Bay-Area Radiation Transport (**BART**), a Research-purpose Parallel Transport Code Framework

Weixiong Zheng[1], Joshua Rehak[1], Rachel Slaybaugh[1]

[1]Nuclear Engineering, University of California, Berkeley

Introductions

What is **BART**?

A open-source research-purpose code

- We hold **BART** on Github with MIT license.
- We build **BART** to be a research-purpose transport code.
- We aim to provide a framework s.t. graduate students only need necessary amount of knowledge on **C++** and third-party libraries to implement new ideas for research

A finite element code based on **deal.II**

- We build **BART** to be a finite element code based on **deal.II**
  - Finite element is wired-shape mesh friendly
  - **BART** computes in general dimension as **deal.II** does.
  - **BART** only call generic functions instead of dimension specified ones.
- Any specs of finite elements are wrapped by **deal.II** s.t. **BART** developers focus only on physical/symbolically mathematical aspects.

A code in parallel

- We build **BART** to be a parallel code computing on distributed memory
  - Even small-size problems (¡10 million DoFs) can be overwhelming for local computers
- It is natural to enable parallelism as **deal.II** has nice wrappers.

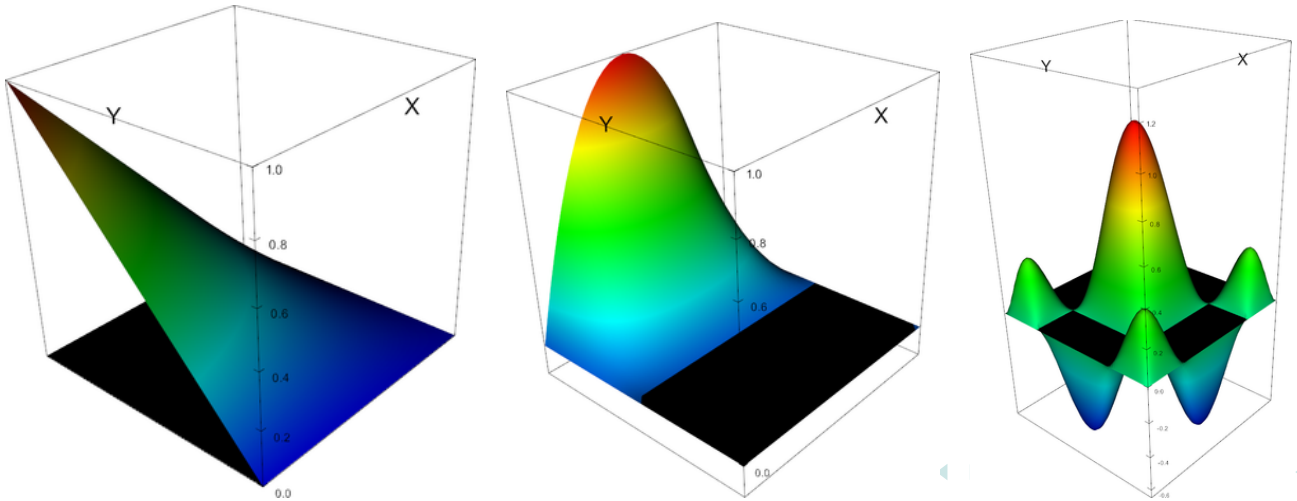
Finite elements in **BART**

Finite elements in general dimensions

- **deal.II** supports finite elements in general dimensions by templates
  - **BART** developers only need to call generic trial functions when implementing weak forms for 1/2/3 D
  - Specs of trial functions are hidden under the hood by **deal.II** for different dimensions.
- **BART** supports DFEM, CFEM, FV and RTk.
  - For high-order-low-order (HOLO), **BART** can assign individual finite elements to different equations.
  - All you need to do is to tell **BART** in input file:

```
set ho spatial discretization = cfem
set nda spatial discretization = dfem
```

- Polynomial orders can be changed in input file as well (see the following demos for Q1(left), Q2(middle) and Q4(right) trial functions)



What can **BART** do?

What approximations can **BART** have?

- Transport approximations that can be decoupled to individual equations
  - Discrete ordinates approximation
  - Diffusion equations
  - Canonical form of simplified spherical harmonics (SPN)
- PN is feasible through extension of current framework.

Solve small-to-median-sized problems

- A transport code doing all real-world large problems with billions/trillions of degrees of freedom is charming, BUT
  - It can require tens/hundreds of man-year of work.
  - It requires tons of optimizations.
  - It is hard for newbies to get started
- We restrict **BART** to small (e.g. one-group) to median sized problems (e.g. C5G7)

Equations/Discretizations

Equations we are solving

We are solving second-order forms of

- Fill this section up.

Parallelism/Linear Algebra/Meshing

BART is designed/implemented to be a parallel code

BART computes on distributed memory

- Message Passing Interface, aka **MPI**, is used for distributed computations.
- Meshing is correspondingly distributed based on **p4est**'s functionality wrapped by **deal.II**.
  - Each processor mainly knows mesh cells on itself
- Linear algebra related objects are distributed as well
  - **PETSc** data structure wrappers in **deal.II** are heavily used to enable the parallel linear algebra.

BART is parallelizing in space

- While extending parallelism to be suitable for other dimensions in phase space, we currently only parallelize in space
  - No special treatment on MPI/scheduling, natural support from **deal.II**
- Computational efficiency in parallel rather depends on solvers/preconditioners, but little on the mesh

Linear algebra in **BART**

Sparse matrix-vector product based computations

- Current implementation of **BART** assembles global matrices and utilize sparse matrix-vector product in linear algebraic solvers.
  - Easy implementation.
  - High computational efficiency with (bi/tri-) linear elements.

BART is interfaced with **PETSc**

- Most **PETSc** solvers/preconditioners wrapped in **deal.II** are used in **PreconditionerSolver** class of **BART**
  - Direct solver: parallel direct solver **MUMPS**
  - Iterative solvers and preconditioners
- Performance remedy: as solving will happen multiple times due to source/power iterations, we initialize the preconditioning/factorization only once then preconditioning/factorization matrices will be stored for reuse.

Meshing capability in **BART**

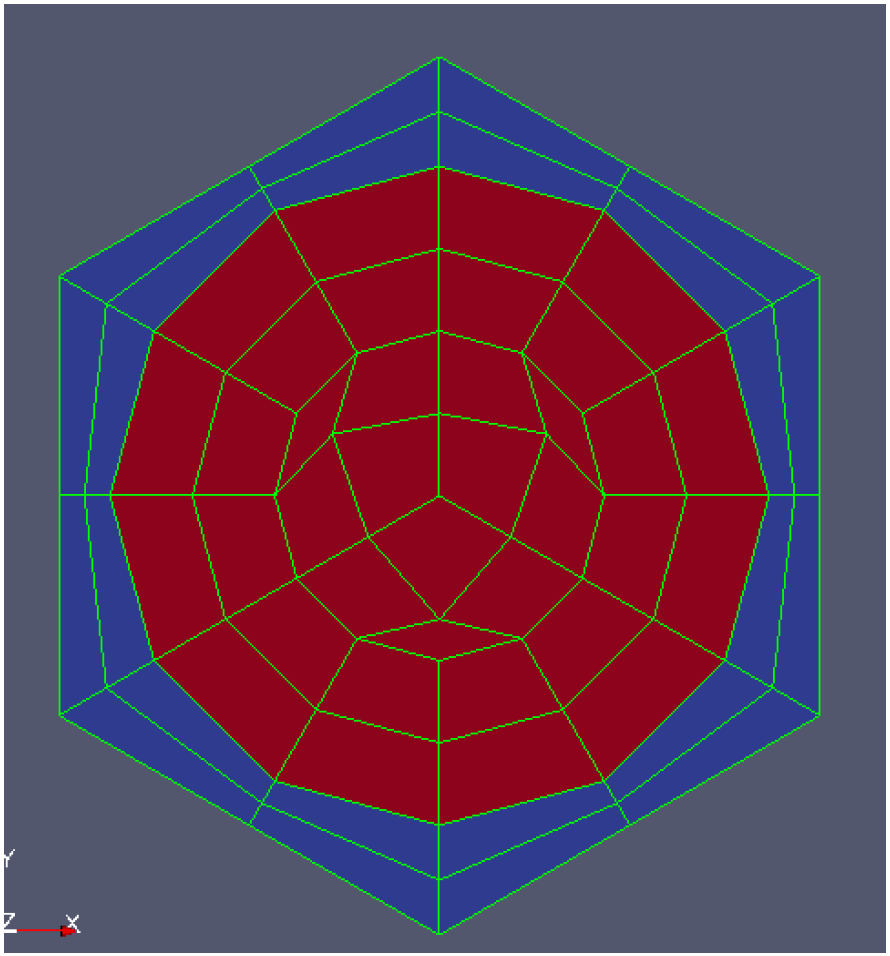
BART was initially implemented for homogenized mesh

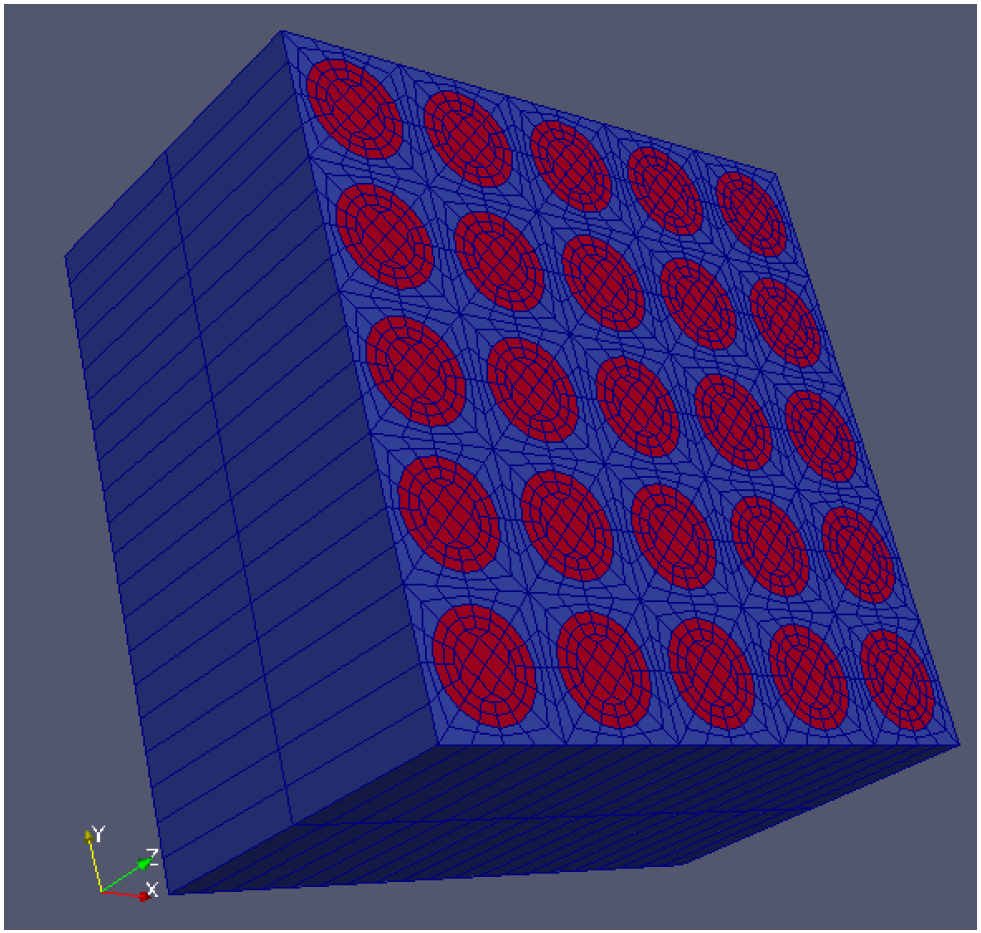
- Hyper-rectangle meshing based on **deal.II**:
  - Lines in 1D, rectangles in 2D and regular cuboid in 3D
  - Material ID assigned to coarsest mesh and stored in cell objects tractable when refining

Pin-resolved meshing

- Recent development enables the use of pin-resolved mesh
  - Rectangular (prism) pin is supported; hexagonal (prism) pin is under development
  - **Goodness:** meshing does **NOT** depend on **Cubit** or **gmsh**. **BART** realizes wrapper functions based on **deal.II** to draw complex geometries.
- We compose different pin models and replicate based on pin types in 2D.
- 3D meshes is realized by extruding 2D mesh.

Pin-resolved mesh demos

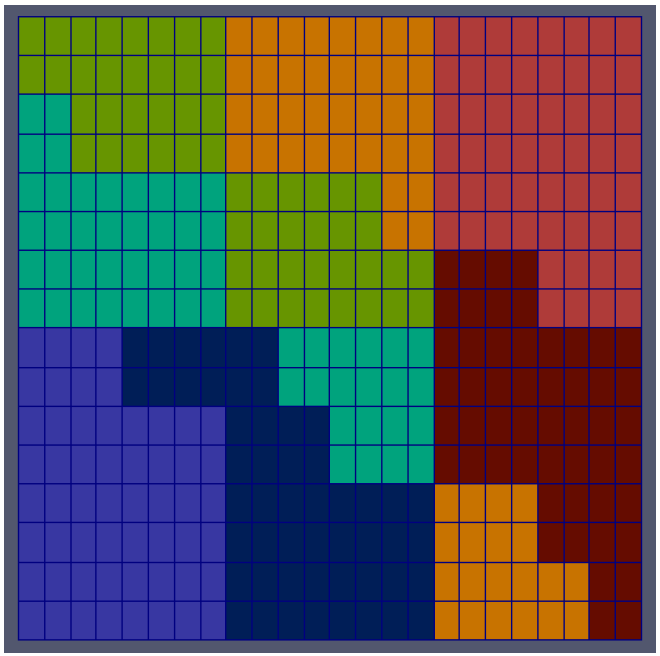


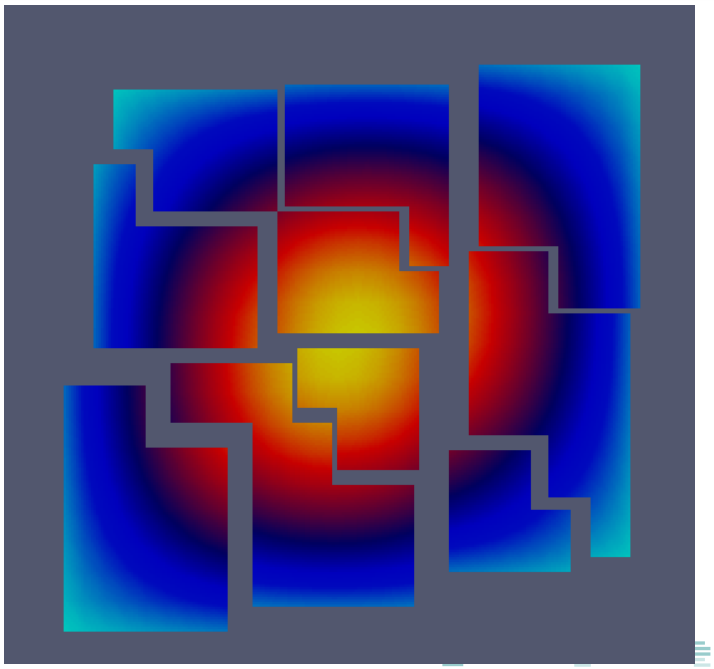


Meshing in Parallel

Distributed triangulation

- Triangulation (meshing) needs to support parallelism for parallel computations.
- **deal.II** supports two ways of triangulation in parallel
  - Shared (**ParMETIS** based): every processor has a copy of the global triangulation.
  - Distributed (**p4est** based): every processor only knows cells living on itself and a layer of neighboring cells from other processors on the local triangulation boundary
- **BART** supports distributed meshing from **deal.II**.
- 1D meshing is serial as **deal.II** has no parallel support





Testing

Unit testing and documentation

We document and test everything possible

- We rewrote **BART** twice:
  - First time, we restructured **BART** and documented everything with **doxygen**.
  - Second time, we added unit testing.
- Philosophy: everything be documented and every function/class be tested if possible.
  - Documentation leads to better understandability of code in the future development.
  - Unit testing ensures new codes do not affect correctness of existing code.

G(oogle)Test and CTest are both used

- We want unit testing to be efficient and compatible with MPI
  - GTest is super efficient but hard to obtain compatibility with MPI.
  - CTest is slow but compatible with MPI.
- Not all the testings require MPI
  - We use GTest for all serial testing
  - We leave all MPI related testings to CTest.

Ongoing Projects

We are conducting projects on **BART**

Ongoing projects

- Advanced spatial discretization methods.
- Advanced energy acceleration methods.

We are designing students' projects in **BART**

- We are designing students' projects based on **BART**
  - **BART** will grow, so intellectually do students.