PTRANSP
Predictive TRANSP Code

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Scientists Involved in Continuation of PTRANSP Project

- **Doug McCune – PPPL**
- **Steve Jardin – PPPL**
- **Rob Andre – PPPL**
- **K. Indireshkumar – PPPL**
- **Don Pearlstein – LLNL**
- **Lynda LoDestro – LLNL**
- **Bill Meyer – LLNL**
- **Tom Casper – LLNL**
- **Lang Lao – GA**
- **Holger St.John – GA**
- **Phil Snyder – GA**
- **Jon Kinsey – GA**
- **Gary Staebler – GA**
- **Arnold Kritz – Lehigh**
- **Glenn Bateman – Lehigh**
- **Alexei Pankin – Lehigh**

PTRANSP Code

- PTRANSP is the TRANSP analysis code used for predictive integrated modeling simulations
  - Code distribution used for TRANSP is also used for PTRANSP
- PTRANSP project has been funded at a level of $600K/year for 2 years
  - Funded as a continuation of NTCC project
  - Institutions involved GA, Lehigh Univ., LLNL (Tech-X), PPPL
- DOE-OFES has indicated that it would consider a three year terminal renewal proposal
  - Goal: Increase level of predictive completeness and usefulness
  - Carry out tasks that support SciDAC FSP prototype projects
- PTRANSP builds on capabilities that exist in TRANSP code
  - TRANSP has a large user base and is well validated

Need for the PTRANSP code

- **PTRANSP will provide a full scale predictive integrated modeling capability during the next 5 to 10 years**
  - **TRANSP has a large world-wide user base**
    - **100 registered users of the PPPL Fusion Grid TRANSP service**
    - **4000 TRANSP simulations are carried out each year at PPPL and JET**
- **PTRANSP effort will combine the models and capabilities that are scattered in other integrated modeling codes**
  - **Reduced models, currently in ONETWO, CORSICA, TSC and BALDUR, are being incorporated into PTRANSP**
  - **Verification and validation will provide a simulation code trusted by a large user base**
- **PTRANSP will provide a link to SciDAC simulation projects**
  - **For example, PTRANSP software being incorporated into the plans of the SWIM and FACETS SciDAC projects**

Vision for PTRANSP

- **Fusion community continues to need a full-featured trusted integrated modeling code such as PTRANSP**
  - For analysis of experimental data
  - For predictive simulations using theory-based and empirical models
  - For understanding the interactions among physical processes in tokamak plasmas
- **PTRANSP will serve as a bridge to full fledged future fusion simulation project capability by**
  - Extending the existing software framework for predictive simulation
  - Providing a prototype for fusion simulations, and
  - Providing rigorous methodology for verification of new modern, high performance, simulation frameworks as these become operational

Integrated SciDAC Projects and PTRANSP

- **Three SciDAC projects (SWIM, CPES and FACETS) are developing new integrated modeling framework prototypes**
  - **These SciDAC projects emphasize integration of first-principles computations**
  - **SWIM (Simulation of RF Wave Interactions with MHD) will improve simulation of large scale instabilities, RF heating and current drive**
  - **CPES (Center for Plasma Edge Simulation) simulating pedestal formation and ELM cycles by coupling edge turbulence and MHD**
  - **FACETS (Framework Application for Core-Edge Transport Simulations) will couple edge and core plasma simulations**
- **Module development for PTRANSP will aid SciDAC projects**
  - **PTRANSP Plasma State module (data structure, interpolation, i/o) will be used directly in SciDAC projects**

TRANSP and PTRANSP Funding

Funding for TRANSP and PTRANSP from a variety of sources

- **Experimental projects**
  - **Need high fidelity source models for diagnostic simulation & analysis**
  - **Several thousand TRANSP runs per year**
- **Continuation of the NTCC project producing NTCC modules and the predictive PTRANSP code**
- **SciDAC projects**
  - **SWIM (Simulation of RF Wave Interactions with MHD)**
    - **Interaction between component codes being developed through the Plasma State module**
  - **FACETS (Framework Application for Core-Edge Transport Simulations)**
  - **RF Wave-Plasma Interactions**

Capabilities Recently Included in PTRANSP

- Newton's method for numerically stable predictions using stiff transport models
  - Used with GLF23 and MMM95 anomalous transport models
- Choice of TEQ, ESC and other equilibrium solvers
  - Facilitates simulation of difficult equilibria
- Predictive pedestal model
  - Scalings for height and width of H-mode temperature pedestal
- ElVis web-based graphical display
  - To view simulations in progress as well as archived simulations
- Object-oriented Plasma State data structure
  - Facilitates connection with other codes
- Variety of NBI and RF heating and current drive sources

Newton's Method Implemented in PTRANSP

- **Formulation of Newton's method developed by Steve Jardin**
  - **This formulation works together with the conventional tri-diagonal finite difference equations resulting from diffusion equations**
- **Currently implemented in PTRANSP and TSC**

$$A_j T_{j+1}^{n+i/N} - B_j T_j^{n+i/N} + C_j T_{j-1}^{n+i/N} + D_j = 0$$

$\Leftarrow$ **Tridiagonal finite difference eqns**

$$A_j = s\theta\Phi_{j+1/2}\left[\chi_{j+1/2} + \left(\frac{\partial\chi}{\partial T'}\right)T'^{\,n+(i-1)/N}_{j+1/2}\right]$$

$$C_j = s\theta\Phi_{j-1/2}\left[\theta\chi_{j-1/2} + \left(\frac{\partial\chi}{\partial T'}\right)T'^{\,n+(i-1)/N}_{j-1/2}\right]$$

$$B_j = 1 + A_j + C_j$$

$$D_j = T_j^n + s(1-\theta)\left\{\left[\Phi_{j+1/2}\chi_{j+1/2}\left(T_{j+1}^n - T_j^n\right)\right] - \left[\Phi_{j-1/2}\chi_{j-1/2}\left(T_j^n - T_{j-1}^n\right)\right]\right\}$$

$$+\Delta t S + s\Phi_{j+1/2}T'^{\,n+(i-1)/N}_{j+1/2}\left(T_j^{n+(i-1)/N} - T_{j+1}^{n+(i-1)/N}\right)\left[\frac{\partial\chi}{\partial T'}\right]$$

$$+ s\Phi_{j-1/2}T'^{\,n+(i-1)/N}_{j-1/2}\left(T_j^{n+(i-1)/N} - T_{j-1}^{n+(i-1)/N}\right)\left[\frac{\partial\chi}{\partial T'}\right]$$

χ = thermal diffusivity, which is a function of temperature gradients

T' = temperature gradient

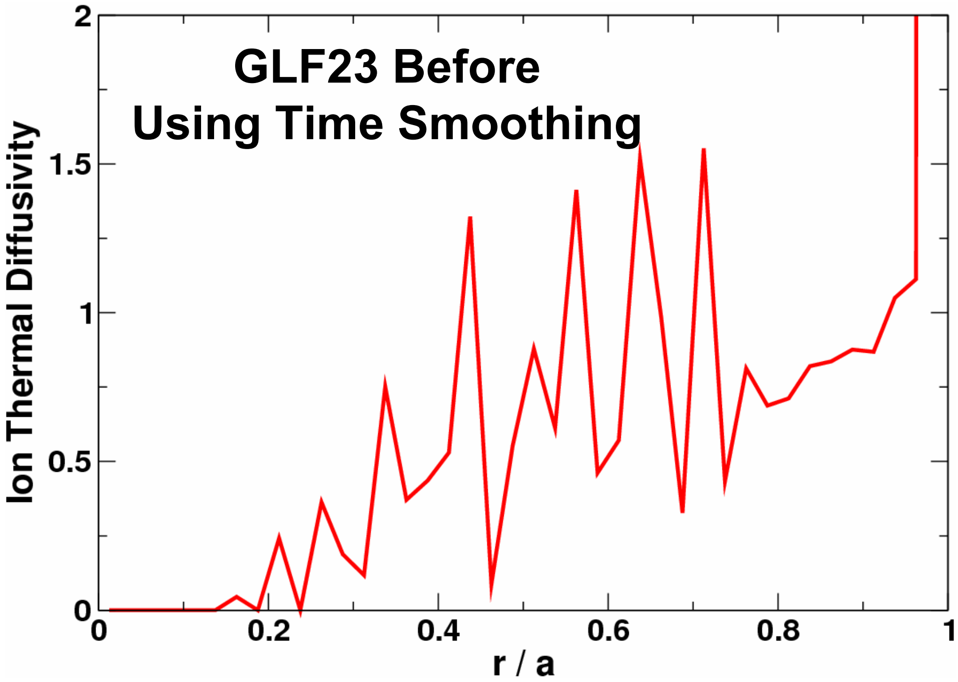
Φ = metric elements in transport eqns

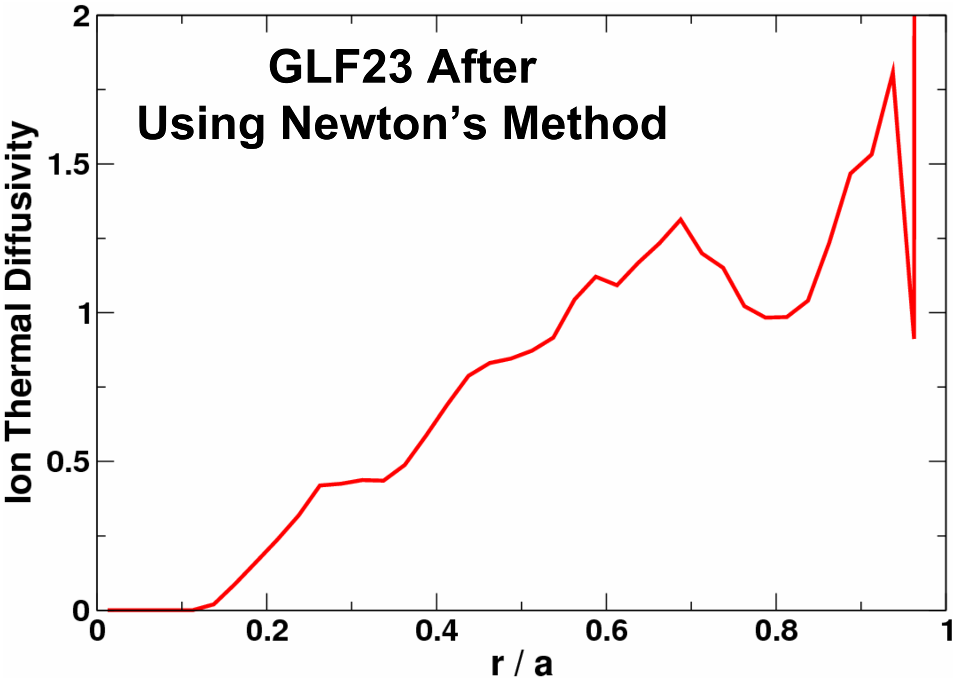
θ = implicitness parameter ≥ ½

$s = \Delta t/(\Delta x)^2$

Effect of Newton's Method in PTRANSP

- **Numerically induced oscillations in the GLF23 and MMM95 thermal diffusivity are eliminated by using Newton's method**
  - **Example below uses 3 Newton iterations per time step with θ = 1.0**
- **In this example, thermal transport model is called 9 times per time step**
  - **Three times per Newton iteration to compute $\partial\chi / \partial\nabla T$ for T_e and T_i**
  - **Three Newton iterations per time step**

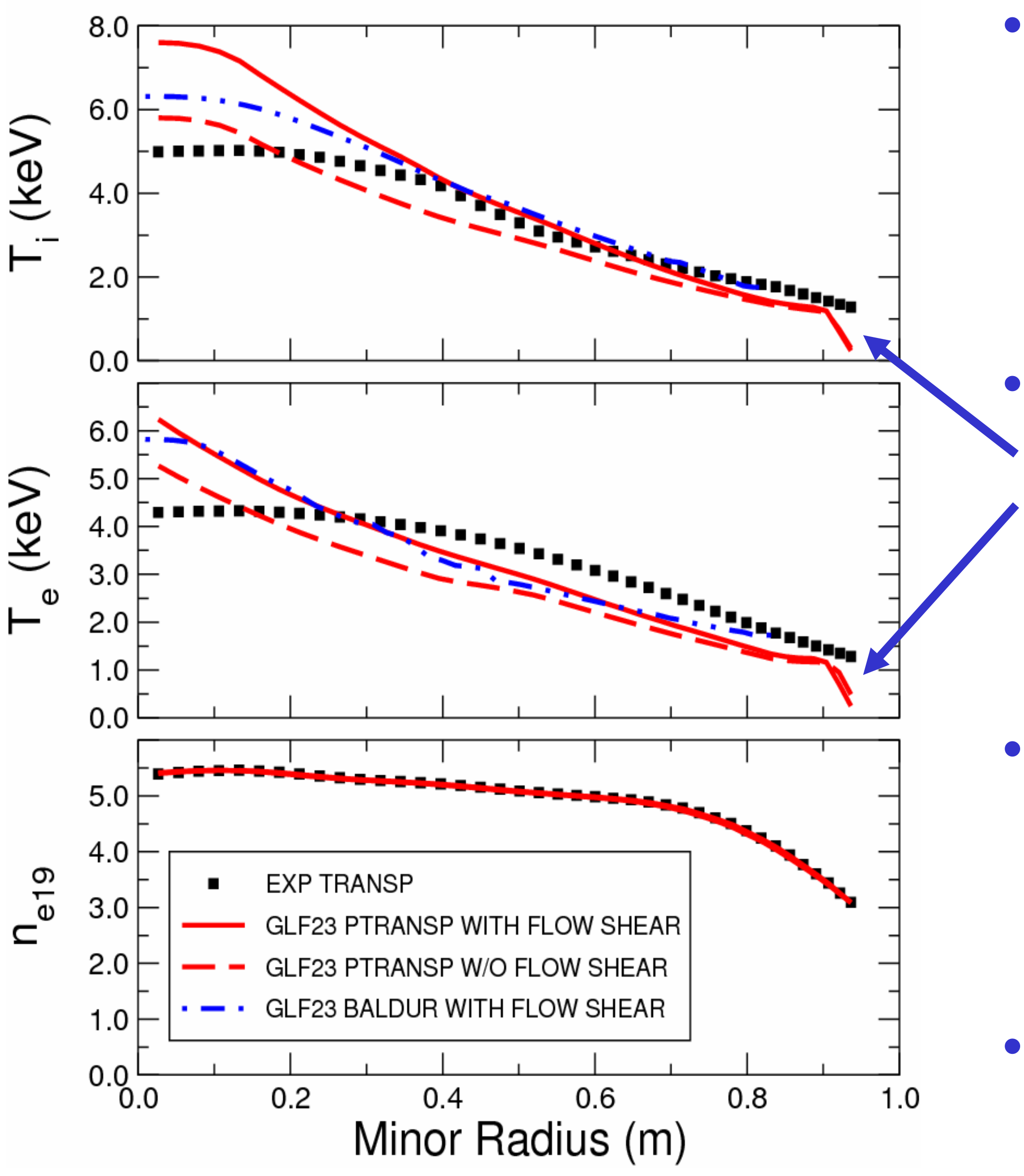




When Implementing Modules the Devil is in the Details

- Implementing complicated models such as the GLF23 anomalous transport model is difficult
  - There are currently 67 input/output variables (scalars and arrays) in the routine that is used to call the GLF23 model
    - It is easy to make a mistake that significantly affects the results
  - Correcting an error in defining radius in a previous implementation of GLF23 reduced predicted temperature profiles by more than 20%
  - Subtle choices, such as the inclusion of fast ion density or the use of alpha stabilization, have a noticeable effect on simulation results
- Sometimes a newly installed module yields unexpected and incorrect results
  - Defensive programming techniques are required
- Important to review, verify and validate all features in the code that relate to the module being implemented

PEDESTAL Module Implemented in PTRANSP

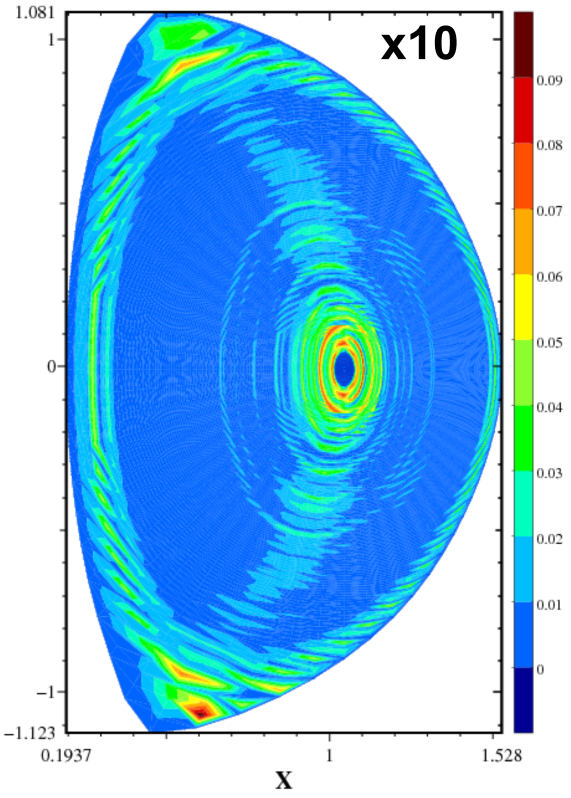


- **The NTCC PEDESTAL module has been implemented in PTRANSP**
  - **Used to compute height and width of temperature pedestal at edge of H-mode discharges**
- **PEDESTAL module provides a predictive boundary condition for temperature profiles in PTRANSP**
  - **Static model for H-mode pedestal is being used at present**
- **It is important to have a predictive model for the pedestal**
  - **Since global confinement and core profiles depend on pedestal height**
- **Predictive pedestal density model will be implemented when density profiles are predicted in PTRANSP**

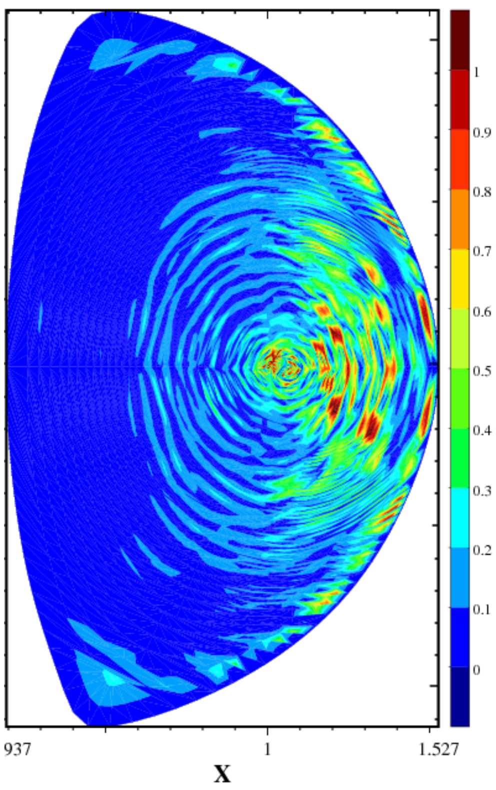
TEQ Module implemented in PTRANSP

- **NTCC TEQ equilibrium module (extracted from CORSICA) now installed in PTRANSP for prescribed boundary equilibria**
  - **TEQ currently most reliable equilibrium solver in PTRANSP**
- **Equilibrium error contour plots shown for different solvers**

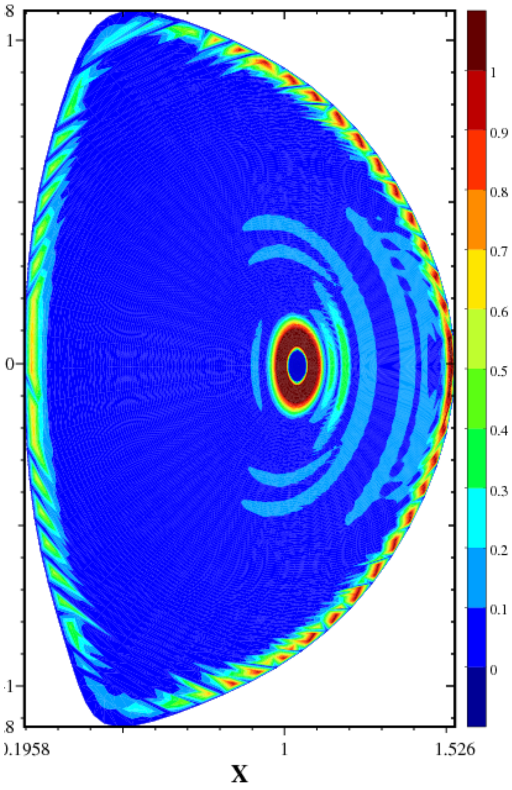
TEQ


Grad–Shafranov equation error

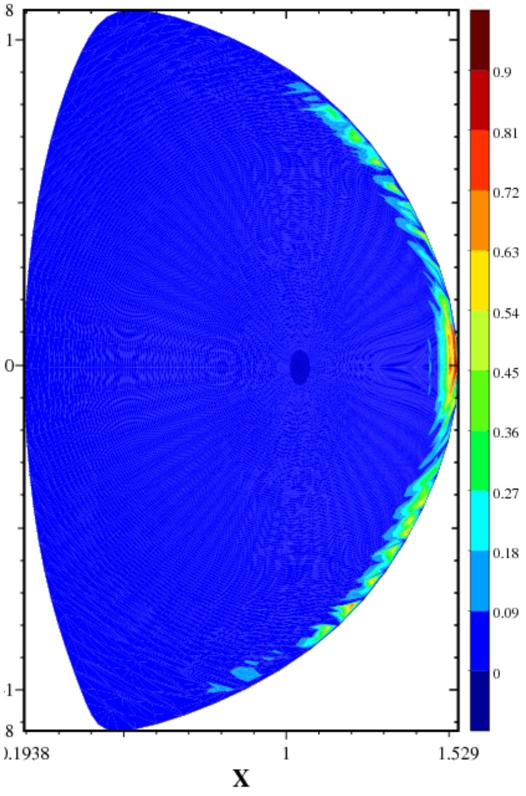
RZSOLVER


Grad–Shafranov equation error

VMEC


Grad–Shafranov equation error

ESC


Grad–Shafranov equation error

From Rob André, APS-DPP 2006

Source Modules Available in PTRANSP

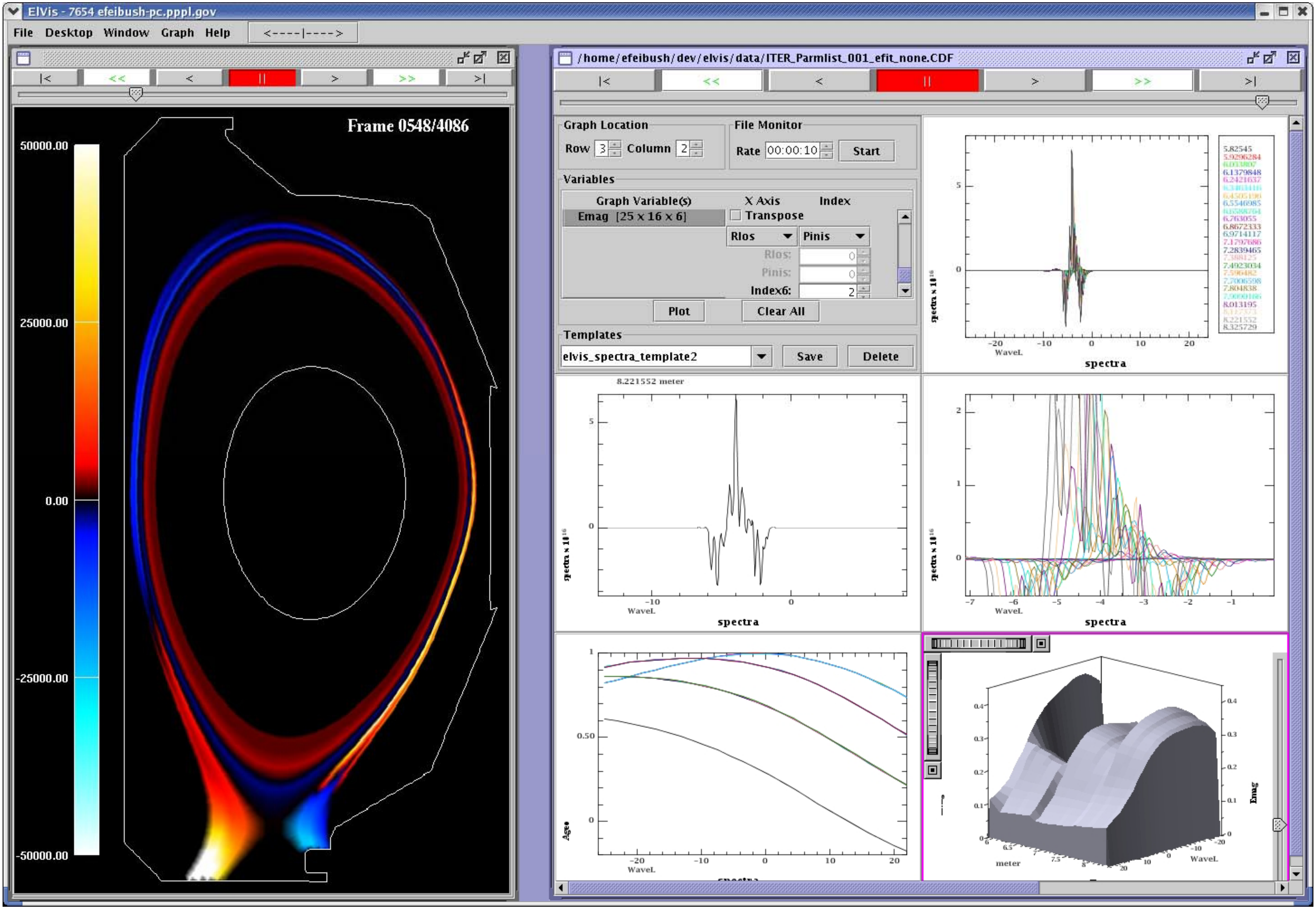
- Neutral beam & fusion product deposition:
  - NUBEAM (Monte Carlo)
- RF sources:
  - TORIC, AORSA: Ion Cyclotron (low and high harmonic), Lower Hybrid: full wave solutions
  - GA-TORAY, LSC, GENRAY: Electron Cyclotron, Lower Hybrid: ray tracing solutions
- Fast ion accumulation; response to RF:
  - NUBEAM (Monte Carlo)
  - CQL3D (Fokker Planck; fast electrons also)
- Inputs to these modules include
  - Beam-line or RF antenna geometries, power, voltage, spectrum, plasma equilibrium magnetic fields, temperatures and densities
- Outputs include source densities of heat, momentum, particles and current drive

ElVis Graphics Package

- **ElVis is a Web/Java enabled graphics package for collaborative scientific work**
  - **See http://w3.pppl.gov/elvis**
- **ElVis can be used for**
  - **Monitoring of running simulations while in progress**
  - **Examining output of completed simulations**
  - **Plotting experimental data**
- **Access using a web browser**
- **ElVis is used in CPES and SWIM SciDAC projects and in the TRANSP/PTRANSP project**

ElVis – Display Sequential Images

Monitor Variables in netCDF Files CPES



ElVis - 7654 efeibush-pc.pppl.gov

/home/efeibush/dev/elvis/data/ITER_Parmlist_001_efit_none.CDF

Frame 0548/4086

Graph Location: Row 3 Column 2

File Monitor: Rate 00:00:10

Variables:

Graph Variable(s): Emag [25 x 16 x 6]

☐ Transpose

X Axis: Rlos

Index: Pinis

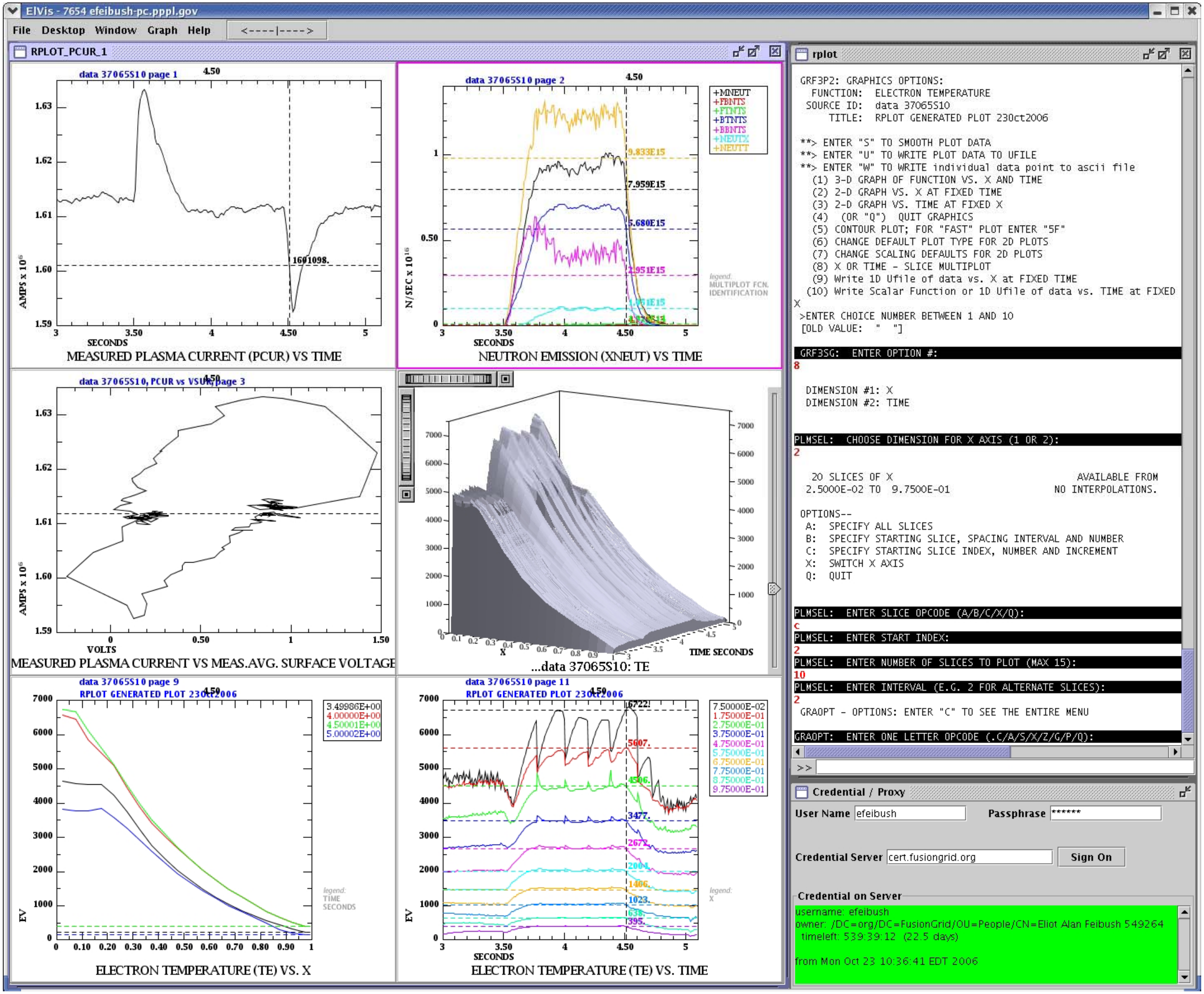
Rlos: 0

Pinis: 0

Index6: 2

Templates: elvis_spectra_template2

Visualization Client in Web Service to TRANSP - RPLOT



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GRF3P2: GRAPHICS OPTIONS:
  FUNCTION:  ELECTRON TEMPERATURE
 SOURCE ID:  data 37065S10
     TITLE:  RPLOT GENERATED PLOT 23Oct2006

**> ENTER "S" TO SMOOTH PLOT DATA
**> ENTER "U" TO WRITE PLOT DATA TO UFILE
**> ENTER "W" TO WRITE individual data point to ascii file
  (1) 3-D GRAPH OF FUNCTION VS. X AND TIME
  (2) 2-D GRAPH VS. X AT FIXED TIME
  (3) 2-D GRAPH VS. TIME AT FIXED X
  (4)  (OR "Q")  QUIT GRAPHICS
  (5) CONTOUR PLOT; FOR "FAST" PLOT ENTER "5F"
  (6) CHANGE DEFAULT PLOT TYPE FOR 2D PLOTS
  (7) CHANGE SCALING DEFAULTS FOR 2D PLOTS
  (8) X OR TIME - SLICE MULTIPLOT
  (9) Write 1D Ufile of data vs. X at FIXED TIME
 (10) Write Scalar Function or 1D Ufile of data vs. TIME at FIXED
X
 >ENTER CHOICE NUMBER BETWEEN 1 AND 10
 [OLD VALUE:  "  "]

 GRF3SG:  ENTER OPTION #:
8

  DIMENSION #1: X
  DIMENSION #2: TIME


PLMSEL:  CHOOSE DIMENSION FOR X AXIS (1 OR 2):
2

   20 SLICES OF X                                   AVAILABLE FROM
  2.5000E-02 TO  9.7500E-01                      NO INTERPOLATIONS.

 OPTIONS--
  A:  SPECIFY ALL SLICES
  B:  SPECIFY STARTING SLICE, SPACING INTERVAL AND NUMBER
  C:  SPECIFY STARTING SLICE INDEX, NUMBER AND INCREMENT
  X:  SWITCH X AXIS
  Q:  QUIT


PLMSEL:  ENTER SLICE OPCODE (A/B/C/X/Q):
c
PLMSEL:  ENTER START INDEX:
2
PLMSEL:  ENTER NUMBER OF SLICES TO PLOT (MAX 15):
10
PLMSEL:  ENTER INTERVAL (E.G. 2 FOR ALTERNATE SLICES):
2
 GRAOPT - OPTIONS: ENTER "C" TO SEE THE ENTIRE MENU

GRAOPT:  ENTER ONE LETTER OPCODE (.C/A/S/X/Z/G/P/Q):
>>
```

User Name efeibush **Passphrase** ******

Credential Server cert.fusiongrid.org

Credential on Server

username: efeibush
owner: /DC=org/DC=FusionGrid/OU=People/CN=Eliot Alan Feibush 549264
 timeleft: 539:39:12 (22.5 days)

from Mon Oct 23 10:36:41 EDT 2006

Plasma State Module

- The “Plasma State”
  - Is an emerging standard to share data time slices
  - Contains data for axisymmetric MHD equilibrium, plasma and source profiles (1-D and 2-D), as well as associated scalar data
  - Includes methods to read and write data
    - Methods can involve interpolation from one grid to another
  - Can be stored in computer memory or as disk files
  - Provides a mechanism for communication between different codes
    - Is not intended to be a restart file for PTRANSP simulations
- Will be possible to construct a time series of Plasma States
  - To provide data communication for time-dependent simulation or experimental results

Plasma State Module -2

- Plasma State will facilitate comparison
  - Between simulation results from different codes
  - Between simulation results and experimental data
- Plasma State to be used for communication between components in the SWIM SciDAC project
  - Loose coupling to distributed source model servers
  - File-based communication scheme will be utilized
- The Plasma State is being prepared as an NTCC Module with support from the PTRANSP project
  - Similar to XPLASMA but with a higher level interface
  - Will conform to NTCC Module standards, particularly documentation

PTRANSP Server

- Other codes can communicate with PTRANSP server
  - PTRANSP server provides unified way to compute sources
  - In server-client mode, each code has its own input and internal state
  - Because of large and complicated inputs/outputs, it is desirable to use components in their own code environment
    - PTRANSP NUBEAM NBI module, for example, requires large amount of input data describing beam lines and large internal state
      - Requires more than 300 input and more than 300 output variables
    - Collectively the source modules contain many 100s of inputs and outputs
  - Each component module has its own control mechanisms
  - Each component module has its own grid structure
- Plasma State developed as a software component to communicate with the PTRANSP server

Proposed Projects for PTRANSP - 1

- Predictive particle transport to evolve density profiles
  - Particle transport coefficients for hydrogenic and impurity ion species computed using MMM95, GLF23, and NCLASS modules
- Free-boundary TEQ equilibrium module with generalized Ohm's law installed in PTRANSP
  - Database of input TEQ specifications for coils, external circuits and structural configurations will support most tokamaks
- Porcelli sawtooth model will be implemented in PTRANSP
  - PORCELLI NTCC module used to trigger sawtooth crashes and the KDSAW module contains Porcelli partial magnetic reconnection
- Globally Convergent Newton Method Parallel (GCNMP) installed in the PTRANSP code
  - GCNMP will be refined for adaptive grids

Proposed Projects for PTRANSP - 2

- TGLF will be installed as a successor to the GLF23 model
  - Since the TGLF model is computationally intensive, simulations will benefit from efficient parallel computing
- A new version of the Multi-Mode model is being developed and will be installed in PTRANSP
  - New Multi-Mode model includes momentum transport, multiple ion species, and improved finite beta effects
- Momentum transport equations for velocity profile evolution
  - Modern transport models such as TGLF and new Multi-Mode modules will be used to compute momentum transport coefficients
- A dynamic model for H-mode pedestal growth and ELM cycles will be implemented in PTRANSP
  - Dynamic ELM cycle model will be patterned after models currently used in ASTRA and JETTO

Proposed Projects for PTRANSP - 3

- ELITE stability code to be installed in PTRANSP
  - ELITE is particularly well suited for computing the onset and width of the MHD instabilities that trigger ELM crashes
- Performance will be improved
  - Equilibration of sources when plasma conditions have not changed
  - Other performance improvements will be identified as code is used
- Improvements to simulation control
  - Options for automated feedback modification of source powers
- Standardized test problems will be developed to facilitate PTRANSP regression testing
  - Standardized time series may be developed for free-boundary equilibria, plasma profile data that is read in from datasets, heating power, current drive, initial & boundary conditions
  - Detailed validation studies will be carried out

Predictive Density Profile Evolution

- Particle transport, sources, and sinks will be used to compute the evolution of density profiles in PTRANSP
  - MMM95, GLF23, and NCLASS modules are used to compute transport for hydrogenic and impurity ion species
  - Particle sources and sinks are already computed in PTRANSP
  - Particle transport equations will be patterned after those already used in BALDUR, JETTO and other transport codes
- Particle transport equations will be used to evolve multiple thermal ion profiles as well as fast ion profiles
  - Quasi-neutrality condition is then used to compute electron density
    - Since all positive ion densities are added, the quasi-neutrality condition can never lead to a negative electron density
    - Normalized density gradients, which are used in MMM95 and GLF23, also satisfy a quasi-neutrality condition
- Greater self-consistency results from predicting evolution of density profiles

Predictive Velocity Profile Evolution

- Momentum transport, as well as sources and sinks of momentum will be implemented to compute the plasma velocity profiles in the PTRANSP code
  - Anomalous momentum transport coefficients will be computed using GLF23 or TGLF or the new Multi-mode transport module
  - NBI momentum sources will be computed using NUBEAM module
  - Boundary conditions will be consistent with models for plasma edge
- The radial gradient of plasma velocity is a part of the ExB flow shear computation
  - The ExB flow shear rate is particularly important in the prediction of transport barriers, where flow shear stabilizes anomalous transport
  - Momentum, thermal and particle transport are needed for self-consistent computations of transport barriers

Free-Boundary TEQ Equilibrium Solver

- **An enhanced free boundary TEQ equilibrium solver will be installed with tight coupling to magnetic diffusion solver**
  - **To be used for start-up and shut-down scenario studies, volt-second computations, simulation of ELM cycles, disruption studies, shape and vertical control system design, and coupling to edge/SOL models**
- **Ohm's law will include hyper-resistive extensions**
  - **Fourth-order magnetic flux diffusion equation to model ELM crashes, neoclassical tearing modes, and sawtooth crashes**
  - **Recent simulations of hybrid DIII-D discharges simulate effects of tearing modes using hyper-resistivity (T. Casper, *et al.*, IAEA 2006)**
- **Database of TEQ input specifications will be available for magnetic coils, external circuits, structural configurations**
  - **Database includes most tokamaks and will be added to as needed**
  - **Input database will facilitate simulations by allowing user simply to name the free boundary configuration to be used**

Globally Convergent Newton Method Parallel (GCNMP)

- **GCNMP: Transport solver module developed by H. St.John**
  - **To be used in SWIM and NTCC/PTRANSP project**
- **Solves a generalized form of diffusive convective equations**
  - **For densities, temperatures, angular velocities and magnetic fields**

$$\underline{\underline{M}}\frac{\partial}{\partial t}\bigg|_{\zeta}\underline{u} - \frac{1}{H\rho}\frac{\partial}{\partial\rho}\left(H\rho\underline{\underline{D}}\frac{\partial}{\partial\rho}\underline{u}\right) + \frac{1}{H\rho}\frac{\partial}{\partial\rho}\left(H\rho\underline{\underline{V}}\,\underline{u}\right) + \underline{\underline{W}}\,\underline{u} = \underline{S_{ext}} \qquad (1)$$

where vector $u \equiv [n_1 \ldots . n_n, T_e, T_i, FGH\rho Bp, \omega]$

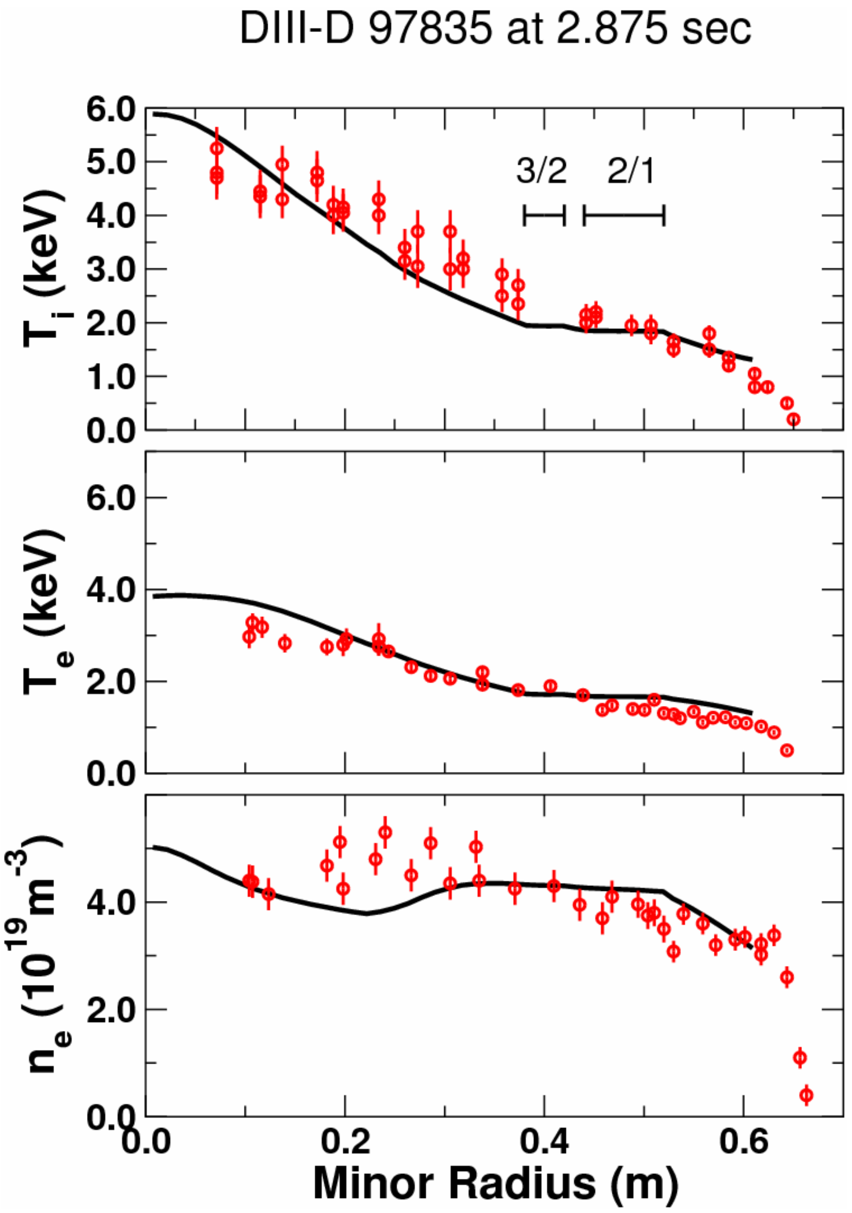
- **Number and subset of equations solved is user selectable**
  - **The remaining equations are run in "analysis mode"**
  - **Boundary conditions can be applied at different radial points**
- **GCNMP solver will use dynamic combination of steepest descent, line search and two trust region strategies**
  - **Switching from one method to next as needed for difficult problems**

Porcelli Sawtooth Model Planned for PTRANSP

- The Porcelli model is a widely used sawtooth model
  - Results using various implementations of Porcelli model have been compared with experimental data
    - Observed effects of NBI and RF heating have been confirmed
- Porcelli trigger model will be implemented in PTRANSP
  - The Porcelli sawtooth trigger module has been installed in the NTCC Module Library after being tested in BALDUR code simulations
    - Sawtooth periods computed in BALDUR simulations are compared with experimental data in Phys. Plasmas 13, 072505 (2006)
  - The trigger model calls the KDSAW module, already implemented in PTRANSP, contains Porcelli partial magnetic reconnection model
    - It was found that the sawtooth period depends on the assumed fraction of magnetic reconnection, which alters the Kadomtsev reconnection model
- Implementation of Porcelli sawtooth trigger model is complicated by the different time step lengths in PTRANSP
  - Triggering at end of long NBI heating time step allows appropriate mixing of fast ions during each sawtooth crash

Model for Neoclassical Tearing Modes Planned for PTRANSP

- The ISLAND module to compute neoclassical tearing mode (NTM) magnetic island widths to be installed in PTRANSP
  - ISLAND module computes multiple island widths in tokamaks with arbitrary cross section and beta
- Transport is enhanced across each island for self-consistency
  - Tested in BALDUR implementation
- Electron Cyclotron Current Drive being implemented to model feedback stabilization of NTMs



New Transport Modules in PTRANSP

- New transport modules will be implemented in PTRANSP as they become available
  - PTRANSP will be used for a careful validation of transport models
- TGLF will be installed as a successor to the GLF23 model
  - TGLF transport is represented in terms of drift mode basis functions that have been calibrated using nonlinear GYRO simulations
  - The TGLF transport model is designed to be accurate from the plasma core to the base of the H-mode pedestal
  - TGLF model computes eigenvalues of 120x120 complex matrix for each toroidal mode number
  - Since the TGLF model is computationally intensive, simulations will probably require efficient parallel computing
- A new version of the Multi-Mode model is being developed
  - New Multi-Mode model includes momentum transport, multiple ion species, and improved finite beta effects

PTRANSP Verification and Validation

- **Standardized collection of plasma state datasets to be used for cross code verification and PTRANSP regression tests**
  - **Time dependent plasma state datasets will facilitate reproducible simulations by different integrated modeling codes**
  - **Standardized plasma state datasets will enable comparison between PTRANSP and first principles computations by SciDAC codes**
    - **For more detailed studies of turbulence, RF heating and MHD instabilities**
- **Detailed comparisons will be made with wide range of scans of tokamak experimental data**
  - **For H-mode and dynamic advanced tokamak scenario discharges**
  - **To test TGLF, GLF23 and Multi-Mode anomalous transport models**
  - **To test other components as well as transport in the context of self-consistent predictive integrated simulations**

Planned Dynamic Edge Model in PTRANSP

- **A dynamic model for H-mode pedestal growth and ELM cycles will be implemented in PTRANSP**
  - Dynamic ELM cycle model will be patterned after models that are currently used in ASTRA and JETTO
  - ASTRA and JETTO simulation results have been compared with experimental data from JET and DIII-D
- **Flow shear and magnetic shear stabilization of anomalous transport results in development of edge pedestal**
  - Different modes of turbulence and different channels of ion and electron thermal transport are treated separately
- **Each ELM crash is triggered by an MHD instability criterion**
  - Initially, parameterizations of the peeling/ballooning MHD instability criterion will be used to trigger ELM crashes
  - Subsequently, ELITE code will be coupled to PTRANSP to compute ELM trigger and to estimate ELM width from eigenfunction structure

Summary

- Predictive simulations are now being carried out with the PTRANSP code based on advances in the past two years
- Significant advances in the physics content will be added during the next three years
  - High-quality widely used modules for transport, equilibrium, sources, sinks and large scale instabilities all interacting together in one code
  - Comparison with experimental data facilitated by extensive data analysis infrastructure already built into TRANSP
- As a result of the effort proposed for the next three years, PTRANSP will become significantly more comprehensive
- PTRANSP will serve as a bridge to high-performance SciDAC Fusion Simulation Projects