Geophysical Research Abstracts
Vol. 18, EGU2016-11042, 2016
EGU General Assembly 2016

Implementation of a flexible and scalable particle-in-cell method for massively parallel computations in the mantle convection code ASPECT

Rene Gassmöller (1,2) and Wolfgang Bangerth (1)

(1) GFZ Potsdam, 2.5 Geodynamic Modelling, Potsdam, Germany (rene.gassmoeller@mailbox.org), (2) Texas A&M University, Department of Mathematics, College Station, USA

Particle-in-cell methods have a long history and many applications in geodynamic modelling of mantle convection, lithospheric deformation and crustal dynamics. They are primarily used to track material information, the strain a material has undergone, the pressure-temperature history a certain material region has experienced, or the amount of volatiles or partial melt present in a region. However, their efficient parallel implementation - in particular combined with adaptive finite-element meshes - is complicated due to the complex communication patterns and frequent reassignment of particles to cells.
Consequently, many current scientific software packages accomplish this efficient implementation by specifically designing particle methods for a single purpose, like the advection of scalar material properties that do not evolve over time (e.g., for chemical heterogeneities). Design choices for particle integration, data storage, and parallel communication are then optimized for this single purpose, making the code relatively rigid to changing requirements.

Here, we present the implementation of a flexible, scalable and efficient particle-in-cell method for massively parallel finite-element codes with adaptively changing meshes. Using a modular plugin structure, we allow maximum flexibility of the generation of particles, the carried tracer properties, the advection and output algorithms, and the projection of properties to the finite-element mesh. We present scaling tests ranging up to tens of thousands of cores and tens of billions of particles. Additionally, we discuss efficient load-balancing strategies for particles in adaptive meshes with their strengths and weaknesses, local particle-transfer between parallel subdomains utilizing existing communication patterns from the finite element mesh, and the use of established parallel output algorithms like the HDF5 library. Finally, we show some relevant particle application cases, compare our implementation to a modern advection-field approach, and demonstrate under which conditions which method is more efficient.
We implemented the presented methods in ASPECT (aspect.dealii.org), a freely available open-source community code for geodynamic simulations. The structure of the particle code is highly modular, and segregated from the PDE solver, and can thus be easily transferred to other programs, or adapted for various application cases.