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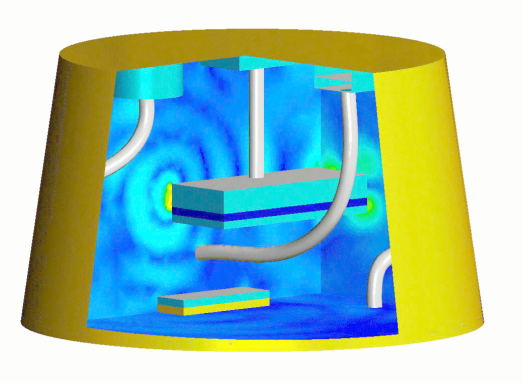

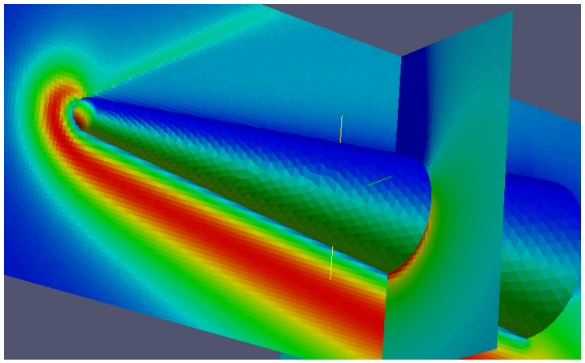

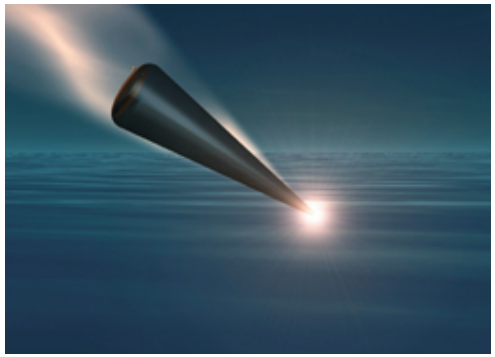

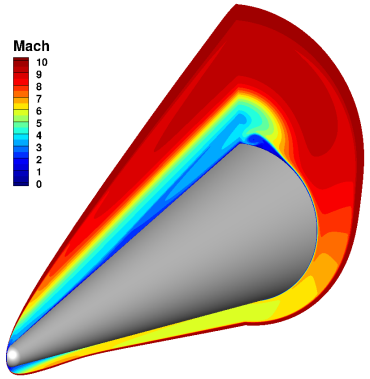

ATDM L2 Milestone

Final Review

Bill Rider & The Milestone Team

August 25, 2016

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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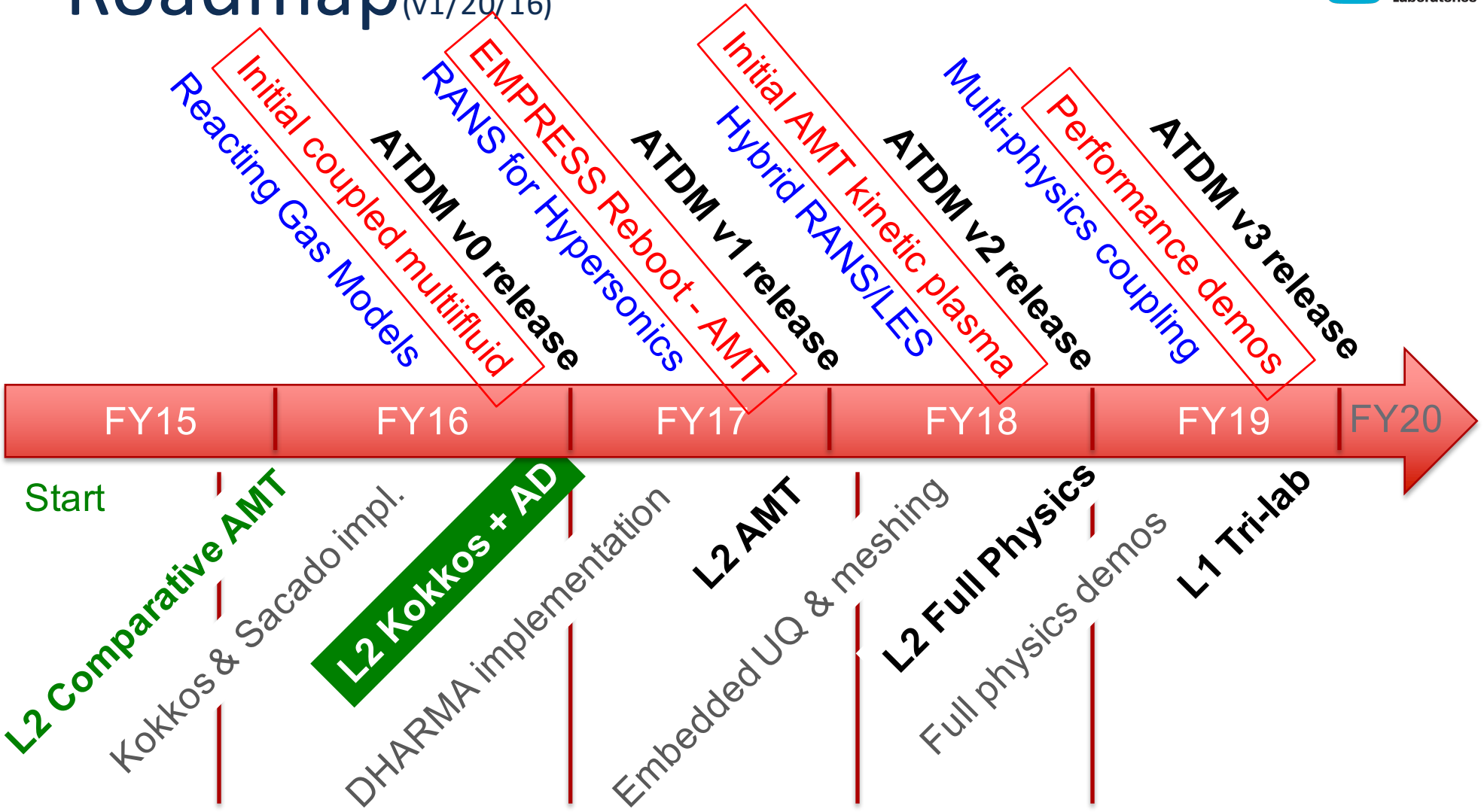
Roadmap (v1/20/16)



Gate 0: App Select

Gate 1: *Kokkos/AD* (ATS-1 Trinity)

Gate 2: *AMT* (ATS-2 Sierra)

Gate 3: *Embedded Workflow* (Pre-exascale testbeds)

Post FY19: hardening, expand turbulence capabilities (WRLES, DNS), …

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Timeline for Q4 FY16 ASC L2 Milestones

Due Date	Action	Role
AUG 31 (WED)	L2M: Complete Milestone Program Review on or before this date	Milestone PI or Lead
SEPT 02 (1st FRI)	1. PLATR: Complete Q4 L2M report to satisfy end-of-year L2M reporting activities **IMPORTANT:** When entering your PLATR write-up for your *completed* L2M, cover performance and accomplishments (and issues/resolutions) for the entire year. PEAR reviewers will only be looking at Q4 write-ups to evaluate milestone performance. Q4 L2 milestone write-ups should be complete enough to fully support and justify the score. There will be no additional information provided to reviewers (via the PEAR, etc.) discussing SNL's performance on the L2 Milestones 2. L2M Documented Evidence: (a) Forward **draft** professional documentation (SAND report or presentation**** **also an executive summary**) to L2M's program element manager (PE Mgr.) (ATDM, CS&SE, FOUS, IC, P&EM, V&V) and Chris Northrop, **and** (b) Submit professional documentation to **formal** R&A ***Requirement: Presentation package will consist of annotated slides. And an executive summary will be provided for both report and presentation*	Milestone Mgr., Lead, or PI
SEPT 09-15 (typically 2nd FRI)	1. Documented Evidence: Forward final professional and program review documentation **complete with displayed SAND # on the cover** to L2M's PE Mgr. and Chris 2. PLATR: Q4 scorecard reporting due. Finalize PLATR report for L2M	Milestone Lead or PI PE Mgr. or Delegate
SEPT 20 (TUES)	Q4 ASC MR1 Quarterly Review *PLATR reporting should be completed prior to the review, including L2M reports*	PE Mgr. or Delegate
SEPT 09-30	Chris will finalize documentation piece in PLATR. She will (1) process the L2M documented evidence into EIMS and (2) add evidence content and links into PLATR. She will coordinate documentation reporting efforts with the NW Ops & Assurance Dept. (00215)	Chris
SEPT 30, or before	Forward finalized documentation to NNSA	PE Mgr. or Delegate (Chris)

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Documented Evidence Types

Evidence Type	Requirement	Review and Approval
SAND Report	SAND report (could contain the executive summary described below)	Complete **formal** R&A. Add the assigned SAND# to the document's cover, and make sure doc displays correct info sensitivity **prior to** forwarding to Chris and others
Presentation	Presentation package will consist of two parts (could be two files): (1) Executive summary and (2) Annotated slides <u>Executive summary:</u> · Think of it as a 2-page news note · Written for NNSA · Could consist of: Introduction, milestone description, impact statement, summary of work done, path forward · Also submit to formal R&A	
Executive Summary	Regardless of the grading criteria identified for the L2M, the Program Office requires a summary of the accomplishment **in MS Word format**. See above for content details	Complete formal R&A
Program Review Document	Usually this is a signed memo from the review team which provides the details of the review, such as: milestone details including exit criteria; acknowledgement that the milestone is completed; summary of the program review (date, review team, attendees, etc.); feedback from the review team	Provide current information sensitivity markings and define access controls for the doc Milestone Mgr. and team will determine whether or not this document will complete R&A

RDT&E FY16 Getting The Job Done List (GTJDL)

DP GTJDL Items

1. Model underground nuclear explosive tests and validate weapons design codes to inform future secondary re-use or remanufacture decisions.
2. Deliver the Trinity-Haswell high performance computing system to do analysis of the most challenging B61-related underground tests.
3. Conduct neutron source tests to enhance diagnostics and inform options for the Enhanced Capabilities for Subcritical Experiments (ECSE).
4. Publish an updated 10-year boost science plan to integrate theoretical, computational, and experimental efforts in support of LEPs and stockpile modernization.
5. **Improve understanding of capabilities and gaps in weapons flight dynamics modeling.**
6. **Publish the Warhead Hostile Environment Survivability Plan outlining experimental and modeling capability requirements to certify all future LEP components for the Stockpile to Target Sequence hostile environment thresholds (both fratricide and adversarial), and describe the future development of survivability features to address an evolving geopolitical environment.**
7. Complete the first-ever Certification Readiness Exercise that will assess new materials for potential use in the W80-4 and a future ballistic missile pit-reuse warhead.
8. Continue Pu aging studies supporting stockpile assessments and analysis of pit-reuse options.
9. Develop research priorities for multi-megajoule thermonuclear fusion at laboratory scale in support of the January 2015 tri-laboratory directors' letter.
10. Document the program needed to achieve 2 subcritical experiments per year by 2019.
11. Model, assemble and test a prototype advanced radiographic injector system for existing NNSA capabilities.
12. Complete an RDT&E facilities study to include smaller-scale and upgrade investments ($5M-$20M).

Virtual Flight Testing for Hypersonic Re-Entry Vehicles*

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Exascale Challenge Problem

- **Virtual flight test simulations of re-entry vehicles from bus separation (exo-atmospheric) to target for normal and hostile environments**
- DSMC-based simulation of exo-atmospheric flight regime with hand-off to continuum Navier-Stokes at appropriate altitude
- Time-accurate wall-modeled LES of high Reynolds number (100k-10M) hypersonic gas dynamics
- **Fully-coupled simulation of re-entry vehicle ablator/thermal (shape change, ablation products blowing) and structural dynamic (random vibration) response**
- DNS and DSMC enhanced reacting gas models and turbulence models via a-priori and on-the-fly model parameter calculations
- **Embedded sensitivity analysis, uncertainty quantification and optimization**

Applications & S/W Technologies

Applications

- **SPARC (continuum compressible Navier-Stokes, hypersonic gas dynamics)**
- SPARTA (direct simulation Monte-Carlo, rarefied gas dynamics)
- Sierra (Aria – thermal response, Salinas – structural dynamics)

Software Technologies Cited

- C++
- MPI, **Kokkos** (OpenMP, Cuda), DARMA (Charm++)
- DataWarehouse, Qthreads, Node-level resource manager
- **Trilinos** (Belos, MuLue, Tpetra, Sacado, Stokhos, KokkosKernels)
- Percept, IOSS, Exodus, CGNS, netcdf, pnetcdf, HDF5
- In-situ visualization (VTK-M, Catalyst)

Risks and Challenges

- *Scalable solvers for hypersonic gas dynamics (multigrid methods for hyperbolic problems)*
- *Extreme-scale mesh generation and refinement*
- Accurate LES models for hypersonic gas dynamics
- **Developing appropriate hypersonic boundary layer/ablator surface interaction models**
- Effective task-parallelism and load balancing of heterogeneous physical model workloads

Development Plan

FY17: Demonstrate extreme-scale mesh generation and refinement; continue UQ development efforts; begin research activity on scalable solvers; develop low-dissipation schemes for unsteady turbulent gas dynamics; document KNL performance on ATS-1 (Trinity)

FY18: Focus on DARMA task-parallelism implementation; continue physics model development and implementation for hypersonic turbulent flows

FY19: Focus on multi-physics coupling and simulation development, including workflows; continue DARMA development activities; document GPU performance on ATS-2 (Sierra)

FY20: Full-physics (SPARTA-SPARC coupling, unsteady hypersonic turbulent flows, ablator & structural response coupling) demonstrations with UQ and optimization; document performance

*PI: Micah Howard (SNL)

Next Generation Electromagnetics Simulation of Hostile Environment

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Exascale Challenge Problem

- **Self consistent simulation from a hostile builder device, radiation transport, plasma generation and propagation to NW system circuits, cables and components with uncertainties**
- **Develop coupled Source Region ElectroMagnetic Pulse (SREMP) to System Generated ElectroMagnetic Pulse (SGEMP) simulation. Physical spatial domain on the order of kilometers down to system geometry down to millimeters**
- Efficient radiation transport and air chemistry through Direct Simulation Monte Carlo (DSMC) in rarified domains and condensed time history in thick regions
- Hybrid meshing (unstructured/regular mesh) for geometric fidelity near geometry and performance in the bulk domain for particle/radiation transport
- **Single integrated code base with efficient execution on diverse modern hardware**

Applications & S/W Technologies

Applications

- EMPRESS
- Drekar

Software Technologies Cited

- C++
- MPI, **Kokkos** (OpenMP, Cuda), DARMA (Charm++)
- DataWarehouse, Qthreads, Node-level resource manager
- **Trilinos** (Solvers, Tpetra, Sacado, Stokhos, Panzer, Tempus, KokkosKernels)
- Percept, IOSS, Exodus, CGNS, netcdf, pnetcdf, HDF5
- In-situ visualization (VTK-M, Catalyst)

Risks and Challenges

- **Embedded uncertainty propagation through stochastic methods such as DSMC research is in its infancy**
- *Scalable solvers for high thread concurrency not available in solver tools, and it is not clear such tools exist in the literature*
- Particle-fluid exchange of moment densities (mass, momentum and energy)
- *Coupling on uncertainties between fluid and particle based codes*
- Load-balancing computing between particle and field codes, AMT technologies

Development Plan

Y1: Complete development on fluid representation of plasma models with simple sources verified – SREMP problem at low altitudes

Y2: Simple radiation transport and PIC coupled to EM/ES fields.

Y3: PIC code verified for simple problems - SGEMP problem at high altitude

Y4: Initial coupled PIC/Fluid approach for plasma simulation – Kinetic SREMP problem at middle to low altitudes

*PI: Matt Bettencourt (SNL)

Milestone Statement

- Given the importance of both **performance portability** abstractions (Kokkos) and the coupled multiphysics and template infrastructure for embedded analysis (Sacado), this L2 milestone is designed to ensure that **the initial versions (v0) of both the aero-reentry safety application and the electromagnetic-plasma hostile environment ATDM application prototypes have demonstrated capabilities** in both these dimensions by the end of FY16.
- Successful completion of this milestone requires a demonstration of **performance portability** on multiple hardware types utilizing the CSSE Advanced Architecture Testbeds. **Completion also requires that the templated automatic propagation of sensitivities be demonstrated for the initial versions of both Sandia ATDM demonstration applications.**

Milestone Deliverables

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- **Documented demonstration of performance portability** and related analysis on v0 of ATDM applications on ASC testbeds including Nvidia, Intel Phi, and traditional CPU architectures.
- Documented demonstration **of templated automatic propagation** sensitivities for coupled multiphysics applications. A transient sensitivity analysis or a rudimentary UQ ensemble propagation will be used to satisfy this requirement.
- Demonstration **for both ATDM applications** (EM & Aero)
- Written detailed **SAND report and slides**
- **Release** of the code and capability demonstration (+input and data files)

Milestone Philosophy Evolution

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- Instead of the milestone being used to measure the successful delivery of a capability, we are changing the philosophy to something more useful.
- The milestone is a package of work that is documented (i.e., evidence) that is used to enable management decision-making
- Given the evidence from this milestone the ATDM management will act to steer the program with respect to the ideas tested in this work.
  - The choice of application targets
  - The utility and performance benefits of embedded sensitivity analysis
  - The use of Kokkos for performance-portability

Milestone Exit Criteria

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- The milestone exit criteria is set in terms of work accomplished from a minimum set (low-bar) and a series of “extra” results.
- Milestone success (passing) is predicated on the low-bar
  - Like getting a “C”
- Accomplishing more than the low-bar will be recognized as providing criteria for judging the milestone as “exceeding”
  - Like getting an “A” or “B”

Overall Status

- We believe that we have passed this milestone
- We have completed a significant number of the additional deliverables beyond the required criteria.
- The milestone has validated the fundamental vision and approach for the SNL ATDM program.
- In the process we have unearthed a number of issues and problems with our execution of the program and begun solving each of them.
- Progress in changing the approach to Trilinos and components to a more production-oriented system is ongoing and proceeding. We are cautiously optimistic.

Overall Successes & Accomplishments

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- Aero
  - Initial release of the application code
  - Kokkos used extensively, portable and tested on multiple platforms
  - Embedded sensitivity analysis
- EM
  - Initial release of the application code
  - Kokkos used extensively including Trilinos components, portable and performance tested
  - Embedded sensitivity analysis
- Sensitivity analysis
  - Utilized Kokkos in the implementation
  - Tested and compared in both application codes with comparisons
- Kokkos
  - Used extensively across all aspects of the milestone execution
  - Used on the full spectrum of ATDM platforms including performance testing

Overall Challenges & Barriers

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- Less technical risk than ideal in certain aspects of code development (model, method,…)
- Effective computing support and troubleshooting.
- Deep engagement with the ECP program; deep overlap in multiple areas (Kokkos, Trilinos, Management,…)
- Tensions between different Sandia Center cultures
- The balance between the research and production cultures
- Trilinos as a production software product
- Issue tracking and coordination
- Lack of software maturity for GPU architectures (lighter cores…)
- Staff is thin leading to gaps and potential delivery delays

Lessons Learned

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- Milestones can be managed to help management with decisions. Under this aegis more risky work may successfully be attempted.
- Manpower and personnel fragmentation is a serious issue that needs to be managed more effectively.
- The hardware testbeds are vital to success; more resources are needed.
- Leveraged software needs to be managed carefully. Without serious attention to the overall planning and coordination the benefits cannot be realized.
- Engagement with ECP provides substantial competition for resources and time. It can reduce the overall focus and energy from ATDM.

Overall Conclusion and Recommendation to Program Management

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- The vision and approach are sound and should continue
- The changes in the approach to milestones are sound and lead to better overall outcomes
- The leading edge computing platforms and environment provide a rather stringent tax on code development
- We need to manage collateral dependencies far better (e.g., Trilinos)
- We need to assure better support for a robust development environment (SEMS)
- We need to encourage a greater degree of risk in the application codes