More on Parabolic PDEs

M.Sc. in Mathematical Modelling & Scientific Computing,
Practical Numerical Analysis

Michaelmas Term 2019, Lecture 9

2D Heat Equation

The heat equation in 2D is given by

$$\frac{\partial u}{\partial t} \;=\; \nabla^2 u \;=\; \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\,,$$

for $t > 0$ and $x \in \Omega \subset \mathbb{R}^2$ with an initial condition

$$u(x, y, 0) \;=\; u_0(x, y)\,,$$

for $x \in \Omega$. We consider Dirichlet boundary conditions

$$u(x, y, t) \;=\; u_D(x, y, t) \quad \text{for } (x, y) \in \partial\Omega\,, \quad t > 0.$$

The Mesh

We define a sequence of uniform timesteps by

$$t_m = m\Delta t$$

for $m = 0, 1, 2, \ldots$ where $\Delta t > 0$ is the constant timestep size.

For the spatial mesh, we assume that the domain Ω is a rectangle, namely $\Omega = (a, b) \times (c, d)$ so that $x \in [a, b]$ and $y \in [c, d]$. We then define a set of uniform mesh points by

$$\begin{aligned} x_i &= a + i\Delta x \ , \\ y_j &= c + j\Delta y \ , \end{aligned}$$

for $i = 0, 1, \ldots, N_x$, $j = 0, 1, \ldots, N_y$ and with the meshsizes $\Delta x = (b - a)/N_x$ and $\Delta y = (d - c)/N_y$.

We write $u(x_i, y_j, t_m) = u^m_{i,j}$ and seek to approximate $u^m_{i,j}$ by $U^m_{i,j}$ for $i = 0, 1, \ldots, N_x$, $j = 0, 1, \ldots, N_y$ and $m = 0, 1, 2, \ldots$.

Finite Difference Schemes

We can write down finite difference schemes in an analogous way to the 1D case. First define

$$\begin{aligned} \delta_x^2 U_{i,j} &= U_{i+1,j} - 2U_{i,j} + U_{i-1,j} \ , \\ \delta_y^2 U_{i,j} &= U_{i,j+1} - 2U_{i,j} + U_{i,j-1} \ . \end{aligned}$$

Then we may write

- Forward Euler (or Explicit Euler)

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^{m}}{\Delta y^2}$$

- Backward Euler (or Implicit Euler)

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\delta_x^2 U_{i,j}^{m+1}}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^{m+1}}{\Delta y^2}$$

Finite Difference Schemes

- θ-Method (Crank Nicolson when $\theta = 1/2$)

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\theta\delta_x^2 U_{i,j}^{m+1} + (1-\theta)\delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{\theta\delta_y^2 U_{i,j}^{m+1} + (1-\theta)\delta_y^2 U_{i,j}^{m}}{\Delta y^2} \quad (1)$$

Finite Difference Schemes

All these finite difference schemes hold for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, N_y - 1$ and $m = 0, 1, \ldots$.

We must also discretise the initial and boundary conditions as

$$\begin{aligned}
U^0_{i,j} &= u_0(x_i, y_j)\ , \quad i = 0, 1, \ldots, N_x,\ j = 0, 1, \ldots, N_y \\
U^m_{0,j} &= u_D(a, y, t_m)\ , \quad j = 0, 1, \ldots, N_y,\ m = 1, 2, \ldots \\
U^m_{N_x,j} &= u_D(b, y, t_m)\ , \quad j = 0, 1, \ldots, N_y,\ m = 1, 2, \ldots \\
U^m_{i,0} &= u_D(x, c, t_m)\ , \quad i = 1, \ldots, N_x - 1,\ m = 1, 2, \ldots \\
U^m_{i,N_y} &= u_D(x, d, t_m)\ , \quad i = 1, \ldots, N_x - 1,\ m = 1, 2, \ldots
\end{aligned}$$

Forward Euler Scheme

The forward Euler scheme is

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^{m}}{\Delta y^2}$$

for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, N_y - 1$ and $m = 0, 1, \ldots$. Writing $\mu_x = \Delta t / \Delta x^2$ and $\mu_y = \Delta t / \Delta y^2$, we may re-arrange the scheme to get

$$\begin{aligned} U_{i,j}^{m+1} &= U_{i,j}^{m} + \mu_x (U_{i+1,j}^{m} - 2U_{i,j}^{m} + U_{i-1,j}^{m}) \\ &\quad + \mu_y (U_{i,j+1}^{m} - 2U_{i,j}^{m} + U_{i,j-1}^{m}) \end{aligned}$$

for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, N_y - 1$ and $m = 0, 1, \ldots$.

As in 1D, this is very simple to implement.

θ-Method

The θ-method is

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\theta\delta_x^2 U_{i,j}^{m+1} + (1-\theta)\delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{\theta\delta_y^2 U_{i,j}^{m+1} + (1-\theta)\delta_y^2 U_{i,j}^{m}}{\Delta y^2}\,.$$

(Recall this includes the backward Euler scheme if we take $\theta = 1$.)

We may re-arrange the scheme to get

$$\begin{aligned}-\mu_x\theta(U_{i+1,j}^{m+1} + U_{i-1,j}^{m+1}) - \mu_y\theta(U_{i,j+1}^{m+1} + U_{i,j-1}^{m+1}) + (1+2\theta(\mu_x+\mu_y))U_{i,j}^{m+1} \\ = \mu_x(1-\theta)(U_{i+1,j}^{m} + U_{i-1,j}^{m}) + \mu_y(1-\theta)(U_{i,j+1}^{m} + U_{i,j-1}^{m}) \\ +(1-2(1-\theta)(\mu_x+\mu_y))U_{j}^{m}\end{aligned}$$

for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, Ny - 1$ and $m = 0, 1, \ldots$.

θ-Method — Linear System

In the case of homogeneous Dirichlet boundary conditions we have $U_{0,j}^{m+1} = U_{N_x,j}^{m+1} = U_{i,0}^{m+1} = U_{i,N_y}^{m+1} = 0$ and we may write the vector of unknowns as

$$\mathbf{U}^{m+1} \;\; = \;\; (U_{1,1}^{m+1}, U_{1,2}^{m+1}, \ldots U_{1,N_y-1}^{m+1}, U_{2,1}^{m+1} \ldots U_{N_x-1,N_y-1}^{m+1})^T \; .$$

We may then write a linear system

$$(I - \theta A)\mathbf{U}^{m+1} \;\; = \;\; (I + (1-\theta)A)\mathbf{U}^m \; ,$$

where A is a matrix with $(N_x - 1)(N_y - 1)$ rows and columns and I is the identity matrix of the same size.

θ-Method — Linear System

The structure of A is

$$A = \left.\begin{pmatrix} B & C & & & \\ C & B & C & & \\ & \ddots & \ddots & \ddots & \\ & & C & B & C \\ & & & C & B \end{pmatrix}\right\} N_x - 1 \text{ blocks}$$

where $B, C \in \mathbb{R}^{(N_y-1)\times(N_y-1)}$ are given by

$$B = \begin{pmatrix} -2(\mu_x + \mu_y) & \mu_y & \\ \mu_y & -2(\mu_x + \mu_y) & \mu_y \\ \ddots & \ddots & \ddots \\ & \mu_y & -2(\mu_x + \mu_y) \end{pmatrix},$$

and $C = \mu_x I_{N_y-1}$ with I_{N_y-1} being the identity matrix of size $N_y - 1$.

Truncation Error

The truncation error for the θ-method is given by

$$T_{i,j}^m = \frac{u_{i,j}^{m+1} - u_{i,j}^m}{\Delta t} - \frac{\theta\delta_x^2 u_{i,j}^{m+1} + (1-\theta)\delta_x^2 u_{i,j}^m}{\Delta x^2} - \frac{\theta\delta_y^2 u_{i,j}^{m+1} + (1-\theta)\delta_y^2 u_{i,j}^m}{\Delta y^2} .$$

It is standard to perform Taylor series approximations about the point $(x_i, y_j, t_{m+1/2})$. This gives

$$T_{i,j}^m = \left(\frac{1}{2} - \theta\right)\Delta t u_{tt} - \frac{1}{12}(\Delta t^2 u_{ttt} + \Delta x^2 u_{xxxx} + \Delta y^2 u_{yyyy}) .$$

Thus for θ independent of Δt and Δx:

- in general, the θ-method is first order in Δt and second order in Δx and Δy;
- for the particular case $\theta = 1/2$, the Crank Nicolson method is second order in Δt, Δx and Δy.

Stability

Stability can be assessed by inserting the Fourier mode $U_{i,j}^m = [\lambda(k_x, k_y)]^m \, \mathrm{e}^{i(k_x x_i + k_y y_j)}$ into the numerical scheme. The scheme is then practically stable if $|\lambda(k_x, k_y)| \leq 1$. Substituting such a Fourier mode into the θ-method (1) and simplifying gives

$$\lambda(k_x, k_y) \;\; = \;\; \frac{1 - 4(1-\theta)(\mu_x \sin^2(k_x \Delta x/2) + \mu_y \sin^2(k_y \Delta y/2))}{1 + 4\theta(\mu_x \sin^2(k_x \Delta x/2) + \mu_y \sin^2(k_y \Delta y/2))}$$

for $k_x \in [-\pi/\Delta x, \pi/\Delta x]$ and $k_y \in [-\pi/\Delta y, \pi/\Delta y]$ and where $\mu_x = \Delta t/\Delta x^2$ and $\mu_y = \Delta t/\Delta y^2$.

Clearly this satisfies $\lambda(k_x, k_y) \leq 1$ for all k_x and k_y. For $\lambda(k_x, k_y) \geq -1$ we require

$$2(\mu_x \sin^2(k_x \Delta x/2) + \mu_y \sin^2(k_y \Delta y/2))(1 - 2\theta) \;\; \leq \;\; 1 \, .$$

This is clearly true for all $\theta \geq 1/2$, but for $\theta < 1/2$ this gives a restriction on Δt.

Stability

Thus for the θ-method we have

- If $\theta \geq 1/2$ the method is unconditionally stable. In particular this means that the backward Euler and Crank-Nicolson schemes are unconditionally stable.
- If $\theta < 1/2$ the method is only conditionally stable. The values of Δt, Δx and Δy must be chosen so that

$$\Delta t \quad \leq \quad \frac{\Delta x^2 \Delta y^2}{\Delta x^2 + \Delta y^2} \frac{1}{2(1-2\theta)} \,.$$

  In particular this means that the forward Euler method is only conditionally stable and, in the case where $\Delta x = \Delta y$, the condition for stability is that $\Delta t \leq \Delta x^2/4$.

Example

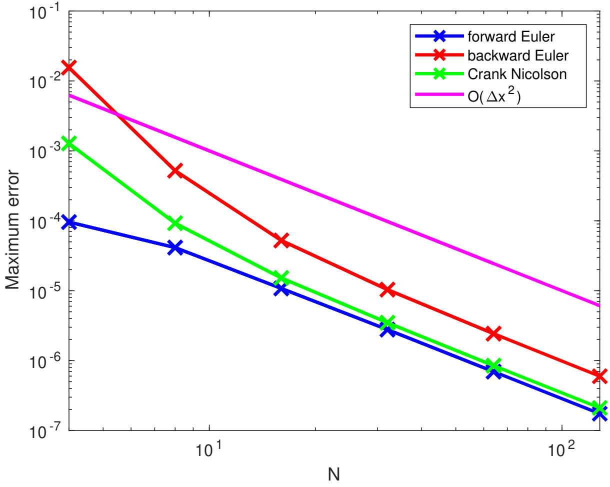
Solve the heat equation $u_t = u_{xx} + u_{yy}$ in the unit square $[0,1]^2$ with homogeneous Dirichlet boundary conditions and initial condition

$$u(x,y,0) \;\; = \;\; \sin(\pi x)\sin(3\pi y)\;.$$

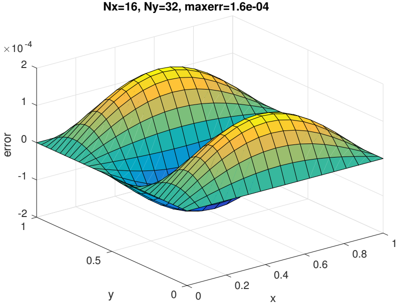
The exact solution is

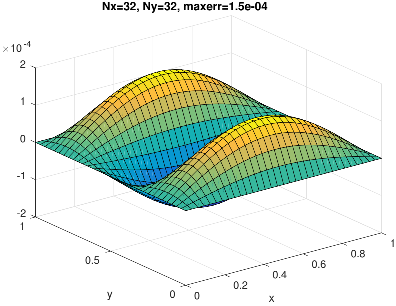
$$u(x,y,t) \;\; = \;\; \mathrm{e}^{-10\pi^2 t}\sin(\pi x)\sin(3\pi y)\;.$$

Results with $\Delta x^2 = \Delta y^2$ and $\Delta t = \Delta x^2/4$



Solution $\Delta x \neq \Delta y$





Method of Lines

What we have done above is to use the method of lines where we first discretise in space to get a system of ODEs and then use a numerical method to solve the ODEs.

So for the 1D heat equation, with homogeneous Dirichlet boundary conditions we can discretise in space using the standard finite difference scheme to get

$$\frac{\mathrm{d}U_j(t)}{\mathrm{d}t} = \frac{U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)}{\Delta x^2}$$

for $j = 1, \ldots, N-1$ and with $U_0(t) = U_N(t) = 0$. We can re-write this as a system of ODEs of the form

$$\frac{\mathrm{d}\mathbf{U}}{\mathrm{d}t} = A\mathbf{U}$$

with initial condition $\mathbf{U}(0) = u_0(\mathbf{x})$.

There is no reason why the spatial discretisation should be via a finite difference scheme — this could be replaced by a finite element method or a spectral method or ...

Coupled Problems

Can use the types of methods already discussed to solve coupled systems of PDEs.

Recall that for the heat equation with homogeneous Dirichlet boundary conditions, we can write the θ-method in matrix form as

$$(I - \theta A)\mathbf{U}^{m+1} = (I + (1-\theta)A)\mathbf{U}^m .$$

Now suppose we want to solve a coupled system of the form

$$\begin{aligned} \frac{\partial u}{\partial t} &= \nabla^2 u + \alpha v , \\ \frac{\partial v}{\partial t} &= \nabla^2 v + \beta u , \end{aligned}$$

for $t > 0$, and $x \in \Omega \subset \mathbb{R}^2$, with homogeneous Dirichlet boundary conditions on both u and v, and initial conditions

$$u(x, y, 0) = u_0(x, y) , \qquad v(x, y, 0) = v_0(x, y) ,$$

for $x \in \Omega$.

Coupled Problems

Using the same mesh and timestep as before, we can write a θ method for the u equation as

$$\begin{aligned}\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} &= \frac{\theta\delta_x^2 U_{i,j}^{m+1} + (1-\theta)\delta_x^2 U_{i,j}^{m}}{\Delta x^2} \\ &\quad + \frac{\theta\delta_y^2 U_{i,j}^{m+1} + (1-\theta)\delta_y^2 U_{i,j}^{m}}{\Delta y^2} \\ &\quad + \theta\alpha V_{i,j}^{m+1} + (1-\theta)\alpha V_{i,j}^{m} \ ,\end{aligned}$$

which can be written in matrix form as

$$\begin{aligned}(I - \theta A)\mathbf{U}^{m+1} - \theta\alpha\Delta t\mathbf{V}^{m+1} &= (I + (1-\theta)A)\mathbf{U}^{m} \\ &\quad + (1-\theta)\alpha\Delta t\mathbf{V}^{m} \ .\end{aligned}$$

Coupled Problems

Writing a similar finite difference equation for v also leads to a matrix form

$$\begin{aligned}(I-\theta A)\mathbf{V}^{m+1}-\theta\beta\Delta t\mathbf{U}^{m+1} &= (I+(1-\theta)A)\mathbf{V}^{m} \\ &\quad +(1-\theta)\beta\Delta t\mathbf{U}^{m}\,.\end{aligned}$$

This can be written as a big matrix system

$$\begin{aligned}&\begin{pmatrix} I-\theta A & -\theta\alpha\Delta tI \\ -\theta\beta\Delta tI & I-\theta A \end{pmatrix}\begin{pmatrix}\mathbf{U}^{m+1}\\ \mathbf{V}^{m+1}\end{pmatrix} \\ &\qquad = \begin{pmatrix} I+(1-\theta)A & (1-\theta)\alpha\Delta tI \\ (1-\theta)\beta\Delta tI & I+(1-\theta)A \end{pmatrix}\begin{pmatrix}\mathbf{U}^{m}\\ \mathbf{V}^{m}\end{pmatrix}\,.\end{aligned}$$

Nonlinear Problems

We can also extend these ideas to nonlinear problems. Consider a problem of the form

$$\frac{\partial u}{\partial t} = \nabla^2 u + f(u) ,$$

for $t > 0$, and $x \in \Omega \subset \mathbb{R}^2$, with homogeneous Dirichlet boundary conditions, and initial condition

$$u(x, y, 0) = u_0(x, y) ,$$

for $x \in \Omega$.

Nonlinear Problems

We can write a finite difference scheme of the form

$$\begin{aligned}\frac{U_{i,j}^{m+1}-U_{i,j}^{m}}{\Delta t} &= \frac{\theta\delta_x^2 U_{i,j}^{m+1}+(1-\theta)\delta_x^2 U_{i,j}^{m}}{\Delta x^2}\\ &+\frac{\theta\delta_y^2 U_{i,j}^{m+1}+(1-\theta)\delta_y^2 U_{i,j}^{m}}{\Delta y^2}\\ &+\theta f(U_{i,j}^{m+1})+(1-\theta)f(U_{i,j}^{m})\ ,\end{aligned}$$

along with the usual initial and boundary conditions. The drawback to this is that, unless the function f is linear, we now have to solve a very large nonlinear system at each timestep. This nonlinear system takes the form

$$\begin{aligned}(I-\theta A)\mathbf{U}^{m+1}-\theta\Delta t f(\mathbf{U}^{m+1}) &= (I+(1-\theta)A)\mathbf{U}^{m}\\ &+(1-\theta)\Delta t f(\mathbf{U}^{m})\ .\end{aligned}$$

Nonlinear Problems

An alternative is to treat the linear terms implicitly and the nonlinear terms explicitly so that the finite difference scheme becomes, in matrix form,

$$(I - \theta A)\mathbf{U}^{m+1} \;\; = \;\; (I + (1-\theta)A)\mathbf{U}^{m} + \Delta t f(\mathbf{U}^{m}) \; .$$

This has the advantage of only requiring a linear solve at each timestep. The approach often works well in practice and it is possible to use a larger timestep size than the simple explicit Euler scheme would have required.

Coupled Nonlinear Example

We consider the Cahn-Hilliard equation which was originally proposed to model phase separation in binary alloys. This is a 4th order problem but can be written as a system of two 2nd order equations

$$
\begin{aligned}
\frac{\partial c}{\partial t} - \nabla^2 w &= 0 \, , \\
w - \frac{1}{\epsilon}\Phi'(c) + \epsilon \nabla^2 c &= 0 \, ,
\end{aligned}
$$

with homogeneous Neumann boundary conditions for both c and w. Usually Φ is a double well potential, e.g. $\Phi(c) = (1 - c^2)^2/4$.

Here c has steady state ± 1 corresponding to pure phase A and pure phase B. In addition, ϵ represents the thickness of the interface between areas where $c = 1$ and areas where $c = -1$.

Coupled Nonlinear Example

If we let A be the matrix representing the Laplacian operator with Neumann boundary conditions (so a slightly different matrix to earlier) then we can use the method of lines to write

$$\begin{aligned} \frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t} - A\mathbf{W} &= 0 \\ \mathbf{W} - \frac{1}{\epsilon}\Phi'(\mathbf{C}) + \epsilon A\mathbf{C} &= 0\,. \end{aligned}$$

Using an implicit scheme for the linear terms and an explicit scheme for the nonlinear terms, we must solve

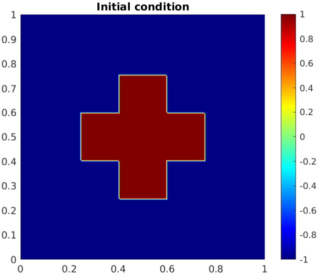
$$\begin{aligned} \frac{\mathbf{C}^{m+1} - \mathbf{C}^{m}}{\Delta t} - A\mathbf{W}^{m+1} &= 0 \\ \mathbf{W}^{m+1} - \frac{1}{\epsilon}\Phi'(\mathbf{C}^{m}) + \epsilon A\mathbf{C}^{m+1} &= 0 \end{aligned}$$

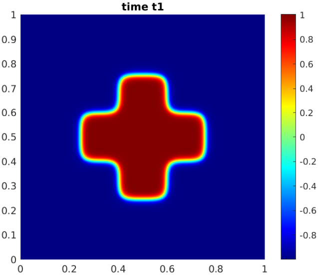
or, as a system we can write this as

$$\begin{pmatrix} I & -\Delta t A \\ \epsilon A & I \end{pmatrix} \begin{pmatrix} \mathbf{C}^{m+1} \\ \mathbf{W}^{m+1} \end{pmatrix} = \begin{pmatrix} \mathbf{C}^{m} \\ \Phi'(\mathbf{C}^{m})/\epsilon \end{pmatrix}.$$

Coupled Nonlinear Example

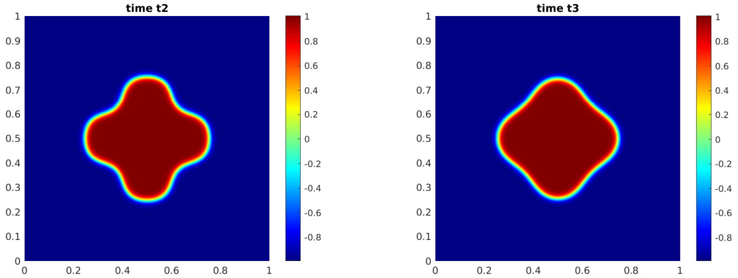
We can take an initial condition where $c = 1$ in a cross in the centre of the domain and $c = -1$ outside this region.





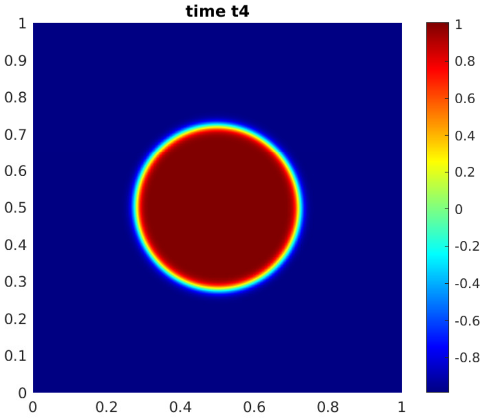
Coupled Nonlinear Example

The edges of the cross smooth out.



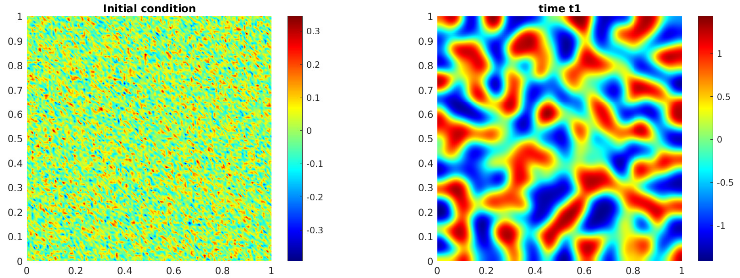
Coupled Nonlinear Example

The steady state has an interface in the shape of a circle.



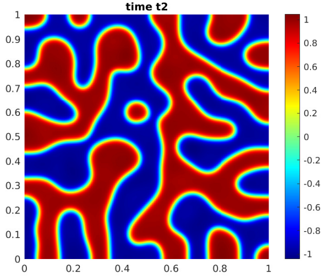
Coupled Nonlinear Example

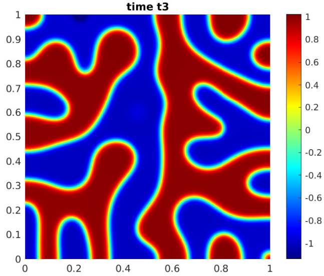
Alternatively we can take a random initial condition. At each grid point we set c to be a number drawn from a normal distribution with mean zero and variance one, then scaled by 0.1.



Coupled Nonlinear Example

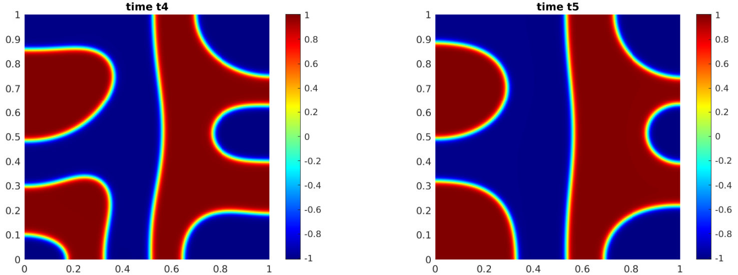
The solution has patches where it is 1 and patches where it is -1 and the boundaries of these regions are preferentially straight edges or circles.



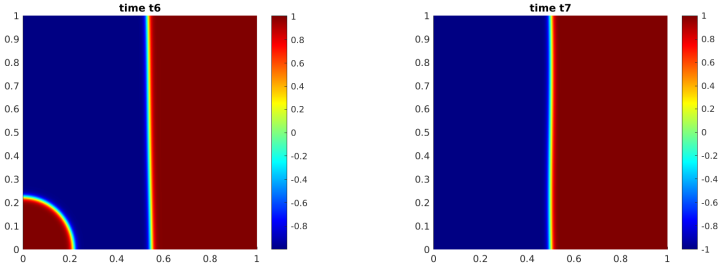


Coupled Nonlinear Example

The solution has patches where it is 1 and patches where it is -1 and the boundaries of these regions are preferentially straight edges or circles.



Coupled Nonlinear Example



The steady state solution (for this initial data) is -1 in the left half of the domain and 1 in the right half of the domain with an interface of size ϵ.