UCRL-JC-130166
PREPRINT

Simulation of Ion-Temperature-Gradient Turbulence in Tokamaks

A.M. Dimits
B.I. Cohen
N. Mattor
W.M. Nevins
D.E. Shumaker
S.E. Parker
C. Kim

This paper was prepared for submittal to
17th IAEA Fusion Energy Conference
Yokohama, Japan
October 19-24, 1998

October 14, 1998

Lawrence Livermore National Laboratory

SIMULATION OF ION-TEMPERATURE-GRADIENT TURBULENCE IN TOKAMAKS[1]

A.M. DIMITS, B.I. COHEN, N. MATTOR, W.M. NEVINS,
D.E. SHUMAKER
Lawrence Livermore National Laboratory
Livermore, CA 94551
USA

S.E. PARKER, C. KIM
University of Colorado
Boulder, CO 80309
USA

Abstract

Results are presented from nonlinear gyrokinetic simulations of toroidal ion temperature gradient (ITG) turbulence and transport. The gyrokinetic simulations are found to yield values of the thermal diffusivity significantly lower than gyrofluid or IFS-PPPL-model predictions. A new phenomenon of nonlinear effective critical gradients larger than the linear instability threshold gradients is observed, and is associated with undamped flux-surface-averaged shear flows. The nonlinear gyrokineic codes have passed extensive validity tests which include comparison against independent linear calculations, a series of nonlinear convergence tests, and a comparison between two independent nonlinear gyrokinetic codes. Our most realistic simulations to date have actual reconstructed equilibria from experiments and a model for dilution by impurity and beam ions. These simulations highlight the need for still more physics to be included in the simulations.

1. INTRODUCTION

The results of nonlinear δf-particle simulations of toroidal ion temperature gradient(ITG) turbulence are reported here. This work is motivated by the need to develop models of the anomalous transport of heat, particles, and momentum in tokamaks and other magnetic plasma confinement devices [1]. Toroidal ITG turbulence is considered to be a likely mechanism to explain thermal and momentum transport, however the quantitative picture is still incomplete.

Tremendous advances both in simulation algorithms and computer power, as well as investments in using this power effectively have made nonlinear δf gyrokinetic simulation a practical tool for studying ITG and other (e.g., trapped-electron) microturbulence for realistic plasma parameter values. This provides opportunities both for direct simulation studies and for better characterization of the turbulence, which may lead to better theories. There are also opportunities for the discovery of new phenomena, both because of limited range of existing nonlinear code parameter studies in the very large ($>$ 7-dimensional) parameter space and because of the limitations of the various reduced treatments of the kinetic processes.

The IFS-PPPL model [2] has attracted attention because of its success in interpreting some plasmas. This model combines nonlinear gyrofluid and quasilinear gyrokinetic calculations into a single transport model. However, we have found that for some relevant experimental conditions, gyrokinetic simulations give a value of the thermal diffusivity χ_i roughly a factor of 3 lower than gyrofluid simulations even though the gyrofluid model is supposed to be an approximation to the gyrokinetic equations. Such differences may have a significant impact on predictions of tokamak (e.g., ITER) plasma performance. It is therefore of great importance and interest to

[1]This work was performed by LLNL for USDoE under contract W-7405-ENG-48, and is part of the US NTTP and Cyclone projects.

assess, and if possible establish, the validity of the gyrokinetic results.

2. NONLINEAR GYROKINETIC SIMULATION CODE AND NUMERICAL PARAMETERS

This paper discusses results from two independent codes (LLNL and U. Colorado, Boulder) which incorporate the advances mentioned above, including δf algorithms [3, 4], field aligned numerical representation [5], and flux-tube simulation domains [6, 7]

The codes used here are toroidal, nonlinear, and electrostatic, with a single fully toroidal nonlinear gyrokinetic ion species [8], and with equilibrium temperature, density, and velocity gradients. The gyrokinetic Vlasov equation is solved using the partially linearized δf particle method [3, 4]. The electron response is taken to be adiabatic, with a zero response to the flux-surface-averaged potential $\langle\phi\rangle_{\theta,\phi}$ [9]. Self-generated turbulent-Reynolds'-stress-driven flows, and equilibrium scale "external flows" are included. The simulation domain used is a flux tube which spans one or more poloidal circuits in the parallel direction. Profile relaxation [9] is prevented by making the simulation volume periodic, with a "twist-shift" radial periodicity condition [4] and parallel periodicity consistent with the mode physics.

Typical numerical parameters are timestep $dt\, c_s/L_T = 0.2$, where $c_s \equiv \sqrt{T_e/m_i}$, T_e is the electron temperature, m_i is the ion mass, L_T is the temperature gradient scale length, perpendicular grid sizes $\Delta_x/\rho_s = \Delta_y/\rho_s = 0.8$–$1.0$, where $\rho_s = c_s/\Omega_i$, and Ω_i is the ion gyrofrequency, grid cell numbers $N_x = N_y = 128$, and $N_z = 32$–64. The thermal diffusivity is defined as

$$\chi_i = 1.5 L_T \langle \tilde{V}_x \tilde{T}_i \rangle / T_i,$$

and is calculated as a suitably weighted sum over the simulation particles. For sufficiently large box sizes χ_i/χ_{GB}, where $\chi_{GB} \equiv \rho_s^2 c_s/L_T$, is finite and becomes independent of the box size. The transport therefore has a clear gyroBohm scaling, irrespective of the magnetic shear.

3. TEMPERATURE GRADIENT SCANS

Figure 1 shows the predictions for χ_i vs. R/L_T, where R is the major radius, for a scan about the "Cyclone DIII-D base case" parameters. This parameter set represents local parameters from an ITER-relevant DIII-D plasma, shot #81499, at time $t = 4000$ms., and $r/a = 0.5$, where r is the minor radius and a is the minor radius of the separatrix. The parameter values, in dimensionless form are $\eta_i \equiv L_n/L_T = 3.114$, where L_n and L_T are respectively the the density and temperature gradient scale lengths, magnetic "safety factor" $q \equiv rB_t/RB_p = 1.4$, where R is the major radius and B_t and B_p are the toroidal and poloidal magnetic field components, $\hat{s} \equiv (r/q)dq/dr = 0.78$, $R/L_T = 6.92$, and $\epsilon_B \equiv r/R = 0.18$. These simulations used circular cross-section model equilibria and a single dynamical (bulk) ion species, as did the nonlinear gyrofluid simulations that underly the IFS-PPPL model.

Shown are the results from our (LLNL and U. Col. Boulder) gyrokinetic simulations and from the IFS-PPPL model, as well as a similar scan (using the LLNL gyrokinetic code) with $\epsilon = 0$. For the base parameter value $R/L_T = 6.92$, the gyrokinetic χ_i is about a factor of 3 lower than that give by the IFS-PPPL-model, which is somewhat larger than was observed for the TFTR "NTP test case" [10]. The relative disagreement between the gyrokinetic results and the IFS-PPPL formula becomes smallest at $R/L_T \simeq 14$, and is largest for smaller values of R/L_T. Part of the disagreement comes from differing values in the critical R/L_T, which is approximately 4.0 for these parameters. It is important to note that these differences cannot be characterized by a simple ratio, or multiplication factor. Beer [11] has verified that for this parameter scan, nonlinear gyrofluid simulations agree reasonably well with the IFS-PPPL model

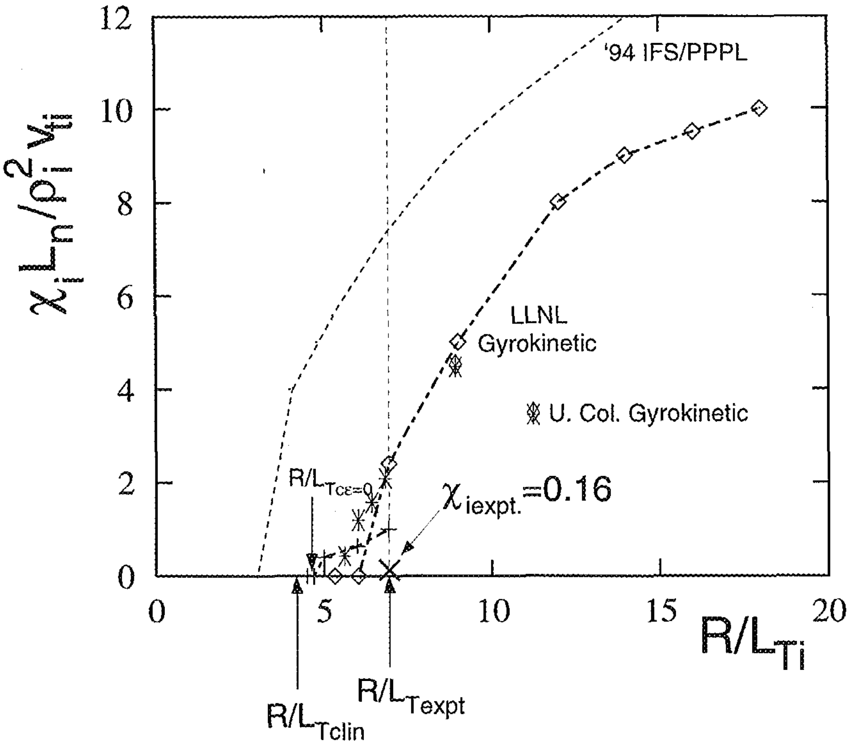

Figure 1: Normalized χ_{i} vs R/L_{Ti} from gyrokinetic simulations, and '94 IFS-PPPL model

(within 27% for $R/L_{\text{T}} = 4.0$–9.0).

4. LINEAR TESTS

In order to establish confidence in the gyrokinetic simulation results, both linear benchmarks and nonlinear tests have been undertaken.

The linear ITG-mode frequencies and growth rates and critical temperature gradients obtained from the LLNL gyrokinetic code have been found to agree very well with independent linear codes [11], both for the Cyclone base case and for a case with the same local parameters, except $\epsilon \equiv r/R = 0$.

A second linear test is based on the linear damping of purely radial modes of the electrostatic potential, i.e., modes which have no variation within a flux surface. This damping is a linear process. A theory for the residual levels of these modes in the collisionless limit has been given by Rosenbluth and Hinton [12]. In the numerical experiment, the gyrokinetic code is initialized with zero δf particle weights. A radially sinusoidal potential with no variation within the flux surfaces, which represents a near poloidal $\boldsymbol{E} \times \boldsymbol{B}$ flow, is imposed. The particle weights evolve, resulting first in geodesic acoustic oscillations which eventually damp. In the large aspect-ratio limit, the theoretical prediction for the ratio of the late-time residual potential to the initial potential is given as a function $0.6h/(1.0 + 0.6h)$ of the single parameter $h \equiv \sqrt{\epsilon}/q^2$ [12].

Figure 2 shows the fractional residual $\boldsymbol{E} \times \boldsymbol{B}$ flows for two scans done with the flux-tube gyrokinetic code, along with the R-H prediction. In one scan, q is varied, while in the other scan ϵ is varied. Very good agreement is observed, lending confidence to both the RH theory and the simulation.

5. EFFECTIVE NONLINEAR CRITICAL GRADIENT

A new result for the gyrokinetic simulations, evident in Fig. 1, is that there is a range of values of the normalized temperature gradient R/L_{T}, between the linear critical gradient R/L_{Tcrit} and an effective nonlinear critical gradient R/L_{Teff} in which the simulations are linearly

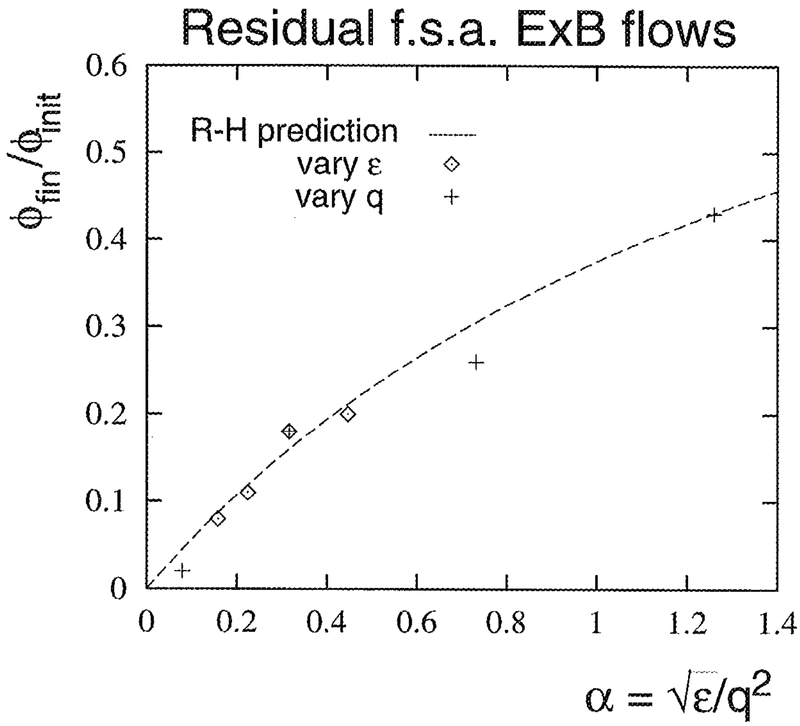

Figure 2: Residual flux-surface-averaged flow fraction vs. Rosenbluth-Hinton parameter $\sqrt{\epsilon}/q^2$. Points are gyrokinetic code results; line is RH prediction.

unstable, but for which the thermal transport at late time becomes essentially zero. This phenomenon appears to be associated with undamped $\boldsymbol{E} \times \boldsymbol{B}$ flows predicted by Rosenbluth and Hinton [12]. A large, very steady flux-surface-averaged potential $\langle\phi\rangle_{\theta,\phi}$ is observed in the cases with $R/L_{\mathrm{Tcrit}} < R/L_{\mathrm{T}} < R/L_{\mathrm{Teff}}$. In contrast, for cases with $R/L_{\mathrm{T}} > R/L_{\mathrm{Teff}}$, the profiles of $\langle\phi\rangle_{\theta,\phi}$ move as time evolves. The peak shearing rates associated with $\langle\phi\rangle_{\theta,\phi}$ are of order three times the growth rate of the fastest growing ITG modes.

In the $\epsilon = 0$ gyrokinetic simulation scan shown in Fig. 1, there is no discernible separation between R/L_{Teff} and R/L_{Tcrit}. This is to be expected if the undamped Rosenbluth-Hinton flows play a key role in the departure of R/L_{Teff} from R/L_{Tcrit}, since the residual flow fraction goes to zero as ϵ goes to zero.

The role of these flows in the gyrokinetic-gyrofluid differences for $R/L_{\mathrm{T}} > R/L_{\mathrm{Teff}}$ will be investigated in the future.

6. NUMERICAL CONVERGENCE

Next, we examine noise in the flux-tube gyrokinetic simulations, and address the possibility of nonconvergence with respect to particle number. Fig. 3 shows χ_{i} vs. time from a particle number scan. The simulations are for different numbers of particles ranging from 5×10^5 to 1.34×10^8. For 10^6 or more particles, χ_{i} at late time does not appear change with increasing particle number. There is some random variation, but this is small, has no systematic dependence on particle number and is most likely due to the initial conditions being different realizations of a random variable. There is some increase in the level of the initial peak which persists even if the scan is done increasing the initial weights (as the square root of the particle number) so as to keep the initial mean noise level fixed. The 5×10^5-particle case shows secular growth in χ_{i} beyond Time = 700. This is due to a noise-driven runaway process in which the detailed δf-particle entropy, most of which is due to noise, increases with the time integral of χ_{i}. The noise causes thermal transport (χ_{i}), both of which increase together. The primary conclusion is

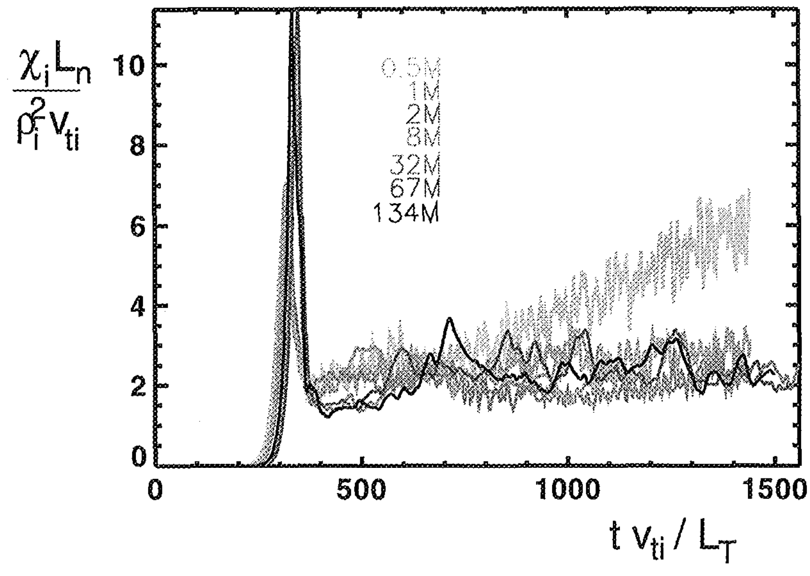

Figure 3: Normalized χ_i vs. tv_{ti}/L_T from gyrokinetic simulations with particle numbers ranging from 5×10^5 to 1.34×10^8.

that χ_i appears to be converged wrt. particle number for 2–4 or more particles per cell.

In order to further assess the impact of particle discreteness, the following scrambling test [13] of the noise level was performed. The gyrokinetic code was run using Cyclone base case parameters, for 8×10^6 and 1.6×10^7 particles, and restart files were saved at selected times. New restart files were formed from these by scrambling the particle δf weight list. The gyrokinetic code was restarted from these scrambled restart files. The scrambled restart eliminates the physical signal but leaves fluctuations whose level is a measure of the noise in the simulation due to particle discreteness. After the restart, the temperature gradient was reduced to slightly below the linear marginally stable value in order to eliminate unstable ITG modes, but to still allow measurement of (noise-driven) diffusion through a transport flux. Shown in Fig. 4 is the time histories of χ_i, both in the absence of scrambling and when the scrambling and gradient reduction is done at three times during the run. χ_i is reduced after the scrambling. The relative reduction is less the later the scrambling is done, indicating a gradual buildup of noise. However, even at the latest time, the post scrambling values are down by an order of magnitude. This indicates that the relative impact of noise is small (or at most moderate at the latest time), and supports the conclusion that the simulations are converged with respect to particle number.

Thus, for the Cyclone DIII-D base case, numerical convergence is achieved with 2–4 particles per cell in our code. An exception has been observed for cases with $R/L_{\mathrm{Tcrit}} < R/L_{\mathrm{T}} < R/L_{\mathrm{Teff}}$. It is found that R/L_{Teff} increases slowly with particle number, so that for the Cyclone base case R/L_{T} scan, for example, $R/L_{\mathrm{Teff}} > 6.0$, but at least ~ 64 particles per cell are needed for an $R/L_{\mathrm{T}} = 6.0$ case to yield zero χ_i.

We have also undertaken simulations that demonstrate convergence with respect to parallel and perpendicular system size and with respect to parallel and perpendicular spatial resolution. The results demonstrate that the values typically used in our simulations are adequate for

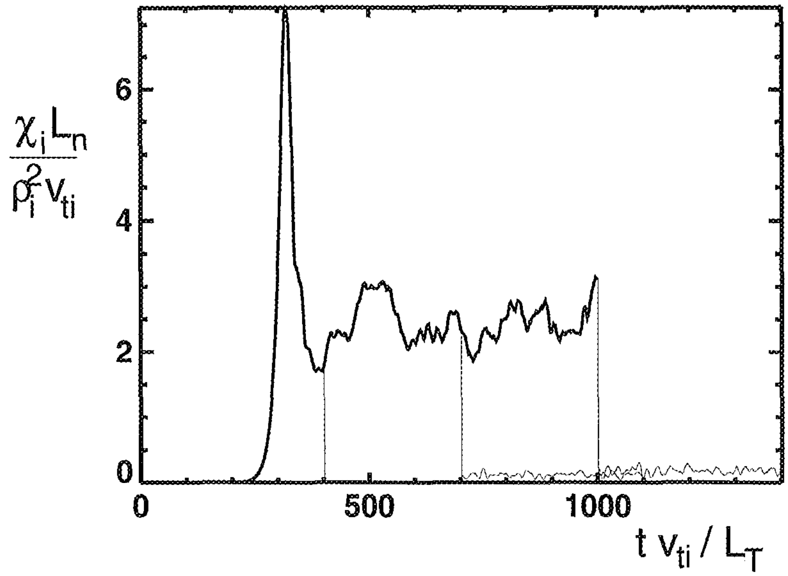

Figure 4: Normalized χ_i vs. time from Cyclone DIII-D base case and three scrambled restarts.

numerical convergence.

7. SIMULATIONS USING REALISTIC EXPERIMENTAL EQUILIBRIA

The LLNL gyrokinetic code has been extended to use realistic equilibra, obtained by direct reconstruction from experimental data, as well as a dilution model for the effects of impurity and beam ion species. Figure 5 shows the χ_i vs. normalized minor radius ρ from such simulations for DIII-D shot #84736 at t=1200ms. This shot is a high-performance negative-central-shear ("NCS") L-mode plasma with an internal transport barrier. The simulations show order-of-magnitude agreement with the experiment, but the wrong trend with minor radius. Several additional physics effects are expected to produce order-one changes in χ_i, including nonadiabatic electrons, active impurity dynamics, collisions, velocity shear, and radial profile variation.

Shown in Fig. 5 is a simulation result, at $\rho = 0.3$, in which the equilibrium scale perpendicular and parallel velocity shear components inferred from the experimental data were included. This reduced the turbulent χ_i to zero, in agreement with the observation that at $\rho = 0.3$, the transport is neoclassical.

8. SUMMARY AND CONCLUSIONS

In summary, in this work some new phenomenology of ITG turbulence has been shown, as were several linear and nonlinear tests and comparisons which add considerably to the for the validity and viability of gyrokinetic simulations. This work supports now widely held views on the physical importance of the effects of shear flows in moderating ITG turbulent transport. While there has been much progress on including many important physical effects in the gyrokinetic codes, much more is needed. Having established some confidence in the method, attention can now be devoted to these important physics enhancements. Some investigations of the effects of realistic equilibria, profile-scale velocity shear and temperature-gradient variation have been made. Nonadiabatic electrons, collision models, and dynamically active impurity species are all important effects that need to be included as self-consistently as possible in the simulation

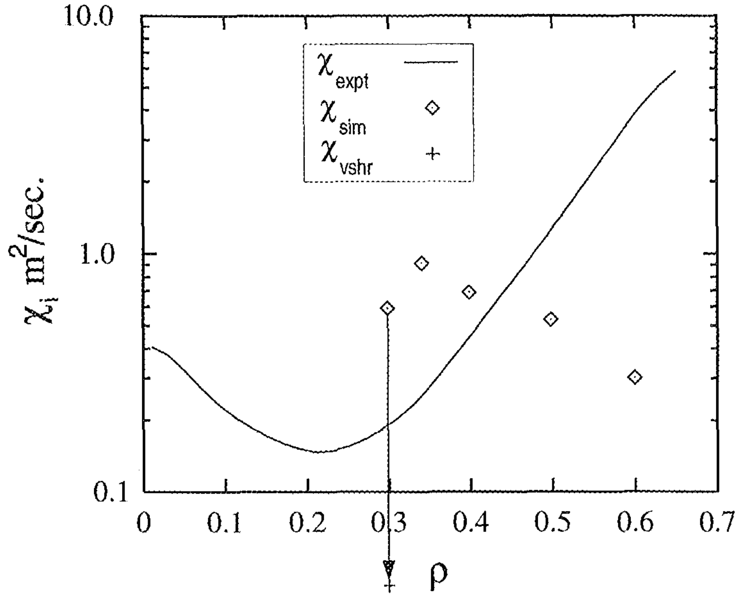

Figure 5: χ_i vs. normalized minor radius from DIII-D shot 84736, t=4000ms. The points are all with zero external velocity shear except the one at the end of the arrow.

model. Work is underway to do so.

ACKNOWLEDGMENTS

The simulations were done on the NERSC T3E. We thank C. Bolton for his encouragement and support, as well the Cyclone team, especially M. Beer, W. Dorland, G. Hammett, M. Kotschenreuther for fruitful discussioins. This work was performed under the auspices of U.S. Department of Energy (DoE) by Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48, and is part of the Numerical Tokamak Turbulence Project supported by the High Performance Computing and Communications Program in the U.S. DoE, as well as the DoE-OFE Cyclone Initiative.

References

[1] See, for example, T.C. Luce *et al.*, in *Proc. 15th. Int. Conf. on Plasma Physics and Controlled Nuclear Fusion* (1995, IAEA), paper A-2-III-2.

[2] W. Dorland, M. Kotschenreuther, M.A. Beer, G.W. Hammett, R.E. Waltz, R.R. Dominguez, P.M. Valanju, W.H. Miner, J.Q. Dong, W. Horton, F.L. Waelbroeck, T. Tajima, and M.J. LeBrun, in *Plasma Physics and Controlled Nuclear Fusion Research, 1994*, paper IAEA-CN-60/D-P-I-6.

[3] A. M. Dimits, Ph.D. thesis, Princeton University, Feb. 1988; A. M. Dimits and W. W. Lee, J. Comp. Phys. **107**, 309 (1993).

[4] M. Kotschenreuther *et al.*, in *Proc. 14th. Int. Conf. on Plasma Physics and Controlled Nuclear Fusion, 1992* (1993, IAEA, Vienna), Vol. 2, 11.

[5] A. M. Dimits, Phys. Rev. E**48**, 4070 (1993).

[6] P.N. Guzdar, J.F. Drake, D. McCarthy, A.B. Hassam, and C.S. Liu, Phys. Fluids B**5**, 3712 (1993).

[7] M. A. Beer, S. C. Cowley, and G. W. Hammett, Phys. Plasmas **2**, 2687 (1995).

[8] E. A. Frieman and Liu Chen, Phys. Fluids **25**, 502 (1982).

[9] B.I. Cohen, T.J. Williams, A.M. Dimits and J.A. Byers, Phys. Fluids B**5**, 2967 (1993).

[10] A.M. Dimits *et al.*, PRL **77**, 71 (1996).

[11] M.A. Beer (1997, private communication).

[12] M.N. Rosenbluth and F.L. Hinton, PRL **80**, 724 (1998).

[13] The scrambling noise test was proposed originally by M. Kotschenreuther, and valuable variations and refinements were suggested by W. Dorland and G.W. Hammett in private communications dating between 1995 and 1997.