

Mathematics and Computer Science for FSP

FSP KickOff Meeting

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Primary areas highlighted in the proposal

- Use of high-performance libraries to improve algorithmic performance; for example
 - Linear and nonlinear solvers
 - Grid generation, adaptive mesh refinement
 - Particle libraries
- Tools for understanding code performance
 - Do components match expectations in terms of serial and parallel performance as well as memory requirements
 - Particularly focus on readiness for LCF
 - Define a suite of tools available for use
- Development of new algorithmic capabilities to fill gaps in components

Assess current status for key codes and identify gaps

- Identify which codes are being (or will be) used or developed
- Identify points of contact
- Determine the mathematical models (equations) being used
- Determine which high performance libraries are already being used (numerical, pre-, post-)
- Evaluate how coupling is being done in proto-FSPs
- Determine which computer science tools are being used for performance, interoperability, tuning, visualization
- Determine the gaps

How can we most efficiently accomplish this assessment? Community Workshop? 1-1 Interactions?

Gaps analysis will pay particular attention to...

- Fidelity to the science drivers
- Stability, accuracy, efficiency and fidelity of coupling techniques
- Accuracy and adaptivity of numerical discretization
- Scalability of numerical algorithms
- Verification methodology and best practices

Filling the gaps

- Identify key tools that can be leveraged from SciDAC, ASC, ASCR base program, and others
 - Which can be leveraged directly?
 - Which need some level of customization?
 - Prioritize development of customized tools
- Identify areas where new development in math and computer science tools is needed specific to FSP needs
 - Sophisticated time integration techniques
 - Asynchronous parallel execution models

This will require substantial interactions between math/cs folks and fusion scientists – limited resources during the planning phase requires we leverage ongoing activities and efficiently facilitate new partnerships

Code verification and uncertainty quantification

- *Verification*: Determining if the component correctly implements the math algorithms
- *Uncertainty Quantification*: Determining the errors associated with the mathematical model, parameterizations, input, etc to determine the degree of confidence we can have in a simulation

- Asses other large projects to determine best practices and lessons learned (e.g. ASC)
- Apply best known practices
- Analytic and asymptotic comparisons
- Method of manufactured solutions
- Forward propagation of uncertainties, model calibration, sensitivity analysis, probabilistic risk analysis
- Ensure transparency to FSP community

Coupling issues will be a rich area for math/cs research and tool development



- Coupling different scales; time and space
 - Novel methods for time scale integration
 - Understanding order of accuracy issues when coupling modules and transferring data
 - Hybrid approaches to modeling and discretization
 - Adaptive methods for multi-physics problems
- Verification and uncertainty quantification of coupled models is very difficult and generally needs research
- Computer science research in interoperability, programming models

We need to identify high priority research areas and start those early so they are ready for FSP use



Interactions with the framework team will be critical

- There are large areas of potential synergy
 - Couplings and data transfer (algorithms, accuracy, framework specification)
 - Verification as it relates to proper software engineering practices
 - Execution (programming) models
 - Algorithms
- Compliance with software standards for FSP components – *how does this apply to independently developed math/cs libraries?*

My biggest question...

- How do we most efficiently and effectively get the FSP community to give us the information we need to do the assessment outlined in the proposal?
 - What are the codes we should target first?
 - Who are the points of contact?
 - Are there workshops/conferences planned where we can target many different code teams with one trip?