GLOBAL RANDOM WALK SIMULATIONS OF DIFFUSION

Calin Vamos, Nicolae Suciu
"Tiberiu Popoviciu" Institute of Numaerical Analysis,
Cluj Napoca Branch of Romanian Academy,
cvamos@ictp-acad.math.ubbcluj.ro, nsuciu@@ictp-acad.math.ubbcluj.ro

Harry Vereecken, Olaf Nitzsche, Horst Hardelauf
Institut für Agrosphäre (ICG-IV), Forschungszentrum Jülich GmbH,
h.vereecken@fz-juelich.de, o.nitzsche@fz-juelich.de, h.hardelauf@fz-juelich.de

Abstract Random walk methods are suitable to build up convergent solutions for reaction-diffusion problems and were successfully applied to simulations of transport processes in a random environment. The disadvantage is that, for realistic cases, these methods become time and memory expensive. To increase the computation speed and to reduce the required memory, we derived a "global random walk" method in which the particles at a given site of the grid are simultaneously scattered following the binomial Bernoulli repartition. It was found that the computation time is reduced three orders of magnitude with respect to individual random walk methods. Moreover, by suitable "microscopic balance" boundary conditions, we obtained good simulations of transport in unbounded domains, using normal size grids. The global random walk improves the statistical quality of simulations for diffusion processes in random fields. The method was tested by comparisons with analytical and finite difference solutions as well as with concentrations measured in "column experiments", used in laboratory study of soils' hydrogeological and chemical properties.

Keywords: diffusion, unbounded domains, random fields

1. Introduction

In this article we present a new numerical method capable of performing simulations for complex transport processes, faster than other similar approaches, and using realistic initial and boundary conditions.

Scientific Computing, Validated Numerics, Interval Methods, Edited by Krämer and Wolff von Gudenberg, Kluwer Academic/Plenum Publishers, New York, 2001

Numerical simulations for diffusion can be obtained by both discrete solutions of diffusion equations and by random walk methods. In the first class enter the well known finite difference and finite element/volume methods. In the second, we quote "fractional random walk method" used by Chorin [1] to solve the viscous terms in Navier-Stokes equations, "particle tracking" methods, as that used by Tompson and Gelhar [10] as model of solute transport in porous media, as well as the more recent "cellular automata" [5] and "lattice gas models" [14]. The common denominator of random walk methods is the use of statistical ensembles of distinct random walkers trajectories to compute the concentration field as average number of particles in a reference volume. For more details and reviews on these methods we refer to [10, 11] and to the handbook in stochastic methods of Gardiner [3]. Besides the simplicity of their algorithms, random walk methods are not affected by numerical oscillations at large Péclet numbers (Pe), as it is the case for finite differences [11], and many diffusion problems benefit from strong proofs of convergence [3, 13].

Related to these methods, we remark: 1) the computation of concentrations requires only statistical ensembles of positions, at given time, for systems of fictitious particles, and 2) the states of this ensemble are invariant under the particles' permutation. Thus, the knowledge of the individual trajectories is not necessary to compute concentrations. This enables us to use a global random walk law: all the particles from a given site are simultaneously scattered following the binomial Bernoulli repartition (the sum of individual random walk probabilities). We propose for this approach the name of "global random walk", hereinafter referred to as GRW.

As a mathematical object, GRW is similar to a "lattice gas model", where "the state of the system is described by specifying the number of particles present at the site x, $n(x)$", the states space is the space of configurations $\Omega = \{\omega = n(\cdot)\}$, and the dynamics is a stochastic process in Ω [12]. "Lattice gas" deals with Markov processes in Ω. It is the same for diffusion processes modeled with GRW, with the difference that the simpler rules (random walk or, more generally, random biased jumps between the grid points) allow the use of Bernoulli repartition to achieve global change of state.

The advantages of the new method are: the computing time is reduced by several orders of magnitude, microscopic processes (reactions, decay, retention) and variable diffusion coefficients can be easily implemented, it describes the diffusion fronts, it allows the simulation of transport in unbounded domains using normal size grids, and it is numerically stable and not sensitive to great Pe numbers.