Parallel simulation of spiral waves in reacting and diffusing media

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Reaction-diffusion equations are ubiquitous in biology, combustion, etc., because of their relevance in pattern formation, ignition and extinction phenomena, etc. [1-3]. Many studies of reaction-diffusion equations have been concerned with equations for activators and inhibitors in one or two spatial dimensions, e.g., the Belousov-Zhabotinskii, Brusselator and Oregonator models [3]. In three dimensions, there have been very few analytical and numerical studies of spiral waves, presumably because of both the large difficulties in examining wave propagation in three-dimensional (3D) space and the cost of such simulations [4].

In this talk, 3D simulations of the propagation of spiral waves in cubes in the presence and absence of extinction sources will be presented. These numerical simulations have been carried out by means of both time-linearized and nonlinearized techniques with and without approximate factorization of the 3D operator into one-dimensional ones.

The numerical methods employed in the discretization of the governing partial differential equations have been implemented in a parallel fashion in both shared- and distributed-memory computers. The parallelization of the approximate factorization technique has been carried out with a block dynamic cartesian decomposition and its efficiency is very near to one. The parallelization of time-linearization methods has been performed in terms of both the overlapping of communications and computations. This overlapping has been carried out by using asynchronous messages in the message-passing version and prefetch directives in shared-memory computers.

The presented model have been applied to study the formation and propagation of spiral waves in three dimensions, as well as their interactions with the boundaries of the computational domain, their local extinction, and the formation of spiral filaments. In the experiments calculations have been performed using 200x200x200 grid points in an Origin-2000 distributed-shared memory (DSM) computer up to 16 processors.

The numerical results indicate that, as the spiral wave approaches the boundaries of the computational domain, its tip describes a curved trajectory and the spiral re-emerges from another place. They also show that local heating may result in local and temporal extinction of the spiral wave and the formation of islands or pockets disconnected from the wave. A study of the isoscalability indicates that it is possible to reach speed-ups of about or higher than 56 with 800x800x800 grid points in a 64-processor computer.

References

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