FINITE DIFFERENCES METHOD part II

Parabolic equations - two (or three) spatial variables

The explicit method

Consider the heat equation in a square domain $D = [0, X] \times [0, Y]$

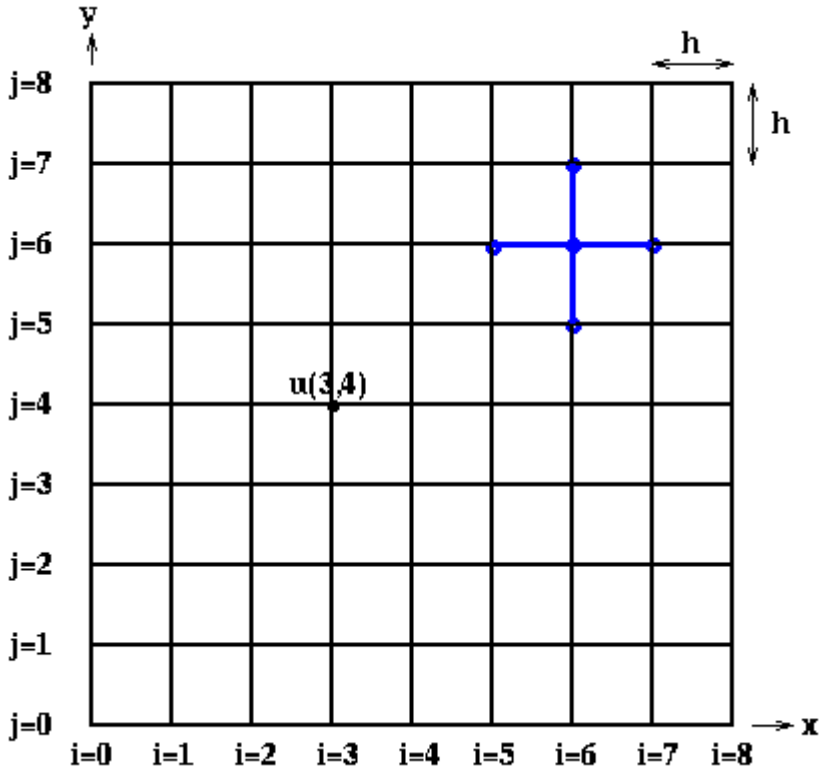
$$\frac{\partial u}{\partial t} = \sigma \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right], \ \sigma > 0$$

along with the Dirichlet type boundary conditions, i.e. the values $u(x, y, t)\big|_{\partial D}$ and $u(x, y, 0)\big|_D$ are known and σ is a constant positive number.

Consider also the mesh with the steps Δx and Δy in Ox and Oy directions:

$$\Delta x = \frac{X}{N_x}, \quad \Delta y = \frac{Y}{N_y}$$

where N_x and N_y represent the nodes number in Ox and Oy directions.



We note the approximation of the initial solution in a point (i, j) of the mesh at the time step n with

$$U_{i,j}^{n} \approx u\left(x_i, y_j, t_n\right),$$
$$i = 0,1,\ldots, N_x, \quad j = 0,1,\ldots, N_y.$$

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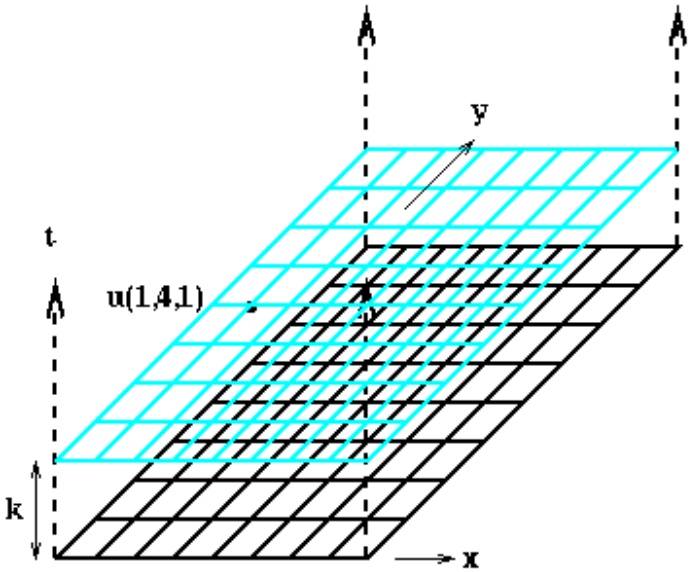
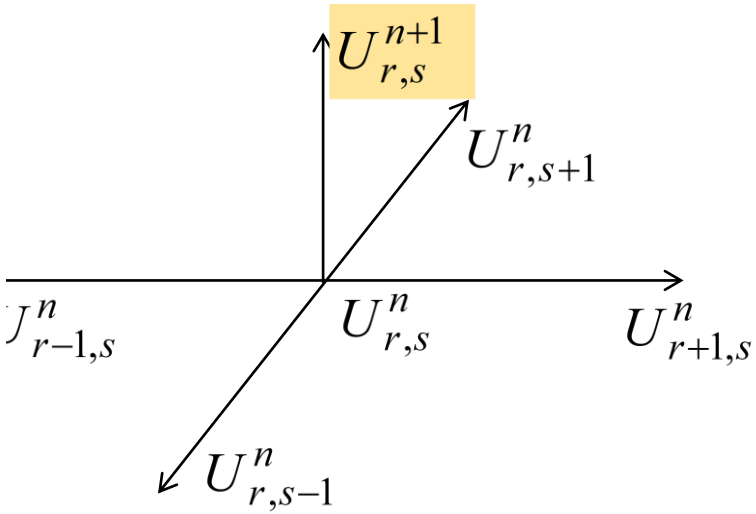
By using progressive finite differences for the temporal derivative and central finite differences for the spatial derivatives the following explicit scheme is obtained:

$$\frac{U_{i,j}^{n+1} - U_{i,j}^{n}}{\Delta t} = \sigma\left[\frac{U_{i+1,j}^{n} - 2U_{i,j}^{n} + U_{i-1,j}^{n}}{\Delta x^2} + \frac{U_{i,j+1}^{n} - 2U_{i,j}^{n} + U_{i,j-1}^{n}}{\Delta y^2}\right] \quad (o)$$





We observe that the unknown value $U_{i,j}^{n+1}$ can be calculated because all values $U_{i,j}^{n}$ are known.

We introduce the truncation error in similar way with the 1D case:

$$T(x,t)=\frac{\Delta_t u(x,t)}{\Delta t}-\sigma\left[\frac{\delta_x u(x,t)}{(\Delta x)^2}+\frac{\delta_y u(x,t)}{(\Delta y)^2}\right]$$

and using the Taylor expansion we get:

$$\Delta_t u(x,t)=u_t\Delta t+\frac{1}{2}u_{tt}(\Delta t)^2+\frac{1}{6}u_{ttt}(\Delta t)^3+\ldots$$

$$\delta_x^2 u(x,t)=u_{xx}(\Delta x)^2+\frac{1}{12}u_{tttt}(\Delta x)^4+\ldots$$

$$T(x,t)=\frac{1}{2}\Delta t\,u_{tt}-\frac{1}{12}\sigma\left[(\Delta x)^2u_{xxxx}+(\Delta y)^2u_{yyyy}\right]+\ldots$$

and the maximum convergence error:

$$E^n\le\left[\frac{1}{2}\Delta t\,M_{tt}+\frac{1}{12}\sigma\left(\Delta x^2\,M_{xxxx}+\Delta y^2\,M_{yyyy}\right)\right]t_F$$

is obtained if the bi-dimensional mesh satisfy the severe condition:

$$\nu_x+\nu_y=\frac{\sigma\Delta t}{\Delta x^2}+\frac{\sigma\Delta t}{\Delta x^2}\le\frac{1}{2}\qquad(*)$$

In order to study the stability we will consider the von Neumann method where the Fourier mode has the form:

$$U^n \approx \lambda^n Exp\left[I\left(k_x x + k_y y\right)\right] \qquad (**)$$

Substituting this form into the numerical explicit scheme the amplification factor is:

$$\lambda = \lambda\left(k_x, k_y\right) = 1 - 4\left[\nu_x \sin^2\left(\frac{1}{2}k_x \Delta x\right) + \nu_y \sin^2\left(\frac{1}{2}k_y \Delta y\right)\right]$$

from where the condition (*) for stability is obtained.

$$\nu_x + \nu_y = \frac{\sigma \Delta t}{\Delta x^2} + \frac{\sigma \Delta t}{\Delta x^2} \leq \frac{1}{2}$$

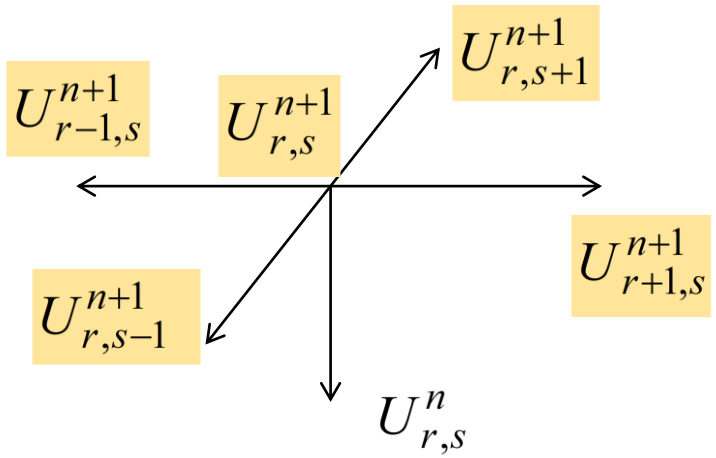
The implicit method

The implicit method is given by:

$$\frac{U_{i,j}^{n+1}-U_{i,j}^{n}}{\Delta t}=\sigma\left[\frac{U_{i+1,j}^{n+1}-2U_{i,j}^{n+1}+U_{i-1,j}^{n+1}}{\Delta x^{2}}+\frac{U_{i,j+1}^{n+1}-2U_{i,j}^{n+1}+U_{i,j-1}^{n+1}}{\Delta y^{2}}\right] \quad \text{(oo)}$$

and it leads to the following system:

$$\nu_x U_{i+1,j}^{n+1}+\nu_x U_{i-1,j}^{n+1}-\left(2\nu_x+2\nu_y+1\right)U_{i,j}^{n+1}+\nu_y U_{i,j+1}^{n+1}+\nu_y U_{i,j-1}^{n+1}=-U_{i,j}^{n} \quad \text{(oo)}$$



It is worth mentioning that the structure of the system (oo) does not allow us to solve it easy.

The implicit scheme (oo) is stable no matter the temporal and spatial steps' dimensions.

In order to find the unknowns $U_{i,j}^{n+1}$ it is necessary to solve an algebraic sparse linear system of dimension $(N_x - 1)\times(N_y - 1)$.

Example: Consider the implicit scheme:
(K. Hoffmann, S. Chiang, Computational Fluid Dynamics, 4th ed, EES, Wichita, 2000)

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{(\Delta t)} = \alpha\left[\frac{u_{i+1,j}^{n+1} - 2u_{i,j}^{n+1} + u_{i-1,j}^{n+1}}{(\Delta x)^2} + \frac{u_{i,j+1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j-1}^{n+1}}{(\Delta y)^2}\right]$$

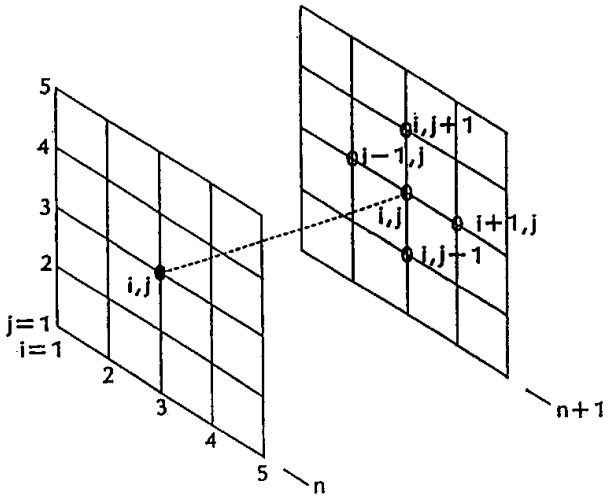
$$d_x u_{i+1,j}^{n+1} + d_x u_{i-1,j}^{n+1} - (2d_x + 2d_y + 1)u_{i,j}^{n+1} + d_y u_{i,j-1}^{n+1} + d_y u_{i,j+1}^{n+1} = -u_{ij}^{n}$$

where

$$d_x = \frac{\alpha \Delta t}{(\Delta x)^2} \qquad d_y = \frac{\alpha \Delta t}{(\Delta y)^2}$$

We note the coefficients with a, b, c, d, e and f:

$$a_{i,j}u^{n+1}_{i+1,j} + b_{i,j}u^{n+1}_{i-1,j} + c_{i,j}u^{n+1}_{i,j} + d_{i,j}u^{n+1}_{i,j-1} + e_{i,j}u^{n+1}_{i,j+1} = f^{n}_{i,j}$$



$$a_{2,2}u_{3,2} + c_{2,2}u_{2,2} + e_{2,2}u_{2,3} = f_{2,2} - b_{2,2}u_{1,2} - d_{2,2}u_{2,1}$$

$$a_{2,3}u_{3,3} + c_{2,3}u_{2,3} + d_{2,3}u_{2,2} + e_{2,3}u_{2,4} = f_{2,3} - b_{2,3}u_{1,3}$$

$$a_{2,4}u_{3,4} + c_{2,4}u_{2,4} + d_{2,4}u_{2,3} = f_{2,4} - b_{2,4}u_{1,4} - e_{2,4}u_{2,5}$$

$$a_{3,2}u_{4,2} + b_{3,2}u_{2,2} + c_{3,2}u_{3,2} + e_{3,2}u_{3,3} = f_{3,2} + d_{3,2}u_{3,1}$$

$$a_{3,3}u_{4,3} + b_{3,3}u_{2,3} + c_{3,3}u_{3,3} + d_{3,3}u_{3,2} + e_{3,3}u_{3,4} = f_{3,3}$$

$$a_{3,4}u_{4,4} + b_{3,4}u_{2,4} + c_{3,4}u_{3,4} + d_{3,4}u_{3,3} = f_{3,4} - e_{3,4}u_{3,5}$$

$$b_{4,2}u_{3,2} + c_{4,2}u_{4,2} + e_{4,2}u_{4,3} = f_{4,2} - a_{4,2}u_{5,2} - d_{4,2}u_{4,1}$$

$$b_{4,3}u_{3,3} + c_{4,3}u_{4,3} + d_{4,3}u_{4,2} + e_{4,3}u_{4,4} = f_{4,3} - a_{4,3}u_{5,3}$$

$$b_{4,4}u_{3,4} + c_{4,4}u_{4,4} + d_{4,4}u_{4,3} = f_{4,4} - a_{4,4}u_{5,4} - e_{4,4}u_{4,5}$$

Matrix form

$$\begin{bmatrix}
c_{2,2} & e_{2,2} & 0 & a_{2,2} & 0 & 0 & 0 & 0 & 0 \\
d_{2,3} & c_{2,3} & e_{2,3} & 0 & a_{2,3} & 0 & 0 & 0 & 0 \\
0 & d_{2,4} & c_{2,4} & 0 & 0 & a_{2,4} & 0 & 0 & 0 \\
b_{3,2} & 0 & 0 & c_{3,2} & e_{3,2} & 0 & a_{3,2} & 0 & 0 \\
0 & b_{3,3} & 0 & d_{3,3} & c_{3,3} & e_{3,3} & 0 & a_{3,3} & 0 \\
0 & 0 & b_{3,4} & 0 & d_{3,4} & c_{3,4} & 0 & 0 & a_{3,4} \\
0 & 0 & 0 & b_{4,2} & 0 & 0 & c_{4,2} & e_{4,2} & 0 \\
0 & 0 & 0 & 0 & b_{4,3} & 0 & d_{4,3} & c_{4,3} & e_{4,3} \\
0 & 0 & 0 & 0 & 0 & b_{4,4} & 0 & d_{4,4} & c_{4,4}
\end{bmatrix}
\begin{bmatrix} u_{2,2} \\ u_{2,3} \\ u_{2,4} \\ u_{3,2} \\ u_{3,3} \\ u_{3,4} \\ u_{4,2} \\ u_{4,3} \\ u_{4,4} \end{bmatrix}
=
\begin{bmatrix}
f_{2,2} - b_{2,2}u_{1,2} - d_{2,2}u_{2,1} \\
f_{2,3} - b_{2,3}u_{1,3} \\
f_{2,4} - b_{2,4}u_{1,4} - e_{2,4}u_{2,5} \\
f_{3,2} - d_{3,2}u_{3,1} \\
f_{3,3} \\
f_{3,4} - e_{3,4}u_{3,5} \\
f_{4,2} - a_{4,2}u_{5,2} - d_{4,2}u_{4,1} \\
f_{4,3} - a_{4,3}u_{5,3} \\
f_{4,4} - a_{4,4}u_{5,4} - e_{4,4}u_{4,5}
\end{bmatrix}$$

The coefficient matrix is pentadiagonal. The solution procedure for a pentadiagonal system of equations is also very time-consuming.

It should be noted that it is possible to obtain many implicit schemes depending on the assumption made on the spatial derivatives. An example is the Crank-Nicolson method (see Morega, 1998):

$$\frac{U_{i,j}^{n+1}-U_{i,j}^{n}}{\Delta t}=\frac{\sigma}{2}\left(\frac{U_{i+1,j}^{n+1}-2U_{i,j}^{n+1}+U_{i-1,j}^{n+1}}{(\Delta x)^2}+\frac{U_{i,j+1}^{n+1}-2U_{i,j}^{n+1}+U_{i,j-1}^{n+1}}{(\Delta y)^2}\right)+$$

$$+\frac{\sigma}{2}\left(\frac{U_{i+1,j}^{n}-2U_{i,j}^{n}+U_{i-1,j}^{n}}{(\Delta x)^2}+\frac{U_{i,j+1}^{n}-2U_{i,j}^{n}+U_{i,j-1}^{n}}{(\Delta y)^2}\right)$$

Alternating direction implicit (ADI) method

Due to the fact that the explicit schemes are restrictive and the implicit schemes are computationally costly, schemes implicit in one spatial direction and explicit in the other directions were looked for.

An example of such a scheme is:

$$\frac{U_{i,j}^{n+1}-U_{i,j}^{n}}{\Delta t}=\sigma\left(\frac{U_{i+1,j}^{n+1}-2U_{i,j}^{n+1}+U_{i-1,j}^{n+1}}{(\Delta x)^2}+\frac{U_{i,j+1}^{n}-2U_{i,j}^{n}+U_{i,j-1}^{n}}{(\Delta y)^2}\right) \text{(ooo)}$$

In order to calculate the solution we have to solve for each step in y direction a tri-diagonal system of order N_x-1. Using (**) into the scheme (ooo) the amplification factor is obtain:

$$\lambda(k_x,k_y)=\frac{1-2\nu_x\sin^2\left(\frac{1}{2}k_x\Delta x\right)-4\nu_y\sin^2\left(\frac{1}{2}k_y\Delta y\right)}{1+2\nu_x\sin^2\left(\frac{1}{2}k_x\Delta x\right)}$$

As expected regarding the stability there is the restriction $\frac{\sigma\Delta t}{(\Delta y)^2}\le\frac{1}{2}$, and for the term $\frac{\sigma\Delta t}{(\Delta x)^2}$ we have no restriction.

It is possible to obtain efficient methods by combining two such methods each of which being implicit in one direction. This is the principle of the alternating direction implicit methods. The first such scheme was proposed by Paceman and Rachford (1955) and was used for solving partial differential equations that model the flow in oil tanks.

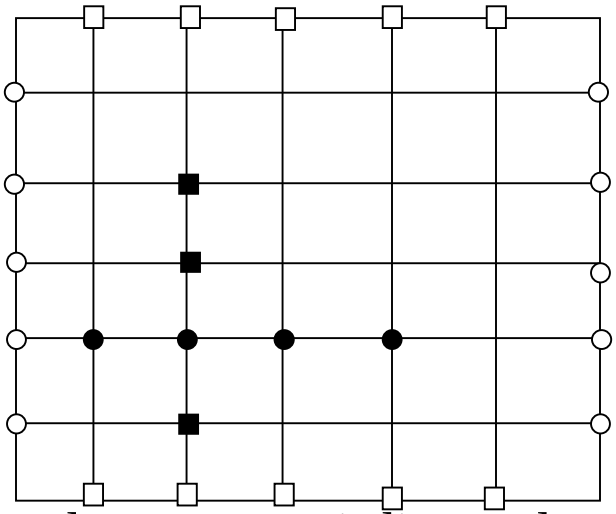
We introduce an intermediary time step, $n+1/2$, and we get:

$$\frac{U_{i,j}^{n+1/2}-U_{i,j}^{n}}{\Delta t}=\frac{\sigma}{2}\left(\frac{U_{i+1,j}^{n+1/2}-2U_{i,j}^{n+1/2}+U_{i-1,j}^{n+1/2}}{(\Delta x)^2}+\frac{U_{i,j+1}^{n}-2U_{i,j}^{n}+U_{i,j-1}^{n}}{(\Delta y)^2}\right) \quad \text{(ADI\_x)}$$

$$\frac{U_{i,j}^{n+1}-U_{i,j}^{n+1/2}}{\Delta t}=\frac{\sigma}{2}\left(\frac{U_{i+1,j}^{n+1/2}-2U_{i,j}^{n+1/2}+U_{i-1,j}^{n+1/2}}{(\Delta x)^2}+\frac{U_{i,j+1}^{n+1}-2U_{i,j}^{n+1}+U_{i,j-1}^{n+1}}{(\Delta y)^2}\right) \quad \text{(ADI\_y)}$$

If the values U^n are known from Eq. (ADI_x) it is possible to calculate $U^{n+1/2}$ and then using (ADI_y) the values of U^{n+1} are found.

In order to calculate $U^{n+1/2}$ we need the values of U^{n} but also the values from the boundary marked with "O", and for U^{n+1} we need the values of $U^{n+1/2}$ and the values from the boundary marked with "□"

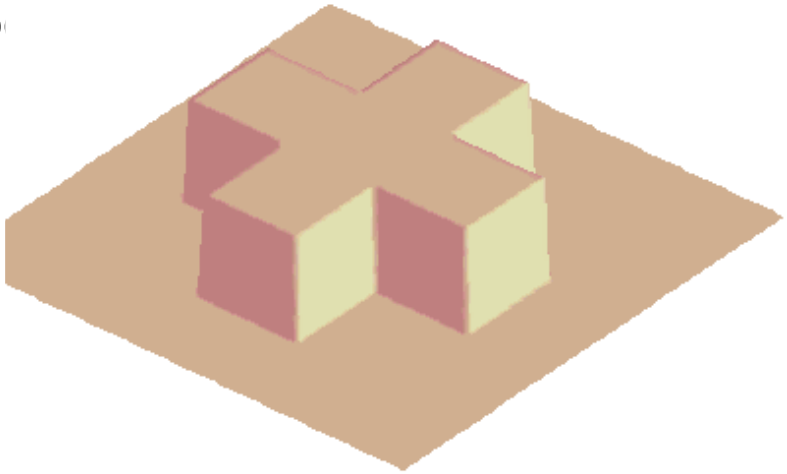


For a time step we have to solve $N_y - 1$ tri-diagonal systems (for the nodes marked with "●") of order $N_x - 1$, and then to solve $N_x - 1$ tri-diagonal systems (for the nodes marked with "■") of order $N_y - 1$. This process needs less time than solving a system of order $(N_x - 1)\times(N_y - 1)$ with a non tri-diagonal structure.

It is worth mentioning that it is possible to demonstrate, using a Fourier analysis, the ADI scheme is unconditionally stable (see Morton and Mayers, 1994).

Solving the heat equation using ADI method

Consider a square plate of length 1 having the boundary maintained at the dimensionless temperature 0. We suppose that at the initial moment (t = 0) a region of the plate having a cross form has the temperature T and the rest of the plate has the temperature 0. For the sake of simplicity we to



The heat equation is discretized using the ADI method for a rectangular mesh with the steps Δx and Δy and the Eqs. (ADI) are obtained. These equations can be written in the form:

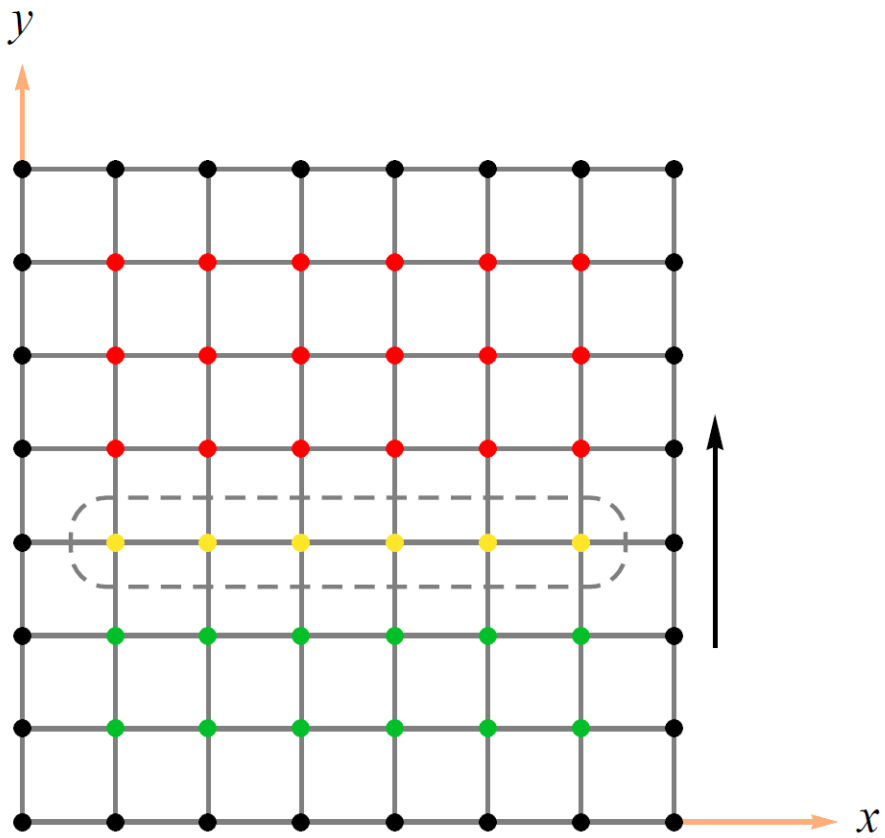
$$-\frac{1}{2}\nu_x U_{i+1,j}^{n+\frac{1}{2}} + (1+\nu_x) U_{i,j}^{n+\frac{1}{2}} - \frac{1}{2}\nu_x U_{i-1,j}^{n+\frac{1}{2}} = C_{i,j}^{n}$$

$$-\frac{1}{2}\nu_y U_{i,j+1}^{n+1} + (1+\nu_y) U_{i,j}^{n+1} - \frac{1}{2}\nu_y U_{i,j-1}^{n+1} = D_{i,j}^{n+\frac{1}{2}}$$

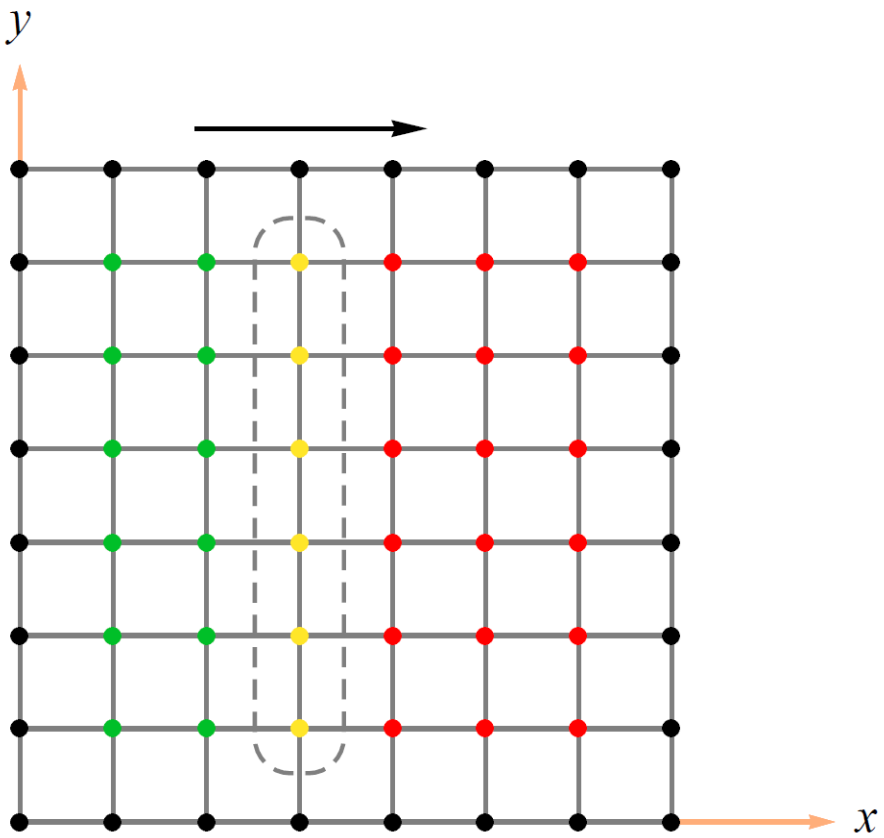
where $\nu_x = \frac{\Delta t}{(\Delta x)^2}$, $\nu_y = \frac{\Delta t}{(\Delta y)^2}$, and:

$$C_{i,j}^{n} = \frac{1}{2}\nu_y U_{i,j+1}^{n} + (1-\nu_y) U_{i,j}^{n+1} + \frac{1}{2}\nu_y U_{i,j-1}^{n+1}$$

$$D_{i,j}^{n+\frac{1}{2}} = \frac{1}{2}\nu_x U_{i+1,j}^{n+\frac{1}{2}} + (1-\nu_x) U_{i,j}^{n+\frac{1}{2}} + \frac{1}{2}\nu_x U_{i-1,j}^{n+\frac{1}{2}}$$



- – boundary nodes
- – nodes at n level
- – current nodes
- – updated nodes at $(n+1/2)$ level



- – boundary nodes
- – nodes at $(n+1/2)$ level
- – current nodes
- – updated nodes at $(n+1)$ level

Matlab program:

```
%Solve the heat equation in a rectangular domain
%[0,X]x[0,Y] using ADI method

X=1;
Y=1;
dt=0.0001;
dx=0.01;
dy=0.01;
Nx=X/dx
Ny=Y/dy
a=-0.5*dt/dx^2;
b=dt/dx^2;
aa=-0.5*dt/dy^2;
bb=dt/dy^2;
A=InitA(a,b,Nx,Ny);
B=InitB(aa,bb,Nx,Ny);
U=InitU(Nx,Ny);
surfl(U);
view(-50,60);
shading interp;
colormap(pink);
axis('off');
pause;
timp=0
while (timp<=0.01)
   timp=timp+dt
   C=InitC(U,Nx,Ny,aa,bb);
   for j=1:Ny-1
      U(:,j)=A\C(:,j);
   end;
   D=InitD(U,Nx,Ny,a,b);
   for i=1:Nx-1
      UU=B\D(i,:)';
      U(i,:)=UU';
   end;
end;
   surfl(U);hold on;
   view(-40,60);
   contour3(U,4);
   view(-50,60);
   shading interp;
   colormap(pink);
   axis('off');
   hold off;
```

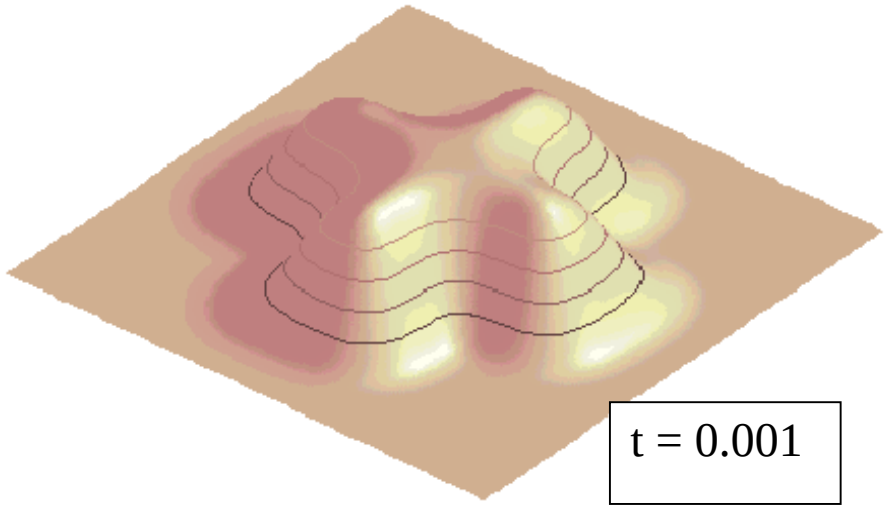
```
function A=InitA(a,b,Nx,Ny)
A=zeros(Nx-1,Ny-1);
for i=1:Nx-1
   A(i,i)=1+b;
end;
for i=1:Nx-2
   A(i+1,i)=a;
end;
for i=1:Nx-2
   A(i,i+1)=a;
end;
```

```
function B=InitB(aa,bb,Nx,Ny)
B=zeros(Nx-1,Ny-1);
for i=1:Nx-1
   B(i,i)=1+bb;
end;
for i=1:Nx-2
   B(i+1,i)=aa;
end;
for i=1:Nx-2
   B(i,i+1)=aa;
end;
```

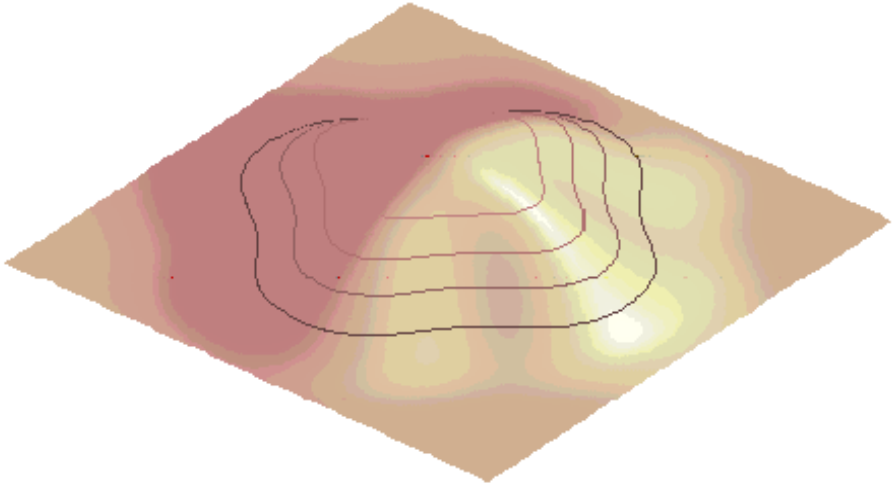
```
function U=InitU(Nx,Ny)
T=0.5
U=zeros(Nx-1,Ny-1);
for i=Nx/5:4*Nx/5
   for j=2*Ny/5:3*Ny/5
      U(i,j)=T;
   end;
end;
for i=2*Nx/5:3*Nx/5
   for j=Ny/5:4*Ny/5
      U(i,j)=T;
   end;
end;
```

```
function C=InitC(U,Nx,Ny,aa,bb)
C=zeros(Nx-1,Ny-1);
for i=1:Nx-1
   C(i,1)=-aa*U(i,2)+(1-bb)*U(i,1);
   C(i,Ny-1)=-aa*U(i,Ny-2)+(1-
bb)*U(i,Ny-1);
  for j=2:Ny-2
    C(i,j)=-aa*U(i,j+1)+(1-bb)*U(i,j)-
aa*U(i,j-1);
  end;
end;
```

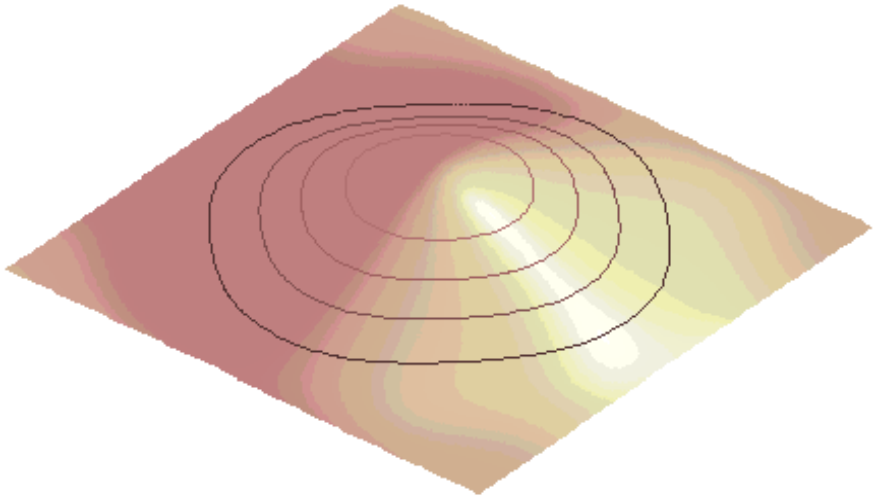
```
function  D=InitD(U,Nx,Ny,a,b)
D=zeros(Nx-1,Ny-1);
for j=1:Ny-1
   for i=2:Nx-2
      D(i,j)=-a*U(i+1,j)+(1-b)*U(i,j)-
a*U(i-1,j);
   end;
   D(1,j)=-a*U(2,j)+(1-b)*U(1,j);
   D(Ny-1,j)=-a*U(Ny-2,j)+(1-b)*U(Ny-
1,j);
end;
```



t = 0.001



t = 0.004



t = 0.01

Fractional step method

An approximation of multidimensional problems similar to ADI (or, in general, approximate factorization schemes) is the method of fractional step. This method splits the multidimensional equation into a series of one-space dimensional equations and solves them sequentially. For the two-dimensional model equation

$$\frac{\partial u}{\partial t} = \alpha \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right]$$

the method provides the following finite difference equations: (Note that the Crank-Nicolson scheme is used.)

$$\frac{u_{i,j}^{n+\frac{1}{2}} - u_{i,j}^{n}}{\frac{\Delta t}{2}} = \alpha \frac{1}{2} \left[\frac{u_{i+1,j}^{n+\frac{1}{2}} - 2u_{i,j}^{n+\frac{1}{2}} + u_{i-1,j}^{n+\frac{1}{2}}}{(\Delta x)^2} + \frac{u_{i+1,j}^{n} - 2u_{i,j}^{n} + u_{i-1,j}^{n}}{(\Delta x)^2} \right]$$

and

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n+\frac{1}{2}}}{\frac{\Delta t}{2}} = \alpha \frac{1}{2} \left[\frac{u_{i,j+1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j-1}^{n+1}}{(\Delta y)^2} + \frac{u_{i,j+1}^{n+\frac{1}{2}} - 2u_{i,j}^{n+\frac{1}{2}} + u_{i,j-1}^{n+\frac{1}{2}}}{(\Delta y)^2} \right]$$

The scheme is unconditionally stable and is of order $[(\Delta t)^2, (\Delta x)^2, (\Delta y)^2]$.

Extensions to three-space dimensions

The ADI method just investigated for the unsteady two-space dimensional parabolic equation can be extended to three-space dimensions, which is accomplished by considering time intervals of n, $n+\frac{1}{3}$, $n+\frac{2}{3}$, and $n+1$. The resulting equations for the model equation

$$\frac{\partial u}{\partial t} = \alpha\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right]$$

are:

$$\frac{u_{i,j,k}^{n+\frac{1}{3}} - u_{i,j,k}^{n}}{\frac{\Delta t}{3}} = \alpha\left[\frac{\delta_x^2 u_{i,j,k}^{n+\frac{1}{3}}}{(\Delta x)^2} + \frac{\delta_y^2 u_{i,j,k}^{n}}{(\Delta y)^2} + \frac{\delta_z^2 u_{i,j,k}^{n}}{(\Delta z)^2}\right]$$

$$\frac{u_{i,j,k}^{n+\frac{2}{3}} - u_{i,j,k}^{n+\frac{1}{3}}}{\frac{\Delta t}{3}} = \alpha\left[\frac{\delta_x^2 u_{i,j,k}^{n+\frac{1}{3}}}{(\Delta x)^2} + \frac{\delta_y^2 u_{i,j,k}^{n+\frac{2}{3}}}{(\Delta y)^2} + \frac{\delta_z^2 u_{i,j,k}^{n+\frac{1}{3}}}{(\Delta z)^2}\right]$$

and

$$\frac{u_{i,j,k}^{n+1} - u_{i,j,k}^{n+\frac{2}{3}}}{\frac{\Delta t}{3}} = \alpha\left[\frac{\delta_x^2 u_{i,j,k}^{n+\frac{2}{3}}}{(\Delta x)^2} + \frac{\delta_y^2 u_{i,j,k}^{n+\frac{2}{3}}}{(\Delta y)^2} + \frac{\delta_z^2 u_{i,j,k}^{n+1}}{(\Delta z)^2}\right]$$

where

$$\delta_x^2 u_{i,j} = u_{i+1,j} - 2u_{i,j} + u_{i-1,j}$$

$$\delta_y^2 u_{i,j} = u_{i,j+1} - 2u_{i,j} + u_{i,j-1}$$

The method is of order $[(\Delta t), (\Delta x)^2, (\Delta y)^2, (\Delta z)^2]$ and is only conditionally stable with the requirement of $(d_x + d_y + d_z) \leq (3/2)$. As a result of this requirement, the method is not very attractive. A method that is unconditionally stable and is second-order accurate uses the Crank-Nicolson scheme.

$$\frac{u^*_{i,j,k} - u^n_{i,j,k}}{\Delta t} = \alpha \left[\frac{1}{2} \frac{\delta_x^2 u^*_{i,j,k} + \delta_x^2 u^n_{i,j,k}}{(\Delta x)^2} + \frac{\delta_y^2 u^n_{i,j,k}}{(\Delta y)^2} + \frac{\delta_z^2 u^n_{i,j,k}}{(\Delta z)^2} \right],$$

$$\frac{u^{**}_{i,j,k} - u^n_{i,j,k}}{\Delta t} = \alpha \left[\frac{1}{2} \frac{\delta_x^2 u^*_{i,j,k} + \delta_x^2 u^n_{i,j,k}}{(\Delta x)^2} + \frac{1}{2} \frac{\delta_y^2 u^{**}_{i,j,k} + \delta_y^2 u^n_{i,j,k}}{(\Delta y)^2} + \frac{\delta_z^2 u^n_{i,j,k}}{(\Delta z)^2} \right],$$

and

$$\frac{u^{n+1}_{i,j,k} - u^n_{i,j,k}}{\Delta t} = \alpha \left[\frac{1}{2} \frac{\delta_x^2 u^*_{i,j,k} + \delta_x^2 u^n_{i,j,k}}{(\Delta x)^2} + \frac{1}{2} \frac{\delta_y^2 u^{**}_{i,j,k} + \delta_y^2 u^n_{i,j,k}}{(\Delta y)^2} + \frac{1}{2} \frac{\delta_z^2 u^{n+1}_{i,j,k} + \delta_z^2 u^n_{i,j,k}}{(\Delta z)^2} \right]$$

Linearization

The investigated models until this moment were linear. However, the real phenomena are not linear and in order to solve them some linearization methods must be used.

Further will give some examples for the non-linear term from Navier Stokes equations:

$$u\frac{\partial u}{\partial x}$$

Lagging method: (a intarzaierii) The non-linear term can be discretized in the following way:

$$u_{i,j}^{n-1}\frac{u_{i+1,j}^{n}-u_{i,j}^{n}}{\Delta x}$$

where $n-1$ is the previous time step, and n is the time step for which the unknown must be calculated.

Iterations method: The linearized term obtained using the lagging method is corrected using an internal iteration until the desired accuracy is reached.

$$u_{i+1,j}^{k} \frac{u_{i+1,j}^{k+1} - u_{i,j}}{\Delta x}$$

For $k = 1$ the value for the previous step is used and then the iterative process continues until a stop criteria is fulfilled:

$$\left| u_{i+1,j}^{k+1} - u_{i+1,j}^{k} \right| \le \varepsilon \quad \text{or} \quad \left| \frac{u_{i+1,j}^{k+1} - u_{i+1,j}^{k}}{u_{i+1,j}^{k}} \right| \le \varepsilon$$

Newton linearization method:

Consider the product $A \cdot B$ and the modification for two successive iterations:

$$\delta A = A^{k+1} - A^k \text{ and } \delta B = B^{k+1} - B^k .$$

Thus:

$$A^{k+1} \cdot B^{k+1} = \left(A^k + \delta A\right)\left(B^k + \delta B\right) = A^k B^k + B^k \delta A + A^k \delta B + \delta A \delta B$$

We suppose that $\delta A \delta B$ is small and we get:

$$A^{k+1} \cdot B^{k+1} = A^k B^k + B^k \left(A^{k+1} - A^k\right) + A^k \left(B^{k+1} - B^k\right) = A^k B^{k+1} + A^{k+1} B^k - A^k B^k .$$

For the Navier-Stokes term we have

$$u \frac{\partial u}{\partial x} \approx u^k \left(\frac{\partial u}{\partial x}\right)^{k+1} + u^{k+1} \left(\frac{\partial u}{\partial x}\right)^{k} - u^k \left(\frac{\partial u}{\partial x}\right)^{k}$$

Using forward finite differences we obtain:

$$\left(u \frac{\partial u}{\partial x}\right)_{i,j} = u^k_{i+1,j} \frac{u^{k+1}_{i+1,j} - u_{i,j}}{\Delta x} + u^{k+1}_{i+1,j} \frac{u^{k}_{i+1,j} - u_{i,j}}{\Delta x} - u^k_{i+1,j} \frac{u^{k}_{i+1,j} - u_{i,j}}{\Delta x}$$

$$= \frac{1}{\Delta x}\left[2u^k_{i+1,j} u^{k+1}_{i+1,j} - \left(u^k_{i+1,j}\right)^2 - u_{i,j} u^{k+1}_{i+1,j}\right]$$