Predictive Integrated Modeling Simulations Using a Combination of NTCC H-mode Pedestal and Core Models

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Outline

- Objectives of predictive integrated modeling
- Codes used by Lehigh Group and collaborators
  - – BALDUR, JETTO, TRANSP, ASTRA, NTCC, HELENA, MISHKA
    - Theory-based core transport models
    - Theory motivated models for H-mode pedestals and ELMs
- Applications of BALDUR code in studies of tokamak discharges
  - – Parameter scans for discharges in a variety of tokamaks under a variety of conditions
    - Explore different discharge scenarios
- Combined core and edge modeling of H-mode discharges
  - – Combine separate core and H-mode pedestal models
  - – Develop continuous, self-consistent model for the core, H-mode pedestal transport barrier, and ELMs
  - – Carry out specialized simulations to develop more sophisticated models for the H-mode pedestal and ELMs
- Development of predictive integrated modeling codes that are more flexible and easier to use
  - – Description of NTCC effort, particularly the NTCC Module Library
- Collaborations

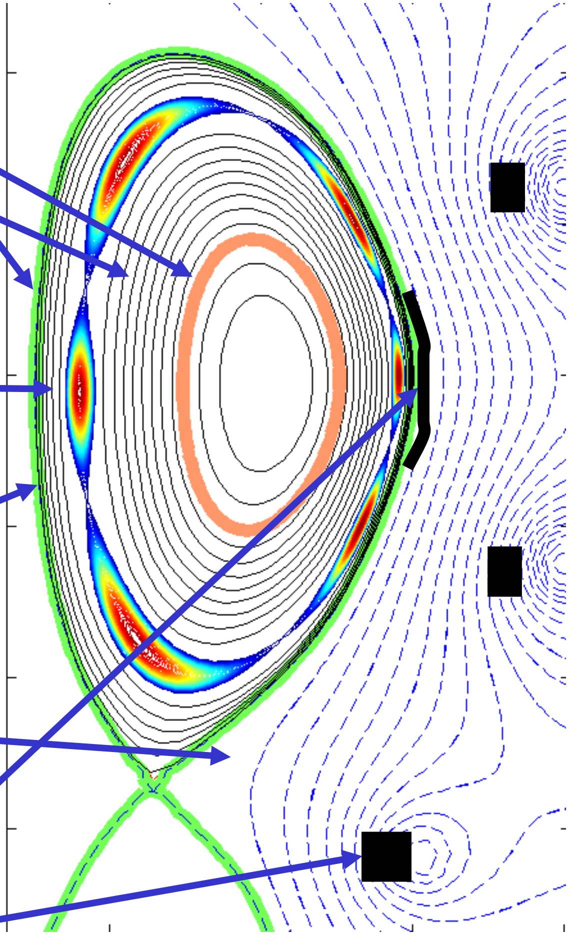
Objectives of Integrated Modeling

Integrated modeling of tokamaks is used for the following reasons:

- **Predict the expected fusion power production in planned burning plasma experiments**
  - **Using theory-based models**
- **Understand the physics of confinement as well as optimize the performance of tokamaks**
  - **Vary operating parameters such as density or auxiliary heating power**
  - **Explore different discharge scenarios**
- **Study the interaction between different physical phenomena, *e.g.:***
  - **Interaction between fusion heating power, transport, and the plasma temperature profiles**
  - **Effect of the H-mode pedestal on global confinement**
- **Provide plasma profiles for more detailed studies**
  - **Such as studies of ELMs, toroidal Alfvén modes, sawtooth oscillations, or other MHD instabilities**

Integrated Modeling of Tokamaks

- Sawtooth Region
- Core Confinement Region
- Magnetic Islands
- Edge Pedestal Region
- Scrape-off Layer
- Vacuum/Wall/ Conductors/Antenna



Core Transport

Edge Transport

Plasma Turbulence

MHD Equilibrium

Plasma-Wall Interactions

Large Scale Instabilities

Radiative Transport

Neutral Gas

Heating Current Drive

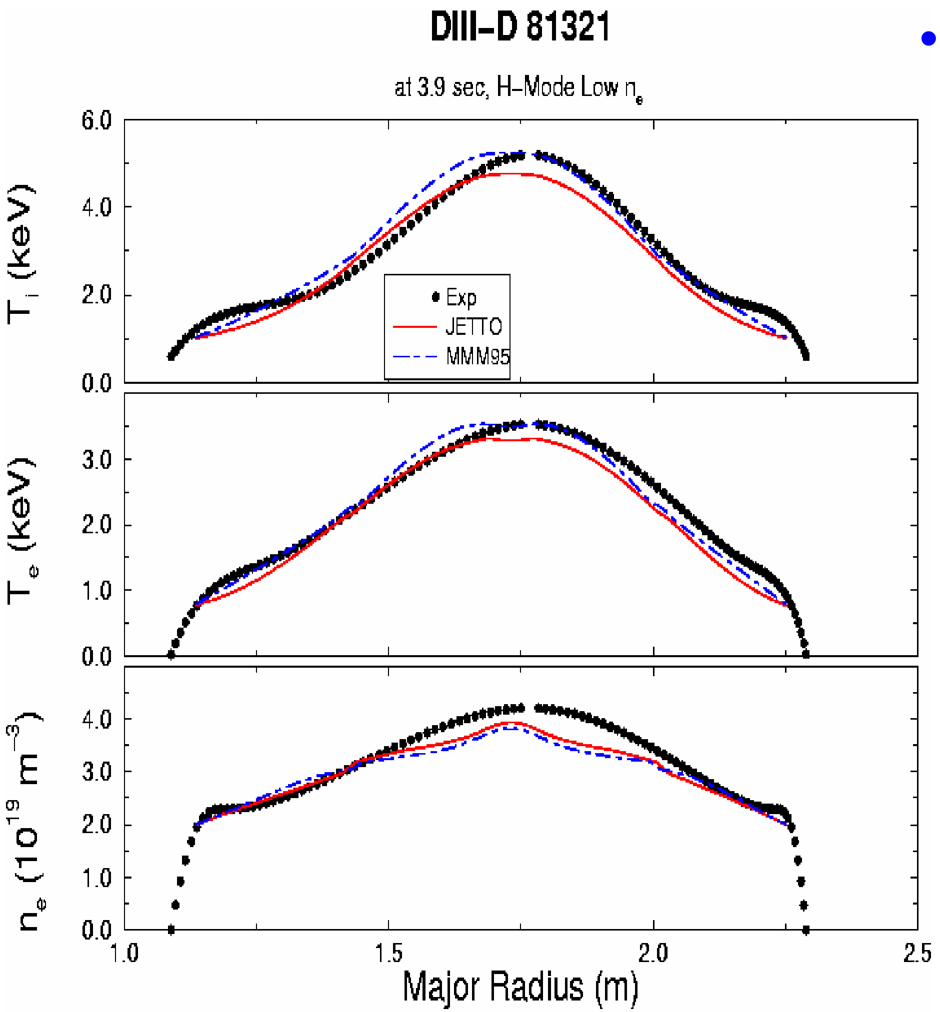
BALDUR Integrated Modeling Code at Lehigh

- Predicts time-dependent profiles for
  - – electron and ion temperature
  - – each ion density (hydrogenic and impurity)
  - – magnetic $q(r,t)$
  - – neutrals
- Self-consistent computations of
  - – sources (such as NBI heating or fusion reactions)
  - – sinks (such as impurity radiation)
  - – transport fluxes
  - – MHD equilibrium
  - – large scale instabilities (such as sawtooth oscillations)

Stiff Transport Models Used in BALDUR Simulations

- Choice of transport models:
  - Multi-Mode transport model (Lehigh)
    - Theory-based transport model that matches a wide range of experimental data for L-mode, H-mode, and other tokamak plasmas
    - Predicts impurity and hydrogenic particle transport as well as electron and ion thermal transport
    - Agrees with non-linear gyro-kinetic turbulence simulations
  - GLF23 transport model (GA)
    - Theory-based transport model that was originally calibrated using non-linear gyro-fluid turbulence simulations
  - Mixed-Bohm/gyro-Bohm (mB/gB) transport model (JET)
    - Empirical transport model
    - Bohm scaling ($\chi \propto \rho c_s$) dominates mB/gB (JETTO) model in most tokamak simulations

Temperature and Density Predictions for L-mode and H-mode Discharges



- **Compare Multi-Mode (MMM95) and mB/gB transport models with experimental data**
  - **Boundary conditions from experimental data**
  - **13 L-mode DIII-D and TFTR discharges, ρ_*, I_P, n_e, and P scans**
    - **Phys. Plasmas 8 (2001) 975**
  - **22 H-mode JET and DIII-D discharges, ρ_* , υ_*, β, isotope, n_e, P, and κ scans**
    - **Phys. Plasmas 8 (2001) 964**

Definitions of Profile Statistics

- **Relative deviation between simulation profile $T^{\text{simulation}}(R_i)$ at each experimental data point $T_i^{\text{experiment}}$**

$$\boxed{\delta_i \equiv \frac{T^{\text{simulation}}(R_i) - T_i^{\text{experiment}}}{T_{\max}^{\text{experiment}}}}$$

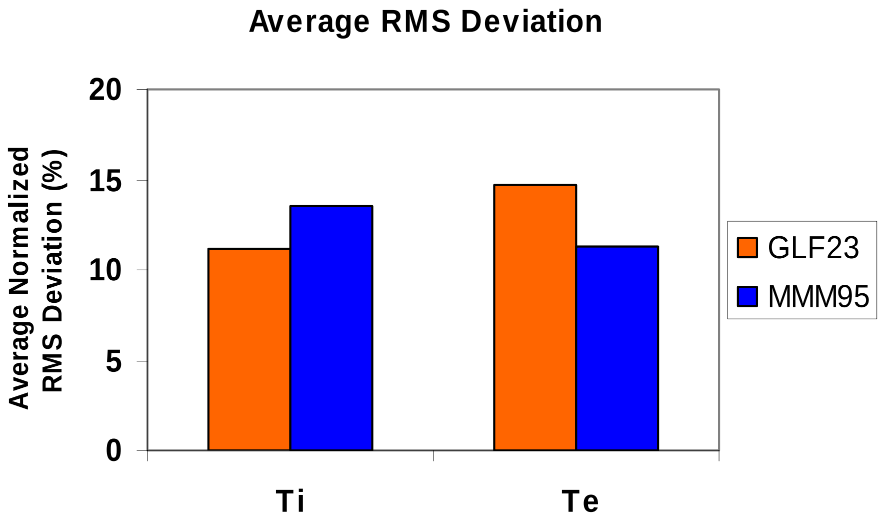
  - **Note that deviation at each data point is normalized by the maximum value for that profile, $T_{\max}^{\text{experiment}}$**
  - **This definition gives equal weight to all data points**
- **Relative RMS deviation for each profile with *N* data points**

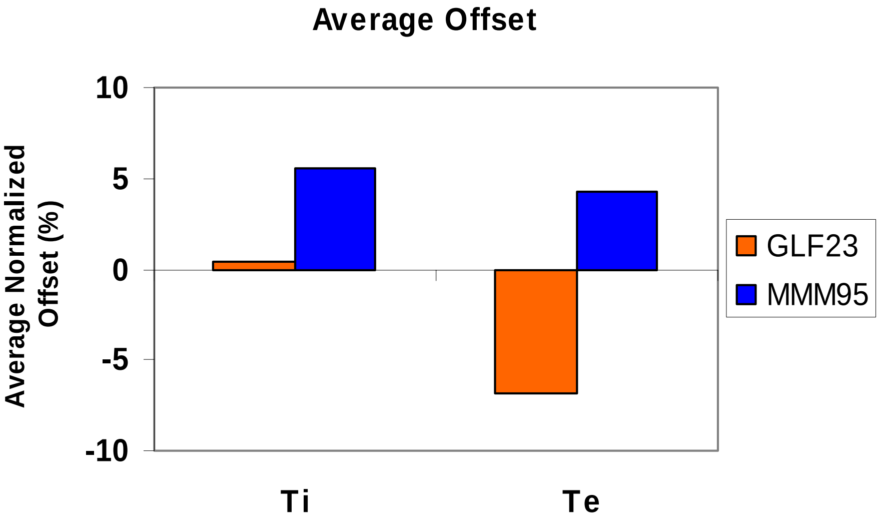
$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\delta_i^2}$$

- **Offset for each profile**

$$\text{Offset} = \frac{1}{N}\sum_{i=1}^{N}\delta_i$$

Comparison of MMM95 and GLF23 Average RMS Deviation and Offset

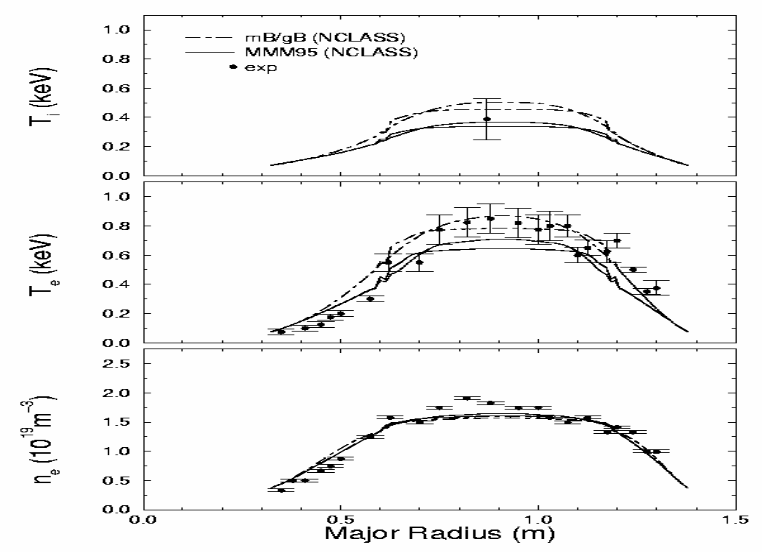




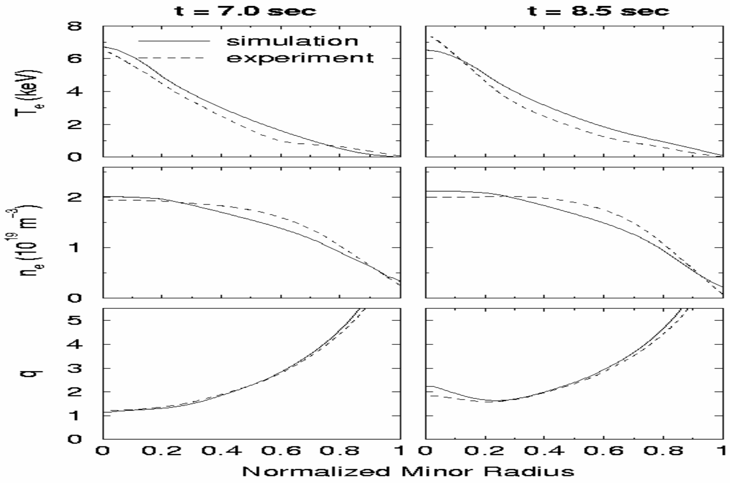
- RMS deviations and Offsets are averaged over 23 JET and DIII-D discharges
  - RMS deviations are between 11% and 15%
    - For both GLF23 and MMM95
    - For both ion and electron temperature
  - Offsets are between –7% and +6%
    - MMM95 model slightly overpredicts T_i and T_e profiles
    - GLF23 model slightly underpredicts the T_e profile
- Errors in this range are probably not significant given the uncertainty in the experimental data

Variety of Simulation Studies Carried out Using the BALDUR Code

- **Mega-Amp Spherical Tokamak (MAST) - low aspect ratio tokamak**
  - **Used both the JETTO (mB/gB) and Multi-Mode (MMM95) transport models together with NCLASS neoclassical, which plays a large role in ion thermal transport**
    Phys. Plasmas 9 (2002) 3930

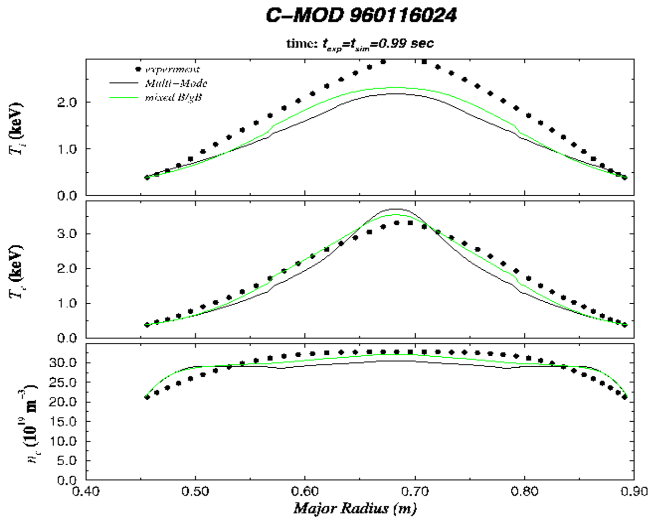


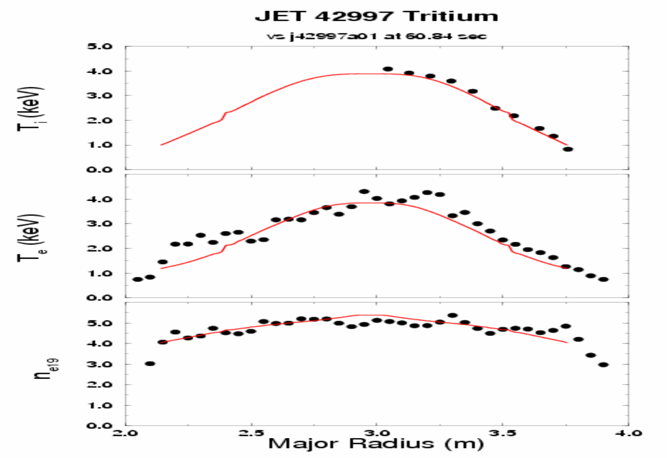
- **MMM95 used in simulations of Tore-Supra**
  - **Lower-Hybrid heating and current drive in a helium plasma with carbon impurity**
    Phys. Plasmas 9 (2002) 4241



Variety of Simulation Studies Carried out Using the BALDUR Code

- **Alcator C-Mod high density ICRH heated ELM-free H-mode discharges**
  - **Used MMM95 and mB/gB model in simulations of seven L-mode and H-mode discharges**
  - **Two models have different dimensionless scaling but match data about equally well Phys. Plasmas 8 (2001) 4403**
- **Effect of Hydrogen isotope mass in JET discharges**
  - **Change in profile shapes effect confinement**
  - **Phys. Plasmas 6 (1999) 4607**





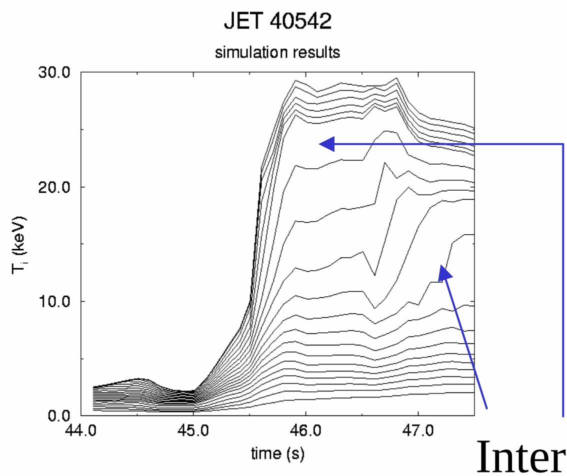
Simulations Predict Formation and Motion of Internal Transport Barriers

BALDUR simulations using Multi-Mode model to predict formation and motion of internal transport barriers (ITBs) in JET and DIII-D

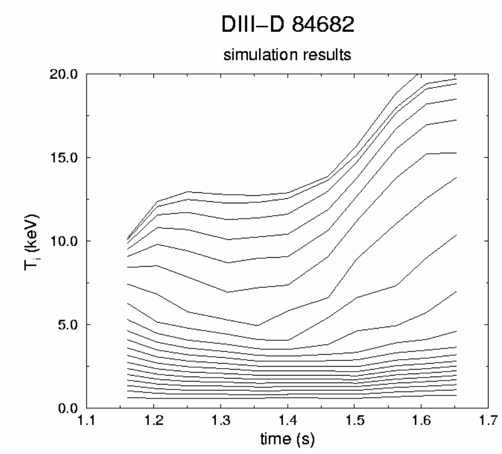
Simulations follow evolution from
Ohmic → L-mode → formation of ITB → H-mode → motion of ITB

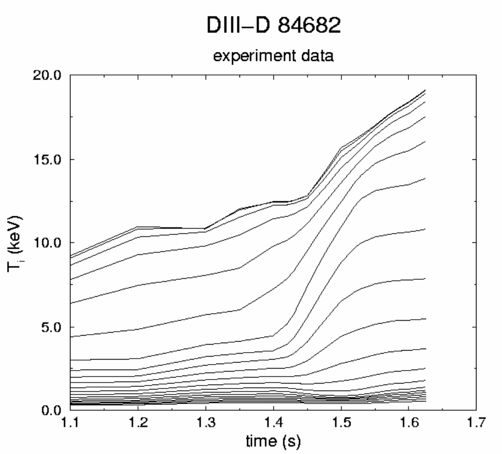
Flow shear and finite β effects both play a role

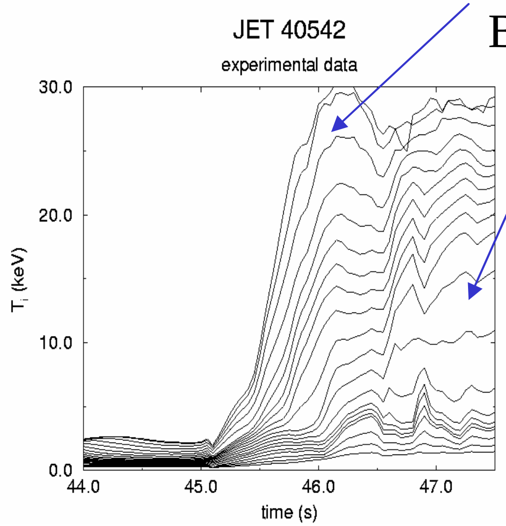
Phys. Plasmas 7 (2000) 2898



Internal
Transport
Barriers







Research Plan for Combined Core Edge Modeling of H-mode Discharges

1. Combine separate core and H-mode pedestal models
   - Pedestal model used for boundary conditions of core simulation
   - No time-dependent model for the ELMs
2. Develop continuous, self-consistent model for the core, H-mode pedestal transport barrier, and ELMs to predict:
   - Height, width, and shape of pedestal
   - Frequency and radial extent of ELMs
3. Carry out specialized simulations to develop more sophisticated models for the H-mode pedestal and ELMs
   - Linear MHD instability codes, HELENA, MISHKA and ELITE, to predict the instability that results in ELM crashes
   - Non-linear MHD instability codes to predict the effect of ELMs
   - Turbulence simulations to predict and understand edge transport

H-mode Pedestal Temperature and Density Models

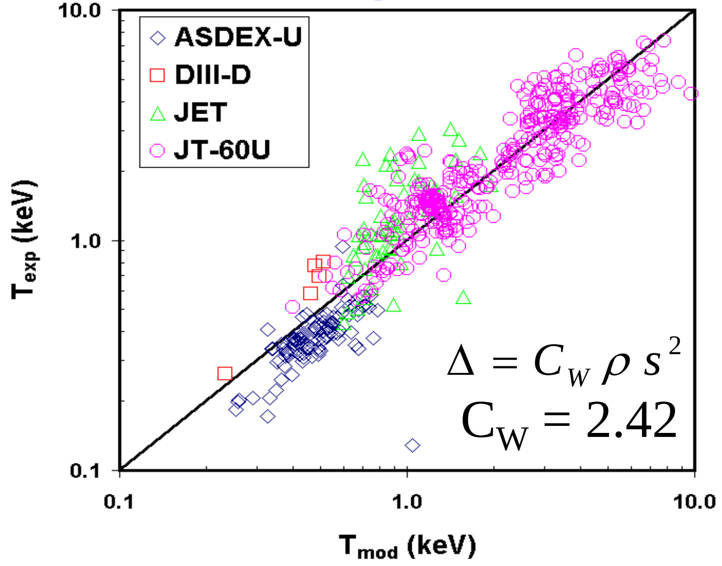
Static models developed at Lehigh for the pedestal temperature and density calibrated against 533 type I ELMy H-mode discharges in the pedestal database

Pedestal width - shearing rate equal to the linear growth rate yields

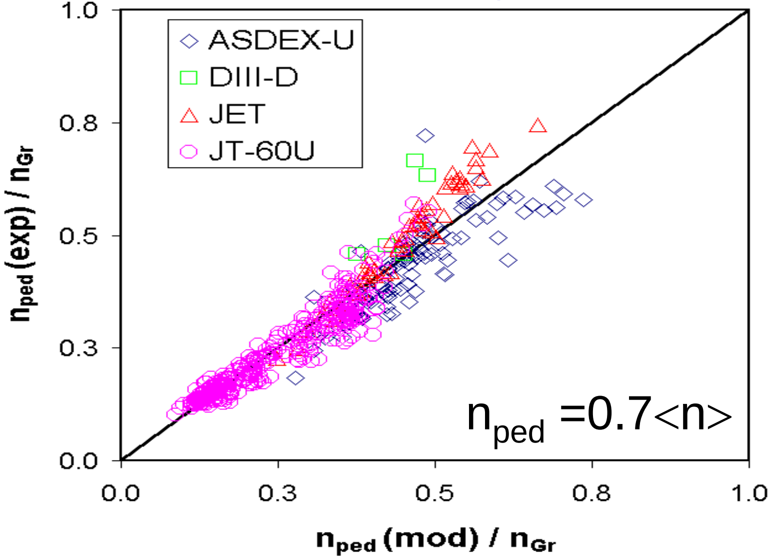
$\Delta \propto \rho_{\mathrm{tor}} s^2$ **M. Sugihara, *et al.*, Nucl. Fusion 40 (2000) 1743**

Pressure gradient limited by first ballooning mode stability condition

Temperature



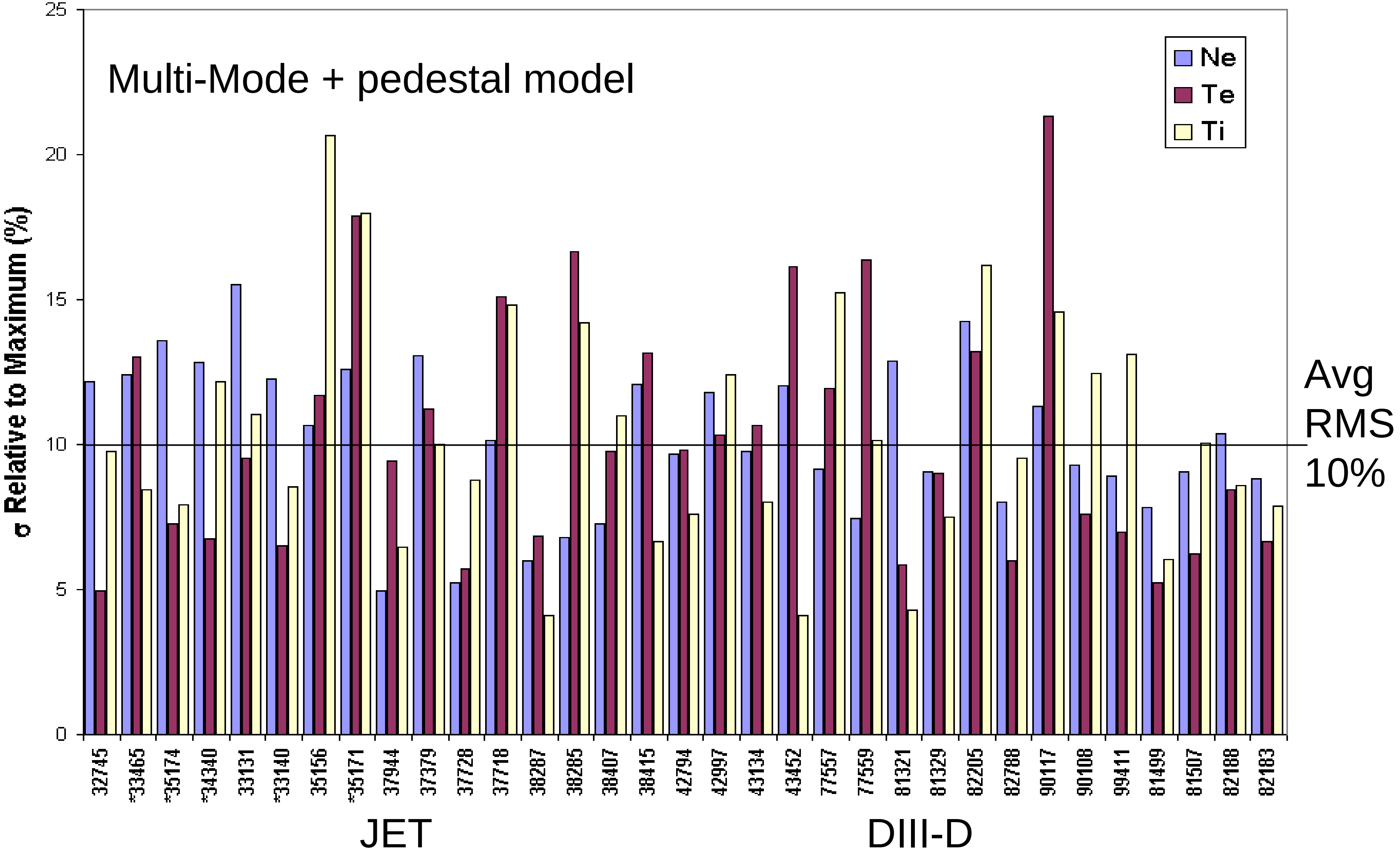
Density



32% Logarithmic RMS deviation 12%

Phys. Plasmas 9 (2002) 5018

Profile RMS Deviations for 33 H-mode Discharges



Self-consistent Model for Pedestal and ELMs

Dynamic models being developed to predict:

Pedestal Profiles

- **Pedestal Width**
- **Pedestal Height**
- **Pedestal Shape**

Dynamics of ELMs

- **ELM Frequency**
- **Width of the region affected by ELMs**
- **Transport between ELMs**
- **Effects of pedestal profiles**

Overall objective is to follow plasma evolution

Ohmic → L-mode → H-mode → ELMs

in integrated predictive time-dependent modeling of tokamak plasmas

Theory-based models being developed for pedestal and ELMs at the edge of H-mode plasmas

- **Flow and magnetic shear stabilization of anomalous transport**
  - **Same transport model used for core and edge**
  - **Local self-consistent calculation of of profiles from core through pedestal**

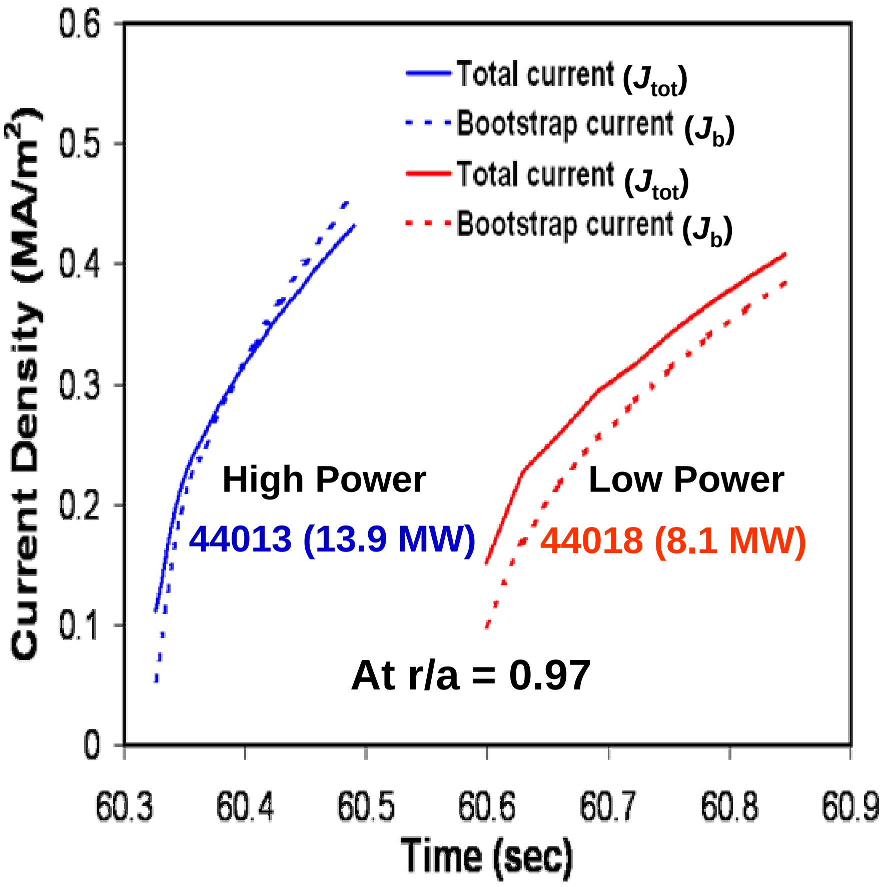
Core/Edge Simulations with JETTO Code
JET Power Scan

- Examine dependence of the height of the H-mode pedestal on the injected power
  - Do the pedestal properties depend on injected power?
    - Compute the MHD mode instability that might trigger ELMs
- Tools used to carry out simulation studies
  - JETTO, integrated predictive modeling code
    - Includes combined core and edge modeling
    - Yields equilibrium profiles for stability analysis
  - HELENA, equilibrium and infinite-*n* stability code
    - Refines equilibrium for use with MISKHA code
    - Establishes region where infinite-*n* ideal ballooning mode is unstable
  - MISHKA, stability code
    - Determine growth rate of most unstable ballooning and current driven modes
    - Applied for toroidal modes with *n*=1 to *n*=14

Integrated Predictive Transport Code (JETTO)

- Evolves plasma core and pedestal profiles, such as I_p, T_e, T_i and n_e, needed for stability analysis
- mB/gB model for core transport
- Transport thought the pedestal is taken to be ion neoclassical transport at the top of the pedestal
  - Turbulent transport is neglected within the pedestal region
  - Neoclassical transport calculated using NCLASS
- An ELM crash occurs when an instability condition is satisfied in the pedestal region
- Simplified stability model used for triggering ELMs
  - ELMs triggered by pressure-driven ballooning mode
    - Check appropriateness of α_c by stability codes
  - ELMs triggered by current-driven peeling mode
    - Details in H. R. Wilson *et al*., Nucl. Fusion, 40, 713 (2000)

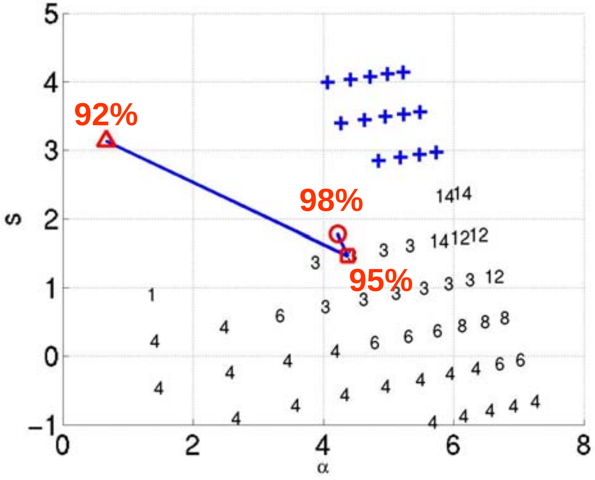
Evolution of Pedestal Current Density Between ELMs



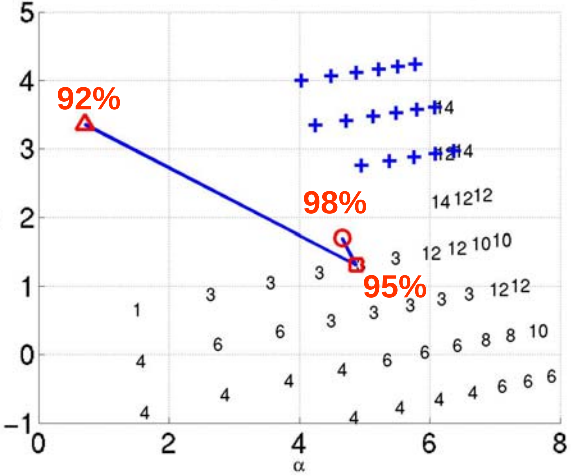
- **Sequence of physical effects as heating power is increased:**
  - **Pedestal pressure gradient and resulting bootstrap current rise more rapidly after each ELM crash as heating power is increased**
  - **Rise in total pedestal current density is impeded by back EMF**
  - **These ELM crashes are caused by current-driven MHD instability**
  - **Hence pedestal pressure gradient can rise to higher values as heating power is increased before the pedestal current can cause ELM crash**

Stability Analysis using HELENA and MISHKA Codes

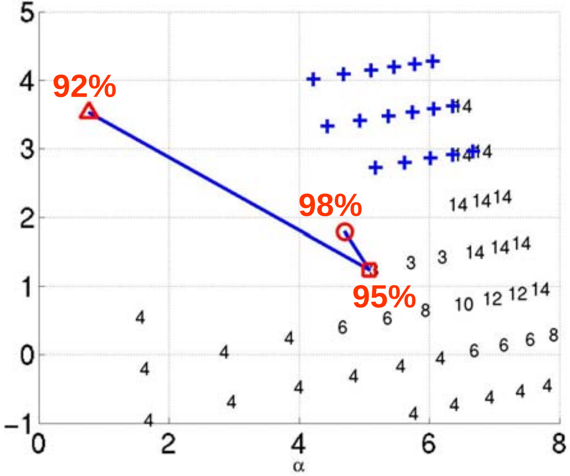
44018 (8.1 MW)



44029 (11.3 MW)



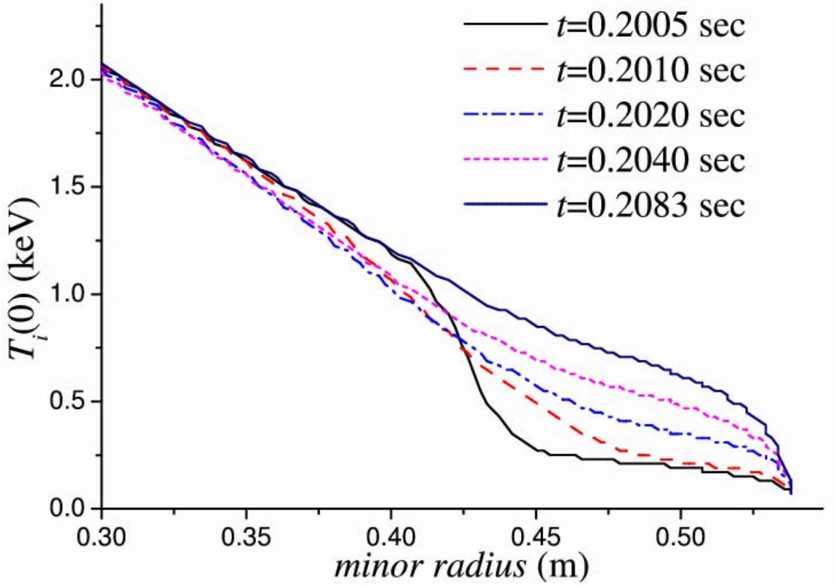
44013 (13.9 MW)



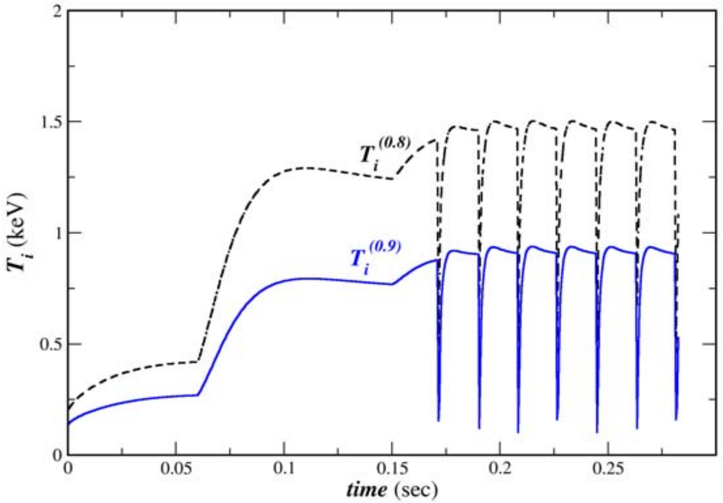
- Stability s-α diagram for 95% flux surface with growth rate greater than 0.03 of Alfven frequency
  - Operational points are indicated for 3 flux surfaces
- Top of barrier is limited by kink/peeling modes
  - Maximum normalized pressure gradient α increases (4.4, 4.9 and 5.2) as P_{heat} increases

Dynamic Simulation of Pedestal and ELMs

- As heating power is increased, ASTRA simulation follows plasma evolution from L-mode → H-mode → ELMy H-mode
  - Flow shear reduces anomalous transport to build H-mode pedestal
  - Steep pressure gradient drives bootstrap current in the pedestal
  - Ballooning or peeling instability triggers periodic ELM crashes

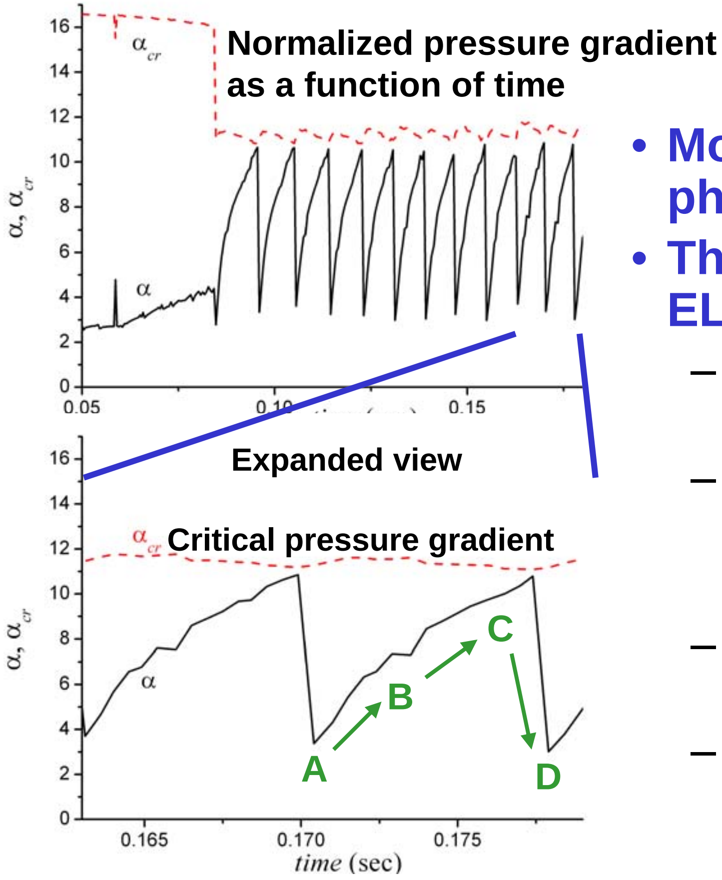


Temperature profile in outer half of the plasma as a function of time through an ELM cycle



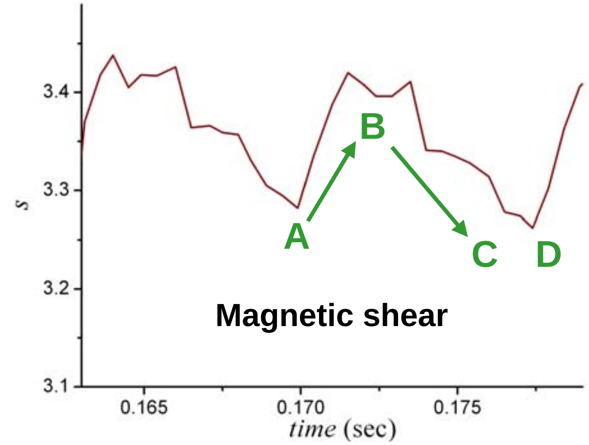
Simulation of an ELM Cycle

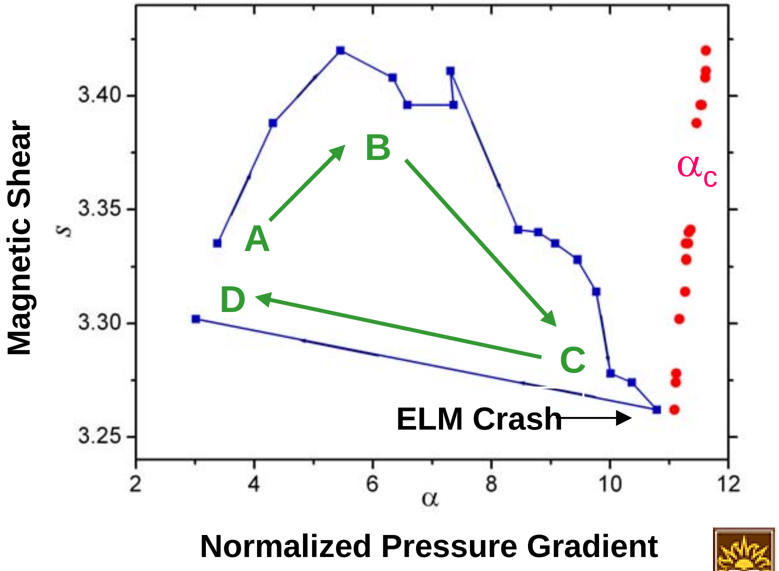
- Model for an ELM cycle illustrating the different physical processes that play a role
- The following sequence of events occur during an ELM cycle, starting just after an ELM crash:
  - – Normalized pressure gradient, α, increases as the pedestal rebuilds
  - – Pedestal current density
    - First decreases, due to high resistivity
    - Then increases, due to bootstrap current
  - – Magnetic shear, s, first increases and then decreases, inversely with pedestal current density
  - – ELM crash occurs when α exceeds α_c


Normalized pressure gradient as a function of time

Expanded view

Critical pressure gradient


Magnetic shear


Normalized Pressure Gradient

LEHIGH UNIVERSITY

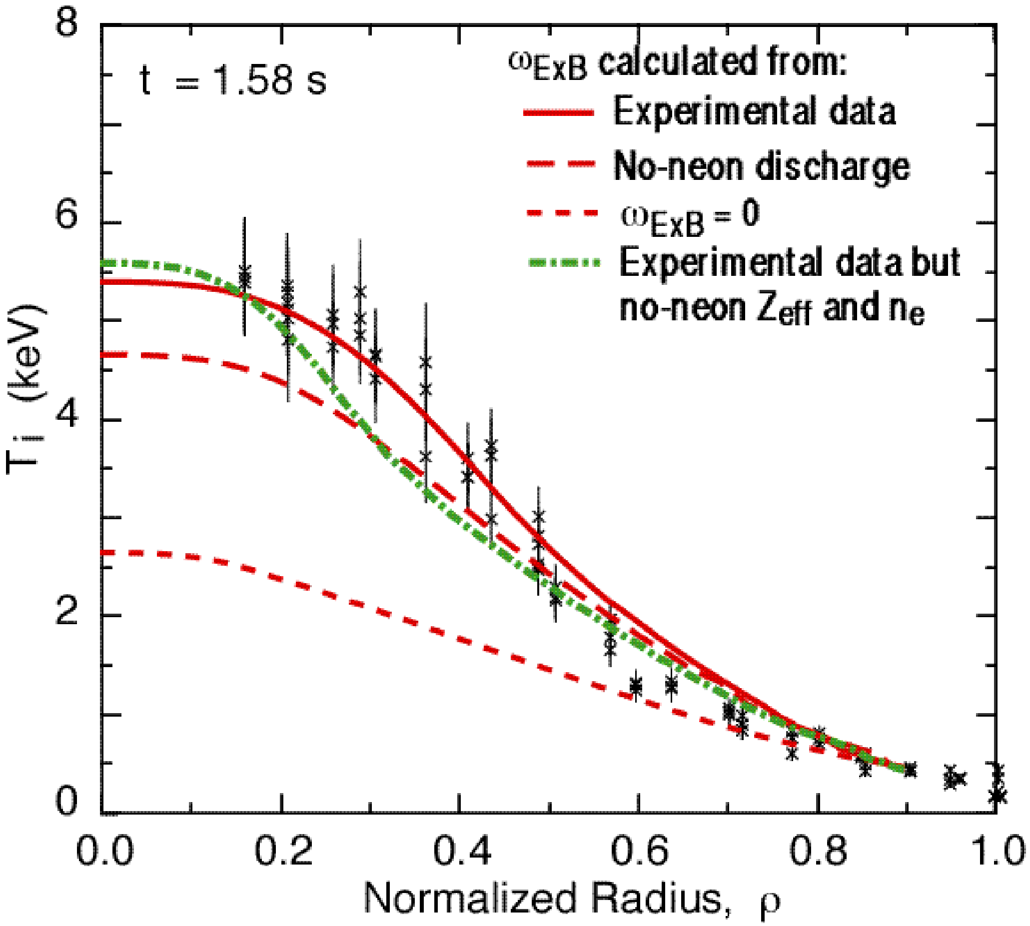
Need Predictive Integrated Modeling Codes that are More Flexible and Easier to Use

- **Issues:**
  - **Integrated modeling codes bring together many different physical processes (transport, sources, sinks, MHD instabilities)**
    - **Hence, integrated modeling codes are large and hard to use**
  - **Most integrated modeling codes are more than 20 years old**
    - **These legacy codes are not up to modern software standards**
  - **Running integrated modeling code is like running an experiment**
- **Future:**
  - **Use modern software engineering to develop new integrated modeling codes**
    - **Modules with clearly defined interfaces for each physical process**
    - **Flexible framework in which modules can be easily switched**
    - **Seamless access to database to store the results of simulations and to access experimental data**
    - **Modern graphical presentation of simulation results**

Improved Integrated Modeling Code – NTCC

- **NTCC team established a path for producing a modern integrated predictive simulation code**
  - **The objective is to have all relevant physics models available in one code**
- **NTCC demonstrated that a geographically distributed community team can function effectively in developing a simulation code**
  - **Object-oriented software aids in this process**
- **Community-owned integrated modeling code must be reliable and user friendly**
  - **A team is needed to maintain the large required infrastructure**
  - **Researchers are more likely to use a community-owned code that has been thoroughly tested, validated, and documented**
- **Predictive integrated simulations will provide an important tool for the design and study of burning plasma experiments**
- **NTCC team developed a Web invocable code using NTCC Library transport modules**

Example of Use of Web-Invocable NTCC Code



NTCC code simulations were used to test:

- **Effects of ExB shearing from experimental ω_{ExB} to no shearing**
- **Effects of changing Z_{eff} (3.2 → 1.4) and $n_e(\rho)$ after the improved state is established**

⇒ Neon injection may be used as a trigger

Nucl. Fusion 41 (2001) 317

NTCC Module Library

- Web-based, community-owned library of modules
- Each module is self-contained software that is:
  - designed to carry out a specific task
    (transport model, heating model, numerical technique, …)
  - isolated, with a clearly defined interface
    (such as an argument list to a procedure or subroutine)
  - with driver program, test cases, and documentation
  - Library modules with different levels of sophistication are encouraged
- NTCC Module Library available at http://w3.pppl.gov/NTCC
- Modules are reviewed and then subject to approval by the six member NTCC Module Library Committee
  - Insures that standards established by the community are satisfied.
- 44 modules now in the library (20 modules reviewed and approved)
- Modules extracted from large integrated modeling codes are now being shared among codes
  - Module development generally results in improved documentation and advances in physics content

Categories of Modules

Category	Number	Comments
Anomalous Transport Models	6	Transport of heat, particles, and momentum
Neoclassical Transport Models	2	Particle, momentum, and thermal transport
Heating	5	Radio Frequency and Neutral Beam heating
Equilibrium and Stability Solvers	7	Force balance and MHD stability
MHD Stability	1	Sawtooth mixing module
Divertor/Edge/Pedestal	1	To compute boundary conditions
Neutral Gas Models	2	Source of ions and radiative losses
Atomic/Nuclear Reaction Rate Data	1	Ionization, recombination, radiation, and fusion reaction rates
Numerical Tools	7	Interpolation, integration, etc
Portability Tools	4	To facilitate transfer of codes from one computer to another
Data Analysis and Visualization	8	To facilitate database and plotting

Advantages of Module Library

- **Reduces the authors' time regarding requests for distribution and installation of modules**
- **Library as origin of shared modules aides version control**
  - **Modules are kept up-to-date in one place**
  - **As upgrades evolve, it is straight-forward to update modules that are being used in codes**
- **Review process helps to improve the quality of modules**
- **Library encourages use of modern coding practices**
  - **Particularly encapsulation and inheritance**
- **High cost of maintaining non-modular legacy code**
  - **Modules help to reduce redundancy**
    - **Particularly when similar physics is used in many codes**
- **Modules encourage community collaboration**
- **Library provides Web-based documentation**

Review Process

- Any researcher can submit a module through the Web page http://w3.pppl.gov/NTCC/guidelines/guide.html
  - As soon as a module is submitted, it is made available on the NTCC Module Library Web page http://w3.pppl.gov/NTCC
- Modules are reviewed to ensure they conform to standards
  - The review process is open, so that the reviewer and the author can communicate as needed to improve the module
    - In some cases, the review process has led to the reorganization or major improvement of the module
    - In most cases, the review process produces improvements in the documentation or results in the repair of minor problems
- Once a satisfactory review has been completed
  - The review is submitted to the Module Library committee
  - Is accepted after an affirmative vote by a majority of the committee members (four out of six)
  - Twenty modules have passed the review process, to date
    - Marked with a green star on the Web page

Module Issues

- The primary goal of the NTCC Module Library is to allow researchers to share parts of computer codes
- Developers have faced the following challenges:
  - Some modules are very large and complex
    - For example, the NUBEAM Neutral Beam Injection module
  - Programmers have very different styles and requirements
    - Most physicists write programs for their own use, rather than learning all the nuances of advanced object oriented programming
    - Hence, many compromises made in the NTCC standards and Module Library standards need to be improved
  - Modules extracted from legacy codes that were run in batch mode have to be adapted for use in more interactive codes
    - Developers and users have gone through a learning curve

NTCC Module Work in Progress

- New modules under development:
  - TEQ : Free-boundary plasma equilibrium
    - Prescribe coil currents rather than prescribing boundary shape
  - TORIC : Full wave treatment of ion cyclotron resonance heating
    - For long wavelengths, where ray tracing is not appropriate
  - IMPRAD : Non-equilibrium coronal impurity radiation
    - Advancing the rate equations using ionization, recombination, and transport of ions with multiple charge states
  - Saturated tearing mode model
    - To predict magnetic island widths in tokamaks
  - Porcelli model to predict the onset of sawtooth crashes
  - Pellet injection module
  - FPPMOD : Fokker-Planck module for slowing down of fast ions
  - GTNEUT : 2-D neutrals code for complicated geometries
  - TOQ : Inverse equilibrium solver for vertically asymmetric plasmas
  - NUT - 1 : Multi-species core neutrals module

Collaborations

- Integrated modeling involves large teams of researchers
  - **Lehigh:** G. Bateman, A. Pankin, J. Kinsey, T. Onjun,
    C. Nguyen, and S. Snyder
  - **Visitors to Lehigh:** I. Voitsekhovitch, V. Parail, J. Weiland,
    P. Strand, T. Davydova, P. Zhu
  - **Other Collaborators:** R. Akers, R. Andre, R. Budny, C. Byrom,
    A. Dnestrovskij, T. Fredian, M. Greenwald, P. Guzdar,
    G. Hammet, W. Horton, G. Huysmans, G. Janeschitz,
    J. Lönnroth, D. McCune, M. Murakami, G. W. Pacher,
    H. D. Pacher, G. Pereverzev, A. Polevoi, F. Porcelli,
    J. Snipes, G. Staebler, A. Sykes, R. Waltz, H. Wilson
  - Lehigh group contributed simulations to the 2002 IAEA papers by:

    X. Garbet; V. Parail; T. Osborne; J. Kinsey; V. Mukhovatov
  - NTCC has involved 24 researchers from 10 institutions
- Integrated predictive modeling capability will be most effectively achieved through international cooperation and collaboration