Advanced Computing Initiative
To Study Methods of Improving Fusion

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Science motivation: Several interesting innovative ideas being pursued to improve fusion power plants (advanced tokamaks and STs, quasi-symmetric stellarators, liquid metals, advanced divertors, …). But only have qualitative / empirical understanding of how they scale to larger devices.

Initiative: Need comprehensive computer simulations to understand how these methods scale, to quantitatively predict performance improvements, and to optimize power plants. Cost-effective way of preparing for next-step decisions, and help make the case for the next steps. Comprehensive predictions also needed to plan shots to avoid disruptions.

Biggest need: Comprehensive simulations of the main core are fairly successful, but new codes needed to handle more complex edge/pedestal region. Challenging, but doable. Naturally synergistic with U.S. computer industry, builds on US leadership in fusion simulations. Partner with DOE Advanced Scientific Computing.

Computational Initiatives Being Proposed in Fusion

- MHD disruptions, …
  (Jardin et al., $2M)
- MHD energetic particle instabilities, …
  (Fu et al., $2M)
- Edge gyrokinetic turbulence, …
  XGC +2-3 new codes (Hammett et al., $3-4M)
- Existing core gyrokinetic codes,
  or reduced transport models.
- Existing source & sink codes
  (beams, rf, neutrals…)

Modular Whole-Device Frameworks:
(Hammett et al., $3M)

Single-code (~XGC+) Whole-Device Model (Chang et al., $4M (half from ASCR))

Total: $13-15M/y (part could be ASCR). Motivation similar to previous FSP proposal ($25M/y), but smaller funding & more modular approach, focusing on key problems first. Similar to VHIMS (Validated, Highly Integrated Models & Simulations, Snyder et al.)

pursue modular & single-code approaches in parallel. Modular approach becomes more integrated as parts are tested.

Improving Confinement Can Significantly ↓ Size & Construction Cost of Fusion Reactor

Well known that improving confinement & β can lower Cost of Electricity / kWh, at fixed power output.

Even stronger effect if consider smaller power:
better confinement allows significantly smaller size/cost at same fusion gain Q ($nT\tau_E$).

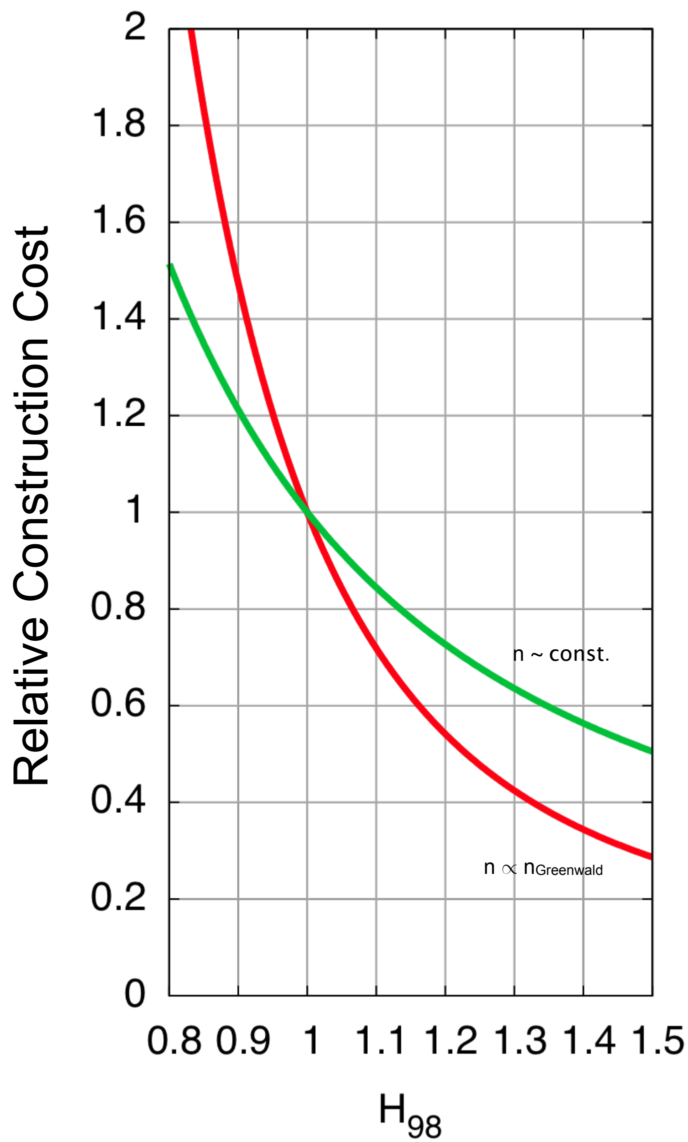
Standard H-mode empirical scaling:

$$\tau_E \sim H\, I_p^{0.93}\, P^{-0.69}\, B^{0.15}\, R^{1.97} \ldots$$

(and assuming fixed $nT\tau_{E,}$ q_{95}, β_N, $n/n_{Greenwald}$):

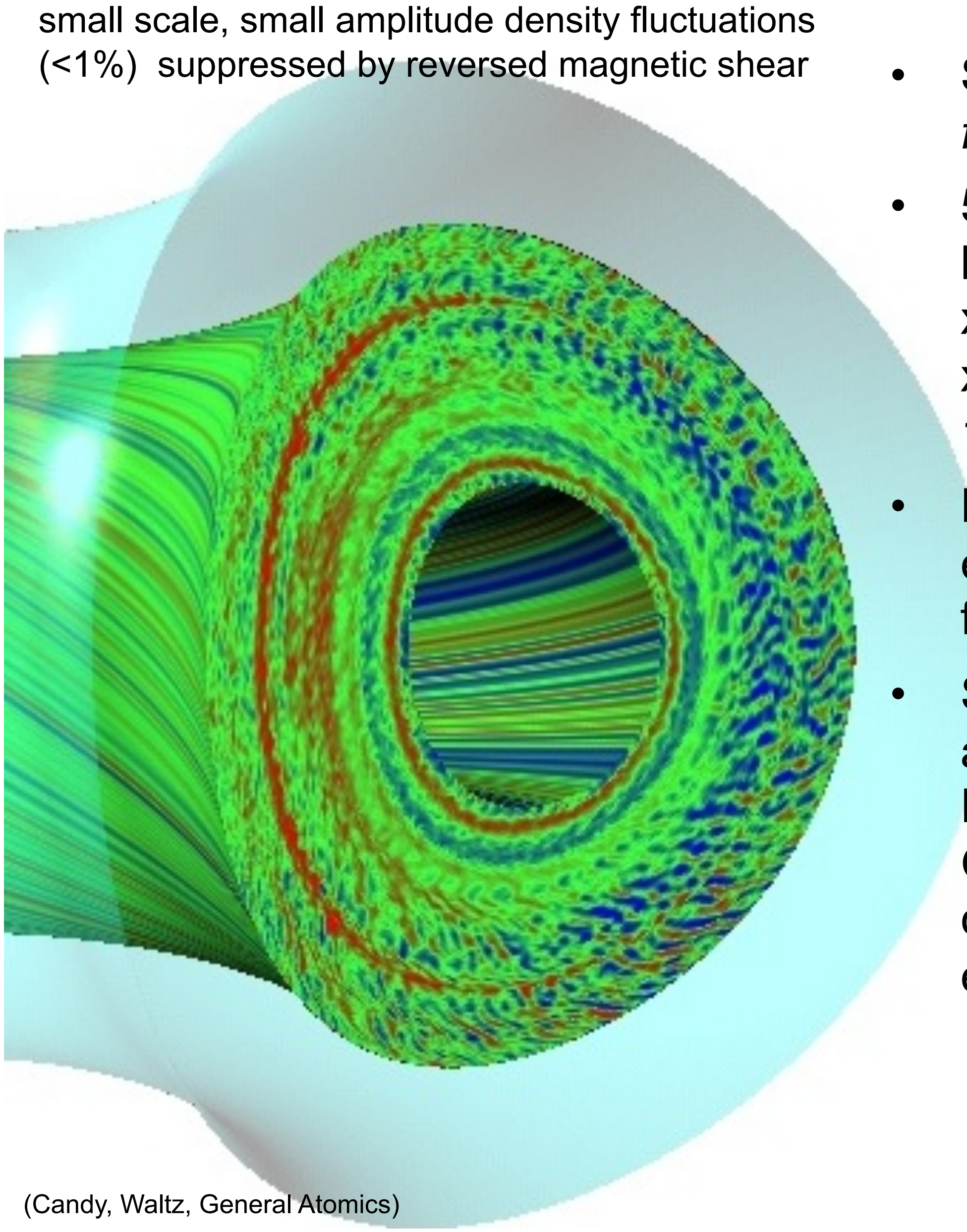
$$R \sim 1 / (H^{2.4}\, B^{1.7})$$

ITER std $H=1$, steady-state $H\sim1.5$
ARIES-AT $H\sim1.5$
MIT ARC $H_{89}/2 \sim 1.4$



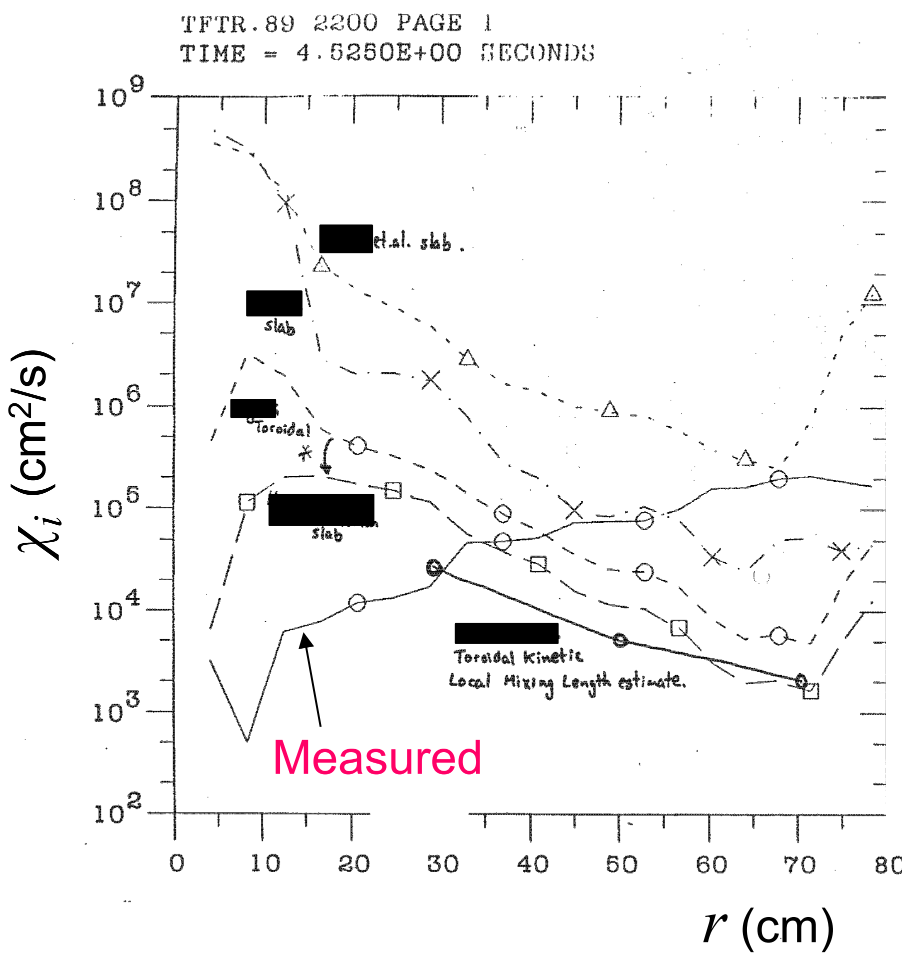
(Plots assumes $a/R=0.25$, cost $\propto R^2$ roughly. Plot accounts for constraint on B @ magnet with 1.16 m blanket/shield.)

Fairly Comprehensive 5-D Gyrokinetic Turbulence Codes Have Been Developed

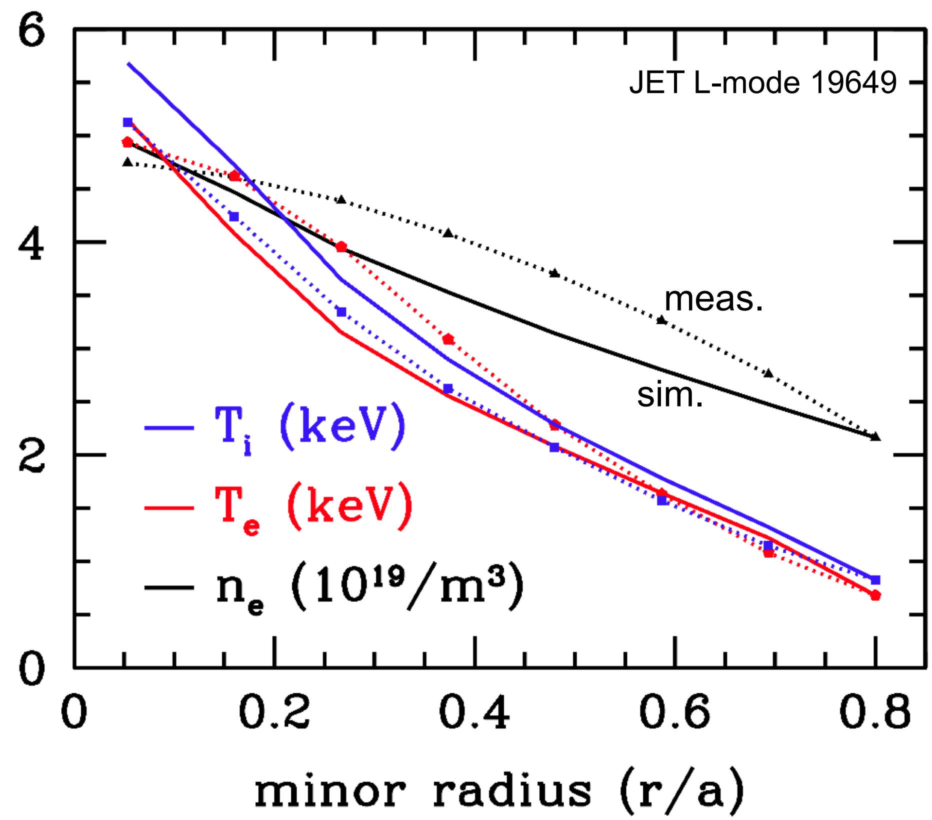


- Solve for the particle distribution function $f(r,\theta,\alpha,E,\mu,t)$ (avg. over gyration: 6D → 5D)
- 500 radii x 32 complex toroidal modes (96 binormal grid points)
  x 10 parallel points along half-orbits
  x 8 energies x 16 $v_{||}/v$
  12 hours on ORNL Cray X1E w/ 256 MSPs
- Realistic toroidal geometry, kinetic ions & electrons, finite-β electro-magnetic fluctuations, full linearized collisions.
- Sophisticated spectral/high-order upwind algorithms. This plot from continuum/ Eulieran code GYRO (SciDAC project), GENE (Garching) similar. These and other codes being widely compared with experiments.

Major breakthrough: Gyrokinetic predictions now much better than 1990 analytic turbulence theories



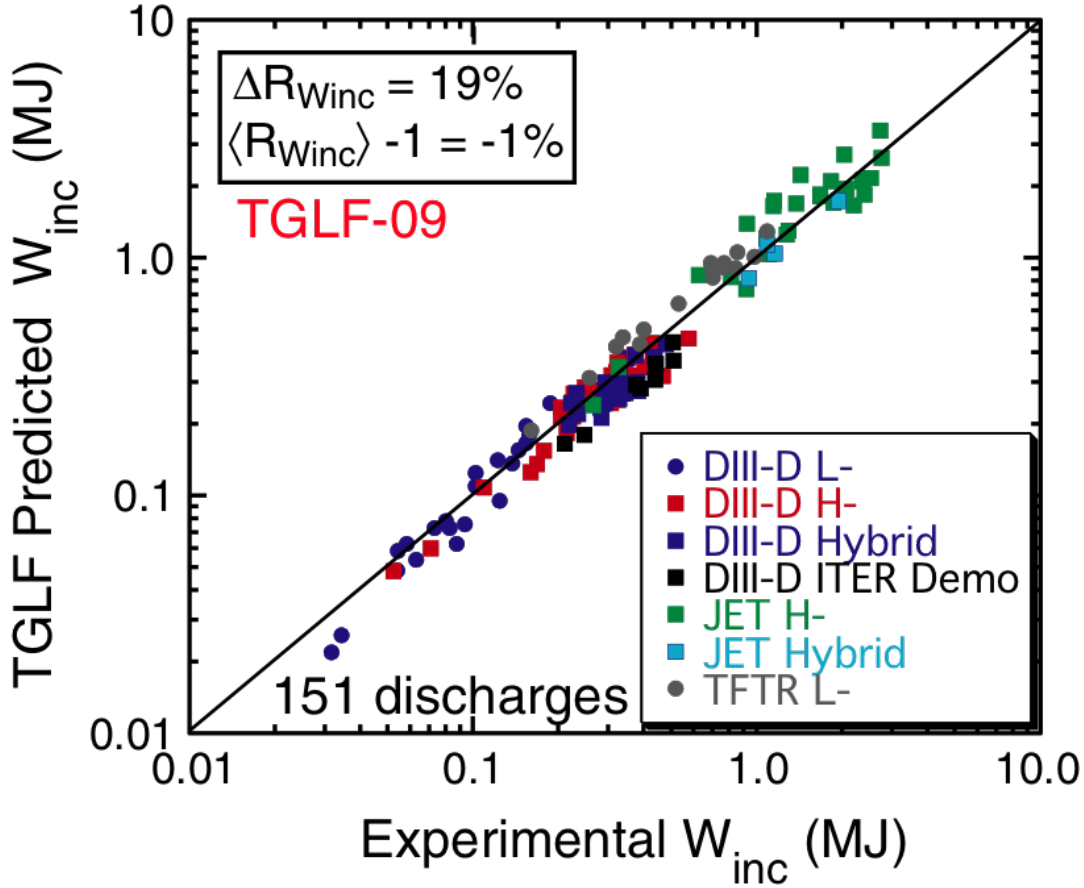
Plot made in 1990. Analytic theories disagreed with measured diffusion coefficients by factors of 100-1000. The importance of thresholds for marginal stability not appreciated then. Explains why the edge effects the core so much.
(see also S.D. Scott et al., Phys. Fluids B 1990)



Gyrokinetic simulations agree fairly well with most experiments. Demonstrates feasibility of directly coupling gyrokinetic turbulence codes to long-time-scale transport codes.

Barnes, Dorland, et al., PoP 2010

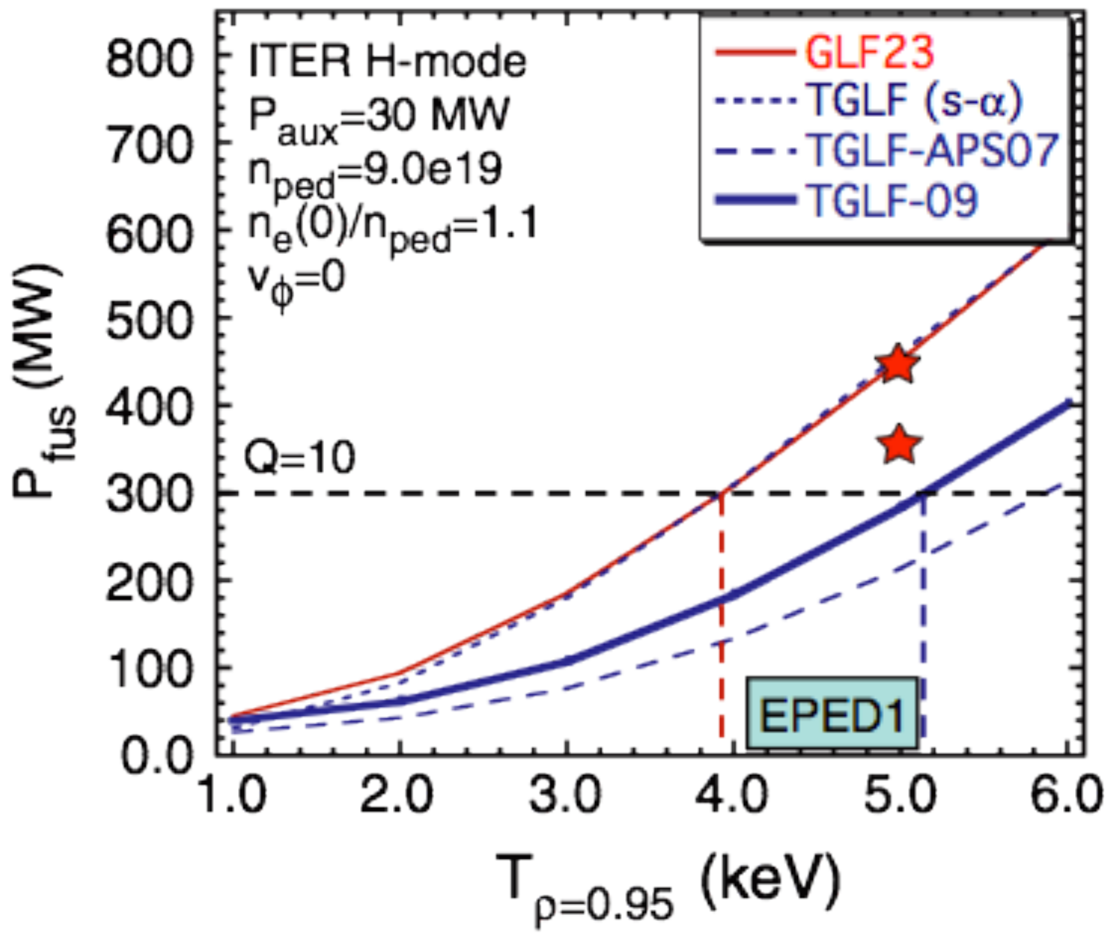
Gyrokinetic-based TGLF transport model compares well with core of many experiments



Biggest gap: doesn't predict edge region (r/a>0.8).

Kinsey et al. Nucl. Fus. 2011 http://stacks.iop.org/NF/51/083001

Motivation: Need comprehensive simulations of edge, because pedestal temperature has big effect on fusion gain Q



Because of marginal stability effects, the edge boundary condition strongly affects the core: the edge is the tail that wags the dog.

Need an edge code to answer many important questions:

height of the pedestal, conditions for H-mode transport barrier formation, effect of RMP coils to suppress ELMs, divertor power handling, improvements with lithium walls...

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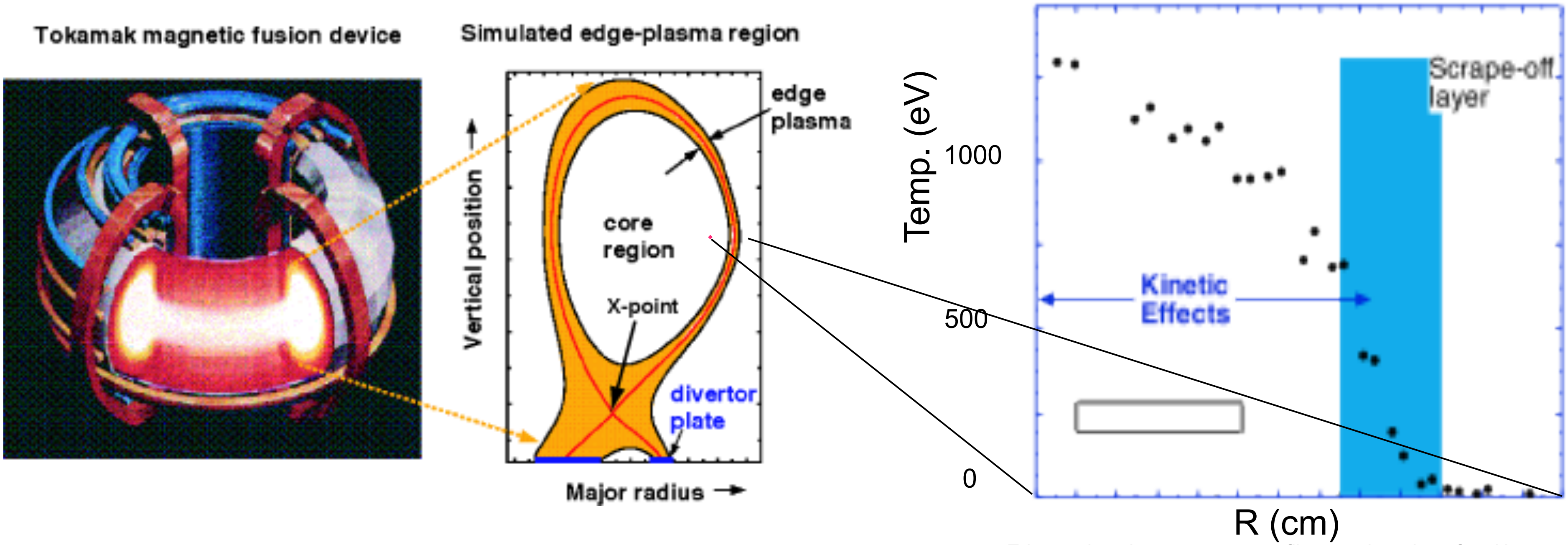
Edge region very difficult



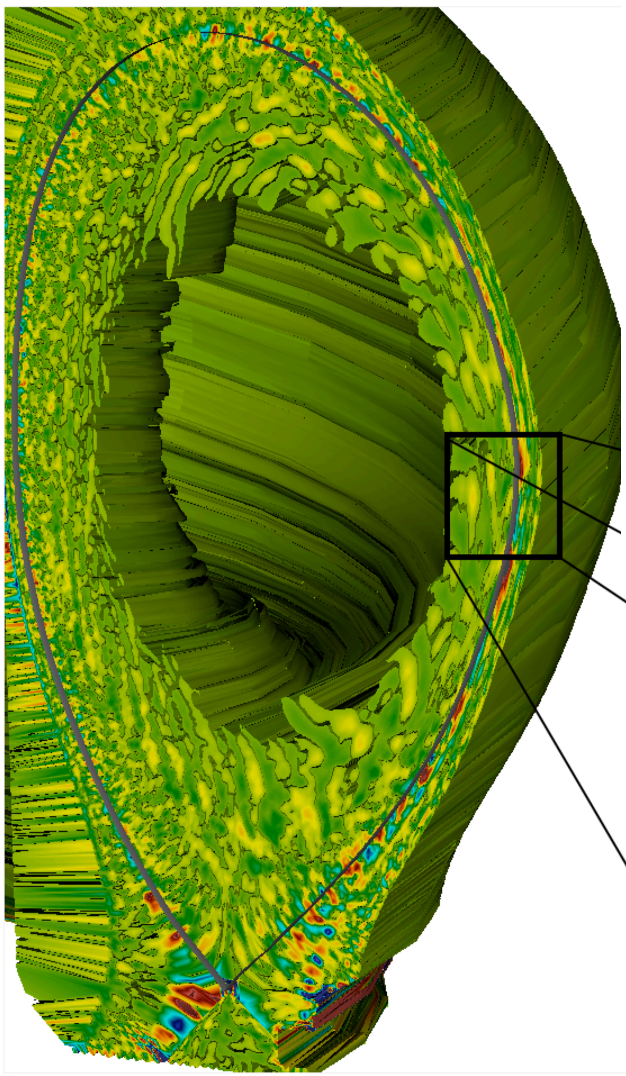
Edge pedestal temperature profile near the edge of an H-mode discharge in the DIII-D tokamak. [Porter*2000*]. Pedestal is shaded region.

Present core gyrokinetic codes are highly optimized for core, need new codes to handle additional complications of edge region of tokamaks (& stellarators):

open & closed field lines, plasma-wall-interactions, large amplitude fluctuations, positivity constraints, atomic physics, non-axisymmetric RMP / stellarator coils, magnetic fluctuations near beta limit…

Hard problem: but success of core gyrokinetic codes makes me believe this is tractable, with a major initiative

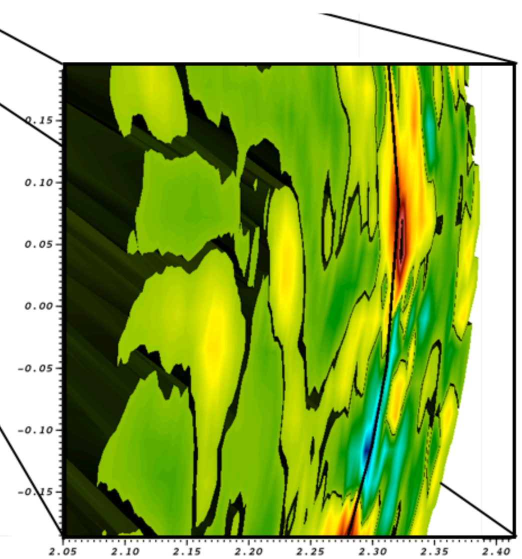
Example of XGC1 Simulation of Edge Turbulence in DIII-D



Encouraging initial electrostatic results, similar blobby edge features & SOL width to this experiment.

Extreme-scale computing: 40B particles, 131k processors & 8k GPUs on Cray XK-7 (ORNL), 6M processor-hours (~5% of yearly allocation) for ~1 ms physics time.

Only gyrokinetic edge turbulence code at present that can handle separatrix, closed & open field lines. Ongoing work to include more physics. Studying different algorithms to include magnetic fluctuations, which are important in edge and have been a long-standing challenge in GK PIC codes.



http://ttf2014.ucsd.edu/TTF_2014/Presentations_files/Ku.pdf, 131

Need Independent Codes to Cross Check

Very important to have independent codes to cross-check each other, particularly for very hard problems like edge turbulence.

Rapid progress in core gyrokinetics made possible by several independent groups developing such codes, exploring different ideas about best algorithms to use, etc. Different algorithms may resolve some physical processes more efficiently.

Silicon Valley-style startups: innovation & initial code development done quickest in small, competing groups.

Widely used core gyrokinetic codes (GYRO, GENE, GS2) use continuum/Eulerian algorithms, so edge codes using continuum algorithms should be developed too. Continuum codes harder to write, but relatively fast & handle magnetic fluctuations fairly well. Advanced algorithms (like Discontinuous Galerkin) could help with challenges of edge turbulence. Propose 2 new continuum gyrokinetic (+ 1 gyrofluid?) edge codes.

Need at least 2 modular framework teams, maybe TRANSP (widely used by expts now) and FACETS/MEMFIS (modern framework including edge models).

- TRANSP: maintenance now: \$1M, propose +\$1.5M/y. MEMFIS +\$1.5M/y

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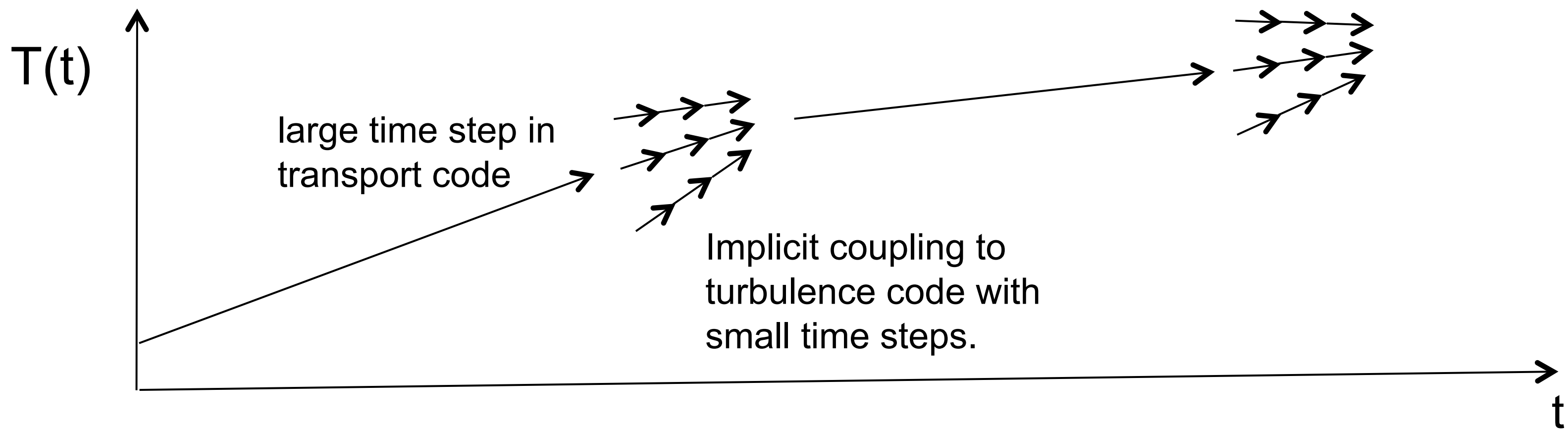
Modular Whole-Device Modelling: Feasibility of coupling long-time transport code with core gyrokinetic turbulence codes has been demonstrated (Trinity, TGYRO, FACETS)



- Multiscale algorithms (using special implicit projective integration). Can simulate a long transport time scales a factor of ~200 to ~10,000 times faster than a brute force simulation (for ion-scale or electron-scale turbulence)
  - Uses ~100,000 CPU hours on leadership-class computers (more CPU time if edge is included) for transport time scale (~10 s). Have done a few cases. Will become more routine over next 5 years.

- At present couples to independent core flux-tube simulations, works well in most cases Eventually upgrade to consider non-local turbulence spreading, important in edge.

- Would be used in extensive validation comparisons with experiments.

Summary: Proposed Computational Fusion Initiatives

- A computational initiative to develop integrated simulations is needed to understand various methods for improving fusion power plant designs, and to plan discharges on future machines to avoid disruptions.

- To develop fully-predictive simulations (at least for MHD quiescent regimes), the biggest need is to develop gyrokinetic turbulence codes that can handle the edge region.

- Comprehensive, well-tested simulations would be a cost-effective way to help make the case for next step fusion experiments.

- Builds on US strengths in the computer industry, and in fusion theory and simulations.

- Opportunity to build on DOE FES and ASCR collaborations (DOE Office of Advanced Scientific Computing) for new joint initiative

EXTRAS

Modular Whole-Device Modelling Initiative

- Current funding: SciDAC has been funding 7 components (MHD, core (& 1 edge) gyrokinetic turbulence, energetic particles) at a modest level:

	SciDAC	**US MFE Theory**
FY12	\$8.3M	\$24.5M
FY13	\$6.6M	\$23.1M
FY14	\$9.3M (+1 new SciDAC)	\$24.0M

- Past funding: 3 Proto-FSP projects were \$2M/y, (full FSP proposed \$25M/y)
- MHD/Disruption/Energetic-particle simulations: +\$4M/y. Disruptions are most important near-term topic to study.
- Need 2 more teams for edge gyrokinetics, 1 for edge gyrofluids. \$1.5M/y each. Edge turbulence simulations is biggest gap in developing complete predictive capability (needed for complete disruption avoidance studies).
- Need at least 2 integrated framework teams, maybe TRANSP (widely used by expts now) and FACETS/MEMFIS (modern framework including edge models)
  - TRANSP: maintenance now: \$1M, propose +\$1.5M/y. MEMFIS +\$1.5M/y
  - Single-code approach (maybe XGC1 expanded, \$4M)

Modular Whole-Device Simulations