

Computational Needs for Reversed-Field Pinch and Spheromak Development

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Introduction. Large-scale numerical computation has been part of Reversed-field Pinch (RFP) and spheromak research for decades. With strong nonlinear dynamics having important consequences for both configurations, we expect that computation will continue to make significant contributions throughout the ITER era. This whitepaper reviews the issues identified in the Toroidal Alternates Panel (TAP, <http://fusion.gat.com/tap/>) report where computation has a role. The review is followed by a discussion of computational requirements, including comparison with modeling for tokamak configurations.

Executive Summary. Theoretical efforts for the RFP and spheromak TAP issues will need large-scale computation. The most important considerations are the following:

1. Nonlinear macroscopic stability computations will have a large role in the issues associated with relaxation, namely current sustainment (steady, AC, and pulsed schemes) and transport scaling in conditions with active relaxation. Achieving dimensionless parameters with cascading fluctuations will continue to be challenging computationally. While implicit methods help address stiffness, they do not alleviate the need for resolving multiple temporal and spatial scales, and computational efficiency with hardware improvement is needed. Two-fluid modeling is needed to address fast reconnection and drift effects during relaxation.
2. Macroscopic simulation will also be important for assessing plasma- β limits, resistive wall, and energetic particle effects. Nonlinear simulations will be able to distinguish hard and soft β -limits, but modeling of fluctuation-induced transport requires spatial representations that are accurate for extreme anisotropy without alignment between the mesh and evolving 3D magnetic topologies. Kinetic models are needed to reproduce physical limits to parallel transport in high temperature plasma. Incorporating energetic-particle modeling is a tractable approach for investigating destabilization of Alfvén eigenmodes and fast-particle effects on magnetic tearing. Incorporating thin-shell and external vacuum models is a tractable approach for resistive wall studies.
3. Transport in high-confinement states, where relaxation is weak or non-existent, will benefit from microscopic turbulence modeling. Application to the RFP is in an early stage, and the applicability of models developed for tokamaks needs thorough review. Nested symmetric flux surfaces are assumed in these models, so computations represent idealized conditions. Combining microscopic and macroscopic computation self-consistently will be a major integration effort for the Fusion Simulation Project (FSP, <http://www.scidac.gov>), and it is essential that the effort produces a general model that addresses RFP and spheromak configurations and not just tokamaks.
4. RF modeling will be important for current sustainment and profile control. Propagation and deposition in conditions with macroscopic fluctuations will need to be considered. Integration with macroscopic dynamics is of interest, particularly for profile control, and also represents a major FSP effort that needs to be sufficiently general.

5. The plasma boundary has a strong influence on RFP and spheromak experiments. Coupling of core and edge models may produce valuable insight on the underlying effects and lead to improved confinement. Again, FSP efforts will be an investment that can have great returns for many confinement configurations if the development is sufficiently general.

Review of TAP Issues. Many of the RFP and spheromak scientific issues listed in the TAP will benefit from large-scale computation. In approximate order from high to low in the tier identification, they are:

- Achieving current sustainment with high confinement: This is Issue #1 (Tier 1) for the spheromak and includes Issues #2 and #3 (Tier 1) for the RFP. Issue #2 (Tier 2) for the spheromak is formation, which is also related to current drive.

The standard RFP is driven inductively and magnetic fluctuations nonlinearly relax the current profile, counteracting the tendency to pinch current at the magnetic axis. The DC-driven spheromak tends to create a pinch at the geometric axis. Fluctuations distribute the current while converting toroidal magnetic flux into poloidal magnetic flux. In principle, DC drive can be sustained, while standard inductive drive cannot. However, like the RFP,¹ high confinement states in spheromak experiments² have only been achieved transiently when inductive effects are important.

- Nonlinear macroscopic computation has contributed to a reasonably detailed description, according to the resistive MHD model, of how fluctuations relax profiles in the standard operating mode of both configurations.^{3,4,5,6,7,8} Extending this work to include more realistic plasma models (two-fluid and kinetic effects) and greater separation of spatial and temporal scales (via larger Lundquist number, for example) is important for characterizing the target plasma of any current-drive method.
- Nonlinear computation has been used to help understand how transients produce high confinement states: pulsed parallel current drive (PPCD) in the RFP⁹ and DC injection with separate formation and sustainment pulses^{10,11} in the spheromak. It is being used to explore current drive methods based on low-frequency oscillation: $F\text{-}\Theta$ pumping or oscillating-field current drive (OFCD) in the RFP¹² and the ‘steady induction’ scheme of HIT-SI.¹³ Initial investigation of pulsed current drive has used the same type of modeling,¹¹ and optimization of pulsed scenarios will benefit from it.
- RF calculations have been used to guide hardware development for current profile control in the RFP.¹⁴ Future efforts in RF current drive will benefit from computational support.
- Calculations of energetic-particle production and deposition from neutral beam injection have been used to investigate control and sustainment of spheromak current profiles.¹⁵ Beam computations do not require large-scale computation, but integration with macroscopic computation would strengthen confidence in possibilities for sustaining high-confinement spheromaks and RFPs.
- Transport and confinement scaling: This is Issue #1 (Tier 1) for the RFP and Issue #3 (Tier 2) for the spheromak.

Laboratory results from the RFP show that parallel transport along magnetic fluctuations dominates energy confinement properties when relaxation is active.¹⁶ Similar conclusions can be inferred from spheromak experiments. In transient conditions when current-profile relaxation is not active, transport properties are largely unknown. It may involve a combination of electrostatic turbulence and pressure-driven MHD. Analytical theory, computation, and laboratory experiment are all needed.

- Nonlinear computations that combine resistive-MHD with fluid-based (Braginskii) closure have been used to investigate how energy confinement changes over different phases of the SSPX experiment.^{10,11} This type of modeling shows synergistic effects of MHD and temperature-dependent transport, and pressure-driven MHD is likely part of the activity reproduced during the quiescent high-confinement phase. It has been used for scaling studies in RFPs,¹⁷ but more can be done for standard, single-helicity, and pulsed operation. Extending the modeling to include kinetic effects that limit parallel heat flow at high temperature¹⁸ is needed for scaling information on fluctuation-induced transport during relaxation. Tearing and interchange modes that are stabilized by drift effects will also require two-fluid modeling.
- Conditions that are not dominated by fluctuation-induced transport may be subject to drift-wave turbulence like tokamaks. Research that applies gyrokinetic simulation to study electrostatic modes and their nonlinear consequences during high-confinement RFP conditions is underway.¹⁹ Similar work is needed for the spheromak configuration to assess cross-field transport in profiles that have been optimized for MHD.
- Separate modeling of the two types of fluctuations is a theoretical convenience, but it does not represent all possible transport scenarios. Magnetic topology-changing macroscopic dynamics and microscopic turbulence may work together over a range of conditions between the limits of large magnetic diffusivity and robust nested flux surfaces. Simulation of conditions between these limits will require integrated modeling that is beyond present-day computational capabilities.
- Plasma- β limits: Determining stability limits associated with pressure is Issue #6 (Tier 2) for the RFP and Issue #4 (Tier 2) for the spheromak.

‘Hard’ β -limits that terminate the discharge and ‘soft’ limits that lead to enhanced transport need better characterization in both devices; though, the nonlinear consequences of the latter can be viewed as part of the transport issue. Both configurations have safety-factor values (q) that are less than unity, hence bad average magnetic curvature. An exception may be RFP single-helicity states,²⁰ where the equilibrium is basically helical. In the case of the RFP, there is large magnetic shear ($q^{-1}dq/dr$), which is good for interchange stability, near the reversal surface. Pellet injection in MST during high confinement has produced β -values as large as 26% without disruption.²¹ Spheromaks have been produced with a range of shear. When the current density on the geometric axis is small, magnetic shear is large. In contrast, flux-core or gun-driven spheromaks with current on open field tend to have weak shear. In SSPX, β -values of roughly 10% were common during high confinement, but the duration of this phase was sensitive to MHD activity resonant at low-order rational surfaces.²²

- Both configurations need better characterization of linear stability with finite pressure. Apart from Suydam stability analysis, linear resistive interchange has been studied for the RFP.²³ This work needs to be expanded to include toroidally symmetric profiles, helical equilibria, and drift effects. Linear stability of pressure-driven modes in spheromaks^{24,25} started many years ago but needs more comprehensive characterization with realistic profiles.
- Nonlinear studies are needed to understand what distinguishes hard and soft limits in both configurations. Resistive MHD predicts instability for $q < 1$ and a centrally peaked pressure profile.²⁶ Whether experimental results reflect linear stability due to effects beyond MHD or a relatively benign saturation of MHD is an open and important question—one that also needs to be addressed for stellarators.
- Energetic particle effects: This is listed as Item #5 (Tier 2) for the RFP and Item #4 (Tier 2) for the spheromak.

The issue is similar to energetic particle effects in tokamaks, but it is less well explored. Energetic particles produced by neutral beams and fusion reactions can resonate with Alfvén eigenmodes and affect their stability. Relative to thermal particles, trajectories and confinement of energetic particles are much less sensitive to global magnetic fluctuations.²⁷ Interaction with tearing instability is a new area of theoretical research²⁸ and may have important consequences for both RFPs and spheromaks.

- Linear computations with simulation particles can be used to assess energetic particle effects on stable oscillations and unstable modes. Linear computation for RFP tearing with energetic particles is underway.²⁹
- Nonlinear simulations can be used to predict interaction between relaxation dynamics and the energetic particle distribution.
- Though not necessarily energetic-particle effects *per se*, numerical research to use simulation particle information to close fluid moments³⁰ has potential for contributing to the study of anomalous ion heating that is associated with magnetic fluctuations.
- Resistive wall mode (RWM) control: There is already a substantial amount of information on RWM and its control for the RFP, hence the lower ranking as Issue #8 (Tier 3). For the spheromak, RWM is listed as Issue #7 (Tier 3).

Macroscopic instabilities in both configurations are sensitive to the location of a conducting wall and become violently unstable without a wall. Effective feedback schemes for resistive walls and multiple modes have been demonstrated experimentally on Extrap-T2R.³¹

- To the author’s knowledge, the first nonlinear MHD simulations of macroscopic modes with resistive walls were performed for the RFP.^{32,33} New studies can be used to help optimize feedback schemes.
- After validation on RFP results, nonlinear simulations of spheromaks with resistive wall can provide design information while experimental efforts concentrate on current drive and transport.
- Plasma boundary interactions: This is listed as Item #4 (Tier 2) for the RFP and has bearing on the particle balance and density control issue (Tier 2) for spheromaks.

Wall conditioning has been important in achieving high performance in both devices. As an example, boronization in MST leads to high confinement states that are comparable to some of the earlier PPCD results.³⁴ So far, large-scale computation has not been applied to these issues, but it may prove useful.

- Development efforts at the Plasma Science and Innovation Center (<http://www.psicenter.org>) are working to couple radiation and neutral modeling in three-dimensional macroscopic simulation. Similar but less general modeling is being used successfully in the study of disruption mitigation techniques for tokamaks.³⁵
- Simulation codes specifically designed for studying edge plasma without coupling to core modeling³⁶ may also prove useful.
- Nonlinear simulation can be used to investigate how different divertor designs affect macroscopic dynamics in the RFP. [Spheromak computation with open flux is well established.]

Computational Requirements. Large-scale numerical computation for magnetic confinement is categorized by its theoretical subfield. The different sets of equations have been most efficiently solved by somewhat different numerical methods, which reinforces the divisions and adds to the challenge of integrated modeling. The following discussion of computational needs uses these traditional categories but also considers integration.

- The vast majority of large-scale simulations applied to both configurations have studied magnetic relaxation, its consequences, or methods of avoiding it. At this point, the only suitable numerical modeling tool is macroscopic or MHD-like computation. Implicit methods for fluid-based algorithms handle the stiffness of profile evolution due to fluctuations that are low frequency relative to MHD waves. Even with tailored algorithms, present-day resistive-MHD computation at Lundquist number of $\leq 10^6$ and Hartmann number of $\leq 10^5$ is one to two orders of magnitude short of experiment. Computational efficiency and improvements in computer hardware are needed. Special considerations for applying macroscopic computation to the RFP and spheromak include:
 - The large aspect ratio, i.e. large toroidal field, ordering is not suitable for either configuration. In addition, some codes developed for tokamaks, such as the original M3D,³⁷ solve sufficiently general systems of equations, but the algorithm expects to take advantage of the large aspect ratio ordering to achieve efficiency. Algorithms based on full models, such as those in DEBS,³⁸ SpeCyl,⁵ NIMROD,³⁹ PIXIE3D,⁴⁰ and HiFi,⁴¹ are more efficient for RFP and spheromak applications.
 - Relative to tokamaks, magnetic fluctuations can be large, generating stochastic regions contained by KAM surfaces or regions of chaotic trajectories that intercept the wall. Adaptive meshing may be useful but will likely be less effective than in tokamak applications where isolated islands are surrounded by nested flux surfaces. High-order spatial representation that can accurately reproduce extreme anisotropy without alignment of the mesh and magnetic field is important for macroscopic computations with transport.

- Cascading of magnetic fluctuations also impacts macroscopic simulation. Conditions may have turbulent properties, and achieving spatial and temporal resolution from global to dissipation scales is challenging. This is also the reason why a code handles lower dimensionless parameters in RFP and spheromak applications than in tokamak applications. Algorithms tailored for more laminar tokamak conditions may not be efficient when many, smaller temporal steps and global spatial resolution are required to reproduce cascading.
- Spheromak computations require a simply connected domain, and codes developed exclusively for toroidal geometry are not suitable.
- For experiments that do not have a direction of symmetry in the geometry, codes constructed with a 2D metric are not applicable. Sufficiently complicated geometries, such as the entire HIT-SI vacuum chamber, require 3D meshing; finite Fourier series in one or more directions is not suitable. The HiFi code is being developed for this need.
- Kinetic extensions to fluid-based modeling are required for modeling a minority species of energetic particles and majority-species parallel transport in moderately collisional to collisionless conditions. The former is the more established of the two for macroscopic modeling,⁴² but the drift-kinetic approximation used for tokamaks is less suitable for RFPs and spheromaks. The ability to use gyrokinetics or full kinetic modeling is important and is being used in RFP computations.²⁹ Incorporating parallel kinetics associated with large effective mean free paths is challenging for all applications.¹⁸ In spheromaks with DC injection, the algorithm additionally needs to handle characteristics that intercept electrode surfaces. Finally, kinetic closure for majority species will likely provide important information on how energy cascading through fluctuations is ultimately converted to thermal energy.
- Validation of macroscopic simulation will require direct comparison with magnetic coil signals and polarimetry information for large-scale fluctuations and time-dependent information on current density profiles. Simulations with transport modeling can additionally be compared with results from Thomson scattering measurements.
- Simulation tools for microscopic turbulence have been an important part of tokamak transport studies for a number of years. They are based on gyrokinetics,⁴³ which limits to reduced MHD at large wavelength ($k_{\parallel}/k_{\perp} \ll 1$), and they use coordinates and meshes that are aligned with a symmetric equilibrium magnetic field. Until recently, the numerical studies have focused on electrostatic turbulence, which underlies cross-field transport in tokamaks, but it is typically small relative to parallel transport during relaxation in RFPs and spheromaks.
 - Flux-tube codes⁴⁴ can be used to investigate local electrostatic modes in ideal high-confinement conditions with nested symmetric flux surfaces.
 - The toroidal flux function is not useful as a coordinate for computations that extend over the reversal surface of a RFP. Global turbulence computations⁴⁵ will not be able to use codes where the toroidal flux function is one of the independent variables.

- Integrating microscopic turbulence with macroscopic dynamics is one of the most challenging tasks for the FSP. In principle, fully kinetic computations can incorporate all of the necessary physical effects including changing magnetic topology, parallel dynamics, profile evolution, and irreversibility due to particle collisions. However, even present-day fluid computations are one to two orders of magnitude short of dimensionless parameters in existing experiments, and they use implicit methods on massively parallel architectures and do not resolve velocity-space dimensions. Ensuring that FSP efforts to integrate microscopic turbulence and macroscopic stability are suitable for configurations other than the tokamak is important for the ReNeW theme of Optimizing the Configuration. It is worth emphasizing that the need is self-consistent integration of three-dimensional and evolving magnetic topology with turbulent transport. Using symmetric profiles as an intermediary between separate macro and micro computations is not sufficient.
- Validation of standalone cross-field turbulence results will need measurements from magnetically quiescent plasma. This may be difficult to achieve, and the modeling will represent ideal conditions with respect to magnetic topology.
- Large-scale computation is needed for RF studies of current drive and heating when ray-tracing (WKB method) is not suitable. In some cases, mode coupling may involve a combination of large and small wavelengths, and multiple scales must be fully resolved in a computation. The wave propagation part of a computation is typically coupled to localized Fokker-Planck calculations,⁴⁶ but other forms of kinetic computation can be substituted, as presently considered in the Simulation of Wave Interaction with Magnetohydrodynamics project (SWIM, http://www.scidac.gov/FES/FES_SWIM.html).
- RFP and spheromak plasmas are overdense for electron cyclotron heating and current drive at the fundamental, i.e. $\omega_{pe} > \Omega_e$ where ω_{pe} is the electron plasma frequency and Ω_e is the electron cyclotron frequency. This is unlikely to be restrictive as far as computational tools, but many existing results may not be applicable.
- The propagation of short wavelength waves will be sensitive to deflection by global fluctuations. Incorporating macroscopic fluctuations in ray-tracing codes should be straightforward. It is expected to be more complicated for full-wave codes^{47,48} and require a major effort under FSP, not unlike integration of macroscopic dynamics and microscopic turbulence.
- Integrated RF/macroscopic modeling can be validated with measurements of current and temperature profile evolution. Integrated models for profile control will also predict changes in magnetic fluctuations, which can be compared with magnetic diagnostics.
- Codes for edge plasma model the interaction of ionized species with neutrals and account for energy loss due to impurity radiation.³⁶ There have been some initial efforts to apply them to spheromaks, but to the author's knowledge, they have not been applied to RFPs.
 - Detailed modeling of edge plasma involved in DC drive (helicity injection) may prove fruitful. Parallel energy loss dominates overall confinement during formation, and anything that can help develop a more detailed understanding of the entire process can lead to improvements in this form of current drive.

- Coupling of macroscopic and edge models will be a major integration effort for the FSP. With many physical processes happening simultaneously, three-dimensional representation of edge plasma is challenging in itself. The motivation for integrated modeling is that macroscopic modes in RFPs and spheromaks lead to parallel transport channels that link core and edge plasma along chaotic trajectories. Edge physics may, therefore, have a large role in regulating the net confinement during periods of relaxation.

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