Implementing particle-based methods with Aboria

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ABSTRACT

Aboria is a C++ library that supports the implementation of particle-based numerical methods, which we define as having three key properties:

1. There is a set of $N$ particles that have positions within an hypercube of $d$ dimensions.
2. The method can be described in terms of non-linear operators on the $N$ particle positions and/or other variables associated to these particles.
3. These operators are defined solely by the particle positions and variables, and typically take the form of interactions between pairs of closely spaced particles (i.e. neighbourhood interactions).

The goal of Aboria is to provide a general purpose library that can be used to support the implementation of particle-based numerical methods. It does this by efficiently abstracting the difficult algorithmic aspects of particle-based methods, such as neighbourhood searches, while still allowing the user complete control of the non-linear operators they wish to apply to the particle set. Aboria is designed as a framework into which different spatial search data structures and fast summation algorithms can be inserted to cater for different use cases.

The online documentation (https://martinjrobins.github.io/Aboria/) provides a set of example programs that illustrate how Aboria can be used to implement different particle-based methods. To date, this set shows simple implementations of Molecular Dynamics, Brownian Dynamics, Discrete Element Model, Smoothed Particle Hydrodynamics, Radial Basis Function Interpolation and the Kansa Method for PDEs.

People interested in using Aboria can clone the git repository at https://github.com/martinjrobins/Aboria. The documentation includes installation instructions, or the authors can be contacted on the email addresses above. People interested in contributing to Aboria should fork the Github repository and create a pull request for their changes.