## **Breakout\_C-4** (can map to issue name later)

Issue: https://github.com/CFDSI/Kickoff Workshop/issues/4

Related Issues:

Issue Statement: What are the best topics for the sub-community workshops for CFDSI?

Discussion topic:

Moderator: Adam Steinberg Note taker: Colin Towery Reporter: Jim Brasseur

Group Members:

- Colin Towery
- Kyle Niemeyer [Oregon State]
- Jim Brasseur [UC-Boulder]
- Adam Steinberg
- Paul Durbin
- Erik Johnson [USC]
- Damian Rouson
- Shawn Shadden [UC-Berkeley]
- PK Yeung
- Lorena Barba [GW]

Please address these topics in your discussion (moderators please make sure that there is enough time to cover all three before the session ends).

## 1. Describe the Big Issues:

From GitHub Issue's comments section (posted by Ken Jansen):

In the original proposal, we envisioned 5 small (O(20) participants) workshops focused on the following activities:

- 1. Software Carpentry for CFDSI
- 2. Data Sources
- 3. Problem Definition and Interfaces
- 4. Error Indication and Adaptivity
- 5. Compression, UQ, and Optimization

Are these the right topics? Should Data Sources be split into experimental/computational streams/databases? Should the Software Carpentry be coordinated with URSSI? Should 3) and 4) be combined?

- This is about conceptualizing the institute, not discussing actual standards/definitions, education workshops, etc.
- What list of services could/will the CFDSI provide? If we have a list of services, we have a list of sub-communities.
- This vision is so broad, it could go in many directions, we need to define boundaries, but the unifying theme is promoting the development of software across the community.
- The final report of this NSF grant is not the proposal for the Institute, it's a white paper that defines community needs to create an RFP for an institute

## 2. What are the possible services the community might need?

- EDUCATION, TRAINING AND OUTREACH
  - Software Carpentry workshops
  - Pedogogy development
- STANDARDS AND PRACTICES
  - Promoting interoperability, convertibility, shareability
  - Promoting reproducibility and reliability
  - Promoting adoption and development of open source science
  - reference standards of algorithms
  - Benchmark problems and data
  - Code/data interfaces
- SOFTWARE DEVELOPMENT & SUSTAINABILITY
  - Solvers for generating data (simulation codes, other PDE/ODE solvers)
  - Analysis, discovery, visualization, and conversion/processing software
  - Knowledge Construction, Model Discovery
  - Outer-loop software: UQ, Inverse/Inference/PE, SA
  - o Inter-analysis and collaboration between experiments and simulations
  - Data storage, maintenance, query, and sharing
- SOFTWARE AND DATA SHARING
  - Supporting exchange and analysis of software and data
    - Data storage, maintenance, querying from central or independent repositories
    - Benchmarking, V&V of software using reference computer system and problems
  - Supporting adoption and development of open source software and data (of all kinds)
  - Supporting interoperability, convertibility, shareability of code and data
- ORGANIZATIONAL STRUCTURE OF INSTITUTE
  - How are we going to support the community (PIs, grad students, etc.)?
  - (not a service)
  - maybe only after we conceptualize, discuss this after the 5 sub-committee workshops

- DEFINING THE BROADER COMMUNITY
  - Problem definition
  - Who is under the umbrella of a CFDSI community? Chemical engineers, Bio, industry, etc.

## 3. Scoping out sub-communities: Services

- 1. SUPPORTING SOFTWARE SHARING AND SUSTAINABILITY
  - o promoting/supporting open source software and open science
  - Improving sustainability (i.e., ensure scalability on new hardware), shareability
  - How would CFDSI interoperate with URSSI and other organizations?
  - (Generic to all types of software, feeds into specific workshops below)
- 2. EDUCATION, TRAINING, AND OUTREACH
  - Workshops (e.g., Software Carpentry, fluid dynamics-specific)
  - Fellowships
  - Policy/culture advocacy, training, etc.
  - Increasing diversity of the research field
  - Teaching ourselves: Self-learning, guides and other wiki-like resources
- 3. SUPPORTING SOFTWARE FOR DATA CREATION
  - CFD simulation codes, solvers
  - Experimental sensor signal processing (e.g. data acquisition and conversion)
  - Error estimation
  - Uncertainty Quantification
  - Manipulation, restructuring and "filtering" of massive datasets
- 4. SUPPORTING SOFTWARE FOR DATA EXCHANGE
  - Compression
  - Transmission
  - Storage
  - Metadata, data descriptions
- 5. SUPPORTING SOFTWARE FOR DATA INQUIRY, INSIGHT, AND DISCOVERY
  - Data inputs (standardization of data storage formats?)
  - o Parameter estimation, model development
  - Integrated analysis of computational and experimental data
  - Knowledge Extraction: integration among data, computer and human cognition
- 4. Misc ideas so they don't get lost (e.g., Did you find new issues? If yes, create the issues on GitHub!):

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5. Summary for report-back (Alternatively, just bold the key points above):