Prototype FSP Center for Plasma Edge Simulation (CPES)

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3 National Labs, 12 Universities, and 1 Private Institution

CPES

Center for Plasma Edge Simulation

Contents

Postdocs and Graduate students

5 postdocs and 9 gradate students + foreign students

- UC Iirvine: **1** postdoc + 1 graduate student
- U Colorado: **1** graduate student
- Columbia: 1 graduate student
- NYU: 1 postdoc + 1 graduate student
- ORNL: 2 postdoc + **1** graduate student
- Rutgers: **3** graduate students
- UTK: **1** graduate student
- LBNL(UC Davis): **1** postdoc

Math
CS
Physics

CPES Meetings after the last PSACI review

- 2006 Fall meeting: APS/DPP, Nov2-3, Philadelphia
- 2007 Spring meeting: April30-May1, Las Vegas

Participating Institutions in CPES

Center for Plasma Edge Simulation

National Laboratories (3)

PPPL, ORNL, LBNL

Academic Institutions (12)

New York U., Columbia U., MIT, Rutgers U.,
U. Tennessee, Lehigh U. U. Colorado Boulder, U. Utah, Auburn U.,
Caltech, UC Davis, UC Irvine.

Private Institution (1)

Hinton Assoc.

Active collaborations with other centers made our progress possible

CMCL **ESL**

CACR PERI ITAPS **NCCS**

Example collaborations with other centers

- **TOPS: Provide solvers, multiscale coupling math**
- **SDM: Kepler work flow and dashboard, Data management**
- **PERI: Performance enhancement**
- **Courant Math and Computational Lab (Greengard): XGC Algorithm**
- **GPSC: Gyrokinetic turbulence techniques**
- **CEMM: M3D and NIMROD code coupling to XGC**
- **NCCS: Incite award for HPC computing**
- **GA: ELITE and EFIT**
- CACR: Software engineering
- SADS (Zoran Budimlic): XGC optimization
- ITAPS: Meshing optimization
- IUV (Ma): Ultrascale visualization
- LOCI: Data sharing
- FACETS: XGC coupling into core-edge framework
- ESL: Code comparison with continuum gyrokinetics

Center for Plasma Edge Simulation
Chang

Advisory Committee

Physics
Lee*

Kinetics
Parker*

- **Theory**
  - Hahm
  - •Hinton
  - •Weitzner
  - •Chang
- **Compute**
  - Lin
  - •Nishimura
  - •Cummings
  - •Ethier
  - •Chen
  - •Ku
  - •Park
  - •Wang

Neutral/Wall
Stotler*

- **Neutrals**
  - Chang
  - •Park
  - •Stotler
- **PSI & Atomic Physics**
  - Schultz
  - •Pindzola

MHD
Strauss*

- **Theory**
  - Weitzner
  - •Hinton
  - •Chang
- **Compute**
  - Sugiyama
  - •Park
  - •Bateman
  - •Pankin
  - •Adams

CS/Math
Keyes*

V&V
Kritz*

- **Validation**
  - Bateman
  - •Stotler
  - •Greenwald
  - •Zweben
  - •Klasky
  - •Maingi
- **Verification**
  - D'Azevedo
  - Greengard
  - •Zorin
  - •Weitzner
  - •Adams
  - •Ethier
  - •Stotler

DM/Viz
Klasky*

- **Code Integration**
  - Parashar
  - •Cummings
  - •Adams
  - •Sugiyama
  - •Lin
  - •Stotler
  - •Parker
  - •Chang
- **Workflow**
  - Shoshani*
  - •Silver
  - •Sugiyama
  - •Stotler
  - •Parashar
  - •Parker
- **Visualization**
  - Silver
  - •Parker
  - •Feibush
  - •Chang
- **Data Access**
  - Beck
  - •Shoshani
  - •Parashar
  - •Kritz
  - •Ethier

Algorithms
Greengard*

- **Linear Solvers**
  - Adams
  - •Keyes
  - •Weitzner
- **Other Algorithms**
  - Zorin
  - •Keyes
  - •Adams
  - •Lin
  - •Chang
  - •Weitzner

Optimization
Worley*

- **Parallel Algorithms**
  - Ethier
  - •D'Azevedo
- **Application specific**
  - Cummings
  - •D'Azevedo
  - •Strauss
  - •Lin
  - •Parker

Physics-CS-Math interface
Samtaney*

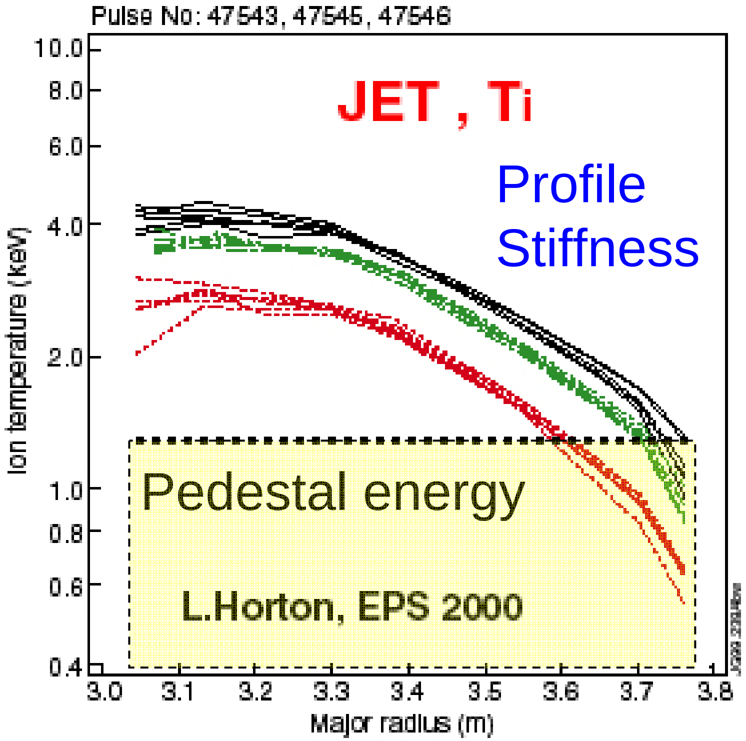
Park, Pankin
Klasky, Adams

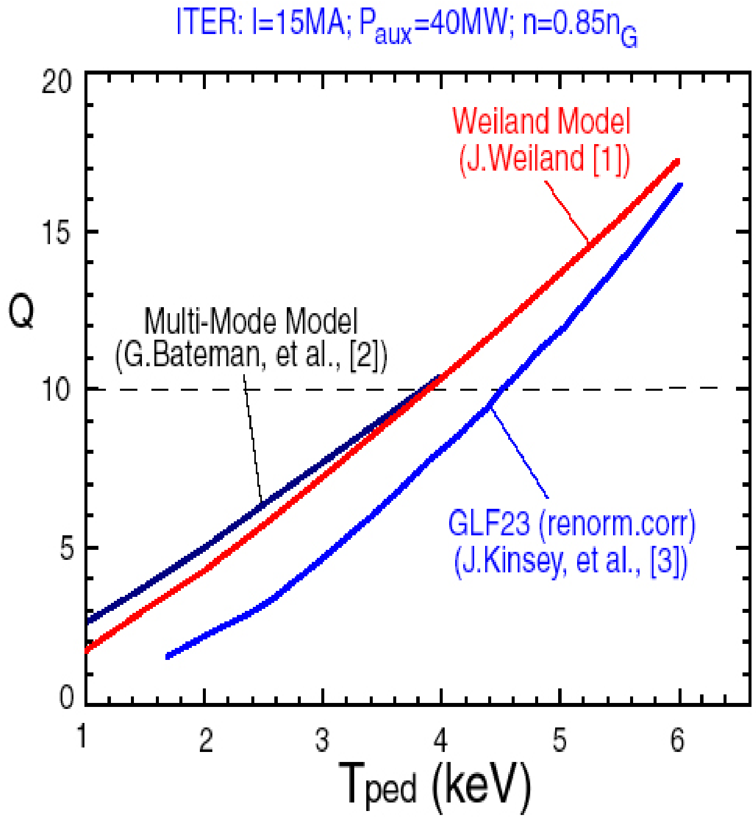
Organizational Chart

Participants are listed once in blue, then, multiply listed in black according to the task connections.

Executive comm. members have * after names

Fusion performance in ITER critically depends on pedestal height – achieve T_{ped}> 4-5 keV?





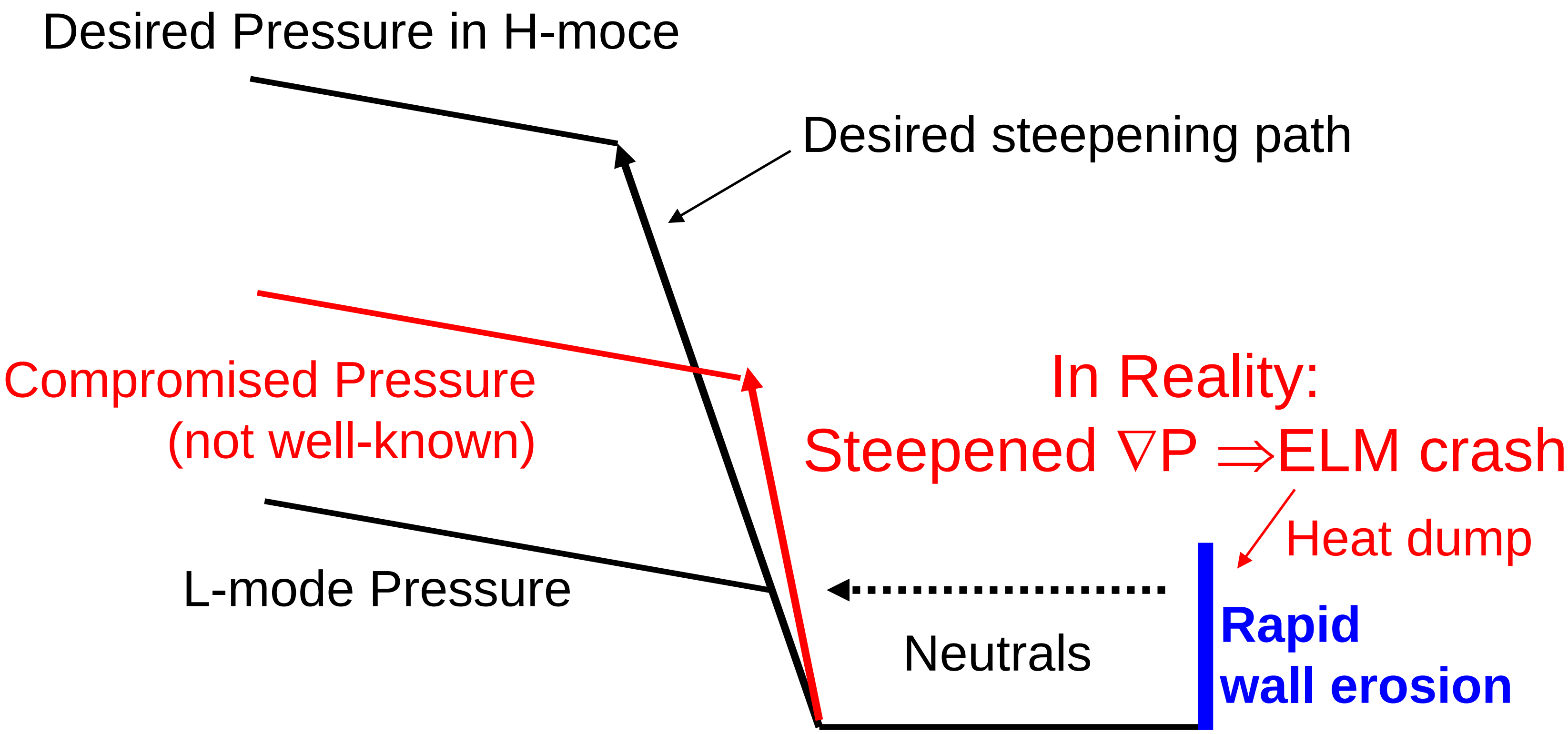
Edge physics (unknown)

Fusion merit: $N_i\tau_E T_i \propto H^{3.2}B^{3.5}/q^3$

Two-faced pedestal issue:

1. **Pedestal must be high enough $\Rightarrow$Induces ELM**
2. **ELM loss should negligible (?)**

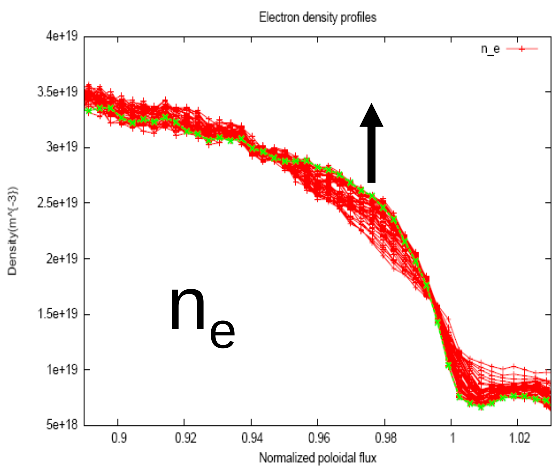
Physics not understood, hence prediction for ITER performance may be uncertain.

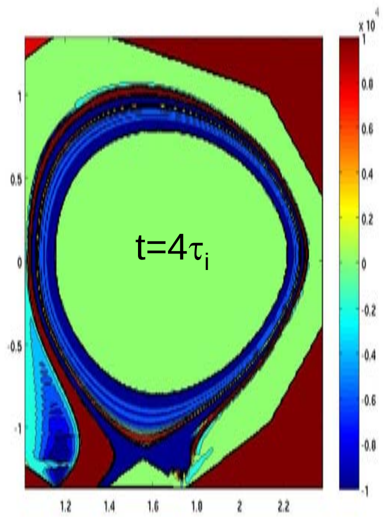


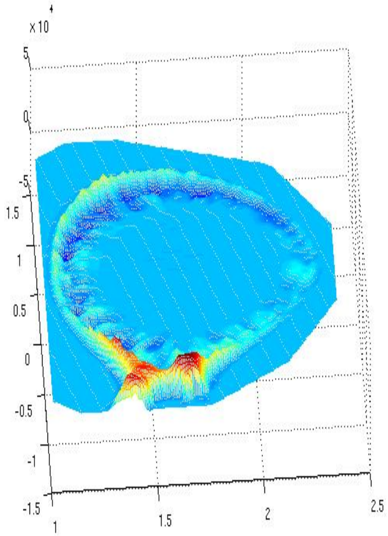
Another issue: Rotation generation, inward propagation, MHD stabilization.

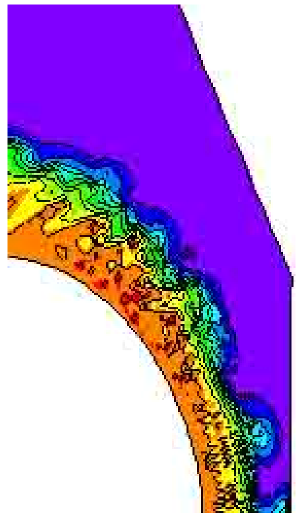
Multi physics in edge requires integrated multiscale simulation (μs–s, 0.1mm–10m)

- Neoclassical and turbulence physics
- Closed and open magnetic field lines with X-point
- Large flux expansion ratio (unstructured mesh)
- Neutral transport
- Plasma-wall interaction and atomic physics
- Edge localized large scale instabilities -ELMs
- Influence from the core plasma (core turbulence, energetic particles, MHD, RF, etc)
- RF-edge interaction
- Impurity transport and radiation physics

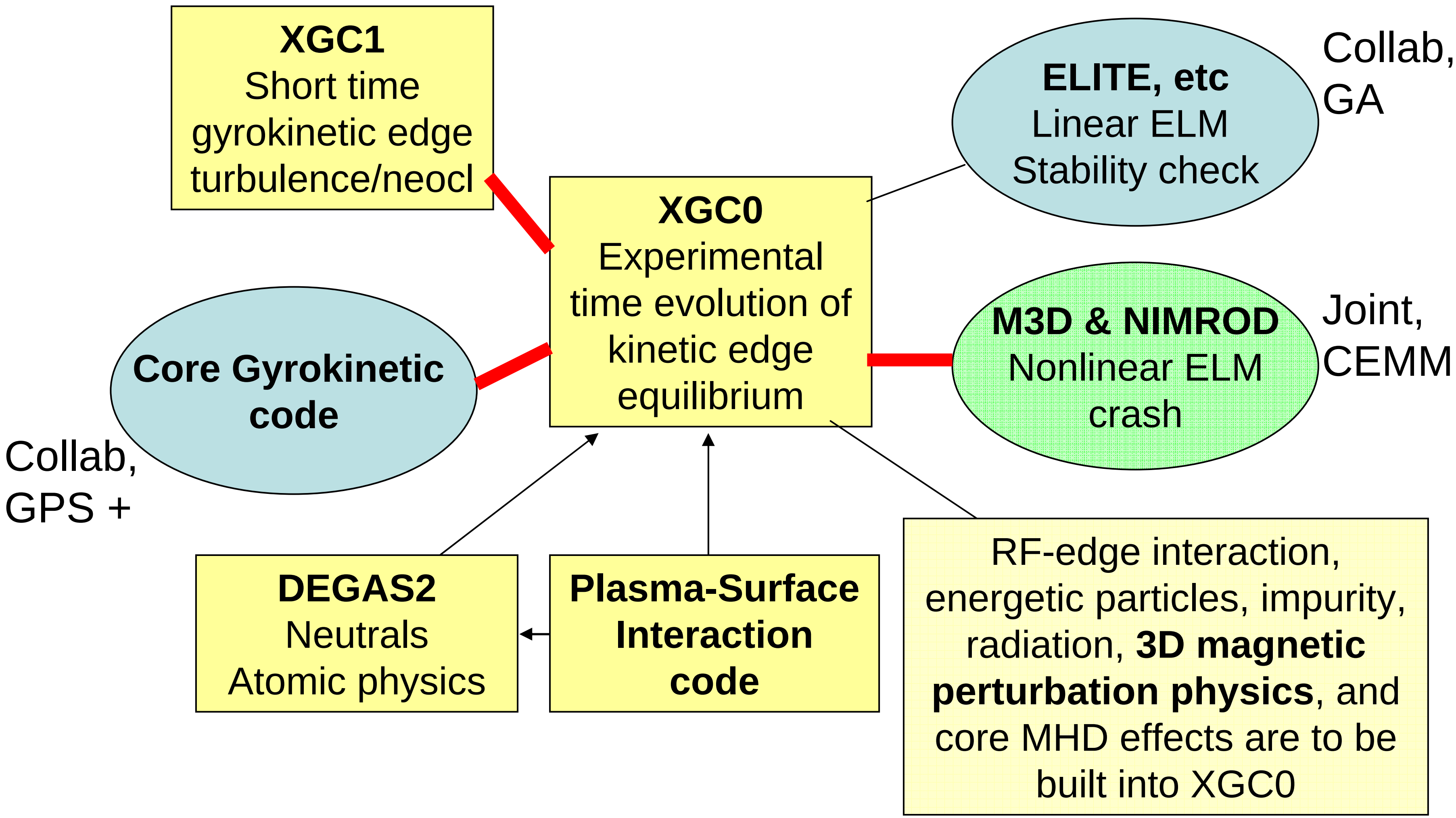








Multiscale code Integration in CPES
in Kepler framework (CS-Math)

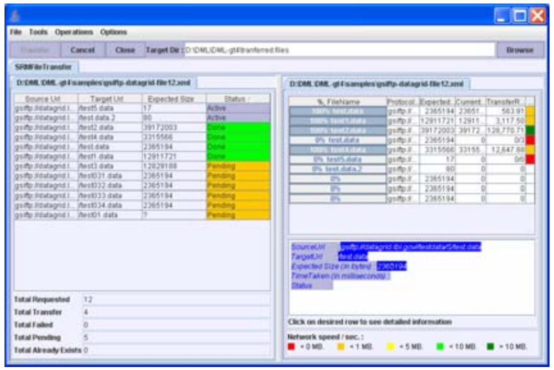


What is the Kepler Workflow Framework?

- Workflow framework.
  - **Kepler is a proven DOE technology for orchestrating scientific workflows which help in the construction and automation** of scientific problem-solving processes.
  - **Captures provenance information for**
    - Data provenance. (Where did my data come from).
    - Data movement, data replication. (during code coupling).
    - Which files are in which tar files on HPSS (NERSC/ORNL).
    - Helps users debug by saving log files.
  - **More powerful than python scripts**.
    - Allows you to do pipeline-parallel with ease!
    - Allows you to continue working even if some scripts/components fails.
    - Allows you to checkpoint/restart the workflow!
    - Makes it easy to modify the workflow for a continuously changing group of scientists.
  - **Excellent Connection to databases**.
    - Allows for easy queries of shots from coupled simulations.
    - **Large SDM effort to save provenance data into DB**.

Fast data transfers!

- **Fast parallel I/O techniques for the Cray XT and Infiniband systems.**
  - **Takes the overhead in large simulations from 20% of the time in I/O down to <3%.**
    - 1 SC2007 paper submission, 2 CUG papers, 1 Grid 2007 paper.
- Logistical Networking
  - With funding from NSF for Research and Education Data Depot Network (REDDnet) and CPES/GPS funding allows for easy data replication.
  - Depots (computers with lots of disk), allow for fast data access and data replication across the grid.
- Storage Resource Manager-light.
  - **Allows for easy data movement taking care of typical problems (network failures, disk failures**).
- All techniques currently being integrated with SDM/CPES Kepler framework.

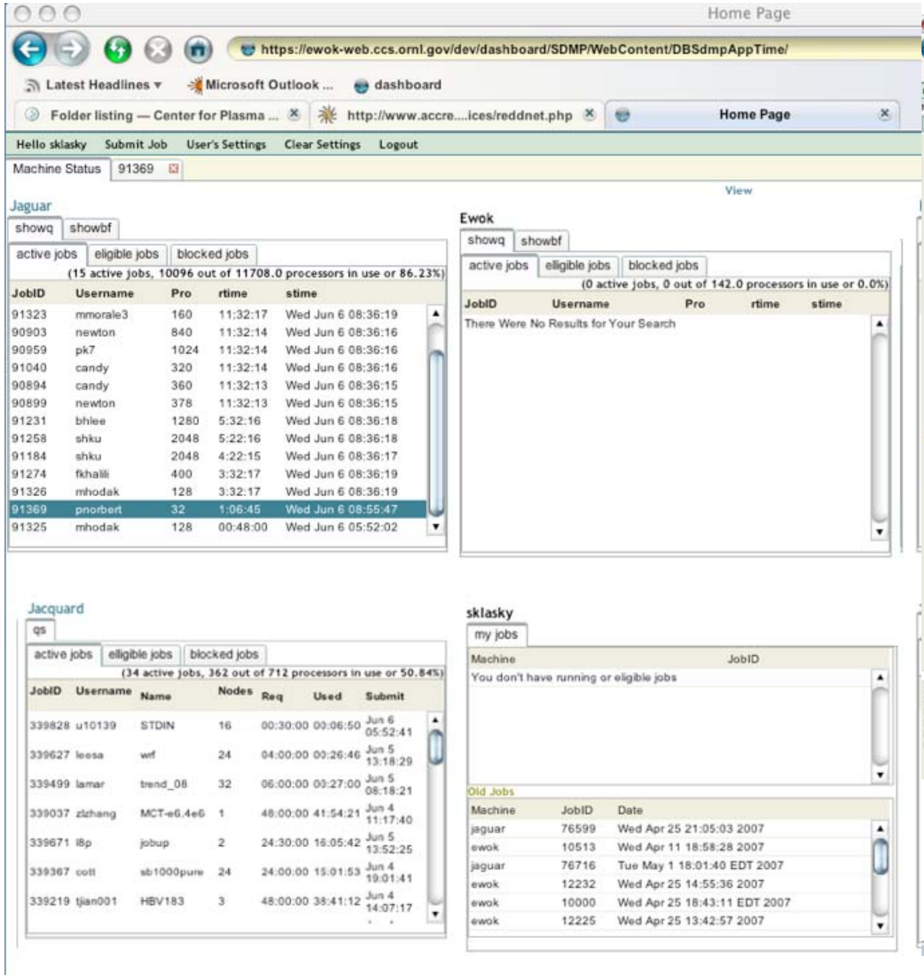


CPES-Kepler coupling/monitoring framework.

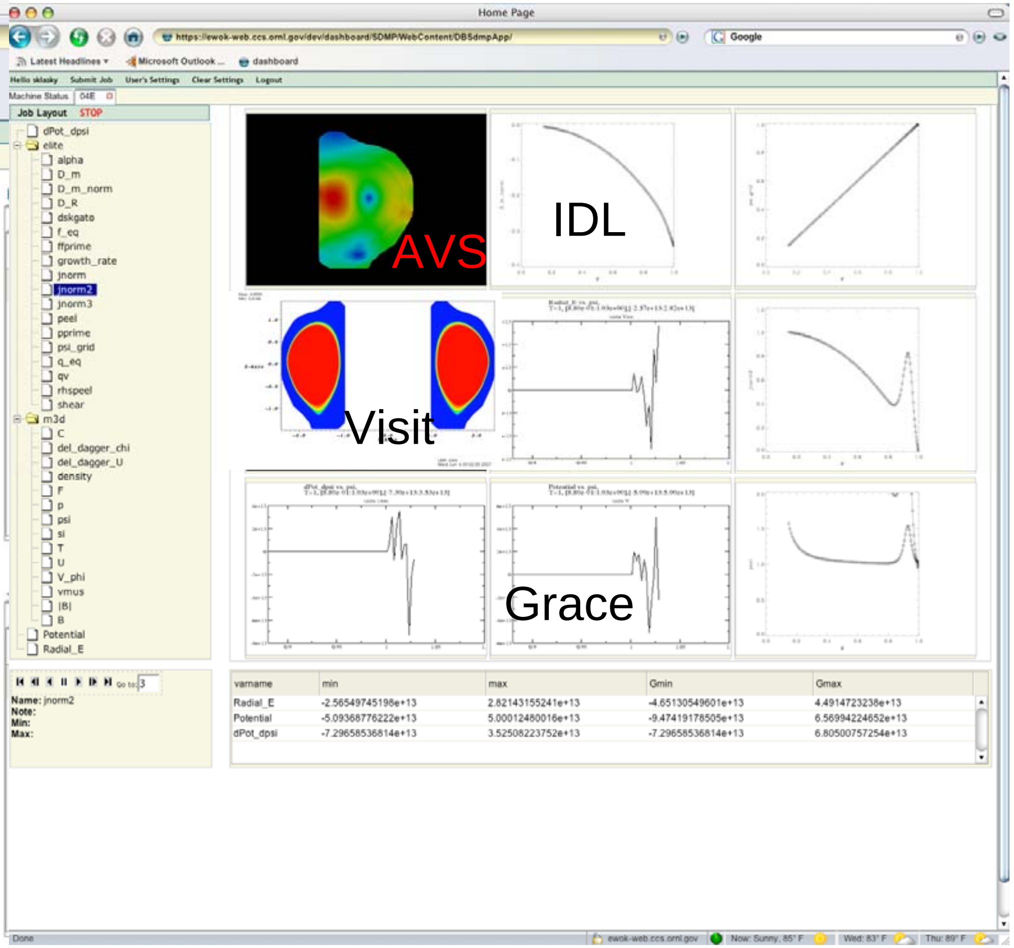
- Job submission.
  - Works for ORNL and NERSC computers, and Grid certificates. [Globus NOT supported by ORNL!]
  - Keeps data streams open with SSL connections.
  - Starts the kepler workflow system during job execution.
- Code coupling. Couples the XGC0 code monitoring routines on the ORNL end to end cluster.
  - Launches the Elite and/or M3D/OMP and or the M3D/MPP codes to check for linear stability.
  - Stops the XGC0 code on jaguar/seaborg if the stability codes indicates it's unstable.
  - Launches the M3D-MPP code.
- Simulation monitoring.
  - Allows any code to produce graphics! (IDL, AVS, Visit, Matlab, gnuplot, Grace).
  - Allows to use for data analysis.
  - Working on 'google-map' technology for display images on dashboard
- **Makes messy and difficult coupling jobs easier!**

Current CPES/SDM Dashboard

Dashboard show simulations at ORNL and NERSC

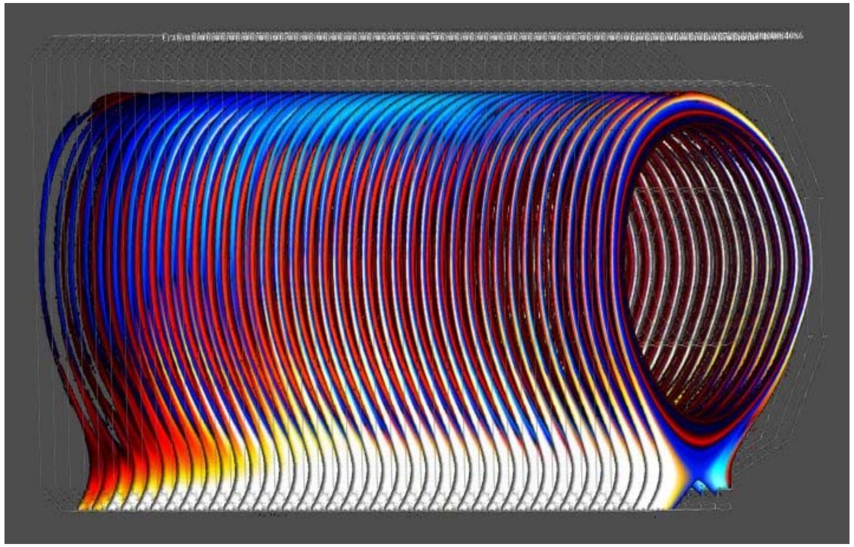


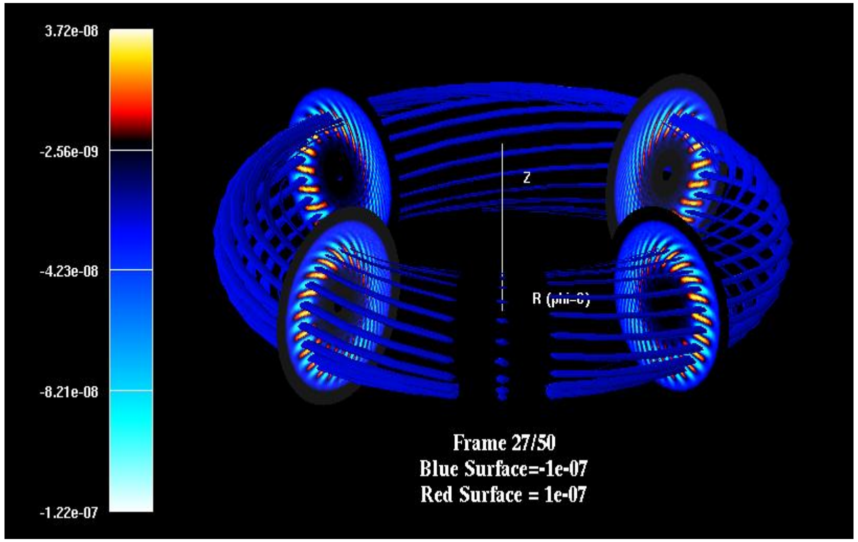
Monitoring of data: Capable for monitoring TB's of Data with efficient communication mechanisms!

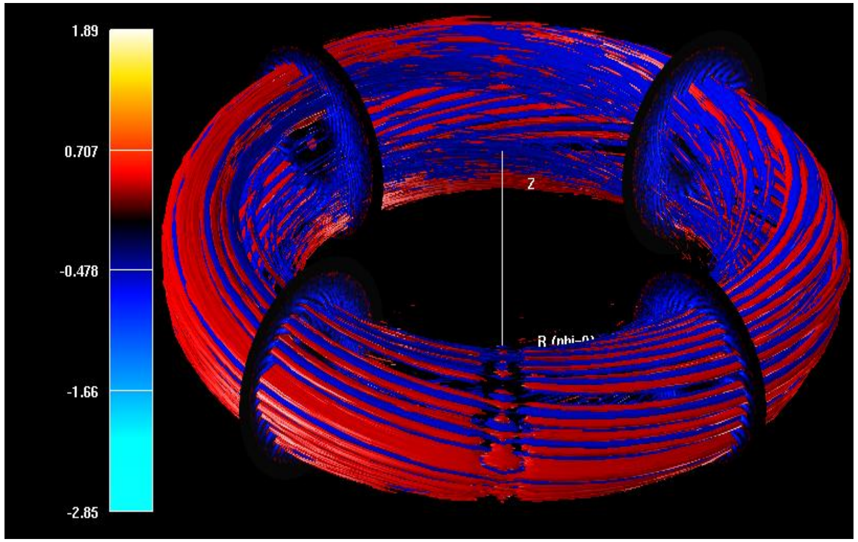


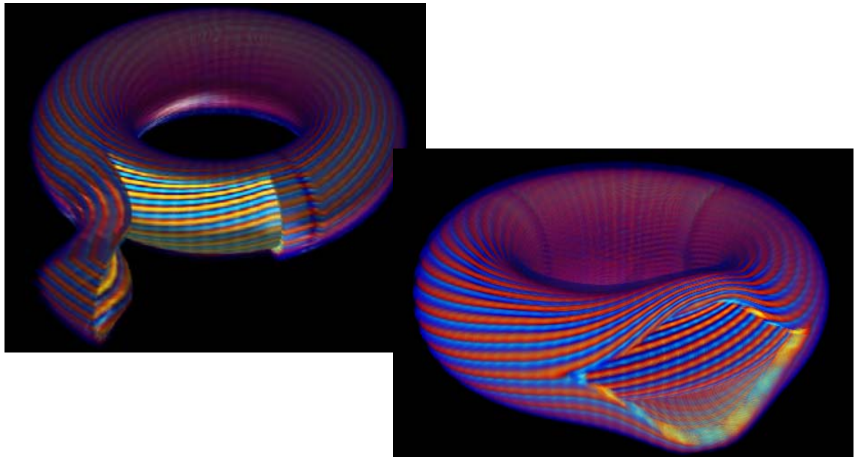
Allows monitoring of ORNL/NERSC machines + jobs on all machines (old + new jobs).
Fully Integrated with SQL Databases.
Uses Enterprise techniques for monitoring and visualizing data.

Community input will make it better



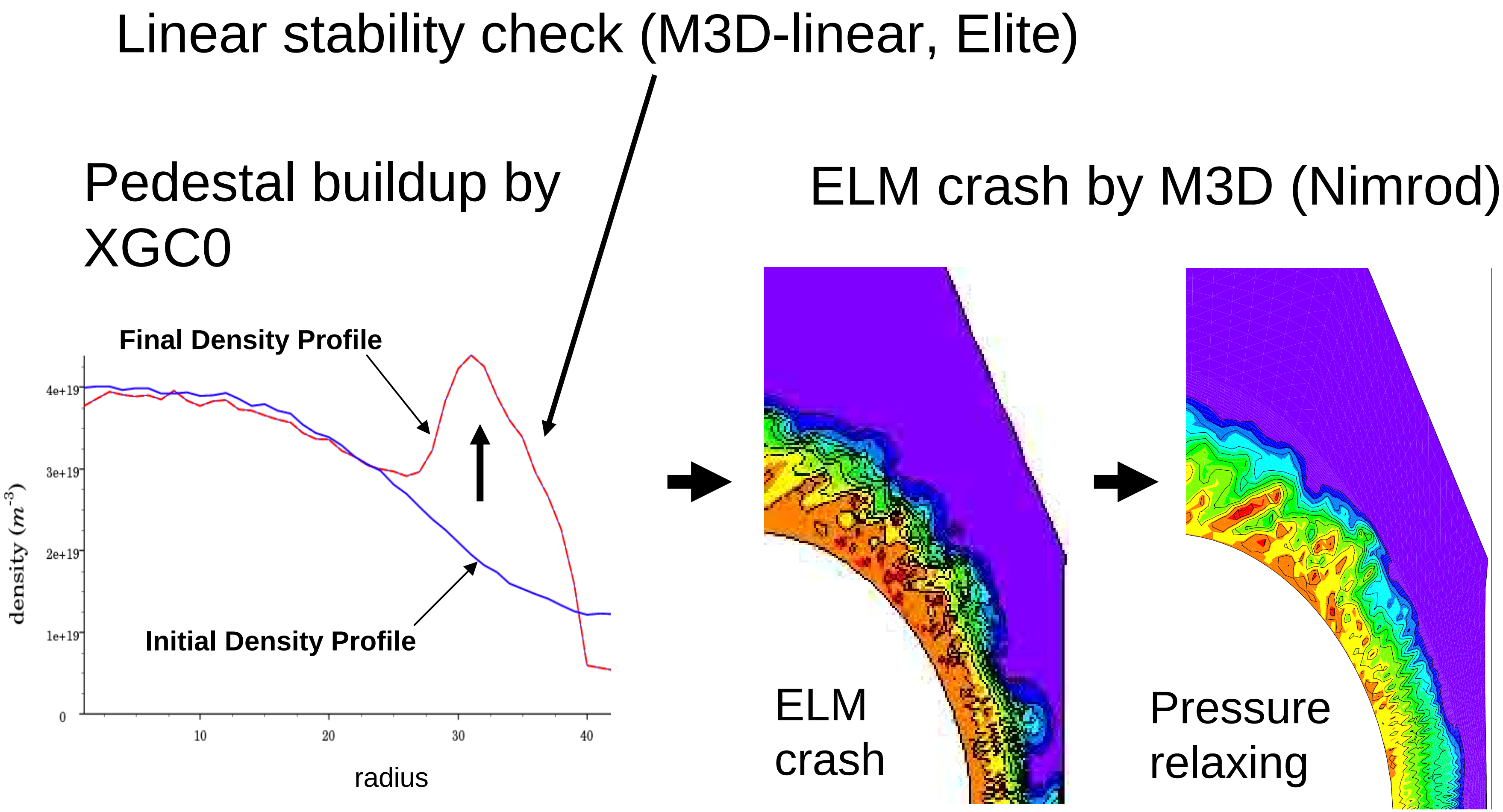






CPES-Kepler demonstration

Coupled XGC0-MHD simulation of ELM cycle on Kepler workflow

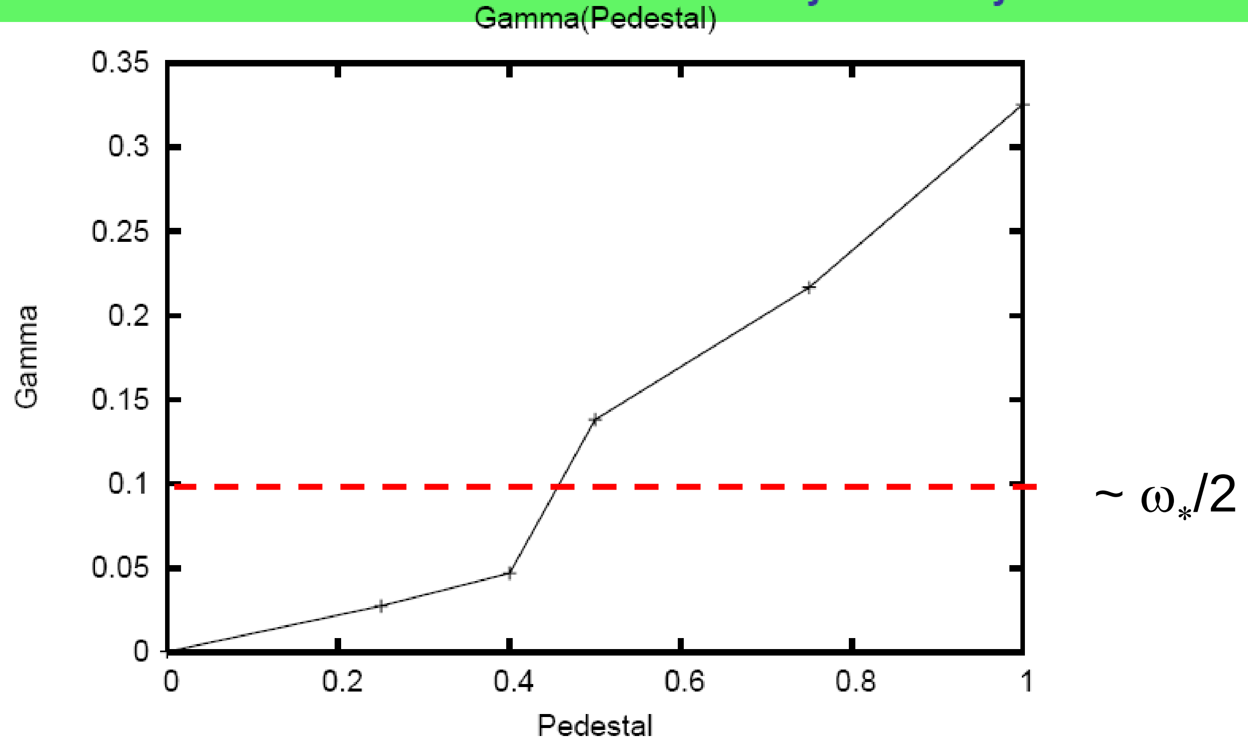


XGC0–M3D coupling: linear stability check

Coupling to ELITE improves the speed.

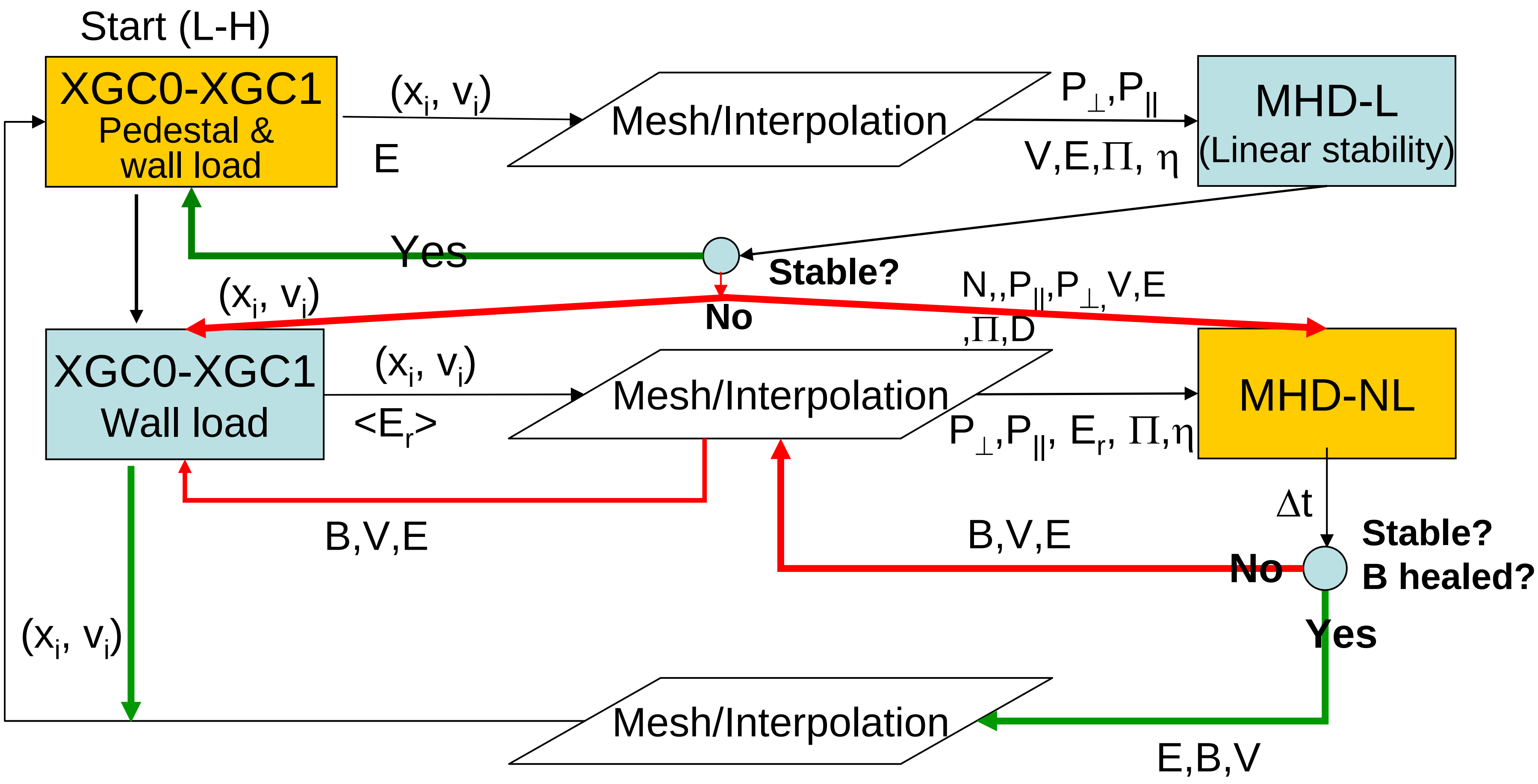
Example of resistive stability

Growth rate of n = 9 mode in a sequence of equilibria
break in curve indicates ideal stability boundary



Fraction of XGC pedestal is varied from 0 to 1 in M3D
Calculate linear stability, resistive MHD model
S = 10^6 at top of pedestal, S = 10^2 at bottom of pedestal

Workflow between XGC and MHD



Orange : Main simulator

XGC evaluates SOL transport during ELM crash.

XGC0 has Grad-Shafranov feedback control coils

2006 PSACI

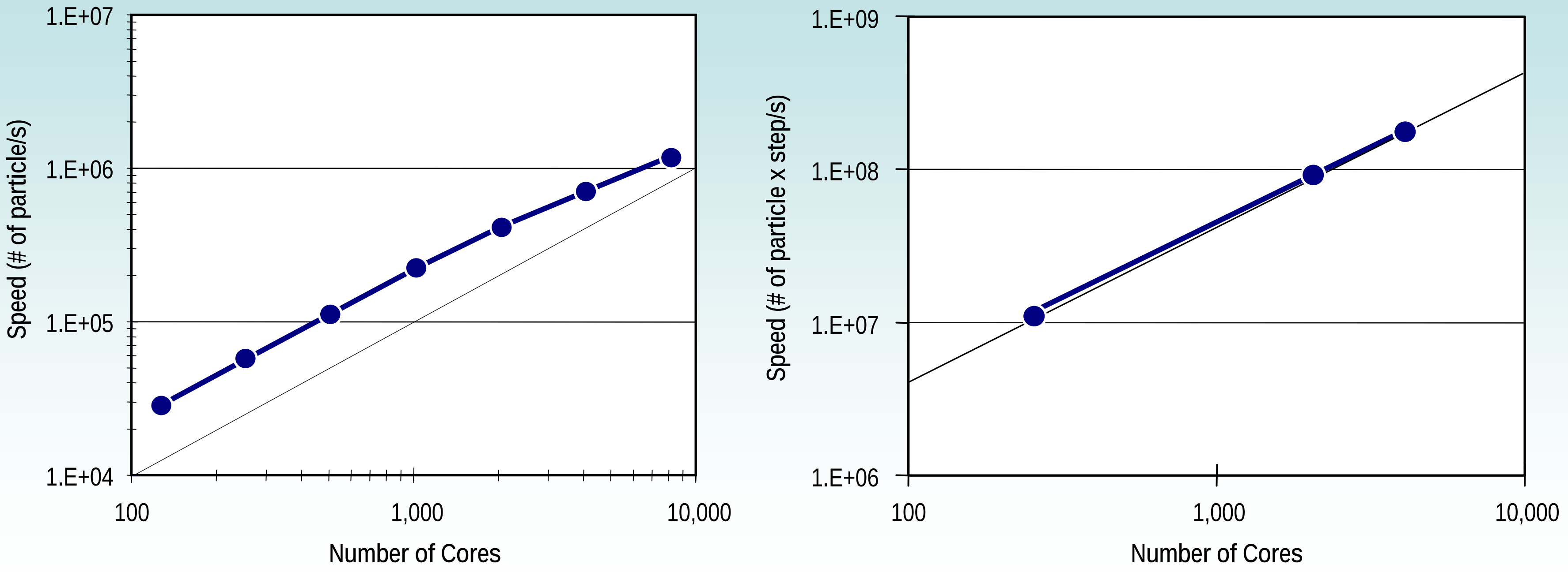
HPC is a required element in CPES

- XGC1 gyro-kinetic edge turbulence code (PIC)
  - Unstructured mesh
  - Spline of numerical magnetic field data to particles
  - Full-f ions (non-Maxwellian)
  - Thousands Cray XT cores for developmental runs
  - Over ten thousands Cray XT cores for production runs

    We have used up to 16,000 cores per job.
- XGC0 kinetic edge equilibrium code (PIC)
  - At least 1,000 times faster than XGC1 due to reduction in cell/particle numbers
  - 1,000 times longer experimental time runs than XGC1 (> 1sec)
- Both XGC0 and XGC1 scale very well with # cores
- XGC0/XGC1 coupling in near future
- Grid coupling of XGC with large memory codes (*eg*, M3D, NIMROD) requires advanced data management..
- **1.1 M Jaguar hours already used in this year.**

Scalability of XGC1 on Jaguar:
Near linear scaling for strong scaling
Linear speedup for weak scaling

XGC Strong Scaling : 131M ions and electrons, 200K grid	XGC Weak Scaling : 50K ions and electrons/core



CPES Physics Goals

Through as much first principles simulations as possible, obtain predictive capability of

- L-H transition (XGC=XGC0 + XGC1 coupling)
- Pedestal growth and ELM cycle (kinetic-MHD/2Fluid)
- ELM control (kinetic and MHD)
- Edge rotation source
- Scrape-off and divertor physics (with impurities)
- Wall heat load
- Core-edge transport coupling (fluxes, pedestal height and rotation boundary condition)
- RF antenna effect on edge plasma
- Effect of core events on edge and heat load

In **Kepler workflow** framework with web-based, user friendly data management and visualization.

Scientific Results

XGC1 edge gyrokinetic code (full-f, 5D)

A full-f kinetic solution of plasma equilibrium across the separatrix (pedestal top to scrape-off), for the first time.

- Large scale convective cell with strong ExB sheared flow has been observed in the whole edge plasma, which may be related to turbulence suppression in H-mode.
- Strong edge rotation source has been observed, which can propagate inward by turbulence pinching (Hahm's analytic theory)

Electrostatic turbulence capability is under verification

XGC0 edge kinetic equilibrium code (mature)

- Full-f ions, electrons, neutrals, conserving collisions
- Verification reported at 2007 US-EU Transport Task Force Workshop
- Existing J_{Boot} formula works unless the density pedestal is very steep.
- Successfully simulated the density drop by Resonance Magnetic Perturbation (RMP), for the first time

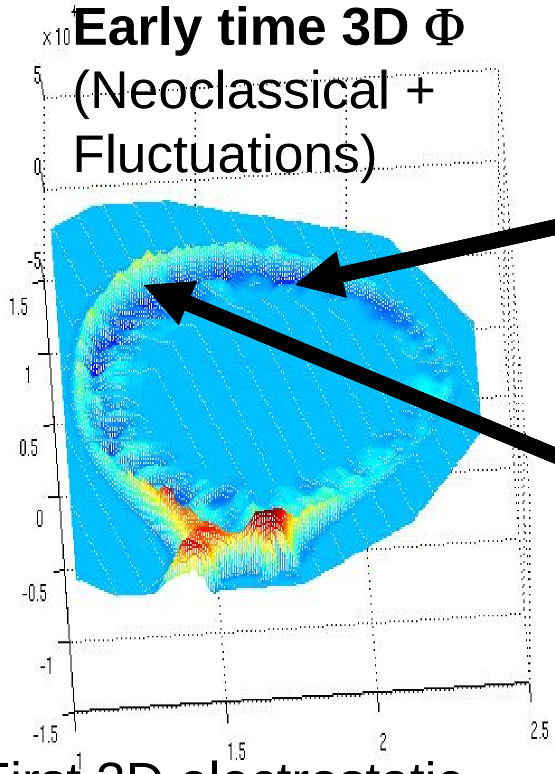
GTC and GEM: preparatory exploration of edge turbulence.

PIC Noise problem is solved (reset, collisions)

Plasma surface interaction data are beginning to emerge

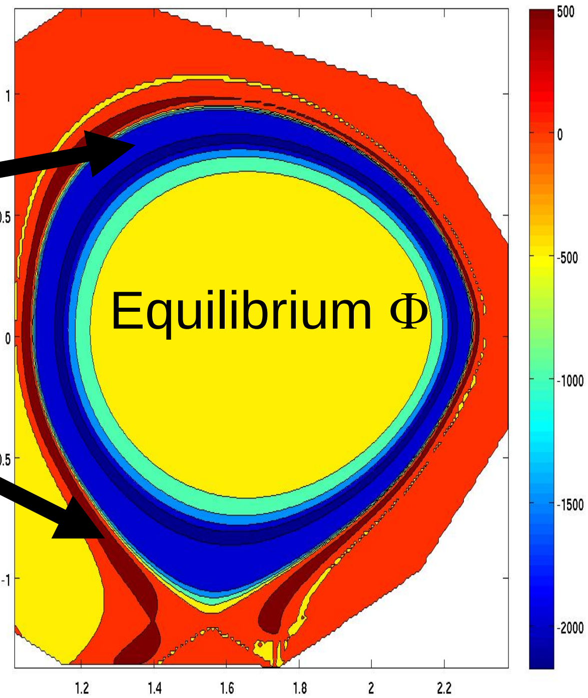
XGC1: Short time Turbulence/Neoclassical gyrokinetic code, will provide turbulence flux to XGC0

Early time 3D Φ
(Neoclassical + Fluctuations)



Negative potential well in H-layer (dark blue)

Positive potential hill in scrape-off (yellow-brown)

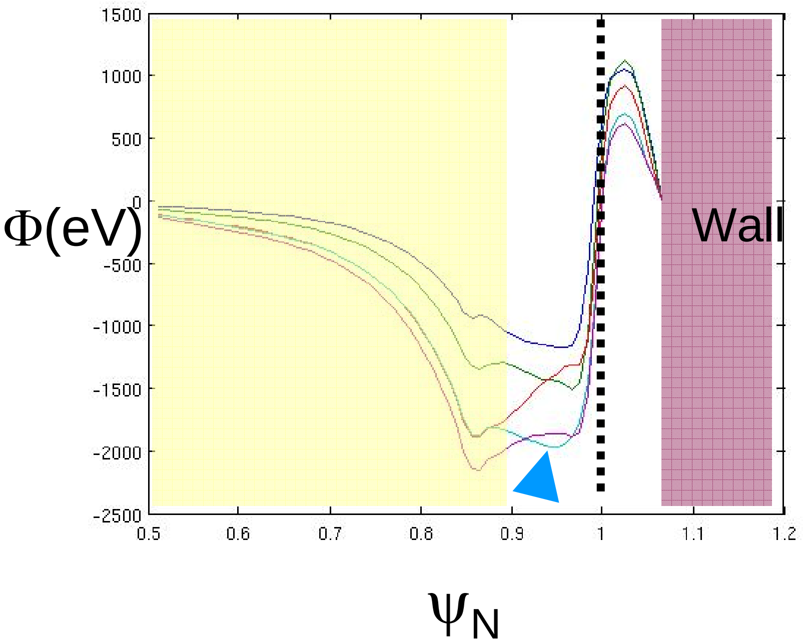


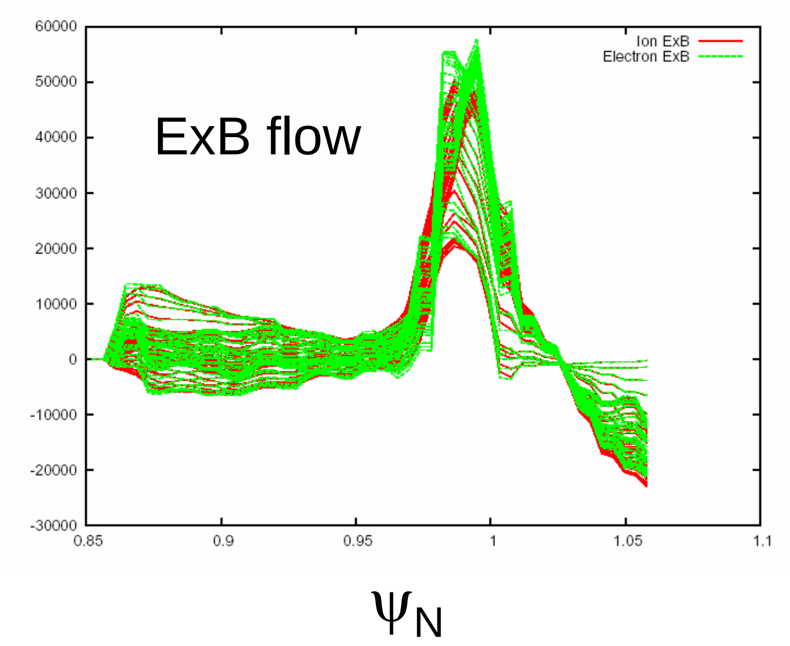
First 3D electrostatic solution across separatrix has been obtained from XGC. What fraction of the fluctuation is numerical?

2D neoclassical potential distribution has been extracted from 3D by toroidal averaging and poloidal-time smoothing

Figures from 2006

Strongly sheared ExB flow profiles in an entire H-mode edge ⇒ Important physics information for fusion





Figures from 2006

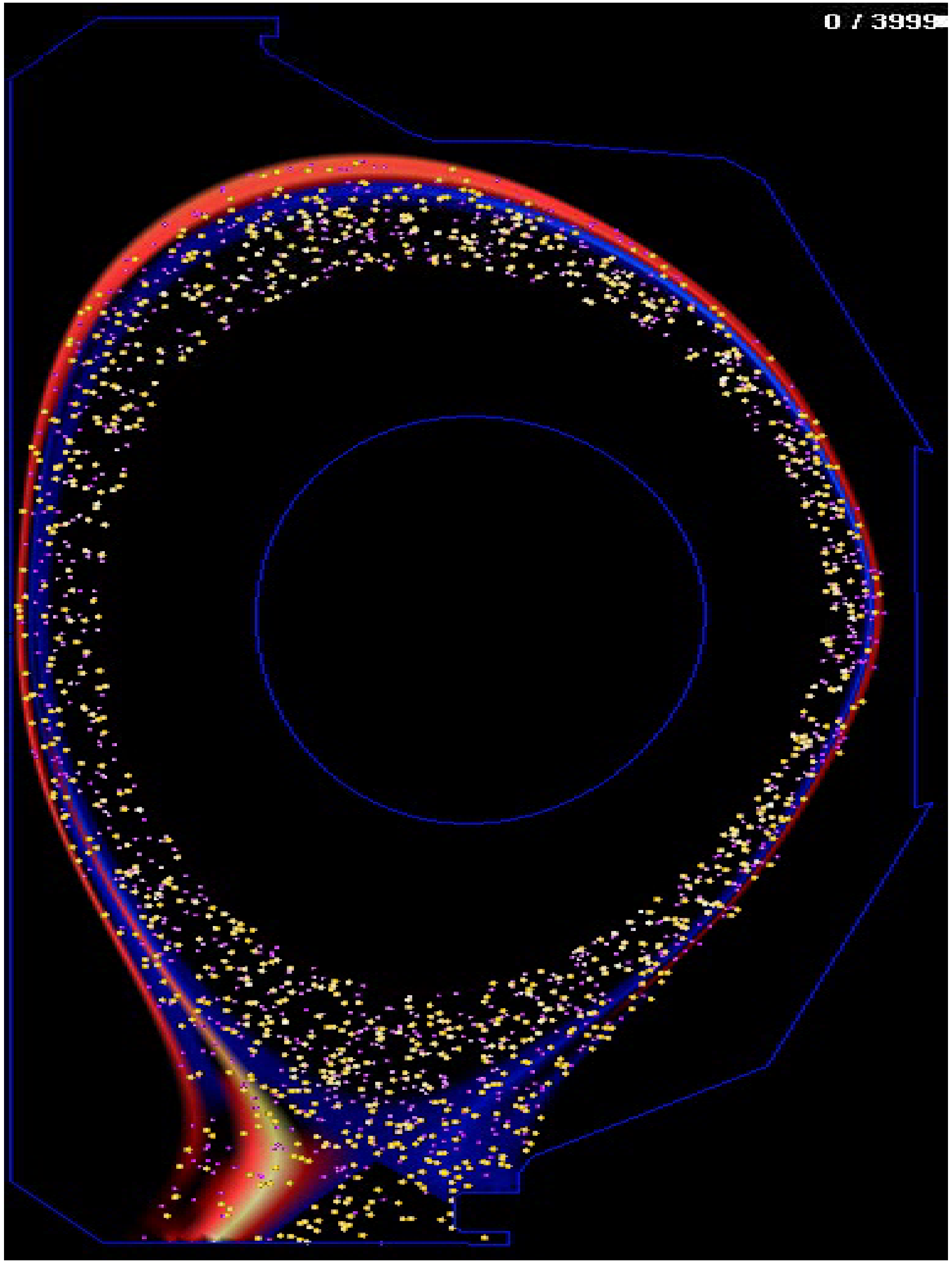
Gyrokinetic particle motions in the poloidal plane

ions

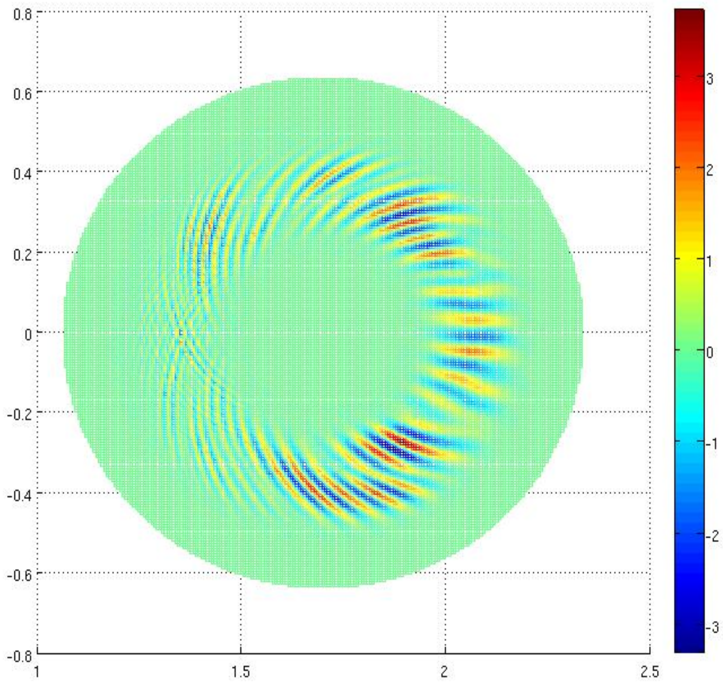
electrons

$V_{||} > 0$

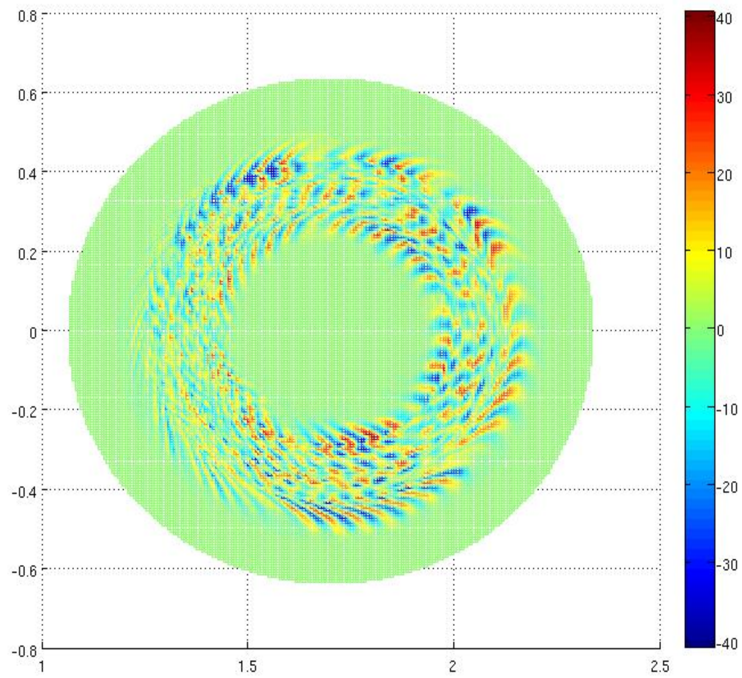
$V_{||} < 0$



Turbulence capability in XGC1 is under careful verification against core cyclone results. Afterwards, XGC1 will return to edge turbulence.



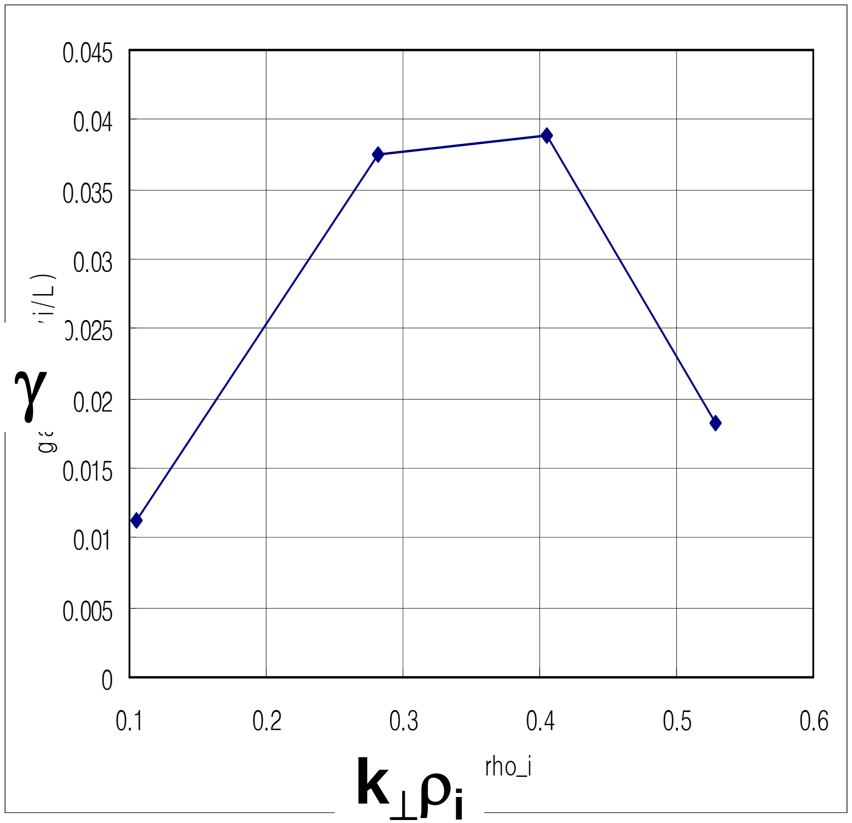
Linear ITG growth rates have been verified.



Nonlinear ITG is under rigorous verification (large scale zonal flow excluded from plot)

Global ITG linear growth rates in XGC1 have been verified in cyclone plasma

XGC



GTC

Z. Lin and T. S. Hahm

Phys. Plasmas, Vol. 11, No. 3, March 2004

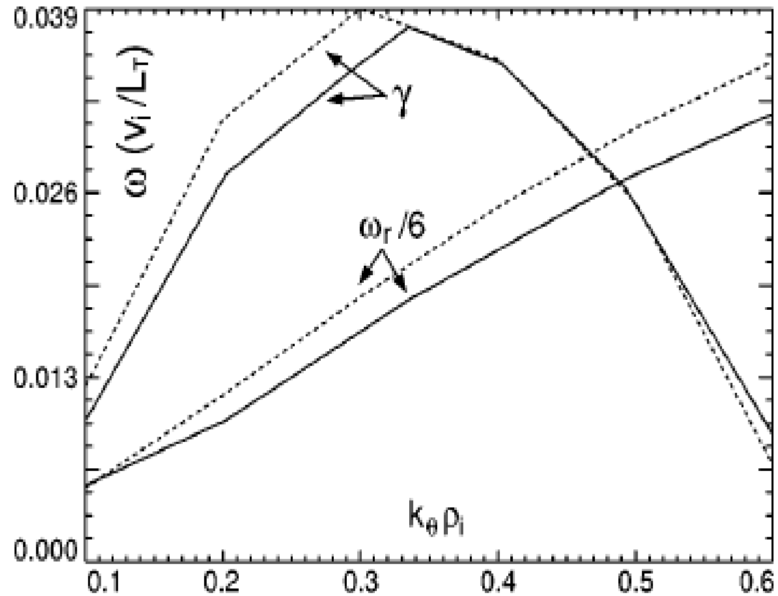
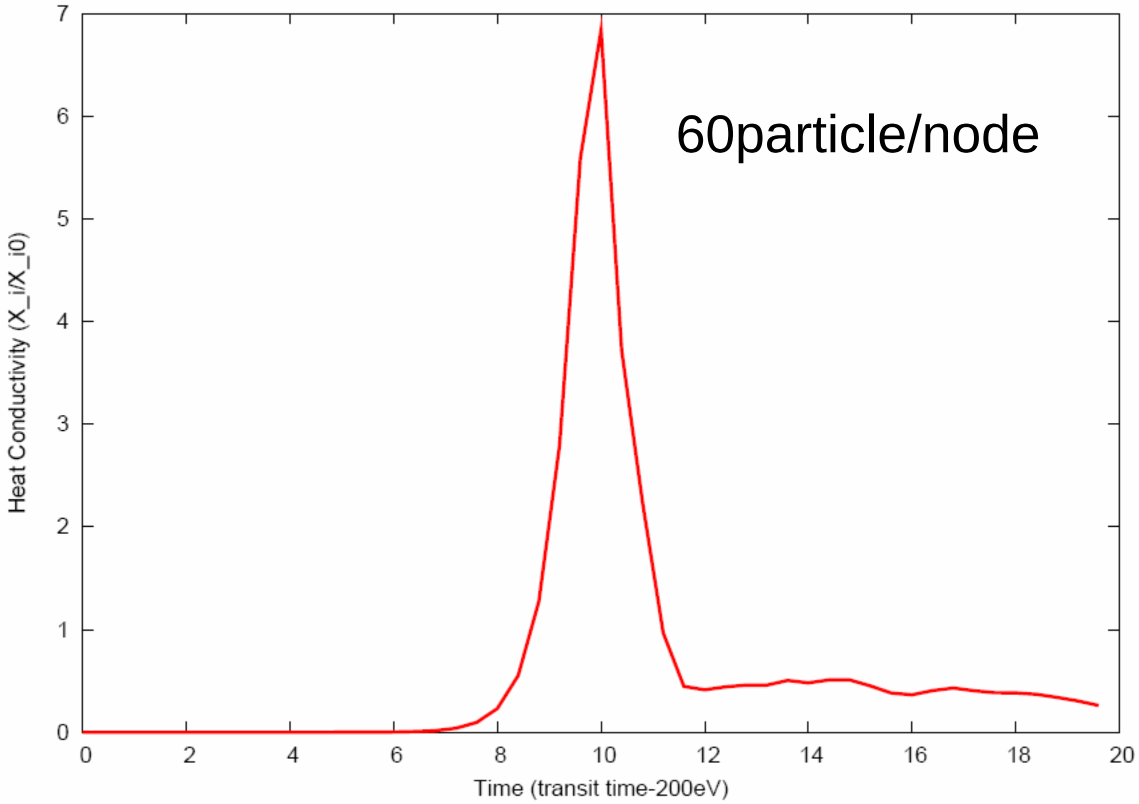


FIG. 1. Linear ITG real frequency ω_r and growth rate γ versus poloidal wave vector from GTC (solid) and FULL (dotted) calculations (upper panel),

Time dependence of ITG turbulence diffusion coefficient in XGC1



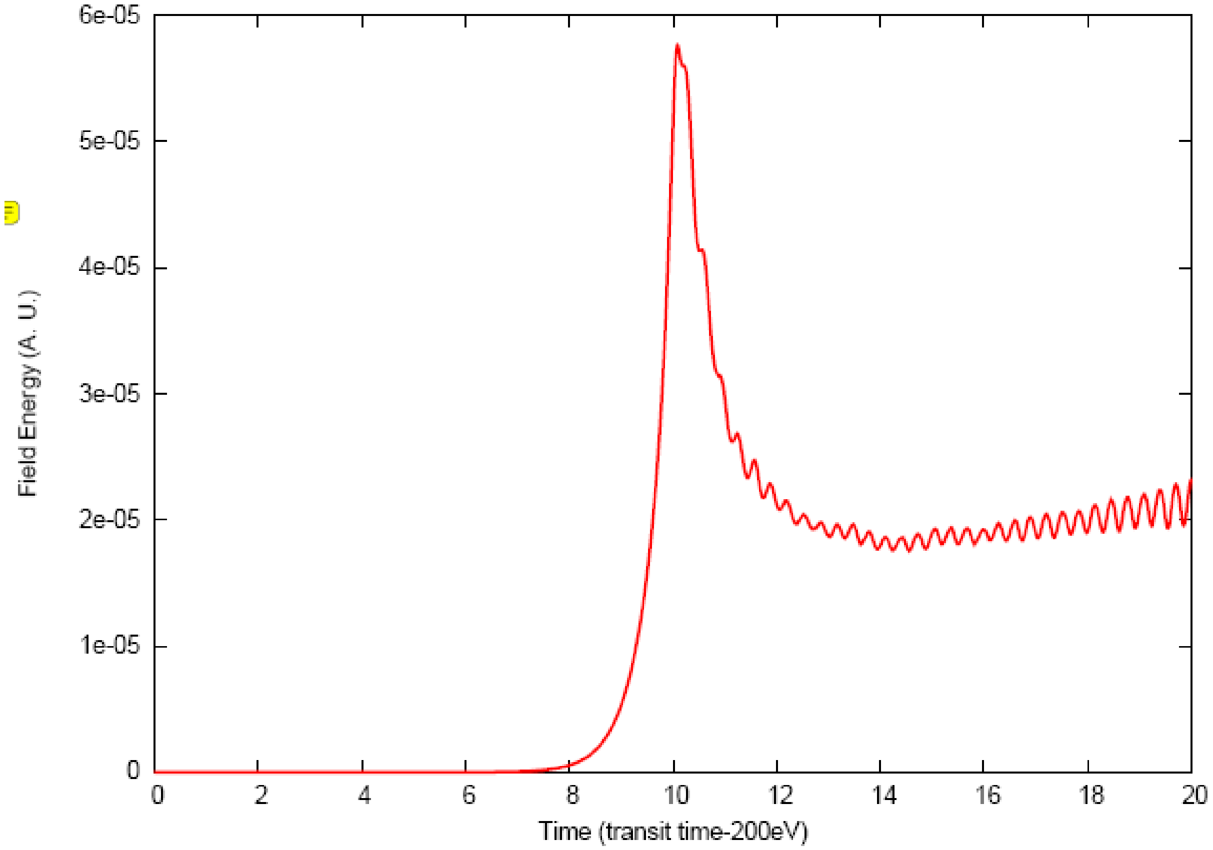
(cyclone geometry, δf_i, adiabatic electrons)

GAM does not decay?

Slow growth of zonal flow?

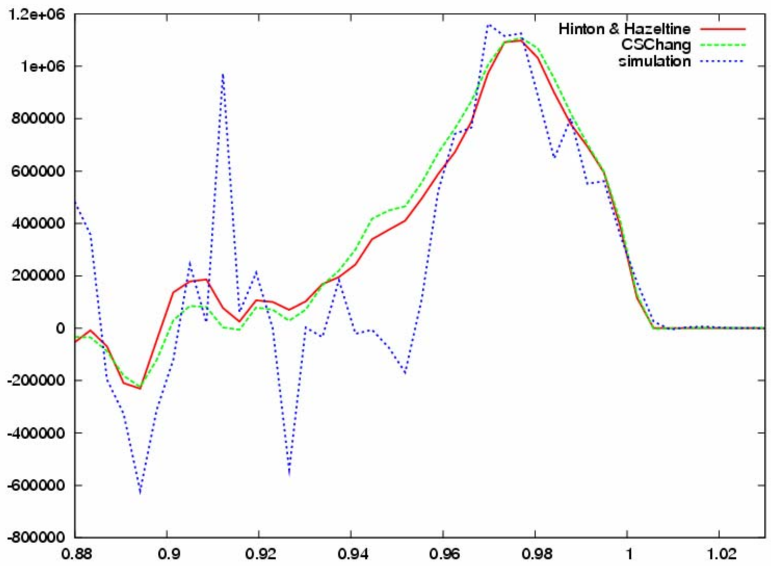
We see finer scale zonal flow with adiabatic electrons?

Need more verification before applying XGC1 to edge.

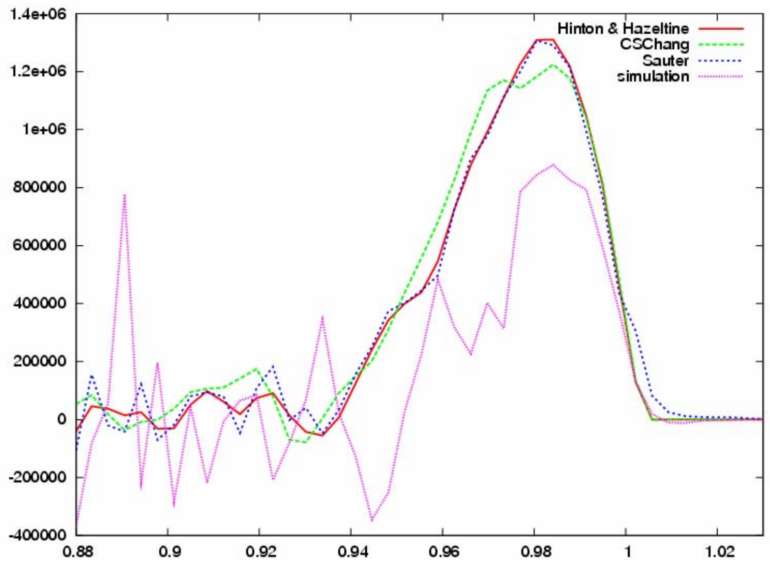


Verification of the analytic bootstrap current models
150K ions and electrons only

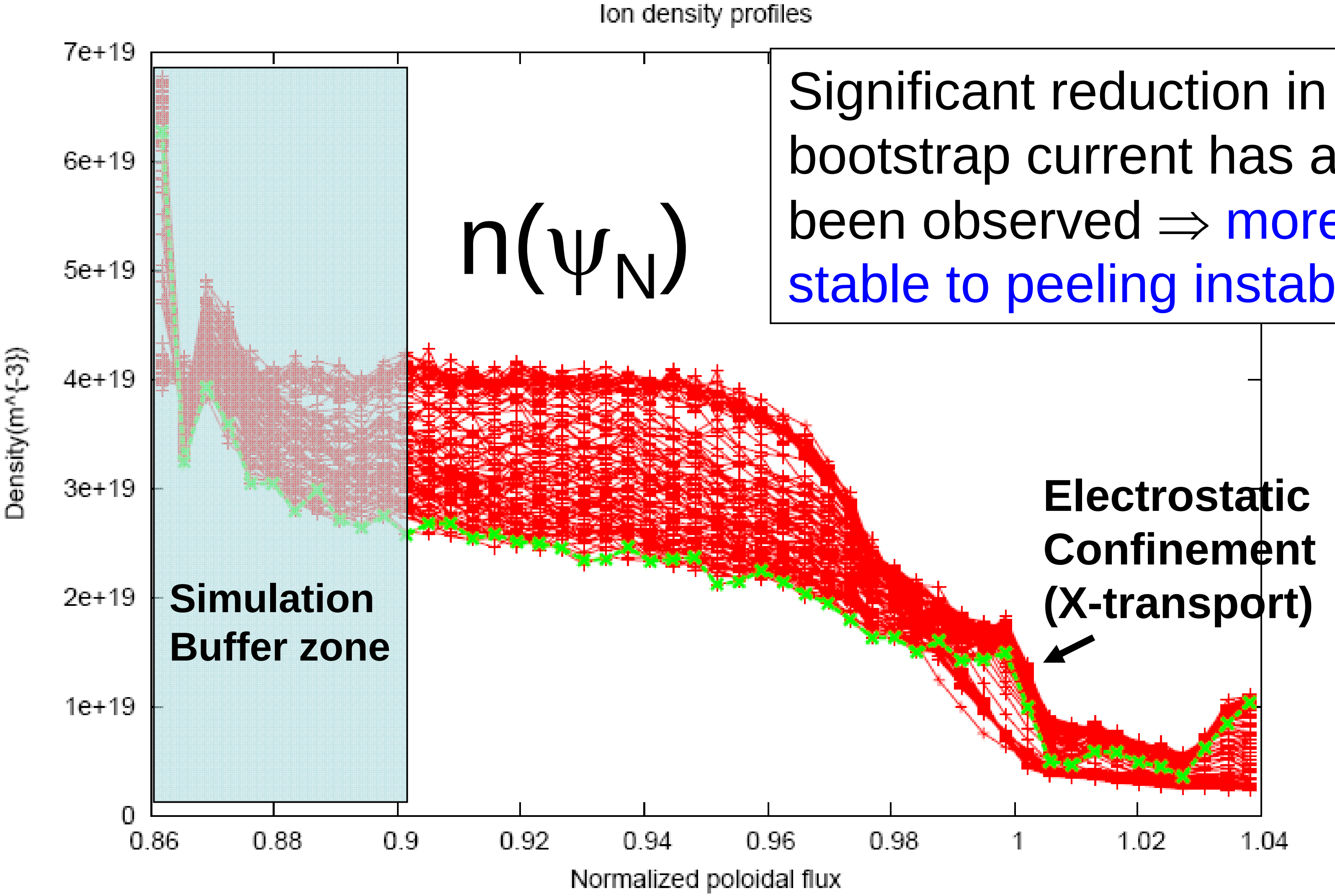
Δ_n = 1.5 cm



Δ_n = 0.75 cm

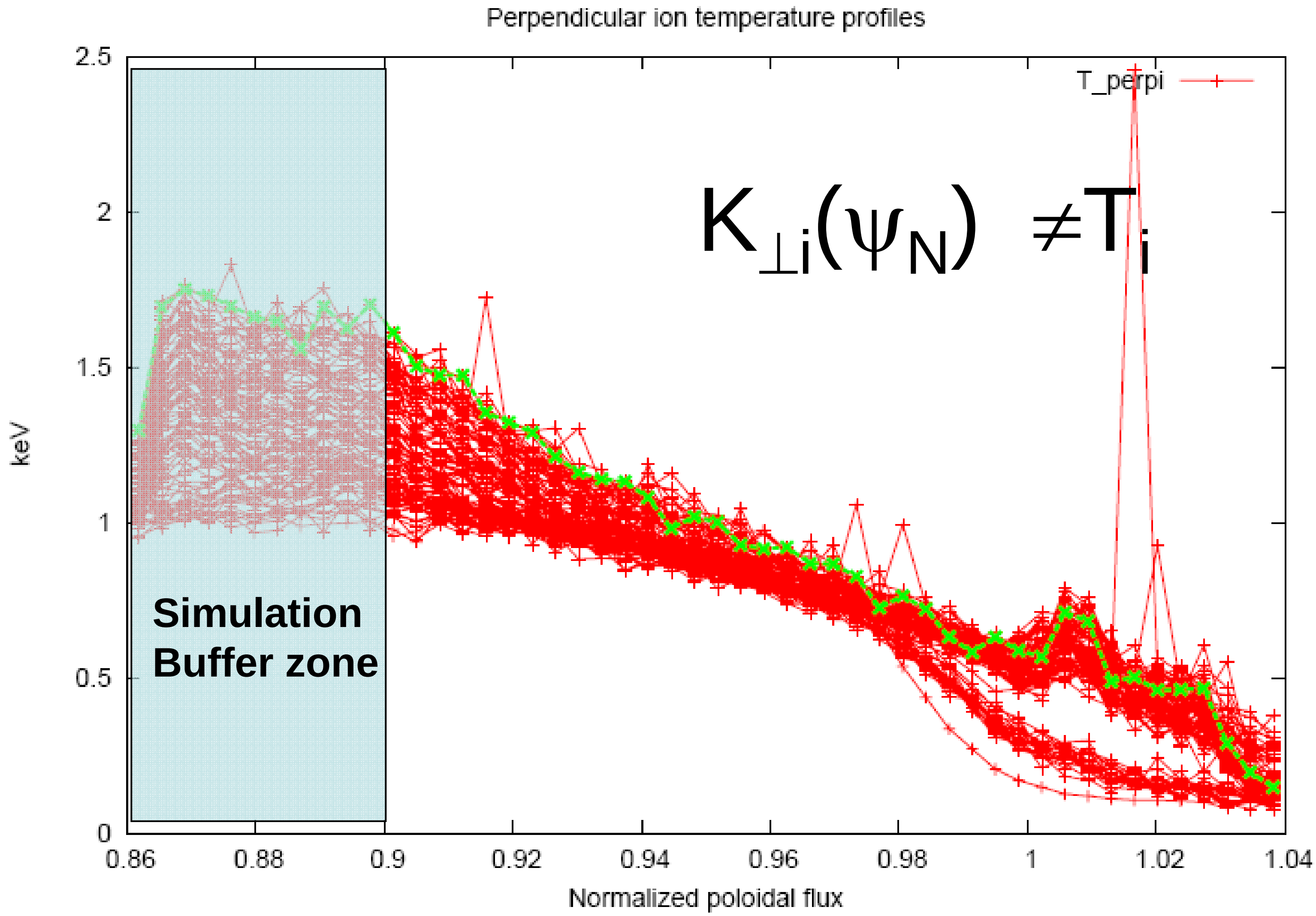


Resonance magnetic perturbation (RMP): Significant density reduction is simulated for the first time
⇒ More stable to ballooning instability

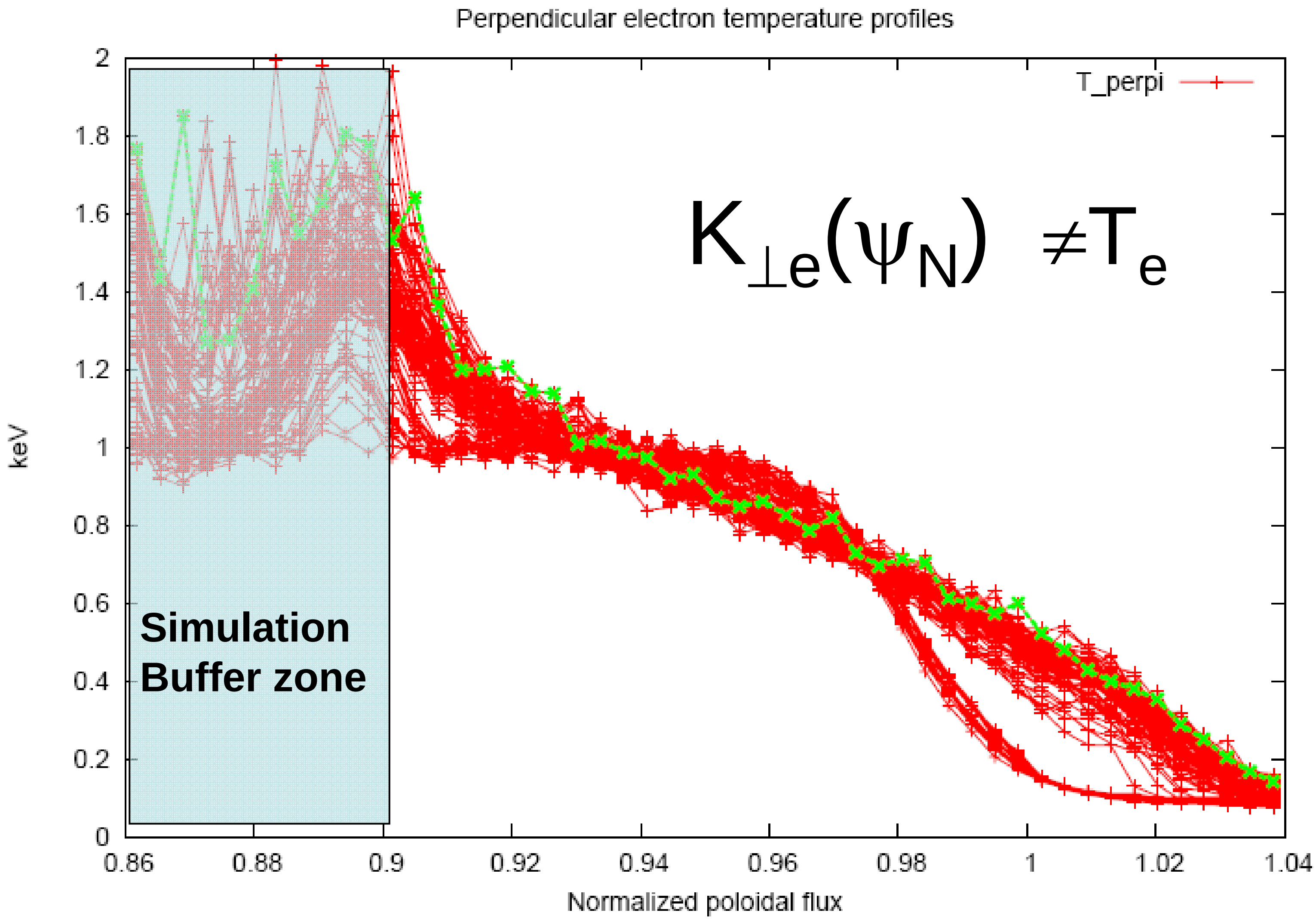


Significant reduction in bootstrap current has also been observed ⇒ more stable to peeling instability

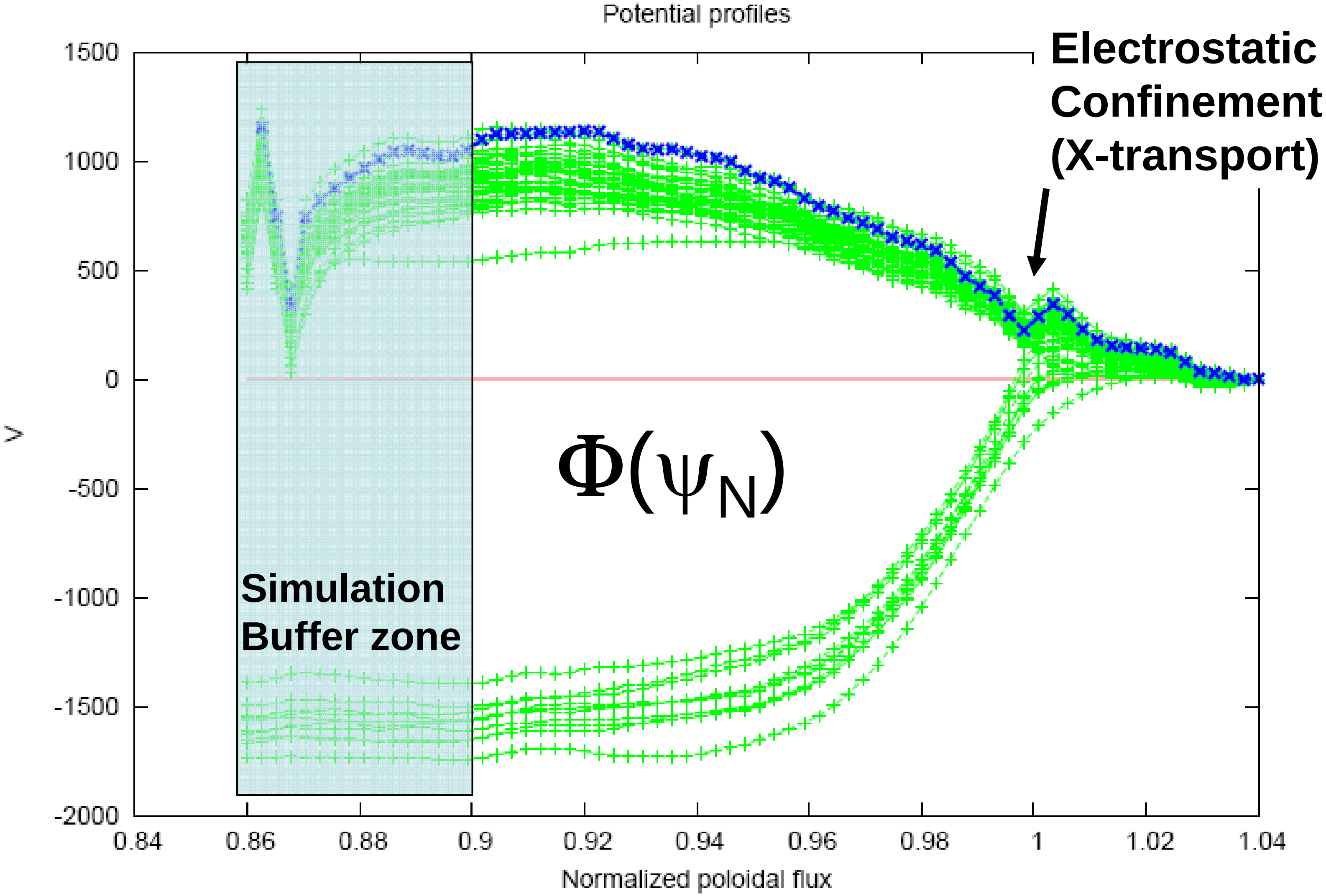
Average ion kientic energy increases due to RMP density reduction in XGC0



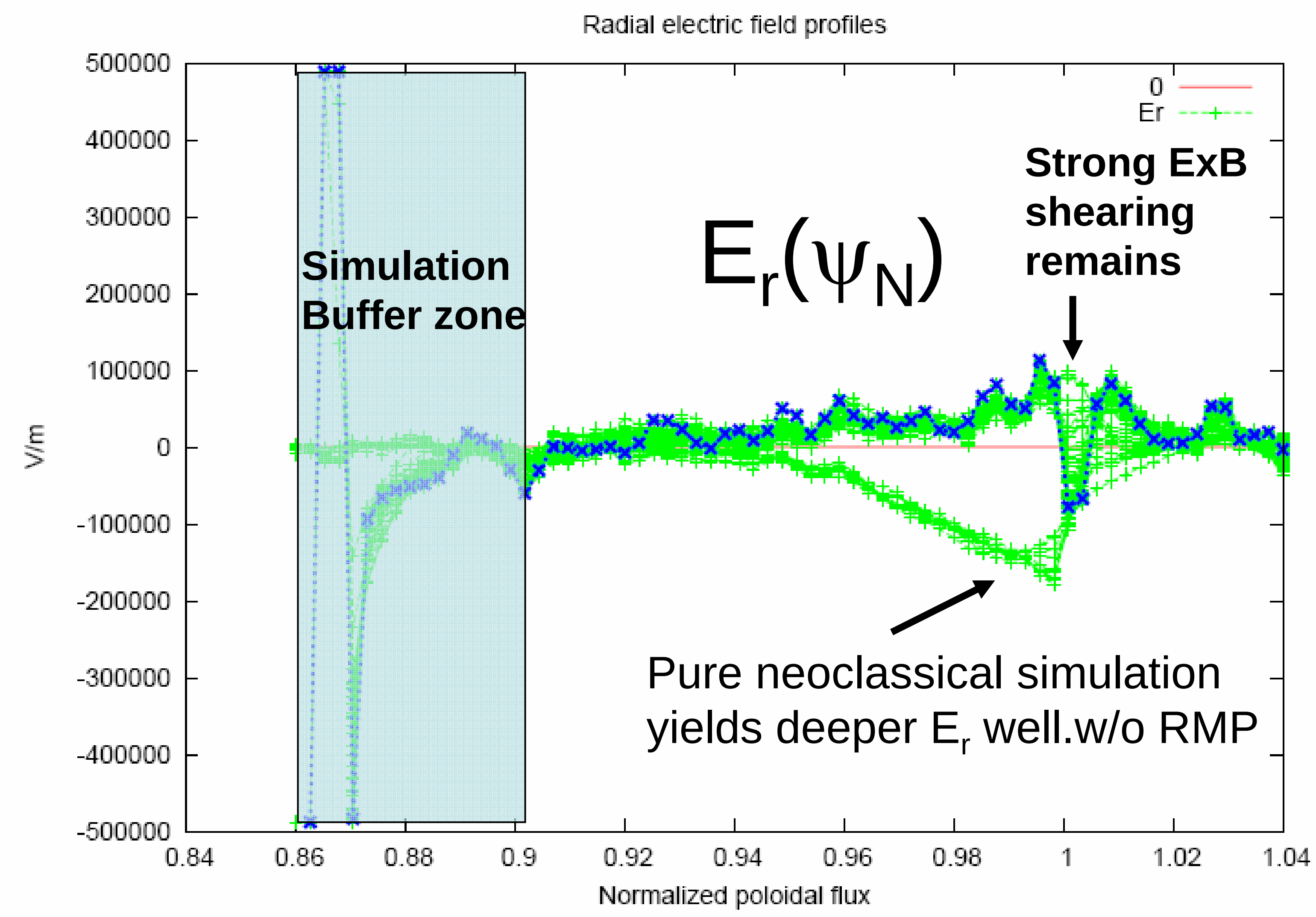
K_e may or may not increase by RMP events depending on power to electrons



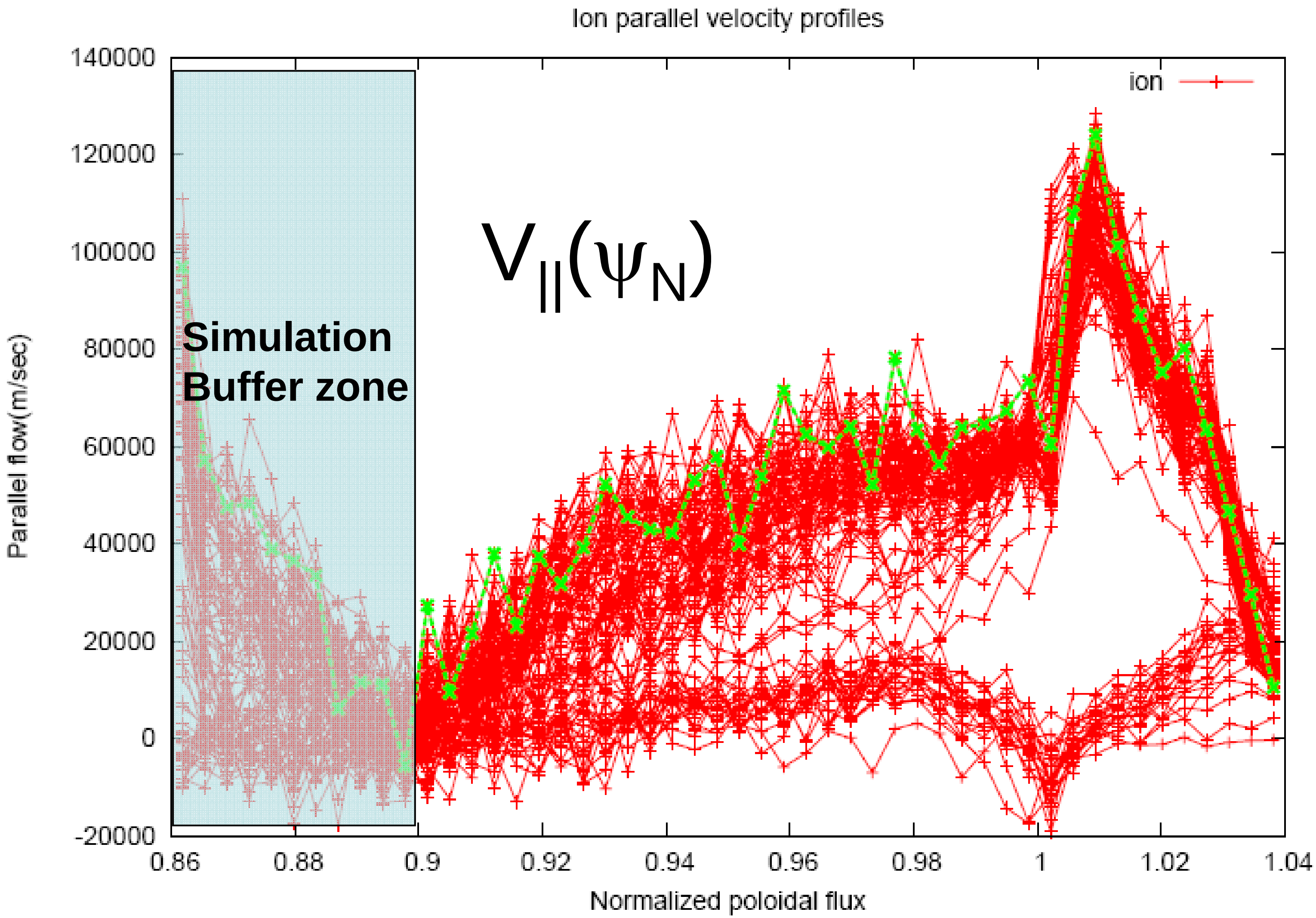
Φ>0 by RMP, but the X-loss remains robust if D_{anom} is small (0.2 m^2/s within ±20º)



E_r>0 by RMP, but the X-loss remains robust if D_{anom} is small (0.2 m²/s within ±20º)

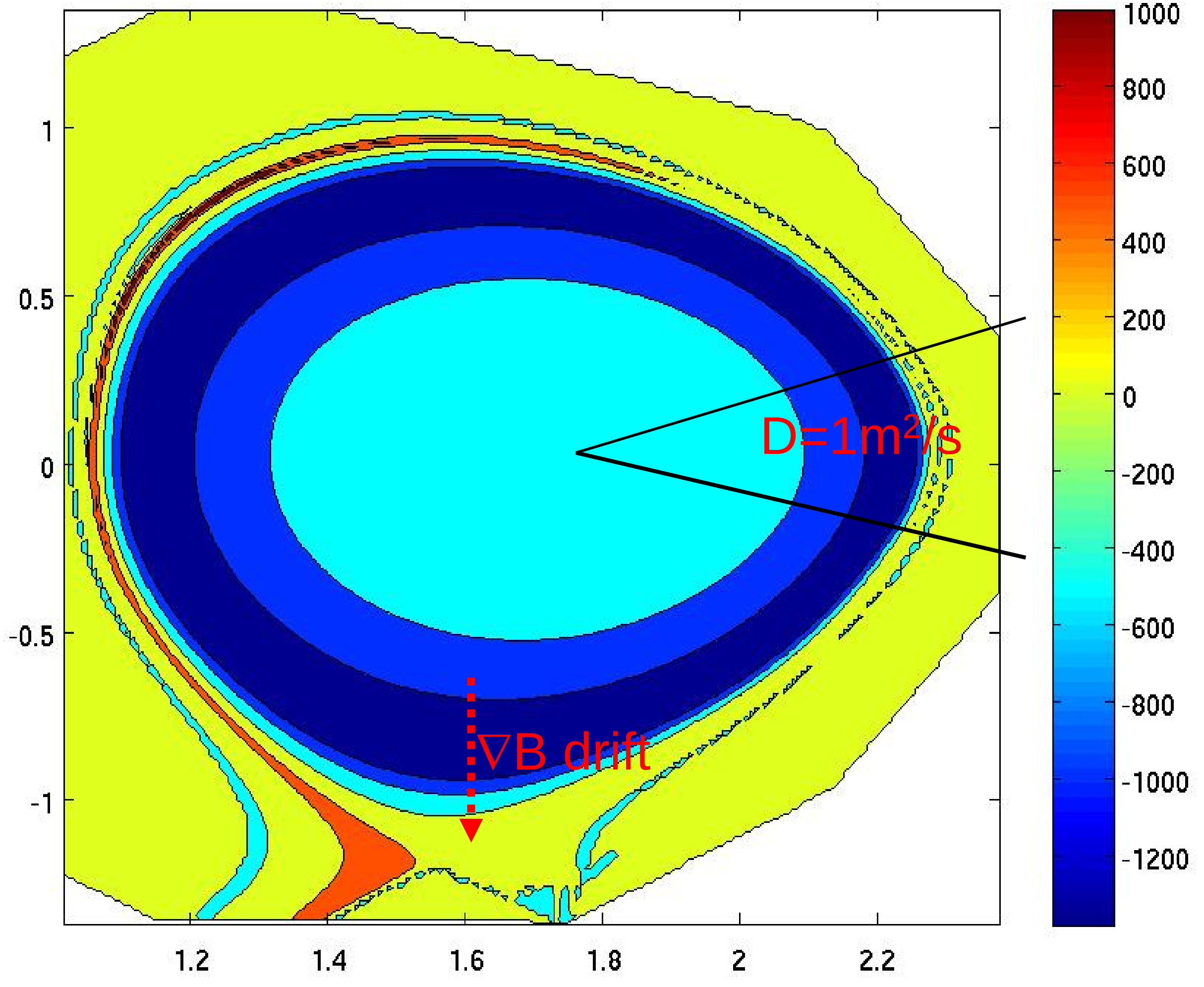


$V_{||}$ increases significantly into co-current direction (to inner divertor) by RMP in XGC0

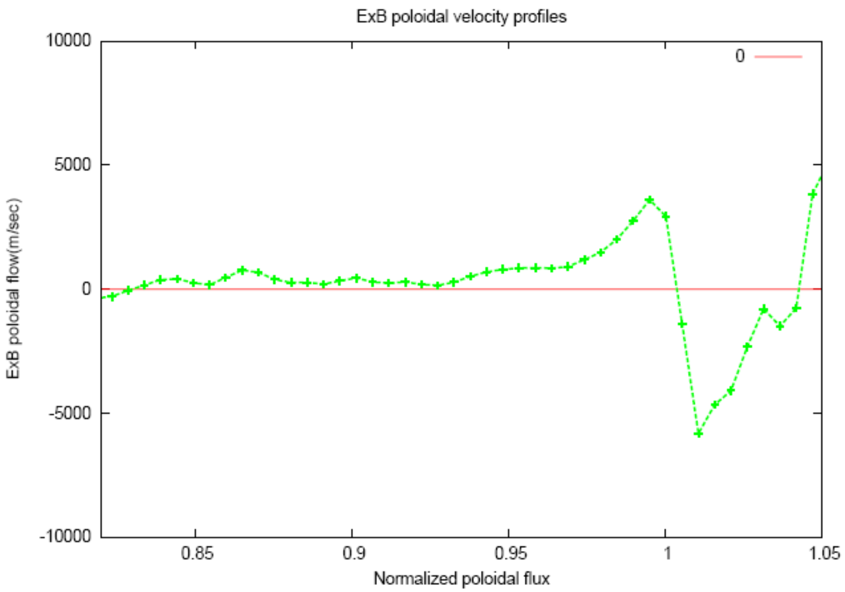


MIT's Relationship between ballooned radial loss and scrape-off physics?

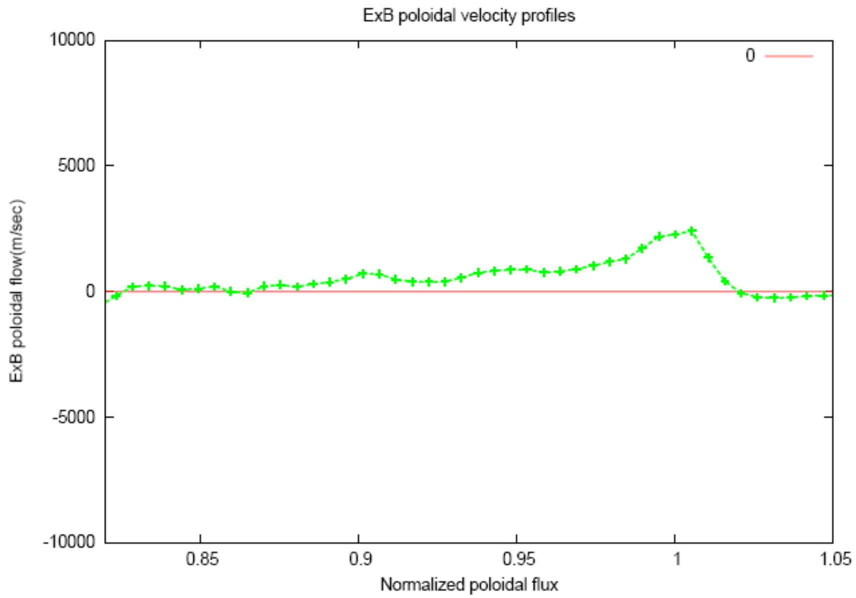
- In-out asymmetric potential observed
- Parallel flow into inner divertor indeed increases!



dV_{ExB}/dr in lower single null is stronger than upper single null (NSTX collaboration)

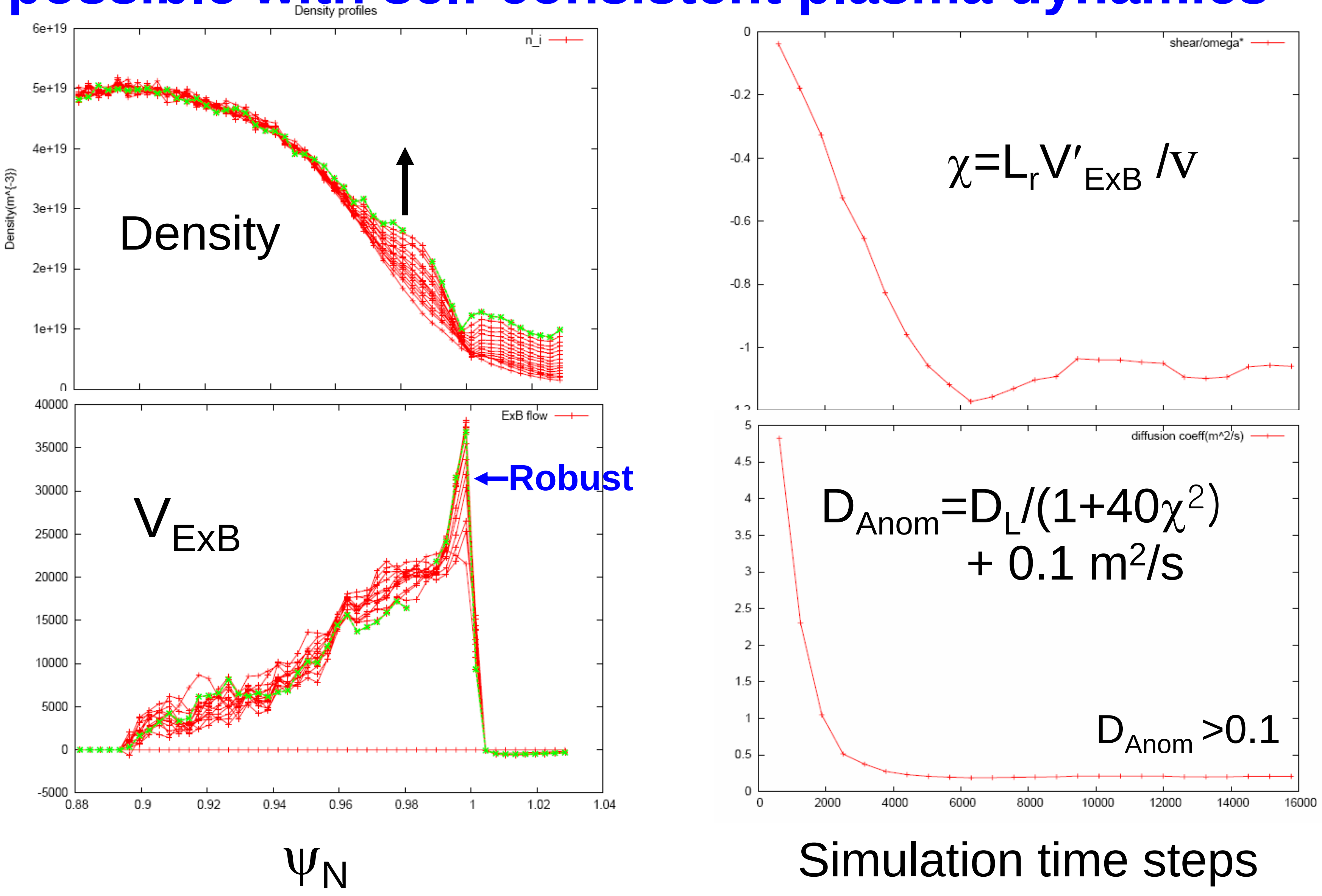


Lower single null,
just before L-H transition



Upper single null,
at identical plasma condition

Test of analytic L-H transition models are now possible with self-consistent plasma dynamics



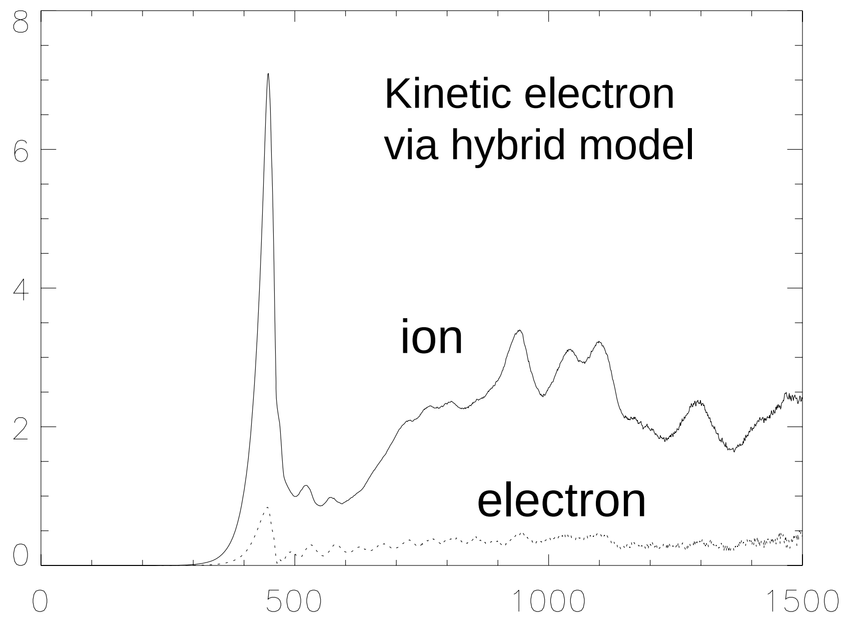
Which turbulence should we investigate first with XGC1?

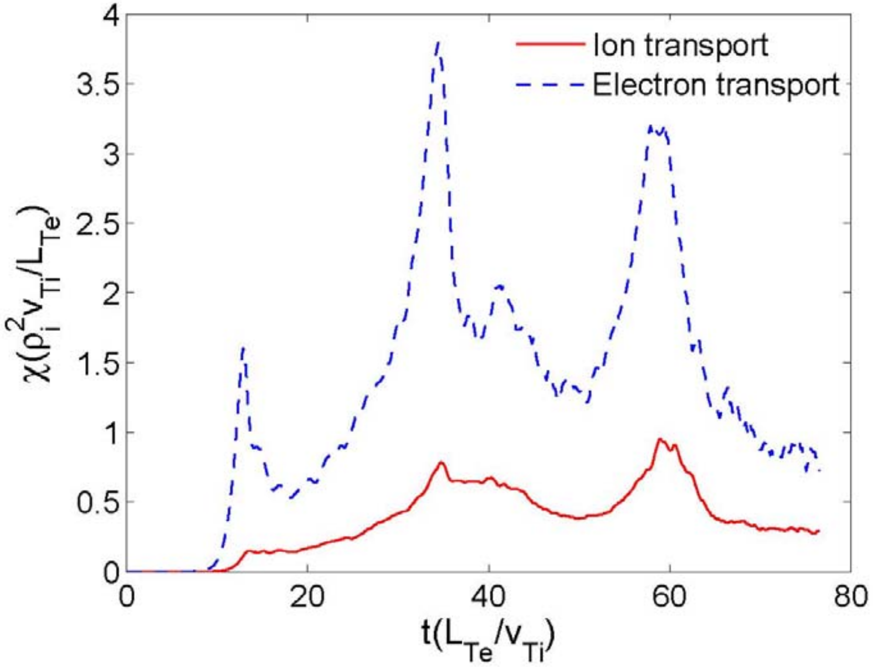
- XGC1 is expensive to run
- For timely progress of edge turbulence studies, we need to plan ahead using the existing core turbulence codes in edge-like plasmas (high q, large r/R, steep gradients)
- GTC and GEM core turbulence codes recommend Trapped Electron Mode and Drift Waves to be focused
  - Effect of magnetic shear?
  - Effect of zonal flow?
  - Effect of density and temperature gradient?

GTC Simulation of Trapped Electron Mode turb.

ITG: R/L_n=2.2, R/L_{Ti}=6.9, R/L_{Te}=6.9, s=0.78, q=1.4

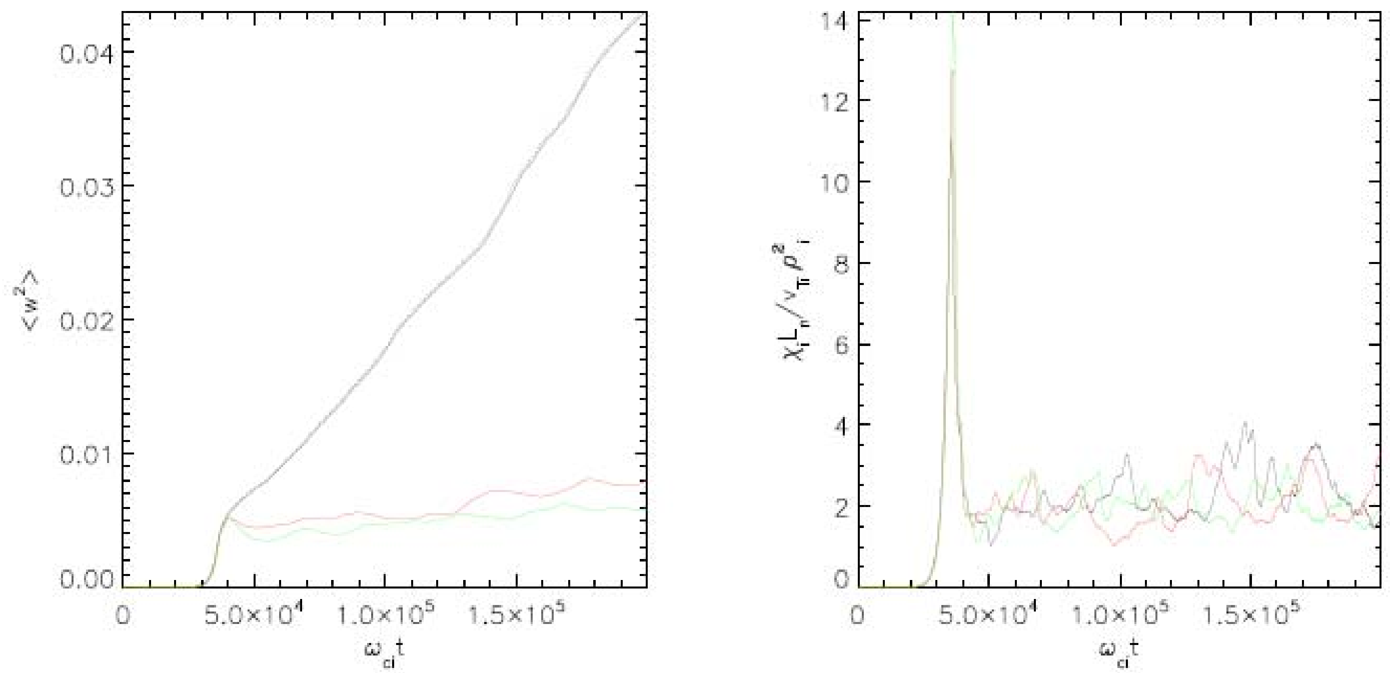
TEM: R/L_{Ti}=2.2





- η_i decrease from 3.1 to 1.0 → transit from ITG to TEM
- ITG turbulence: Trapped electrons mostly do not respond to ITG: low χ_e
- TEM turbulence: electron transport dominates & bursty, zonal flows as dominant saturation mechanism for this parameter set.
- **GEM study shows drift wave is important with steep density pedestal, and the strong TEM may not actually contribute much to transport.**

Growing-weight problem in δf-PIC simulation is solved by averaging weights of near-by particles in 5D phase space



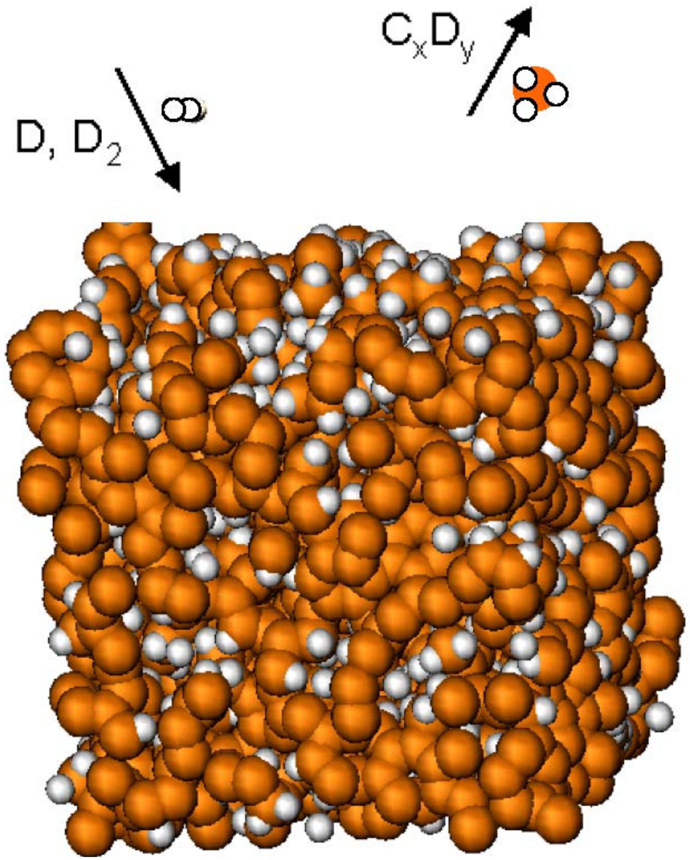
black–no resetting red–resetting with $\delta = 0.05$, $N_s = 10$ green–resetting with $\delta = 0.1$, $N_s = 10$

Reset only small fraction δ of particles in every N_s time step

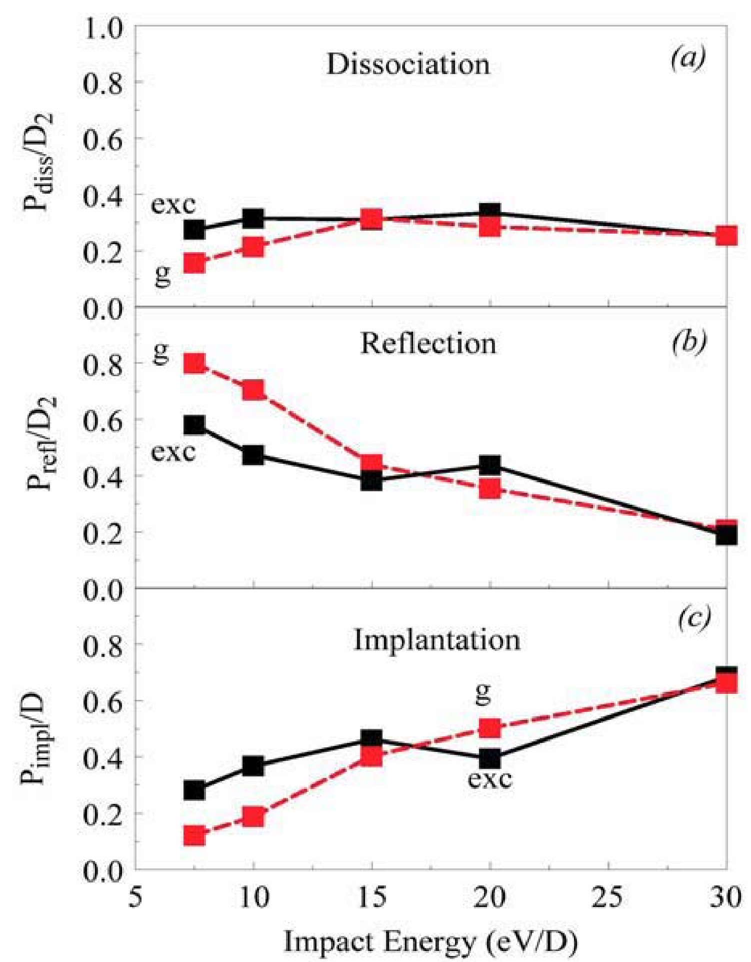
(U. Colorado at Boulder)

Progress in simulation of particle-wall interactions
(Example)

Very large scale Molecular Dynamics simulations



Data production for D_2 + deuterated amorphous carbon



Example International Collaborations

In addition to the usual domestic collaboration with NSTX, DIII-D, CMOD, and others,

we are requested for active international collaboration as follows:

- ITPA/ITER: ELM control by non-axisymmetric B
- JET/JT60U: Ripple effect on Pedestal (A young scientist from JET stayed at NYU for a month to learn and take a copy of XGC0 code.
- ASDEX-U: ELM effect on divertor heat load (a copy of XGC0 is requested)
- KSTAR: Active development of XGC-rf and implementation of rf into NUBEAM (one KSTAR employee is at PPPL for two years)

CPES Achievement, in comparison with the original schedule

Year 1

All items accomplished as scheduled except "Integrate DEGAS-2 into XGC" (To be accomplished soon)

Most other items are ahead of schedule

Notables:

- **The 5D particle reset scheme for δf noise reduction has been well-verified using GEM code.**
- **Electrostatic gyrokinetic equations for steep gradient has been published**

Year 2 (Ahead of schedule, Blue color shows largely accomplished items, and red means focused items in Year 2)

Code development

Implement non-linear collisions into XGC (Semi-nonlinear already in XGC, New nonlinear presented)
Add electron kinetics to XGC (Already running)
Optimize improved M3D version (M3D has already produced deep nonlinear crash)
Start code interface by running XGC and M3D together (Simple coupling is accomplished)
Add delta-f drift-kinetic electrons to XGC-ET (Done, Under verification)
Improve hydrogen molecule physics data used by neutral transport module (Significant improvement)

Computer Science and Applied mathematics

Develop parts of the Elvis system from PPPL into Kepler actors (25%)
Integrate geometry-based shared space with application codes and evaluate and integrate with Kepler
Develop semantic database of features
Create "easy-to-program" workflow actors
Develop a data movement actor for Kepler using Logistical Networking (30%)
Optimize linear solver used in MHD code (left to CEMM)
Implement FMM solver to XGC [toroidal geometry still under development]

Physics research

Improve gyrokinetic equation for steep gradient plasmas (Electrostatic eqns published)
Improve two-fluid equations for M3D in edge (collaboration with CEMM)
Preparatory exploration of electromagnetic turbulence parameter space for edge-like plasmas
Study nonlinear phase of ELM crashes with stand-alone M3D (IAEA2006)
Study simplified pedestal-ELM cycle from coupled M3D- XGC (IAEA2006)
Study electrostatic turbulence with XGC-ET (In verification stage)

Year 3 (We do not anticipate much problem in achieving the goal if given enough HPC time, Blue shows items ahead of schedule)

Code development

Add fluid/kinetic hybrid electron routine with intermittent scheme

Interface M3D with XGC-ET (Change of plan to XGC0, done)

Implement particle-reset noise reduction scheme into XGC-ET (ready to implement)

Optimize XGC-ET

Upgrade surface physics data in DEGAS-2

Implement non-linear collision algorithm into XGC-ET

Computer Science and Applied mathematics

Develop prototype framework of autonomic control. Integrate with simulations.(40%)

Design feature database, and incorporate in workflow for automatic detection.

Incorporate Logistical Networking techniques into our simulation database framework.

Further develop the monitoring system and IDAVE for experimental/simulation comparison.

Implement FEM solver to XGC-ET (done).

Implement FMM solver method to XGC-ET.

Optimize parallel performance of XGC-ET code.

Physics research

Develop gyrokinetic equation for steep gradient plasmas

Study electrostatic turbulence using XGC-ET

Study pedestal-ELM cycle from coupled M3D and XGC-ET (DOE 2009 milestone)

Study neoclassical electron transport due to neutral ionization

Compare and validate XGC with B2-Irene

CPES Physics Research Roadmap

	Pre-CPES	2006	2007	2008	2009	2010
Edge Kinetic code	XGC0, Full-f ions with 1D E_r solver	**XGC1, Full-f ions & electrons, 2D solver (E_r, E_θ) + 1D solver parallel to B**	XGC1, Full-f, electrostatic turbulence in the entire edge XGC0-MHD ELM cycle **Enhance XGC0 with Electrons,**	Multiscale XGC0-XGC1 coupling	XGC2, full-f E&M edge Turbulence code Develop XGK: Multiscale XGC0-XGC2 Integration framework	Develop coupling to core code
Physics Research	First 1D neoclassical ion edge solution, with pedestal buildup by neutrals	**First 2D neoclassical kinetic solution in the entire edge**	Edge Rotation physics. Ripple and error field effects on pedestal, rotation & ELM	Study L-H transition Study pedestal-ELM cycle with concurrent turbulence capability (in integration with MHD/ELM codes)		Study core-edge coupled physics

Summary

We are mostly ahead of the original schedule

Current Achievement

- Equilibrium particle kinetic code XGC0 [$\Phi(\psi)$] is in production stage, and beginning to produce new physics.
- First version Kepler Workflow is at work for XGC0-Elite-M3D coupling
- Turbulence PIC kinetic code XGC1 is in the verification stage, and will move to the edge soon.
- Equilibrium XGC1 version [$\Phi(\psi,\theta)$] is beginning to produce new discoveries.
- Growing weight problem in δf-PIC solved
- Preparatory exploration of edge turbulence is beginning to show important results
- Edge rotation source (XGC) and inward pinch mechanism (analytic) identified.
- New PSI data are beginning to emerge

Plan for the Coming Year

- DEGAS2 into XGC0
- Non-axisymmetric B effect on pedestal
- Kinetic $\leftrightarrow$ MHD coupling for pedestal height
- Wall load
- Study electrostatic turbulence in edge (including L-H transition)
- XGC1-XGC0 coupling
- Edge rotation physics

HPC usage is essential. We have used up to 16,000 Jaguar cores and spent 1.1Mhrs.

Active collaboration with other centers made our progress possible.

Active international and domestic collaborations (ITPA-ITER, JET-JT60-ASDEX, DIII-D-CMOD-NSTX) are beginning.