NTCC
(National Transport Code Collaboration)

ECC
(Edge Coordinating Committee)

Presented by

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NTCC Project Initiated in 1998

- NTCC has involved 29 researchers from 11 institutions:
- Effort has been focused on
  - Developing a Modular Transport Code
  - Developing a Data Accessor
  - Establishing a Module Library
- Project Funding during past 7 years
  - Approximately $4.8 M
- Focus during past 3.5 years has been on producing modules for the NTCC Module Library
  - Extracting Modules from Legacy Codes
  - Advancing Physics Content of Modules in Library

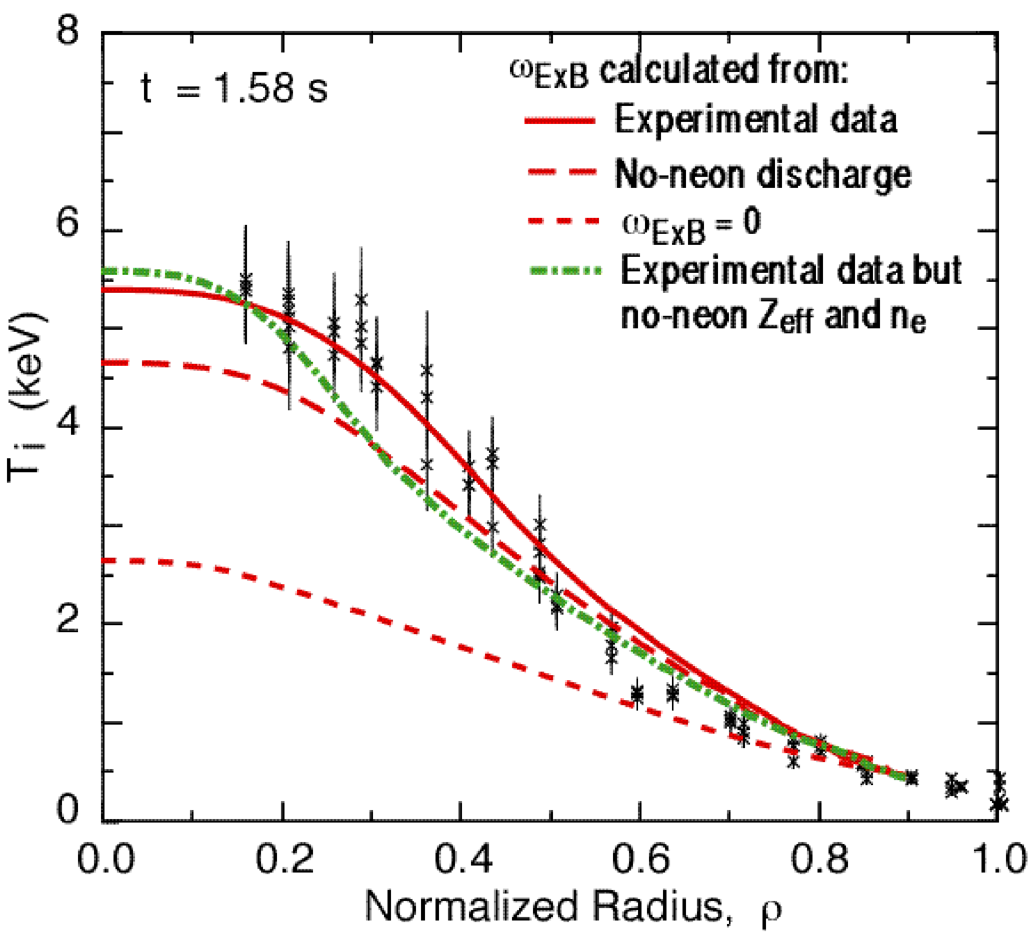
NTCC Motivated by Need for Predictive Integrated Modeling Codes that are Flexible and Easy to Use

- **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 $\rightarrow$ 1.4) and $n_e(\rho)$ after the improved state is established**

$\Rightarrow$ Neon injection may be used as a trigger

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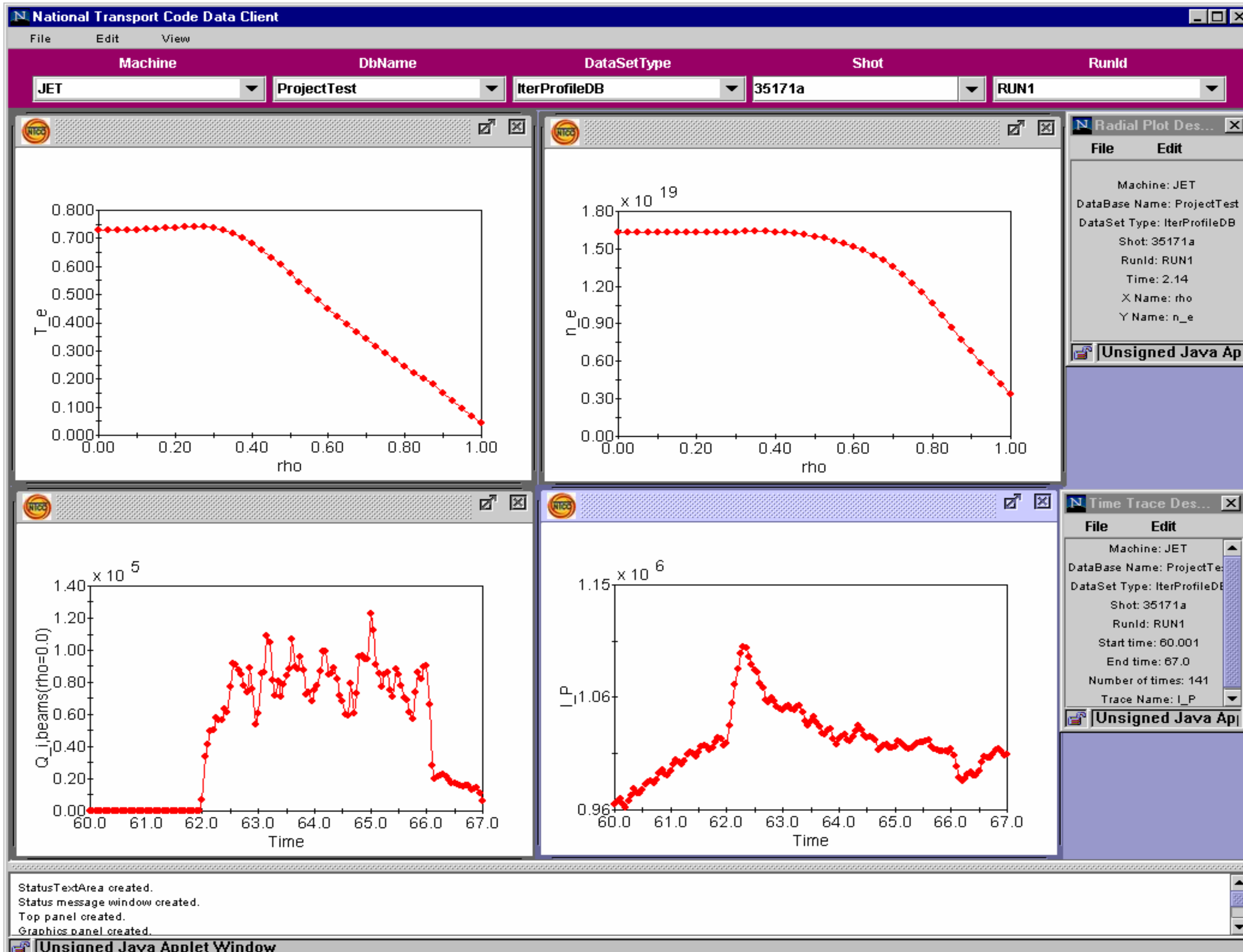
NTCC Data Accessor

- NTCC Code accesses data through Data Accessor
- Web-invocable NTCC data accessor provides uniform standardized access to databases regardless of source
  - International (ITER) Profile Database
  - MDSplus trees
- Data Accessor applies rules for missing data
  - For example, computes impurity density from Z_{eff}, n_e and Z_{imp}
- Brings data together in a uniform way
  - With standardized set of names and units
  - Interpolated in time and radius to a prescribed radial grid
- Web-based documentation
  - With definitions and units for all variables
- Allows single transfer of complex, composite data
  - Connected to the NTCC transport code
- Recently installed at Culham to provide access to ITPA Confinement Database

Data Accessor Plots



NTCC Module Library

- Web-based, community-owned modules http://w3.pppl.gov/NTCC
- 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
- Modules extracted from legacy codes has resulted in re-use
  - Often with improved documentation and physics content
- Library as origin of shared modules aides version control
  - Modules are kept up-to-date in one location
  - Straight-forward to include improved modules as they become available
- 47 modules now in the library (21 modules reviewed and approved)
  - Library Standards and Review Procedure helps to improve module quality
  - Modern coding practices encouraged – inheritance and encapsulation
  - Modules encourage community collaboration and help reduce redundancy

Anomalous Transport Models

- GLF23 — Gyro-Landau-Fluid drift wave model
  - Full featured model quasi-linear drift wave models
  - Multiple channels of transport
- MMM95 — Multi-Mode transport model
  - Drift wave transport combined together with other modes
  - Multiple channels of transport
  - Transport from the center of the plasma to the edge
- JETTO transport model
  - Mixed Bohm/gyro-Bohm anomalous transport model
- IFS/PPPL transport model
  - Thermal transport based on non-linear turbulence simulations of the Ion Temperature Gradient (ITG) mode
- Ottaviani-Horton-Erba transport model
  - Thermal transport driven by ITG modes
- CYTRAN
  - Transport of thermal energy caused by emission and absorption of electron cyclotron radiation

Neoclassical Transport

- **NCLASS**
  - **Sophisticated, full-featured model for neoclassical transport**
    - **Multiple species of hydrogenic and impurity ions**
    - **Arbitrary aspect ratio, geometry, and collisionality**
    - **NBI-driven neoclassical effects**
  - **Widely used within integrated modeling codes in the US and abroad**
- **KAPISN**
  - **Neoclassical ion thermal transport from several models**
    - **including the Rutherford, modified Hazeltine-Hinton, Bolton, Chang-Hinton (1982) and modified Chang-Hinton (1986) models**

NBI Heating Modules

- **NUBEAM Neutral Beam Injection extracted from the TRANSP code**
  - **Largest and most complex code in the NTCC Module Library**
  - **Monte-Carlo numerical technique to compute**
    - **Neutral deposition from multiple NBI sources**
    - **Slowing down of fast ions**
    - **Comprehensive atomic and nuclear physics**
    - **Effects of large scale instabilities such as sawtooth crashes and fishbone instabilities**
    - **Effects of magnetic ripple and finite Larmor radius**
- **NBEAMS**
  - **Analytic approximations in simplified geometry**
  - **Heating, particle deposition, and current drive**

The Tokamak Monte-Carlo Fast Ion Module NUBEAM in the National Transport Code Collaboration Library, Comput. Phys. Comm. **159,** 157 (2004), by Alexei Pankin, D. McCune, R. Andre, G. Bateman, and A. H. Kritz.

Numerical Techniques Used in Neutral Beam Injection Modules, in press Comput. Phys. Comm, by Alexei Pankin, G. Bateman, R. Budny, A. H. Kritz, D. McCune, Alexei Polevoi, and Irina Voitsekovitch

RF Heating Modules

- **CURRAY**
  - Ray tracing for ion cyclotron and lower hybrid wave heating and current drive
  - This code has evolved since the 1980's with many co-authors
- **TORAY**
  - Ray tracing for electron cyclotron wave heating and current drive
  - Evolved over decades with several co-authors
  - Includes relativistic effects
- **LSC**
  - Lower hybrid ray tracing for power deposition
  - 1-D Fokker-Planck approximation
  - Including effect of DC electric field

MHD Equilibrium Modules

- ESC
  - Efficient prescribed-boundary MHD equilibrium code
  - Computes harmonic representation of flux surfaces
    - $R = R(\psi, \theta)$ and $Z = Z(\psi, \theta)$, where ψ is a flux surface label and θ is a poloidal angle-like variable
- JSOLVER
  - Prescribed-boundary MHD equilibrium code using an iterative numerical technique
  - Computes harmonic representation of flux surfaces in equal arc poloidal angle coordinates

Divertor/Edge

- PEDESTAL
  - Model to predict the pedestal temperature and density height for type I ELMy H-mode plasmas

Modules Related to MHD Equilibrium

- **XPLASMA**
  - **Converts equilibrium from one representation to another**
- **I2MEX**
  - **Standard MHD equilibrium representation for metric elements**
- **TRXPLIB**
  - **To load and XPLASMA equilibrium from a TRANSP archive**
- **TRACK**
  - **Compute the intersection between a given trajectory and equilibrium magnetic surfaces in 3-D toroidal plasmas**
  - **Used, for example, in neutral beam and pellet injection modules**

MHD Instability Modules

- **PEST3**
  - Non-ideal version of the Princeton Equilibrium and Stability code
  - Growth rate and spatial structure of resistive MHD instabilities, such as resistive and neoclassical tearing modes
  - Ideal MHD stability
- **KDSAW**
  - Kadomtsev sawtooth mixing model to compute the mixing radius and mixing produced by a sawtooth crash

Neutral Gas Modules

- **FRANTIC**
  - Fast 1-D, circular cross section, neutral gas transport module
  - Includes charge exchange and ionization atomic reactions
  - Multiple species particle, momentum, and energy sources
- **NUT**
  - Semi-analytic 3-D neutral transport in a 3-D plasma
- **PREACT**
  - Ionization, recombination, radiation, and fusion reaction rates
  - Table look-up and interpolation

Numerical Tools - 1

- **PSPLINE**
  - Spline and Hermite interpolation routines for 1-D, 2-D, and 3-D data sets on rectilinear grids
  - Full control over boundary conditions — such as periodic, "not a knot", 1st derivative, 2nd derivative, or divided difference
- **MELKES**
  - Reduced Hermite piecewise cubic polynomial interpolation for data in an arbitrary number of dimensions
  - Data may be mix of values, gradients, or Hessians
- **RNG**
  - Portable, parallel random number generator
  - To produce the same sequence of random numbers on all platforms
- **R8SLATEC**
  - Double precision routines for elementary and special functions
  - From the SLATEC library http://www.netlib.org/slatec/toc
- **LSODE**
  - Double precision version of ODE solver
  - From http://www.netlib.org/odepack/opkd-sum

Numerical Tools - 2

- **GRIN**
  - C++ package to solve 2-D elliptical PDEs using Green's functions
- **NSCRUNCH**
  - To compute rapidly converging Fourier harmonic representation of 2-D nested contours such as flux surfaces in tokamaks
- **GACO**
  - Solve ODEs and PDEs based on expanding the solution in Gabor wave packets
- **SupraLu**
  - Solve sparse matrix problems in C, Fortran90 and Python
  - Solve linear systems, compute determinants, eigenvalues/eigenvectors

Data Analysis Modules

- **EZCDF**
  - **Easy to use interface to the NetCDF library**
- **UFILES**
  - **Routines to read and write Ufiles, which are a self-documenting data file format developed at PPPL**
- **TRREAD**
  - **Routines to facilitate access to data produced by the TRANSP integrated modeling code developed at PPPL**
- **UREAD**
  - **To facilitate the development of interactive Fortran codes**

Data Visualization Modules

- PPPL-UTILITIES
  - Collection of utilities designed to study experimental data
- SGLIB
  - Scientific Graphics Library to generate plots that are compatible with the Tektronix 4014 or 4105 terminal classes
- TEK2PS
  - Converts SGLIB Tektronics formatted plot files to PostScript
- XTC
  - X-window display of SGLIB Tektronix 4014 or 4105 plots
- TRGRAPH
  - For the interactive display of data
  - Built on the UREAD and SGLIB modules

Portability Tools

- **FPREPROC**
  - **PERL script for preprocessing Fortran-77 codes**
- **FTOKEN**
  - **To facilitate strong typing in Fortran-77 codes**
- **MPPL**
  - **To allow programmers to write in a free-form, structured Fortran-like computer language**
- **PORTLIB**
  - **To standardize system calls within Fortran programs**

***The National Transport Code Collaboration Library**, in press, Comput. Phys. Comm., by A. H. Kritz, G. Bateman. J. Kinsey, A. Pankin, T. Onjun, A. Redd *et al*.

NTCC Module Work in Progress

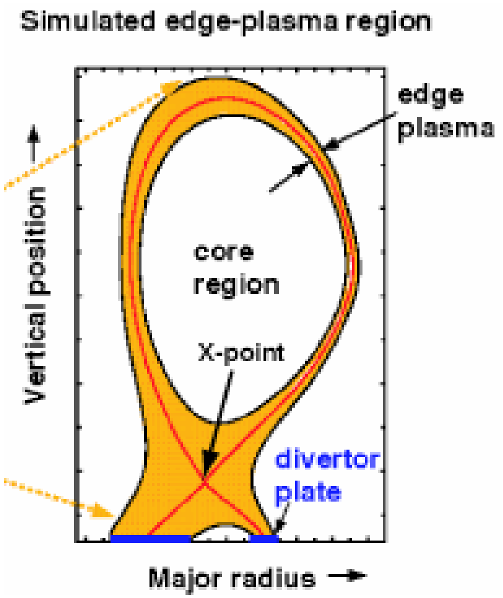
- New modules under development:
  - TEQ : Free-boundary plasma equilibrium
    - Prescribe coil currents rather than prescribing boundary shape
  - TORIC : Full wave treatment of ion cyclotron resonance heating
    - For long wavelengths, where ray tracing is not appropriate
  - IMPRAD : Non-equilibrium 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

Utilization of Module Library

- Experimental and theoretical fusion research programs have benefited significantly by the availability of well benchmarked, efficient, and extensively validated modules
  - Standards and review process help insure module quality
  - Numerous examples of module use at PPPL, GA, Lehigh, LLNL, ORNL
  - Modules have been used in European codes: ASTRA and JETTO
- Modules have been used in science programs outside fusion
  - In the US as well as in Europe
  - More than 45 examples of applications of NTCC modules
- Majority of NTCC modules are applicable for study of burning plasmas and provide components needed for the development of a predictive integrated modeling code
  - Key test of the utility and applicability of the NTCC library will be its use in developing a modern integrated modeling code for use in ITER studies
- Integrated predictive modeling capability will be most effectively achieved through international cooperation and collaboration
- Formation of an International ITER Code Collaboration
  - Utilize modern framework and NTCC modules to develop ITER predictive modeling code

ECC (Edge Coordinating Committee)

- **Mission http://www.mfescience.org/ecc**
  - Advance US fusion science through technical assessment, prioritization, and coordination of edge plasma theory and modeling in close partnership with national experimental groups and international fusion programs.
- **Scope**
  - Physics of everything from the top of the pedestal into the plasma-facing material
  - Theory, computational and experimental partnerships
  - International collaboration



- **Initial Committee Meeting**
  - July 14-15, 2004 Germantown, MD
  - Fusion Scientists met to discuss establishing a road map for tokamak edge plasma science research during next 5 years

ECC Objectives

- Strengthen the edge community
  - Workshops
  - Web site http://www.mfescience.org/ecc
  - Conference calls
- 5-year roadmap of technical goals and needs
- Promote edge research cooperation between theory, modelers, experiments, and computer scientists
- Promote implementation of standards for verification and validation
  - Establish database of modeling results
  - Verification -> code does what you think it should do
  - Validation -> code results compare correctly with reality
- Advocate international collaboration in high priority areas

Draft of ECC By-Laws

- By-Laws to be reviewed and adopted at ECC meeting next week
  – http://www.mfescience.org/ecc/bylaws.html
  – Committee membership
    - 3-year terms, 1/3 new each year (after initial 2 years)
  – Decision-making process
    - Affirmative vote of a majority present
  – Meetings (each year)
    - Two physical committee meetings
    - At least two electronic meetings
    - One technical Edge meeting/workshop

ECC Membership

Charter members of ECC selected by OFES, July 2004

- **Glenn Bateman, Lehigh University**
- **Curt Bolton, Office of Fusion Energy Science, ex officio member**
- **Choong-Seock Chang, New York University**
- **Max Fenstermacher, Lawrence Livermore National Lab**
- **Parvez Guzdar, University of Maryland**
- **Taik Soo Hahm, Princeton Plasma Physics Lab**
- **Sergei Krasheninnikov, University of California, San Diego**
- **Arnold Kritz (Vice Chair), Lehigh University**
- **Thomas Rognlien (Chair), Lawrence Livermore National Lab**
- **Dalton Schnack, Science Applications International Corp**
- **David Schultz, Oak Ridge National Lab**
- **Philip Snyder, General Atomics**
- **Daren Stotler, Princeton Plasma Physics Lab**
- **James Terry, Massachusetts Institute of Technology**
- **Michael Ulrickson, Sandia National Lab**

ECC Initial Working Groups, Coordinators

- **Elm Growth and Crash (Phil Snyder)**
- **Pedestal Profile Reconstruction between Elms (Choong-Seock Chang)**
- **L-H Mode Transition (Parvez Guzdar)**
- **Scrape-off Layer Dynamics and Density Limit (Sergei Krasheninnikov)**
- **Plasma/Material Interactions (Mike Ulrickson)**
- **Atomic/Molecular Data Needs (Dave Schultz)**
- **Fundamental Equations for the Edge (Taik Soo Hahm)**
- **Integrated Edge Simulations (Glenn Bateman)**
- **Computational Techniques (Dalton Schnack)**
- **Validation and Verification of Codes (Daren Stotler)**
- **Partnerships with Experimentalists and International Programs (Jim Terry)**

ECC Working Draft Documents and Meetings

- The Coordinator of each working group has prepared a draft document
  - Topical draft documents can be obtained from
    http://www.mfescience.org/ecc/wg.html
    by clicking “summary” at the end of each topic line
- The draft documents will provide, at least in part, the basis for discussion at the ECC meeting to be held next Monday and Tuesday
- Future ECC meetings
  - September 27-28, 2004: Planning and organizational meeting
    General Atomics, San Diego, CA: Draft Agenda
    http://www.mfescience.org/ecc/ECC_agenda_Sept27_28_TRc.htm
  - Nov. 14, 2004: Planning and informational meeting
    Satellite meeting of APS-DPP
    7 p.m., Grand Ballroom E, Westin Hotel, Savannah, GA
  - April 6-9, 2005: Tentative 2-day technical meeting
    coordinated with the TTF meeting; Napa, CA

Edge Community Program Goals

- **Develop and implement predictive fundamental physics models for the tokamak plasma edge**
  - **L-H Transition**
  - **Pedestal and Scrape off layer dynamics during ELM cycle**
  - **Plasma-Materials interactions and their impact on surface morphology and boundary/core plasmas**
- **Develop partnerships among theorists, modelers, experimentalists and international community to facilitate comparison between experimental and simulation data**
  - **Evaluate and extend experimental and simulation data sets**