ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

High Performance Computing for Science and Engineering I

Spring semester 2015

Prof. Dr. P. Koumoutsakos
ETH Zentrum, CLT F12
CH-8092 Zürich

Project 3

Issued: 2015
Hand in: 2015

ADI

Alternating Direction Implicit (ADI) is a finite difference scheme based on the idea of operator splitting. The ADI method applied to the diffusion equation

$$\frac{\partial \rho(\mathbf{r},\, t)}{\partial t} \;=\; D\nabla^2 \rho(\mathbf{r},\, t) \tag{1}$$

is summarized in the following two steps:

Step 1 Implicit Euler in x direction; Explicit Euler in y direction:

$$\rho_{i,j}^{n+\frac{1}{2}} = \rho_{i,j}^{n} + \frac{D\delta t}{2}\left[\frac{\partial^2 \rho_{i,j}^{n+\frac{1}{2}}}{\partial x^2} + \frac{\partial^2 \rho_{i,j}^{n}}{\partial y^2}\right] \tag{2}$$

Step 2 Explicit Euler in x direction; Implicit Euler in y direction:

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{n+\frac{1}{2}} + \frac{D\delta t}{2}\left[\frac{\partial^2 \rho_{i,j}^{n+\frac{1}{2}}}{\partial x^2} + \frac{\partial^2 \rho_{i,j}^{n+1}}{\partial y^2}\right] \tag{3}$$

The algorithm takes advantage of both implicit and explicit schemes and results in an integration scheme which is unconditionally stable and second order in space and time.

Moreover, the implicit integration step, which usually requires iterative methods in order to invert a matrix, consists in a tridiagonal system of equations which can be efficiently solved by the Thomas algorithm.

In order to use the latter method for the implicit step in x direction, we need to rewrite for each row j the implicit step

$$\rho_{i,j}^{*} = \rho_{i,j}^{n} + \frac{\delta t}{2}\frac{D}{\delta x^2}\left(\rho_{i-1,j}^{*} - 2\rho_{i,j}^{*} + \rho_{i+1,j}^{*}\right) \tag{4}$$

in the form $\mathbf{A}\boldsymbol{\rho}^{*} = \boldsymbol{\rho}^{n}$, where $\mathbf{A}$ is a tridiagonal matrix of coefficients a_i (lower diagonal, $i = 1..n$), b_i (main diagonal, $i = 0..n$) and c_i (upper diagonal, $i = 0..n-1$), $\boldsymbol{\rho}^{*}$ is the unknown

vector of $\rho^*_{i,j}$ with $i = 0..n$ and $\boldsymbol{\rho}^n$ is the corresponding solution vector of $\rho^n_{i,j}$ with $i = 0..n$ at time n for row j.

An implicit step of ADI in x direction therefore consists in solving m tridiagonal systems of equations, where m is the size of the grid in y direction.

For the implicit Euler step in y direction we proceed analogously by writing a m systems of equations, where m is the size of the grid in x direction.

Thomas Algorithm

The Thomas algorithm[1], named after Llewellyn Thomas, is an $\mathcal{O}(n)$ algorithm used to solve a tridiagonal system of equations and can therefore be used to solve the implicit component of ADI.

In the following, a C code is given for the Thomas algorithm as a reference (from Wikipedia):

```c
void solveMatrix(int n, double *a, double *b, double *c,
  double *v, double *x)
{
    /**
     * n - number of equations
     * a - sub-diagonal (means it is the diagonal below the
       main diagonal) -- indexed from 1..n-1
     * b - the main diagonal
     * c - sup-diagonal (means it is the diagonal above the
       main diagonal) -- indexed from 0..n-2
     * v - right part
     * x - the answer
     */
    for (int i = 1; i < n; i++)
    {
        double m = a[i]/b[i-1];
        b[i] = b[i] - m*c[i-1];
        v[i] = v[i] - m*v[i-1];
    }

    x[n-1] = v[n-1]/b[n-1];

    for (int i = n - 2; i >= 0; i--)
        x[i] = (v[i] - c[i] * x[i+1]) / b[i];
}
```

Note that the algorithm is not parallel due to dependencies between iterations.

[1] from Wikipedia

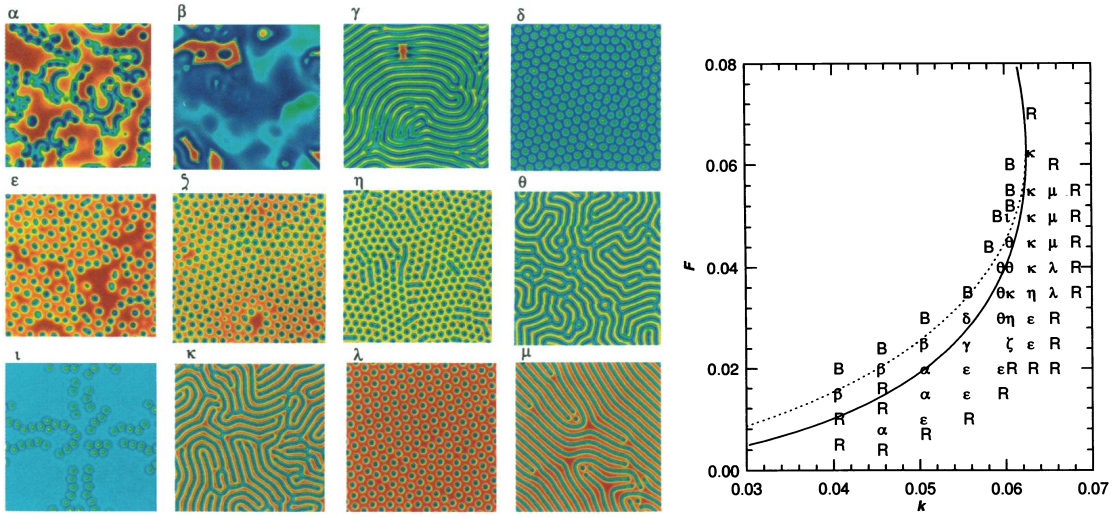

Figure 1: *On the left, different patterns obtained with Gray-Scott system. The Greek letters on the right figure indicate the locations in the parameter space which correspond to the patterns on the images on the left. Both figures are taken from "Complex Patterns in a Simple Systems" by J.E. Pearson.*

Reaction Diffusion

Reaction-Diffusion processes describe the evolution of concentrations of one or more substances distributed in a space. The substance concentrations are modified by chemical reactions and their distribution is governed by diffusion. The corresponding reaction-diffusion equation for M different species with respective concentration fields u_i and diffusion coefficients D_i has following form:

$$\frac{\partial u_i}{\partial t} = D_i \Delta u_i + f_i(\mathbf{u}),\ \forall i = 1 \cdots M, \tag{5}$$

where $\mathbf{u} = (u_1, u_2, \cdots u_M)$. The terms f_i describe creation or consumption of species i caused by reactions. Note that since each concentration field u_i depends on the reaction term $f_i(\mathbf{u})$ (with possible different form for the term f_i), we are dealing with a system of coupled PDEs.

We will consider Gray-Scott system, a reaction-diffusion system consisting of two chemical species with respective concentrations u and v and corresponding diffusion terms D_u, D_v, which are subjects to the following reaction-diffusion equation:

$$\frac{\partial u}{\partial t} = D_u \Delta u - uv^2 + F(1-u), \tag{6}$$

$$\frac{\partial v}{\partial t} = D_v \Delta v + uv^2 - (F+k)v. \tag{7}$$

The terms F and k are model parameters. The Gray-Scott system results in a formation of various patterns, see Figure 1 for few examples, where different pattern modes are obtain by different combination of values for model parameters F and k.

ADI for Reaction-Diffusion Equation

We can use ADI to simulate the reaction-diffusion equation. Since now we are solving a system of coupled PDEs (Equation 5), each grid point will carry a vector of concentrations, with one entry for each chemical species. Assuming the Gray-Scott system with two species with respective concentrations u, and v, given in Equations 6-7, we will define for each grid point a vector of corresponding concentrations as:

$$\mathbf{u}_k^n = (u_k^n, v_k^n) = (u(\mathbf{x}_k,\, n \cdot \delta t), v(\mathbf{x}_k,\, n \cdot \delta t))\,. \tag{8}$$

Each grid point carries the concentration values of all species in vector $\boldsymbol{u}_k^n$.

The diffusion can be simulated as described above. We also observe that the reaction terms $f_i(u_k^n, v_k^n)$, where $i = 1, 2$ in the Gray-Scott system, only depend on (u_k^n, v_k^n) at the location of the corresponding grid points. Reactions are thus purely local operations and require no neighborhood interactions at all.

Question 1: Diffusion

We define the domain Ω in two dimensions as $x, y, \in [0,\, 1]$. We will use periodic boundary conditions and an initial density distribution

$$\rho(x, y, 0) = sin(x \cdot 2\pi) \cdot sin(y \cdot 2\pi), \tag{9}$$

for which the analytical solution is given by

$$\rho(x, y, t) = sin(x \cdot 2\pi) \cdot sin(y \cdot 2\pi) \cdot e^{-8D\pi^2 t}. \tag{10}$$

Question 2: Reaction-Diffusion

Extend your implementation of ADI to handle the Gray-Scott system. Consider the simulation domain $[-1, 1]^2$, with periodic boundary conditions and initial conditions $(u, v) = (1, 0)$ everywhere except within the square $A = [-0.2, 0.2]^2$, which should be set to $\left(\frac{1}{2}, \frac{1}{4}\right)$ and perturbed with $\pm 1\%$ random noise in order to break the square symmetry, i.e:

$$u(x, y, 0) \;=\; (1 - \chi_A(x, y)\,) + \chi_A(x, y) \left(\frac{1}{2} + \frac{r_1}{100}\right), \tag{11}$$

$$v(x, y, 0) \;=\; \chi_A(x, y) \left(\frac{1}{4} + \frac{r_2}{100}\right), \tag{12}$$

where r_1, r_2 are random numbers from a normal distribution $\mathcal{N}(0, 1)$ and χ_A is the characteristic function:

$$\chi_A(x, y) = \begin{cases} 1 & \text{for } (x, y) \in [-0.2, 0.2]^2, \\ 0 & \text{otherwise.} \end{cases}$$

The diffusion coefficients are $D_u = 2 \times 10^{-5}$, $D_v = 10^{-5}$ and time step dt is chosen according the stability condition

$$dt \leq \frac{dh^2}{2 \max\{D_u, D_v\}} \tag{13}$$

where dh is a spacing between particles.

Chose any combination of parameters F and k based on the parameter space in Figure 1. Visualize the results and report the used parameters. Can you get the expected pattern?

Run your simulation sufficiently long so that you reach a steady state, meaning that you will have a pattern that is not changing with time.

Summary

Summarize your answers, results and plots into a PDF document. Furthermore, elucidate the main structure of the code and report possible code details that are relevant in terms of accuracy or performance. Send the PDF document, source code and related movies to your assigned teaching assistant.