinec, "Extended MHD Analysis of the Gravitational Interchange," International Sherwood Fusion Theory Conference, New York, New York, March 16-18 (2015).

19. E. C. Howell and C. R. Sovinec, "Two-Fluid Calculations of the 1/1 Internal Kink," presentation BAPS.2015.DPP.NP12.16, Bull. Am. Phys. Soc. **60**, No. 19 (2015).

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21. C. R. Sovinec, "Advection-Dominant MHD Computation for External Kinks and Edge-Localized Modes," presentation BAPS.2016.DPP.BP10.5, Bull. Am. Phys. Soc. **61**, No. 18 (2016).

22. K. J. Bunkers and C. R. Sovinec, "Nonlinear External Kink Computing with NIMROD," presentation BAPS.2016.DPP.GP10.77, Bull. Am. Phys. Soc. **61**, No. 18 (2016).