

Numerical Methods in Geophysics: The Finite Difference Method



Explicit Methods

Implicit Methods





Numerical solution to first order ordinary differential equation

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

We can not simply integrate this equation. We have to solve it numerically! First we need to discretise time:

$$t_j = t_0 + jdt$$

and for Temperature T

$$T_j = T(t_j)$$





Let us try a forward difference:

$$\left. \frac{dT}{dt} \right|_{t=t_j} = \frac{T_{j+1} - T_j}{dt} + O(dt)$$

... which leads to the following explicit scheme :

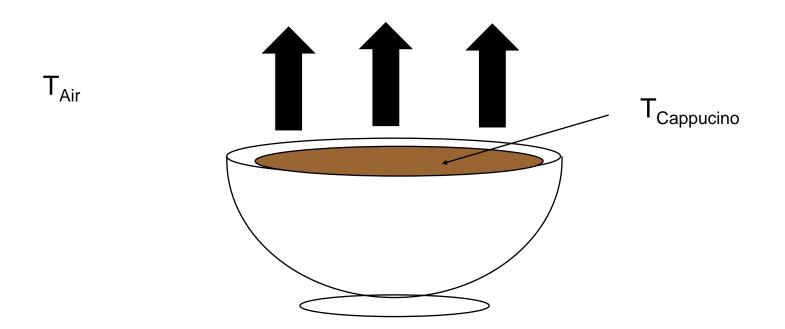
$$T_{j+1} \approx T_j + \mathrm{dt}f(T_j, t_j)$$

This allows us to calculate the Temperature T as a function of time and the *forcing* inhomogeneity f(T,t). Note that there will be an error O(dt) which will accumulate over time.





Let's try to apply this to the Newtonian cooling problem:



How does the temperature of the liquid evolve as a function of time and temperature difference to the air?





The rate of cooling (dT/dt) will depend on the temperature difference $(T_{cap}-T_{air})$ and some constant (thermal conductivity). This is called **Newtonian Cooling**.

With $T = T_{cap} - T_{air}$ being the temperature difference and τ the time scale of cooling then f(T,t)=-T/ τ and the differential equation describing the system is

$$\frac{dT}{dt} = -T / \tau$$

with initial condition $T=T_i$ at t=0 and $\tau>0$.





This equation has a simple analytical solution:

$$T(t) = T_i \exp(-t/\tau)$$

How good is our finite-difference appoximation? For what choices of dt will we obtain a stable solution?

Our FD approximation is:

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





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

Does this equation approximation converge for dt -> 0?
 Does it behave like the analytical solution?

With the initial condition $T=T_0$ at t=0:

$$\begin{split} T_1 &= T_0(1-\frac{dt}{\tau}) \\ T_2 &= T_1(1-\frac{dt}{\tau}) = T_0(1-\frac{dt}{\tau})(1-\frac{dt}{\tau}) \\ \text{leading to :} \quad \boxed{T_j = T_0(1-\frac{dt}{\tau})^j} \end{split}$$





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

Let us use $dt=t_j/j$ where t_j is the total time up to time step j:

$$T_{j} = T_{0} \left(1 + \left[-\frac{t}{j\tau} \right] \right)^{j}$$

This can be expanded using the *binomial theorem*

$$T_{j} = T_{0} \left[1^{j} + 1^{j-1} \left[-\frac{t}{j\tau} \right] \binom{j}{1} + 1^{j-2} \left[-\frac{t}{j\tau} \right]^{2} \binom{j}{2} + \dots \right]$$





... where

$$\binom{j}{r} = \frac{j!}{(j-r)!r!}$$

we are interested in the case that dt-> 0 which is equivalent to j->@

$$\frac{j!}{(j-r)!} = j(j-1)(j-2)...(j-r+1) \to j^r$$

as a result

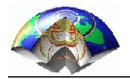
$$\binom{j}{r} \to \frac{j^r}{r!}$$





substituted into the series for T_i we obtain: $T_{j} \rightarrow T_{0} \left| 1 + \frac{j}{1!} \left[-\frac{t}{j\tau} \right] + \frac{j^{2}}{2!} \left| -\frac{t}{j\tau} \right|^{2} + \dots \right|$ which leads to $T_{j} \rightarrow T_{0} \left| 1 + \left[-\frac{t}{\tau} \right] + \frac{1}{2!} \left[-\frac{t}{\tau} \right]^{2} + \dots \right|$... which is the Taylor expansion for

$$T_j = T_0 \exp(-t/\tau)$$





So we conclude:

For the Newtonian Cooling problem, the numerical solution converges to the exact solution when the time step dt gets smaller.

How does the numerical solution behave?

$$T_j = T_0 \exp(-t / \tau)$$

The analytical solution decays monotonically!

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

What are the conditions so that $T_{j+1} < T_j$?





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

$$T_{j+1} < T_j \text{ requires}$$

$$0 \le 1 - \frac{dt}{\tau} < 1$$

or
$$0 \le dt < \tau$$

The numerical solution decays only montonically for a limited range of values for dt! Again we seem to have a *conditional stability*.





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

$$\text{if } \quad \tau < dt < 2\tau \qquad \text{then} \qquad (1 - \frac{dt}{\tau}) < 0 \\ \end{array}$$

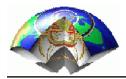


if $dt > 2\tau$ then $dt / \tau > 2$



1-dt/ τ <-1 and the solution oscillates and diverges

... now let us see how the solution looks like



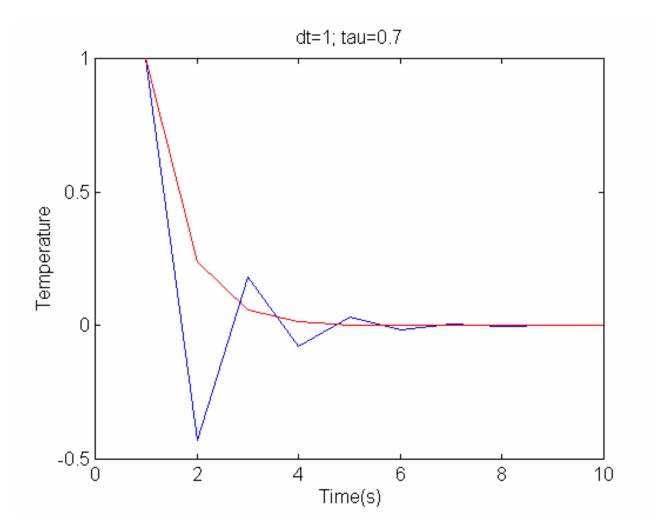


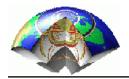
% Matlab Program - Newtonian Cooling

```
% initialise values
nt=10;
t0=1.
tau=.7;
dt=1.
% initial condition
T=t0;
% time extrapolation
for i=1:nt,
T(i+1)=T(i)-dt/tau*T(i);
end
% plotting
plot(T)
```



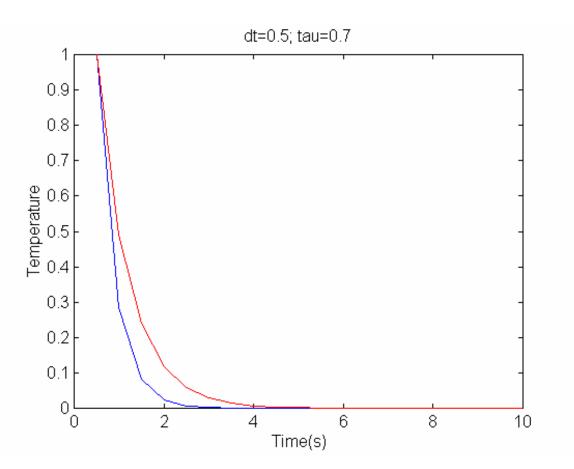


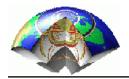






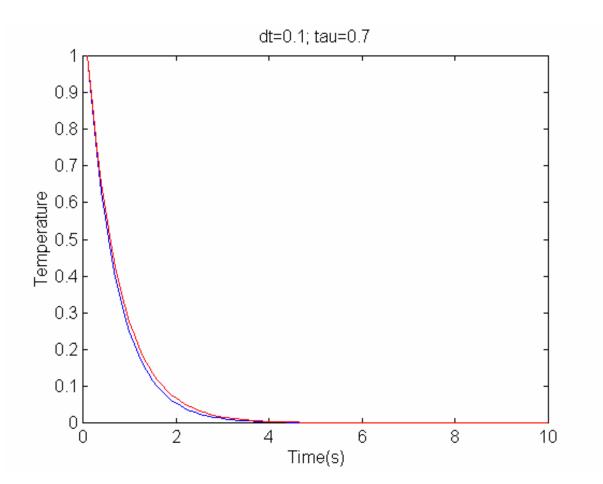
Solution converges but does not have the right time-dependence







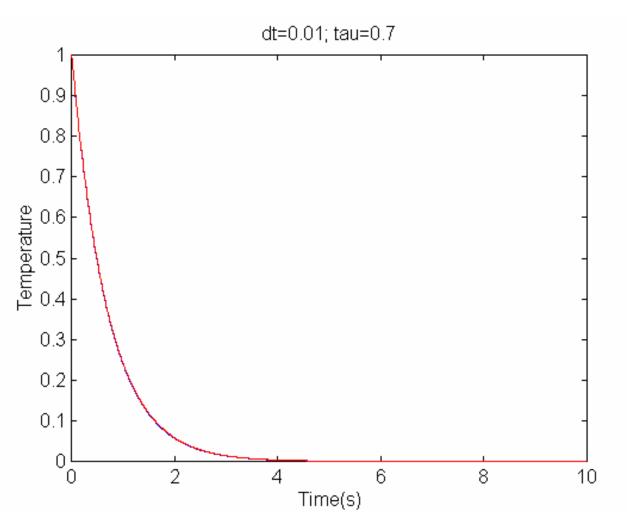
... only slight error of the time-dependence - acceptable solution ...

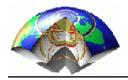






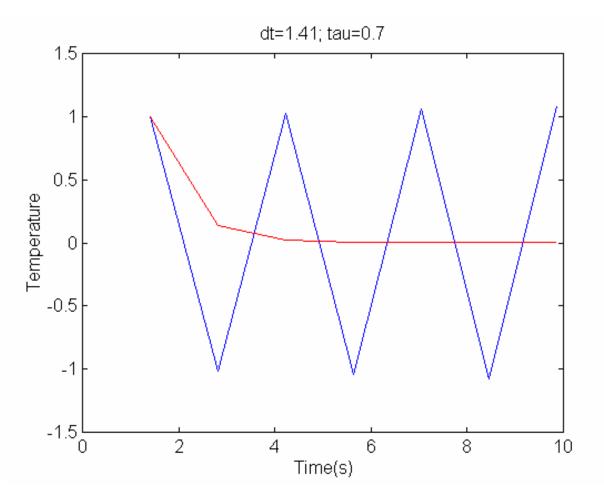
.. very accurate solution which we pay by a fine sampling in time ...







... this solution is wrong and unstable !







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



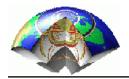


Let us recall the ODE:

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

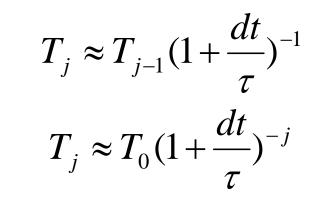
Before we used a forward difference scheme, what happens if we use a backward difference scheme?

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





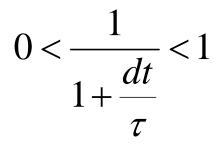




Is this scheme convergent?

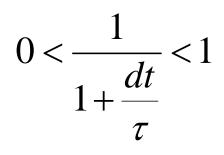
Does it tend to the exact solution as dt->0? YES, it does (exercise)

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









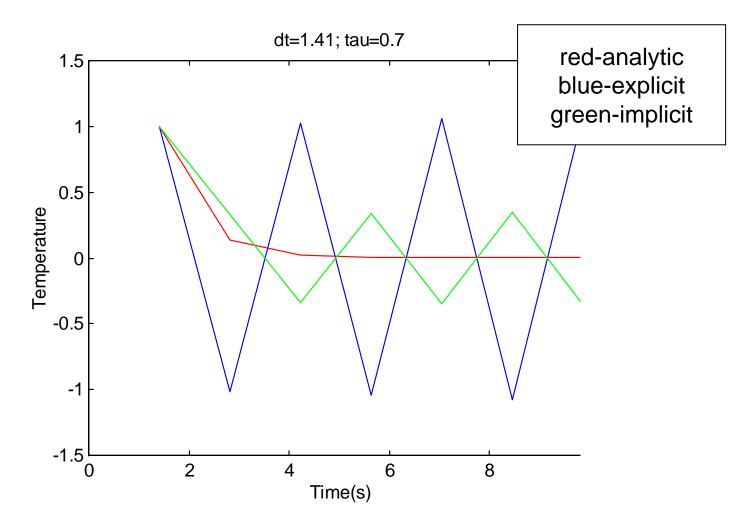
This scheme is always stable! This is called unconditional stability

... which doesn't mean it's accurate! Let's see how it compares to the explicit method...



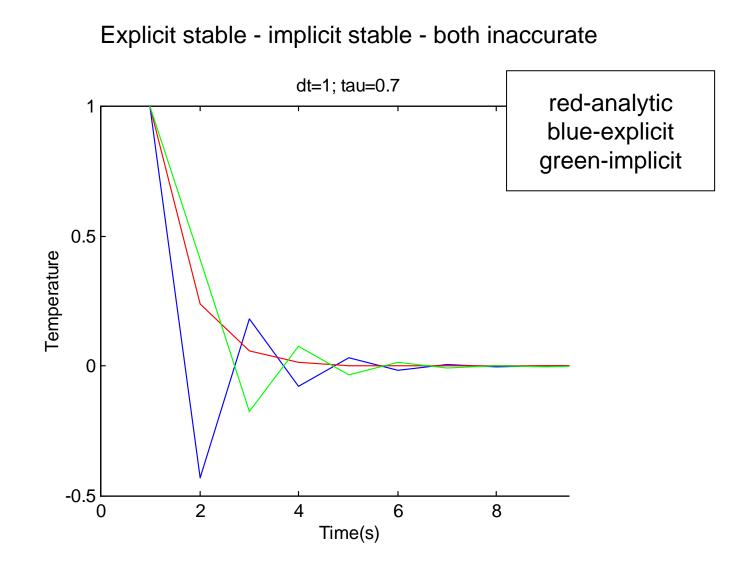


Explicit unstable - implicit stable - both inaccurate



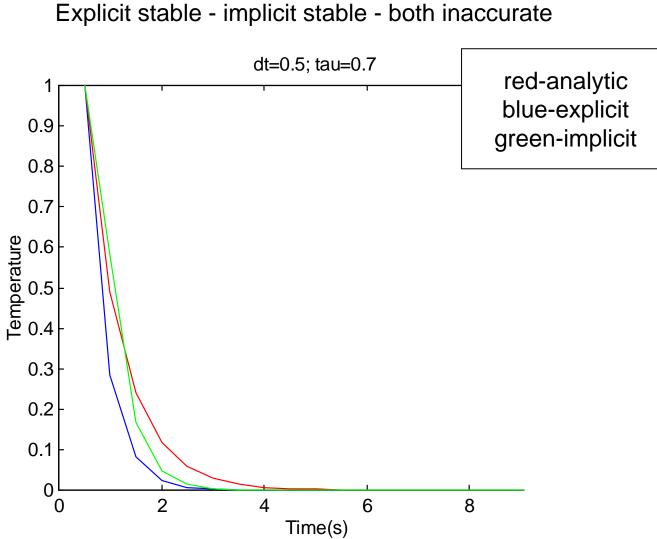






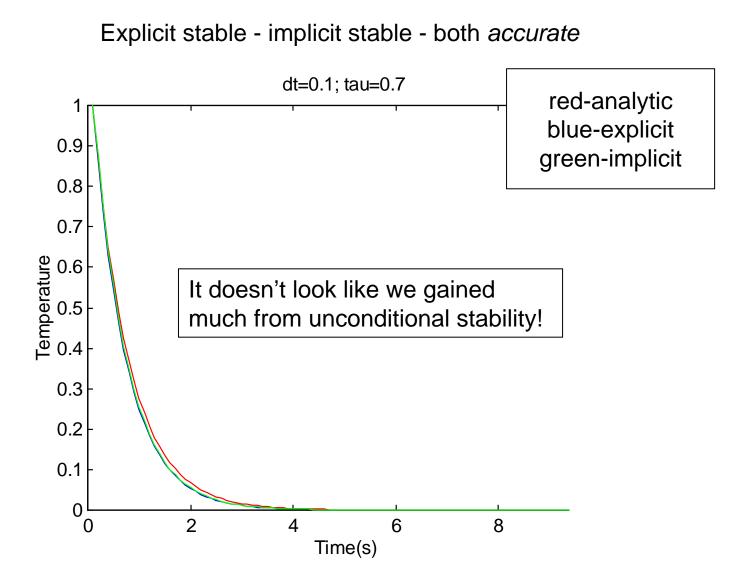
















We start again with ...

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

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 ...

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

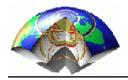
... also the interpolation can be written as ...

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

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

since

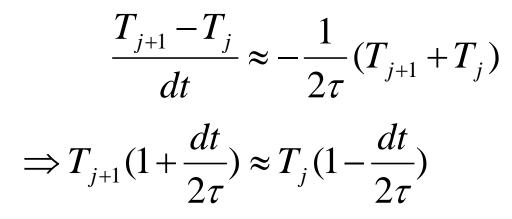
dt





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

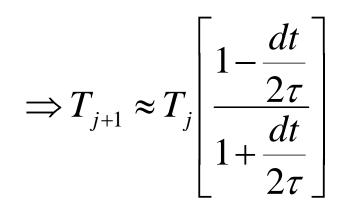
Now our cooling experiment becomes:



leading to the extrapolation scheme





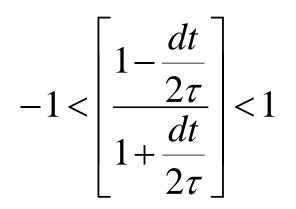


How stable is this scheme? The solution decays if ...

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







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.

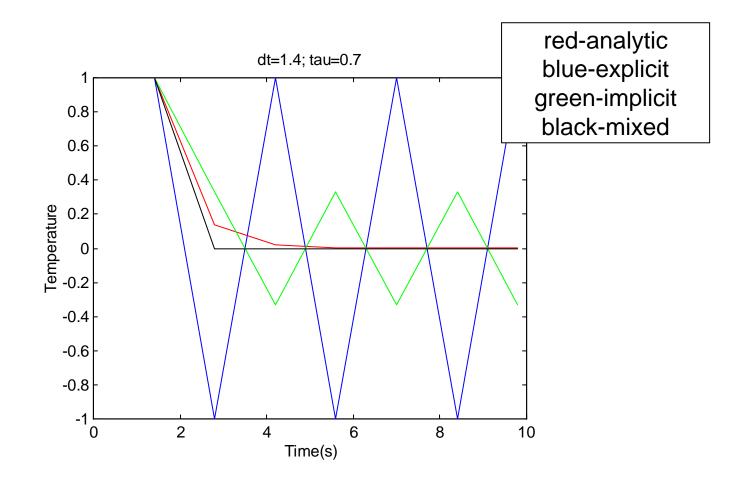




```
t0=1.
tau=.7;
dt=.1;
dt=input(' Give dt : ');
nt=round(10/dt);
T=t0;
Ta(1)=1;
Ti(1)=1;
Tm(1) = 1;
for i=1:nt,
t(i)=i*dt;
T(i+1)=T(i)-dt/tau*T(i);
                                            % explicit forward
Ta(i+1)=exp(-dt*i/tau);
                                            % analytic solution
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),'q-',t,Tm(1:nt),'k-')
xlabel('Time(s)')
ylabel('Temperature')
```

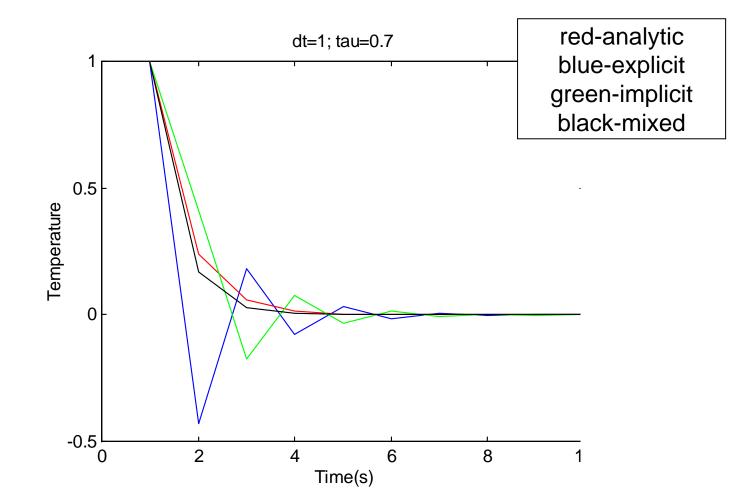






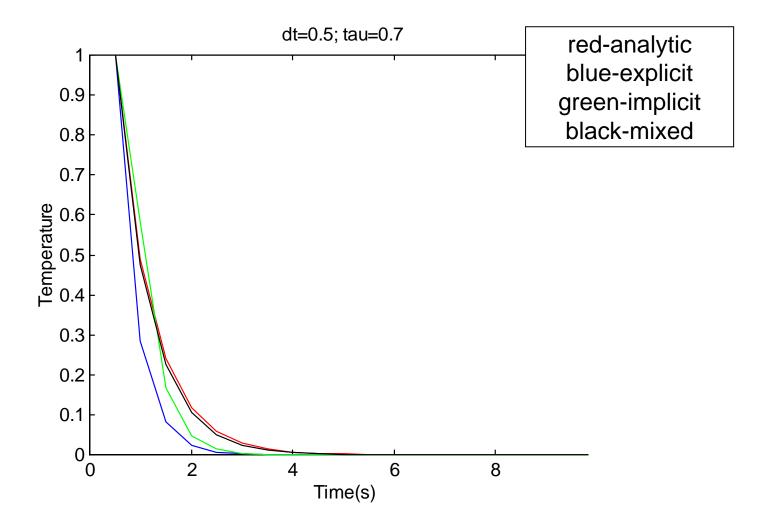






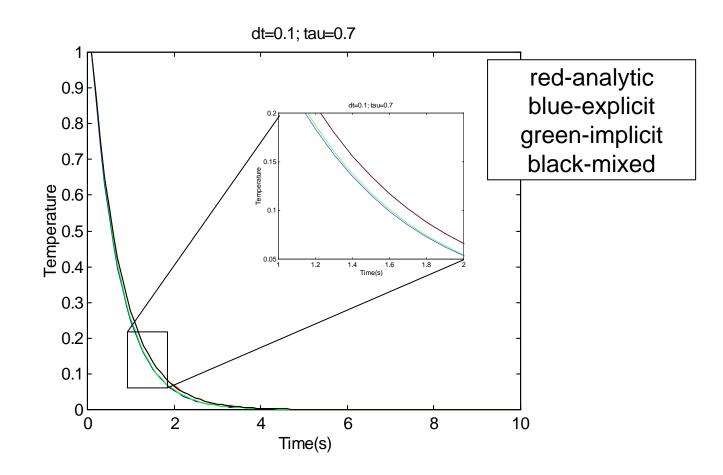












The mixed scheme is a clear winner!





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.