Summary of

Track 4: Computational Physics, Applications, Etc…

Track 4: Topic Areas

- Establish goal target
  - Speed vs. accuracy
  - Cost
- Numerical and computational methods
  - verification
- Code structure
  - Modular, object-oriented
  - Framework (i.e., micro, meso, macro)
  - Accuracy driven
  - Open source
  - User-friendly
- Validation
  - Data quality
  - Test problems & challenge problems
- Fundamental physics
- Funding
- Education
  - Teaching
- Communication / collaboration / coordination
  - Documentation
  - Stakeholder gaps (industry / university / labs)

Roadmap: Short-Term (2009)

Objectives

1) higher-fidelity, transient, 3D, PSD (no density variations), hydrodynamic-only for any 2 phases for transport reactor & TRDU-scale gasifier; simulation to run on 2009 workstation overnight

2) develop reduced-order, ~real-time models of (1: hydro) that can be linked to process simulators

Technical Challenges

- Funding levels
- Fundamental physics (other tracks)
- Numerical: stability, stiffness, efficiency
- parallel efficiency
- robust computational framework with eyes toward expansion (breadth & depth – modular & layering, respectively)
- model & experimentalists communication network
- disparity in time & length scales

Roadmap: Short-Term (2009)…continued

Approaches

- Communication: newsletter, web page, template for regular workshop
- Communication: Identifying what is wrong with current models (assessment of where we are at).
- Expert system for identifying "current best approach", state-of-the-art
- Code structure: detailed plan for integration of various codes
- Common component architecture for open source management
- Education: curriculum for modular university courses, 10% increase in grad. students; on-line example problems
- Validation / Data quality: detailed plan for test cases, identify challenge problems, identify fund. experimental problems, transient data
- Verification plan: identify standard approach

Roadmap: Mid-Term (2012)

Objectives

1) heat & mass transfer, 3D, phase transformation, scale of at least 12.5 MW or 800 lbs/hour transport reactor and gasifier (overnight simulation) for any 2 phases

2) same hydrodynamics as 2009, with addition of density differences (multiple species)

3) develop reduced-order, ~real-time models of (1: heat & mass) that can be linked to process simulators

Technical Challenges

- Radiation model
- correlation for heat and mass transfer
- Framework should be different than open source code (framework with multiple codes working together)
- Framework: DNS vs. continuum vs. both
- Coarse-graining
- Process models
- disparity in time & length scales
- numerical issues with PSD (eg, DQMOM)
- validation data at high T, P

Roadmap: Mid-Term (2012)…continued

Approaches

- Communication: different entities working on same code, system-wide open source, committee available for oversight, version control

- Challenge problems for heat & mass transfer; correlations for heat & mass transfer based on highly-resolved simulations

Roadmap: Long-Term (2015)

Objectives

1) reactive, 3D code for ~25 MW system

2) develop reduced-order, ~real-time models of (1: reaction) that can be linked to process simulators

Technical Challenges

- Numerical stiffness of added physics (reaction, radiation, density jumps, etc)
- Parallel efficiency
- disparity in time & length scales
- detailed, local validation data
- identifying minimum set of input parameters

Approaches

TBD

Additional Issues

- Data Mining
- Integrators: temporal and spatial
- Quantifiable Visualization?
- Boundary Conditions (e.g., law of the wall)
- Pre-conditioning?
- Parametric studies
- Resolution (CPU vs. accuracy)
- Numerics of additional physics (e.g., PSD, turbulence, shear stress)