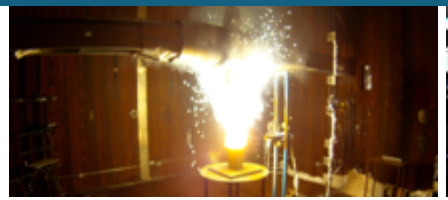
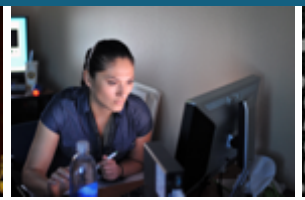
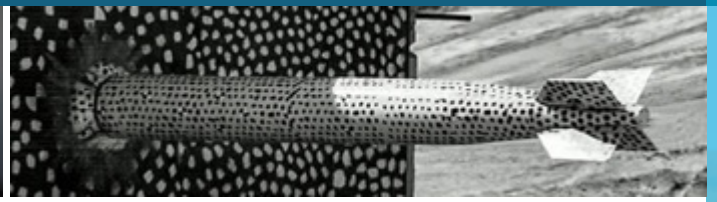
SAND2021-15104PE

Sandia National Laboratories

Sierra Thermal Fluids use of Trilinos and FY21 GPU porting milestone recap







Jonathan Clausen

Trilinos User Group meeting, December 1, 2021

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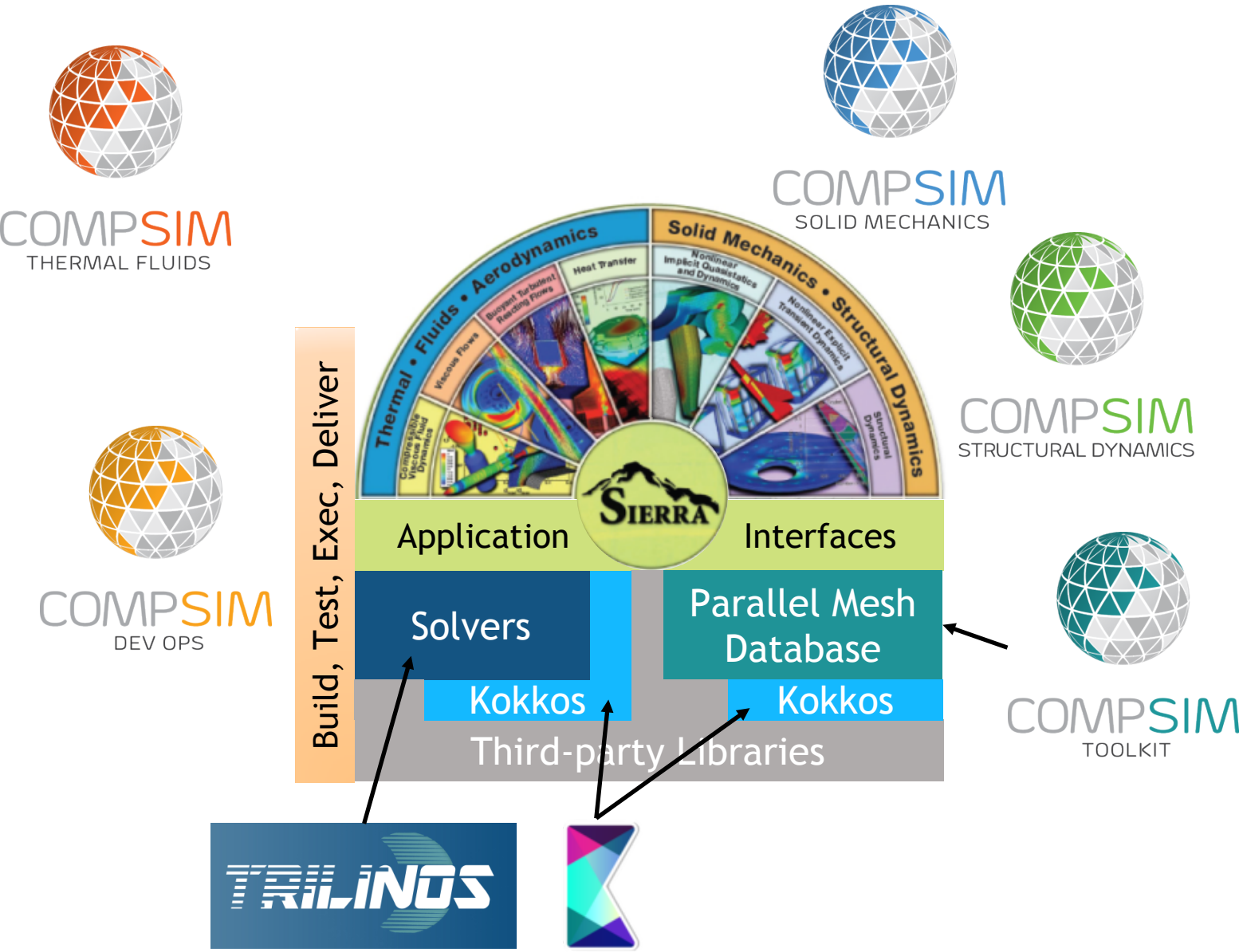
Discussion outline

1. Overview of Sierra and TF codes
2. Sierra/TF TPLs
3. Collaboration areas
4. FY21 L2 milestone recap
5. FY22 milestone needs

SIERRA Mechanics Overview



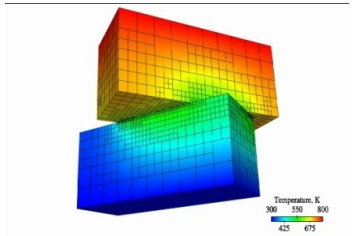
Focus evaluation on CTS-1 and ATS-2 platforms

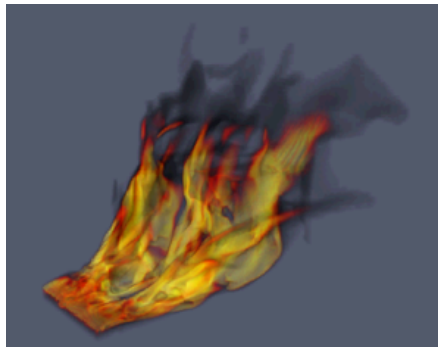
CTS-1

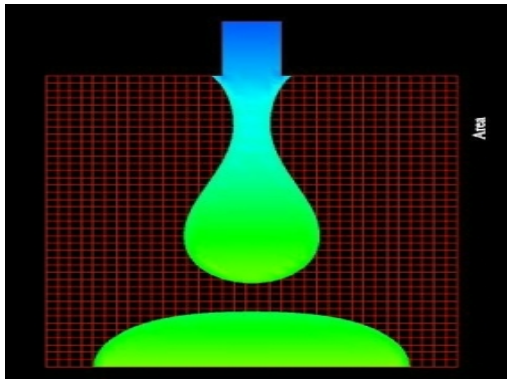
ATS-2

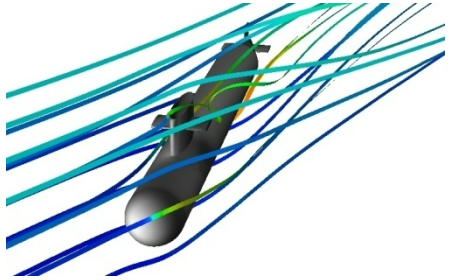
Computational Thermal & Fluid Mechanics

- **Thermal** – Heat Transfer, Enclosure Radiation and Chemistry
  - Dynamic enclosures
  - Element birth death
  - Contact
- **Aero/Sparc** – Compressible Fluid Mech.
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh
- **Multiphase** – Non-Newtonian, Multi-physics, and Free Surface Flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes
  - Pressurization models
- **Fire/Combustion** – Low Speed, Variable Density, Chemically Reacting Flows
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh









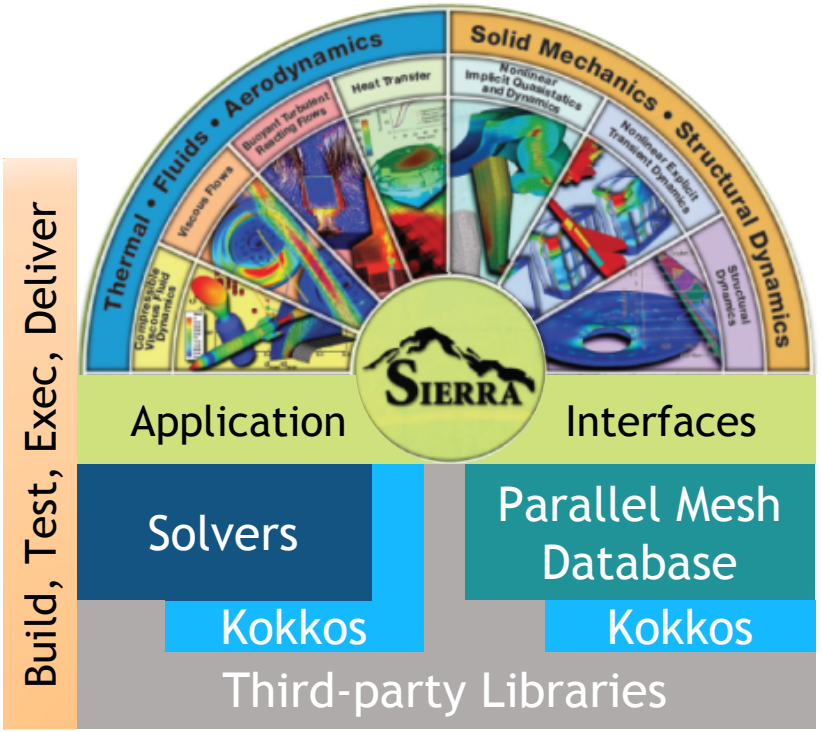
Sierra/TF codes

Sierra/TF primary codes

- **Aria**
- Fuego
- Sparc
- Nalu

Thermal/fluids/aerodynamics

- Compressible fluid mechanics with subsonic through hypersonic flows
- Non-newtonian reacting flow with free surfaces and complex material response
- Low mach number turbulent reacting flow participating media radiation
- Heat transfer with limited convection, chemistry, and enclosure radiation



Third party libraries & Trilinos usage

Trilinos packages:

- STK
- Kokkos
- Krino
- Tpetra
- Sacado
- Zoltan2
- Teko
- ROL
- FEI (Fuego only; deprecated)
- Solvers/preconditioners
  - Belos
  - Amesos2, ifpack2
  - Muelu

Other packages:

- Sierra
- Sierra Utilities
- Framework
- Apublic
- Contact
- Seacas (NetCDF/HDF5)
- Boost
- Gtest

Current collaboration areas between Sierra/TF and Trilinos

1. Sierra/TF successfully using many Trilinos TPLs
2. Frequent integration of Trilinos into Sierra (needs improvement)
3. Kokkos used extensively as abstraction layer
4. Kokkos ODE solver library
5. FY21 and FY22 joint L2 milestones
6. Trilinos – Sierra/TF meetings, every 3 weeks
7. Teko block preconditioning research

FY21 Milestone Goals

Enable production normal environment Qualification Evidence Report (QER) simulations on ATS-2

Improve GPU-solver performance and scaling to support SIERRA applications on ATS-2

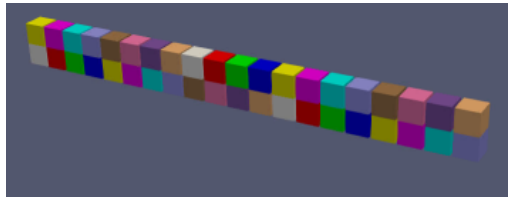
Milestone Problems

<u>Thermal Fluids Development Team</u>
Victor Brunini
Sam Subia
Alex Kucala
Dan Moser
Justin Lamb
Lincoln Collins
Mike Hansen
Neil Matula
Phil Sakievich
Robert Knaus
Stephen Lin
Tom Ransegnola
Tyler Voskuilen
Yaro Vasyliv

COMPSIM
THERMAL FLUIDS

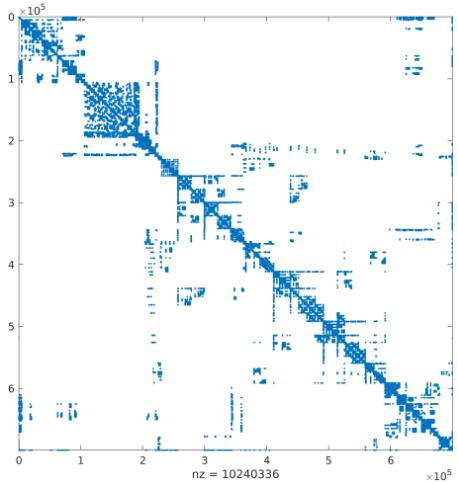
Classified Model

Normal Thermal



Surrogate

TRILINOS



Representative systems of eqs. from apps

COMPSIM
THERMAL FLUIDS

FY21 Milestone Goal: Enable production normal environment QER simulations on ATS-2

Meets:

Correct simulation of analyst provided system model on ATS-2 hardware

Exceeds:

4x end-to-end simulation performance improvement when comparing ATS-2 to CTS-1 hardware

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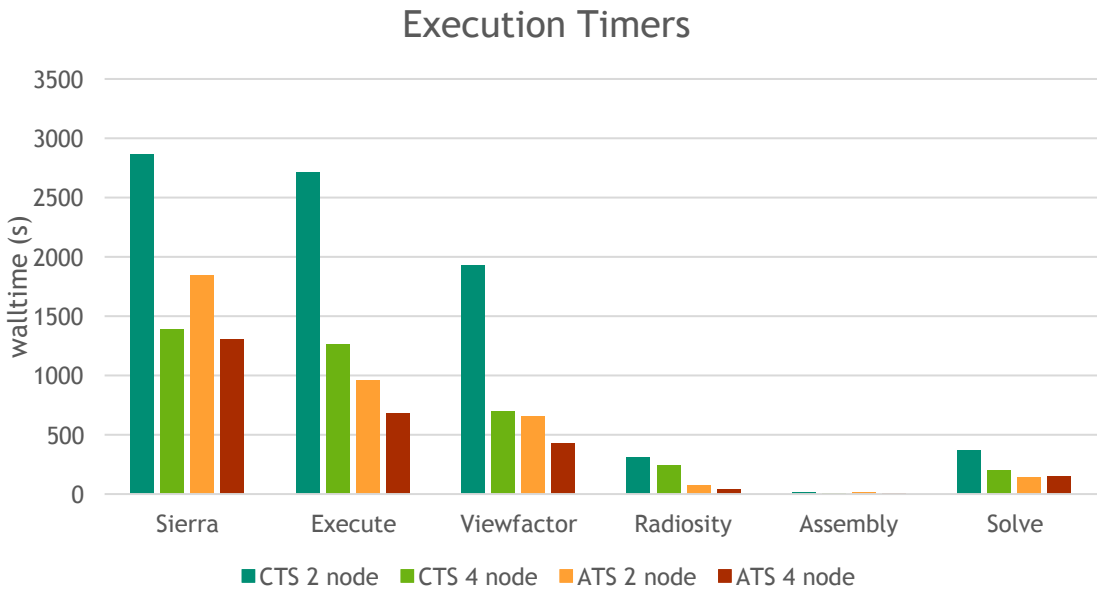
THERMAL FLUIDS

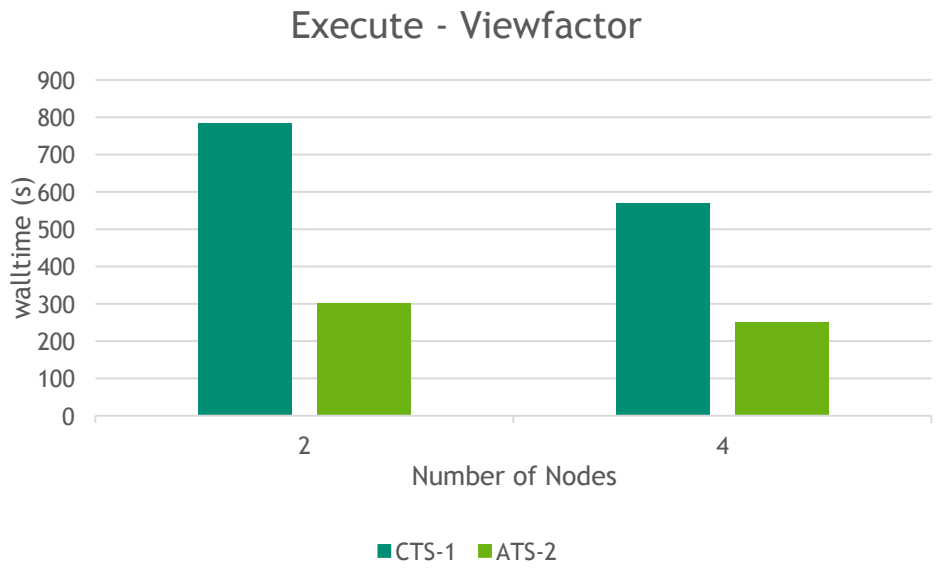
FY21 SIERRA/TF Milestone Problem

- Classified Normal thermal model as of Q1FY21 (frozen)
- 6.7 M Elements (FY20 milestone was 3.9 M)
- Radiation enclosures were biggest surprise
  - 80 enclosures
  - largest: 109,090 facets @ 73% dense (~70 GB of data!)
  - FY20 milestone had 63 K, 40K and smaller at ~25% dense
- Uses contact (late realization)
- Correctness demonstrated on ATS-2 hardware (Meets)
- Surrogate generated for performance monitoring and development

FY21 Sierra/TF Milestone Problem

COMPSIM THERMAL FLUIDS





Comments & Challenges:

- steady state
- large enclosures
  - memory constraints
  - poor solver scalability

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FY21 SIERRA/Production Readiness

- Integrated latest Trilinos changes and delivered for 5.2 Sierra release
- Improved testing on ATS-2
  - Nightly testing of normal thermal regression & verification tests
  - GPU continuous integration (CI) testing
- Significant porting of Aria capabilities
  - Encore postprocessing
  - Additional physics
  - Contact
  - Initialization (particularly mesh read & solver setup)
  - Viewfactor optimization
  - Radiosity solve performance

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THERMAL FLUIDS

FY22 Milestone Goal: Enable production abnormal environment QER simulations on ATS-2

Meets:

Correct simulation of analyst approved system model surrogate on ATS-2 hardware

Exceeds:

4x end-to-end simulation performance improvement when comparing ATS-2 to CTS-1 hardware

Correct execution on classified model with performance data

FY22 Milestone Goal: Enable production abnormal environment QER simulations on ATS-2

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- all normal physics from last-year's milestone
- level set burn front model
- chemistry solver infrastructure

TRILINOS

- ODE solver library as backend for chemistry solves
- much "harder" linear solves (dd-ilu/GMRES)

Questions?

Backup Slides

Milestone Goal: Improve GPU-solver performance and scaling to support SIERRA applications on ATS-2

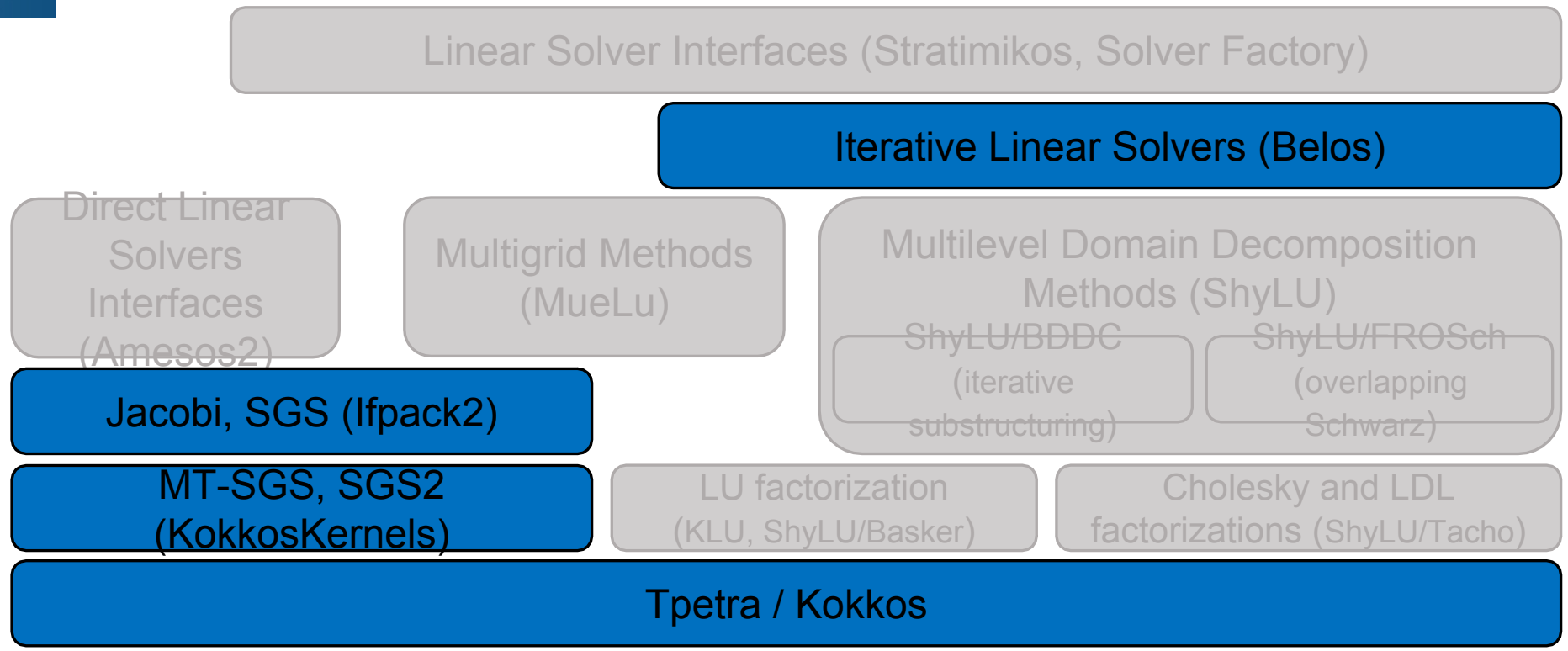
Meets:

- ✓ Support SIERRA application needs for bug fixes and performance improvements
- ✓ Demonstrate >=4x linear solver performance on ATS-2 relative to CTS-1 for CG, BiCGSTAB and GMRES solvers with Jacobi preconditioner
- ✓ Any performance improvements to TRILINOS will be available for SIERRA build/installation

Exceeds:

- Demonstrate >= 4x linear solver performance on ATS-2 relative to CTS-1 for CG, BiCGSTAB and GMRES solvers with SGS and DD-ILU preconditioners
- Demonstrate >= 4x in-situ performance of solver/ preconditioner on ATS-2 relative to CTS-1 for system model

Relevant Components for Milestone



Solver methods

Krylov methods

- Conjugate gradients, GMRES, BiCGStab

Algebraic preconditioners

- Jacobi, symmetric Gauss-Seidel (SGS)
- Domain decomposition / ILU(k)

- Fundamental reliance on Tpetra and Kokkos
- Not all solver/preconditioner combinations are valid
  - CG theoretically requires symmetric preconditioner

Relevant Components shown in blue.

Final Accomplishments/Status

Performance comparisons on CTS-1 (Eclipse) and ATS-2 (Vortex)

- Representative linear systems from SIERRA/TF thermal solve
  - 699,466 rows and 10,302,620 non-zeros
  - Systems have a few non-sparse “bulk” rows
    - Two rows with 40K and 30K entries, respectively
    - One row with 5K entries
- Using matrix reading for initial experiments
  - Initial testing prior to milestone problem being defined

Bulk Nodes:

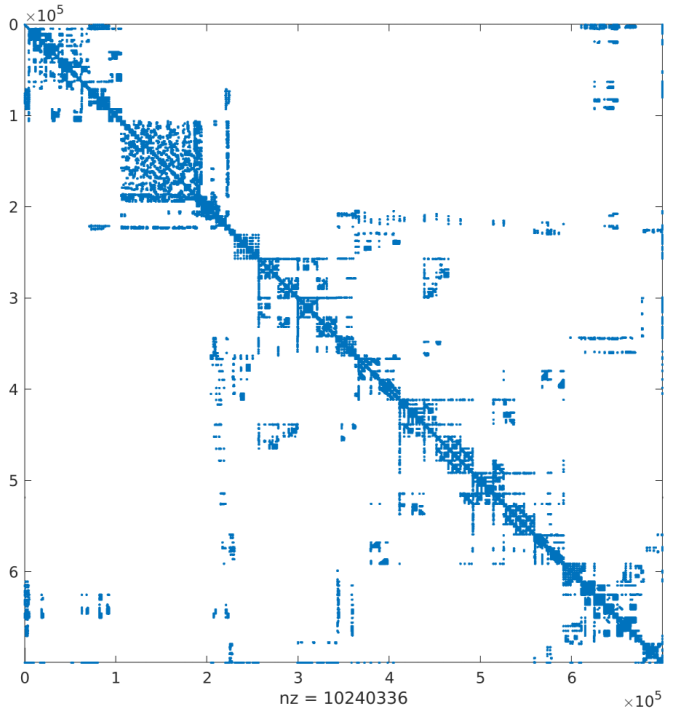
- Couples a node/DOF with all the faces on a surface.
- Example – bulk-node temperature (T_∞) for enclosed space to calculate convective heat transfer, $h(T - T_\infty)$.
- Generates non-sparse rows.

Final Accomplishments/Status

Eclipse and Vortex results, Trilinos develop branch (SHA e726b6aff)

Krylov method	Preconditioner	CTS-1* (seconds)	ATS-2 (seconds)	Speedup
GMRES	Jacobi	4.60	0.76	6x ✓
	SGS	2.55	1.02	2.5x
	DD-ILU(0)	0.41	1.1	<1
BiCGStab	Jacobi	2.3	0.53	4.3x ✓
	SGS	1.72	1.13	1.5x
	DD-ILU(0)	0.38	2.0	<1
CG	Jacobi	1.22	0.29	4.2x ✓
	SGS	1.32	0.91	1.45x
	DD-ILU(0)	0.20	breakdown	--

*using uniform rowmap



Meets
Exceeds

Meets: Achieved >4x for all Krylov methods using Jacobi.
Exceeds: Made progress in SGS & ILU(k), but didn't achieve 4x.

FY21 Improvement of Trilinos Performance on ATS-2

Krylov method	Preconditioner	Trilinos release 13 Nov. 2020 (seconds)	Trilinos develop e726b6aff (seconds)	Speedup
GMRES	Jacobi	3.86	0.76	5x
	SGS	5.52	1.02	5.4x
	DD-ILU(0)	1.18	1.08	1.1x
BiCGStab	Jacobi	5.62	0.53	10.6x
	SGS	7.75	1.13	6.86x
	DD-ILU(0)	2.08	1.96	1.1x
CG	Jacobi	3.34	0.29	11.5x
	SGS	5.95	0.91	6.5x
	DD-ILU(0)	Did not converge	Did not converge	-

- Specialized SGS kernels for matrices with bulk rows (B. Kelley)
- Tpetra, Ifpack2 UVM removal (Tpetra and SAKE teams)
- Fused residual, SpMV communication optimizations (C. Glusa)
- *Myriad of other changes throughout Tpetra stack*