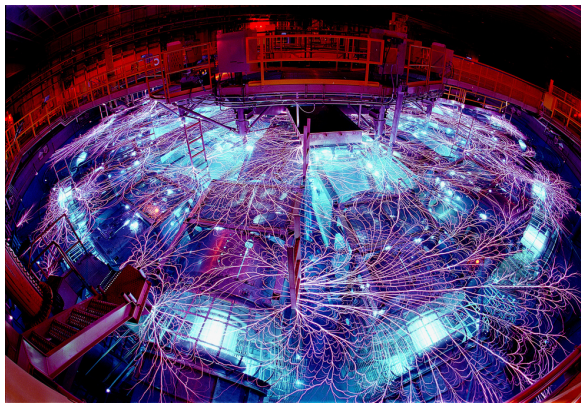
Exceptional service in the national interest

Sandia National Laboratories

SAND2017-11739C





ICERM - 2017

COMPADRE: An open-source massive scale meshfree library

Nathaniel Trask

Center for Computer Research, Sandia National Laboratories

8/10/17

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-mission 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.

Outline

Sandia National Laboratories

ComPadRe - Compatible particle discretization

Contributors - Pavel Bochev (PI), Pete Bosler, Paul Kuberry, Mauro Perego, Kara Peterson

- Second generation code built on existing work developing SPH+AMG solvers
- A brief sketch of ongoing meshless work in our group
- Code structure

Sandia National Laboratories

Many similarities to reproducing kernel particle methods

- **Apply convolution to obtain nonlocal approximant to derivative**

$$\hat{u(x)} = \int u(y)\delta_\epsilon(||x-y||)dy$$

$$\nabla\hat{u}(x) = \int u(y)\nabla\delta_\epsilon(||x-y||)dy$$

- **Discretize using point quadrature**

$$\nabla\tilde{u(x_i)} = \sum_j u(x_j)\nabla\delta_\epsilon(||x_i-x_j||)V_j$$

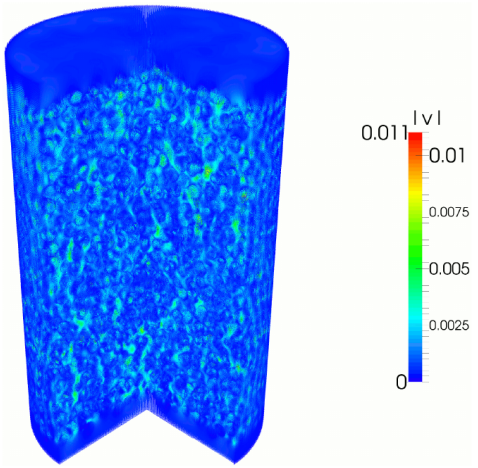
- **Introduce correction matrix to kernel to enforce polynomial reproduction**

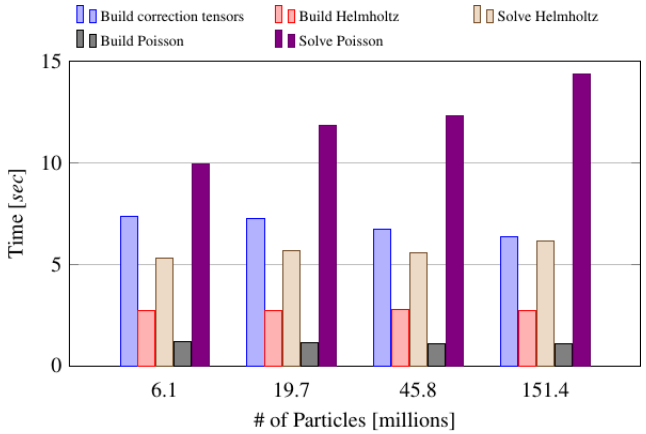
$$\nabla_c\tilde{u}(x_i) = \sum_j u(x_j)\mathbf{B}_i\nabla\delta_\epsilon(||x_i-x_j||)V_j$$

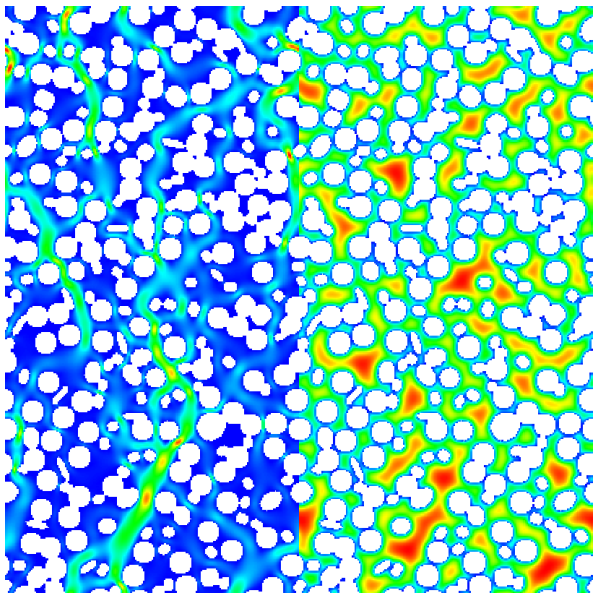
Old work developing a massive-scale implicit SPH solver

1. LAMMPS offers embarrasingly parallel strong scaling for particle methods - meshless discretization goes here
2. Trilinos provides gives suite of algebraic multigrid libraries to achieve $O(N)$ matrix solves

Discretization			Per Processor		
N	dx	# Particles	# Processor	# Particles	Load balance
128	6.875e-05	6,083,687	432	14,083	1.0003
192	4.583e-05	19,701,287	1,440	13,682	1.0004
256	3.437e-05	45,803,537	3,432	13,347	1.0007
384	2.291e-05	151,438,991	11,376	13,313	1.0006



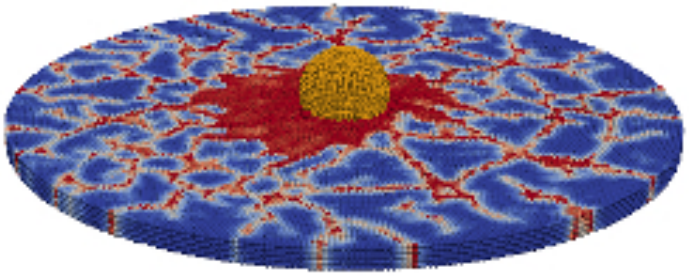


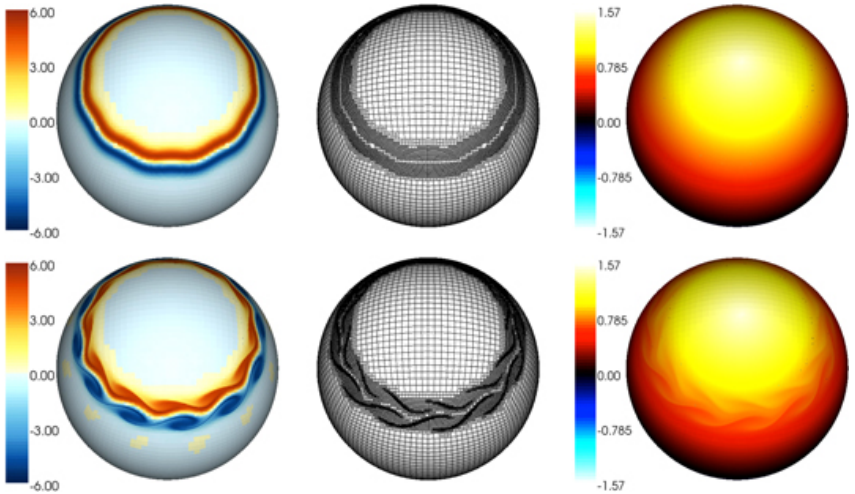


Refs: Trask JCP 2016, W Pan JCP 2017

An incomplete list of meshless projects in the lab

- Problems in fracture mechanics (particle distretization of peridynamics)
- RBF + vortex particle methods for problems in climate science
- Development of new meshfree discretizations for material science problems

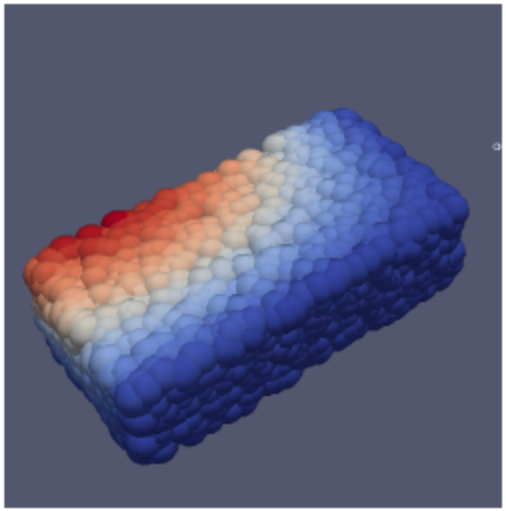




The Compadre library

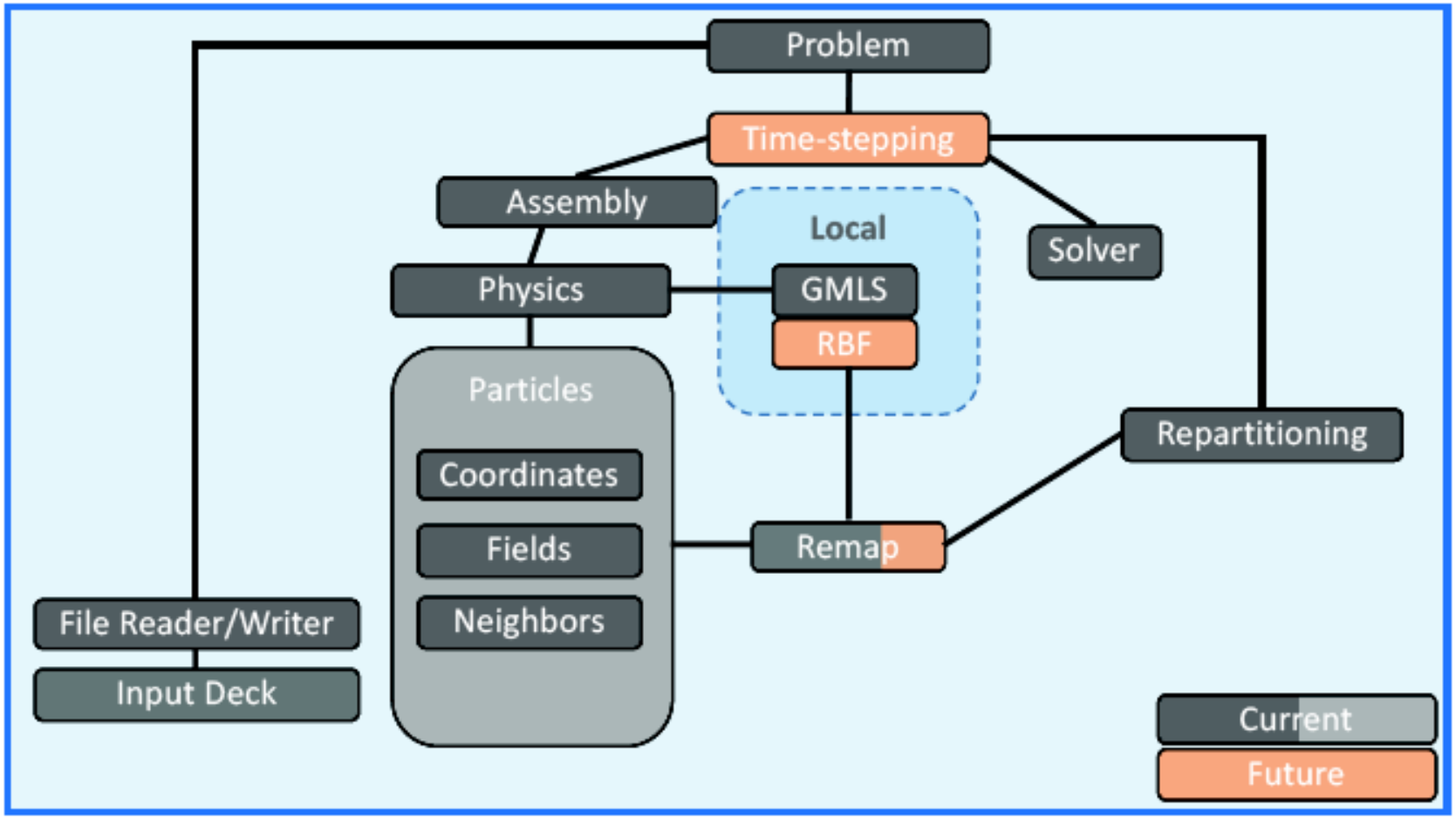
Sandia National Laboratories

- **Supports**
  - Various coordinate systems (Euclidean, Spherical, etc..)
  - Lagrangian (future) and Eulerian simulations
  - Strong and weak-form (future) model solution
- **Managing**
  - Fields of various dimensions (pressure, velocity, etc..)
  - Sets of particles
    - Data transfer between sets (remap) (in progress)
    - Time-stepping over sets (future)
    - Partitioning/repartitioning particle sets over multiple processors
- **Leveraging**
  - **GMLS interpolation library (compatible discretizations)**
  - Trilinos Zoltan2 particles over processor partitioning
  - Trilinos solvers (Amesos2, Ifpack2, MueLu, and Belos)



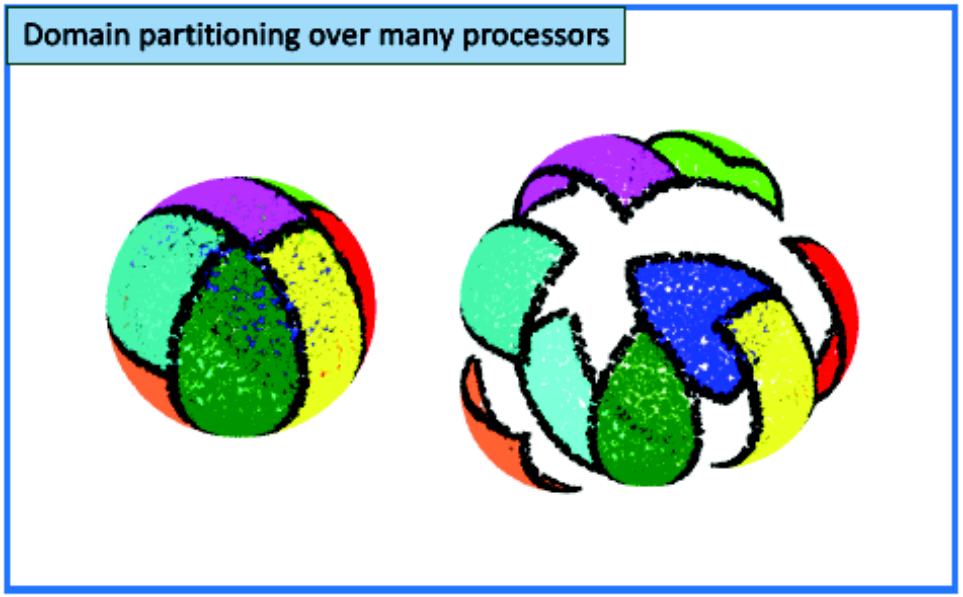
- Combines MPI parallelism with thread-parallelism (MPI + Kokkos) using Trilinos, Tpetra, and Kokkos
- Manages importing/exporting data in the form of VTK files
- Input deck driven simulation (XML / YAML)

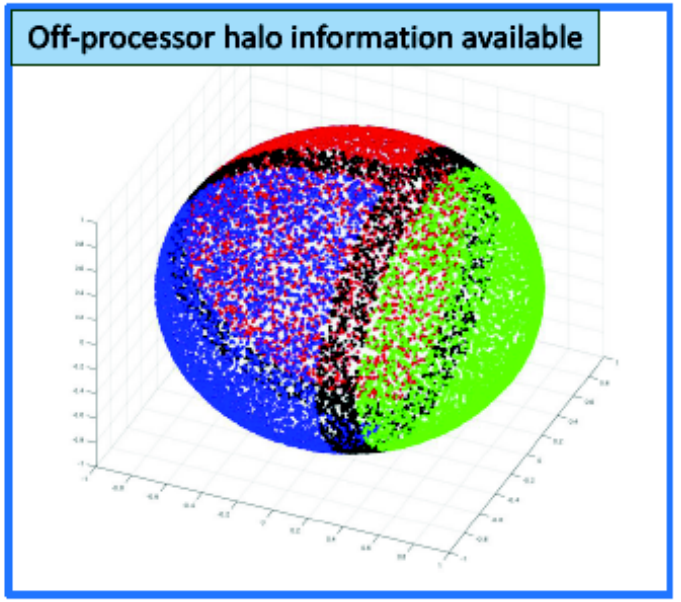
Code layout - local and global modules



Dynamic domain partitioning using Zoltan 2 in Trilinos

Sandia National Laboratories

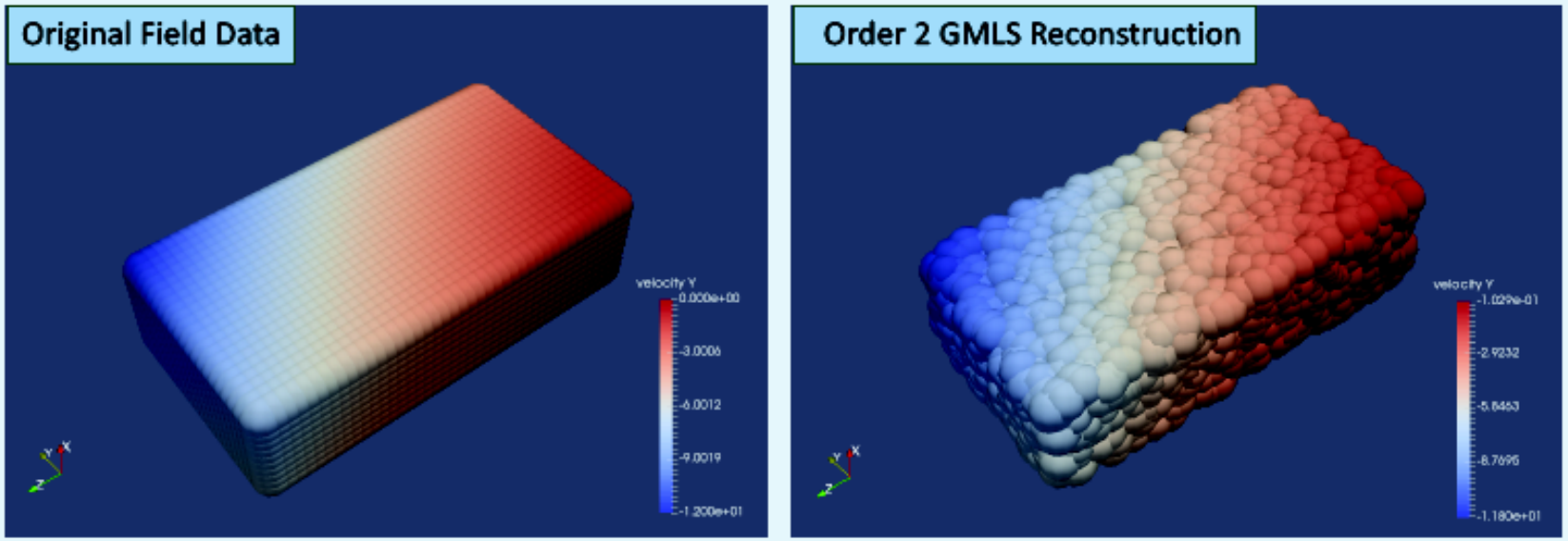




Adaptive particle insertion and removal using remap

Sandia National Laboratories

Insertion requiring interpolation from existing field data using GMLS



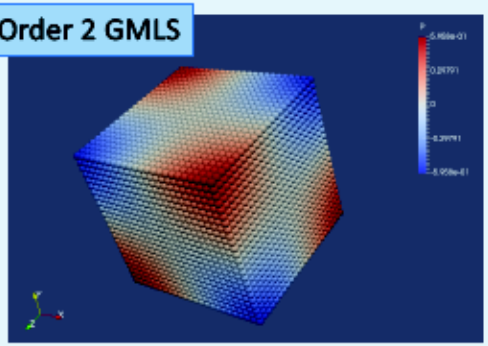
Error < 1e-16

Sandia National Laboratories

Manufactured Solution (Convergence):

$$\sin(x) \cdot \sin(y) \cdot \sin(z)$$

Order 2 GMLS

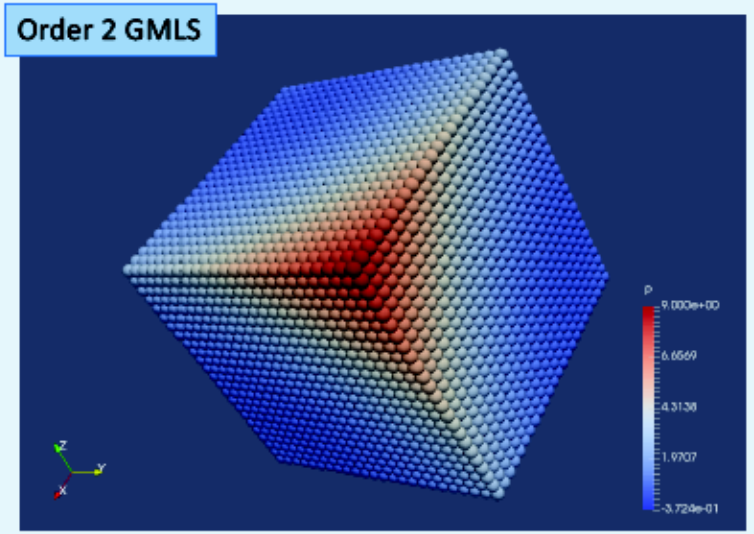


Spacing	L^2 Error	Rate
1/3	8.23e-4	-
1/6	1.390-4	2.57
1/12	3.22e-5	2.11
1/24	7.88e-6	2.03
1/48	1.97e-6	2.00

Manufactured Solution (Exact):

$$x(1+x+y+z)+y(1+y+z)+z(1+z)$$

Order 2 GMLS



L^2 Error: 9.25978e-17

The Compadre library

Sandia National Laboratories

- How can you utilize the Compadre toolkit?
  - Local reconstruction of functionals (completely local work)
  - Perform neighbor searches, reconstruction of functionals, transfer of information between particle sets
  - Manage fields, generate and repartition particle sets, load input decks and export data for visualization
  - Complete package for simulating multi-physics problems

Moving forward

Sandia National Laboratories

- Year one of three year project - current code architecture in place
- Not yet released for general consumption but great time to get in on the ground floor
- Stay posted!