Proposed Software R&D in Support of the Fusion Simulation Program (FSP)

Prepared by D. McCune

Presented by M. Zarnstorff

FSP Kickoff Meeting, PPPL

July 16, 2009

Key FSP Needs Addressable by Proposed FSP-0 R&D

- Practical near term deliverables based on specific user requirements.
- Vehicle for validation, leveraging existing coupling to the experimental data.
- Risk Mitigation: deliverables built on known, well understood software platforms to help mitigate risk for proposed FSP plan.
- Path to new capabilities: leverage major past investments in the best software.

  -- no need for FSP to “start from scratch.”

  -- new physics components tested using FSP-0 drivers.

FSP Software Should Leverage Existing Capability

- A conceptual organization of the software suite:
  - FSP-0: workstation and cluster applications; significant enhancement of legacy code base (PTRANSP, ONETWO,…):
    - Run on workstations, clusters, Ncpu <~ 100s.
  - FSP-1: midrange supercomputing applications; further development of SciDAC Proto-FSP code base (SWIM, FACETs, CPES):
    - e.g., currently run on capacity machines, Ncpu ~ 1000s.
  - FSP-2: high end supercomputing applications; development of integrated advanced modules from most aggressive DNS codes
    - e.g., run at peta/exascale, Ncpu ~ 100000s.

All FSP Levels Important

- Unique FSP-2 applications may be possible through advent of peta/exascale computing, but…
- The vast majority of users/customers live at FSP-0. Present focus of validation.
- Success of FSP critically depends on maintaining confidence of users/customer base
- Acceptance of FSP-1 and FSP-2 capability will involve benchmarking against FSP-0.
- FSP-0 results will be well known & validated.

FSP-0 Development is a Key Element of the FSP

- Most easily accessible test bed for FSP component physics at all levels;
- Most mature user support, production and data management systems;
- Established validation track record;
- Independent development and validation of FSP-1 and FSP-2 will require several more years of work.

User Base

FY-2009 estimates	FSP-0 (legacy)	FSP-1 (SciDAC)	FSP-2 (TBD)
Users making runs*	~100	<10	0
Users of run results*	100s	<10	0
Production* runs/year (user)	~5000	<10	0
Test runs/year (developer)	100s	100s	0

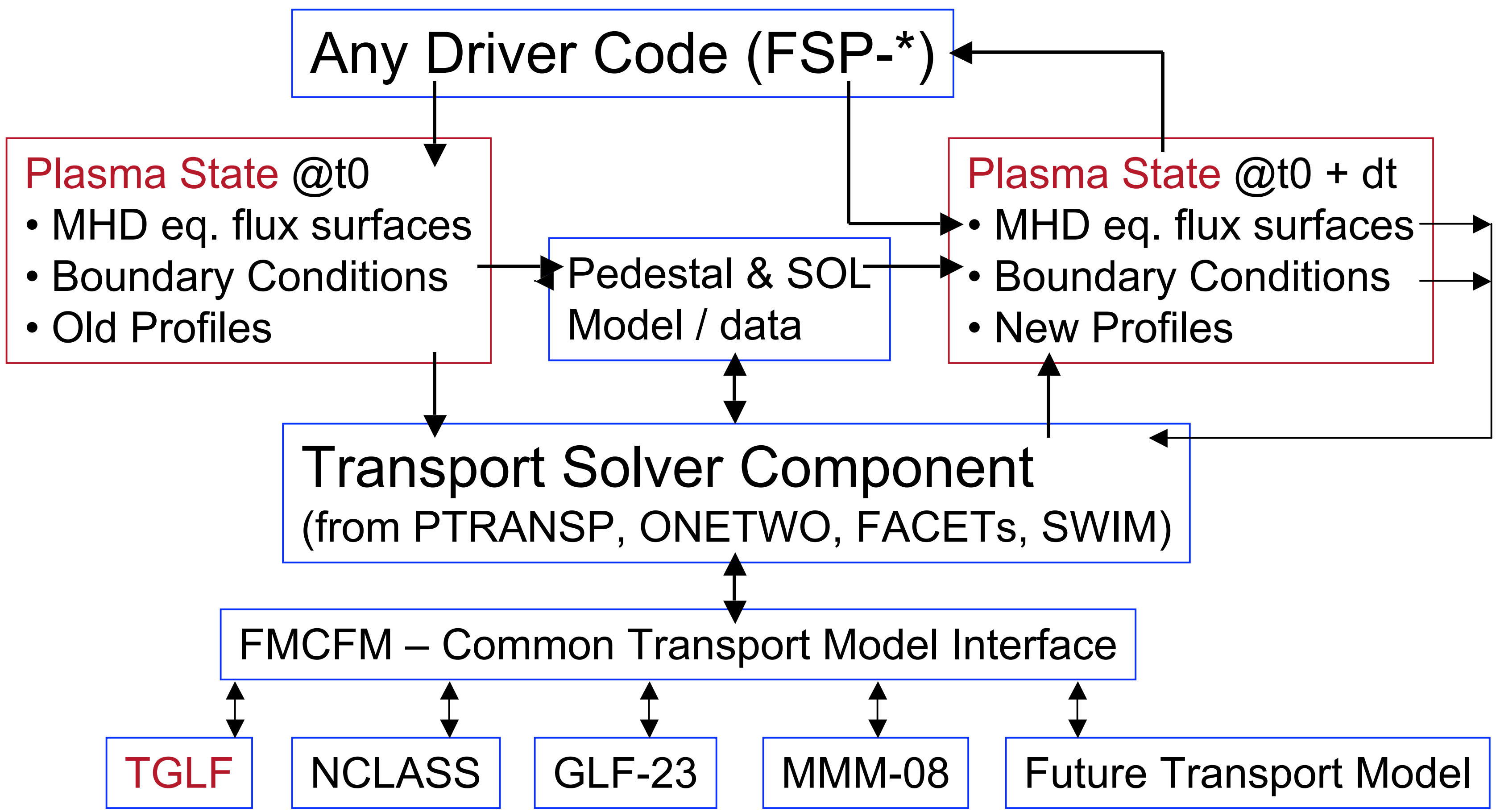
*For research applications – not code development or testing

Specific User Requirements for Tokamak Modeling (e.g. ITER)

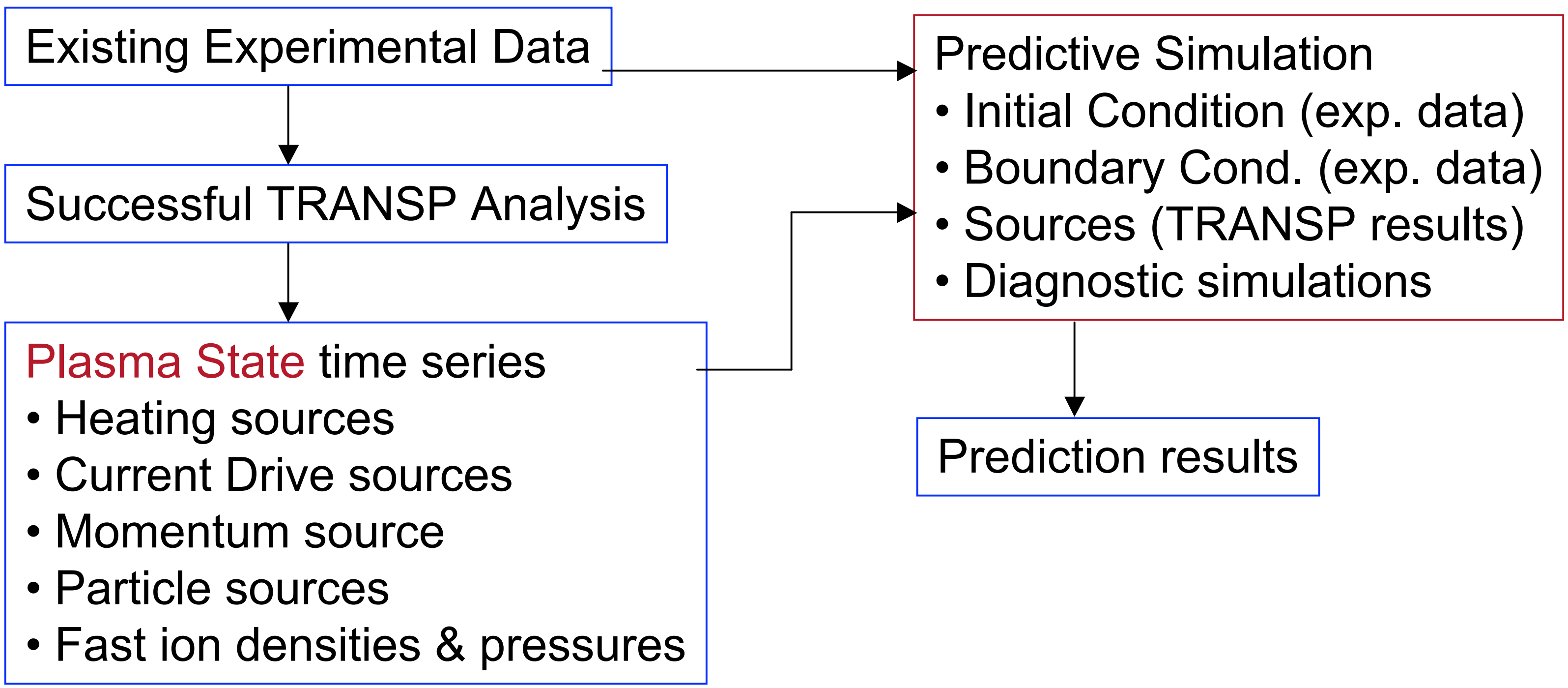
- Flexible, well validated, efficient, robust predictor of core profile evolution: Te, Ti, density, toroidal angular momentum.
  - Cluster level MPI coupling to TGLF
  - Flexibility to combine/compare predictive models:
    - Transport; pedestal boundary condition; equilibrium; MHD activity etc.
- Free boundary equilibrium
- Clear validation procedure– coupling to experimental data and analysis results.

Attainable Using FSP-0 R&D

Component development now in FSP-0, eventual use in FSP-1,2.



FSP-0 Validation Framework



Results directly comparable to experimental data, testing predictive models.

Well Defined, Achievable Tasks

- Plasma State interfaces in Pedestal boundary condition models.
- Plasma State interfaces in Solvers.
- Maturation of FMCFM:
  - Coupling all predictive transport models.
- Cluster level MPI parallelization of system.
- Initial testing and verification.
- Validation through research comparisons and applications.

Experienced R&D Team

- General Atomics (Lang Lao, H. St. John)
  - TGLF, GCNMP solver, EPED1 pedestal height model (Snyder, 2008 APS).
- Lehigh University (A. Kritz, G. Bateman)
  - FMCFM, PTRANSP Solver, Pedestal module.
- PPPL (D. McCune, TRANSP team)
  - PTRANSP, Plasma State, validation system.
- Tech-X Corp. (J. Cary, A. Pletzer)
  - FMCFM, FACETs core solver

Resources

- PTRANSP R&D funding expected to end in FY-2009
  - Approx. $600k/year.
- Recommend continuation as FSP-0 R&D project within the FSP Project Definition/Planning activity
  - Focus on standardizing interfaces, addressing needs, parallelization
  - Team of GA, Lehigh U., PPPL, Tech-X Corp.
- Helps address concerns about near-term deliverables and risk mitigation.
- Lays groundwork for full FSP.
- Provides continuity in producing technical R&D needed for FSP.
  - Especially important with expected end of PTRANSP R&D activity

Track Record: Effective PTRANSP/SciDAC Collaboration

- Plasma State developed by SWIM, FACETs, and TRANSP/PTRANSP.
  - Any TRANSP archive time slice extractable as a Plasma State;
  - Such Plasma States applied to facilitate verification e.g. TORIC vs. AORSA ICRF results in ITER simulations, by SWIM.
- NUBEAM component adapted to Plasma State data exchange.
  - Version shared by TRANSP, SWIM, FACETs.

Mutual Benefits

- NUBEAM component MPI-parallelization for SWIM & FACETs also running now in TRANSP/PTRANSP.
  - FSP prototypes, tested to Ncpu = ~1000;
  - Now in routine (P)TRANSP production use
    - Modest cluster use, typically Ncpu = 4-16;
    - Still enough for much improved simulation statistics.
- TRANSP testing paved way to SciDAC use.
- Example of effective collaboration between PTRANSP and SciDAC FSP prototypes.

Strong FSP-0-Type Coupling to Tokamak Research Program -- Examples

- MDS+ based data preparation for TRANSP; source for Plasma States.
- Numerous tools for extraction of TRANSP and PTRANSP results data.
  - Inputs to first principles physics models:
    - MHD Stability
    - Turbulent transport
    - Fast Ions, TAE modes, etc.
    - Wave particle interactions, high resolution RF.

Summary

- FSP-0 will leverage major past investments and then build-on and enhance the capabilities of those legacy codes (e.g., PTRANSP) that are a resource and benefit to FSP generally.
- Continue & expand beneficial collaborations between PTRANSP and the SciDAC & Proto-FSP developers. Nurture them into the the FSP-0 and FSP-1 activities.
- Maintain continuity at FSP-0 level for continued verification, validation, and production of new physics results.
- This proposed R&D effort, within the FSP Project Definition/Planning activity, will build on the best capabilities developed to date, leverage the recognition and trust from the established large user base, and generally help mitigate risk via early delivery of useful products -- all to demonstrate the attractiveness and viability of the FSP activities.