NSCI SI2-S2I2 Conceptualization of ***CFDSI***: Model, Data, and Analysis Integration for End-to-End Support of Fluid Dynamics Discovery and Innovation

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2018 NSF SI² PI Meeting

Prior Community Effort

1. Cyber Fluid Dynamics workshop held in Arlington, VA in July of 2007.
2. Fluid Mechanics Community Software and Data Resources workshop held in Austin, TX in March of 2010.

Pre-conceptualization Abstract of CFDSI

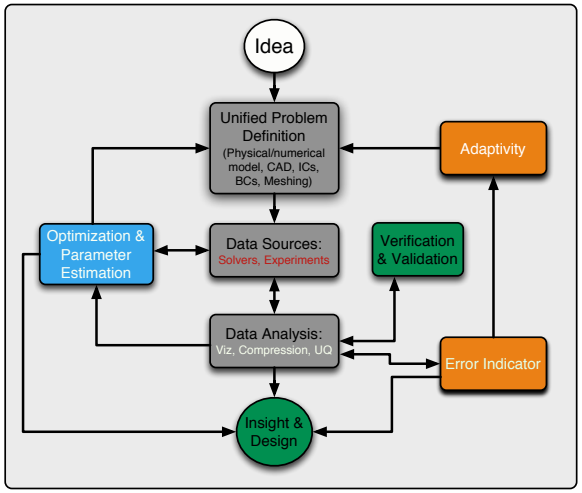
The conceptualized institute will make a wide variety of powerful simulation, data, and analysis resources available to the fluid dynamics research community by lowering or eliminating barriers associated with the adoption and use of these resources. The software infrastructure will have a number of positive impacts on the fluid dynamics research community. To do so, CFDSI will connect the best research in fluid dynamics to the best research in data science/analytics within a highly sustainable software development environment. Specifically, CFDSI will:

1. enhance the dissemination of fluid dynamics data resources and advances in CFD modeling,
2. facilitate collaboration in fluid dynamics research, especially between computational and experimental researchers,
3. enable detailed comparisons between different data sources and detailed validation of computational models,
4. ease the use of advanced CFD models, methods, and codes in new and complex applications,
5. facilitate advanced analytics, such as uncertainty quantification, data compression, and optimization,
6. provide students access to advanced CFD methods and data resources, both computational and experimental, to enhance both graduate and undergraduate education in fluid dynamics, and
7. improve the sustainability of current and future CFD software and facilitate the management of the growing body of fluid dynamics data sets.

These outcomes will greatly enhance the effectiveness and productivity of research in fluid dynamics. In particular, they will transform the conduct of fluid dynamics research by:

1. making it more collaborative,
2. enhancing the credibility of research results,
3. enabling discovery,
4. reducing the cost of pursuing new research questions, and
5. diversifying and widening the fluid dynamics community through lowering the barriers associated with accessing and adopting CFD codes and large data sets.

Software components will be designed for both analysis of experimental and computational databases as well as direct integration into CFD codes. The latter will enable *in situ* data analytics to address the growing chasm between data creation rate (solver performance) and data storage rate/volume (IO resources). After conceptualization and implementation, CFDSI will enable more effective fluid dynamics research and thus impact the wide variety of application domains in which fluid dynamics is critical including climate, environment, health, transportation, propulsion, and power generation (including conventional, alternative, and nuclear sources) which will, in turn, strongly impact our economy. Additionally, CFDSI will provide the capability for immersive simulations and experiments that will close the loop on idea, insight, discovery, and design through establishing links to in situ data analytics and problem redefinition during ongoing simulations or experiments. Finally, CFDSI will impact other problem domains governed by partial differential equations (e.g. solid mechanics) by serving as a model and starting point for similar domain-specific software infrastructures.



- To create an end-to-end fluid dynamics analysis capability with a common user interface requires carefully defined interfaces that link the necessary components together in an efficient and reliable way.
- At a bare minimum, there are three components that must be linked (grey boxes):
  - Problem Definition,
  - Data Sources: solver and/or experiment, and
  - Data Analysis.
- The community has tremendous existing solvers and experimental facilities to create data as streams or databases.
- The goal of CFDSI is not to develop new, community solver, or to promote one data source, rather to make to make interfaces to these data sources more unified so as to lower the barrier to competent use.
- CFDSI could add a collection of share-developed components:
  - data analysis beyond visualization (viz) to include data reduction and regression (compression), and uncertainty quantification (UQ),
  - error indicators and adaptivity, and
  - optimization and parameter estimation.
- During the conceptualization phase, the community will be engaged to evaluate our team's update of the 2010 vision and set a community-driven course for development and integration of these components.
- CFDSI's overarching goal is to improve the science and engineering community's ability to efficiently and accurately transform an *idea* about a physical process related to fluid dynamics into *insight, discovery, and verified/validated design*.

Conceptualization Plan (subject to community feedback)

- Kickoff Conceptualization Workshop May 16-17 in Boulder Colorado.
  - 60 confirmed participant
  - 60% fluid dynamicists, 40% data analysts
  - Format: Discussion Groups (4 sessions) and presentations from SI2 Institutes
- Sub-Community Workshops, five meetings Summer of 2018
  - Preliminary topics (subject to community feedback)
    - Software Carpentry/Sustainable Development for CFDSI
    - Data Sources
      - Streams (live)
        - Experiments
        - Solvers
      - Databases (both computational and experimental)
    - Problem Definition
    - Error Indicator/Adaptivity
    - Compression, Uncertainty Quantification, Optimization, Visualization
- Prototyping Summer School – Priming : Last 4 weeks of Summer 2018
- Mid-term Workshop November 2018
  - Preliminary report to community on
    - Community feedback from Kickoff
    - Sub-Community Workshops
    - Prototyping Summer School progress
  - Gather community feedback on adjustments to the conceptualization path
- Present evolving vision of CFDSI at all conferences that have sessions relevant to CFDSI
- Prototyping Summer School – Delivery : First 4 weeks of Summer 2018
- Conceptualization Closure Workshop Summer of 2019

Kickoff Workshop: Goals and Outcomes

In this workshop, we want to:

- Introduce CFDSI
- Bring together leaders across the many software components that define, create, and analyze data from both computations and experiments
- Discuss what needs are currently unmet or underserved
- Discuss what analysis capabilities hold promise but need development to be more broadly used
- Discuss how the community can better share its existing software
- Discuss how an institute can facilitate improvement in all of the above,
- Discuss the five Sub-Community Workshops that will follow
- Discuss goals to achieve by the Mid-term Workshop to be held the Saturday before APS-DFD-18 in Atlanta, GA

The specific outcomes we hope to achieve from this workshop are:

- A refined vision for CFSI that reflects intense community engagement
- A passionately engaged set of attendees that form not only the foundation for the CFDSI community, but represent strong advocates to communicate this vision through their colleagues to grow the community further
- A set of long term goals for the institute
- A set of near-term goals for the conceptualization that demonstrate the promise of the full institute so as to grow confidence within the community in its success
- Define the five Sub-Community Workshops that will follow in Summer of 2018

https://www.colorado.edu/events/cfdsi/

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