MULTI-PHYSICS FOR NATIONAL SECURITY

Sandia's Advanced Technology Development and Mitigation (ATDM) components vision has enabled apps like EMPIRE and SPARC to build on foundational capabilities developed and deployed by other teams, providing great leverage and potential for reuse and increased impact.

EMPIRE: Preparing Electromagnetic Plasma Physics Codes for Exascale

Ionizing electro-magnetic pulse (IEMP) environments comprise both system-generated and source-region-generated electromagnetic pulse conditions. To meet mission requirements, these IEMP environments must be extrapolated from what can be realized with test facilities, and hence, validated computational simulation tools become critical. To meet this need, EMPIRE will deliver advanced electromagnetic and plasma physics code capabilities, will be performant on next-generation hardware architectures, and will provide analysis tool suites.

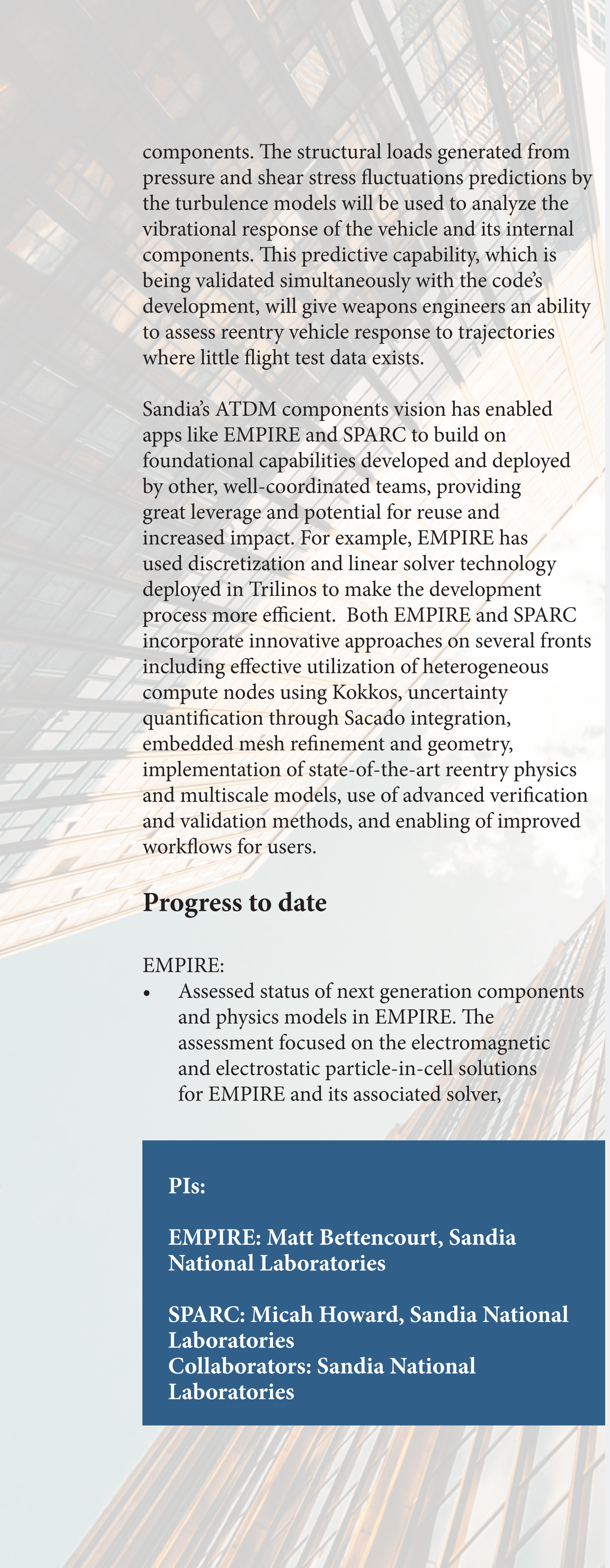
The team will focus on computing electronic effects induced by ionizing radiation interacting with materials under various reentry flight conditions. The project will develop a self-consistent plasma simulation including the radiation output of a hostile builder device, radiation transport, plasma generation and propagation down through the effects on nuclear system electronics.

The team will demonstrate the capabilities in EMPIRE with a simulation of an experiment that is relevant to the team's qualification mission: modeling a high-energy beam with particles and the background gas with a fluid at a higher fidelity than has been possible before. For the performance and code comparison metrics, the team will expand upon the validation work already performed and simulate a cavity plasma experiment. The EMPIRE results will be compared to legacy-code simulations of the same problem to show the performance and portability enhancements that have been enabled by the ATDM and ECP program.

SPARC: Sandia Parallel Aerodynamics and Reentry Code Virtual Flight Testing

Engineering and physics applications for hypersonic reentry have multiple national security implications and represent complex modeling of physical phenomena and engineering responses that significantly drive exascale computing requirements. SPARC will provide nuclear weapon qualification evidence for the random vibration and thermal environments created by reentry of a warhead into the earth's atmosphere. This state-of-the-art hypersonic flight simulation capability on next-generation hardware will include thermo-chemical nonequilibrium gas ablation models and hybrid RANS-LES turbulence models.

The pacing science challenge problem for SPARC is to perform a virtual flight test of a reentry vehicle, in its entirety, and to predict the structural and thermal response of the vehicle's components under simulated reentry environments. Performing this analysis includes simulation of the flow field around the vehicle (including the aft end and its wake) using a turbulence model suited for hypersonic, unsteady turbulent fluid dynamics. The thermal loads generated from the computational fluid dynamics simulation will be used to predict the ablation and thermal response of the vehicle's thermal protection system and internal components. The structural loads generated from pressure and shear stress fluctuations predictions by the turbulence models will be used to analyze the vibrational response of the vehicle and its internal components. This predictive capability, which is being validated simultaneously with the code's development, will give weapons engineers an ability to assess reentry vehicle response to trajectories where little flight test data exists.



Sandia's ATDM components vision has enabled apps like EMPIRE and SPARC to build on foundational capabilities developed and deployed by other, well-coordinated teams, providing great leverage and potential for reuse and increased impact. For example, EMPIRE has used discretization and linear solver technology deployed in Trilinos to make the development process more efficient. Both EMPIRE and SPARC incorporate innovative approaches on several fronts including effective utilization of heterogeneous compute nodes using Kokkos, uncertainty quantification through Sacado integration, embedded mesh refinement and geometry, implementation of state-of-the-art reentry physics and multiscale models, use of advanced verification and validation methods, and enabling of improved workflows for users.

Progress to date

EMPIRE:

- Assessed status of next generation components and physics models in EMPIRE. The assessment focused on the electromagnetic and electrostatic particle-in-cell solutions for EMPIRE and its associated solver, time integration, and checkpoint-restart components. The assessment included code verification, performance, and portability across available HPC architectures.
- Next-generation readiness was based on the incorporation of portable performance abstractions such as Kokkos (MPI+X), high performance I/O (FAODEL), and time integration libraries that allow for embedded sensitivity analysis (Tempus). Performance was tested on roughly half of each Trinity partition (KNL and HSW). The core PIC algorithm was shown to have nearly perfect weak and strong scaling, on up to 256k cores on Trinity and problems with up to 1.3B elements and 66B particles.

PIs:

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SPARC:

- Assessed the code performance and portability across Trinity-Haswell, Trinity-KNL, and GPU test platforms. Algorithmic improvements have led to significant strong-scaling speedups since the start of FY19 (e.g., ~4× for GPU performance).
- A new structured mesh refinement capability that honors CAD geometry has been integrated. By honoring the CAD geometry, each refinement of the mesh more accurately captures the shape of curved surfaces, which helps achieve more accurate simulation results. Embedding the refinement process in the application will allow SPARC to read in a coarse mesh and refine in parallel to produce dramatically larger meshes for detailed analyses on large problems.
- Conducted a comprehensive verification and validation study of hypersonic flow in SPARC validated by several experiments and reviewed an external review committee. The V&V process was thorough, including applicable frameworks, professional standards, code and solution verification, calibration, sensitivity analysis, and parametric uncertainty, and has provided a basis for using SPARC as credible analysis tool for hypersonic reentry flows.