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Title: CERT TST December 2015 Visit Summary

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Report

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CERT TST December 2015 Visit Summary

LA-UR-16-?????

The annual PSAAP II TST visit to Texas A&M's CERT Center was held on December 1-3, 2015. The agenda for the visit is attached. Non-TAMU attendees were:

- TST Members – Teresa Bailey (LLNL), Todd Gamblin (LLNL), Bob Little (LANL) – Chair, Chad Olinger (LANL), Shawn Pautz (SNL), Alan Williams (SNL)
- Other Lab staff – Skip Kahler (LANL), Ana Kupresanin (LLNL), and Rob Lowrie (LANL)
- AST Members – Nelson Hoffman (LANL) and Bob Voigt (Leidos)

The TST wishes to express our appreciation to all involved with CERT for the high-quality posters and presentations and for the attention to logistics that enabled a successful visit. We have broken our comments into four sections: (1) Kudos, (2) Recommendations, (3) Feedback on Priorities for April Review, and (4) Follow-Up Activities with Labs.

1. Kudos

- We appreciate viewgraphs 5 and 6 from Morel's Overview Talk – "Project Components and Integration" and "Project Roadmap to Year 5 Experiments." These charts go a long way toward addressing TST feedback from the December 2014 visit. Speakers identifying their area of contribution on the "Project Components and Integration" chart was helpful.
- Initial IM-1 experiments, simulations, and calibration have been completed using PDT "brick" geometry.
- Completion of IM-1 experiments overcame previous issues with facility power variations, and drift and fluctuations within the MCA.
- Planning to incorporate neutron detectors to monitor details of each neutron pulse (including symmetry) in out-year experiments is wise.
- Boric acid experiments were completed with known Boron concentrations. These experiments will be used to test the IM-1 calibration model.
- Initial IM-1 validation experiments have been performed.
- Careful attention to simulation details (e.g., geometry, material compositions, cross sections, and discretizations) has resulted in 4% agreement between PDT and MCNP for IM-1 using PDT brick geometry.
- Center attention to pedigree of every runset is important. We appreciate acknowledgment of needs for automated tools for problem setup and QOI extraction. Script to take MCNP input and generate PDT input is a good example of progress in this area.
- Very good to see initial IM-1 calibration results using real experimental data and simulation results, including predicted distributions for source radius, axial location, and impurity distribution.
- Arbitrary grid capability in PDT is advancing. Extruded triangular meshes complete (and in process of being used for IM-1 simulations), more advanced representations planned for future.
- Iterative load-balancing scheme for arbitrary meshes has been implemented.

- Mixed-mode parallelism supported by STAPL runtime has been employed with no changes required in PDT.
- Excellent PDT scaling has now been shown to > 1 million cores.
- Work to QA NJOY output through sanity checks and detailed comparisons between continuous-energy MCNP and multigroup PDT is impressive, and has already resulted in improvements to capability. Remaining issues have been clearly identified through such comparisons, and suggestions for fixes have been made.
- Plans for imminent Tri-Lab release of STAPL are appreciated.
- Attention to reducing algorithmic redundancy and communication in STAPL have resulted in performance improvements.
- Preliminary Kripke / STAPL implementation is completed, including both mixed-mode and nested parallelism. Overhead issues have been identified and are being addressed.
- NERT (neutron-equivalent radiative transfer) capability implemented in PDT for non-fissionable, isotropic scattering. This has allowed PDT radiative transfer runs to be equivalent to PDT neutron transport runs for certain cases. We applaud the planned documentation of exactly what has been required to produce a NERT capability.
- Progress to address slow iterative convergence in optically thick configurations (such as within group scattering and thermal upscattering) is impressive and important for being able to simulate out-year experiments. Initial results indicate improvements of 1-2 orders of magnitude in solution time using the two-grid methodology.
- We appreciate the poster session on night one of the visit, and thank all the students for their efforts put in to the posters, and for their time to meet and discuss with us.
- Student engagement at all three Labs continues to be excellent.

2. Recommendations

- We recommend enhancing the projects overview charts to communicate dependencies and yearly goals.
- Develop contingency plans for pulsed neutron source in case current procurement path is not successful.
- It was asserted that lower observed count rates at the ends of the graphite bars results from neutron leakage. We recommend confirming this by a simple experiment and / or simulations.
- We request a presentation next year on CERT code development processes.
- Suggest planning parallel deep-dive sessions for next TST visit. Contingent on expected attendees, these could allow more in-depth discussion on specific topic (such as UQ methodology and practices) as well as a chance to delve in to real issues the Center is facing (for example, in exponential Monte Carlo).
- Understand why prismatic grid version of PDT compares less favorably with MCNP than brick grid geometry.
- Slides such as # 4,5 in McClarren's talk are useful as reminders of what the stated objective was during last visit and what has been accomplished since that visit. Such information begins to address a recommendation from the April 2015 review that "for future reviews, it would be useful to the team if each presenter would not only show how their work fits in with the overall

CERT vision, but would also summarize clearly what work was done in the past year with CERT funding and what work is planned for the upcoming year."

- Prepare for using computing resources at all three Labs (in addition to ORNL, ANL) as runsets become more complex.
- We are interested in the roadmap for general STAPL release – what events must occur?
- When Kripke / STAPL implementation is improved, we would like to compare performance with other tools and methods.
- Communicate how UC Boulder work serves as risk mitigation for other efforts, and how results would impact PDT / CERT.
- Consider the likelihood that simulations of more complex experiments will result in negative angular fluxes and begin to develop a plan to address.
- Suggest putting publications resulting from this project on the CERT Web site.
- CERT should consider hosting a transport Deep-Dive to include all relevant PSAAP II Centers and the Laboratories.

3. Feedback on Priorities for April Review (as proposed during Adams' presentation)

- TST view of highest priorities:
    - Complete IM-1 runset using prismatic grids, and use these results for updated IM-1 calibration and prediction of IM-1 validation experiments.
    - Complete the IM-1 validation experiments and simulations and assess predictions.
    - Perform initial simulation of "Year-5" experiment.
    - Review recommendations from April 2015 review and be prepared to address.
- TST view of lower priorities:
    - Addressing the stretch goals associate with planned runsets.
    - Demonstrating scaling on 3 million parallel processes.
    - Work required to ascertain whether IM-2 impurity model is required.
- TST comment on proposed priority # 7, "Develop detailed plan to implement parallel arbitrary-grid uncollided flux algorithm."
    - We applaud the desire to "do this right" as such a capability in PDT would be not only important, but complex. Working through requirements and testing plan before turning to implementation plan might be considered.
    - Whether this can be accomplished before April or not, it is an important goal for the Center.

4. Follow-Up Activities with Labs

- More in-depth technical interaction with the TST is recommended in general.
- Enhanced capability and resolution of potential numerical issues regarding NJOY processing of thermal scattering data.
- Discussion with SMEs on appropriate neutron scintillator technology to consider for pulse monitoring.
- Help from Labs on formal software processes used that may be beneficial for CERT to adopt. This can also include debug and performance tools and validation practices.

- Interact with Lab SMEs to discuss current obstacles being faced in exponential Monte Carlo.
- Provide specific example of existing roadblocks students are facing with regards to bringing software they develop at the Labs back to the university.
- Interact with Lab SMEs on methods for choosing regions for angular adaptation.

CERT
Center for Exascale Radiation Transport

# Agenda for CERT TST Meeting

## Texas A&M University

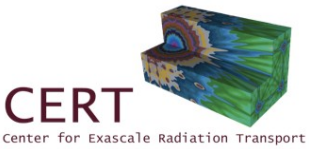
### Emerging Technologies Building (ETB), Room 2005
### &
### Thomas G. Hildebrand, Equine Center, Wagonhound Land and Livestock Education Building 0117, Room 708A

## Tuesday, December 1, 2015
**ETB 2005**

| | | |
|---|---|---|
| 6:00 – 7:00 pm | Poster Session | |
| 7:00 – 8:00 pm | Dinner | |

## Wednesday, December 2, 2015
**Equestrian Center, Wagonhound Land and Livestock Education Building 0177, Room 708A**

| | | |
|---|---|---|
| 8:30 – 9:00 am | Breakfast | |
| 9:00 – 9:30 am | TST/AST private meeting, | |
| 9:30 – 10:00 am | Overview of CERT status, | Jim Morel |
| 10:00 – 10:10 am | Status of accelerator and equipment purchases | Les Braby |
| 10:10 – 10:40 am | Initial IM1 experiments | Delia Perez-Nunez |
| 10:40 – 11:00 am | Break | |
| 11:00 – 11:20 am | IM1 calculations | Daryl Hawkins |
| 11:20 – 12:00 pm | UQ methodology, analysis, and results for IM1 | Derek Bingham |
| 12:00 – 1:00 pm | TST lunch with students | |
| 1:00 – 1:30 pm | Discussion of IM1 | |
| 1:30 – 1:50 pm | Latest scaling results, mixed-mode parallelism<br>Plans for PDT, resource usage | Daryl Hawkins |
| 1:50 – 2:10 pm | Break | |
| 2:10 – 2:40 pm | STAPL improvements, KRIPKE/STAPL status and future plans | Lawrence Rauchwerger |
| 2:40 – 3:00 pm | PDT-MCNP comparisons and NJOY data | Yunhuang Zhang |
| 3:00 – 3:45 pm | Least-Squares weighting, LL*, and multigrid | Thomas Manteuffel |
| 3:45 – 5:00 pm | Discussions/breakouts | All |
| 5:00 pm | Return to hotel before dinner | |
| 7:00 – 8:00 pm | Dinner | Madden's |




## Thursday, December 3, 2015

**Equestrian Center, Wagonhound Land and Livestock Education Building 0177, Room 708A**

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|---|---|---|
| 8:30 – 9:00 am | Breakfast | |
| 9:00 – 9:20 am | Neutron-equivalent thermal radiation calculations | Ryan McClarren |
| 9:20 – 9:35 am | Upscatter acceleration and parallel AMG diffusion solver | Jean Ragusa |
| 9:35 – 10:05 am | Planned accomplishments before review | Marvin Adams |
| 10:05 – 11:30 am | Discussions/Breakout | |
| 11:30 – 12:00 pm | Wrap-up with TST chair, AST, and center leaders | |
| 12:00 pm | Adjourn (boxed lunches provided for TST and AST) | |