

ExMatEx All-hands meeting Sept 23-25, 2014

Klaus Advanced Computing Building, Room 1116W
Georgia Tech, Atlanta GA

<http://www.cc.gatech.edu/about/directions#klaus>

Tuesday, Sept 23 morning

- 8:30 Welcome: Introductions, Logistics & Meeting Goals..... Tim Germann
Los Alamos National Laboratory
Jim Belak
Lawrence Livermore National Laboratory
Jeff Vetter
Oak Ridge National Laboratory & Georgia Tech
- 8:50 ExMatEx Overview..... Tim Germann
Los Alamos National Laboratory
Project goals, objectives, overall 5-year (agile) plan and where we are in it (including Y3 milestones for upcoming report and Y4 plans being re-evaluated this week)
- 9:20 Adaptive Sampling for Materials Science/Engineering..... Nathan Barton
Lawrence Livermore National Laboratory
Ricardo Lebensohn
Los Alamos National Laboratory
- 9:30 CoEVP proxy application..... Milo Dorr
Lawrence Livermore National Laboratory
Embedded ViscoPlasticity Scale-Bridging Proxy Application, representing the adaptive sampling scale-bridging workload. Available at: <https://github.com/exmatex/CoEVP>
- 10:00 CoHMM proxy application..... Kipton Barros
Los Alamos National Laboratory
Simplified elastodynamics scale-bridging workload, based on the Heterogeneous Multiscale Method. Available at: <https://github.com/exmatex/CoHMM>
- 10:20 Break
- 10:30 External co-design and stakeholder engagements..... Moderator: Jim Belak
Lawrence Livermore National Laboratory
Brief summaries (5-10 minutes each) from partners & stakeholders attending in person or remotely. As appropriate, these summaries may include project goals and objectives, & experiences and/or expectations of application co-design centers.
- Noon Lunch (provided)
Queue up afternoon CS discussion topics

Tuesday, Sept 23 afternoon

- Main conference room (w/ BlueJeans videoconference): discussion of materials science & engineering challenge problems and use cases (with external domain science stakeholders), following the suggested agenda below.
- Two small classrooms (each with Polycom) will be available for parallel side discussions on CS topics, including programming models and tools and techniques for performance, power, and resilience (P2R) optimization. WebEx conferencing may also be available for remote participants (contact Martin Schulz).

1:30 ExMatEx single-scale proxy applications..... David Richards
Lawrence Livermore National Laboratory

2:00 ExMatEx Y4 scale-bridging challenge problem(s)..... Nathan Barton
Lawrence Livermore National Laboratory
Ricardo Lebensohn
Los Alamos National Laboratory

2:30 Open Discussion

What aspects of more general materials science & engineering workflows expected over the next 5-10 years do our proxy apps and target problem capture (or miss) for other application areas, including (but not limited to): integrated experiment/simulation (e.g. DCS@APS, MaRIE), materials genome/ICME, additive manufacturing, etc.

5:00 Adjourn (dinner on your own)

Wednesday, Sept 24 morning

- Main conference room (w/ BlueJeans videoconference): discussion of programmability, usability, and tools (with external CS stakeholders), following the suggested agenda below.
- Two small classrooms (each with Polycom) will be available for parallel side discussions. WebEx conferencing may also be available for remote participants (contact Martin Schulz).

8:30 Summaries of CS side discussions.....Allen McPherson
Los Alamos National Laboratory

9:00 Recap of 2013-14 co-design summer schools Jim Belak
Lawrence Livermore National Laboratory
Christoph Junghans
Los Alamos National Laboratory

9:30 Open Discussion.....Moderator: Jim Belak
Lawrence Livermore National Laboratory

Discussion of programmability and usability: What are the emerging themes/lessons learned regarding X-stack and other programming models evaluated in the context of our applications? What should X-stack 2.0 look like to be useful to real-world application developers? What is the role and future of DSLs?

10:30 Open Discussion.....Moderator: Allen McPherson
Los Alamos National Laboratory

Tools and techniques for performance, power, and resilience (P²R) optimization.

Noon Lunch (off-site, with continued discussions from morning)

End of public session

Wednesday, Sept 24 afternoon

Begin internal team status updates and planning: where we are, and open discussion of where we should be, and will include in annual review report. Discussion organized according to:

(a) Karen's organizing structure from last year:

- Applications & algorithms
- Programming & systemware
- Hardware-interfacing tools

(b) Our Year 3 milestones:

- Y3.1. Scale-bridging target problem and prototype
- Y3.2. Requirements/implementation of single-physics and scale-bridging programming models
- Y3.3. Uncertainty for scale-bridging
- Y3.4. Power/resilience analysis
- Y3.5. Aspen for scale-bridging and SST coupling
- Y3.6. Reborn proxy apps (& analysis tools) release(s)

1:30pm – Programming & systemware (and milestone Y3.2) focus: What have we learned in terms of requirements (or desiderata) for programming models (continuing programmability/usability discussions from morning)?

3:00pm – Applications & algorithms (and milestone Y3.1-3) focus: Discussion of Y4 target problem, logistics (this includes systemware requirements for Y3.2), and how (or whether) we can best integrate all project efforts as part of it, including mod/sim tools, DSLs, etc.

PM Team Dinner Location TBA

Thursday, Sept 25 morning: hardware-interfacing tools focus

8:30 GREMLIN development, release (Y3.6), and use for power/resilience analysis (milestone Y3.4)

10:30 Aspen for scale-bridging and SST coupling (Y3.5)

Noon Lunch (off-site, with continued discussions from morning)

Thursday, Sept 25 afternoon: G4 and task area leads strategy session

- Report structure, content (including remaining work to be done), and writing schedule and assignments
- Review and reassessment of Y4 milestones
- Discussion of out-year plans: best use of advisory committee and Y5 plans as we look ahead to potential renewal/follow-on

7:10 Pittsburgh Pirates vs. Atlanta Braves Turner Field