Green's functions of the diffusion equation for simulation of chemical species in biological systems

I. Plante[1,2*], F.A. Cucinotta[2]
[1]Universities Space Research Association, [2]NASA Johnson Space Center.
*e-mail: Ianik.Plante-1@nasa.gov

GREEN'S FUNCTIONS OF THE DIFFUSION EQUATION

The simulation of systems comprising different types of molecules is of great interest in several fields, notably in chemistry and in biological sciences. The conventional approach to the simulation of biological networks is to write macroscopic rate equations and solve the corresponding differential equations numerically. In this method, the evolution of the system is deterministic, and it is implicitly assumed that the concentrations are large and that fluctuations can be neglected. However, in most biological systems, the interactions of molecules are highly stochastic. Recently, various techniques have been developed to take into account the spatial distribution of the molecules and the stochastic character of the reactions between them [1-2]. Several of these techniques are based on the Green's functions of the Diffusion Equation (DE), and they offer the advantage of being able to follow all the particles in time and space.

GENERAL-PURPOSE GRAPHIC PROCESSING UNITS

The approaches based on Green's function are usually limited by the computational time, which can be problematic even in simulations of systems comprising a small number of particles. However, in the recent years, the increase of the computer hardware performance made it possible to use the Green's functions to simulate particle systems. A significant development is a new type of cards called general-purpose graphic processing units (GPGPU), which have been designed to carry out computations traditionally handled by central process units (CPU). GPGPU perform simple operations, but can process them simultaneously. Nowadays these GPGPU have hundreds of processor cores and can execute thousands of threads concurrently. This is particularly interesting for the stochastic simulation of particles using Green's functions, because the sampling of the Green's function is repeated a large number of times. By submitting the sampling threads simultaneously to the GPGPU, it will be possible to simulate the evolution of the biologically-relevant systems in a reasonable time.

APPLICATIONS

The Green's functions of the DE in different geometries in 1D, 2D and 3D are well known; most of them were obtained from the propagation of heat in solids [3]. With appropriate modifications, these Green's functions represent the probability distribution of particles in the system; therefore, their sampling allows the simulation of the motion of particles and has the advantage of taking the stochastic effects and the geometry into account. Many of the algorithms used today to sample the Green's functions use look-up table methods, which can use a significant amount of memory and are difficult to implement on a GPGPU. We have recently developed sampling algorithms which do not require much memory and therefore, are well suited to implement on a computer comprising a GPGPU. Two applications of the approach based on the Green's functions are discussed. The first is the simulation of a particle near a membrane comprising receptors and the initiation of signal transduction [4]. This application was developed to investigate the action of the molecule "Transforming Growth Factor β" (TGF-β) in irradiated biological systems, but the approach may eventually be generalized to study other ligand-receptors system. The second application is the simulation of bi-molecular reactions [1]. These reactions are of particular importance in radiation chemistry, because the radiolytic species are created by the radiation in a non-homogeneous manner, the so-called radiation track structure. These simulations may be of crucial importance to investigate the indirect effect of ionizing radiations, i.e. the damage caused to the DNA by the •OH radical. In this case, the time evolution of the inter-particle distance vector is described by the DE. Therefore, these reactions may be investigated by using the Green's functions of the DE in 3D.

REFERENCES

[1] van Zon, J.S. and ten Wolde, P.R. (2005) *J. Chem. Phys.* 123, 234910. [2] Park, S. and Agmon, N. (2008) *J. Phys. Chem. B* 112, 5977-5987. [3] Carslaw, H.S. and Jaeger, J.C. *Conduction of Heat in Solids*, 2nd ed.. Oxford University, London. [4] Plante, I. and Cucinotta, F.A. (2011) *Phys. Rev. E*, 051920