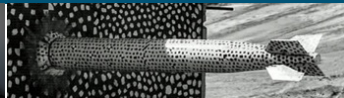




National
Laboratories

The ALEGRA Finite Element Code and Trilinos



Presented by:

Tim Fuller



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Overview

What is ALEGRA?

Applications

Trilinos usage in ALEGRA

Conclusion



What is ALEGRA?



What is ALEGRA?

ALEGRA began development circa 1996 to solve the transient equations of Lagrangian solid dynamics (balance laws)

- conservation of mass

$$\frac{d}{dt}(\rho \, dv) = \frac{d}{dt}(dm) = 0$$

- conservation of momentum

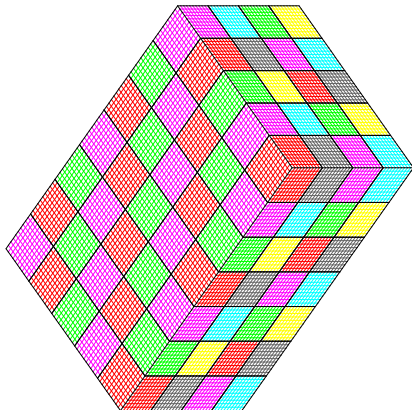
$$\rho \frac{d}{dt} \dot{U} = \rho \ddot{U} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}$$

- conservation of energy

$$\rho \frac{d}{dt} e = \rho s = \boldsymbol{\sigma} : \mathbf{D} - \nabla \cdot \mathbf{q}$$

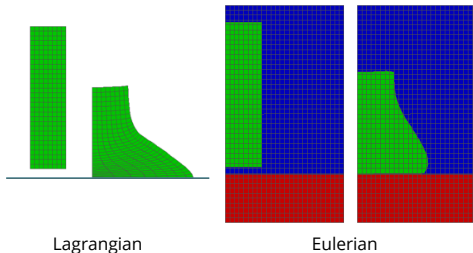
What is ALEGRA?

... using a finite element discretization ...



What is ALEGRA?

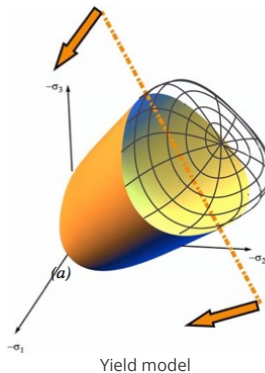
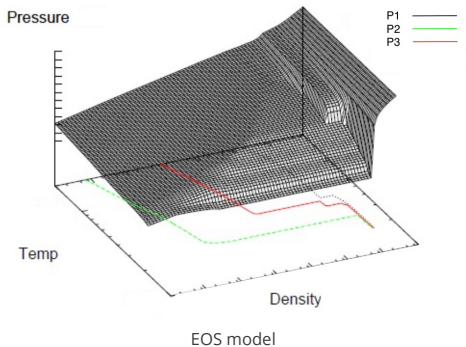
... with Lagrangian, Eulerian, Arbitrary Lagrangian-Eulerian (ALE), or XFEM capability ...



ALEGRA = **A**LE General Research **A**pplication

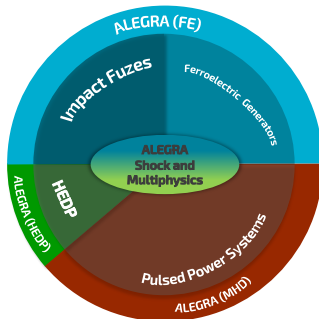
What is ALEGRA?

... using material data to close the system ...



What is ALEGRA?

... and operator splitting to add multiphysics.



Who uses ALEGRA?

Analysts developing models for

- Solid mechanics
- Shock hydrodynamics
- Electromagnetics
- Radiation hydrodynamics

Physicists and engineers interested in

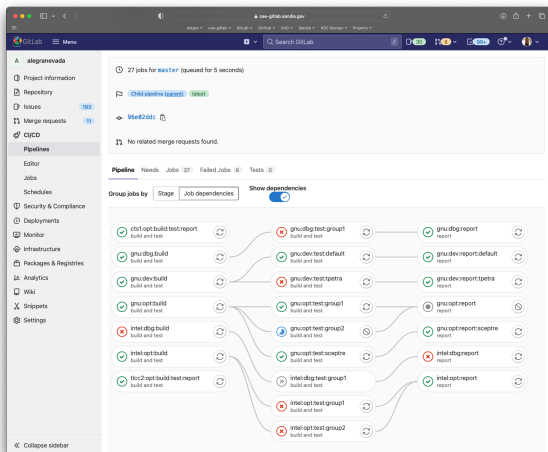
- Pulsed power
- Terminal ballistics
- Radiation effects

Civil servants and contractors in DOE and DoD physics/engineering R&D institutions

ALEGRA devops

- Git repository served on GitLab
- Spack for dependency management
- vvtest for testing
- CMake build system
- GitLab runners for CI/CD
- Toolset to glue it all together
- Toolset is python library used by developers and users to build, run, and test ALEGRA

ALEGRA Devops



ALEGRA Devops

The screenshot displays the GitLab CI/CD interface for a project named 'alegranevada'. The left sidebar contains a navigation menu with options: Project information, Repository, Issues (193), Merge requests (11), CI/CD, Pipelines (selected), Editor, Jobs, Schedules, Security & Compliance, Deployments, Monitor, Infrastructure, Packages & Registries, Analytics, Wiki, Snippets, and Settings. The main content area shows the details of a pipeline triggered 19 hours ago by Jason James Sanchez. The pipeline is titled 'Merge branch 'gmg_eos' into 'master'' and has a status of 'passed'. It includes a job named 'fs16714c' and a related merge request '1873 Consolidate GMG EOS Algorithms'. The pipeline summary shows 2 jobs for 1873 with 'gmg_eos' into 'master' in 18 seconds (queued for 1 second). The pipeline stages are: Setup (generate_merge_request_config), Merge_request (merge_request), and Downstream (merge_request #1697933).

alegranevada

- Project information
- Repository
- Issues 193
- Merge requests 11
- CI/CD
- Pipelines**
- Editor
- Jobs
- Schedules
- Security & Compliance
- Deployments
- Monitor
- Infrastructure
- Packages & Registries
- Analytics
- Wiki
- Snippets
- Settings

alegranevada

source code

Pipelines #1697930

passed Pipeline #1697930 triggered 19 hours ago by Jason James Sanchez

Delete

Merge branch 'gmg_eos' into 'master'

Consolidate GMG EOS Algorithms

See merge request 1873

2 jobs for 1873 with gmg_eos into master in 18 seconds (queued for 1 second)

fs16714c

1 related merge request: 1873 Consolidate GMG EOS Algorithms

Pipeline Needs Jobs Tests

Setup	Merge_request	Downstream
generate_merge_request_config	merge_request	merge_request #1697933

generate_merge_request_config merge_request merge_request #1697933

collapse sidebar

ALEGRA Devops

The screenshot displays the GitLab CI/CD interface for a project named 'alegranevada'. The left sidebar contains a navigation menu with options: Project information, Repository, Issues (193), Merge requests (11), CI/CD, Pipelines (selected), Editor, Jobs, Schedules, Security & Compliance, Deployments, Monitor, Infrastructure, Packages & Registries, Analytics, Wiki, Snippets, and Settings. The main content area shows the details of a pipeline triggered 19 hours ago by Jason James Sanchez. The pipeline is titled 'Merge branch 'gmg_eos' into 'master'' and has a status of 'passed'. It includes a summary of 8 jobs for '1873 with gmg_eos into master' in 116 minutes and 50 seconds. A job named 'f516714c' is highlighted. Below, the pipeline structure is shown with a 'Upstream' section containing a job 'alegranevada #1697930' and a 'Parent' link. The main pipeline consists of two parallel stages: 'gnu:opt:build' (build and test) and 'gnu:opt:test' (build and test), both of which are successful. The final job is 'gnu:opt:report' (report), which is also successful. The interface includes a 'Delete' button for the pipeline and a 'Show dependencies' toggle.

alegranevada

Project information

Repository

Issues 193

Merge requests 11

CI/CD

Pipelines

Editor

Jobs

Schedules

Security & Compliance

Deployments

Monitor

Infrastructure

Packages & Registries

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Snippets

Settings

alegranevada

source code

Pipelines

#1697933

passed Pipeline #1697933 triggered 19 hours ago by Jason James Sanchez

Delete

Merge branch 'gmg_eos' into 'master'

Consolidate GMG EOS Algorithms

See merge request 1873

8 jobs for 1873 with gmg_eos into master in 116 minutes and 50 seconds (queued for 1 second)

Child pipeline (parent) latest

f516714c

1 related merge request: 1873 Consolidate GMG EOS Algorithms

Pipeline Needs Jobs Tests

Group jobs by Stage Job dependencies Show dependencies

Upstream

alegranevada #1697930 Parent

gnu:opt:build build and test

gnu:opt:test build and test

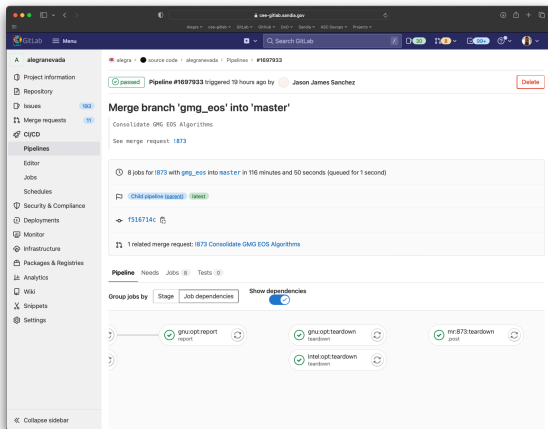
gnu:opt:report report

intel:opt:build build and test

intel:opt:report report

Collapse sidebar

ALEGRA Devops

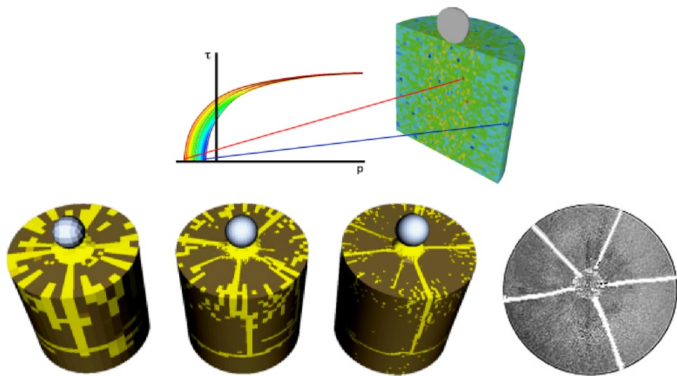




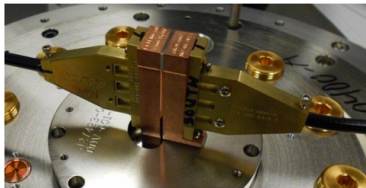
Applications



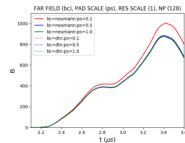
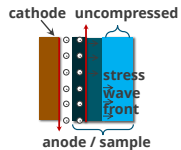
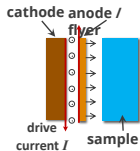
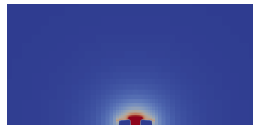
Validating theories of brittle damage



Dynamic material properties (DMP)



Compute Accurate Magnetic Field Drive History in the Gap at the Material Surface



MRTI mitigation via screw pinch mechanism

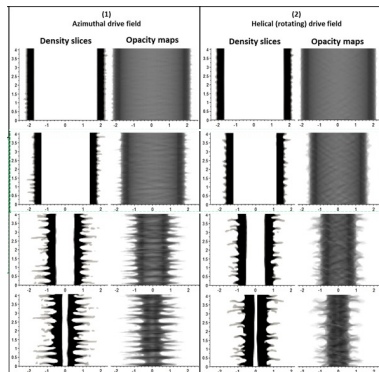
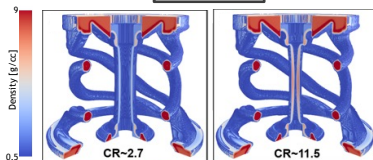
Azimuthal drive field implosion

vs.

Helical (rotating) drive field produced
by Z design return current structure

$$\beta = \frac{B_z}{B_\phi} \sim 0.5$$

3D ALEGRA

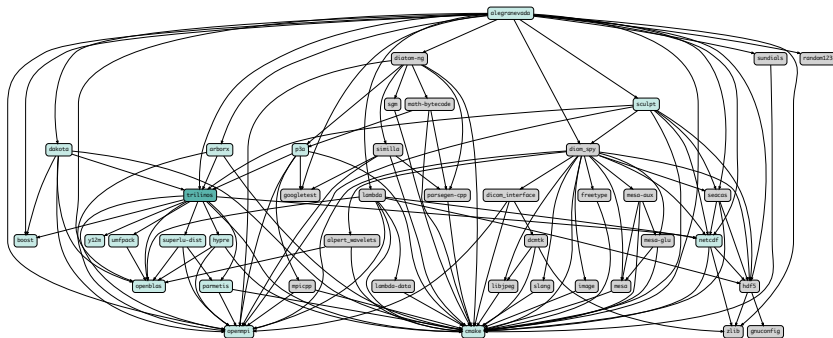




Trilinos usage in ALEGRA

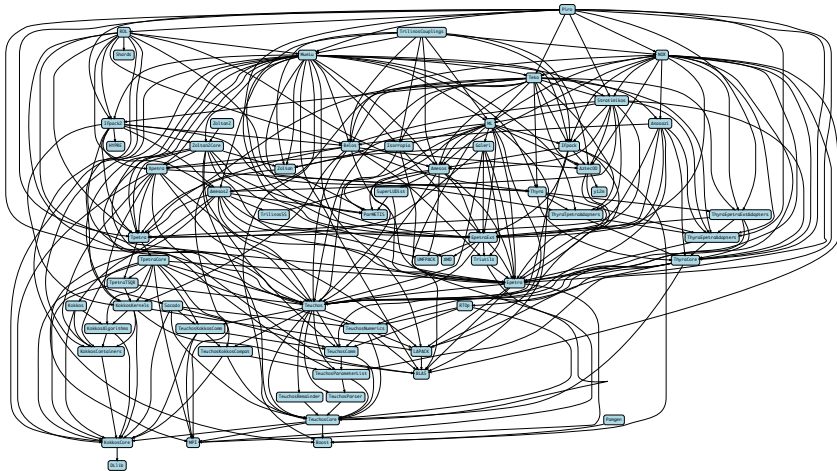


ALEGRA depends on many third-party libraries



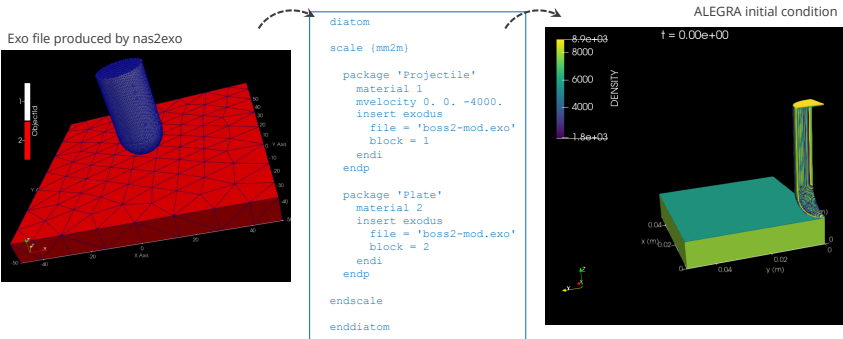
Trilinos plays a central role in ALEGRA by providing data structures and solvers required by key physics capabilities.

ALEGRA depends on many Trilinos packages



CAD insertion through SEACAS

The SEACAS `nas2exo` tool converts Nastran bulk data files to Exodus files that can be imported into an ALEGRA simulation



Epetra to Tpetra migration in MHD physics

Requirements

- Transition Epetra/AztecOO/ML to Tpetra/Belos/MueLu
- Enable 64 bit global indices to enable 2^{32} (or more) unknowns
- Ensure same results using Tpetra stack as Epetra stack

Strategy

- Support both Epetra and Tpetra via runtime switch
- Work with Trilinos developers to develop missing functionality in Tpetra stack
- Develop IO capabilities to compare results between Epetra/Teptra stacks
- Nightly regression testing of both stacks

Lessons learned

- Epetra does a lot of work under the hood that users of Tpetra must do themselves
- Tpetra_FECrsGraph, Tpetra_FECrsMatrix, and Tpetra_FEMultiVector had a non-intuitive interface (fixed)
- Belos and MueLu lack(ed) implementations for several solvers and preconditioners implemented in AztecOO/ML that users of ALEGRA depend on

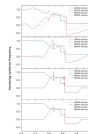
3D GMHD(XMHD) ALEGRA

1) Original implementation of GMHD equations (Hall term) was found to contain a near null space but included non-physical oscillatory modes complicating scalable linear solves.

$$\int \left(\frac{\epsilon}{\Delta t} + \underbrace{\chi_{\beta} \sigma^{n+1} \Pi_P}_{\text{when Hall term dominates, } \approx \frac{1}{3} \text{ of spectrum is nearly 0}} \right) \mathbf{E}^{n+1} \cdot \Psi \, d\Omega + \int \frac{\Delta t}{\mu} \operatorname{curl} \mathbf{E}^{n+1} \cdot \operatorname{curl} \Psi \, d\Omega$$

when Hall term
dominates, $\approx \frac{1}{3}$ of
spectrum is nearly 0

solve for \mathbf{E}^{n+1}



2) Reformulated into 2x2 system which avoids element projections in Ohm's law to produce a matrix more amenable to solver technology.

Block edge
element matrix

$$\begin{bmatrix} \mathbb{A}_{11} & \mathbb{A}_{12} \\ \mathbb{A}_{21} & \mathbb{A}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{E}^{n+1} \\ \mathbf{J}^{n+1} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix},$$

$$\mathbb{A}_{11}(\hat{\mathbf{E}}_i, \hat{\mathbf{E}}_j) = \frac{\epsilon}{\Delta t} \int_{\Omega} \hat{\mathbf{E}}_i \cdot \hat{\mathbf{E}}_j \, d\Omega + \frac{\Delta t}{\mu} \int_{\Omega} \operatorname{curl} \hat{\mathbf{E}}_i \cdot \operatorname{curl} \hat{\mathbf{E}}_j \, d\Omega$$

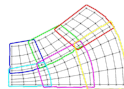
$$\mathbb{A}_{21}(\hat{\mathbf{J}}_i, \hat{\mathbf{E}}_j) = - \int_{\Omega} \sigma^{n+1} (\hat{\mathbf{J}}_i \cdot \hat{\mathbf{E}}_j) \, d\Omega$$

$$\mathbb{A}_{12}(\hat{\mathbf{E}}_i, \hat{\mathbf{J}}_j) = \int_{\Omega} \hat{\mathbf{E}}_i \cdot \hat{\mathbf{J}}_j \, d\Omega$$

$$\mathbb{A}_{22}(\hat{\mathbf{J}}_i, \hat{\mathbf{J}}_j) = \int_{\Omega} \left(\left(1 + \frac{\tau}{\Delta t} \right) (\hat{\mathbf{J}}_i \cdot \hat{\mathbf{J}}_j) - \frac{e\tau}{m_e} [\hat{\mathbf{J}}_i \cdot (\mathbf{B}^n \times \hat{\mathbf{J}}_j)] \right) d\Omega$$

3) Designed **patch** preconditioners to resolve near null space errors and complement existing algebraic multigrid preconditioners.

Tuminaro Led Late Start LDRD – “Composing preconditioners for multiphysics PDE systems with applications to Generalized MHD”
SAND2022-12164R



3D GMHD(XMHD) ALEGRA

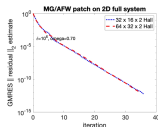
ALEGRA GMHD Solver Strategy going Forward

- 1) Devise and implement a production 3D algebraic multigrid software strategy based on MatLab based geometric multigrid analysis of sample Alegra matrices.

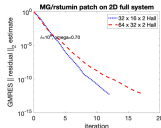
Two types of patch preconditioners have been investigated:

Arnold-Faulk-Winter (MG/AFW) and Adjacent Elements (MG/rstumin)

Scalable



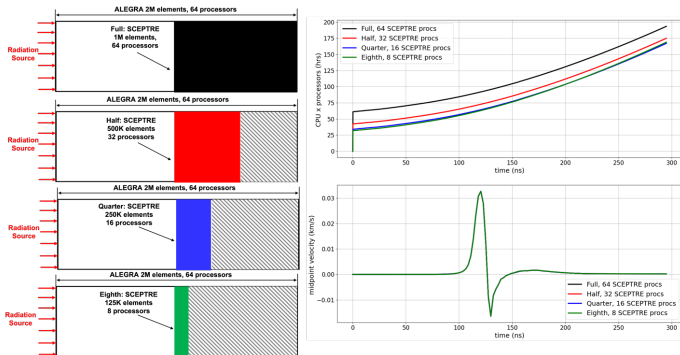
Faster



- 2) Trilinos impact: work should result in a better patch preconditioner infrastructure useful for dealing with multiple near null space preconditioning issues.
- 3) Will also investigate additional XMHD model extensions and the associated impact on discretization and solver strategy.

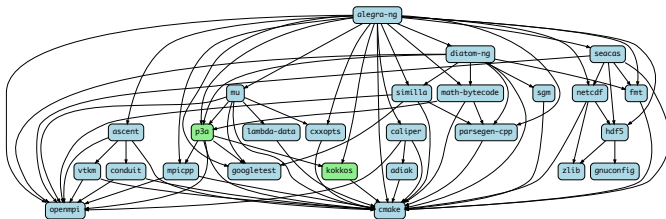
ALEGRA-SCEPTRE coupling through STK

- ALEGRA-SCEPTRE interface allows radiation transport physics subdomains, for which SCEPTRE is only applied to relevant parts of a problem
- Coupling achieved via STKSearch, STKTransfer, and MPI MPMD interfaces



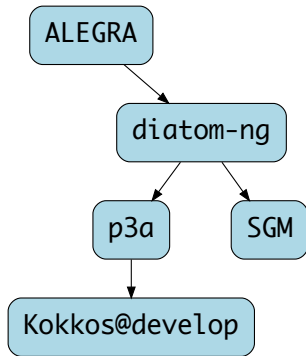
ALEGRA performance portability through Kokkos

The ALEGRA project has a performance portability effort to rewrite ALEGRA functionality using Kokkos and modern C++17

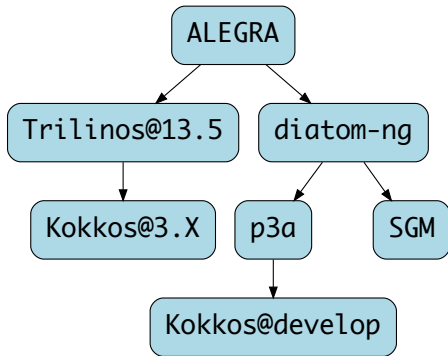


- Achieved across Intel CPUs, NVIDIA V100 GPUs, and NVIDIA A100 GPUs
- Developed SIMD types for guaranteed efficient outer loop vectorization on Intel and ARM CPUs
- SIMD types are being moved into Kokkos to benefit other Sandia applications
- Kokkos built standalone and for GPUs uses the built-in CMake support for CUDA, not the Kokkos compiler wrappers

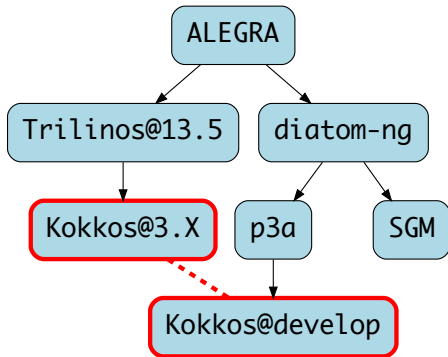
Next-gen geometry insertion



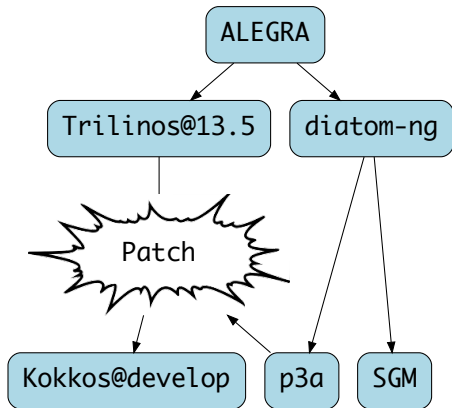
Next-gen geometry insertion



Next-gen geometry insertion



Next-gen geometry insertion





Conclusion



Conclusion

- ALEGRA depends on over 4 dozen Trilinos packages
- Trilinos is a key component to ALEGRA delivering to its customers
- ALEGRA uses both the Epetra and Tpetra stack and is currently migrating to fully Tpetra
- Infrequent Trilinos releases causes issues in a Spack eco system
- Inability to use intrinsic CMake CUDA support is an obstacle for ALEGRA's GPU strategy
- Inability to link external Kokkos causes significant devops issues