

SNL ATDM Math Libraries – Data Propagation Components

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Overview

Combines algorithmic R&D with delivery of interoperable software components that focus on enabling advanced analysis workflows

- Sensitivity analysis
- Uncertainty quantification (UQ)
- Model calibration
- Design and shape optimization

Focus on embedded workflows for next-generation architectures

- Embedded derivative propagation through Automatic Differentiation (AD)
- Embedded, large-scale optimization

Approach

Sacado AD package in Trilinos provides analytic derivative capabilities for C++, large-scale simulation codes:

- Forward and Adjoint sensitivities
- Hessians
- Tightly integrated with Kokkos for efficient differentiation of Kokkos parallel kernels (OpenMP, Cuda, ...)
- Resulting analytic derivatives provide foundation for a variety of embedded analysis workflows:
 - Local sensitivity analysis
 - Derivative-based optimization and calibration
 - Derivative-enhanced UQ



ROL Rapid Optimization Library is a C++ package for large-scale, derivative-based optimization

- Optimal design, optimal control and inverse problems.
- Image processing and image enhancement.
- Computational mesh generation and mesh optimization.
- Embeds directly in applications through generic interfaces to applications data structures and linear algebra
- Implements a variety of state-of-the-art algorithms:
 - Constrained and unconstrained optimization
 - Optimization under uncertainty
 - Risk-averse optimization



Dakota delivers state-of-the-art, robust software for optimization and UQ including

- Global sensitivity analysis
- Forward uncertainty propagation
- Deterministic and Bayesian calibration

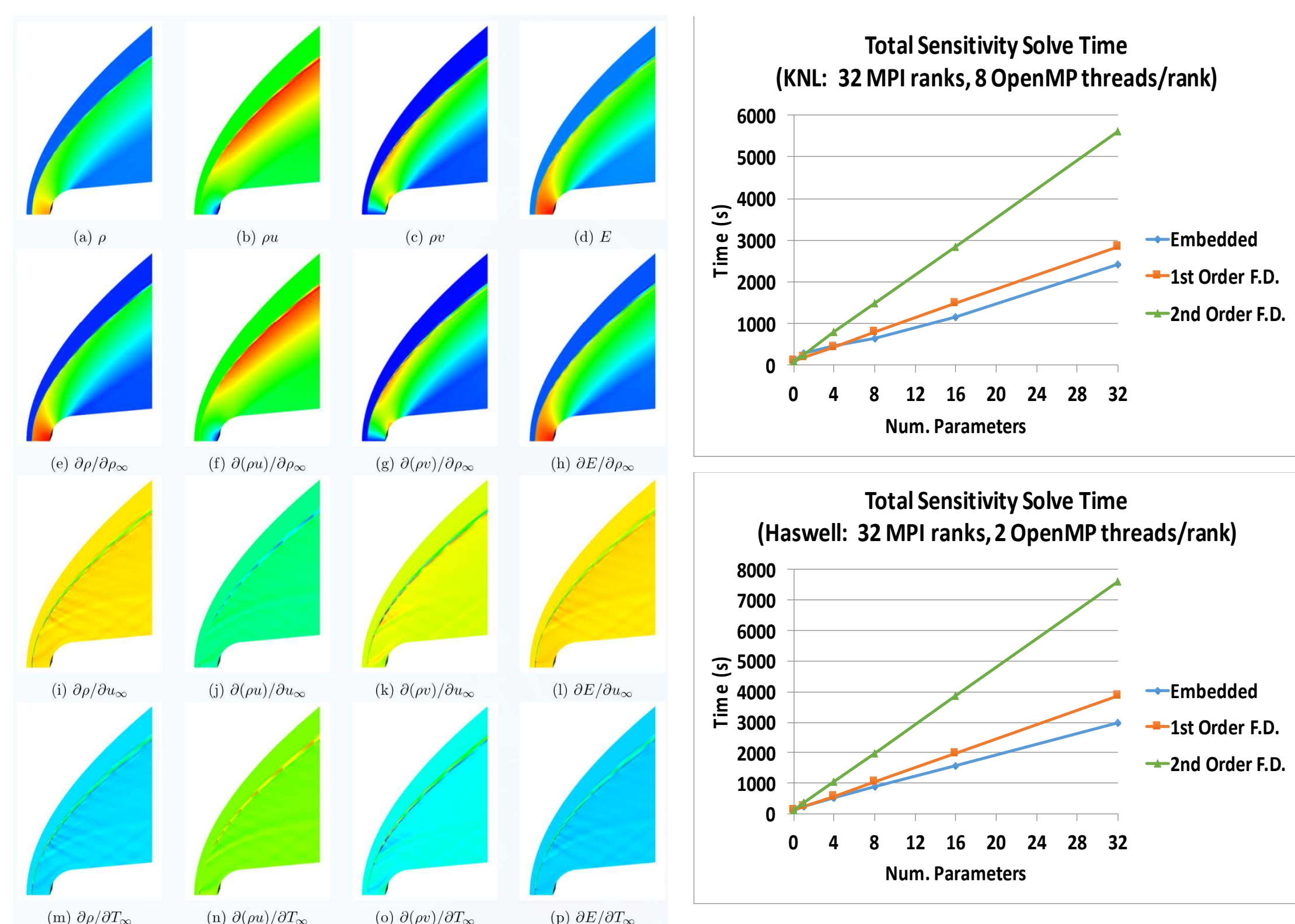


Tools integrated with ATDM SPARC and EMPIRE application codes enabling advanced embedded analysis workflows

Accomplishments

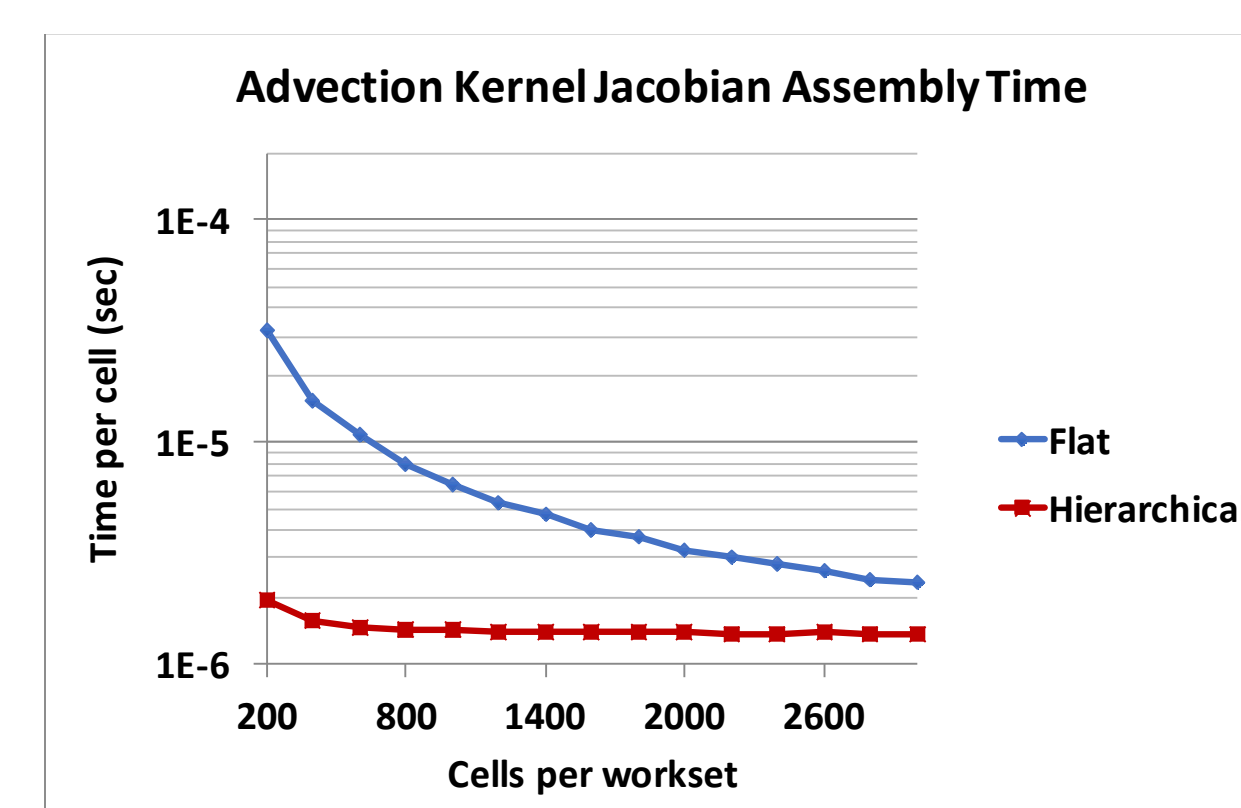
Sacado-based sensitivity analysis for hypersonic flows in ATDM/SPARC

- Demonstrates substantially improved performance compared to traditional finite differences
- Provides robust, efficient and simple-to-use sensitivities that can be visualized and explored



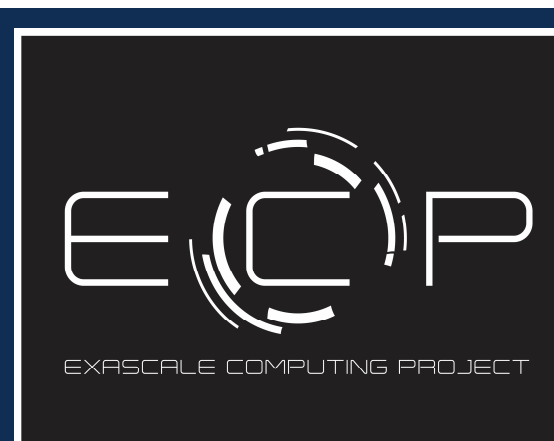
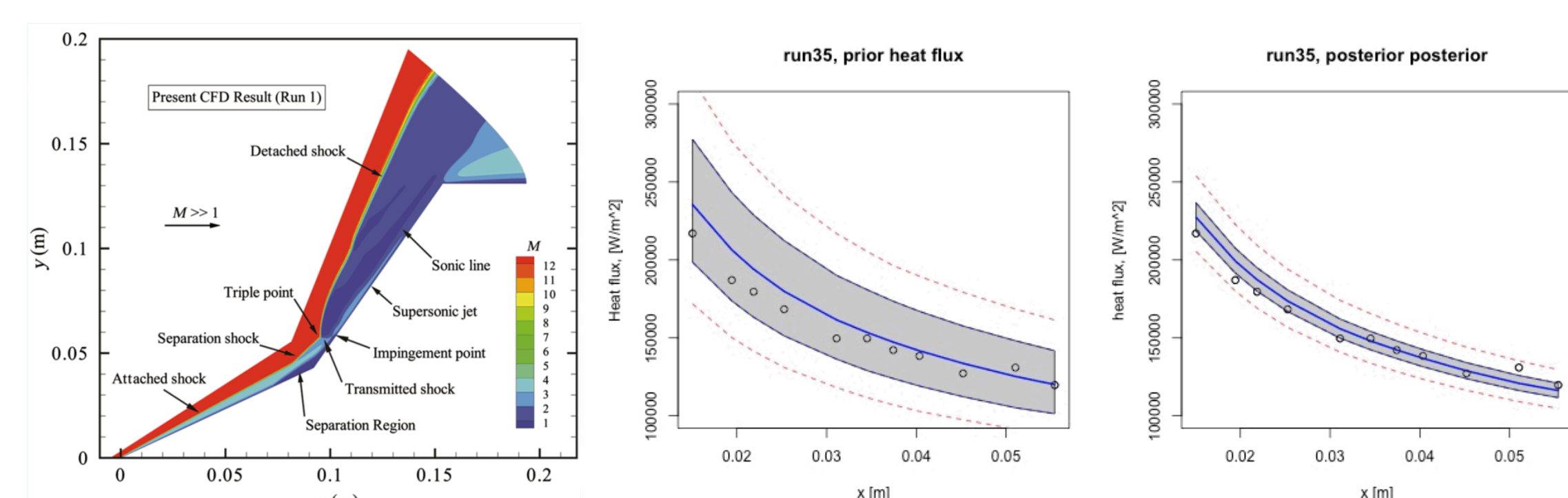
Hierarchical parallelism with Sacado enables substantially improved EMPIRE PDE Jacobian assembly performance

- Map Cuda fine-grained threads across derivative evaluation through Sacado overloaded operators
- Enables effective use of hierarchical parallelism while allowing developers to write simpler assembly kernels



Bayesian calibration with Dakota reduces uncertainties for validation of SPARC hypersonic flow models

- Calibration of hypersonic flow boundary conditions against ground-test data generated at CUBRC LENS facilities for on-going validation studies



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