ICiS Institute for Computing in Science

Multiphysics Simulations: Challenges and Opportunities

Breakout on Opportunities & Leverage

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Group 2

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Opportunities and Leverage

Identify opportunities based on needs of applications and limits of current approaches.

Questions for Breakout Sessions:

1. Based on the workshop proceedings to date, where do you see opportunities for new innovations to impact multiphysics simulations, especially in:
   - Algorithms
   - Software engineering
   - Hardware
2. What challenges do you see that have not been well handled by current methods or software?
3. Are there innovations that have been very successful in one application that can be applied to others?
4. What multiphysics integration would your community like to perform today that by conventional wisdom is out of reach, but might be crackable with a specific breakthrough?

Based on the workshop proceedings to date, where do you see opportunities for new innovations to impact multiphysics simulations, especially in:

- Algorithms
  - Multiphysics simulation is an opportunity to change the computing paradigm from moving data to code to moving code to data.
  - Create algorithms that automatically measure coupling between models (ensemble PDEs, stochastics)

- Software/Software Engineering
  - While multiphysics simulation is running other parts of a machine could be used to calculate the adjoint information to give overall confidence of simulation
  - Education role to help application writers understand ways to structure their code to increase opportunities for multiphysics
    - Let go of MAIN
    - Use actual communicator instead of MPI Comm_World - allows putting different physics on different parts of a machine
    - Driven by math – develop prototypes and counter examples
  - Multiphysics is an opportunity to think in parallel for new programming paradigms

Based on the workshop proceedings to date, where do you see opportunities for new innovations to impact multiphysics simulations, especially in (cont):

- Hardware
  - Industry is looking for next design of HPC systems within certain constraints e.g. power, multi-core, etc. the multiphysics community should communicate their future needs
  - Random number hardware would be especially useful for atomistic multiphysics models
  - Multiphysics codes should not rely on cache coherency at the Exascale because it won't be there.
- Formulation
  - Need to define coupling terminology from the physics and implementation to frame the discussion (e.g. tightly/loosely coupled algorithms, strong/weak interactions)
  - With advanced in HW opens the door to new first principles based multiphysics modeling
  - Impact of tight vs loosely coupled models (simulations) on performance, programming models, scheduling and hardware design.

What challenges do you see that have not been well handled by current methods or software?

- Need more rigorous and generalizable mathematical analysis for coupling of continuum and discrete (and even discrete models themselves) – exists in specific domains.
- Coming up with validation metrics for simulations of non-deterministic multiphysics process e.g., bubble formation in foams, surface tensions effects, cracks, etc.
- Estimation and control of temporal error and stability in multiphysics simulations.

Are there innovations that have been very successful in one application that can be applied to others?

- Mathematical coupling approaches in some areas could be applied to wider range of potential multiphysics applications
  - Define a set of interfaces (Implicit-IMEX-Explicit) to guide application developers - - “Multiphysics Primer”
    - Elucidate coupling requirements
    - Advantages and disadvantages of each approach

- Analysis is needed of current coupling in multiphysics codes
  - Develop a suite of test cases designed to exposed numerical characteristics – not just the scientific questions
    - Provide prototypes and counter examples
    - It was suggested this suite be used to prove a code’s worthiness for publication and/or funding
      - See e.g. http://journaltool.asme.org/Content/JFENumAccuracy.pdf
    - Provide input for vendors in the design of new machines
  - Funding agencies should support correctness of multiphysics

What multiphysics integration would your community like to perform today that by conventional wisdom is out of reach, but might be crackable with a specific breakthrough?

- Mathematical understanding of accuracy and stability of coupling between different methods e.g., particle and PDE
- Exploration of new scales that will be only be feasible with coupled continuum and particle methods @ Exascale and the analysis to do this
  - Atomistic
  - Particle-in-Cell
- Cultural breakthrough toward support and funding of interdisciplinary work – multiphysics is a prime exemplar
  - Formal working group/committee to coordinate cross disciplinary interactions and report on agencies support
  - Potential example to emulate is NCI – PS-OC

Other Topics not in the Questions

- Validation & Verification
  - Stronger emphasis
    - Practioners
    - Funders
  - Need for hierarchy of regression tests for multiphysics problems
  - Creation of manufactured solutions to verify code.

- UQ, specifically how uncertainty in experimental measurement gives rise to multiphysics simulation uncertainties – math help for understanding how errors propagate

- Multiphysics algorithms will need to be more adaptable and asynchronous with hardware to support this.
  - Can HW or SW tells us when there is a problem to allow fault tolerant multiphysics simulations to correct themselves

- Document and give concrete examples of multiphysics algorithms that get close to peak performance on multi-core systems.

Some opportunities heard during the week
Questions used to start Breakout session

- The discussion on Helicopter flutter - how do you know it is really numerical dissipation or due to the physics?
- Coupling between PDEs and particle methods - do we need more mathematical foundation?
- Verification of multiphysics codes when experiments are difficult to perform, is there a way to develop verification tests?
- Build regression tests into multiphysics codes? Hierarchical test for multiphysics codes?
- How do multiphysics codes pass data? Is multiphysics an opportunity to move code to data?
- For a particular problem how do we measure coupling mathematically, collection of sensitivities?
- Define terminology - strong & weak for physics, tight & loose for implementation?
- Carry error - i.e. on massively parallel systems can we simultaneously compute adjoint to improve error or avoid going astray?
- UQ for multiphysics - match numerics & experiments; manufactured solutions?
- For modern architectures, do we need to rethink the problems from the math (first principles) and is multiphysics an opportunity to drive new approaches as new class of problems that new architectures enable?
- Coupling and scheduling single multiphysics codes that operate on different grids. Should they be tightly coupled so that MPI is called for the group together? or can they be more loosely coupled with their own MPIcomworld and exchange data through files or RDMA?
- How can we best insert on node (intranode) parallelism models into coupled or multifphysics codes that individually use different methods of MPI parallelism (or can we)?
- Is particles the way to go for exascale architectures or will there still be room for fluid approaches?
- Control time errors?