GA–A27743

EDGE SIMULATION LABORATORY

GENERAL ATOMICS ANNUAL REPORT

FOR GRANT YEAR 2013
APRIL 1, 2013 THROUGH MARCH 31, 2014

by
PROJECT STAFF

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DISCLAIMER

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GENERAL ATOMICS

Edge Simulation Laboratory

General Atomics Annual Report

Grant Year 2013 (April 1, 2013 - March 31, 2014)
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1 Annual Progress Highlights

- NEO has been used to analyze the accuracy and limitations of bootstrap current models for experimental edge plasmas, including the effects of extreme aspect ratio, large impurity fraction, energetic particles, and high collisionality.
- Integrated modeling of MHD equilibrium reconstruction, which couples kinetic EFITs with direct NEO bootstap current simulations, has been implemented via the OMFIT framework for use in routine experimental analysis.
- A novel 3D local equilibrium solver has been developed for use in fast systematic shaping studies of non-axisymmetric effects on neoclassical transport.
- Non-axisymmetric effects have been added in NEO. The neoclassical toroidal viscosity (NTV) with full kinetic dynamics, as well as the non-ambipolar particle fluxes, have been verified and the so-called $1/\nu$ collisionality regime of 3D transport has been identified.
- A preliminary framework for a linear direct implicit 5D gyrokinetic solver with more advanced collision models has been completed. The multi-species reduced Hirshman-Sigmar collision operator has been implemented and tested with full cross-species collisional coupling
- Advances in physics understanding of the pedestal, including ESL contributions to the EPED model, were recognized by the 2013 John Dawson Award for Excellence in Plasma Physics Research http://www.aps.org/programs/honors/prizes/prizerecipient.cfm?last_nm=Snyder&first_nm=Philip&year=2013

The above work has been presented in invited talks at the 2013 Sherwood, APS-DPP, and International Toki Conferences. Further information on research accomplishments is given in Sec. 3, and a list of presentations and publications in Sec. 5. Coordination with the multi-institutional ESL project has been achieved via a full group meeting in Livermore CA, August 26-27, 2013, and via conference calls and subgroup meetings during major conferences.

2 Background

The purpose of the Edge Simulation Laboratory (ESL) project is to bring to bear a coordinated effort, utilizing modern computing resources, advanced algorithms, and ongoing theoretical development to progress toward a fundamental, quantitative and predictive understanding of the edge plasma. A key component of ESL is the development, verification and validation of kinetic simulations, employing Eulerian methods and modern numerical techniques to the solution of the drift- and gyro-kinetic equations, in the complex geometry of the edge plasma, complete with sophisticated collision operators required to accurately treat the broad range of collisionality across the edge region.

The efforts in the General Atomics (GA) group have focused on 4D (NEO) and 5D (GYRO) kinetic studies of the closed field line pedestal and near-pedestal region, as well as the development of the EPED model to predict the pedestal height and width. Work on NEO and the new VGEN tool have been supported primarily by ESL, while work on GYRO and EPED leverage substantial development efforts within the GA theory and SciDAC programs. The work plan is described in detail in the 2012 ESL renewal proposal.

3 ESL Accomplishments

3.1 Bootstrap current studies with NEO

NEO [1, 2] is an Eulerian code that solves the 1st-order (in the drift-ordering parameter $\rho_* = \rho_i / a \ll 1$) drift-kinetic-Poisson equations. In NEO, no approximations beyond the drift-ordering are made. Full sonic toroidal rotation and centrifugal terms are retained, and general flux-surface shape, including up-down asymmetry, is treated (although the code is limited to the closed flux-surface region). The full linearized Fokker-Planck collision operator is used for the collision dynamics, with complete cross-species collisional coupling for arbitrary mass ratio and an arbitrary number of ion species. NEO has been extensively benchmarked with analytic theories, as well as with NCLASS, over a wide range of parameters and in various asymptotic limits. The equations solved in NEO complement those solved in gyrokinetic codes such as GYRO [3] insofar as together they represent the complete first-order deviation of the plasma from a local Maxwellian.

NEO has been used to explore the accuracy and limitations of two bootstrap current models: (1) the Sauter model [4, 5] and (2) the KCK12 model [6] (a modification of the Sauter model proposed by Koh *et al.*). The results for representative experimental DIII-D and NSTX H-mode plasmas are shown in figure 1. For DIII-D, we find that the differences between the Sauter and KCK12 formulas are negligible, such that both agree well with NEO. For a range of experimental DIII-D discharges, it is observed that the Sauter model overestimates the bootstrap current at low collisionality, $\nu_{*e} < 1$, with increasing error toward the banana regime, and largely underestimates the bootstrap current at high collisionality, with increasing error toward the Pfirsch-Schlüter regime. In contrast to the DIII-D results, a large difference is found between NEO and the KCK12 formula in the NSTX pedestal, with the NEO results qualitatively following the Sauter model. Further analysis finds that this is essentially due to a failure in the KCK12 formula at large inverse aspect ratio for large collision frequency ($\nu_{*e} \sim 1$). We have demonstrated that the origin of this fitting error is a pathology related to the use of a non-analytic function in the KCK12 fitting-formula.

We have also analyzed errors associated with simplified forms of the ion-electron collisional dynamics (to our knowledge only NEO retains the exact electron-ion coupling). This analysis revealed a large inaccuracy of the simplified operators deep in the Pfirsch-Schlüter regime. Specifically, significant errors in both the transport coefficients and individual ion and electron parallel flows are observed. The key physical effect is the electron-ion energy exchange, which when correctly retained, reduces the ion transport to the electron scale. This process cannot be modeled without the full, cross-species field-particle operator. Remarkably, we also observe the fortuitous result that reduced models may still recover a sensible bootstrap current (via cancellation of errors in the subtraction of ion and electron parallel velocities) as long as the associated collision operator conserves momentum.

For impure plasmas, comparisons with NEO find that the Sauter model is able to accurately capture the electron-impurity interaction through the use of $z_{\rm eff}$ in ν_{*e}, but does not accurately model the ion-impurity collisional interaction. However, the latter, which enters as a term proportional to the ion temperature gradient, is often a sub-dominant contribution to the bootstrap current compared with the pressure gradient and electron temperature gradient terms representing the former. Analysis of the Sauter model for energetic impurities shows that it largely overestimates the collisional effect of the energetic species on the ion and electron dynamics. This may have implications for the modeling of reactors like ITER that are expected to have a significant concentration of α particles.

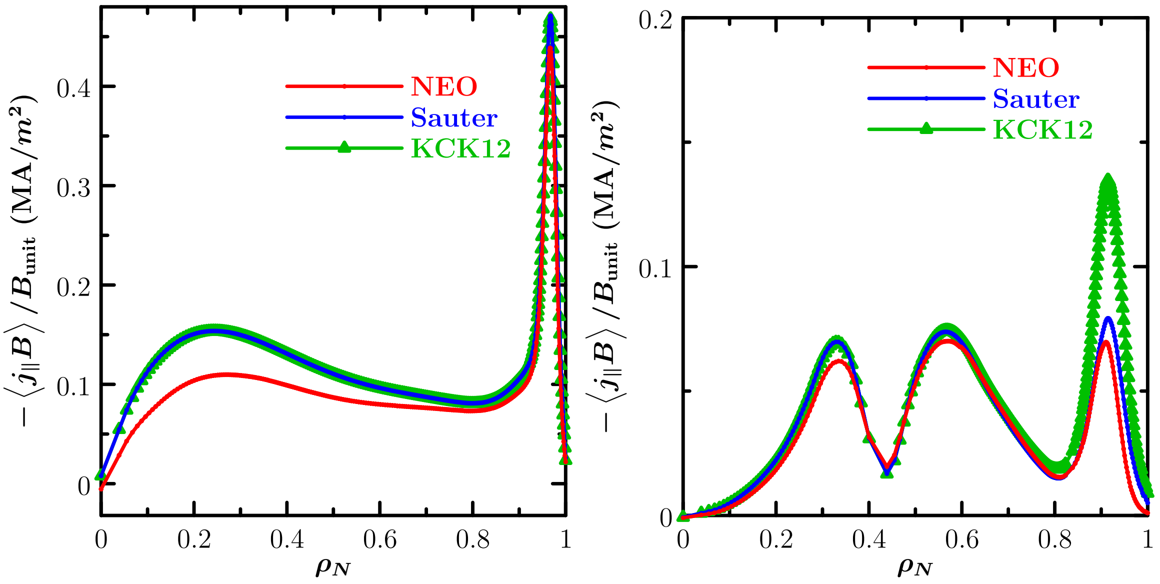

Figure 1: Bootstrap current profile for DIII-D H-mode shot #145421 at t=2283ms and NSTX H-mode shot #129015 at t=409ms, comparing the NEO simulation results with the Sauter model and the KCK12 formula. The KCK12 modification is insignificant for DIII-D plasmas, but deviates largely from Sauter in the NSTX pedestal, which is inconsistent with NEO.

3.2 Integrated modeling of NEO with kinetic EFIT

Integrated modeling of MHD equilibrium reconstruction, which couples kinetic EFITs with direct NEO simulations, has been demonstrated for the first time. Using the OMFIT framework, a comparison of the EFIT reconstruction obtained using NEO and Sauter bootstrap currents embedded into the EFIT edge total current constraint for a high collisionality DIII-D H-mode case (shown in figure 2) found a lower χ^2 value for NEO. This indicates that the current constraint from NEO is more consistent with the pressure and magnetics measurements. The differences in the equilibrium reconstruction using NEO versus the Sauter model were found to be largest at the inboard midplane and near the X-point.

3.3 3D equilibrium solver

A novel 3D local equilibrium solver, LE3, has been developed for use in studying non-axisymmetric effects in neoclassical transport and gyrokinetic turbulence simulations. The method is analogous to a 3D extension of the Miller formalism for shaped axisymmetry equilibria [7]. Yet, unlike Miller, which can be computed straightforwardly, the 3D solver requires solution of a difficult nonlinear PDE. The advantage of the local method is that, unlike a global equilibrium solve, it allows for fast systematic studies of the effects of 3D flux-surface shaping parameters. In addition, it guarantees a valid magnetostatic equilibrium with good flux surfaces, i.e. without any islands or other stochasticity, which is essential for use in our $\mathcal{O}(\rho_*)$ kinetic calculation.

Like the method developed by Hegna [8], LE3 constructs a local 3D equilibrium by solving the magnetostatic equilibrium equations in the neighborhood of a reference flux surface. Momentum balance and

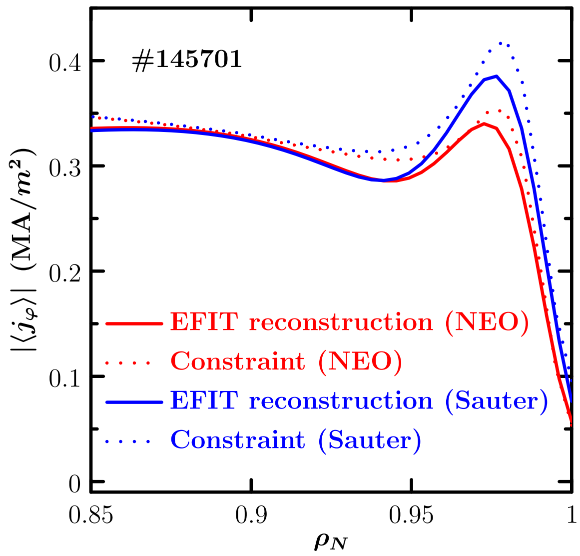

Figure 2: The edge total toroidal current profiles used as a constraint and the values obtained for the EFIT reconstruction for DIII-D #145701 comparing use of the NEO versus the Sauter model bootstrap current embedded into the EFIT total current constraint.

Ampère's law determine the basic equations of magnetostatic equilibrium, which yield scalar conditions for the metric elements, physically representing (1) zero radial current and (2) radial force balance. The method proceeds by specifying the local flux surface parameterization (R, Z) as a function of the toroidal angle ϕ and undetermined parametric angle $\bar{\theta}$ (equivalent in 2D to the poloidal arc length). We then use the zero-radial-current equation to determine the mapping between the parametric angle $\bar{\theta}$ and the straight field line angles θ and ϕ. This involves solving a complex nonlinear PDE for which there may not be a solution for an arbitrary (R, Z) parameterization. Once this mapping is known, we then linearize the radial current and force balance equations about the chosen magnetic surface and solve the resulting linear magnetic differential equations. In this process we avoid singularities associated with rational surfaces by selecting values of q for which the condition $nq = m$ is not satisfied anywhere in the solution space.

Our method differs from Hegna's approach in which one specifies the flux-surface parameterization (R, Z) as a function of the straight field line angles, and then uses the radial current equation to determine the Jacobian. This Jacobian will not in general be the same as the Jacobian computed from radial derivatives of R and Z, and thus, unlike the Miller approach, shape effects like the derivative of the elongation or the Shafranov shift cannot be controlled explicitly.

3.4 Non-axisymmetric effects in NEO

The effects of toroidal non-axisymmetry (e.g. due to magnetic field ripple, caused by the discreteness of the toroidal field coils, or imposed resonant magnetic perturbations) on the flows and transport are being explored using a new 3D extension of NEO. The NEO drift-kinetic equation solve has been upgraded to includes the toroidal angle dependency, retaining all of the 2D physics features of NEO in the diamagnetic ordering limit. In principle, the NEO DKE solver can be coupled with any numerical equilibrium, such as from VMEC, though presently NEO is coupled directly with our new local equilibrium solver LE3 for fast 3D shaping studies.

For verification, NEO has been benchmarked with an analytic formula that we have derived for the case of a single ion species in the Pfirsch-Schlüter regime. For this case, while in the axisymmetric limit, the particle and energy fluxes are zero, we find that even small 3D magnetic perturbations give rise to non-ambipolar transport. The results show excellent agreement with the analytic theory at high collisionality, where the fluxes scale as $1/\nu$. 3D NEO can also be used to compute the neoclassical toroidal viscosity (NTV) with full kinetic corrections. This is shown in figure 3. The kinetic NTV from NEO is even more physiclly accurate than that from similar recent 3D neoclassical particle codes due to full FP collision model and multiple ion physics without mass ratio approximations. Verfication of the NEO NTV calculation has also been successfully demonstrated with our Pfirsch-Schlüter analytic calculations and the expected δB^2 dependence independent of collisionality was shown.

For physics studies, results including kinetic electrons with full collisional coupling have identified physically interesting collisionality regimes of 3D transport. The results are shown in figure 3. At high collisionality, the Pfirsch-Schlüter particle flux Γ_i exhibits the exact 2D axisymmetric ambipolar (i.e. $\Gamma_i = \Gamma_e$) ν scaling since collisions, rather than the non-axisymmetry, dominate the dynamics. As collisionality decreases, the ions and electrons undergo a plateau-like regime and then we see the strongly enhanced $1/\nu$ transport at low collisionality, first for the ions and then for the electrons by about a square root of the electron to ion mass ratio later in ν_{*e}. This regime exists only for finite nonaxisymmetry and arises when the bounce average of the drift velocity acting on the Maxwellian is no longer nonzero and must balance the collision term. The $1/\nu$ divergence is clearly unphysical, and points to a breakdown of the drift ordering in the limit of very weak collisions. In this limit, we expect the transport to approach a finite limiting value determined by stochastic motion of particles in the nonaxisymmetric field.

A common approach to regularize the transport in this regime is to add the $\mathbf{E}\times\mathbf{B}$ drift velocity to the drift-kinetic equations. With the addition of this term in NEO, we find that both the ion and electron $1/\nu$ regimes disappear and transition to a ν-scaled regime at very low frequency. We emphasize that the theory for the transport in this region is not rigorous since the $\mathbf{E}\times\mathbf{B}$ drift is a higher-order term in the drift-kinetic theory. In reality, the transport in this regime should be determined by orbit stochasticity. A proper reformulation of drift-kinetic theory for this regime has not yet been developed.

3.5 Gyrokinetics with Advanced Collision Operators (CGYRO)

The algorithmic design of GYRO focused on optimality for the collisionless limit and uses a coordinate system appropriate for this limit. The focus of gyrokinetic studies in ESL, however, has been the plasma region near the top of the pedestal (nonlinearly) as well as deep into the pedestal region (linearly). In both cases, collisions play a more critical role than in the core and now there is concern that more accurate collision operators, as well as numerical methods optimized for the strong collisionality regime, are appropriate. These considerations have motivated the plan to develop CGYRO.

A preliminary framework for a linear direct implicit gyrokinetic solver with more advanced collision models has been completed. This new approach uses the NEO (ξ,ε) velocity-space coordinate system rather than the standard GYRO/GS2 (ε,μ) coordinates to optimize the accuracy of the collision dynamics, particularly for multi-species collisions and including energy diffusion. The multi-species reduced Hirshman-Sigmar collision operator has been implemented with full cross-species collisional coupling.

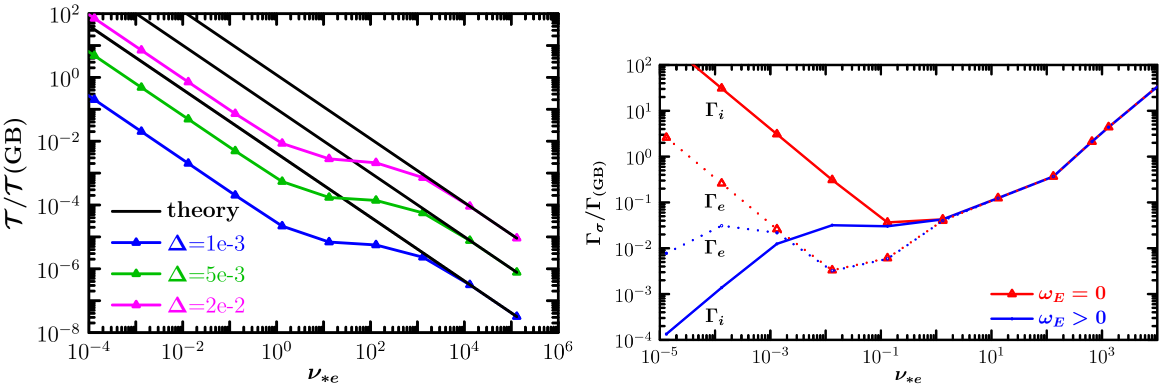

Figure 3: Verification of NEO calculation of the ion neoclassical toroidal viscosity (torque density, $\mathcal{T}$) with Pfirsch-Schlüter analytic theory for various values of $\Delta \sim \delta B$. Also, variation of the 3D non-ambipolar particle fluxes from NEO for $\Delta = 10^{-3}$. Addition of the $\mathbf{E}\times\mathbf{B}$ drift velocity (blue) removes the unphysical $1/\nu$ scaling at low collisionality but is theoretically *ad hoc*.

With this model we have been able to recover linear ITG growth rates and the collisional GAM test at moderate collision frequency. Work continues to improve the behavior in the collisionless regime, particularly for developing better methods to handle the trapped/passing particle boundary physics for kinetic electrons.

3.6 ELITE and the EPED Pedestal Model

ELITE [9, 10, 11] is a highly efficient MHD code aimed at the study of nonlocal, intermediate to high toroidal mode number (n) MHD instabilities of the tokamak edge transport barrier region. ELITE provides an efficient tool for quantifying and testing the peeling-ballooning model of ELMs, which holds that the pedestal height is constrained, and ELMs triggered, by intermediate wavelength (typically $4 < n < 30$) MHD modes driven by a combination of pressure and current gradients in the edge barrier region.

The EPED model combines peeling-ballooning calculations with ELITE with an integrated kinetic ballooning mode (KBM) constraint to predict the pedestal height and width [12, 13, 14], with no free or fit parameters. EPED has been extensively and successfully tested against a broad range of experiments on several tokamaks [15, 16, 13, 17, 18, 12] .

While ELITE and the EPED model were largely developed outside the ESL project, ESL has developed an improved diamagnetic stabilization model for EPED [13], and is engaged in further improving the model by inclusion of NEO-calculated bootstrap current and GYRO-calculated improvements to the KBM constraint.

In 2013, the physics understanding generated by work with ELITE and the EPED model, and its validation in an extensive series of experiments on DIII-D, was recognized by the John Dawson Award for Excellence in Plasma Physics Research.
http://www.aps.org/programs/honors/prizes/prizerecipient.cfm?last_nm=Snyder&first_nm=Philip&year=2013

Within ESL, ELITE stability analysis has been conducted on equilibria with NEO-calculated bootstrap current, with equilibrium reconstruction via the OMFIT framework (Figure 2)). For high collisionality cases it is found that the reduced bootstrap current calculated by NEO (relative to the Sauter model, which was previously used) moves the equilibrium toward the pressure-gradient driven part of the peeling-ballooning stability diagram, with the pedestal expected to be limited by somewhat higher-n instabilities.

Work is ongoing to directly couple NEO calculations of the bootstrap current into the EPED model, which uses sets of approximately100 equilibria per case to calculate the P-B and KBM constraints and predict pedestal height and width.

4 Near Future Plans

- 3D NEO will be parallelized for more extensive neoclassical studies, including examination of the effects of non-axisymmetries due to edge magnetic field ripple on the bootstrap current, including impurities.
- NEO bootstrap current calculations will be directly coupled to EPED.
- Develop tool to extract 2D equilibrium and small perturbations from numerical 3D MHD solution
- Further compare 3D NEO results and behavior with analytic results
- Develop more refined version of CGYRO with advanced (Sugama or full FP) collision operator

5 Presentations and Publications

- E.A. Belli, “Neoclassical Flows, Bootstrap Current, and Non-Axisymmetric Effects in the Plasma Edge”, 55th Annual APS Meeting of the Division of Plasma Physics, Denver, CO, Invited Talk, PI2 4, (Nov 2013).

- E.A. Belli, “Neoclassical Flows and Transport in the Tokamak Plasma Edge and Extensions to Include Non-Axisymmetric Effects”, 2013 International Sherwood Fusion Theory Conference, Santa Fe, NM, Invited Talk, (Apr 2013).

- E.A. Belli, J. Candy, O. Meneghini, and T.H. Osborne “Limitations of Bootstrap Current Models". Submitted to Plasma Phys. Control. Fusion (Nov 2013).

- M. N. A. Beurskens *et al.* (including P. B. Snyder), “Comparison of Hybrid and Baseline ELMy H-Mode Confinement in JET with the Carbon Wall," Nucl. Fusion **53** 013001 (2013).

- R. J. Groebner, C. S. Chang, J. W. Hughes, R. Maingi, P. B. Snyder *et al.*, “Improved Understanding of Physics Processes in Pedestal Structure, Leading to Improved Predictive Capability for ITER," Nucl. Fusion **53** 093024 (2013).

- J. W. Hughes, P. B. Snyder, J. R. Walk *et al.* “Pedestal Structure and Stability in H-Mode and I-Mode: A Comparative Study on Alcator C-Mod," Nucl. Fusion **53** 043016 (2013).

- M. J. Leyland (including P. B. Snyder), “Pedestal Study Across a Deuterium Fuelling Scan for High Delta ELMy H-Mode Plasmas on JET with the Carbon Wall," Nucl. Fusion **53** 083028 (2013).

- X. Litaudon *et al.* (including P. B. Snyder), “Modelling of Hybrid Scenario: from Present-day Experiments Towards ITER," Nucl. Fusion **53** 073024 (2013).

- P.B. Snyder, “Predicting and Optimizing Pedestal Structure in Existing and Future Devices," Transport Task Force Workshop, Santa Rosa CA (April 2013).

- P.B. Snyder, “Update on the EPED Model and Predictions for ITER," ITPA Pedestal Meeting, Garching, Germany (April 2013).

- P.B. Snyder, “The Use of EPED Pedestal Predictions in Integrated Modeling," ITPA Pedestal Meeting, Fukuoka, Japan (Oct 2013).

- P.B. Snyder, “Implications of Edge Stability and the EPED Model for RMP ELM Suppression," ITPA Pedestal Meeting, Fukuoka, Japan (Oct 2013).

- P.B. Snyder, “Optimizing Pedestal Performance with the EPED Model," APS/DPP Conference, Denver CO (Nov 2013).

- P.B. Snyder, “How the Tail Wags the Dog: Understanding the Physics of the H-Mode Pedestal and ELMs in Tokamaks," invited talk, 23rd International Toki Conference, Toki, Japan (Nov 2013).

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