UCRL-PRES-231533

Edge Simulation Laboratory (ESL)

Progress and Plans

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edge
simulation
laboratory

PSACI Meeting, PPPL
June 7-8, 2007

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Work at UC LLNL performed under the auspices of the U.S. Department of Energy under contract No. W-7405-Eng-48

OUTLINE

Edge Simulation Laboratory

- ESL at a glance
- ESL components: recent progress
- Plans

Some recent publications:

- X.Q. Xu, K. Bodi, J. Candy, B. I. Cohen, R. H. Cohen, P. Colella, M. R. Dorr, J. A. Hittinger, G. D. Kerbel, S. Krasheninnikov, W. M. Nevins, H. Qin, T. D. Rognlien, P. B. Snyder, M. V. Umansky, Z. Xiong, "Continuum Edge Gyrokinetic Theory and Simulations", in Fusion Energy 2006 (Proc. 21st Int. Conf. Chengdu, 2006) (Vienna: IAEA) CD-ROM file TH/P6-23 and http://wwwnaweb. iaea.org/napc/physics/FEC/FEC2006/html/index.htm
- H. Qin, RH Cohen, WM Nevins and XQ Xu, Contrib. Plasma Phys., **46**, 477 (2006)
- H. Qin, RH Cohen, WM Nevins and XQ Xu, Phys. Plasmas, 14, 056110 (2007).
- X.Q. Xu , Z. Xiong, M.R. Dorr, J.A. Hittinger, et al., "Edge Gyrokinetic Theory and Continuum Simulations", accepted by Nuclear Fusion.
- Z.Xiong, R. Cohen, T. Rognlien and X. Xu, "A high-order finite-volume algorithm for Fokker-Planck collisions in magnetized plasmas", submitted to J. Comp. Phys.
- X.Q. Xu, A. Xiong, W. Nevins and G. McKee, "TEMPEST simulations of collisionless damp-ing of GAM and neoclassical residual in edge plasma pedestal", submitted to Phys. Rev. Lett.
- R.H.Cohen and X.Q.Xu, (2007), "Progress in Kinetic Simulation of Edge Plasmas" , submitted to Contrib. Plasma Phys.

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What is the ESL?

- Edge Simulation Laboratory (ESL): a project to develop gyrokinetic simulation for MFE edge plasmas based on continuum (Eulerian) techniques
- Why continuum?
  - Concerns about PIC noise in environment where there are large density variations and where full f is required
  - Exploit advanced numerical methods from fluids community
  - Build on successes of continuum core codes (GYRO, GS2, GENE)
- ESL is a collaboration:
  - LLNL, GA, UCSD, LBNL, PPPL, Lodestar, CompX. Others welcome.
  - Present funding: OFES
    - 0.8 FTE LLNL
    - Postdoc + ε FTE GA
    - Grad student at UCSD
    - Associated math activity in algorithm research, 1/2 FTE each at LBL, LLNL

ESL has three funded components

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- TEMPEST code (outgrowth of LLNL LDRD project; full geometry, full-f, E-μ finite difference.)
- EGK: prototyping code, $v_{||}$-μ, simple geometry; finite difference; presently linear
- Math component: develops and implements algorithms for a next-generation code
- Not funded, but needed: a computer science component which would develop software infrastructure, provide user support, and address needs for data handing and analysis

TEMPEST is a full-f, full-geometry edge kinetic code

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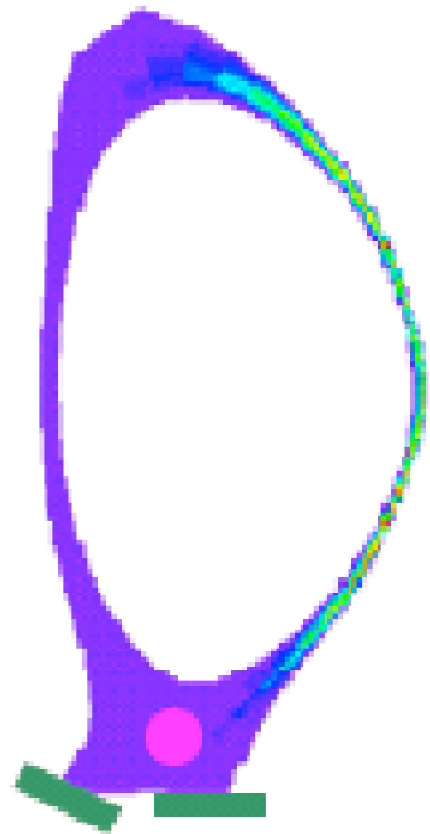
- 5D ($\psi,\theta,\zeta,E_0,\mu$); results here 4D
  - E_0-μ choice for accurate || streaming
- Full f, but also δf option
- Electrostatic (EM deferred to next gen. code)
- Geometry options:
  - Shifted circle core
  - Full single-null diverted, closed-flux-surface + SOL
- Implicit backward-differencing time advance; Newton-Krylov iteration
- 4th-order upwinded finite-difference spatial discretization, and Weno
- Low-order finite-volume discretization for collisions
- Collision options
  - Krook
  - Lorentz with full v dependence
  - Full collision op. with test-particle or fully nonlinear Rosenbluth potentials



EGK is a simple-geometry rapid-prototype code

- “Rapid-prototype code” to explore physics, coordinate, and algorithm issues associated with edge simulation
- Geometry: circular, no SOL
- Currently:
  - δf
  - $v_{||}$-μ coordinates
  - Lorentz collisions
  - Electrostatic
  - Adiabatic or gyrokinetic electrons
- Themes for exploration:
  - Tradeoffs of $v_{||}$-μ representation (vs. E-μ for TEMPEST, E_k, $v_{||}/v$)
    - Plusses: simple volume element; simple representation of parallel nonlinearity
    - Minuses: $\mu \, \partial B/\partial s \, \partial f/\partial v_{||}$ trapping term bridging passing-trapped boundary can be numerically challenging
  - Unified treatment of neoclassical transport and turbulence

Next-generation ESL code will build on experiences from TEMPEST, EGK and core codes

- Conservative form of GK equations
- 4th order finite-volume (conservative) discretization
- $v_{||}$-μ coordinates (tentatively)
- Arbitrarily mapped multiblock grids, field-aligned on block (allowing for shifts at any box boundary), to handle magnetic shear
- AMR capability
- Electrostatic initially; subsequently EM
- Math team developing algorithms to enable this

TEMPEST and EGK have been tested by simulating geodesic acoustic modes (GAMs)

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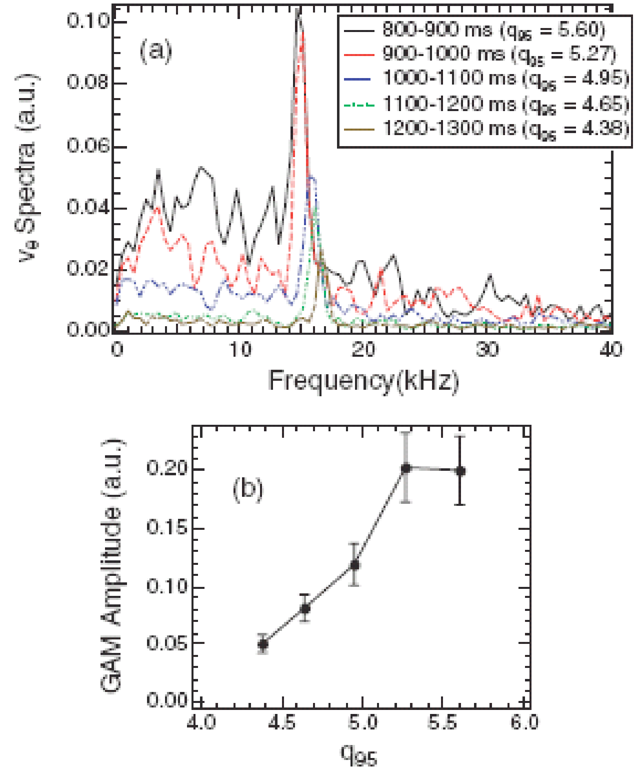
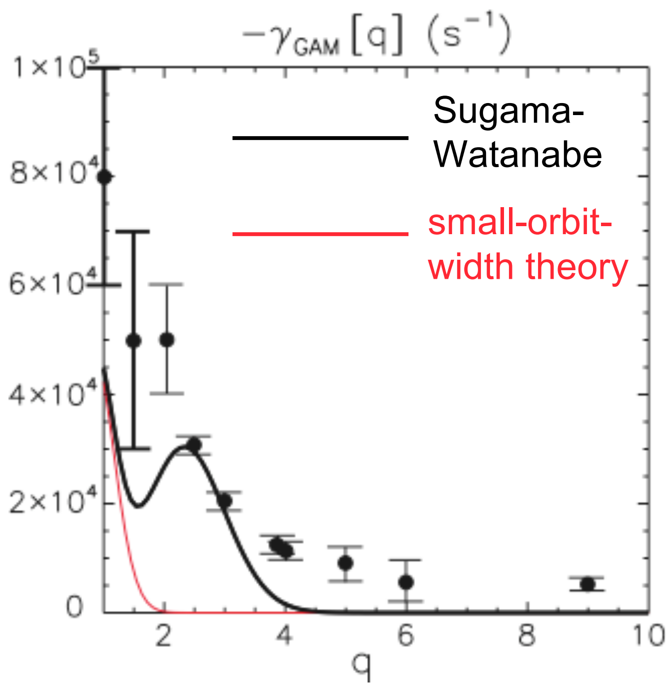
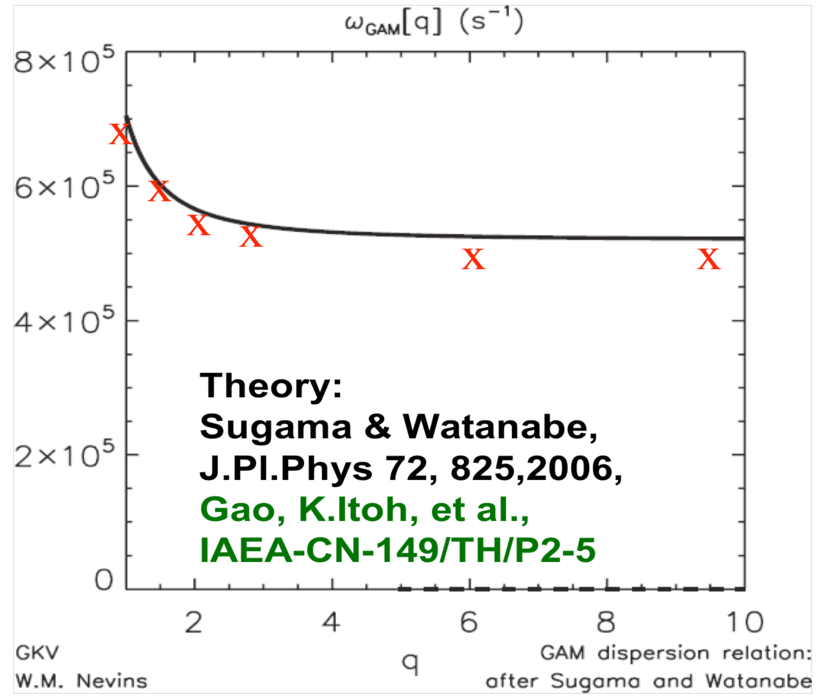
- Geodesic acoustic modes (GAMs): a coherent poloidal flow oscillation
- Why we are interested:
  - A good test problem
  - Clearly identified experimentally
  - May dominate in edge
- Setup:
  - TEMPEST: Full-f, nonlinear
  - EGK: δf, linear
  - Both codes: drift-kinetic ions, Boltzmann electrons
  - "Ring" geometry, periodic radial b.c.'s
  - Homogeneous plasma with initial sinusoidal perturbation



DIII-D BES GAM expt.
Mckee, PPCF, 48, s123(2006)

TEMPEST results for GAM decay rate and real frequency agrees reasonably with Sugama-Watanabe theory





Note DIII-D experimental result (previous slide) suggests significant damping for q < 5.

TEMPEST and EGK scan of GAM residual versus ε agree with each other and with Xiao-Catto

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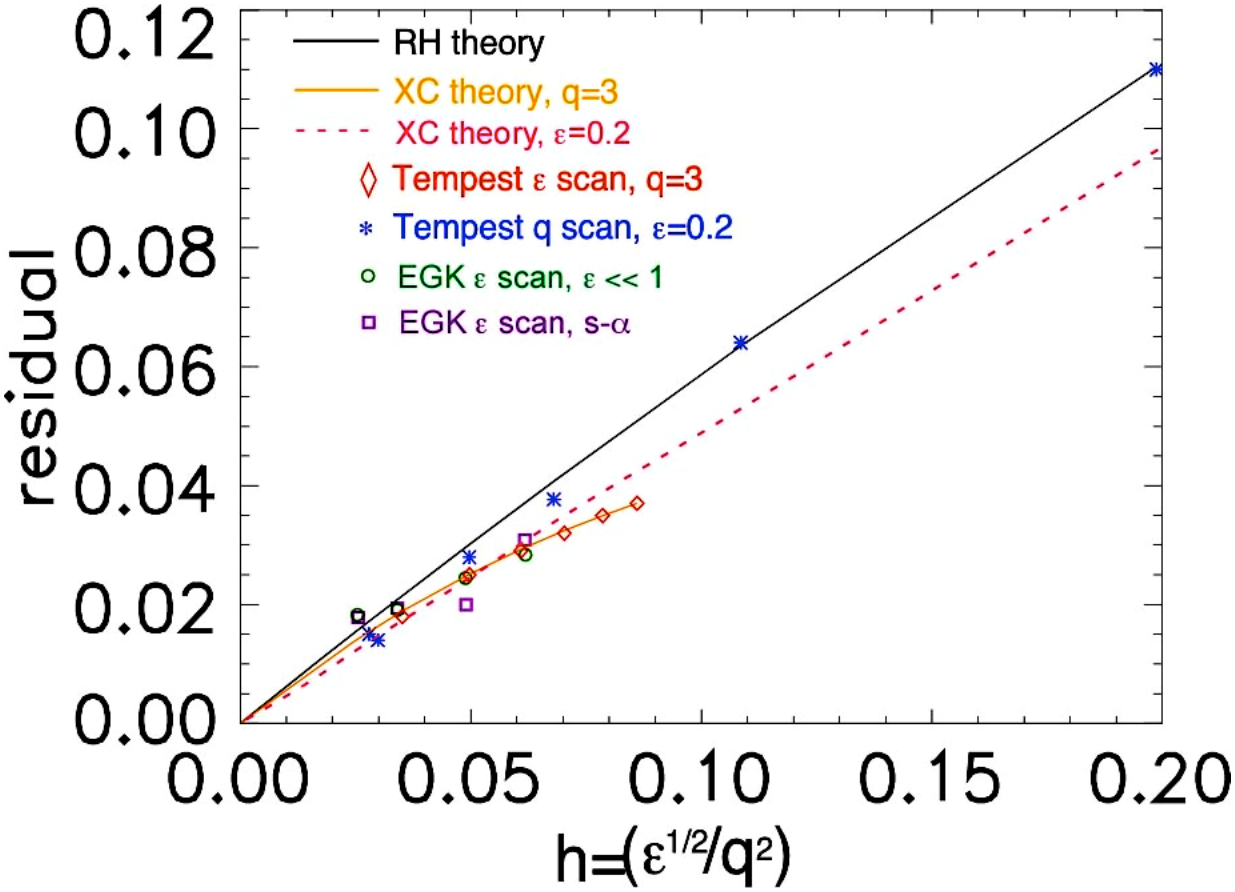
- But TEMPEST q scan agrees somewhat better with older (Rosenbluth-Hinton) result.



TEMPEST and EGK are both exploring neoclassical transport with goal of unified treatment of NC and turbulence.

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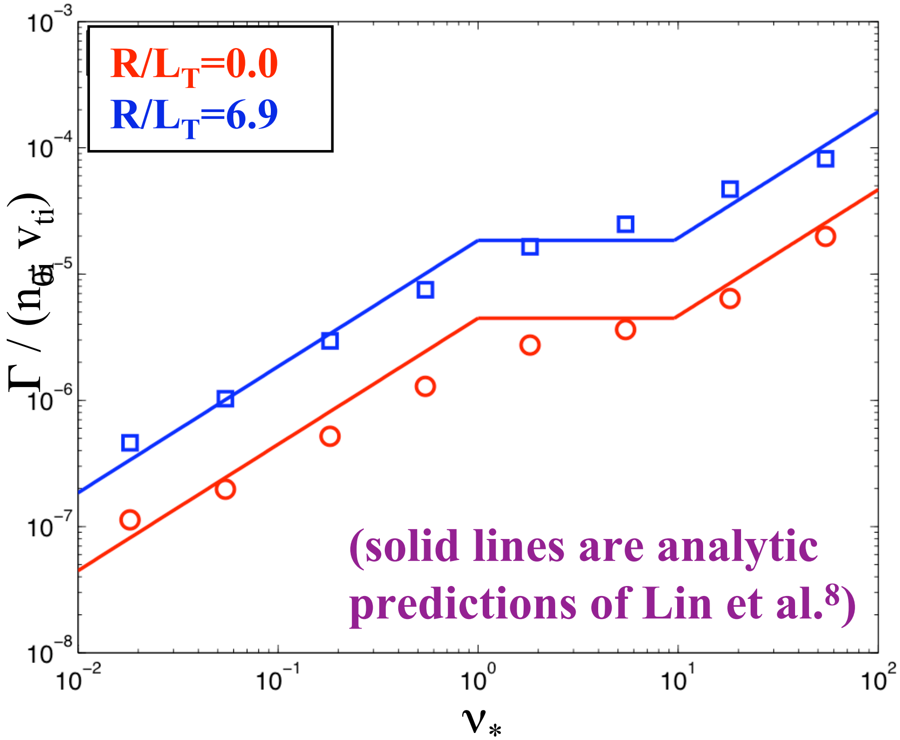
- EGK studies: δf with neoclassical driving terms; Lorentz collisions with constant ν with momentum-conserving corrections.
  - Current thrusts: 2D potential solution; electron heat flux
  - Approach: recognizing that in k_r=0 limit GK-Poisson has no explicit phi dependence (just statement of quasineutrality), treat parallel free-streaming implicitly.
- TEMPEST studies: full-f. Lorentz collisions with energy-dependent ν.
  - Current thrusts: solution with large gradients; solution in diverted geometry; comparison with XGC.

Radially local EGK has been benchmarked against neoclassical results

$E_r^0=0$

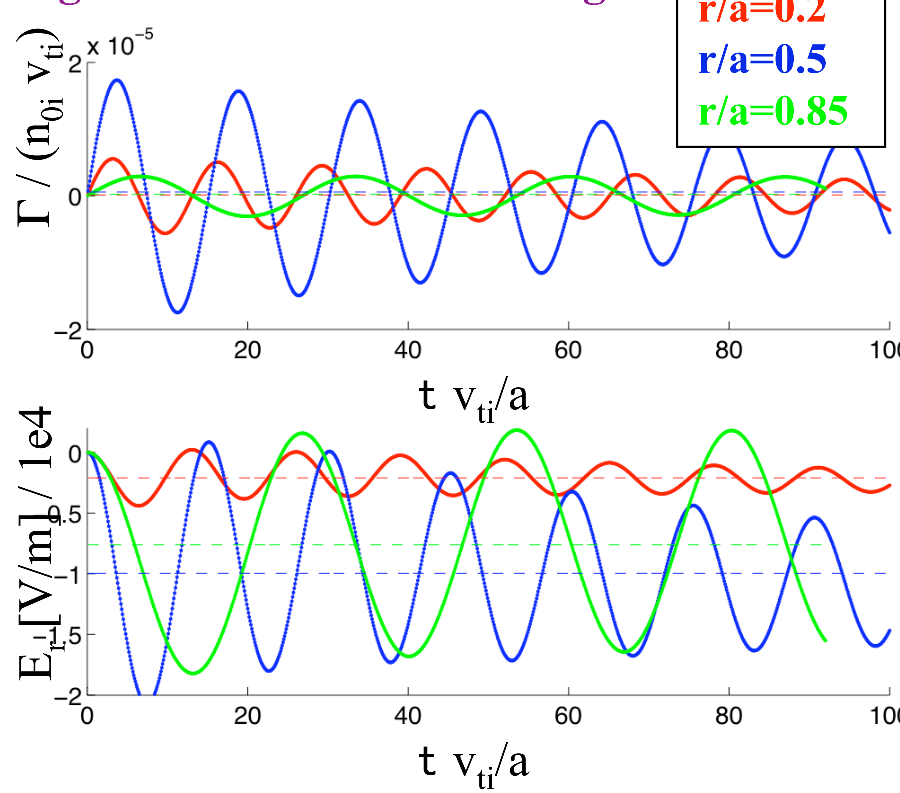


$r/R=0.18$ $\rho/R=0.001$
$q=1.388$ $R/L_n=2.2$

8) Phys. Plasmas **2**, 2975 (1995)

Including E_r^0 (vorticity eqn coupling)

Agrees with Satake et al.[7] fig. 4



$R/a=4.0$ $\rho/a=0.0039$ n, T vary
$q=3.0$ $\nu/v_{ti}/a=0.1$ R/L_n, R/L_T vary

Preliminary EGK results ⇒ while $\Phi = \Phi(\theta)$ does not significantly affect ion dynamics, it does produce enhanced electron heat flux.

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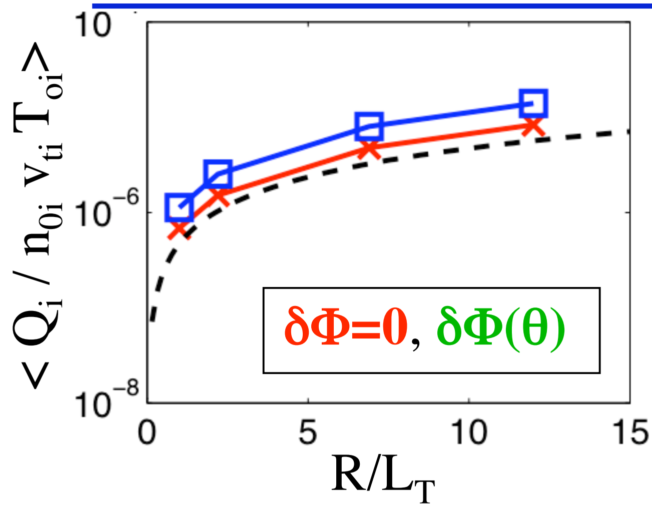
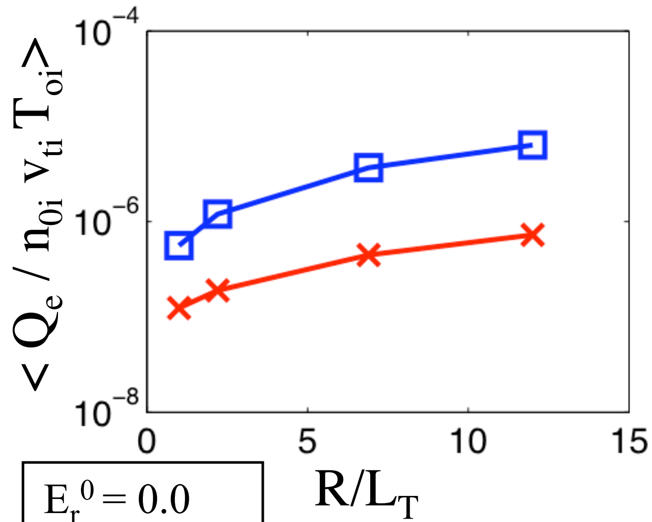
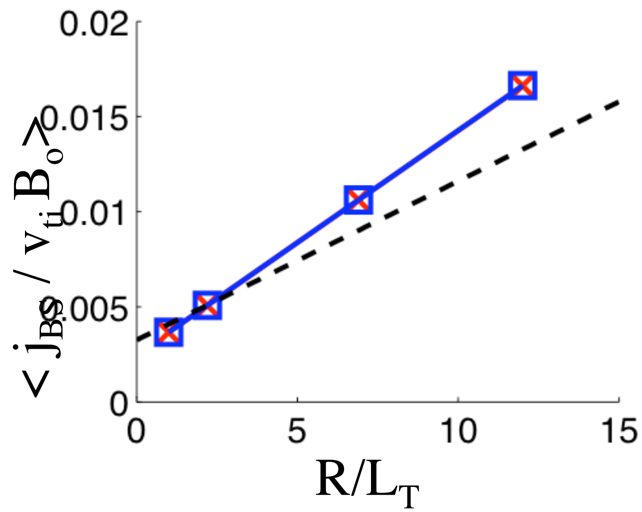


This effect on Q qualitatively agrees with the analytical prediction of Stringer et al.[10]





$E_r^0 = 0.0$
$\nu_* = 0.18$

The ion heat flux and the bootstrap are also in agreement with theory. Here we show the models of Chang-Hinton[11] and Sauter et al. [12] in the $\nu_*=0$ limit. For direct comparisons with analytical neoclassical theory, a more realistic collision operator is needed. This will be explored next.

10) Phys. Fluids B **3**, 981 (1991) 11) Phys. Fluids **25**, 1493 (1982) 12) Phys. Plasmas **6** 2834 (1999)

We have done cross-code comparisons of TEMPEST with XGC-0 (divertor geometry)

- Simulations based on common EFIT files (DIIID #096333)
- Tanh initial T_i and n radial profiles, centered at $\psi_N = 0.99$, half width 0.02; $T_{i,max} = 1$ keV, $n_{i,max} = 0.5 \times 10^{14}$ cm^{-3}; T_i, n_i min 0.1 times max. Poloidally constant on separatrix.
- $\Phi = 0$; Lorentz collisions
- For Tempest: resolution npol*nrad*nE*nμ = 50*40*40*50
- Caveats:
  - Different versions of Lorentz collisions:
    - Tempest run is with Lorentz with constant n and T (= values at inner bounary).
    - XGC run is with Lorentz with local (and periodically updated) n and T.
  - Different boundary conditions, and this should matter!
    - Tempest: specify f_{in} on boundary
    - XGC: continued collisionless orbits on boundary
  - VERY preliminary. 1st run-of-kind for TEMPEST.
- Have also done in comparisons in closed-flux-surface geometry, collisional scans a la EGK, and 2D field solve (Krook collisions in plateau regime; kinetic electrons)

TEMPEST-XGC Divertor comparison: results similar to expected degree

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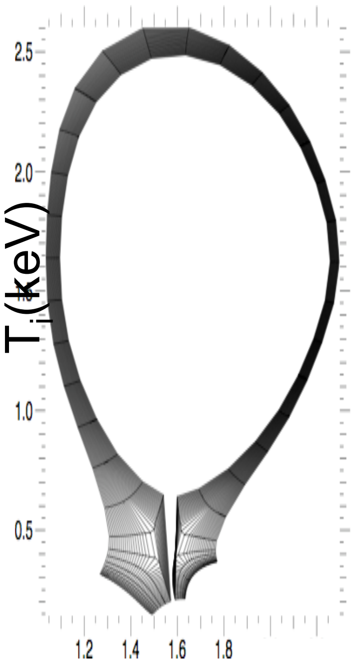
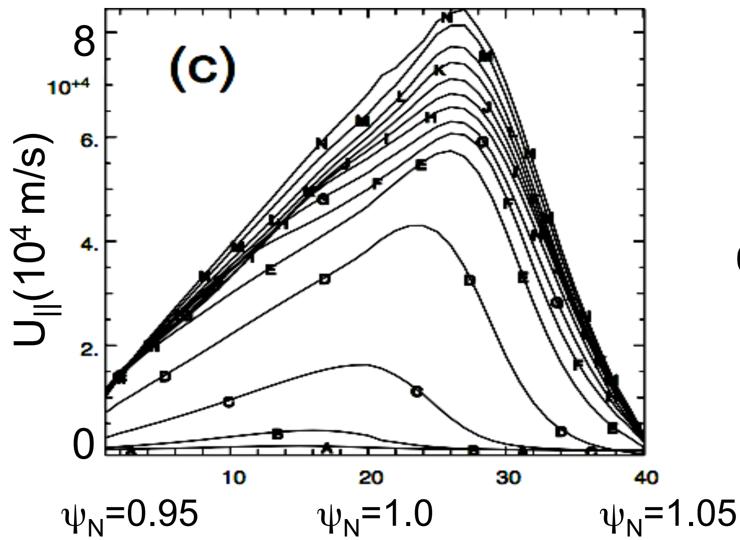
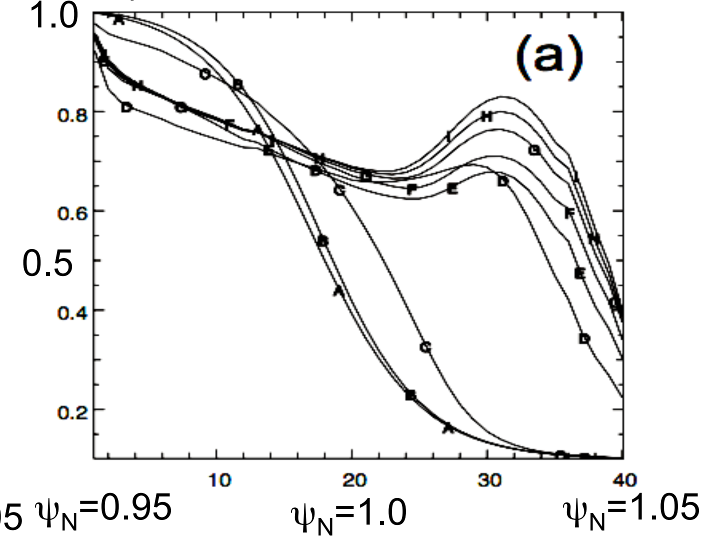
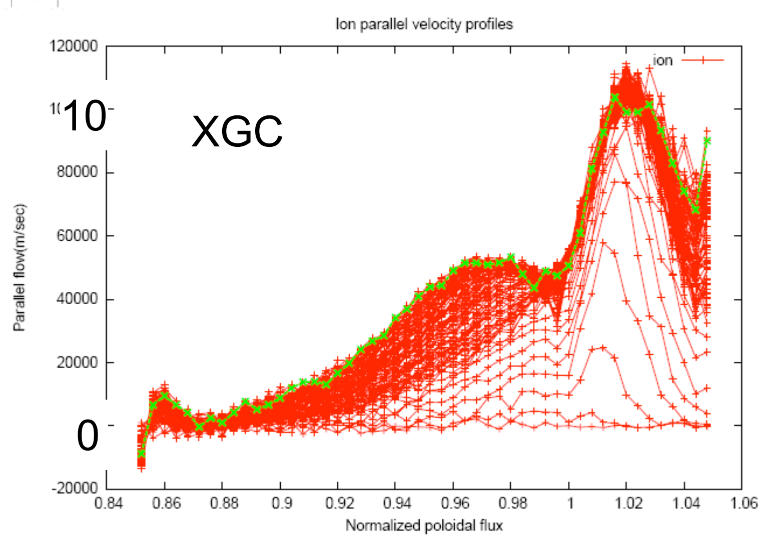


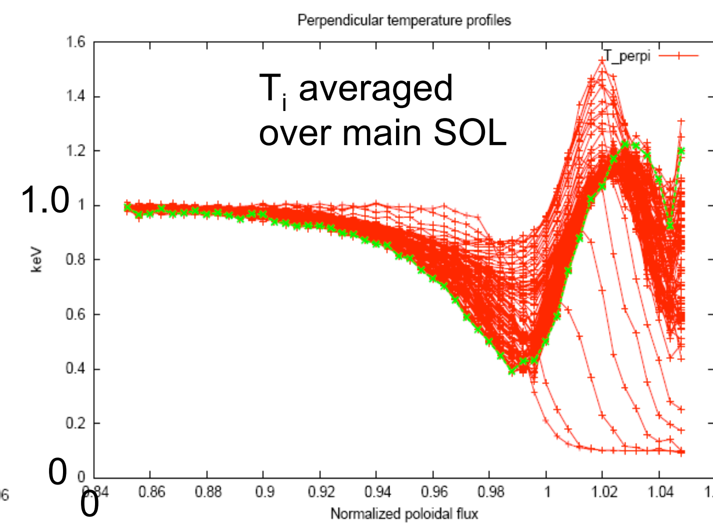
$-u_{||}$ (m/s, pol av above xpt)



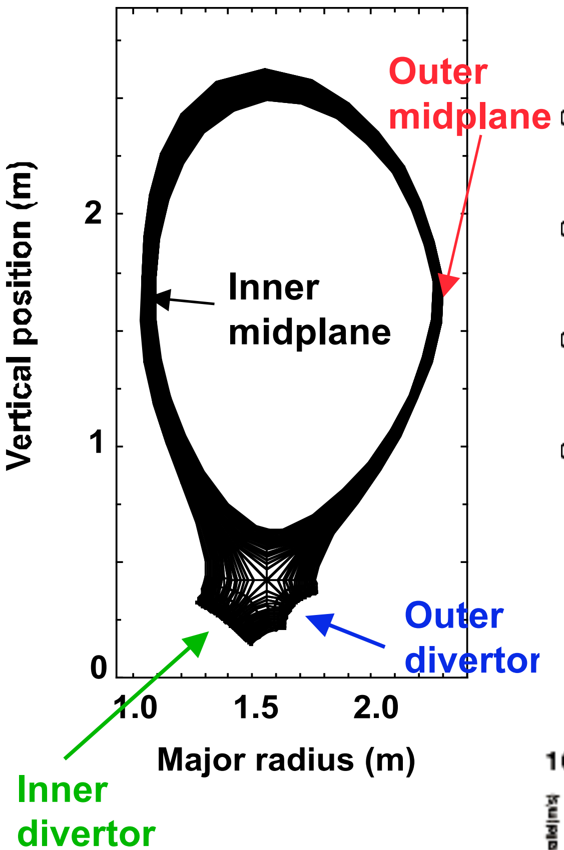
T_i (keV, outer midplane)

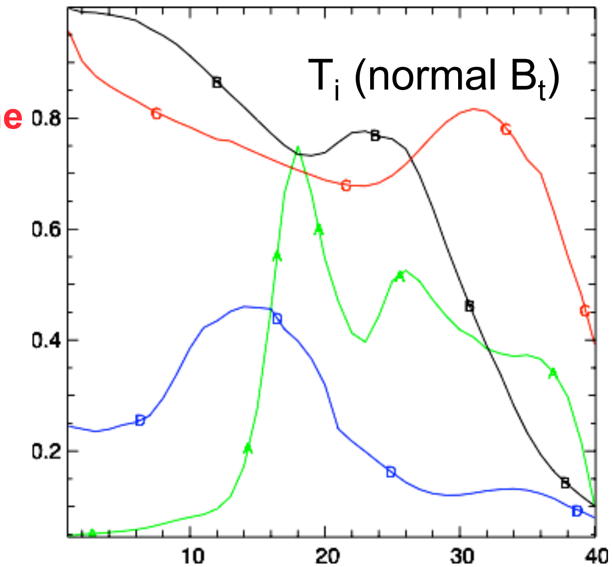


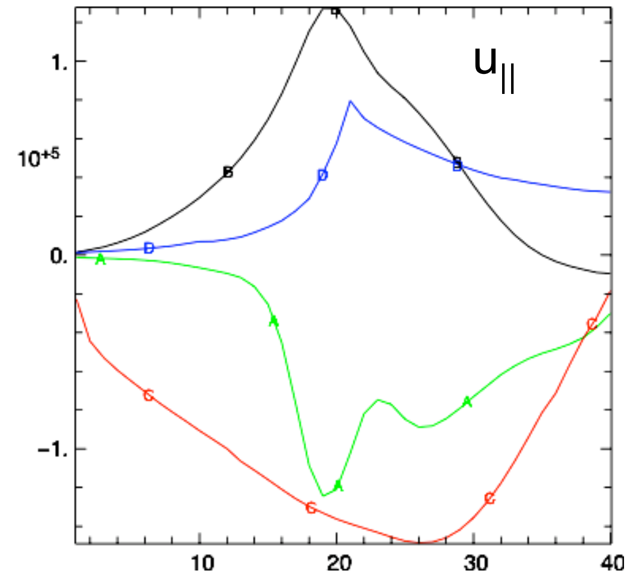


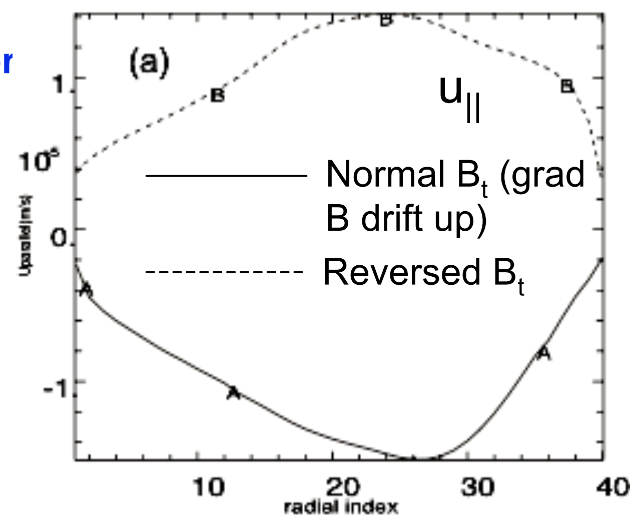


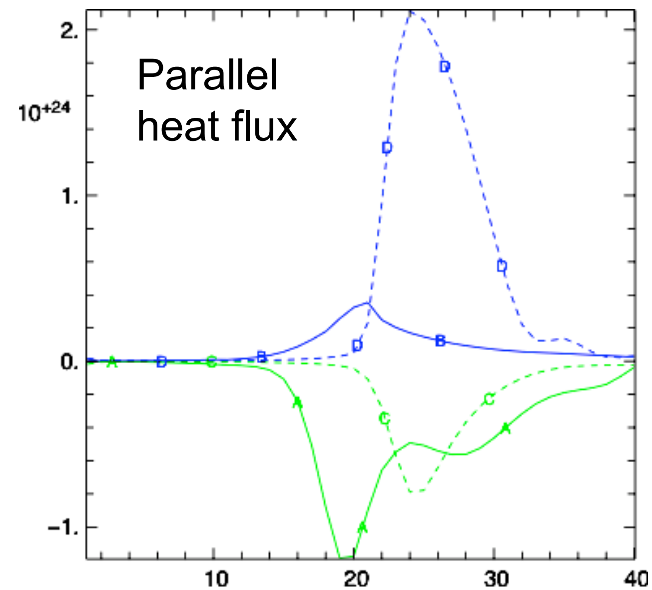
Tempest divertor neoclassical test shows reasonable poloidal dependence and intuitive asymmetries











Down (up) grad B drift loads inner (outer) divertor, consistent with direction of bananas

We are adding a velocity-dependent diffusion operator to TEMPEST

- Why? To do long-timescale simulations modeling effects of turbulence; a “kinetic UEDGE”.
- Add a term:

$$\frac{1}{V}\frac{\partial\left(V\,\Gamma_{\mathrm{a}}/h_{\psi}\right)}{\partial\psi}\bigg|_{\theta,\mathrm{v}}$$

with:

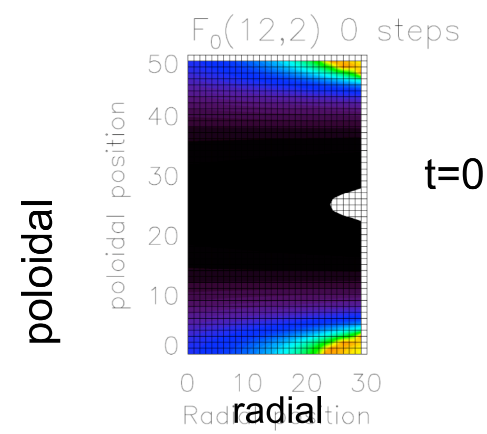
$$\Gamma_a = U_a f - \frac{D}{h_\psi}\frac{\partial f}{\partial\psi}\bigg|_{\theta,\mathrm{v}}$$

$$V = 2\pi R h_\psi h_\theta$$

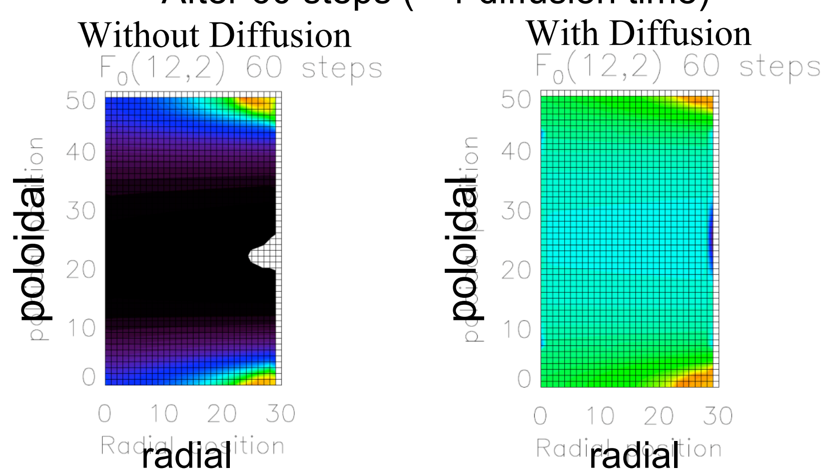
D, U fns of **x** and **v**, and above terms chain-ruled to derivs at const E and μ

- With proper choice of velocity dependence of D and U can mock up an extended matrix of transport coefficients

First results (Bodi)



After 60 steps (~ 1 diffusion time)



Associated math activities

- Starting with conservative form of GK equation

$$\frac{\partial(B_{\|}^{*} f)}{\partial t} + \nabla_{\mathbf{R}} \cdot \left(\dot{\mathbf{R}} B_{\|}^{*} f\right) + \frac{\partial}{\partial v_{\|}} \left(\dot{v}\| B_{\|}^{*} f\right) = 0$$

- And long-wavelength conservative form of GK-Poisson:

$$\nabla \cdot (D \nabla \Phi) = e \left(n_e(\mathbf{x}) - \sum_i Z_i \bar{n}_i(\mathbf{x}) \right)$$

- and complicated edge geometry, develop strategy for conservative discretization and edge connectedness

We are applying a finite volume, mapped grid formalism to discretize the GKV and GKP equations in edge geometries

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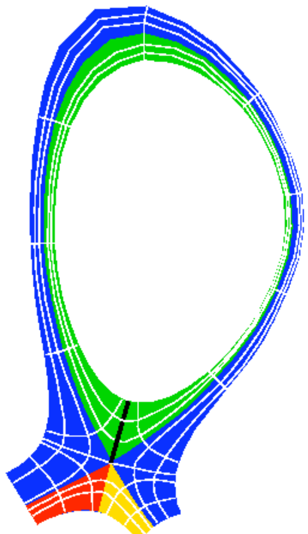
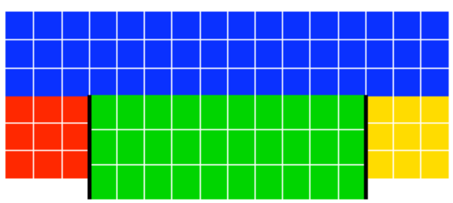
2D Case: A poloidal slice of the plasma edge is mapped to a multiblock, locally rectangular grid

Physical coordinates: $\mathbf{X}$



Mapping $\mathbf{X} = \mathbf{X}(\xi)$

Mapped (computational) coordinates: $\xi = (\psi,\theta)$



Flux surface label ψ

Poloidal angle θ

Key result: Fourth-order accurate flux divergence averages are obtainable from fourth-order accurate cell face averages:

$$\frac{1}{vol(X(V_{\mathbf{i}}))}\int_{\mathbf{X}(V_{\mathbf{i}})} \nabla_{\mathbf{x}} \cdot \vec{F} d\mathbf{x} = \frac{1}{h}\sum_{d=1}^{D}\sum_{\pm=+,-} \pm F^d_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} + O(h^4),$$

$$F^d_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \equiv \sum_{s=1}^{D} \langle N^s_d\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \langle F^s\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{12}\sum_{s=1}^{D}\left(G_0^{\perp,d}(\langle N^s_d\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\right)\cdot\left(G_0^{\perp,d}(\langle F^s\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d})\right).$$

$G_0^{\perp,d}$ = second-order accurate centered difference of $\nabla_\xi - \mathbf{e}^d \frac{\partial}{\partial \xi_d}$

$$\langle q\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \frac{1}{h^{D-1}}\int_{A_d} q(\xi) dA_\xi + O(h^4)$$

Math component: status and current activities

- GKV and GKP discretizations have been formulated and documented.

  GKV:
  - Fourth-order, multidimensional, flux-corrected transport (FCT) with hyper-viscosity and limiting
  - RK3 or RK4 time integration

  GKP:
  - Fourth-order, compact (5x5) stencil
  - Multigrid linear solver
- A suite of test problems for the hyperbolic integrator has been specified. Implementation and testing are underway.
- Support for the mapped grid formalism has been added to *Chombo* and tested on common mappings (example at right).
- Fourth-order accuracy of the elliptic discretization has been verified on some analytically manufactured solutions.
- Implementation of GKP stencils in *Hypre* is underway.
- Goal: A coupled GKV and GKP prototype by the end of the year.

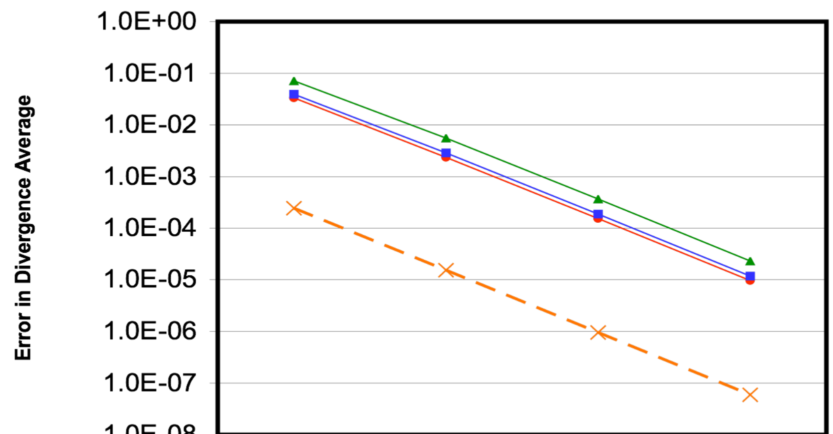
Mapped grid infrastructure test:

$$\mathbf{F}(r,\theta,z) \equiv \left(r^2, r\sin(\theta), z^2\right)^T$$

Mapping: cylindrical coordinates

$$\mathbf{x} = (\mathbf{r},\theta,\mathbf{z}) \rightarrow \xi = (\xi_1,\xi_2,\xi_3)$$

Error in $\frac{1}{vol(V_i)}\int\int_{V_i} \nabla\cdot\mathbf{F}(r,\theta,z)\,r\,dr\,d\theta\,dz$:



	8	16	32	64
L1 Norm	3.321E-02	2.358E-03	1.529E-04	9.648E-06
L2 Norm	3.926E-02	2.872E-03	1.873E-04	1.183E-05
Max Norm	7.169E-02	5.531E-03	3.663E-04	2.326E-05
N^{-4}	2.441E-04	1.526E-05	9.537E-07	5.960E-08

Grid Dimension N = 1 / h

Plans for next year:

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- We plan to move effort from TEMPEST and EGK to the next-generation code when the math team has prototype ready (expected Jan 08). Physics and math teams will collaborate to add collisions, gyro-averaging, neutrals, and eventually EM. Physics teams will also begin V&V.

MEANWHILE:

- TEMPEST:
  - Return to 5D V&V (drift-wave, ITG tests begun last fall; dormant since)
    - Core first, then edge
  - Divertor geometry neoclassical solutions with field solve
  - Complete debug and V&V of anomalous diffusion model
- EGK:
  - Demonstrate solutions combining neoclassical + turbulence
  - Explore efficient treatments for solving equilibrium and fluctuations together
    - Consider approach with equilibrium treated implicitly, fluctuations explicitly
  - Examine physics of parallel nonlinearity under edge-like conditions

Remarks on capability computing and CSETs

- Capability computing:
  - We haven't needed it in 4D. Runs on ~ 10-20 CPU of a cluster suffice for problems so far.
  - We WILL need it for 5D (in coming year).
  - TEMPEST and next generation codes "born parallel" courtesy of framework (was SAMRAI, now Chombo)
- CSETs:
  - Project heavily interwoven with APDEC
  - Also using IDA from Sundials for time integration and Hypre for field solve, both part of TOPS.