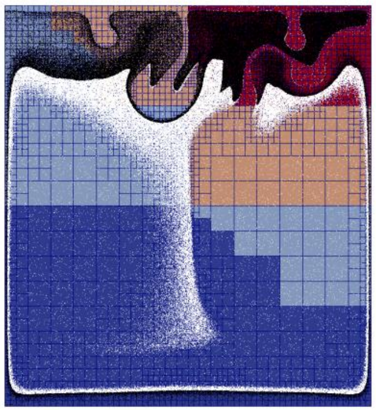
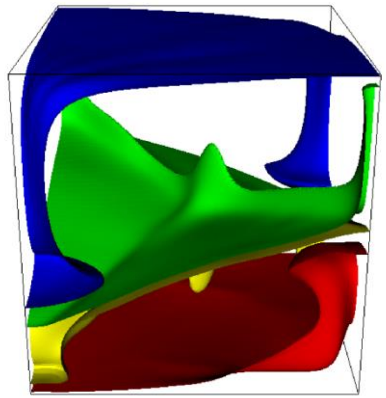
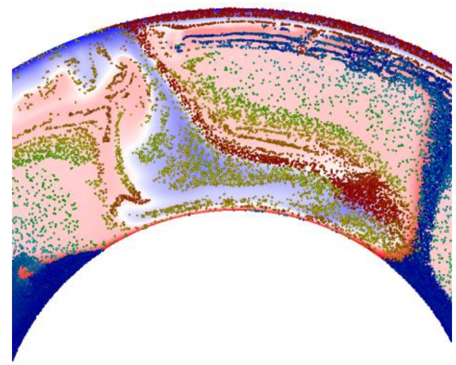
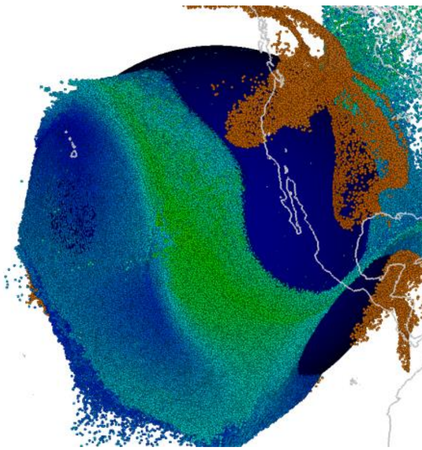
Particle Methods in deal.II

Rene Gassmoeller, Shahab Golshan, Bruno Blais

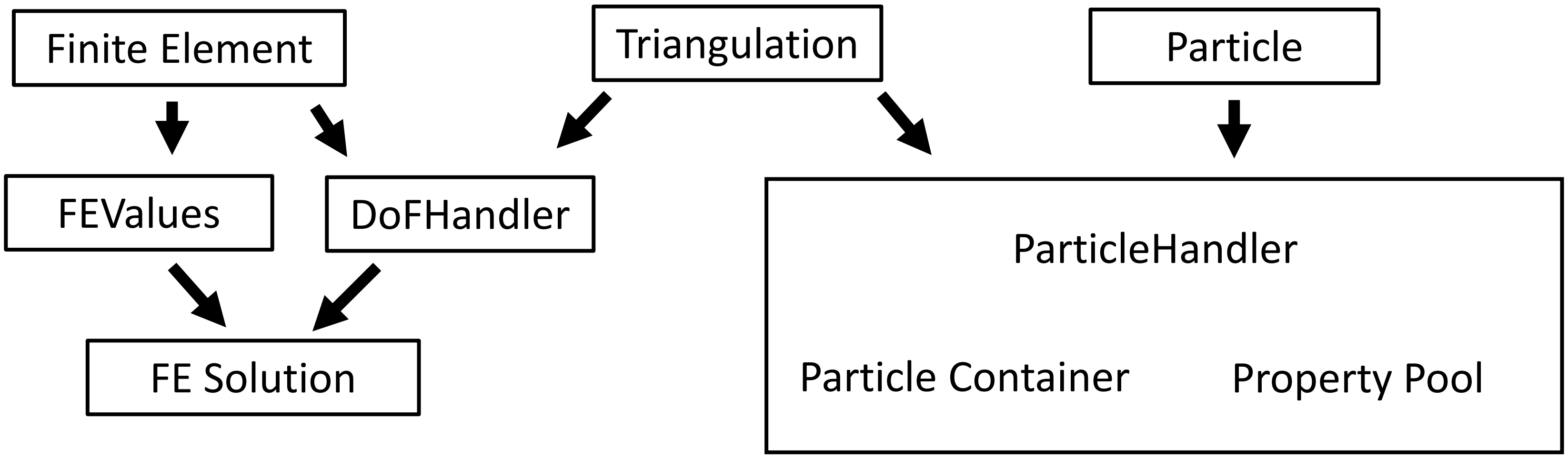
With work by: Wolfgang Bangerth, Elbridge Gerry Puckett, Luca Heltai, and many deal.II contributors

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

PARTICLE METHODS IN DEAL.II

- deal.II is a finite-element library; solution domain is a continuum
- Often knowing properties at discrete locations is useful
- deal.II contains functionality to create and track a set of discrete particles (/tracers/markers)
- How these particles are used is left to the application
- There are many applications and variants of particle methods (e.g. Particle-in-cell; Marker-and-cell; Discrete Element Method; Smoothed Particle Hydrodynamics; Fluid-structure interaction)

PARTICLE METHODS IN DEAL.II



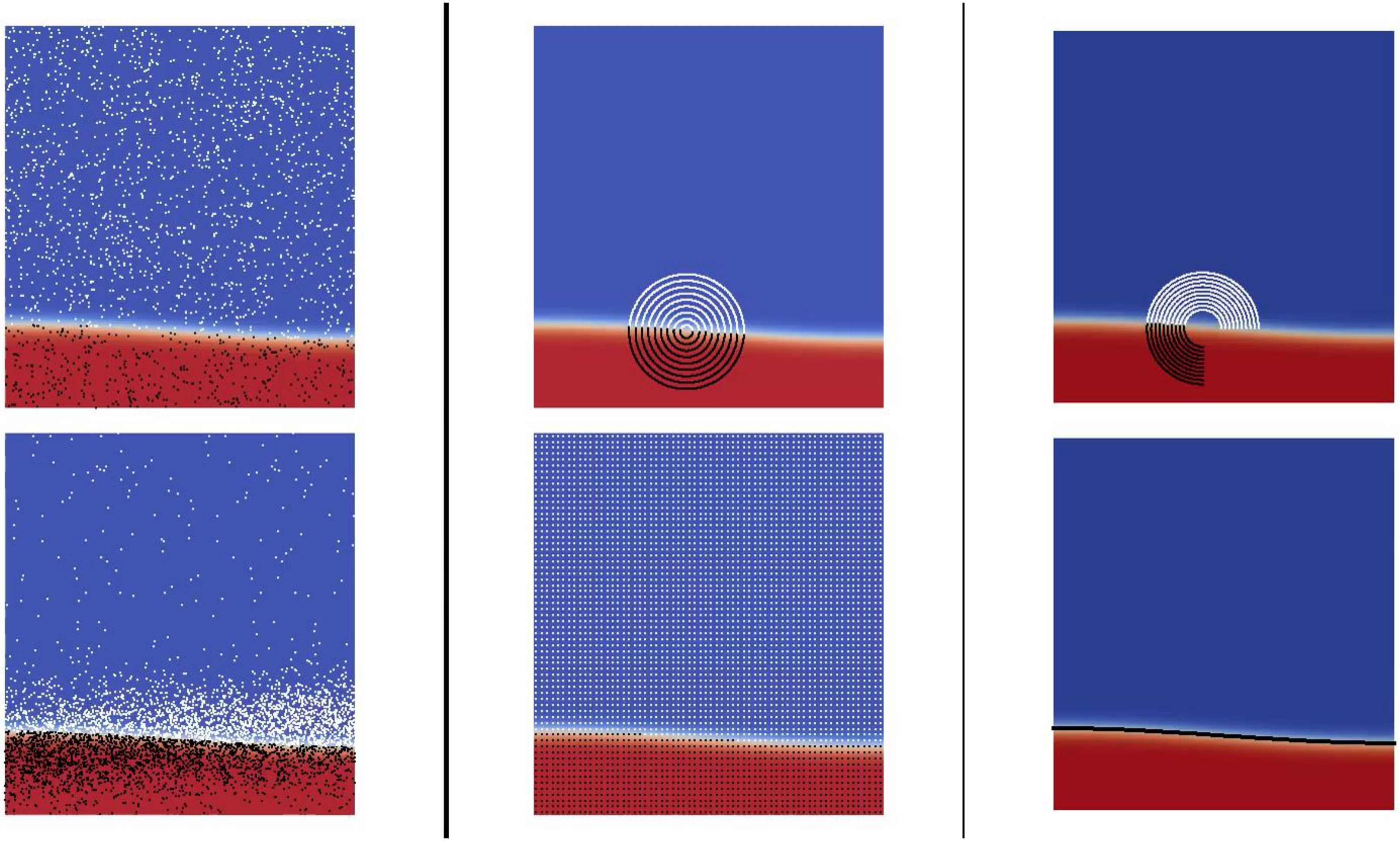
- Managing particles inside deal.II happens in the ParticleHandler class, and works similar to the DoFHandler class plus the solution vectors
- I.e. the particle handler knows where particles are, provides iterators to access them, and functions to change them

PRACTICAL IMPLEMENTATION IN DEAL.II

```
{
  Triangulation<dim, spacedim> triangulation;
  GridGenerator::hyper_cube(triangulation);

  MappingQ<dim, spacedim> mapping(1);

  Particles::ParticleHandler<dim, spacedim>
    particle_handler(triangulation, mapping);

  Functions::ConstantFunction<2> uniform_distribution(1.0);
  Particles::Generators::probabilistic_locations(
    triangulation, uniform_distribution, false, 16,
    particle_handler, mapping);

  for (const auto &particle: particle_handler)
    std::cout << particle.get_location() << std::endl;

  Particles::DataOut<dim, spacedim> particle_output;
  particle_output.build_patches(particle_handler,
                                data_names,
                                data_interpretations);
  particle_output.write_vtk(deallog.get_file_stream());
}
```

- Create a triangulation
- Generate the grid
- Create a mapping
- Create a particle handler
- Generate some particles
- Access individual particles
- Write particle output file

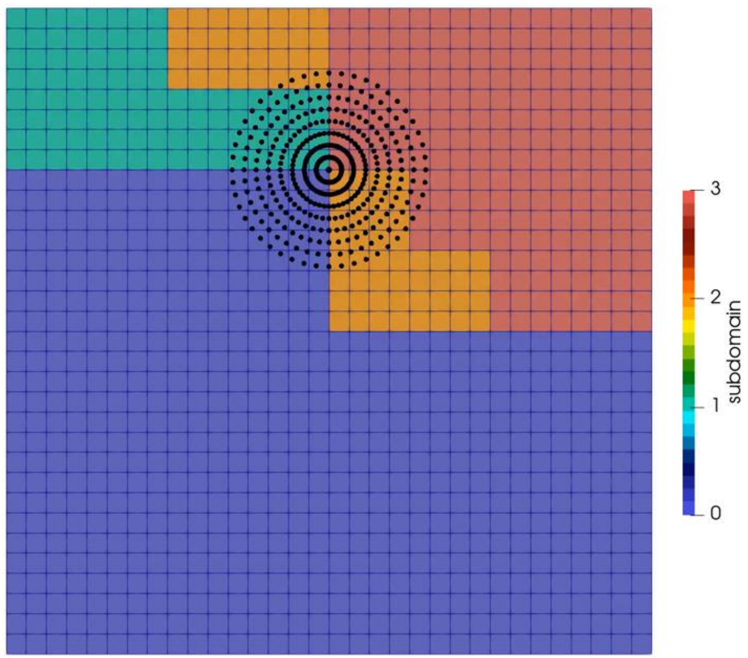
PARTICLES::GENERATORS



Statistical distributions   Regular distributions   Arbitrary distributions

SCALABILITY: LOAD BALANCING

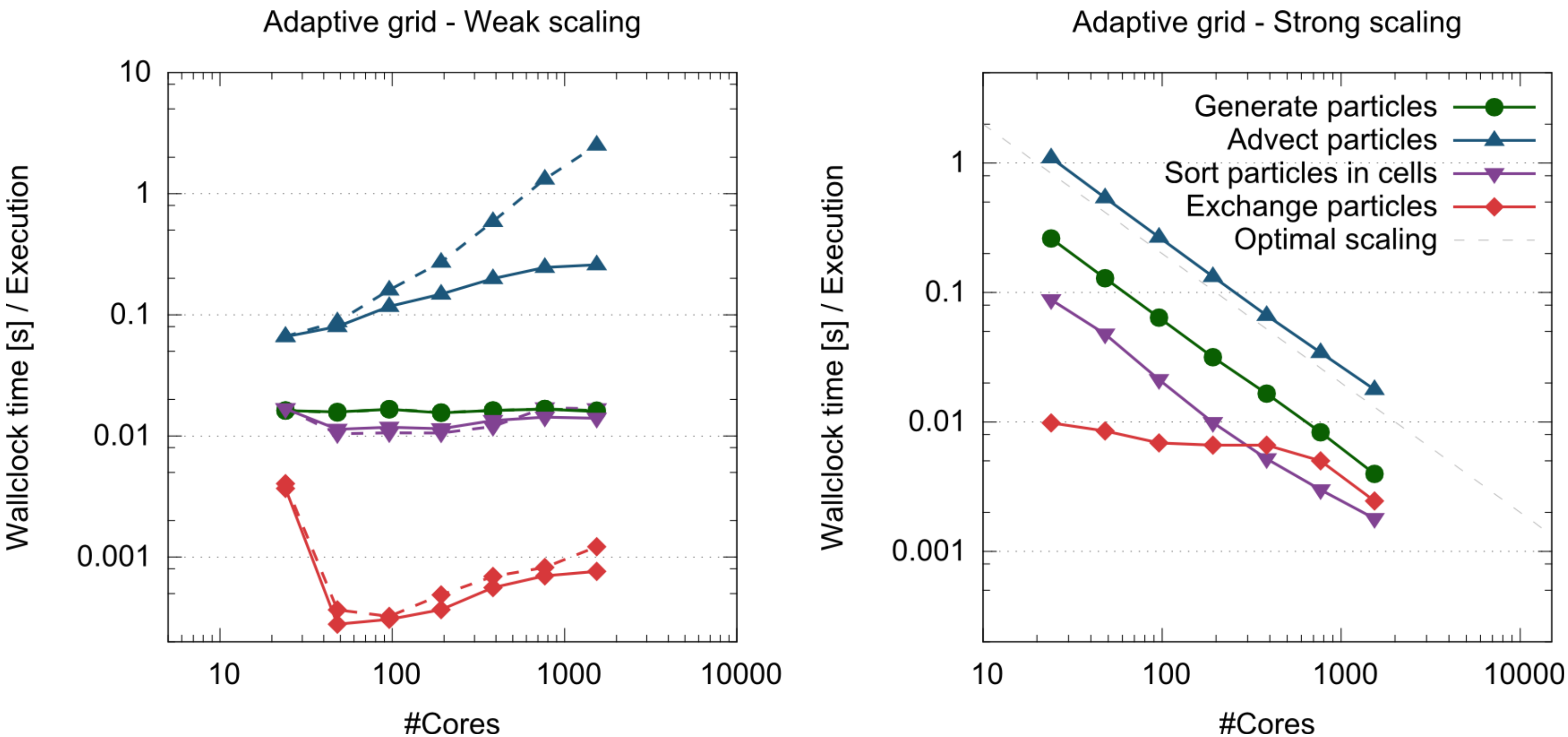
How to balance the computational load for particles and cells?



Animation by Bruno Blais, Step-68

- Partitioning of domain by number of cells per process
- For uniform particle density large imbalance in particle work
- Imbalance grows with number of mesh levels
  - ➢ Limited scalability
- ➢ Solution: Balance by number of particles instead

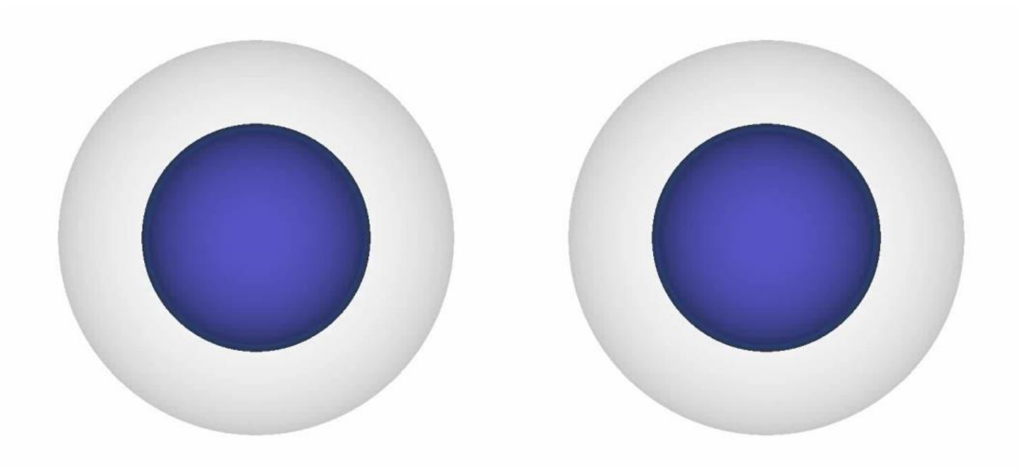
SCALABILITY: LOAD BALANCING

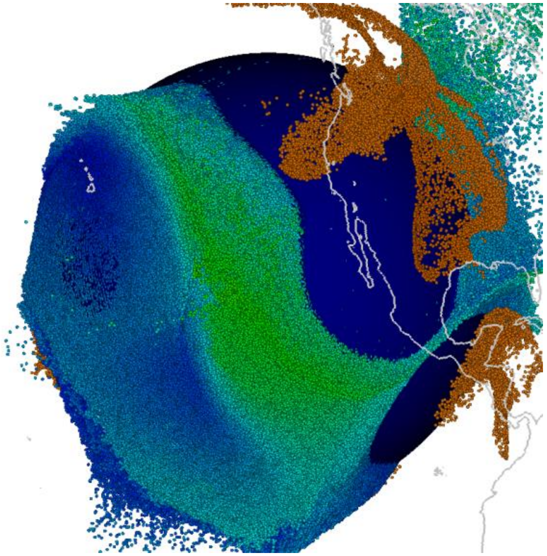


Gassmoeller et al., 2017

- Weak scaling dependent on load balancing technique
- Optimal strong scalability independent of technique

APPLICATIONS (ASPECT)

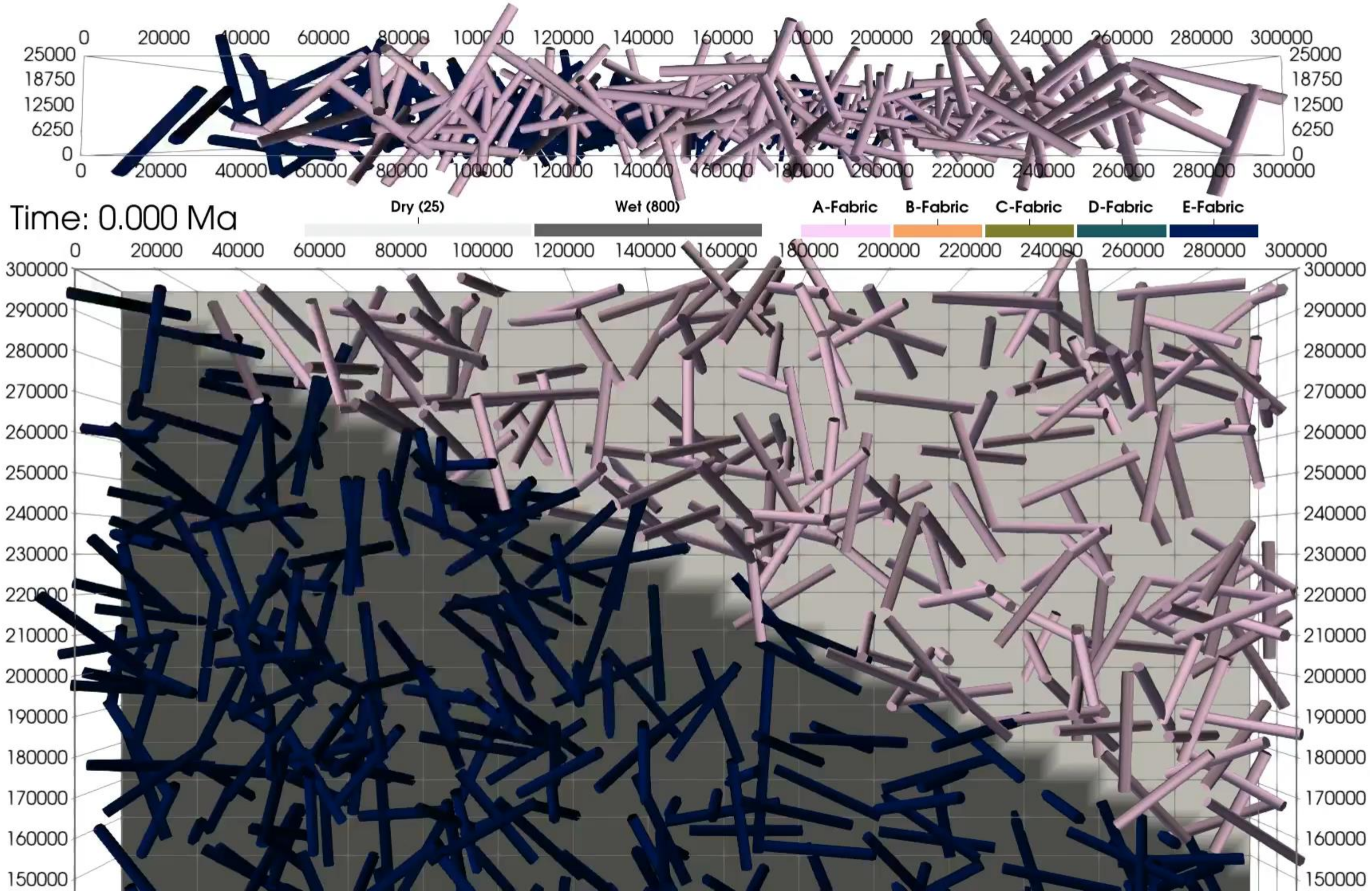




Gassmoeller et al., 2017

- Convection in the Earth's mantle:
  - Track origin of material
  - Track composition of material

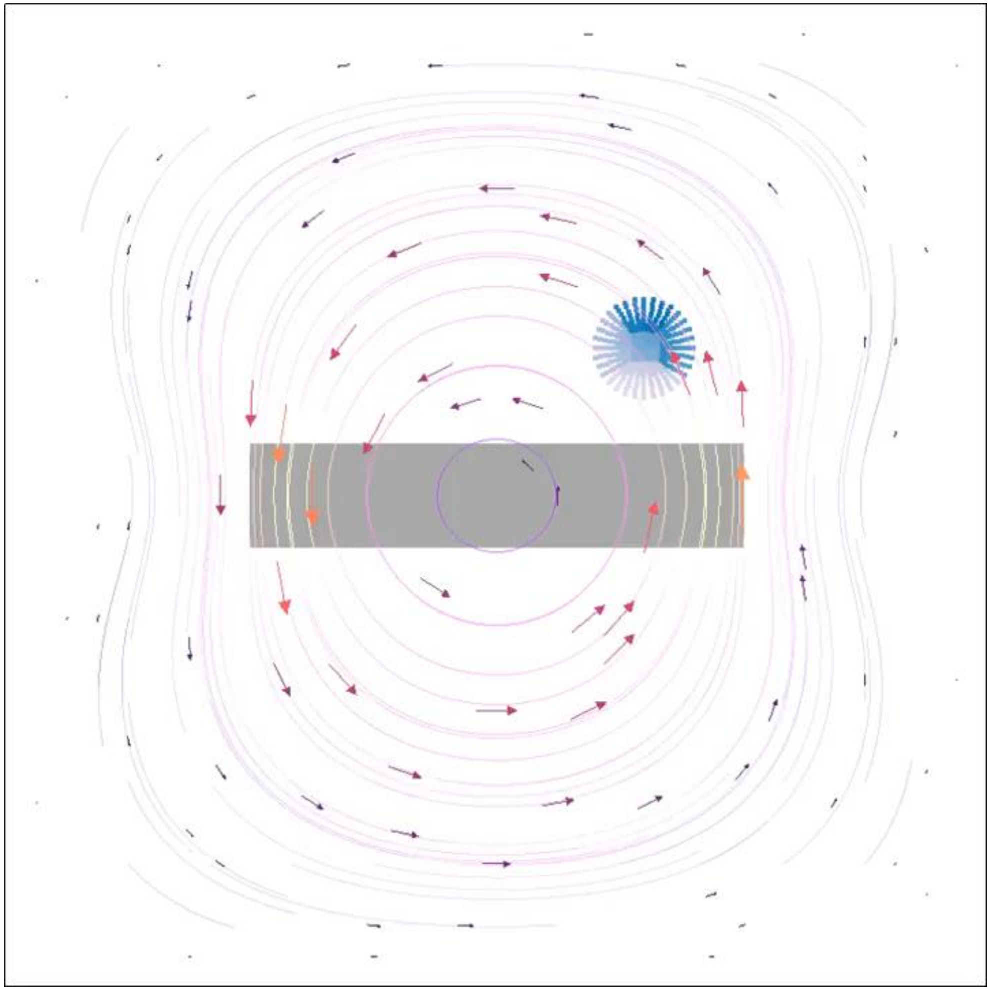
APPLICATIONS (ASPECT)



Animation and work by M. Fraters

- Deformation of crystalline material:
- Track deformation tensor
- Solve ODE for anisotropic material properties (crystal orientations)

APPLICATIONS (STEP-70)



Animation of Step-70, Luca Heltai, Bruno Blais, Rene Gassmoeller

- Interaction between a solid impeller and and a flowing fluid
- Particles are used both for embedding the impeller into the flow (gray), and to track deformation of the fluid (blue)

FURTHER INFORMATION

- Example steps that explain and utilize the particle features:
  - Step-19 (electrons in a cathode tube) provides an introduction for how particles and a field interact
  - Step-68 (chemical heterogeneities in fluid flow) uses particles as tracers in distributed triangulations
  - Step-70 (fluid-structure interaction) uses particles to transfer information between two non-matching triangulations
- Tests for usage examples are in deal.II/test/particles/

○ **Reference***:* Gassmöller, et al. "Flexible and Scalable Particle-in-Cell Methods With Adaptive Mesh Refinement for Geodynamic Computations." *Geochemistry, Geophysics, Geosystems* 19.9 (2018): 3596-3604.