Defense Programs

Solvers, Algorithms and Libraries (SAL)

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Working Group Description

- Scope: SAL addresses technical challenges and near-term R&D topics necessary for successful execution of PEM and IC application codes on future architectures:
  - Full range of linear and nonlinear solvers and preconditioners (libraries).
  - Embedded Optimization and UQ.
  - Multiphysics coupling / time integration including dynamic scale-bridging (more predictive).
  - Parallel algorithm patterns / abstractions, load balancing, mesh generation
  - We are not OS and run time libraries (e.g. MPI). We are not "physics models" libraries.
- Key dependencies on other working groups (from our view)
  - Applications
  - Programming Models
  - Hardware Architectures
  - Connections to other as well (Co-design)

Exascale Challenges

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- **Common technical challenges across all SAL activities**:
  - migration to scalable manycore
  - management of data
  - use of hybrid programming models,
  - communication-reducing or avoiding approaches
  - Increase algorithm concurrency
  - fault tolerance
  - Prediction of performance potential bottlenecks
- Specific issues related to Krylov solvers, preconditioners, and multigrid methods (see white paper). Specific issues related to IC code multiphysics coupling algorithms (see white paper)
- Performance portability across a range of platforms
- Mini-app development along with good metrics and a reliable methodology to analyze algorithms and codes to exascale-related issues
- Creating a "computational Co-design code team" and getting better at team software engineering

Path Forward

- **Linear solves on scalable manycore architectures**
- Initial next steps: develop manycore preconditioners
- Timeline: Phase I, Communication management, minimization, avoiding technology and physics-based methods, Phase II. Implementation in solver libraries and deployment to Apps, Phase III, New strategies that make communication and computation concurrent
- Required Partnership: OASCR
- Risks: IC codes currently use this technology heavily.

Path Forward

- **Mini-apps and related "apps" development for understanding patterns in co-design with Apps, PM, Hardware**
- Initial next steps; Detailed interaction with Apps to extract important design points and build supporting mini apps
- Timeline: Phase I, Interact with PM and Apps to define requirements for, and develop mini-apps and extract patterns, Phase II, Impacting application code , hardware and software stack development with pattern-aware SAL advancements
- Required Partnership
- Risks: Being forced to characterized important patterns with complex codes

Path Forward

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- **Multiphysics coupling algorithms (more concurrency)**
- Initial next steps: Initial algorithm R&D. Interaction with Apps to extract compact- apps. Initiate algorithm testing and analysis
- Timeline, Phase I, Extract compact-apps with Apps WG and pose initial ideas, test and numerical analysis. Develop mini-apps to interact with PM and HW WGs, Phase II, Extend compact apps, numerical analysis of proposed algorithms and verification of algorithm properties.
- Required Partnership: OASCR
- Risks: Expecting standard sequential operator splitting to perform well on exascale platforms

Path Forward

- **Scale bridging algorithms (more predictive simulation and new system-scale formulation of same physics problem**)
- Initial next steps: Detailed interaction with Apps to extract compact apps and initiate algorithm development and numerical analysis
- Timeline, Phase I, Extract compact-apps with Apps WG and pose initial ideas and test. Develop mini-apps to interact with PM and HW WGs, Phase II, Extend compact-apps, numerical analysis of proposed algorithms and verification of algorithm properties.
- Required Partnership: OASCR
- Risks: Going to exascale, but not increasing predicative nature of simulation

Path Forward

- **Advanced Analysis (UQ, Optimization, Sensitivity Analysis)**
- Initial next steps: Partner with Apps to define requirements
- Timeline: Phase I: Apply existing technology for embedded optimization, Phase II, Apply existing technology for embedded UQ. Developing scalable algorithms for a broader class of optimization and UQ problems
- Required Partnership: OASCR
- Risks: Limiting ASC access to modern UQ, optimization and sensitivity analysis

Path Forward

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- **Resilient solvers (Fault tolerant algorithms)**
- Initial next steps: work with PM and systems software to incorporate resilience features.
- Timeline: Phase I, Continue development of algorithms, Phase II, deploy in solver libraries
- Required Partnership: OASCR
- Risks: Apps WG folks will be very unhappy

Recommended Co-Design Strategy

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- Critical steps/activities
  - Defining a co-design processes
  - Defining a co-design "code team"
- Role of skeleton/compact apps
  - A critical "tool" in co-design
  - A method to expose patterns
  - A method to interact with hardware vendors
  - A method to verify performance of new algorithms
- Concerns/suggestions
  - Define a glossary
  - Important to document what is not included in a mini-app
  - Hardware vendor NDA
  - Required level of effort (fractional person) in a co-design effort. Communication efforts must go up !

Some Specific Co-Design Teaming

- Applications WG
  - Resiliency
  - Data management and algorithm concurrency (linear solvers and multiphysics coupling)
  - Embedded UQ methods
  - New formulations for improved predictivness and innovative use of exascle resources (scale-bridging)
  - Compact-apps and mini-apps
  - Defining a co-design “code team” (tighter coupling of Apps and SAL)
- Hardware Architectures WG
  - SAL provides a window to Application (mini-apps)
  - Focused studies to present insight to hardware vendors in a timely fashion (mini-apps)
- Program Models WG
  - Abstractions
  - Patterns
  - Data management
  - Mini-apps !

ASC

Big Picture Comment

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- Thanks to NNSA / ASC for standing up the SAL WG, it is important to the success of the Exascale Initiative.
- Applied math efforts will be key in developing, and characterizing, advanced algorithms with increased concurrency and reduced memory footprint.
- The ASC SAL path forward can benefit from many possible joint efforts with similar SAL activities within OASCR