

Particle swarms for numerical wave equation

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Summary

Randomly moving particles may be used as a computational model for a numerical simulation of partial differential equations in several spatial variables. We demonstrate examples in one and two spatial dimensions to show how a Green's function for the heat equation, and the acoustic wave equation, can be approximated by a simulation with many random particles. We considered a simple case of a coupled system of first order partial differential equation in one spatial dimension that can be modelled by a branching process of super Brownian particle motion, and showed the limiting density of the particles forms a solution to the PDEs. This system required a model with two types of particles. In three spatial dimensions, four types of signed particles are required. Examples are presented, and GPU computation discussed.

Mathematical formulation

A significant computational challenge that arises in seismic imaging is creating a numerical simulation of seismic waves propagating through a complex, three dimensional media. Whether one uses finite difference, finite elements, Galerkin, pseudospectral or Fourier transform methods, there is typically a computational grid where all the wavefields are computed, which can become very large even for modest problems.

However, there are other models for computation worth considering. A very familiar physical model of Brownian motion involves tracking a large number of particles moving randomly in a medium, resulting in a diffusion process that is accurately described by the heat equation.

Some useful references on these models of the heat equation appear in Kozdron (2008) and Lawler (2010). More recently, researchers have been using random particle motion as models for a wide variety of stochastic processes that extend such models to equations beyond the heat equation. In the works of Crisan and Lyons (1999), Quer-Sardanyons and Tindel (2007), Toomey and Bean (2000), and Yang and Li (2015) we see these stochastic models applied to the wave equation, other hyperbolic equations, and more exotic partial differential equations. Beyond Brownian motion, one can also consider super Brownian motion as in Slade (2002), in which the randomly moving particles may also undergo branching processes where new particles may be born, and old ones may dies. This allows for a richer class of processes.

Following Zauderer (1989) we can build a particle model for the 1D wave equation by defining the density of particles as a sum of left-going and right-going particle densities:

$$v(x, t) = \alpha(x, t) + \beta(x, t).$$

Dynamics are given as probabilities for particles to continue in the same direction, or reverse:

$$\alpha(x, t + \tau) = p\alpha(x - \delta, t) + q\beta(x - \delta, t)$$

$$\beta(x, t + \tau) = p\beta(x + \delta, t) + q\alpha(x + \delta, t),$$

where τ, δ are step sizes in time and space. With appropriate assumptions on the probabilities p, q , the limiting distribution for this system satisfies the Telegrapher's wave equation:

$$v_{tt} - c^2 v_{xx} + 2\lambda c v_t = 0.$$

A similar derivation in 2D, with particles that have a finite probability of changing direction, results in a numerical performance that is very similar to the 2D acoustic wave equation. However, we lack a mathematical proof for this correspondence between particles and wave.

We can use branching processes to simulate the wave equation in its representation as a hyperbolic system of first order partial differential systems. Namely, with $P(x, t)$ as acoustic pressure and $U(x, t)$ as fluid flow, the wave equation is represented as a 2x2 system

$$\begin{aligned} P_t + BU_x &= 0 \\ U_t + \frac{1}{\rho_0} P_x &= 0 \end{aligned}$$

where parameters B and ρ_0 come from the state equation and median density.

To model this first order system, we consider a swarm of particles made up of two types: type P and type U. These particles will each have a sign attached to them, a ± 1 . We step in time with step size τ and step in space with step size δ . A particle of type P at x will generate a particle of type U in the next time step, at location $x + \delta$, with probability p' . It will also generate a particle of type $-U$ in the next time step, at location $x - \delta$, with probability q' . Similarly, a particle of type U will generate particles of type $\pm P$ to the right and left of its position in the next time step, with corresponding probabilities p'' , q'' .

Now let $v(x, t)$ equal the sum of particles of type P at point x , at time t , where the sum takes into account the sign of the particles, and $w(x, t)$ the corresponding sum for the particles of type U. We now have difference equations for v, w that tells us how many particles are present in the next time step. From the difference equations, we expand as a Taylor series to linearize and obtain the system of equations

$$\begin{aligned} v_t(x, t)\tau &= -2p''w_x(x, t)\delta \\ w_t(x, t)\tau &= -2p'v_x(x, t)\delta. \end{aligned}$$

Choosing the ratio δ/τ and probabilities p', p'' appropriately, in the limit as $\delta, \tau \rightarrow 0$ we obtain the desired system of PDES,

$$\begin{aligned} v_t &= -Bw_x \\ w_t &= -\frac{1}{\rho_0}v_x. \end{aligned}$$

From this we conclude that a simulation with particles following the generating process above will result in a numerical solution to the first order PDE system. Note however, that this is an example of a branching process, as new particles are potentially created at each time step. This may lead to some computational difficulties, as the number of particles will be expected to increase over the duration of the simulation.

In three spatial dimensions, four types of particles would be required: one representing acoustic pressure (type P) and three of type U, say U_1, U_2, U_3 , representing each component of the fluid flow. This will lead to a larger computational system, but again free of grids and finite difference simulation.

Computational speedups

The goal of this exercise is to get a method that can rapidly compute Green's functions, and consequently calculate wave propagation from source to receivers in a typical seismic simulation. Some features we intend to exploit:

1. Each particle moves independently of the others. Thus the computational burden of following many particles can be distributed across many processors, which do not need to communicate with each other. This is a significant advantage over finite difference methods, where computational cells must communicate with their neighboring cells.

2. The computations are simple, mainly involving additions and multiplications, thus well suited for graphical processing units (GPUs). A graphics card running CUDA may be a very efficient way of achieving a highly parallel, accelerated computation.
3. There are no computational boundaries. We do not have to worry about implementing numerical absorption of a particle at a computational boundary, as the particles can move without bound, or at least up to the numerical range of IEEE floating point numbers. Indeed, once a particle has travelled too far, we can remove it from the simulation since it will not have time to return to a receiver. Exiting particles free up computational resources for other particles.
4. There is considerable flexibility in choice of parameters: number of particles, step sizes, correlations between steps. We may be able have choices that give both high accuracy as well as speed.

Numerical Results

We compute the Green's function for the acoustic wave equation in 2D, which will have a singularity along the wave front that includes a trailing tail. In Figure 1 we compare the cross section of an initial pulse of particles at the origin, modeling an impulsive source of a wavefront as it travels out to a circle of radius 6000 meters. The computed results does have the tail, behind the sharp front at 6000 meters, as expected.

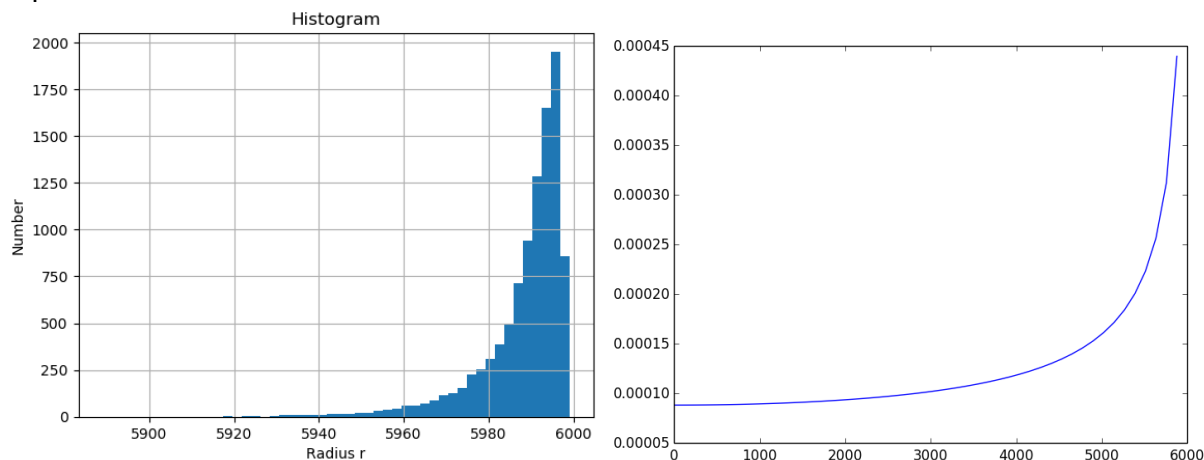


Figure 1: Comparison of particle density with exact Green's function for 2D, showing the trailing edge behind the wavefront.

Not shown here are results from additional experiments with 1D and 2D acoustic wave simulations in the particle formulation, with inhomogeneous media. Again these show promising results, although the mathematical formulations are lacking.

Summary

Motivated by the possibility of computation speed-ups using massive parallelization on fast graphical processing units, we have begun an investigation of the use of particle swarms to produce a numerical simulation of seismic wave motion in heterogeneous media in 2D and 3D.

It is well known that Brownian motion of particles bouncing about at random forms a useful model for diffusion of heat. In the limit as particle numbers go to infinity, the Brownian motion leads to the diffusion equation: a second order, linear, parabolic partial differential equation. A similar model with correlated, but still random, particle motion leads to the acoustic wave equation in dimensions one, two and three.

Focusing on the Green's function for individual source and receiver pairs in a seismic experiment, we tested a numerical simulation of wave propagation using large numbers of independently acting particles without modelling the entire seismic waveform in the experiment. We presented the mathematics behind the theory of the particle simulation and suggested some potential computational advantages in this approach.

Novel Information

It is a curious phenomenon that the wave equation results in a Green's function that has no waves in it – it is actually a “transport” equation. We anticipate numerical simulation on GPU-based computers will result in rapid computation, with particles transporting the wave energy.

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