NEAMS Enabling Computational Technologies

This work performed under the auspices of the
U.S. Department of Energy by
Lawrence Livermore National Laboratory under
Contract DE-AC52-07NA27344
10/19/2010

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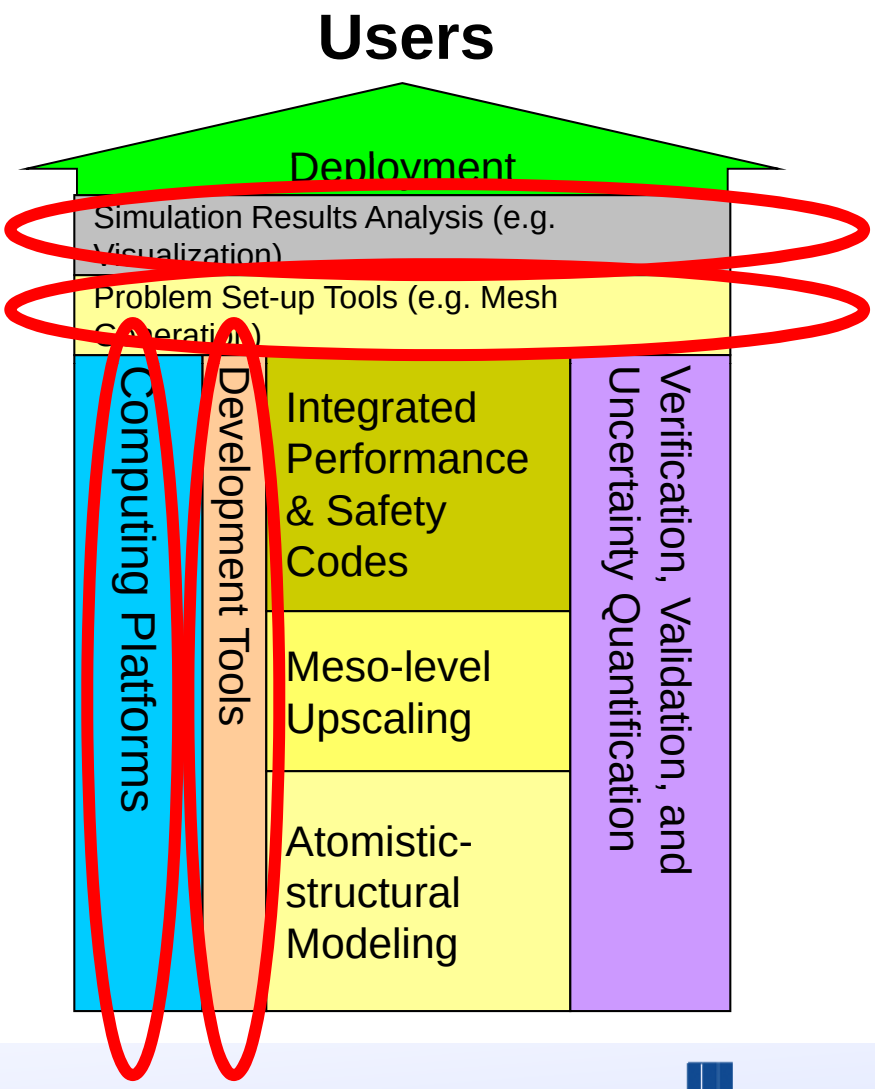
The NEAMS program relies on enabling computational technologies

***ECT Strategic Vision**:* Deliver a comprehensive set of enabling computational technologies required to achieve the NEAMS vision of creating new, advanced capabilities



The ECT program element can result in significant efficiencies for the NEAMS program

- Eliminate duplication of effort across IPSCs
  - Software identification and deployment
  - Duplicated expertise in problem set up, data analysis, SQA, etc.
- Reduce scientist team ‘distractions’
- Provide a clearinghouse of ECT information
  - Create a team intimately familiar with ongoing related efforts (e.g. SciDAC, ASC)
  - Deploy a single web portal with collected information
  - Work with IPSCs to develop customized solutions as necessary

The FY10 scope for ECT spans several areas

Software Quality Assurance

Goal: *Provide the e*
necessary to ens
the highest quali

Approach:

- Understand the
provide guidance
- Synthesize and
- Provide best pra

FY10 Activities:

- Complete draft S
- Risk-based asse
- Demonstration a

Cross-cut libraries and tools

Goal: *Increase the effi*
program by providin
and libraries for sim
the IPSCs

Approach:

- Understand requirer
NEAMS program el
- Use existing softwa
develop customized
- Disseminate tools to

FY10 Activities:

- Customize Overlink
- Coordinate with Ca
NEAMS framework
- NEAMS framework

Computing Platforms

Goal: *Provide access to the necessary computer resources to accomplish NEAMS program goals*

Approach:

- Understand program needs for compute resources
- Evaluate capacity computing resources available in the DOE complex
- Improve accessibility and usability
- Provide guidance on additional options (e.g. INCITE, NERSC)

FY10 Activities:

- Instantiate early adopters program at INL
- Gather user feedback to improve accessibility

ECT FY10 activities span the NEAMS program

- Software quality assurance
  - All IPSCs participated in Risk-based assessments
  - SQA tools demonstrated and used for Reactors, Fuels, SafeSep
  - SQA plan relevant to entire NEAMS program
- Cross-cut libraries
  - Overlink coupling demonstration focused on Reactors IPSC in FY10; will extend to Reactor/Fuels if successful
  - Frameworks discussions in close collaboration with CT; input solicited from entire NEAMS program
- Computing platforms
  - Early adopters program offered to entire NEAMS program
  - Initial users from SafeSep IPSC

ECT session talks will focus on several of these topics

- Dissemination of ECT technologies:
  - "**The ECT Web Portal**", Laura Schulz (LLNL)
- Software Quality Assurance:
  - "**Draft NEAMS SQA Plan**", Greg Pope (LLNL)
- Computing Platforms:
  - "**Current and Future HPC Capabilities at Idaho National Laboratory**", Eric Whiting (INL)
- NEAMS Framework Survey:
  - "**NEAMS Survey and Report on HPC Frameworks**", John Magerlein (IBM)

FY10 mesh-to-mesh coupling effort in ECT builds on Overlink software library

- **Mesh coupling identified as a high priority area in FY09**
- **Overlink provided a good starting point for the solution**
  - Remaps zone and node centered field data, defined on a given mesh, to a different, unrelated mesh
  - Mesh Types: Domain decomposed, block structured and unstructured general polyhedral meshes
  - Specialized high performance software for cartesian grids
  - Operates on thousands of processors; handles billions of elements
- **FY10 focused on customizations necessary for NEAMS**
  - Inline functionality rather than file based; required development of new communication templates
  - Interfaces developed to MOAB and Sharp framework
- **FY11 work will complete the demonstration and deliver open source library to NEAMS**

Significant discussions and meetings about NEAMS 'frameworks' occurred in FY10 (w/ Capability Transfer)

- **April PI meeting, presented ECT/CT view of frameworks**
  - Significant discussion which resulted in a broadened view of "frameworks"
  - IBM presented preliminary results of a survey on existing frameworks
  - Determined that resources are best focused on creating a consistent end user experience across the IPSCs
    - *Release and distribution*
    - *Build and configure*
    - *Mesh generation/problem set up*
    - *Visualization and results analysis*
    - *Data management*
    - *Workflow and job execution*
  - Determined that more information on physics components used by IPSCs is required to analyze the cost/benefit trade-offs for an interoperable mesh and software backplane
- **July frameworks meeting**
  - ECT, CT, the 4 IPSCs, VU and IBM
  - Discussed needs in more detail resulting in FY11 work package

Several elements for the NEAMS frameworks are being investigated in FY11

- **FY10 framework efforts in CT/ECT combined into ECT program element for FY11 (led by David Bernholdt)**
- **Significant effort will focus on**
  - **RSICC** for release and distribution of export-controlled code
  - **Cmake and Ctest** for configure, build, and test harness
    - Will leverage significant experience at SNL using these tools for Trilinos
    - Provide help for teams to migrate to these systems as needed
  - **CUBIT** for mesh generation and problem set up
    - Key issues are licensing, availability to end users, and ensuring NEAMS developers can add necessary functionality
  - **VisIt** for visualization and results analysis
  - **NICE** tool development for job execution and work flow

The scope for ECT in FY11 spans 4 areas

Software Quality Assurance

- Finalize NEAMS SQA Plan
- Update IPSC risk assessments
- Provide best practices and tools
- Centralized server of SQA tools and consulting expertise

Cross-cut libraries

- Pre-processing tools such as geometry and meshing - CUBIT
- Post-processing tools such as visualization and data analysis – VisIt
- Materials properties library

Common Frameworks

- Evaluate tools for deployment across all NEAMS program elements
  - Release/Distribution (RSICC)
  - Configure/build
  - Workflow and execution
  - Data and information
  - Code coupling
- Propose and develop solutions

Computing Platforms

- Roadmap of NEAMS program needs
- Evaluate INL/ORNL capacity computing resources
- Improve accessibility /usability
- Provide guidance on additional options (e.g. INCITE, NERSC)

Collect and release information on ECT web portal