Sandia National Laboratories

SPARC Leveraging of Trilinos Components

December 1, 2021

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Trilinos User Group Meeting 2021

Albuquerque, NM

SAND2021-14972 C

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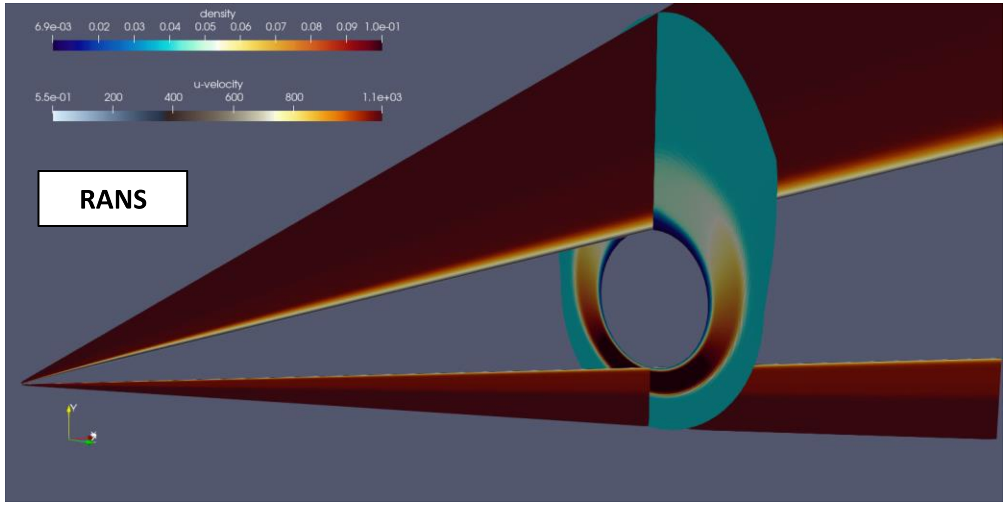
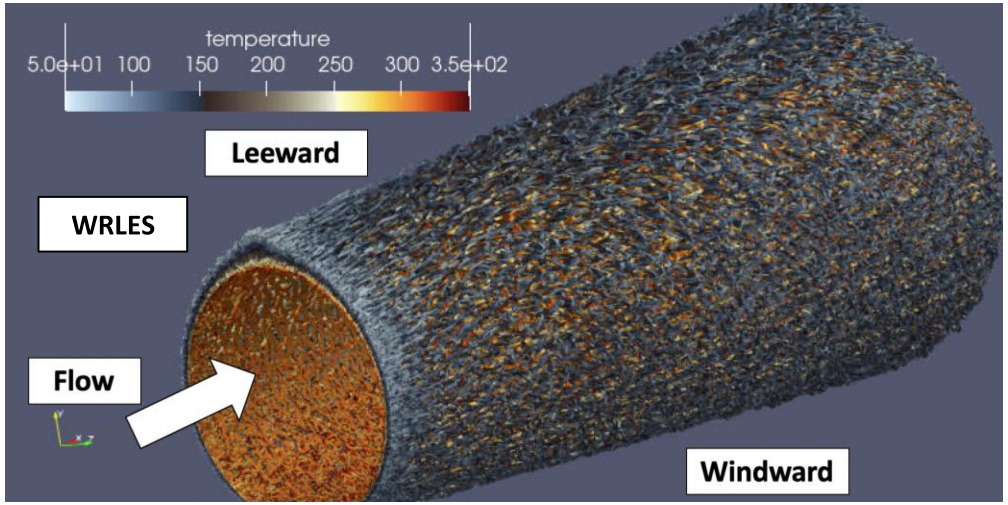
SPARC Overview

Goal: Create a credible full-system virtual flight-testing platform for hypersonic vehicles

- Modeling
  - Perfect and non-equilibrium thermal and chemical gas models
  - Euler, Laminar, RANS, Hybrid RANS/LES, LES, and DNS
  - Structured and Unstructured Finite Volume methods
  - R&D in structured and unstructured high-order methods
  - Simulate coupled ablation
  - Couples to SIERRA for full-system thermal and structural analyses
- Performance and Portability
  - Performance Portability through Kokkos
  - Good performance on x86, Arm, and GPU platforms
  - Uses performance portable/scalable linear solvers from Trilinos
  - Uses embedded geometry and inline mesh refinement
- Credibility
  - Validation with UQ against wind tunnel and flight test data
  - Visibility and peer review by external hypersonics community



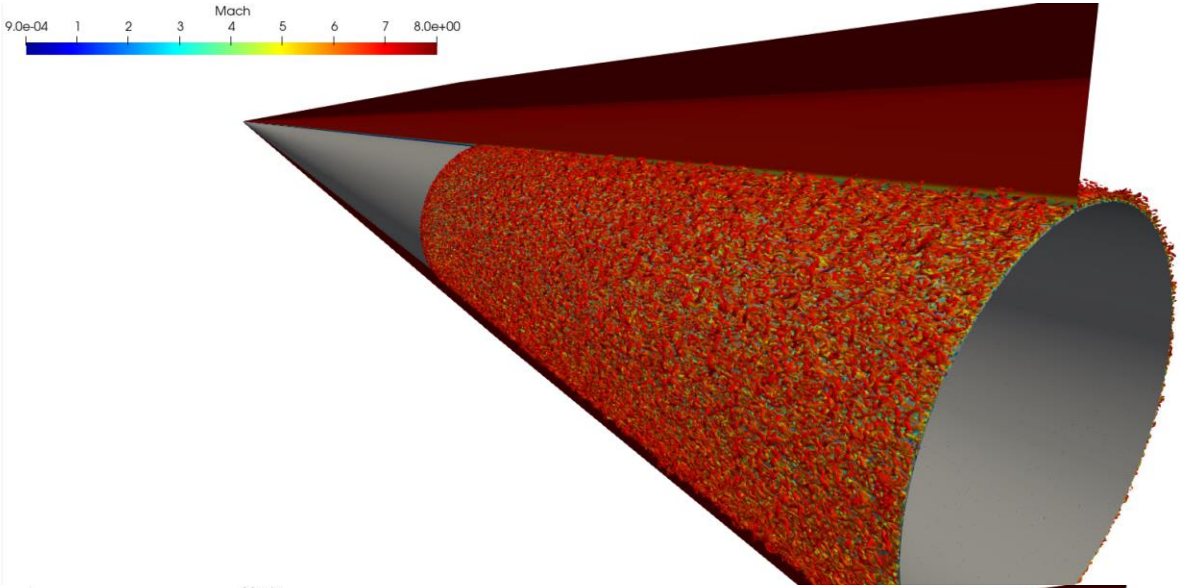


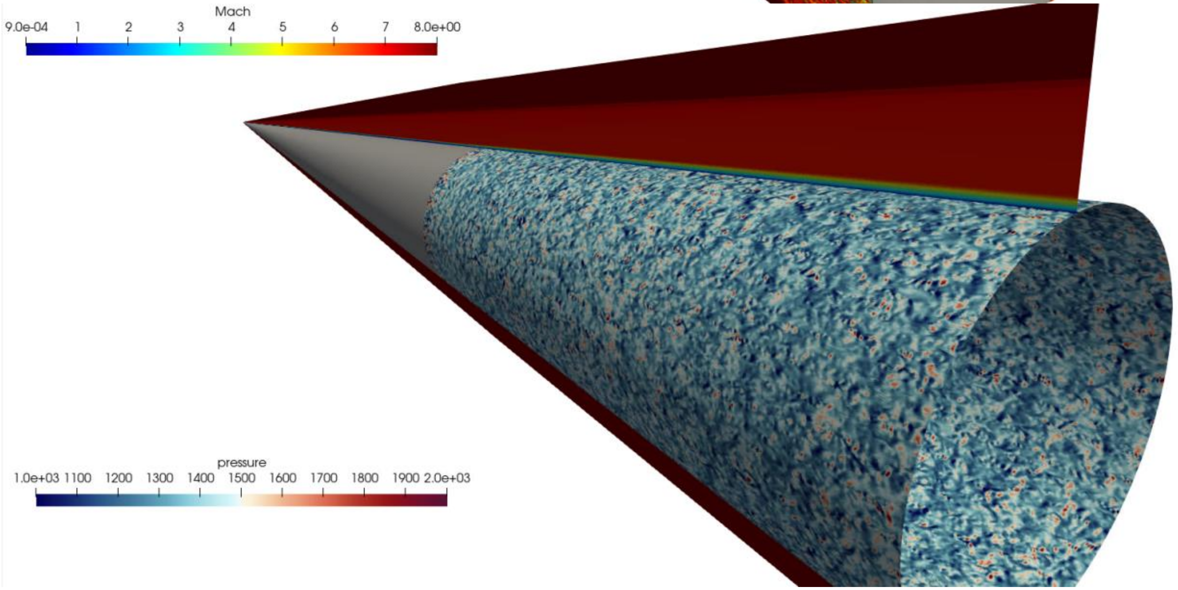
SPARC and Trilinos

- SPARC's success is dependent on several Trilinos components
  - Kokkos/Tpetra for nonlinear residual and Jacobian assembly
  - Seacas for IO
  - Kokkos Kernels/Ifpack2/Belos/Teko for linear solvers
  - STK for mesh transfers and coupling
  - Sacado for low-level sensitivity computations
- Others show promise but need more investment from application, component, or both
  - MueLu for improved steady state solvers
  - NOX/LOCA for trajectory continuation methods
  - Tempus for forward and adjoint sensitivities

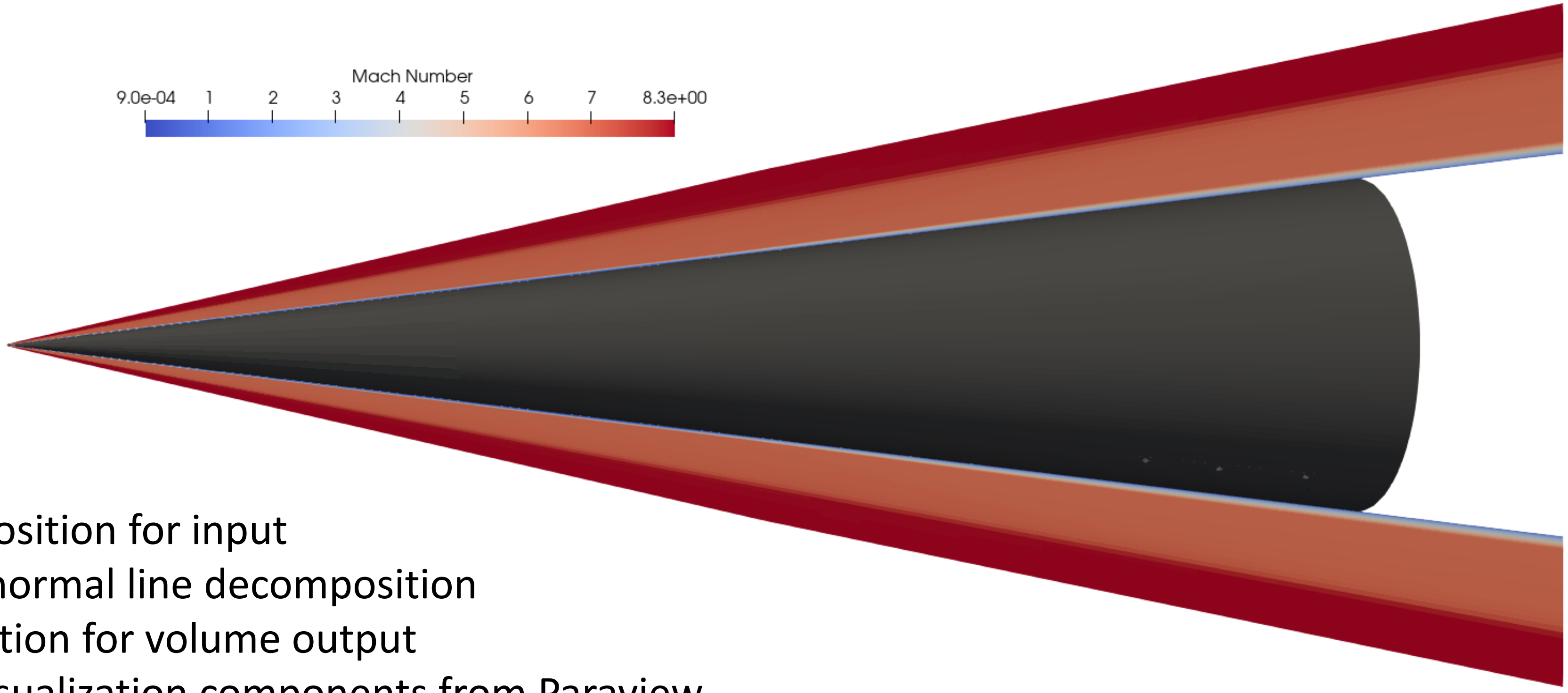
An Illustrative Example

- Unsteady scale resolving simulations are the main exascale driver for SPARC
- Assess a Mach 8 Hypersonic Wind Tunnel flow around an instrumented cone
  - Simulate turbulent boundary layer random vibration loading
  - RANS is performed around the whole cone
  - LES is performed in the turbulent boundary layer along a portion of the cone
  - Problem has a variety of scaling options
    - Wall-modeled LES vs Wall-Resolved LES
    - Streamwise and azimuthal resolution
    - Azimuthal domain extent (5 deg to 360 deg)





Production RANS Technologies



Parallel mesh IO using Seacas

- Uses automatic decomposition for input
- Native support for wall-normal line decomposition
- Uses automatic composition for volume output
- Can connect to in-situ visualization components from Paraview

Residual assembly using Kokkos and Tpetra

- Runs on x86, ARM, and GPUs
- Block data structures in Tpetra are leveraged for all aero computations

Linear solver using Ifpack2 block-tridiagonal solver

- Performance portable
- Superior convergence compared to block Jacobi solver

"Production" LES Technologies

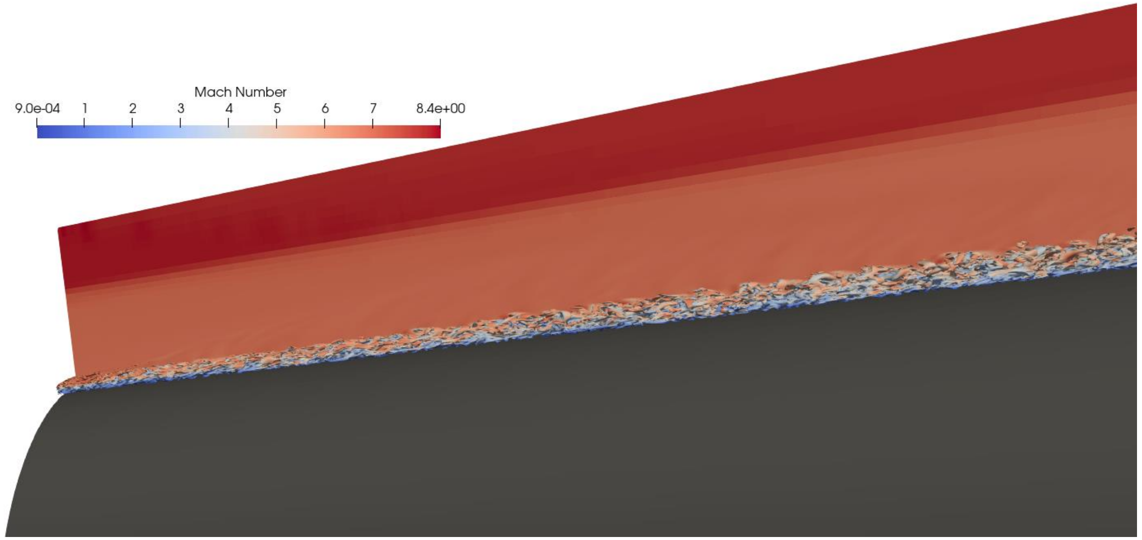
Seacas/IOSS for mesh decompose/recompose
Kokkos and Tpetra for assembly
Ifpack2 block-Jacobian solver (performance portable)
STK transfer

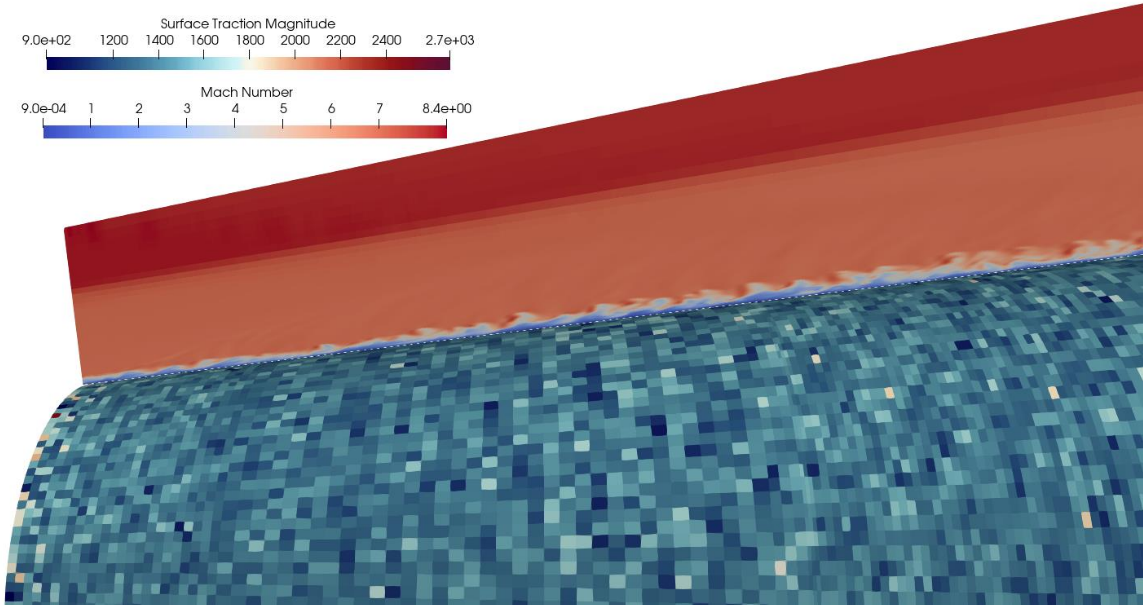
- Parallel transfer initial condition from RANS solution
- Parallel transfer boundary data from RANS solution
- Parallel transfer output extraction of subsets and transfer surface loads to structural dynamics cone mesh

STK coupling (*new*)

- MPMD coupling to Sierra/SD for passing loads when file coupling infeasible
- Provides consistency checking facilities to reduce parallel hangs during development

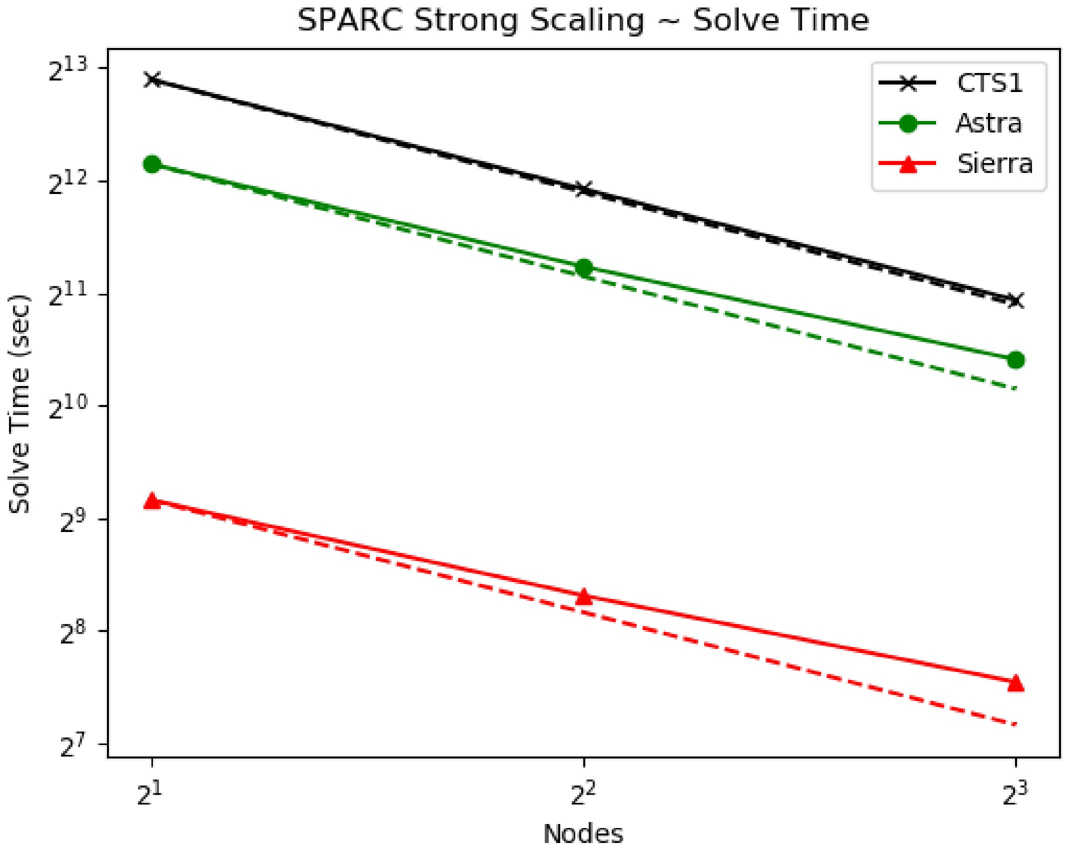
STK mesh for file coupling to Sierra/SD





Large Eddy Simulation Performance – Strong Scaling

- Initial FY22 focus on lower node counts
- CTS1 (X86) has good strong scaling
- Astra (Arm) nearly twice as fast at lower node counts
- ATS-2/Sierra (V100) is 12x faster
  - Can be further improved
  - Expose more concurrency
  - Limit register spillage



Evaluating Matrix Free Solvers in SPARC

Inexact Newton
- 7-pt stencil
- First-order inviscid Jacobian
- Neglect viscous cross-terms
- Linear convergence

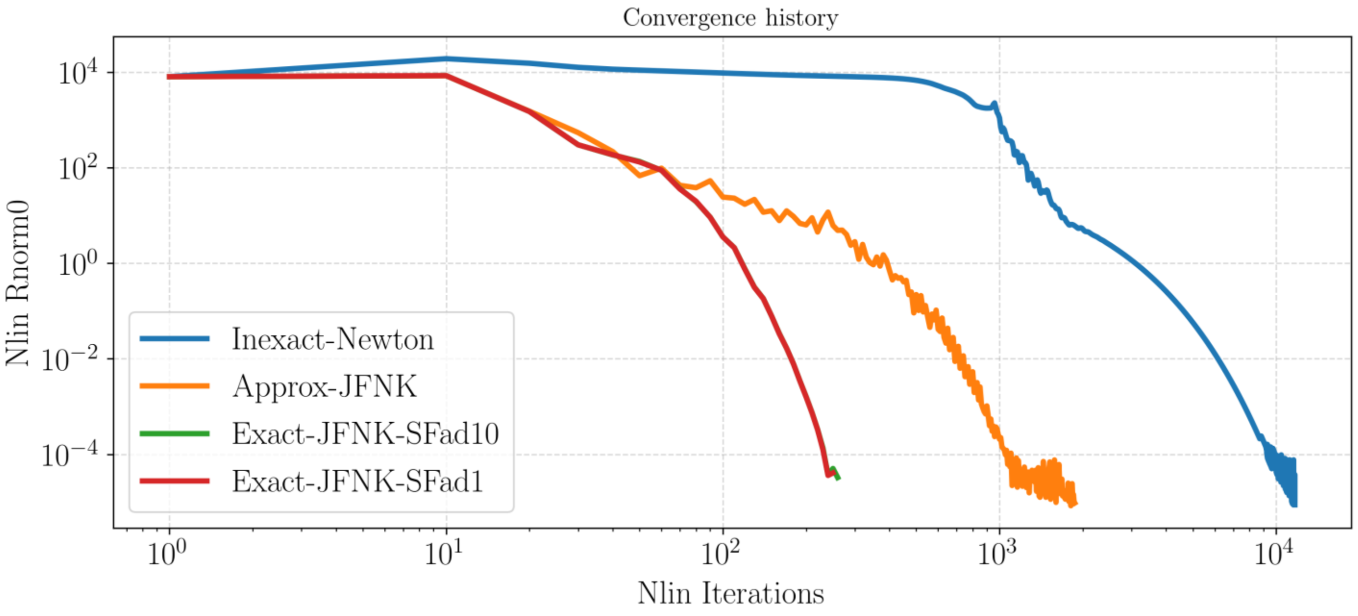
Matrix Free Approximate
- Use inexact Newton matrix for preconditioning
- Use Frechet derivative approximation
- Quadratic convergence in ideal conditions
- Nonlinear evaluations scale as number of linear iterations

Matrix Free Exact
- Use inexact Netwon matrix for preconditioning
- Use Sacado/AD for matrix-vector product
- More robust quadratic convergence
- Nonlinear evaluation w/AD scales as number of linear iterations

- Advantages of AD over Frechet Derivative
  - No perturbation constant
  - Insensitive to equation scaling
  - Can neglect sensitivities easily (e.g. SST turbulence model terms)
- Disadvantages
  - Slower!
  - Requires templated code
  - Increases build time
  - May be harder to solve

Enabled and Performance Portable courtesy of Sacado and Belos

Success story: M = 0.2 Turbulent Flat Plate BL



	Nlin Iterations	Problem Solve Time (s)	Belos Solve Time (s)
Inexact-Newton	11684	109.216	58.7482
Approx-JFNK	1873	51.9301	43.1881
Exact-JFNK-SFad10	262	46.3098	44.2337
Exact-JFNK-SFad1	256	15.2841	13.4616

- Spalart Allmaras turbulence model
  - Second-order finite volume
  - Aggressive CFL schedule
  - Exact matrix-free leads to 7x speedup
- SST turbulence model
  - Approx matrix free doesn't work
  - Exact matrix free can work if code is added to neglect terms
  - Inexact Newton still preferred

Success of exact Jacobians for real problems is more challenging and still being worked