FACETS: Framework Application for Core-Edge Transport Simulations

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for the
FACETS TEAM

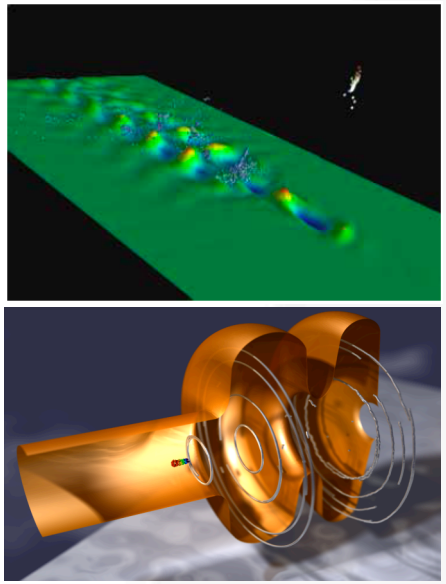
https://www.facetsproject.org/facets

Plasma Science Advanced Computing Institute (PSACI)
Program Advisory Committee
June 8, 2007

framework application: an application designed to allow a series of computations with ever increasing fidelity and, therefore, to include successively more sophisticated models, in particular of each of the aspects of a fusion confinement device.

In-reach:
Fang (Cherry) Liu, Bramley/IU, Dist components
Mahmood Miah, Jardin/PPPL, MHD Eq.

Old news:
Plasma 2010



Self-consistent SRF

Argonne NATIONAL LABORATORY
Colorado State University
OAK RIDGE National Laboratory
ParaTools
PPPL PRINCETON PLASMA PHYSICS LABORATORY
UCSD
GA
LBNL
IU
MIT
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SciDAC Scientific Discovery through Advanced Computing

FACETS Background

- Part of SciDAC portfolio of the Office of Fusion Energy Sciences
- Proposed in April, 2006
- Funded January 1, 2007
- Multi-institutional main project: Tech-X (Physics, CS/AM); LLNL (Physics, CS/AM); PPPL (Physics); ANL (CS/AM); UCSD (Physics); CSU (AM); ORNL (CS, perf); ParaTools (CS, perf)
- Appended SAP: GA, ORNL
- Advisory: Columbia; LBNL; IU; MIT; NYU; Lodestar
- In collaboration with the CETs: TOPS, TASCS, VACET

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FACETS Goals

- Provide coupled core-edge-wall computational capability to the fusion community
  - at various levels of detail
  - serial and **parallel**
- Make impact on ITER and existing/new machines
  - Device selection (heating)
  - Scenario development
  - Operation
  - Analysis
- Maximal reuse of existing (legacy) software
- Take advantage of petascale computing facilities: **a priori parallel**
- Have FACETS broadly installed and in use (move beyond "users = developers")

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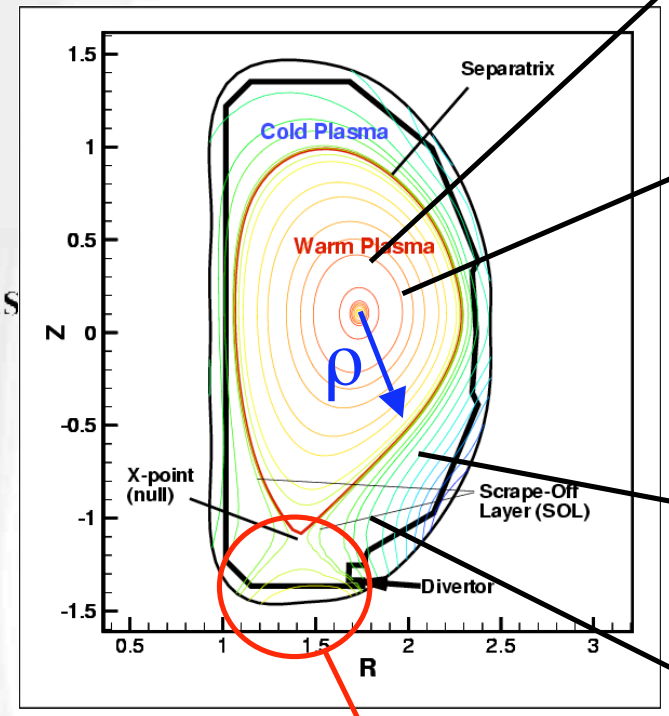
Core-edge-wall integration involves multiple dimensionalities



Closed field lines: slow perpendicular + fast parallel transport
⇒Quantities 1D
Hot plasma
⇒Collisionless, no significant atomic physics (except beams)

Open field lines: so parallel transport must balance perpendicular
⇒Quantities are 2D
Cool plasma
⇒Collisional, atomic physics is important

Plasma-wall interaction is 2D

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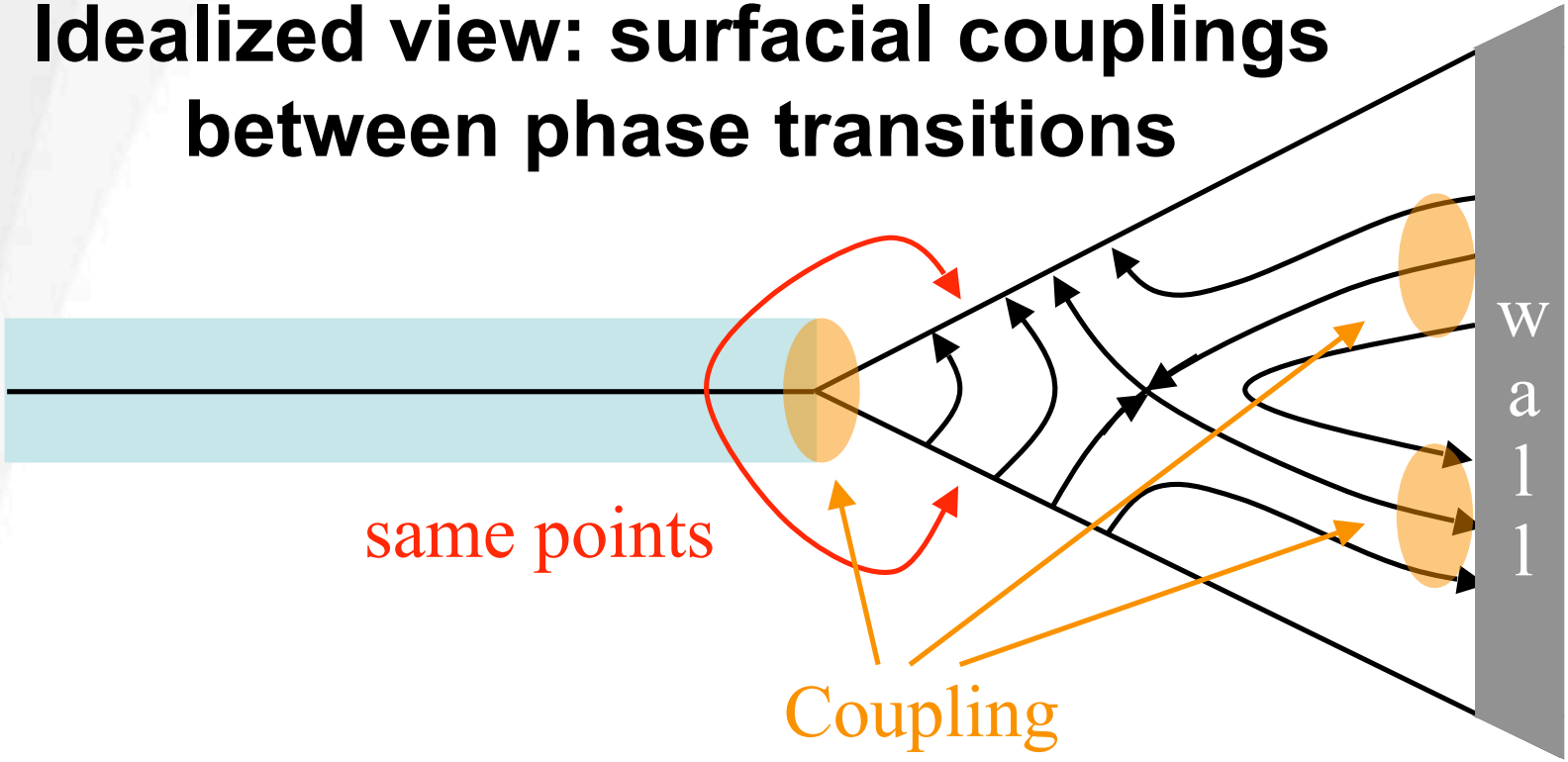
Idealized view: surfacial couplings between phase transitions



- Core is a collisionless, 1D transport system with local, only-cross-surface fluxes
- Edge is a collisional, 2D transport system
- Wall: beginning of a particle trapping matrix

Surfacial couplings

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FACETS: distinct part of the SciDAC portfolio

- Single-physics SciDACs
  - RF
  - CEMM
  - GKT
    - particle
    - continuum
  - Energetic particles
- FIIs (proto-FSP's)
  - SWIM (RF + MHD: volumetric; diagnostic → mutual; file transfer)
  - CPES (Edge + MHD; volumetric; diagnostic; data flow)
  - FACETS (Core + Edge + Wall; surfacial; implicit; message passing)

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Management: FACETS approach via teams

Framework, Components, Research, Engineering

- Framework (Cary): Tech-X, LLNL, ParaTools, all
  - main(…)
  - generic components, including core driver
- Core sources (McCune): PPPL, Tech-X
- Edge (Rognlien): LLNL, ANL, ORNL (perf)
- Wall (Pigarov): UCSD, Tech-X
- Embedded turbulence SAP (Fahey, Candy): ORNL, GA
- Algorithms (McInnes): ANL
- Performance (Kuehn): ORNL, ParaTools
- Coupling (Estep): LLNL, CSU, ANL
- Infrastructure (Wade-Stein):
  - build, regression, repo, doc system)
- V&V (early, but starting)

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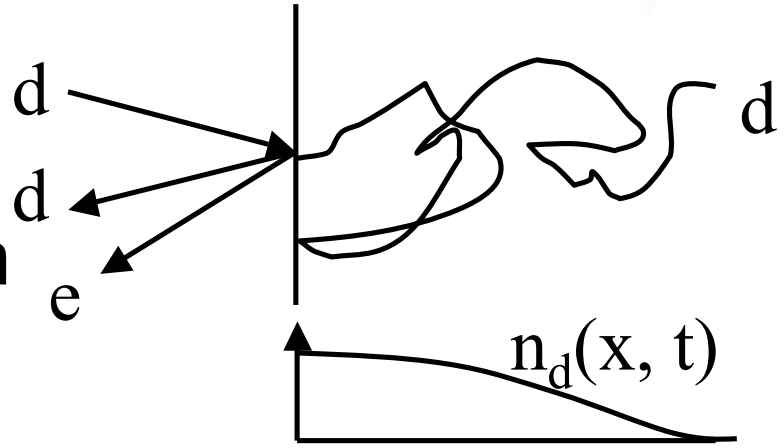
Surfacial coupling: scientific basis and numerical issues

Idealized view common for edge-wall interaction



- Edge-plasma/wall analogous to atmosphere/ocean
- Wall acts as a boundary condition for edge plasma
  - Sputtering
  - Secondary electron/ion emission
- Refinement needs wall model to account for internal state
  - Wall has embedded H/D density
  - H/D diffuses in metal, both in and out
  - Impact of electrons, ions, and neutrals can cause release of embedded H/D

Valid basis for independent components

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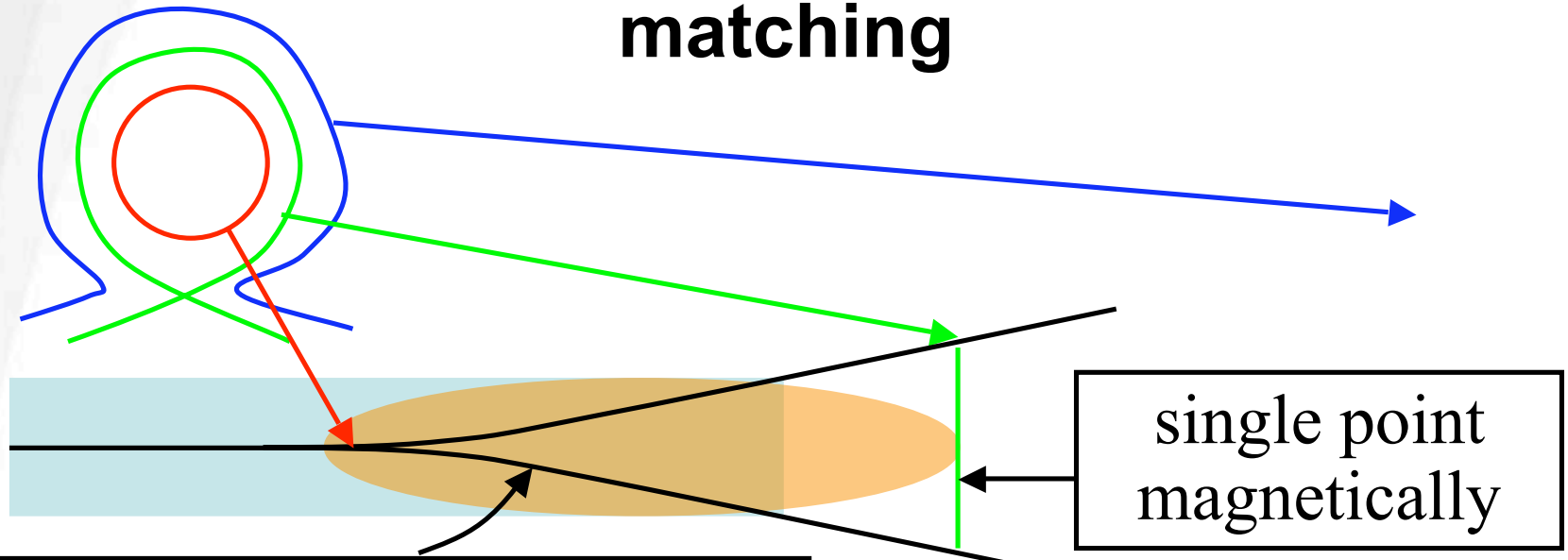
Justification for core-edge coupling needs matching



- Sufficiently inside the last closed flux surface, 2D effects are small
- Moving out, plasma becomes more collisional
- Both approximations exist - allows matching

Basis requires matching theory

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Relaxation times very different

- Core energy relaxation time (energy confinement time)
  - ~ s
  - Gradient relaxation means local relaxation very fast
- Edge relaxation times very short
  - Collide into scrape-off layer
  - Stream to walls
- Implicit solver needed for coupling the two systems

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How do we choose among the ways to solve these systems?

- Core gives $\mathbf{F_c}(Q_e, t+\Delta t)$
- Edge gives $\mathbf{Q_e}(F_c, t+\Delta t)$
- Which? (Parametric dependence on $t+\Delta t$ dropped)
  - $\mathbf{Q_e}(\mathbf{F_c}(Q_e)) - Q_e = 0$ (edge dictator)
  - $\mathbf{F_c}(\mathbf{Q_e}(F_c)) - F_c = 0$ (core dictator)
  - Coupled (component democracy)
    - $\mathbf{F_c}(Q_e) = F_c$
    - $\mathbf{Q_e}(F_c) = Q_e$
  - Global solver for all residuals (residual democracy)

Which way to solve?

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Project goals

- Overall goals
- Year 1: Ad hoc coupling of core and edge
- Year 2: Core and edge coupled within framework
- Year 3: Wall and equilibrium coupled in with core and edge
- Years 4 & 5: Core turbulence added into framework

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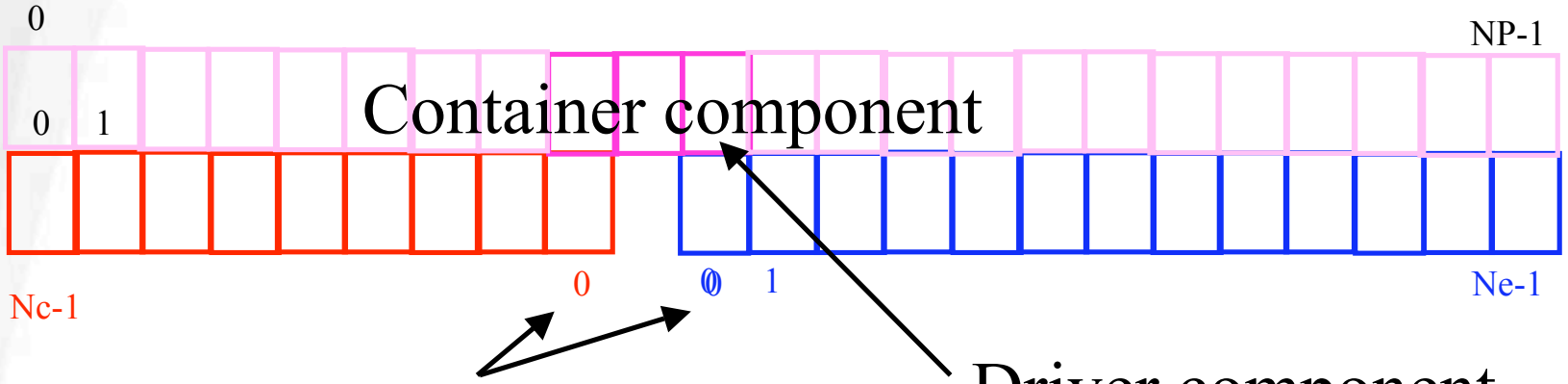
Coupling of two parallel components uses server component concept



- The coupler communicates through the server component running on rank 0 of sub-components (red and blue in diagram).
- Server listens for calls from driver (purple) and redirects them to the appropriate ranks in its communicator set.

With fast Newton solve, high degree of parallelism through concurrency

Independent components through one interface

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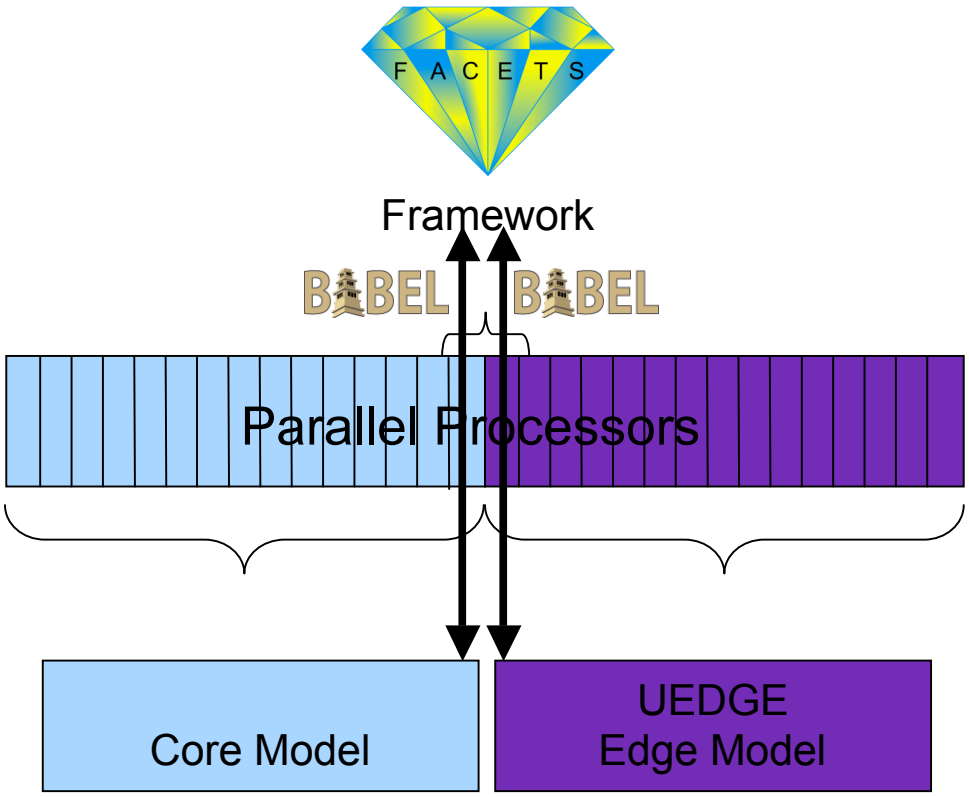
Interlanguage accomplished through Babel



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Generic component interface

- Librarify so can run entirely through methods (functions, subroutines), namespacing
- Create driver to use library calls
- Supply input file
- readParams() (Reads input file)
- setComm() (if parallel)
- initialize() (allocated memory, set initial values) OR startServer()
- setData() (various, see next slide)
- getData() (various, see next slide, gets appropriate to tentative new state)
- advance(double t)
- acceptState()
- dump()
- restore() (read restart file)

LATER

- getRankOfInterface()

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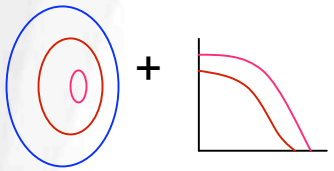
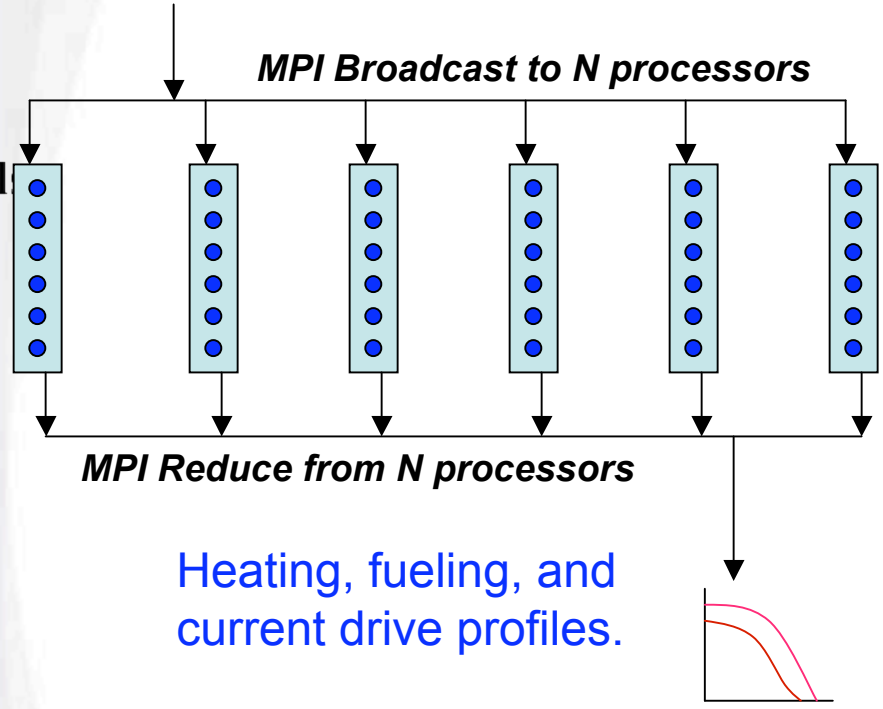
Interface walked through for implicit and explicit coupling

CORE Sources (McCune)
PPPL NUBEAM in FACETS



Core plasma MHD equilibrium, temperatures and densities.



Heating, fueling, and current drive profiles.

Progress Since 1-Jan-2007:

- MPI NUBEAM running on small Linux Clusters.
- Tech-X "autotools" NUBEAM version builds and runs.
- Serial NUBEAM verified on:
  - SGI (intel fortran 9.0)
  - Linux (LF fortran 32 or 64)
- N to M mapping of MPI-distributed particle state files.

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Fast ion deposition, orbiting, and losses computed over N processing elements. Each PE handles (1/N) of the Monte Carlo ions.

Progress and plans for edge simulation team

- Completed tasks
  - script to automatically convert any UEDGE to full F90 source
  - utilize Forthon & F90 UEDGE to build portable Python-UEDGE
  - PyUEDGE & test cases to algorithm & performance teams
  - begin developing interface wrapper to core model

Near-team tasks (six months)

  - complete interface wrapper to core and wall models
  - aid algorithm group in assessing solver enhancements
  - aid performance group in identifying/fixing bottlenecks
  - re-establish UEDGE parallel capability with 2D domain decomp

- One-year tasks
  - implement & test initial coupling algorithms with core & wall
  - aid algorithm/perform. teams to assess parallelization/coupling

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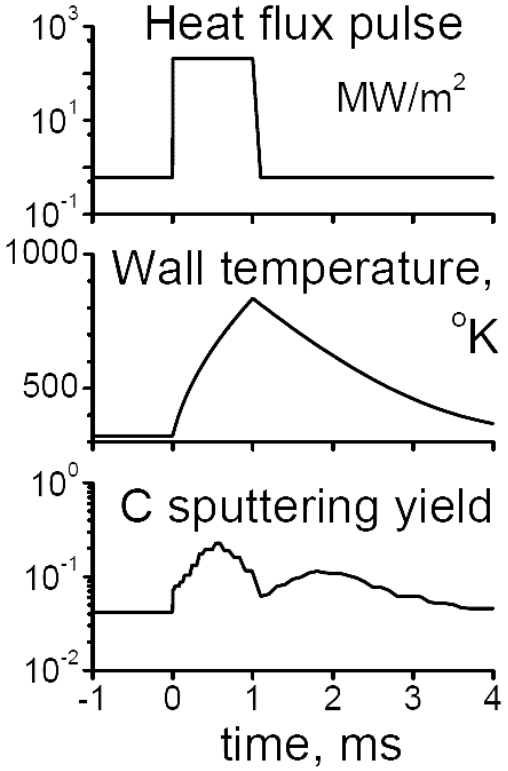
Plasma-wall interaction

- We developed **WALLPSI** which is the **0-D two-point (surface and bulk) "wall" model** to calculate: (i) wall temperature, (ii) trapped and mobile hydrogen concentrations in the wall, (iii) erosion rates.

- Current work on WALLPSI includes:
  (i) benchmarking the code by solving some standard physics problems,
  (ii) incorporation of extensive data on various elementary processes describing the hydrogen kinetics in wall and on surface,
  (iii) coupling WALLPSI and UEDGE.

- The development of the **1-D "wall" model** has started.

- Simple **1-D plasma transport model** is under development and it will be coupled to 1-D "wall" model for further studies of basic physics of plasma-wall interactions and plasma stability analysis.



Results of WALLPSI calculation (0D) of wall temperature and effective erosion rate on the response to the heat and particle plasma pulse ("ELM"). As seen, there is strong coupling of temperature and erosion.

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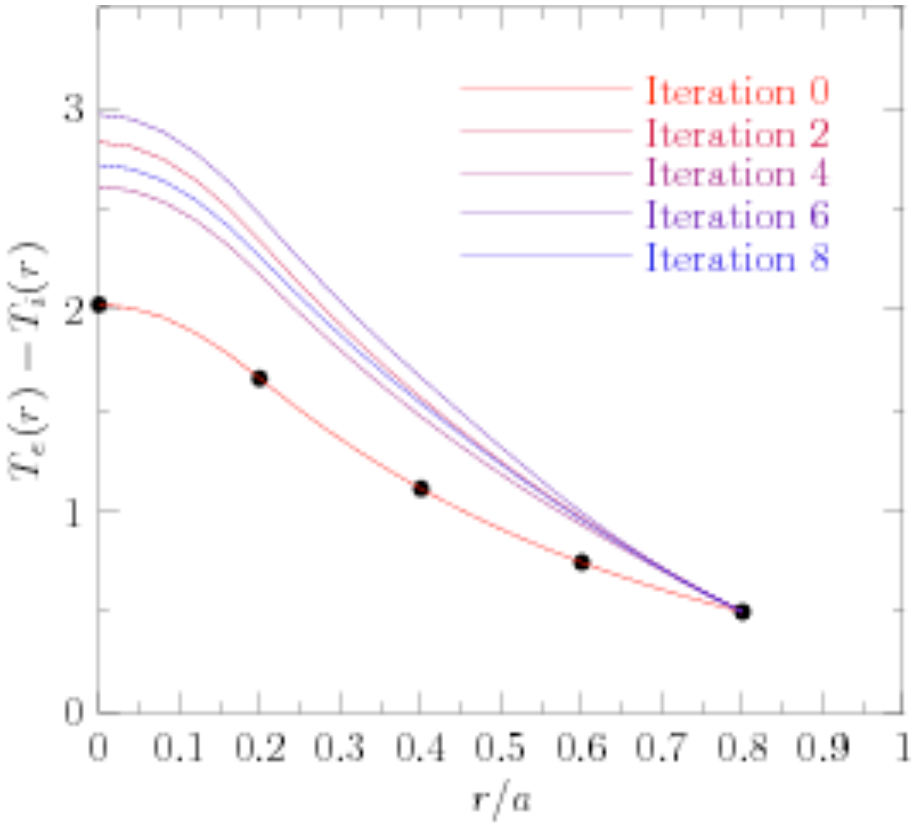
Out-year efforts: embedded, higher-fidelity

- Embedded SAP: callable GYRO
  - Using fixed-profile GYRO gyrokinetic simulations, we
    - perform transport-timescale simulations
    - adjust profiles to achieve steady-state power balance
  - Find the unique plasma profile for which losses due to core turbulence are balanced by sources
- Higher-fidelity edge models
  - TEMPEST
  - XGC{0,1}



Steady-state profiles using 4 instances of GYRO with radii r=(0.2, 0.4, 0.6, 0.8) and 16 processes for each instance

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Coupling Team Activities

- Organization of activities and information gathering
  - Series of presentations covering the algorithms of the UEDGE 2D edge code, the coupling of UEDGE to core transport, and mathematical tools for measuring the goodness of coupling algorithms
- Development and initial analysis of simplified test models
  - The test models are targets for algorithm development and instrumentation
  - the first model is a coupled point model for core and edge transport and the second is a set of coupled 1-dimensional ODEs describing profiles in the core, central edge, and divertor legs
  - Initial analysis of the test models using applied mathematics tools has begun
- Current activities
  - Explore the self-consistent coupling of turbulence and transport
  - Development of testbed code for mathematical analysis of core-edge coupling and testing of new coupling strategies
  - Elucidating the organizing principles of coupling and parallel coupling

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Progress in performance

- Demonstrate TAU performance instrumentation, measurement, and analysis tools with FACETS
  - Python and C++ FACETS framework
- Design FACETS⇔TAU performance interface
- Design global performance access support
- Integration of performance support in components
  - NUBEAM
    - Lahey Fortran under Linux x86_64
  - UEDGE
  - WALL
- Creation of FACETS performance database
- Review of software licensing and recommendation of the modified Eclipse license
- Working with SciDAC PERI group with Shirley Moore, UTK

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Much of the basic engineering infrastructure in place

- Layering
- Revision control: subversion
- Build system: autotools
- Communication: conf. calls, 2 meetings/year
- Issue tracking: TRAC.
- Testing: See next page
- Versioning/release management: protocol in use elsewhere
- Documentation: only API (doxygen)
- Interface design: some

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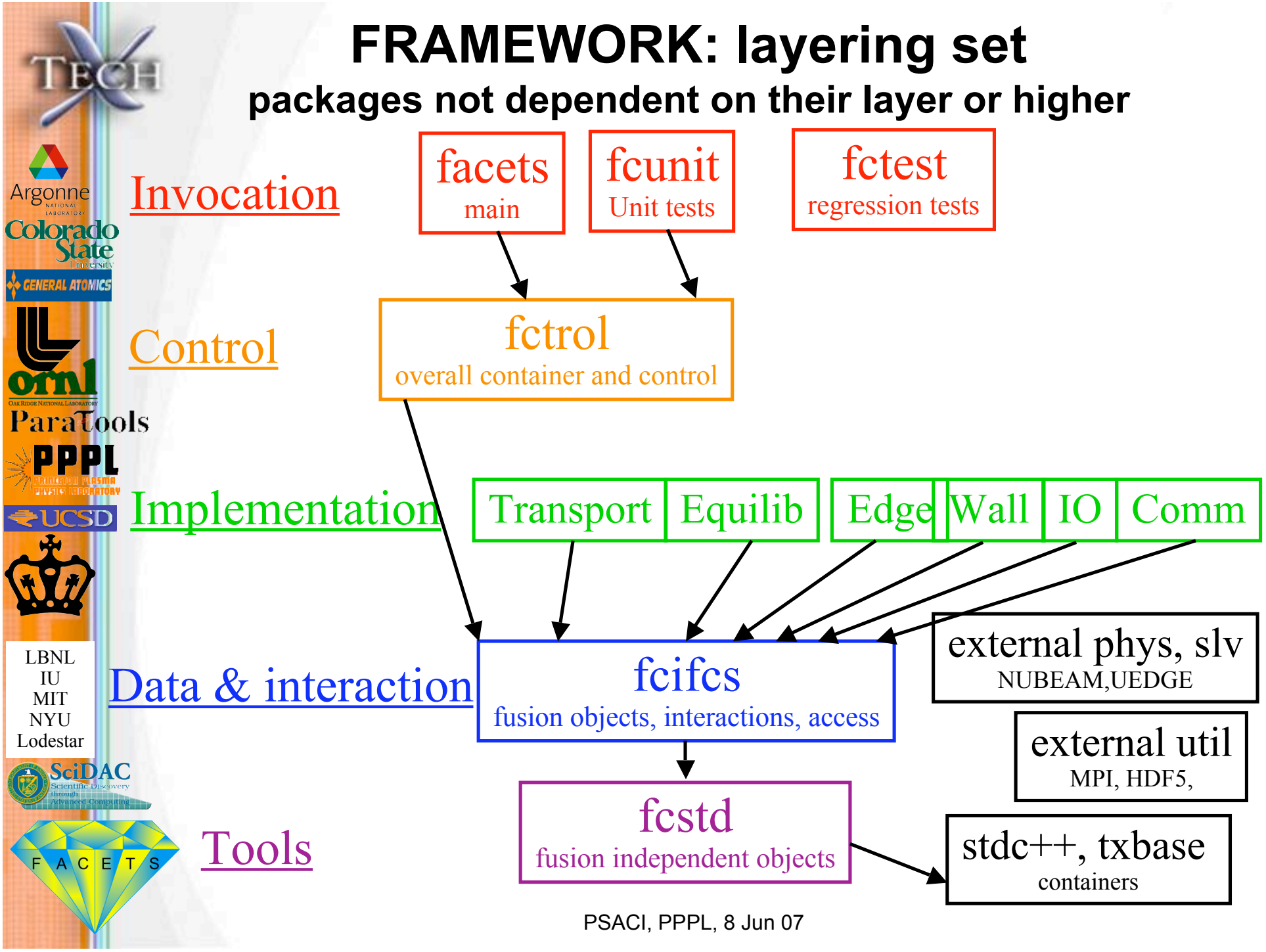
FRAMEWORK: layering set

packages not dependent on their layer or higher



Who dreads reading the morning email?

```
Subject: [Facets-internal] FACETS nightly test results (3 FAILURES)

facets test results: FAILED
        Serial configure passed.
        Serial build passed.
        Parallel build passed.
        Unit tests passed.
        ==> Serial distcheck failed.
        ==> Parallel distcheck failed.
        ==> Integrity check failed.
Output from unit tests...
        fcany-parallel: PASSED = 18. FAILED = 0
        fcbox-parallel: PASSED = 89. FAILED = 0
        fcboxcmp-parallel: PASSED = 2. FAILED = 0
        fcboxneigh-parallel: PASSED = 16. FAILED = 0
        <snip>
        fcdecomp-serial: PASSED = 6189. FAILED = 0
        fcindexer-serial: PASSED = 596. FAILED = 0
        fcsequencer-serial: PASSED = 760. FAILED = 0
        fctypelist-serial: PASSED = 4. FAILED = 0
layercheck.pl finds no layering violations
reform.sh finds formatting violations in the following files:
     fcifcs/FcCutCellGrid.h
     fctrol/FcSimulation.cpp
     facets/facets.cxx
reform.sh finds no non-virtual destructors
integcheck.sh finds no Doxygen errors
```

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Risk evaluation: simplest, well-studied components may need rethinking as we move to the petascale

- Equilibrium depends on core currents, potentially halo currents
- Equilibrium provides geometry for core and edge
- In a parallel code, how do these collocated components communicate?
  - Single equilibrium solver answering requests from 1000 other ranks?
- If parallel, to minimize communication, how?
  - Solution natural in R-Z
  - Core wants per flux surface
  - Edge has different domain decomposition

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FACETS has started outreach program

- Want user set > developer set
- Delicate balance on first delivery
  - too soon wastes time
  - too late delays input gathering
- Established communications with modelers at PPPL, MIT, GA, LLNL
- First release before year end for input gathering

Advisory committee

Bill Nevins, Chuck Kessel, Dennis Whyte,
Lori Diachin, Andrew Siegel, Jim Drake

Team meetings

Nov 30-Dec 1, 2006
Aug. 9-10, 2007

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- Surfacial, implicit coupling via message passing
- First cut at organization complete
- Framework coming together
  - Infrastructure
  - Superstructure
- Components (core sources, edge, wall) coming together
- Embedding of CS/AM partners has occurred.
- Research proceeding.
- Engineering and communication infrastructure in place
- Outreach activities started

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