Perspectives on Integrated Whole-Device Modeling at NERSC

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Integrated Whole-Device Modeling of Tokamak Plasmas

Studies in isolation of elements that describe plasma behavior (plasma heating, MHD equilibria, large scale instabilities, core and edge transport ...)

- **Do not capture interactive nature of physics described in whole-device integrated modeling simulations**
  - ➢ **It is important that we understand effects that result from interactions between various physical processes in tokamak plasmas**

Predictive whole-device modeling helps avoid costly design mistakes

- **Facilitates the optimization and control of experimental scenarios in order to make the most effective use of expensive experiments**
  - ➢ **It is important that we understand effects that result from interactions between various physical processes in tokamak plasmas**

Validation of whole-device modeling simulations and uncertainty quantification studies requires large number of simulations

- **Consequently there is an expanding need for computational facilities required for carrying out whole-device modeling simulations**
  - ➢ **Components of codes now being parallelized**
  - ➢ **Codes used to carry out both interpretive and predictive simulations**

Challenges of Integrated Whole-Device Modeling

Broad range of spatial and time scales

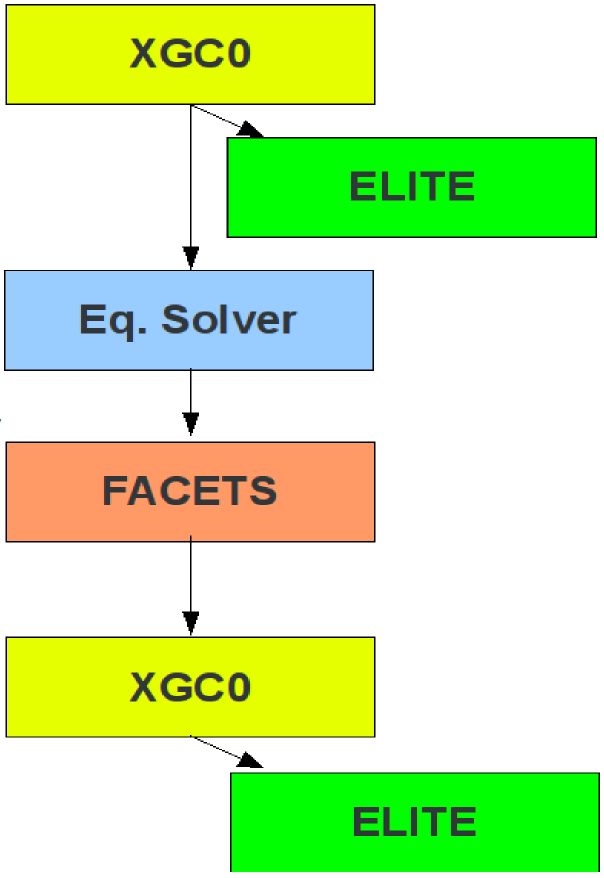
- RF, MHD, equilibrium, transport, atomic physics

Failure-free robust operation required for long pulse simulation

- Order of 3000 sec for ITER
- Development of real time control algorithms within integrated modeling
- Exception handling

SciDAC projects related to integrated modeling

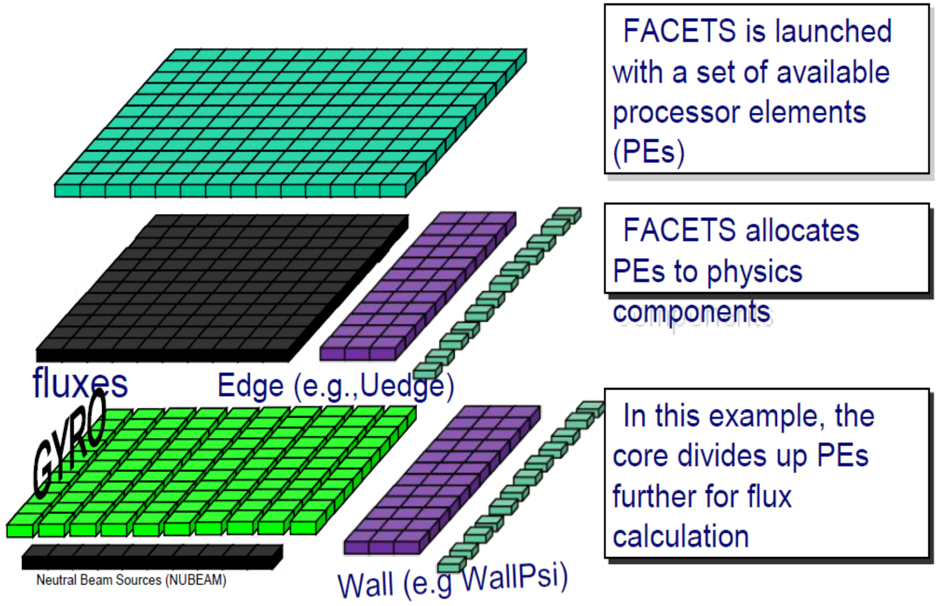
- FACETS, CSWIM, CPES (EPSI)
  - Elements of code coupling frameworks from all three SciDAC projects used in study of effects of transient fluxes on the H-mode pedestal stability
    - Kinetic neoclassical XGC0 code from CPES used to model H-mode pedestal buildup
    - Facets solver has been used for modeling of internal kink modes triggering and transient flux propagation in the plasma core



Experience from SciDAC Projects Relavant to Integrated Whole-Device Modeling

Mechanisms for code coupling have been tested

- Workflows were examined
- Optimization of load balancing
- Restart capabilities
  - Hdf5 based in FACETS
  - PlasmaState in CSWIM
  - Several options for restart in CPES including parallel Adaption IO system (ADIOS)



Load balancing in FACETS: FACETS creates a recursive communicator splitting framework to allow for such distributions/connectivities

Portability and regression tests

Run time control and visualization

- FacetsComposer in FACETS
- EFFIS in CPES

These experiences can be used to improve older whole device integrated modeling codes

Whole-Device Integrated Modeling Codes

FSP (Fusion Simulation Project) as joint FES-ASCR Project

- Two-year planning process but FSP not funded

Codes currently used

- TRANSP/PTRANSP, ONE-TWO, CORSICA, TSC, ASTRA…
- Newer codes with more modern computational techniques and numerical algorithms
  - More limited selection of physics models and synthetic diagnostics and limited user base: TGYRO, TRINITY, ...

Large user base and large number of TRANSP/PTRANSP runs

- Ongoing effort to parallelize, to improve components and advance predictive capability
  - Implementation of Uncertainty Quantification tools
- Focus on understanding evolution of plasma including the evolution of temperatures, current density and toroidal rotation profiles

Recent and continuing advances in TRANSP/PTRANSP

- Significantly increase computational requirements

Coupling of TRANSP/PTRANSP and DAKOTA codes

DAKOTA toolkit developed at Sandia National Laboratory

- **Sensitivity analysis; Uncertainty quantification (UQ); Parameter optimization; and Calibration**

DAKOTA coupled with TRANSP/PTRANSP: Study uncertainties in fusion Q related to different predictions of pedestal shape in ITER

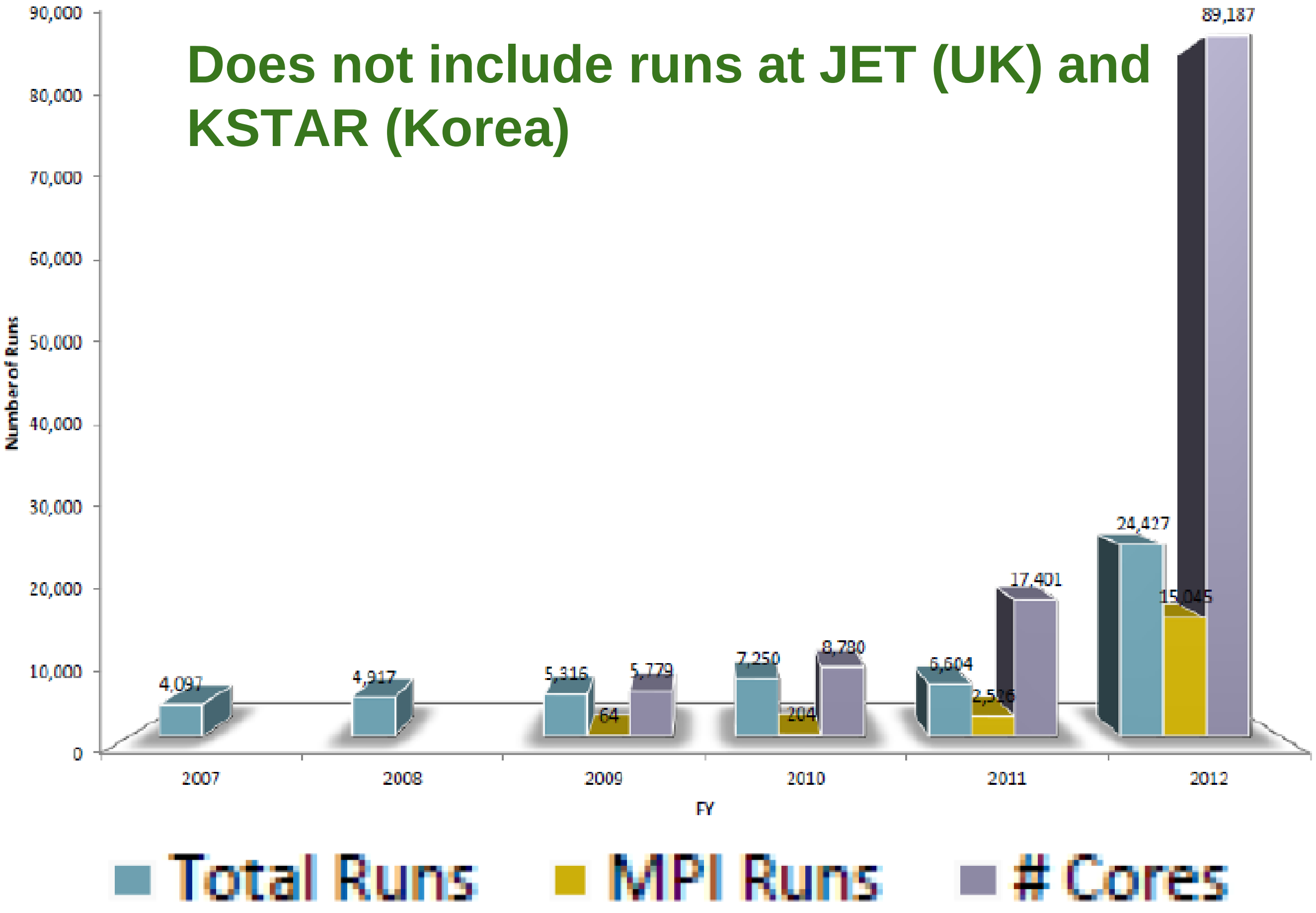
- **Several dozen simulations were performed in automatic way without user interference**
- **Use of DAKOTA framework may result in a tenfold increase of runs even without any increase in the user base**

DAKOTA toolkit can be used for analysis of uncertainties in experimental data

- **Experimental data comes with experimental error bars**
- **Interpretive TRANSP run is a complex multi-parameter problem that can be automated using UQ technique**

Use of DAKOTA for predictive and analysis runs will significantly increase computational requirements in TRANSP/PTRTANSP

Number of TRANSP/PTRANSP Runs per Year



S. Jardin
TRANSP APS meeting
Providence, RI (2012)

- Number of runs has grown exponentially during last three years
- Currently number of runs is limited by computational capabilities at PPPL and ability to analyze the results

TRANSP/PTRANSP Simulaiton in 2017

Level of fidelity of integrated modeling will increase

Selection of various modules, with widely varying computation requirements, for each physics component

- **H-mode pedestal buildup and pedestal stability**
  - **Reduced models for H-mode pedestal**
  - **2D fluid modeling with UEDGE or kinetic modeling with XGC0**
- **Triggering and nonlinear dynamics of internal kink modes**
  - **Reduced models (Kadomtsev, Porcelli, ...)**
  - **Extended MHD simulations with NIMROD or M3D**
- **Heat pulse propagation and turbulence response**
  - **Quasilinear drift-wave models (MMM, TGLF)**
  - **Gyrokinetic simulations (GYRO, XGC1)**
- **ELM dynamics and pedestal response**
  - **Reduced models for ELMs**
  - **Extended MHD simulations of ELMs with neoclassical sources from XGC0**

Use of HPC resources will be based on modules required for the appropriate physics conditions in a particular simulation

TRANSP/PTRANSP Integrated Modeling in 2017

Need dedicated cluster for integrated modeling at NERSC with ability to launch jobs on Hopper and other resources

- **Number of runs expected to triple (75,000 per year) and number of CPU hours for TRANSP runs will increase tenfold**

Some components parallelized and parallelization is continuing

- **Neutral Beam (NUBEAM), RF (TORIC), transport solver (PT_Solver) and anomalous (TGLF) and neoclassical (NEO) models**
  - ➢ **PT_Solver with TGLF will utilize 128-1024 CPU cores**
  - ➢ **NERSC resources can help to resolve the limitation on the computational capability at PPPL**

TRANSP/PTRANSP currently compiled and being tested at NERSC

DAKOTA toolkit can be used with TRANSP/PTRANSP for investigating uncertainties in analysis of experimental data