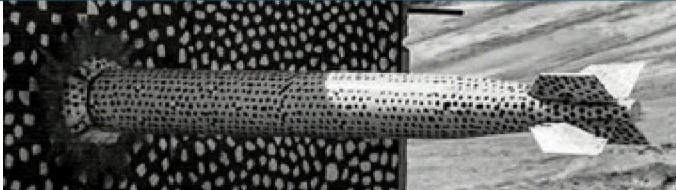


Gemma: an ATDM Electromagnetics Code



PRESENTED BY

Salvatore Campione



SAND2019-5312PE



SAND2019-XXXX

Sandia National Laboratories is a
multimission laboratory managed and
operated by National Technology and
Engineering Solutions of Sandia LLC, a wholly
owned subsidiary of Honeywell International
Inc. for the U.S. Department of Energy's
National Nuclear Security Administration
under contract DE-NA0003525.



- Gemma is a new electromagnetic radiation modeling application written for modern heterogeneous compute architectures tailored toward nuclear deterrence

FY19

- Identify Plan Forward on Gemma UI/UX
- MPI Implementation and Demo on CPU/MIC or CPU/GPU
- First Demo of Representative Coupling Simulation
- Implement time history of unit test coverage/regression test timing
- Iterative Physical Optics (IPO) Implementation and Demo

Motivation:

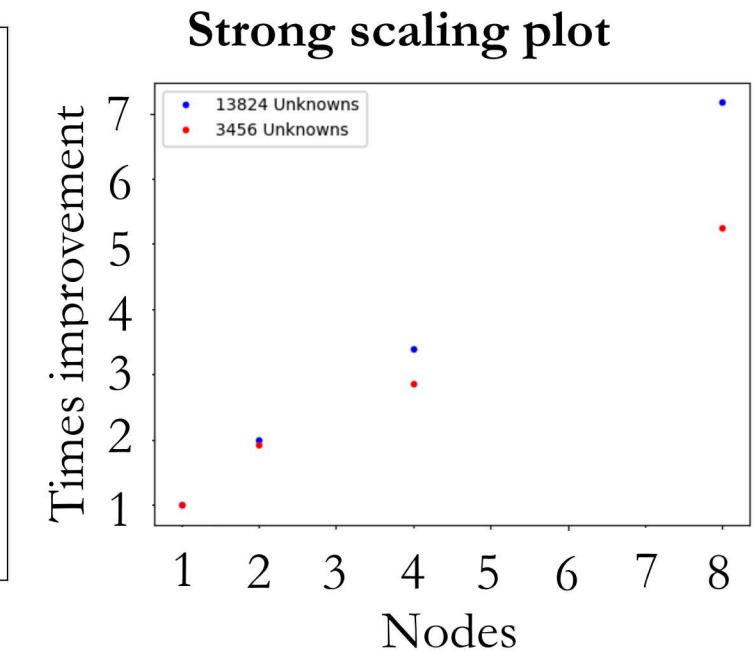
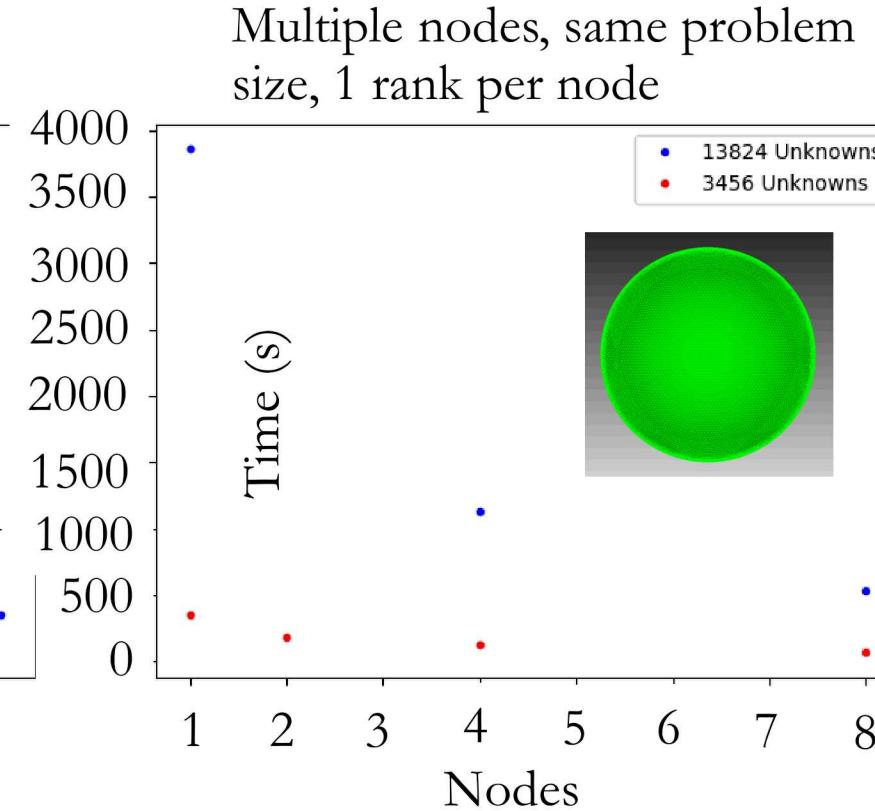
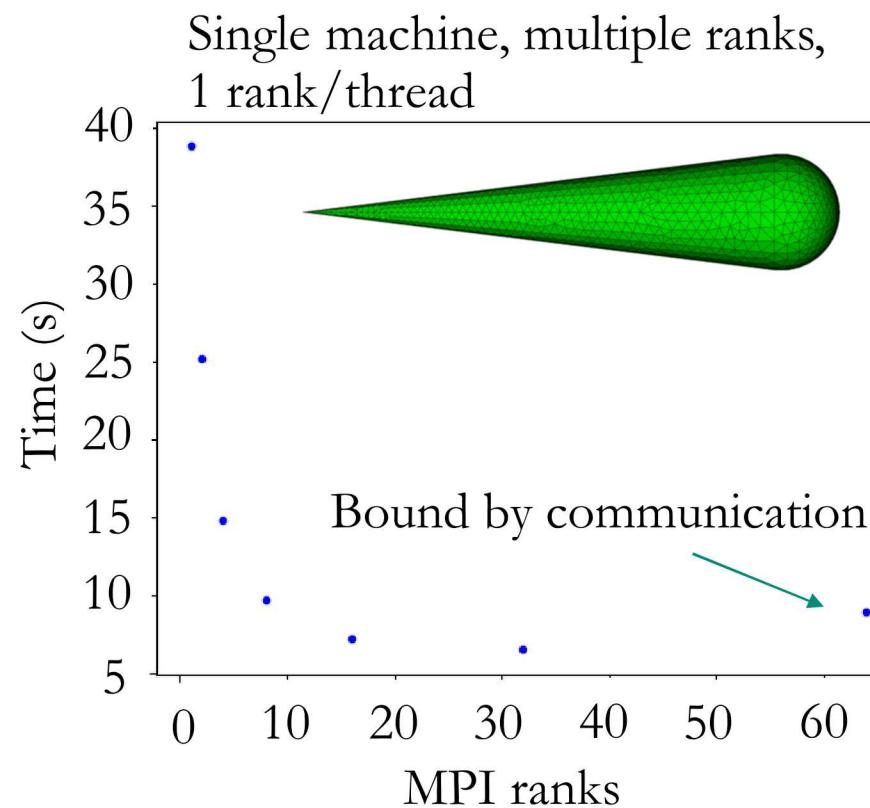
- Establish physics capabilities for Sandia use cases
- Establish V&V early in code lifecycle
- Enable parallel simulations across multiple nodes/ranks
- Demonstrate candidate alternative modeling methods

3 Gemma: Recent Progress



Gemma

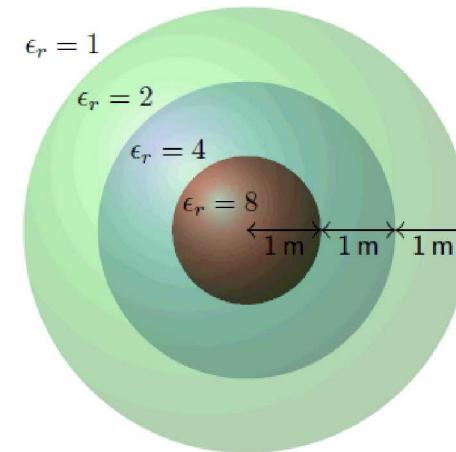
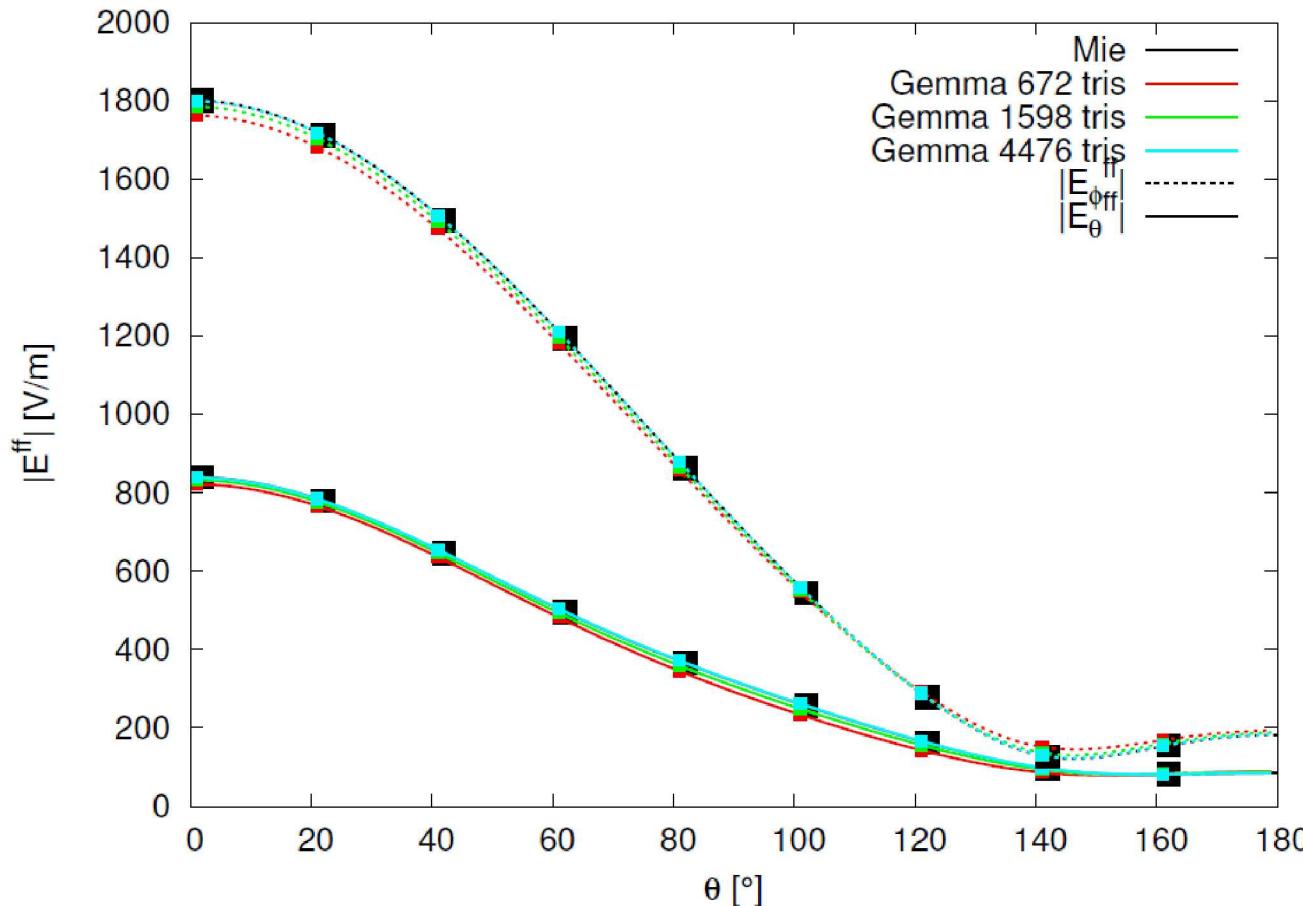
- Gemma has a working MPI version that has been tested on small problems on between 1 and 8 nodes. Work is ongoing to validate performance on larger problem sizes and increased node counts.



Reasonably good scaling on
Mutribo (CPU)

- Currently bound by memory for increasing problem size; taking steps to improve this as function of node count

- Initial implementations for multiple regions and dielectrics have been completed paving the way for initial coupling simulations.

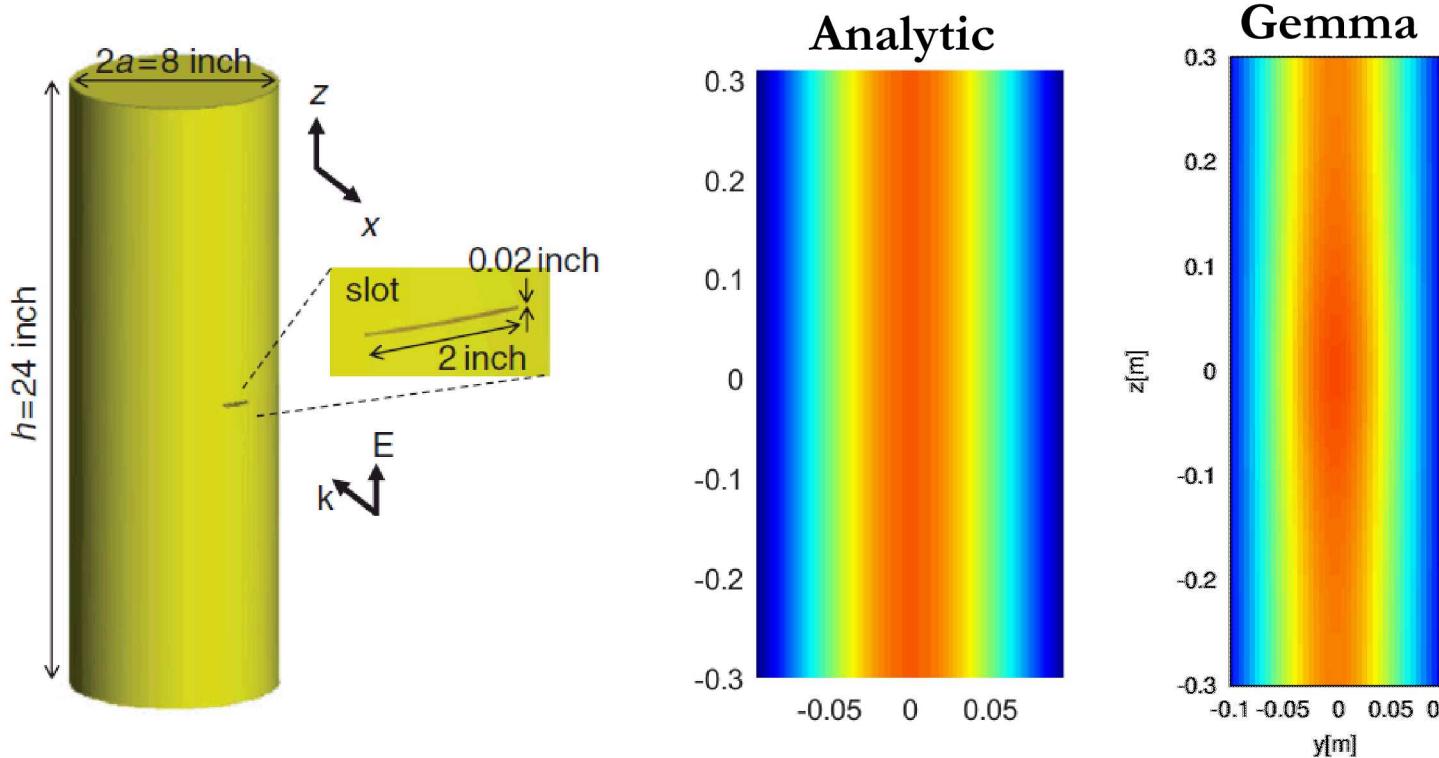


- $+z$ -traveling wave,
 $\mathbf{E} = 377 \text{ V m}^{-1} \hat{x}$
- Frequency 30 MHz
- Far-field scattered \mathbf{E}
 computed at $\varphi = 65^\circ$

5 Gemma: Recent Progress



- Very first coupling simulation in Gemma shown for a canonical cylindrical slotted cavity



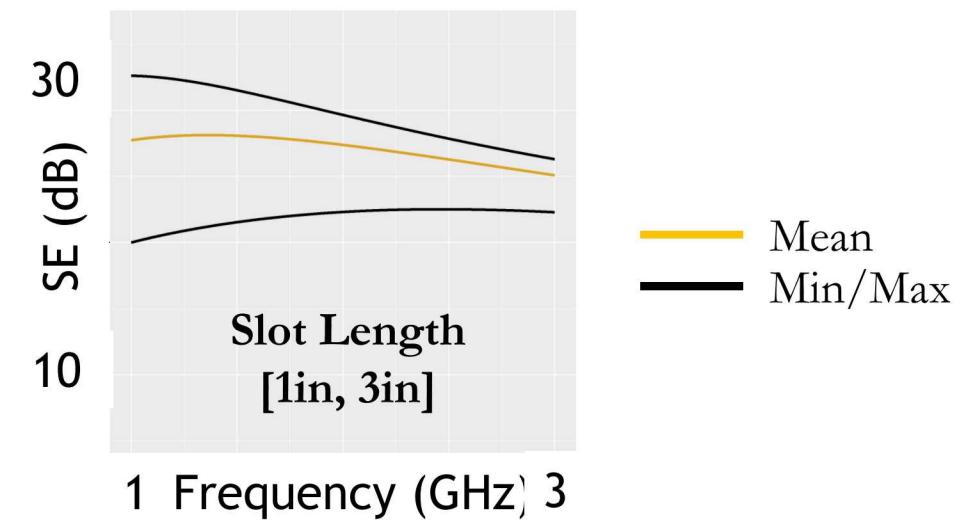
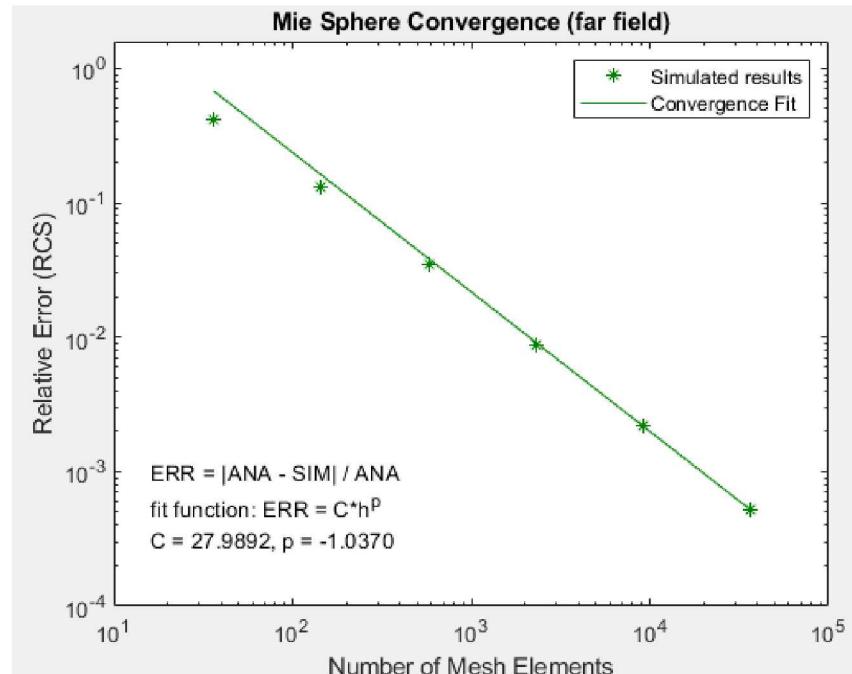
- Gemma shows proper field distribution within the cavity
- More work is needed to verify accuracy

- Development of Pliris direct solver for GPUs together with Kokkos Kernels
- Tracked timing for gcc, clang, and cuda based builds
- Initial Iterative Physical Optics code implementation is being tested to verify correct results and limitations for coupling to analytical power balance codes.

6 Gemma: Recent Progress



- Integrated Workflow (TWF) is proceeding with EIGER testing for both serial and parallel simulations. This activity will inform the Gemma UI/UX development.
- Collaboration with Trilinos has allowed us to use Trilinos-maintained cmake and testing. This has streamlined building and testing on new machines.
- Initial V&V (with 1544) against analytical solutions initiated and providing expected convergence rates. Drafting a V&V and UQ plan
- Initial sensitivity analysis (with 9136) using analytical power balance code

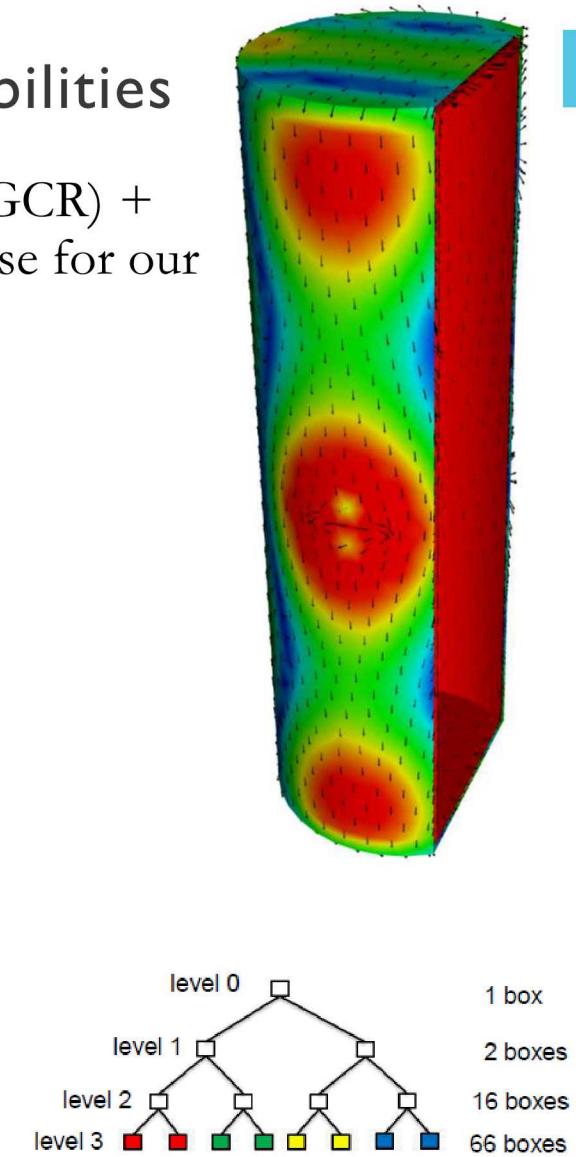
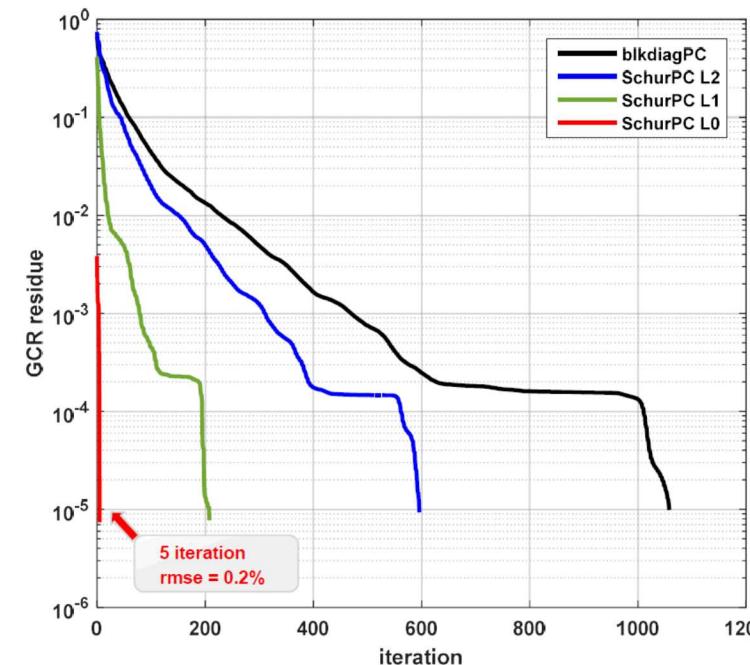
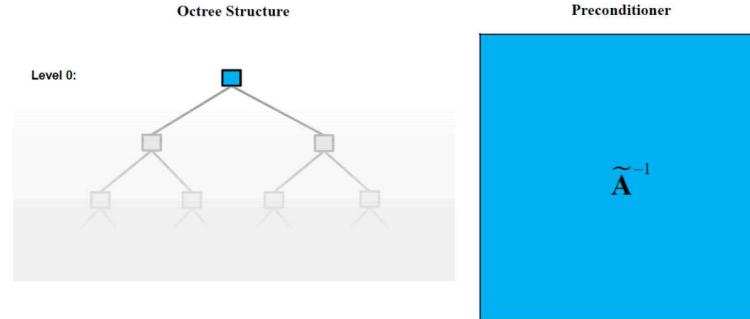
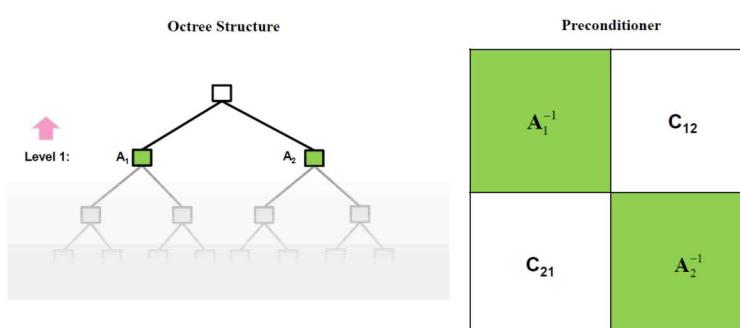
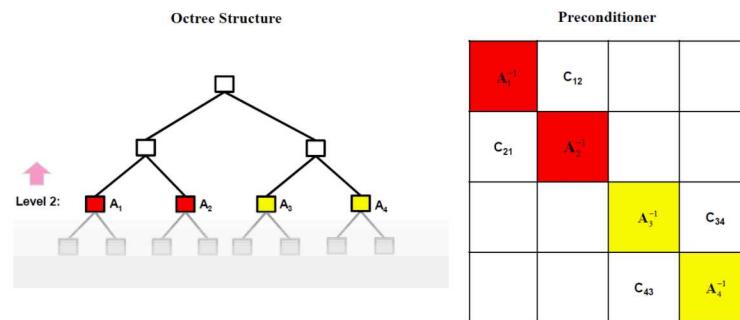
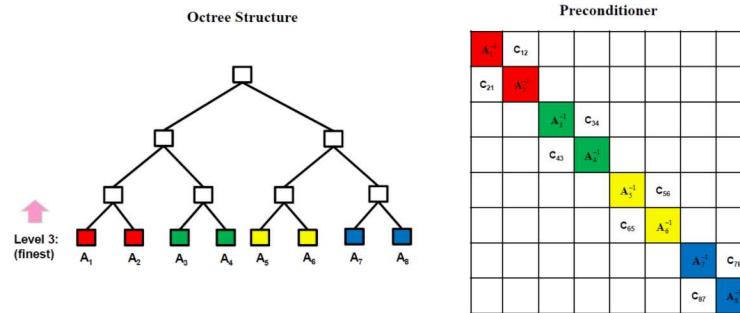


Dependencies on other ATDM Capabilities and Services

- Primary dependency is on Kokkos. Planned future interaction with Kokkos to see where Gemma's performance can be improved
- We plan on increasing our dependence on Belos and possibly a preconditioner library
- We use a handful of helpful features from Teuchos

8 Linkages and Contributions to ATDM Applications or Capabilities

- In collaboration with Ohio State University, the Generalized conjugated residual (GCR) + Schur- Principle Component Analysis (PCA) preconditioner has shown great promise for our applications. This could be developed in collaboration with Trilinos



$$rmse = \frac{\sqrt{\iint_S |J_{ref}(\mathbf{r}) - J_{appx}(\mathbf{r})|^2 dS}}{\sqrt{\iint_S |J_{ref}(\mathbf{r})|^2 dS}}$$

Usage and Impact across ASC, ECP, Sandia Mission Areas, etc.

- Gemma has applications across multiple mission areas and divisions:
 - ND support (9400 and 2000)
 - LDRD support (both inside and outside of 1000)
 - ASC PEM and V&V dependencies and support
 - RCS support (Sandia missions outside of 1000)
 - Design support for antennas and microwave/electromagnetic devices (kHz → THz)