FSP Framework Design

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For the FSP Frameworks Team

Mission
Team
Communication
Terminology
Breaking up the work
Sequencing the work
Risks
End products

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Fusion community is increasingly facing integrated computation but lacks the tools

- Core-edge modeling currently consists of
  - Core
    - Fix value of temperatures and densities close to edge
    - Take sources of particles and density from analysis code (e.g., NUBEAM/TRANSP)
    - Compute profiles using some model for fluxes
  - Edge
    - Compute outgoing power at some flux surface from integrated sources
    - Compute edge (2D) profiles from using 2D transport (from 1^{st} principles code or interpreted diffusivities)
- Problems
  - Not self-consistent: both models rely on sources from interpretation
  - Requires human intervention (data values on input files)
  - Can fail to include real physical effects (energy storage rate)

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The frameworks effort will facilitate the complete modeling process

requires

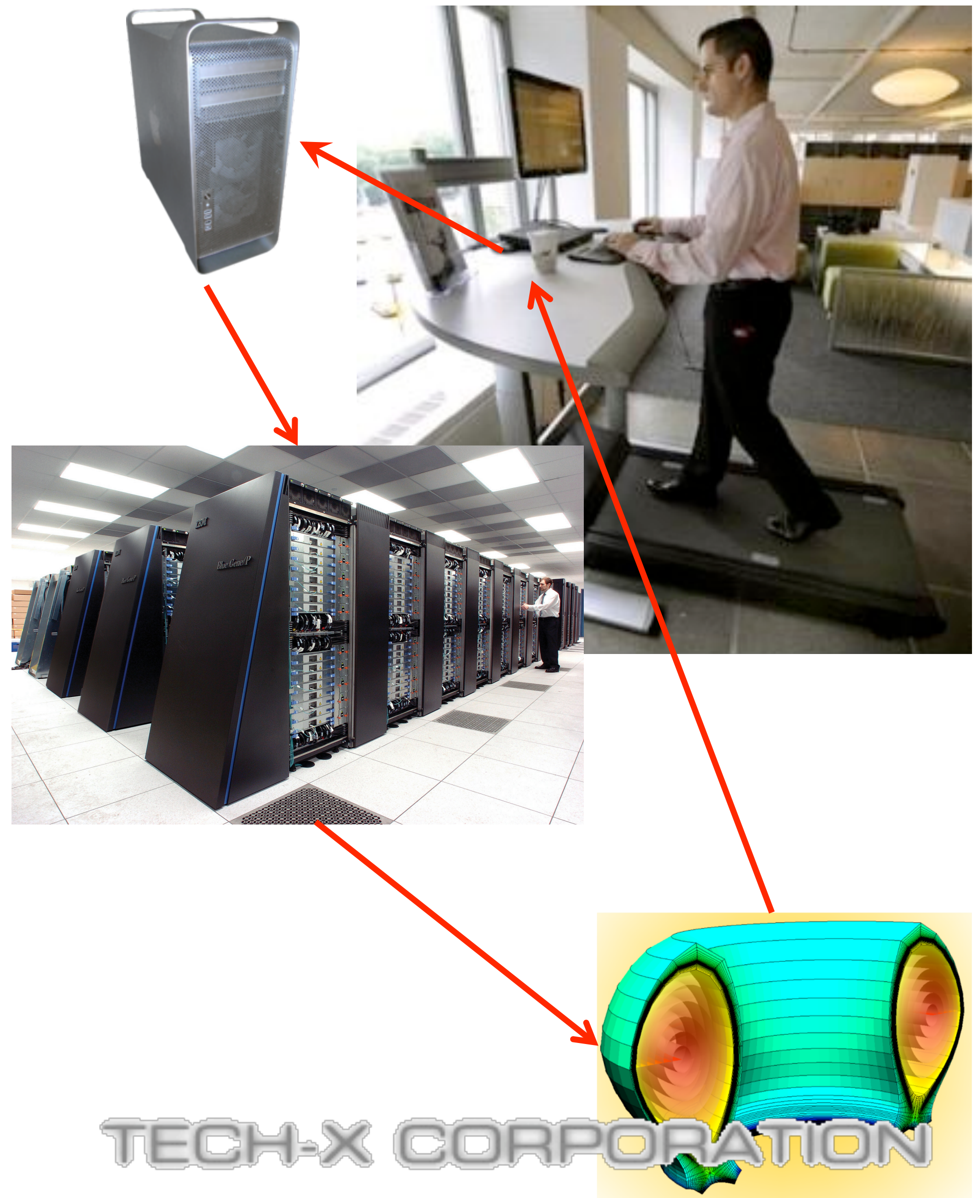
- Needs assessment
- Physics composition
- Workflow
- Software engineering

provides

- Transparency
- Standards

reduces

- Redundancy



Framework team mission

- The Frameworks Planning Group (of the Fusion Simulation Project/Program) has the mission of designing the FSP Composition Software Suite for multiphysics, integrated computations and support of the same to meet the research goals of the Office of Fusion Energy Sciences
- Meeting this mission will require:
  - Working with the Science Drivers team to determine highest priority computations and the requirements those impose on the framework software suite
  - Development of an understanding of the needs of users and how they work: the entire flow from research problem conception to publishable physics result
  - Developing initial designs and prototyping them to see if they meet user needs.
  - Developing rigorous software engineering practices that ensure software reliability and usability.
  - Developing software distribution mechanisms for dissemination to all target platforms and institutions.
  - Developing standards for verification.
  - Developing standards for data management

The framework team combines physics, app math, and comp sci expertise

- JR Cary, U. Colo and Tech-X, theoretical and computational physicist, publish in CS/AM
  - Prof. Physics and CEO, Tech-X (65 employees, 2/3 PhD, 6 SciDACs)
- RH Cohen, LLNL, Theoretical and computational plasma physicist
  - Former FES theory group leader
- B Norris, ANL, Computer Scientist
  - ANL PI for the Performance Engineering Research Institute SciDAC project
- B Van Straalen, LBL, Computer Scientist
  - Lead architect, APDEC

Framework team have assigned primary responsibilities

- JR Cary
  - Management
  - Physics composition
- RH Cohen
  - Science drivers liaison
  - Identification of users and their needs
- B Norris
  - Processes and engineering
- B Van Straalen
  - Work flow and interaction with non physics components and services
  - Interaction with validation

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Established communication methods for community and team

- Team mailing list
  - fspfrmwrkpi@ice.txcorp.com
- Public mailing list
  - fspfrmwrkplan@ice.txcorp.com
- Wiki
  - https://ice.txcorp.com/trac/fspfrmwrkplan
- Webex
  - Interactive presentations as needed

Our goal is to maximize openness and deal with the difficult issues of collaboration early

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Terminology is particularly challenging

- There are no broadly accepted definitions of
  - component
  - service
  - framework
  - workflow
  - (during public input, 48 emails Sep 1-14 discussing software terminology)
- But we have to break up the work
  - By area
  - Assessment
  - Decision

The FSP Composition Software Suite must contain

- **Physics composition** (driven 1st by science)
  - Physics component composition
  - Infrastructure
- **Workflow** (driven 1st by modelers)
  - Problem setup
  - Visualization
  - Data management
- **Development processes** (driven 1st by developers)
  - Verification: standards, methods, transition
  - Documentation
  - Distribution
- **Determined by Stakeholder Needs**
  - Science drivers
  - Users
  - DOE

Work plan for the definition phase contains 9 basic elements:

- Gather information (from the Science Drivers team) on the highest priority research areas and defining use cases from those.
- Gather information on existing software and practices that have been developed either inside or outside of the fusion community - including information on gaps: missing software for greater robustness or for workflows.
- Identify the potential users.
- Gather information from potential users (including Validation Analysts) on the tools and methods they need (by priority) for their work.
- Design prototypes
- Prototyping all aspects of the framework software suite, including build systems, workflows, utilities, and computational framework, data management, ...
- Review
- Complete initial design of all elements of the framework software suite.
- Estimate the costs of providing all elements of the framework software suite for an initial period

Planning stage (next two years)

	Stakeholder	Physics	Workflow	Processes
Q1	Initialization: set up communication, set mission			
Q2	Id stakeholders, workshop on science drivers	Id components needed to address science drivers	Id users in fusion and outside, set up workshop	Id successful projects in fusion and outside, set up workshop.
Q3	Design physics use cases in detail – what must be coupled	Assess components in terms of data flow, computational time, …	Assess status of workflows; workshop, document: what exists, how to test.	Assess status of processes; workshop; document: what exists, how to test
Q4	Engage with other teams; hold stakeholder review	Set component standards (I/O), develop model physics components	Assess status of validation process and data management	Prototype component engineering, incl. I/O and library invocation
Q5		Prototype coupling mechanisms.	Prototype workflow engines for validation, discovery	Determine effort to bring components to engineered state
Q6	Hold stakeholder review	Review findings, initial document	Review findings, initial document	Review findings
Q7		Create WBS for Physics engine	Create WBS for Workflow	Create WBS for processes
Q8	Contingency and review			

Neither rigid nor cross-coordinated

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07/09 thru 09/09: Initialization

- Communications set up
  - Wiki
  - Mailman list
- Presentations from the protoFSPs
  - Boulder, Aug 6-7
  - Begin on assessment questions
- Multiple conference calls of the framework team
- Multiple conference calls for public input
  - Aug 21: Mission, timetable
  - Aug 25: Discussion of CD process
  - Sep 4: Interactions with the Science Drivers and Validation groups
  - Sep 11: Timeline for framework design, WBS

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Q2: Identify stakeholders, start analysis of science drivers (RHC)

- Identification
  - Obtain initial list of science drivers
  - Identify users (modelers, experimentalists, designers)
  - Identify experimentalists for validation prototyping
- Convert first science drivers to use cases
  - Develop set of coupling types needed at first
    - Relevant time scales
    - Surfacial, volumetric, temporal, concurrent, sequential, linear, nonlinear
  - Data needed to describe a problem
    - Initial conditions
    - Static data (machine description)
- December workshop on drivers and description
  - Results: well described science drivers

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Q3: Detailed analysis of workflows

- **Develop results desired from workshop**
- **Workshop to understand work flows and data management needs**
  - **Users to discuss how they work (transformation software, viz, ...)**
  - **Presentations on needs for validation**
  - **Presentations on existing and proposed solutions**
    - Practices in the fusion community
    - Practices outside the fusion community (e.g., ESMF)
  - **Results**
    - Superset of user practices
    - Use cases for testing workflow tools
  - **Follow on**
    - Prototype application of workflow tools

○ **Document workflow needs, community review**

Q3-4: Understand engineering processes

- **Set desired results from workshop**
- **Workshop on processes for computational software,**
    - Communication systems (mailings, wikis)
    - Verification processes
    - Software management: package management, revision control, build systems, test systems, release process
  - **Presentations on what is done (library providers have good examples)**
  - **Discussion of advantages, disadvantages and identify primary candidates**
  - **Results**
    - Top candidates for tools
    - Candidates for the evaluation of tools (E.g., apply autotools and cmake to GYRO)
    - Identification of gaps: needs without a suitable tool
- **Develop document on processes, review**

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Risks of the framework planning process

- Components not delivered for prototyping processes
- Community unwilling to participate
- Insufficient time to complete prototypes
- Tools not identified, so low-accuracy cost estimates cannot be made

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Possible risks for the FSP

- Computational architectures make approach invalid (layered design)
- Component sampling not representative
  - Many components take much more work than expected (identify multiple components for any one capability)
  - Any one component has much smaller region of validity than advertised
- Team building too difficult with distributed team (have local subteams with definitive responsibilities)
- Integrated codes have numerical problems not observed in prototypes

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Frameworks team has an aggressive plan; 3 mo. for slippage and refinement

- Have completed the startup with communications, public input mechanisms in place
- Plan brings in science drivers
- Plan allows for input from users and potential providers
- Plan covers the major areas of software engineering, including determining the costs for bringing legacy components to a modern state

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