Analysis of a Parallel Solver for the Gray-Scott Reaction-Diffusion System

Parallel Programming for Large-Scale Problems SF2568
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Problem description

The subject of this report is the parallelization of a numerical method for a two-component reaction-diffusion system known as the Gray-Scott model. Originally introduced by Gray and Scott [1], the model is a system of two partial differential equations for the concentration of two generic chemical species, which are reacting with each other as they diffuse through a medium.

Pattern formation resulting from the Gray-Scott model is a rich area of research, with applications to a variety of physical, chemical, and biological phenomena, as well as cellular automata and the pattern formation of other partial differential equation systems [2]. We investigate a parallelization strategy for the two-dimensional case. We make a series of trials, running the solver in parallel on 4, 16, 36, and 64 processes, and perform a speedup analysis using the results of these trials. Finally, we show a few of the various patterns that emerge from the Gray-Scott model with various input parameters.

Mathematical Formulation

The Gray-Scott model involves the reaction and diffusion of two generic chemical species, U and V, whose concentrations are described by the functions $u(x, y, t)$ and $v(x, y, t)$, reacting according to the chemical equations

$$\begin{aligned} U + 2V &\to 3V, \\ V &\to P, \end{aligned}$$

where P is an inert byproduct. This system is governed by the following system of partial differential equations:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1 - u), \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 u + uv^2 - (F - K)v. \tag{2}$$

Here, D_u and D_v are the diffusion constants for u and v respectively, and F and K are constants which govern the replenishment of the chemical species.

Numerical Method

In order to discretize (1) and (2) we let....

...thus we can write the fully discretized equations as

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t[A\mathbf{u}^n + f_u(\mathbf{u}^n, \mathbf{v}^n)], \tag{3}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \Delta t[A\mathbf{v}^n + f_v(\mathbf{u}^n, \mathbf{v}^n)], \tag{4}$$

and we have an exact update formula for each time step.

Stability Conditions

In order to ensure numerical stability for the differential operator A in (3), we must conform to the restriction

$$\Delta t \lambda_k \in \mathcal{S},\ \forall k,\ k = 1, 2, \ldots \text{N},$$

where λ_k is the k-th eigenvalue of A, and $\mathcal{S}$ is the stability region of the forward Euler method: a circle in the complex plane centered at -1 with unit radius [3]. The maximum eigenvalue, λ_{max} for the chosen parameters has a strictly negative real value, and thus we must choose a timestep such that $\Delta t \cdot \lambda_{max}$ is at least -2. The maximum eigenvalue is computed using Matlab as:

$$\lambda_{max} = -2.547,$$

which provides the limitation on the timestep:

$$\Delta t \leq \frac{-2}{-2.547} = 0.7852.$$

Since the timestep also has a damping effect on the replenishment term and reaction rate, we must consider these as well when choosing the timestep. We settle on

$$\Delta t = 0.25.$$

This is well within the stability bounds of A, and provides suitable damping on the replenishment and reaction rate terms for Gray-Scott pattern formation as studied in [2].

Psuedo-code algorithm description

Theoretical performance evaluation

Implementation details

Testing with different cases

Experimental speedup investigation with meaningful data

References

[1] Gray P, Scott SK. *Sustained oscillations and other exotic patterns of behavior in isothermal reactions.* J Phys Chem 1985;89:22–32.

[2] Weiming Wang, Yezhi Lin, Feng Yang, Lei Zhang, Yongji Tan, *Numerical study of pattern formation in an extended Gray–Scott model*, Communications in Nonlinear Science and Numerical Simulation, 16 (2011).

[3] Lennart Edsberg *Introduction to Computation and Modelling for Differential Equations*, 2008, John Wiley and Sons, pp 50.