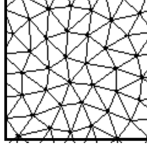
Numerical Methods in Geophysics:
Implicit Methods



What is an implicit scheme?

Explicit vs. implicit scheme for Newtonian Cooling

Crank-Nicholson Scheme (mixed explicit-implicit)

Explicit vs. implicit for the diffusion equation

Relaxation Methods

What is an implicit method?

Let us recall the *ODE*:

$$\frac{dT}{dt} = f(T,t)$$

Before we used a forward difference scheme, what happens if we use a backward difference scheme?

$$\frac{T_j - T_{j-1}}{dt} + O(dt) = f(T_j, t_j)$$

$$\Rightarrow \boxed{T_j \approx T_{j\text{-}1} + \mathrm{dt} f(T_j, t_j)}$$

What is an implicit method?

or

$$T_j \approx T_{j-1}(1+\frac{dt}{\tau})^{-1}$$

$$T_j \approx T_0(1+\frac{dt}{\tau})^{-j}$$

Is this scheme *convergent*?

Does it tend to the exact solution as dt->0? YES, it does (exercise)

Is this scheme *stable,* i.e. does T decay monotonically? This requires

$$0 < \frac{1}{1+\frac{dt}{\tau}} < 1$$

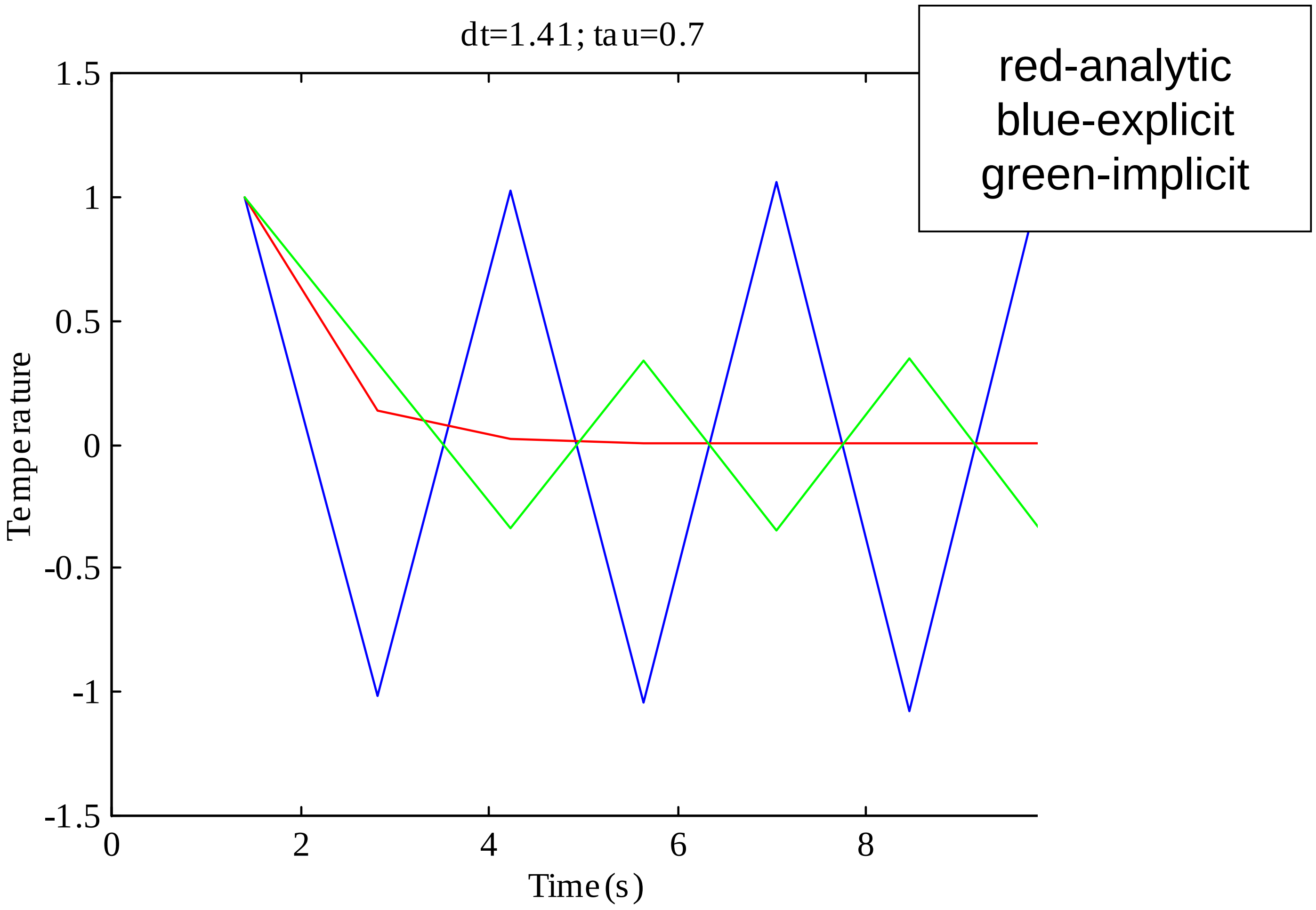
What is an implicit method?

$$0 < \frac{1}{1+\frac{dt}{\tau}} < 1$$

This scheme is always stable! This is called
unconditional stability
... which doesn't mean it's accurate!
Let's see how it compares to the explicit method...

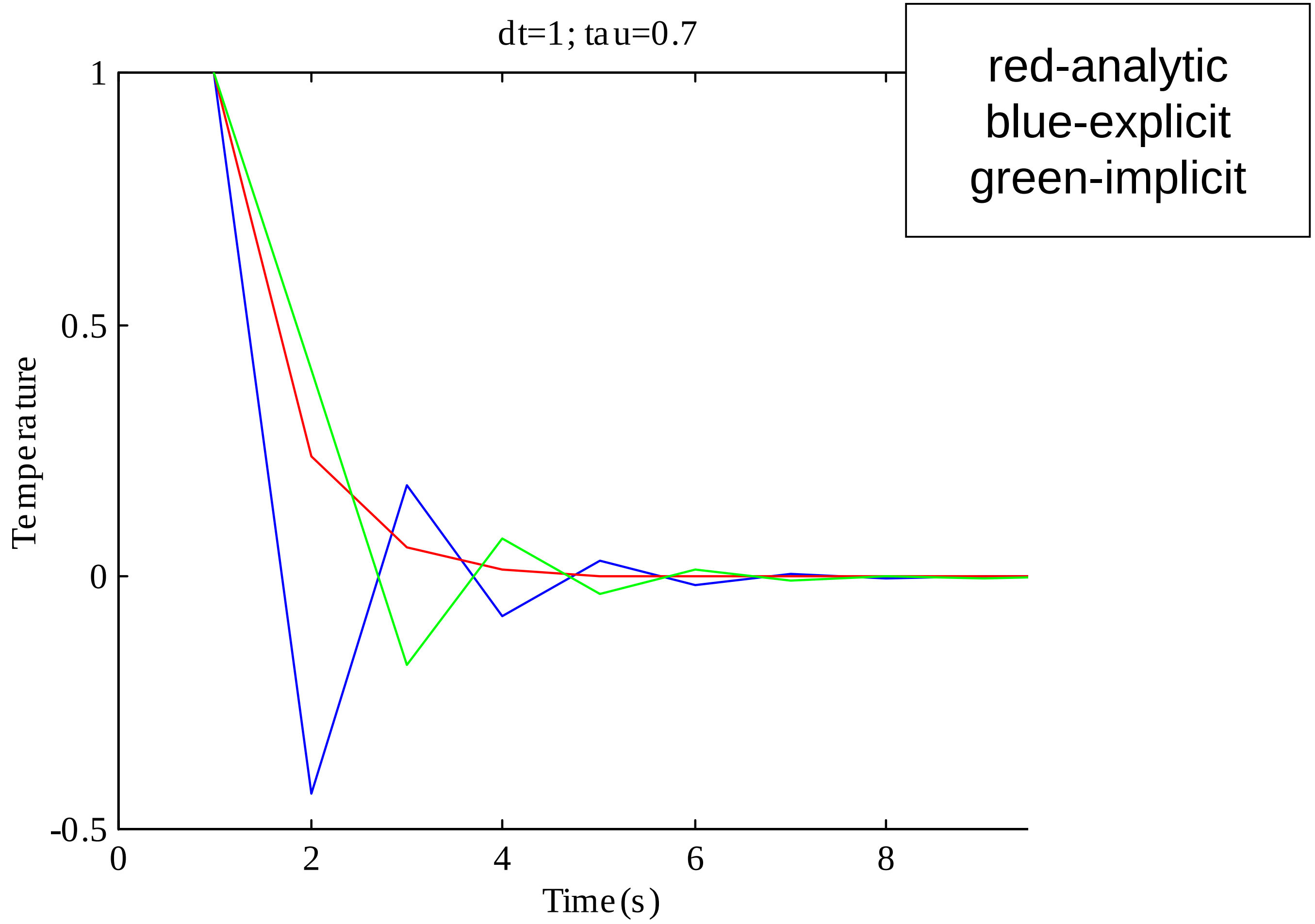
What is an implicit method?

Explicit unstable - implicit stable - both inaccurate



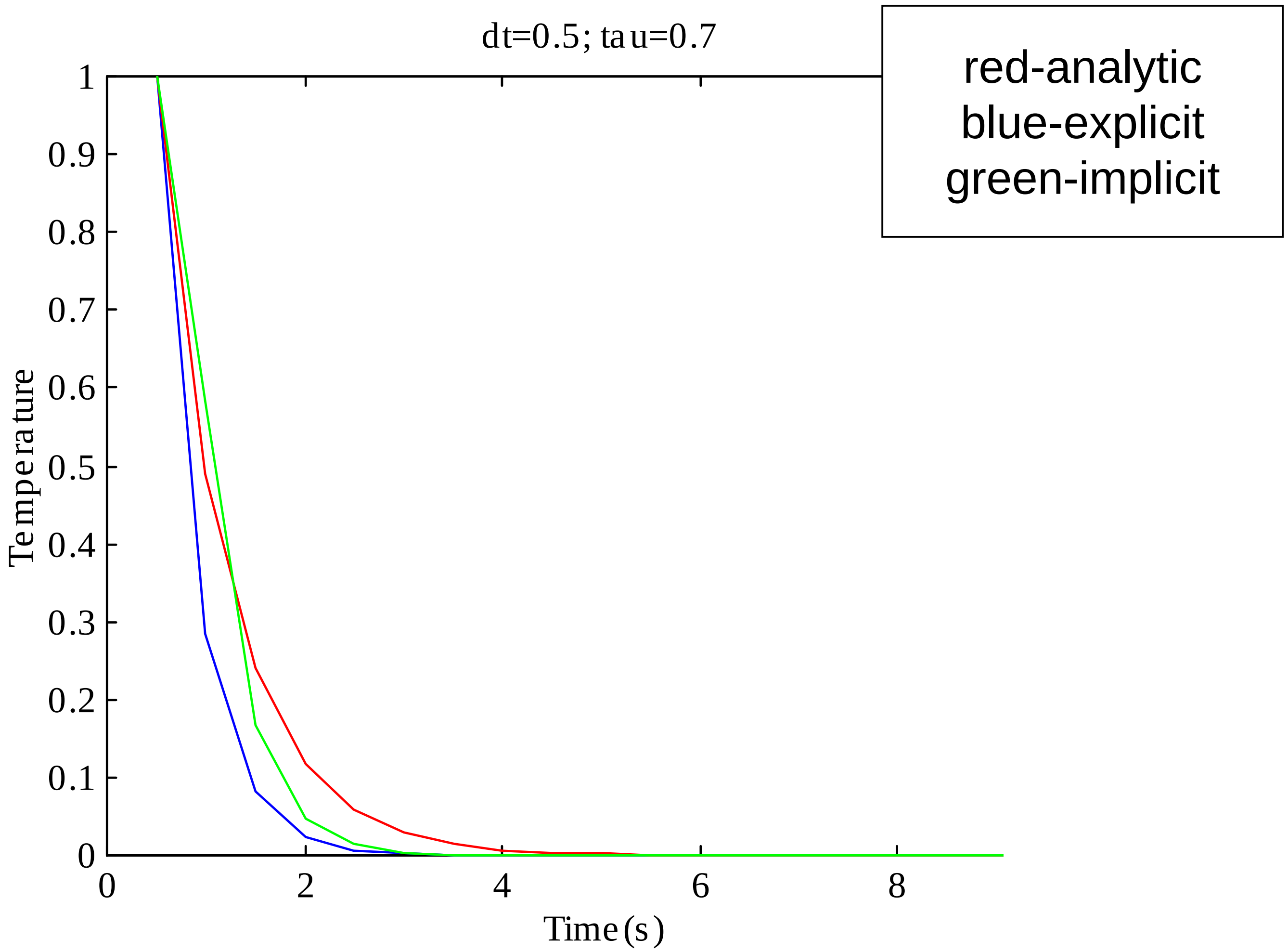
What is an implicit method?

Explicit stable - implicit stable - both inaccurate

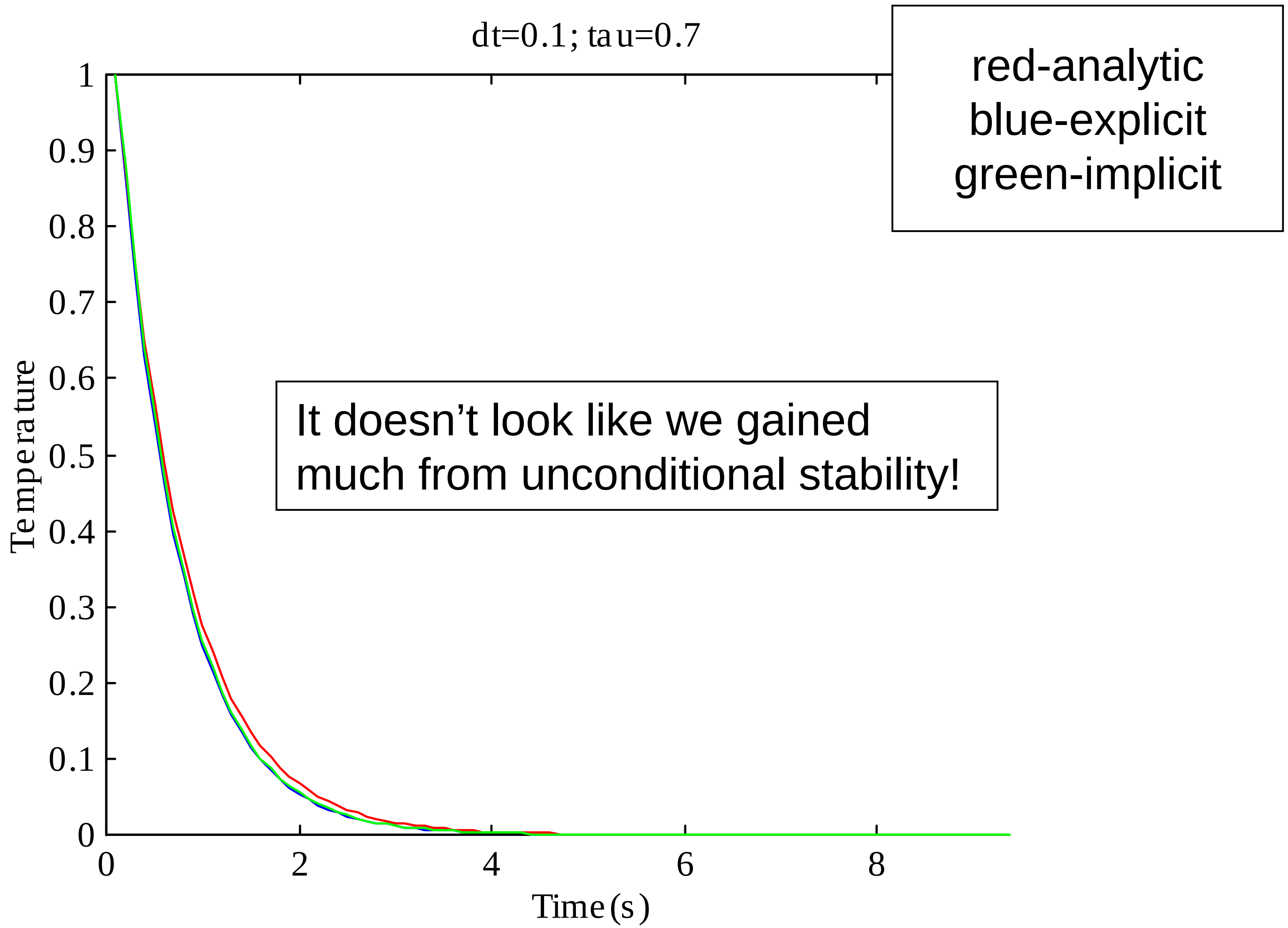


What is an implicit method?

Explicit stable - implicit stable - both inaccurate



Explicit stable - implicit stable - both *accurate*



Mixed implicit-explicit schemes

We start again with ...

$$\frac{dT}{dt} = f(T,t)$$

Let us interpolate the right-hand side to j+1/2 so that both sides are defined at the same location in time ...

$$\frac{T_{j+1} - T_j}{dt} \approx \frac{f(T_{j+1}, t_{j+1}) + f(T_j, t_j)}{2}$$

Let us examine the accuracy of such a scheme using our usual tool, the *Taylor series*.

... we learned that ...

$$\frac{T_{j+1}-T_j}{\Delta t}=\left(\frac{dT}{dt}\right)_j+\frac{\Delta t}{2}\left(\frac{d^2T}{dt^2}\right)_j+\frac{\Delta t^2}{6}\left(\frac{d^3T}{dt^3}\right)_j+O(\Delta t^3)$$

... also the interpolation can be written as ...

$$\frac{1}{2}\left(f_j+f_{j+1}\right)=\frac{1}{2}\left[2f_j+\Delta t\left(\frac{df}{dt}\right)_j+\frac{\Delta t^2}{2}\left(\frac{d^2f}{dt^2}\right)_j+O(\Delta t^3)\right]$$

since $\frac{dT}{dt}=f(T,t)$ => $\frac{d^2T}{dt^2}=\frac{df(T,t)}{dt}$

Mixed implicit-explicit schemes

... it turns out that ...
this mixed scheme is accurate to **second** order!
The previous schemes (explicit and implicit) were all first order schemes.

Now our cooling experiment becomes:

$$\frac{T_{j+1} - T_j}{dt} \approx -\frac{1}{2\tau}(T_{j+1} + T_j)$$

$$\Rightarrow T_{j+1}(1+\frac{dt}{2\tau}) \approx T_j(1-\frac{dt}{2\tau})$$

leading to the extrapolation scheme

Mixed implicit-explicit schemes

$$\Rightarrow T_{j+1} \approx T_j \left[\frac{1 - \frac{dt}{2\tau}}{1 + \frac{dt}{2\tau}} \right]$$

How stable is this scheme?
The solution decays if ...

$$-1 < \left[\frac{1 - \frac{dt}{2\tau}}{1 + \frac{dt}{2\tau}} \right] < 1$$

Mixed implicit-explicit schemes

$$-1 < \left[\frac{1 - \frac{dt}{2\tau}}{1 + \frac{dt}{2\tau}} \right] < 1$$

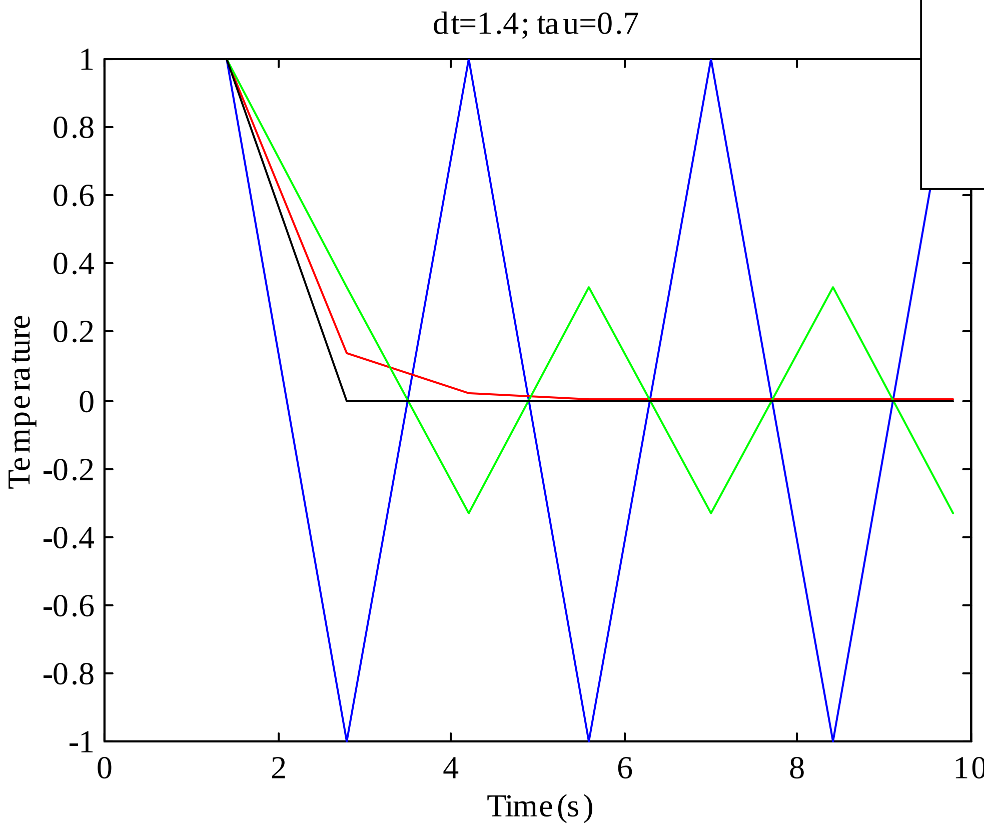
This scheme is always stable for positive dt and τ!
If dt>2 τ, the solution decreases monotonically!

Let us now look at the Matlab code and then
compare it to the other approaches.

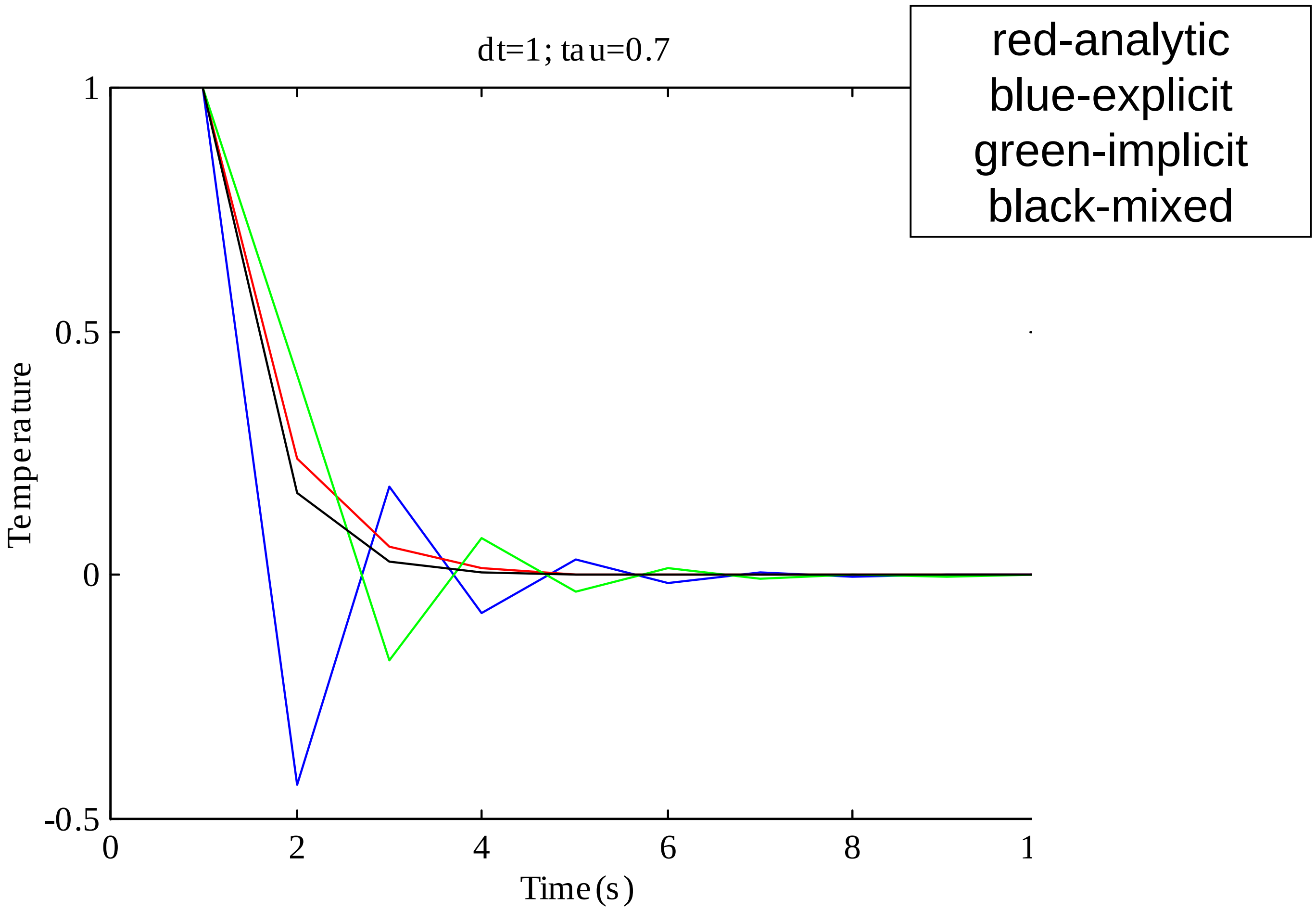
Mixed implicit-explicit schemes

```
t0=1.
tau=.7;
dt=.1;
dt=input(' Give dt : ');

nt=round(10/dt);

T=t0;
Ta(1)=1;
Ti(1)=1;
Tm(1)=1;

for i=1:nt,
t(i)=i*dt;
T(i+1)=T(i)-dt/tau*T(i);                      % explicit forward
Ta(i+1)=exp(-dt*i/tau);                       % analytic solution
Ti(i+1)=T(i)*(1+dt/tau)^(-1);                 % implicit
Tm(i+1)=(1-dt/(2*tau))/(1+dt/(2*tau))*Tm(i); % mixed
end

plot(t,T(1:nt),'b-',t,Ta(1:nt),'r-',t,Ti(1:nt),'g-',t,Tm(1:nt),'k-')
xlabel('Time(s)')
ylabel('Temperature')
```

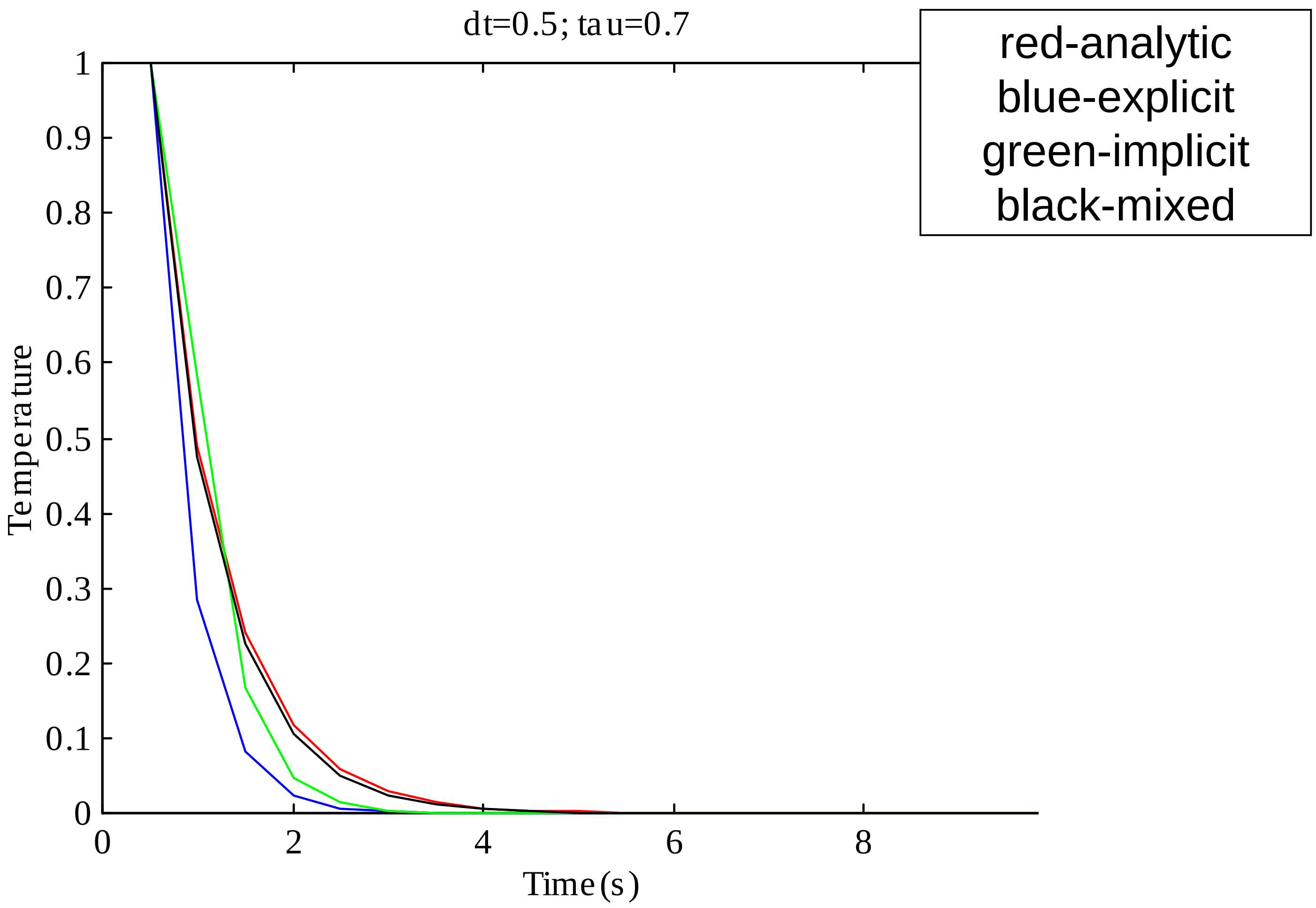
Mixed implicit-explicit schemes

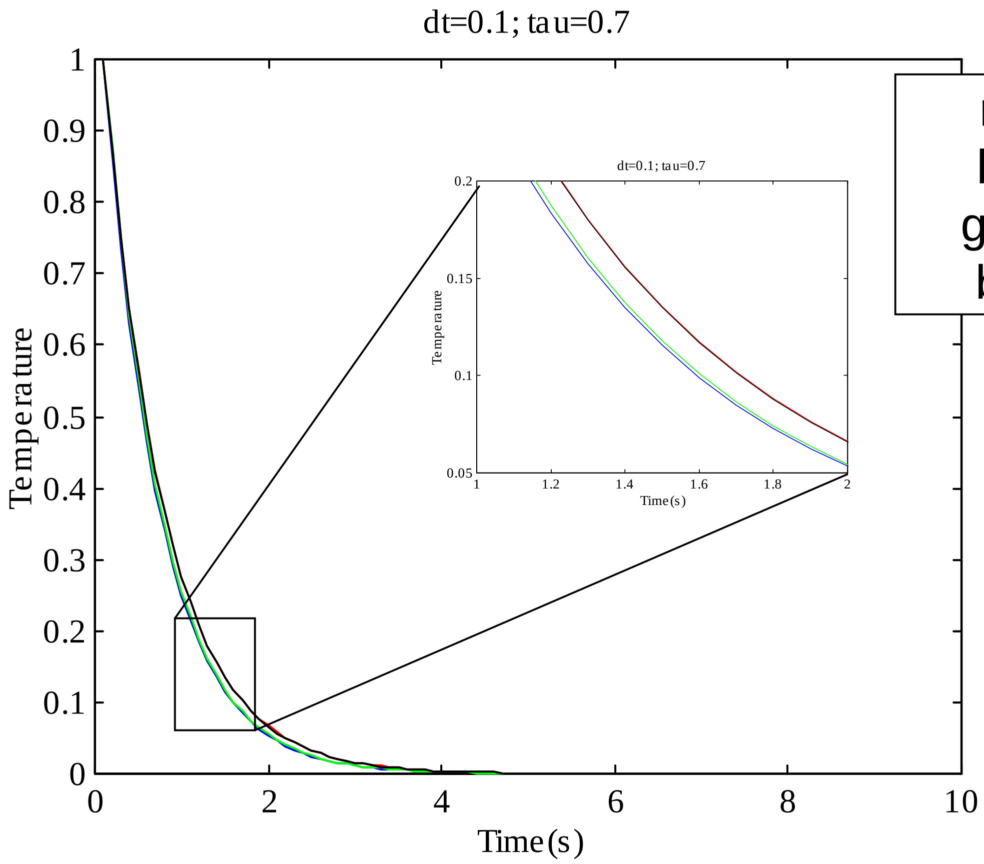


red-analytic
blue-explicit
green-implicit
black-mixed


dt=1; tau=0.7
1
0.5
0
-0.5
0
2
4
6
8
1
Time (s)
Temperature
red-analytic
blue-explicit
green-implicit
black-mixed

Mixed implicit-explicit schemes





red-analytic
blue-explicit
green-implicit
black-mixed

The mixed scheme is a clear ***winner***!

The Diffusion equation

$$\frac{\partial C}{\partial t} = k \frac{\partial^2 C}{\partial x^2}$$

k diffusivity

The diffusion equation has many applications in geophysics, e.g. temperature diffusion in the Earth, mixing problems, etc.

A centered time - centered space scheme leads to a **unconditionally unstable** scheme!

Let's try a forward time-centered space scheme ...

$$C_j^{n+1} = C_j^n + s(C_{j+1}^n - 2C_j^n + C_{j-1}^n)$$

where

$$s = k\frac{dt}{dx^2}$$

how stable is this scheme? We use the following *Ansatz*

$$T = e^{i\omega dt} \qquad X = e^{-ikdx}$$

after going into the equation with

$$C_m^n = e^{i(\omega n dt - kmdx)} = X^m T^n$$

The Diffusion equation

... which leads to ...

$$T-(1+sX^{1}-2s+sX^{-1})=0$$

and

$$|T|\leq|1-4s|$$

so the stability criterion is

$$s\leq\frac{1}{2}\Rightarrow dt\leq dx^{2}/(2k)$$

This stability scheme is impractical as the required time step must be very small to achieve stability.

The Diffusion equation (matrix form)

any FD algorithm can also be written in matrix form, e.g.

$$C_j^{n+1} = C_j^n + s(C_{j+1}^n - 2C_j^n + C_{j-1}^n)$$

is equivalent to

$$\begin{bmatrix} C_1^{n+1} \\ \vdots \\ C_j^{n+1} \\ \vdots \\ C_J^{n+1} \end{bmatrix} = s \begin{bmatrix} \ddots & \ddots & & & \\ \ddots & \ddots & \ddots & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} C_1^{n} \\ \vdots \\ C_j^{n} \\ \vdots \\ C_J^{n} \end{bmatrix}$$

The Diffusion equation (matrix form)

... this can be written using operators ...

$$\underline{c}^{n+1} = \underline{c}^{n} + \underline{\underline{L}}\,\underline{c}^{n}$$

where L is the tridiagonal scaled Laplacian operator, if the boundary values are zero (blank parts of matrix contain zeros)

The Diffusion equation

... let's try an implicit scheme using the interpolation ...

$$C(x, t + \frac{dt}{2}) \approx \frac{C(t+dt) + C(t)}{2}$$

and

$$\frac{C_j^{n+1} + C_j^n}{dt} = \frac{k}{2dx^2}\left(C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1} + C_{j+1}^n - 2C_j^n + C_{j-1}^n\right)$$

... so again we have defined both sides at the same location
... half a time step in the future ...

The Diffusion equation

... after rearranging ...

$$-(s/2)C_{j+1}^{n+1}+(1+s)C_j^{n+1}-(s/2)C_{j-1}^{n+1}=(s/2)C_{j+1}^{n}+(1-s)C_j^{n}+(s/2)C_{j-1}^{n}$$

... again this is an implicit scheme, we rewrite this in matrix form ...

$$\begin{bmatrix} \ddots & \ddots & & & \\ \ddots & \ddots & \ddots & & \\ & -(s/2) & (1+s) & -(s/2) & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{bmatrix}\begin{bmatrix} C_1^{n+1} \\ \vdots \\ C_j^{n+1} \\ \vdots \\ C_J^{n+1} \end{bmatrix}=\begin{bmatrix} \ddots & \ddots & & & \\ \ddots & \ddots & \ddots & & \\ & (s/2) & (1-s) & (s/2) & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{bmatrix}\begin{bmatrix} C_1^{n} \\ \vdots \\ C_j^{n} \\ \vdots \\ C_J^{n} \end{bmatrix}$$

... or using operators ...

$$\underline{\underline{U}}\,\underline{c}^{n+1}=\underline{\underline{V}}\,\underline{c}^{n}$$

The Diffusion equation

... and the solution to this system of equations is ...

$$\underline{c}^{n+1} = \underline{\underline{U}}^{-1}\underline{\underline{V}}\,\underline{c}^{n}$$

... we have to perform a tridiagonal matrix inversion to solve this system. Stability analysis using the Z-transform yields

$$T((1+s)-s/2(X^{1}+X^{-1})) = T((1-s)+s/2(X^{1}+X^{-1}))$$

$$\Rightarrow T = (1-\beta)/(1+\beta)$$

$$\beta = s(1-\cos\theta)$$

... where we used ...

$$\cos\theta = \cos k\Delta x = (X^{1}+X^{-1})/2$$

The Diffusion equation

$$\Rightarrow T = (1-\beta)/(1+\beta) \qquad \beta = s(1-\cos\theta)$$

... T describes the time-dependent behaviour of the numerical solution, as before we find ...

$$|T| = |(1-\beta)/(1+\beta)| \leq 1$$

... which means the solution is unconditionally stable ...

... this scheme implies that the FD solution at each grid point is affected by all other points. Physically this could be interpreted as an infinite interaction speed in the discrete world of the implicit scheme!

The Relaxation Method

Let us consider a space-dependent problem, the Poisson's equation :

$$(\partial_x^2 + \partial_z^2)\Phi = -F$$

applying a centered FD approximation yields ...

$$\frac{1}{dx^2}\left(\Phi_{i,j-1} - 2\Phi_{i,j} + \Phi_{i,j+1} + \Phi_{i-1,j} - 2\Phi_{i,j} + \Phi_{i+1,j}\right) = -F$$

rearranging ...

$$\Phi_{i,j} = \left(\frac{\Phi_{i,j-1} + \Phi_{i,j+1} + \Phi_{i-1,j} + \Phi_{i+1,j}}{4}\right) + \frac{Fdx^2}{4}$$

... so the value at (i,j) is the average of the surrounding values plus a (scaled) source term ...

The Relaxation Method

... the solution can be found by an iterative procedure ...

$$\Phi_{i,j}^{m+1} = \left(\frac{\Phi^{m}{}_{i,j-1} + \Phi^{m}{}_{i,j+1} + \Phi^{m}{}_{i-1,j} + \Phi^{m}{}_{i+1,j}}{4} \right) + \frac{Fdx^{2}}{4}$$

... where m is the iteration index. One can start from an initial guess (e.g. zero) and change the solution until it doesn't change anymore within some tolerance e.g.

$$| \Phi_{ij}^{m+1} - \Phi_{ij}^{m} | < \varepsilon$$

If there is a stationary state to a diffusion problem, it could be calculated with the time-dependent problem, or with the relaxation method, assuming dC/dt=0. What is more efficient? (Exercise)

Implicit Methods - Summary

Certain FD approximations to time-dependent partial differential equations lead to implicit solutions. That means to propagate (extrapolate) the numerical solution in time, a linear system of equations has to be solved.

The solution to this system usually requires the use of matrix inversion techniques.

The advantage of some implicit schemes is that they are unconditionally stable, which however does not mean they are very accurate.

It is possible to formulate mixed explicit-implicit schemes (e.g. Crank-Nickolson or trapezoidal schemes) , which are more accurate than the equivalent explicit or implicit schemes.