# FSP Advanced Physics Component: mission and work plan

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# Mission & Tasks

- Mission:
  - develop a plan for the identification, improvement, and creation of advanced software components to be used as modules in the integrated FSP framework.
- Tasks:
  - Assembling a team of experts in computational physics, applied math and computer science to carry out the planning exercise.
  - Performing an analysis of the science drivers to determine the needed physics capabilities and advanced code features.
  - Analyzing existing codes and libraries for their ability to meet the needs of science drivers and their readiness for incorporation into FSP.
  - Assessing and developing adequate verification methods.
  - Developing an effective management plan to address the gaps and produce a “living-scientific-road-map” that identifies viable deliverables.
  - Producing an implementation plan with initial technical approaches and milestones, estimate of manpower, computing resource, and funding.

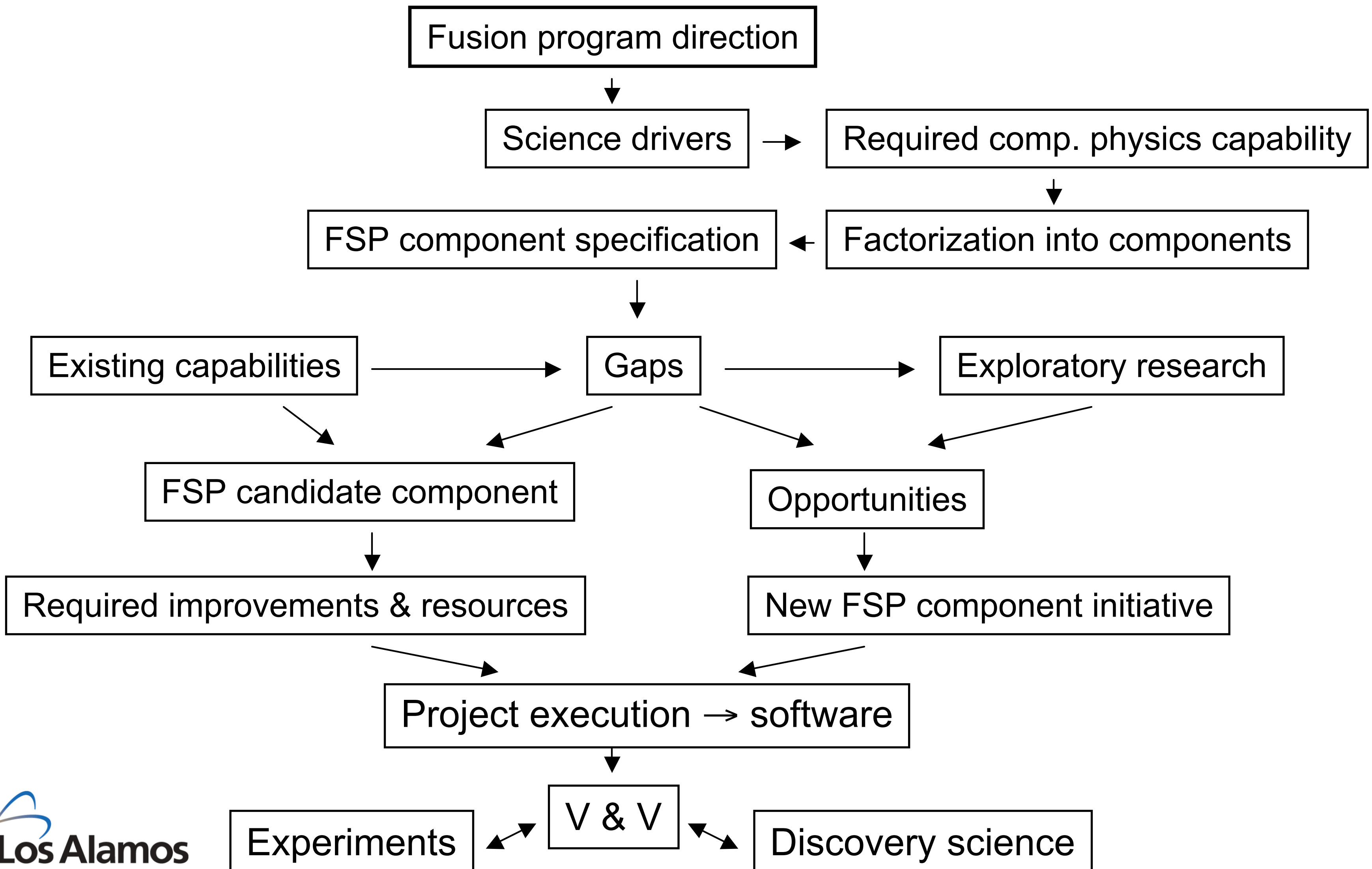
# Key characteristics of a FSP component

- Provide the simulation of key physical processes in the same or different physical domains.
- Have well-defined inputs and outputs that are clearly documented.
- Clearly documented to have been verified and validated for the regimes of physical parameters intended and open to retrospective verification review as needed.
- Conform to software development and management practices defined and accepted by FSP team.
- FSP component spans a wide range of fidelity and resolution requirements.

# Workplan: (1) team leads and approaches

- Component activities organized in four thrusts, emphasizing cross-integration.
  - (1) Plasma/materials interaction (lead: Jeff Brooks; co-lead on edge physics: C.S. Chang)
  - (2) Turbulence & transport (lead: Jeff Candy; co-leads: W-X. Wang & C.S. Chang)
  - (3) Extended MHD (lead: Xianzhu Tang; co-lead: Luis Chacon)
    - (2) and (3) share integration with RF (lead: Paul Bonoli) and energetic particle physics (lead: Nikolai Gorelenkov)
  - (4) Math and computer science (lead: Lori Diachin; co-lead on verification: Leslie Greengard)
- Approaches: focused workshop, interviews, and solicitation of reports
  - Engaging the broader FES and ASCR communities.
  - Involving FES SciDAC centers: GPS-TTBP (P. Diamond); CSPM (W. Nevins); CEMM (S. Jardin); CSWPI (P. Bonoli); GSEP (Z. Lin).

# Workplan: (2) determining component specification from science drivers

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# Workplan: (3) Assessing current capability and performing gaps analysis

- (3.a) Assessing existing physics component capabilities and their readiness for FSP integration
- (3.b) Assessing mathematical and computer science infrastructure needs for FSP components
- (3.c) Gaps analysis to provide prioritization for FSP component program directions

# Workplan: (3.a) Readiness of current physics component capabilities

- Objectives:
  - Determine the initial set of physics component codes to be integrated into FSP framework
  - Determine the additional FSP work scope and hence cost estimate in terms of necessary software engineering and physics/algorithm upgrade beyond their SciDAC and base program support.
- Topical areas and candidate codes
  - Turbulence & transport
    - PIC: GTC/GTS, GEM,XGC; continuum: GYRO, GS2, Tempest; etc
  - MHD & two-fluids
    - NIMROD, M3D, BOUT, and various Newton-Krylov codes.
  - Auxiliary heating & RF
    - AORSA, TORIC. CQL3D, NUBEAM, ORBIT-RF, XGC, etc
  - Energetic particles
    - MHD-particle hybrid codes and gyrokinetic codes
  - Plasma/materials interaction
    - SOL codes, 6D sheath codes, and materials response codes (e.g. MD).

# Workplan: (3.b) Mathematical and computer science needs for physics components

- Objectives:
  - Define the requirements for applied math and computer science infrastructure required for physics components
  - Plan to meet these requirements
    - New development specifically for FSP and/or adaptation of existing tools from SC, NOAA, NSF, and ASC programs.
- Focus areas:
  - Verification and uncertainty quantification (separated out for their importance)
  - (3.b.1) Use of high-performance libraries to improve algorithmic performance
  - (3.b.2) Tools for understanding code performance
  - (3.b.3) Development of new algorithmic capabilities

# Workplan: (3.c) Gaps and opportunities analysis for FSP investment prioritization

- Objectives:
  - Provide the basis to identify additional resource requirements for new initiatives in FSP component development.
- Tasks:
  - Gaps and opportunities analysis
    - Fidelity of physics and mathematical models in relation to science driver requirements
    - Stability, accuracy, efficiency, and fidelity of coupling technique I multiphysics and multiscale integration.
    - Accuracy and adaptivity of numerical discretization
    - Scalability of numerical algorithms to petascale and exascale cmputing
  - Develop criteria and process for prioritization in FSP investment
    - Balance the need for short term deliverables and strategic necessity of high risk/high reward exploratory research.
    - Transparent mechanism for resource allocation and re-allocation.
  - Develop process and strategies for risk mitigation
    - Programmatic changes in fusion development path
    - Task failure in component development initiatives
    - Computer architectural and software tools evolution/revolution.

# Workplan: (4) Robust verification and uncertainty quantification strategies for FSP components

- Integration into a whole device modeling framework is meaningful only if the components are validated and verified.
  - Code verification: determining if the component correctly implement the mathematical algorithm as specified.
  - Uncertainty quantification: determining the errors associated with the mathematical model, parameterizations, input data, and numerical solution, etc.
- Tasks:
  - Assess existing verification and uncertainty quantification methodologies to determine best practices and lessons learned in other large projects.
  - Design common processes for verification in component development.
  - Define process coordinating component development and experimental validation, and facilitating discovery science activities to guide V&V design.

# Workplan: (5) Develop the FSP component program execution plan

- Objectives:
  - Ensure the successful execution of a committed component project
- Tasks:
  - Assess and define the life cycle of component development
    - Risk mitigation requires accountability, responsibility, and a large degree of transparency.
    - Provide a reference map for tracking project progression, updating milestones, and planning contingencies.
  - Define software engineering standards for components
    - For both new development and re-engineering of existing components.
  - Develop the FSP component deliverables and schedule
    - 5, 10, 15 years perspective from the three prior FSP reports.
  - Ensure community assimilation and distribution
    - Acceptance standards and user support for scientific discovery.
  - Determining the resource requirements

# Work breakdown

| Task | Year 1 (percentage) | Year 2 (percentage) |
|---|---|---|
| Overall coordination | 15 | 15 |
| Science driver to component requirement | 20 | 5 |
| Assess present capabilities | 20 | 5 |
| Gaps and opportunities analysis | 15 | 20 |
| Prioritization and design initial approaches | 5 | 15 |
| Verification strategy | 20 | 20 |
| Roadmap + implementation plan + deliverables | 5 | 20 |
| **Total** | **$460K** | **$460K** |

# Focus of the First Quarter

- Thrust leaders to identify subject experts and form working groups.
- First pass of science driver to component specification
  - Case study of component factorization in peer programs.
  - Produce an initial (short) list of FSP components.
- Solicitation of reports on current capabilities by topical areas
  - Physics codes from FES SciDAC program
  - HPC libraries from ASCR SciDAC program
- Assess existing verification methodologies
- Assessing existing uncertainty quantification methodologies

# Focus of the Second Quarter

- Second pass of science driver to component specification
  - Produce a detailed specification for the initial list of FSP components.
  - Continuing science driver to component specification analysis.
- Comparing component specifications with current capabilities
  - Working groups solicit additional information according to component specification
  - Produce an initial gaps analysis
- Produce a case study of how an existing verification methodology can be applied to an FSP component
- Produce a case study clarifying the issues associated with uncertainty quantification in the case of an FSP component.