Numerical Methods in Geophysics:
The Finite Difference Method

What is a finite difference?

Forward-backward-centered schemes

Higher Derivatives

Taylor Series

Partial Derivatives

Newtonian Cooling

Explicit finite-difference scheme: the wave equation

Consistency

Stability

Dispersion

What is a finite difference?

Common definitions of the derivative of f(x):

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x) - f(x-dx)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x-dx)}{2dx}$$

These are all correct definitions in the limit dx->0.

But we want dx to remain **FINITE**

What is a finite difference?

The equivalent ***approximations*** of the derivatives are:

$$\partial_x f \approx \frac{f(x+dx) - f(x)}{dx}$$ forward difference

$$\partial_x f \approx \frac{f(x) - f(x-dx)}{dx}$$ backward difference

$$\partial_x f \approx \frac{f(x+dx) - f(x-dx)}{2dx}$$ centered difference

What about the second or higher derivatives?

Higher Derivatives with FD

$$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx}$$

$$\partial_x f^- \approx \frac{f(x) - f(x-dx)}{dx}$$

$$\partial_x^2 f \approx \frac{\partial_x f^+ - \partial_x f^-}{dx}$$

$$\partial_x^2 f \approx \frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2}$$

Second Derivative

Other derivation via Taylor Series (Exercise).

The **big** question:

How good are the FD approximations?

$$\approx \neq =$$

This leads us to Taylor series....

Taylor Series

Taylor series are expansions of a function f(x) for some finite distance dx to f(x+dx)

$$f(x \pm dx) = f(x) \pm \mathrm{dx} f'(x) + \frac{dx^2}{2!} f''(x) \pm \frac{dx^3}{3!} f'''(x) + \frac{dx^4}{4!} f''''(x) \pm \ldots$$

What happens, if we use this expression for

$$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx}$$

?

Taylor Series

... that leads to :

$$\frac{f(x+dx)-f(x)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^2}{2!}f^{''}(x)+\frac{dx^3}{3!}f^{'''}(x)+\ldots\right]$$

$$=f^{'}(x)+O(dx)$$

The error of the first derivative using the *forward* formulation is *of order dx*.

Is this the case for other formulations of the derivative?
Let's check!

Taylor Series

... with the *centered* formulation we get:

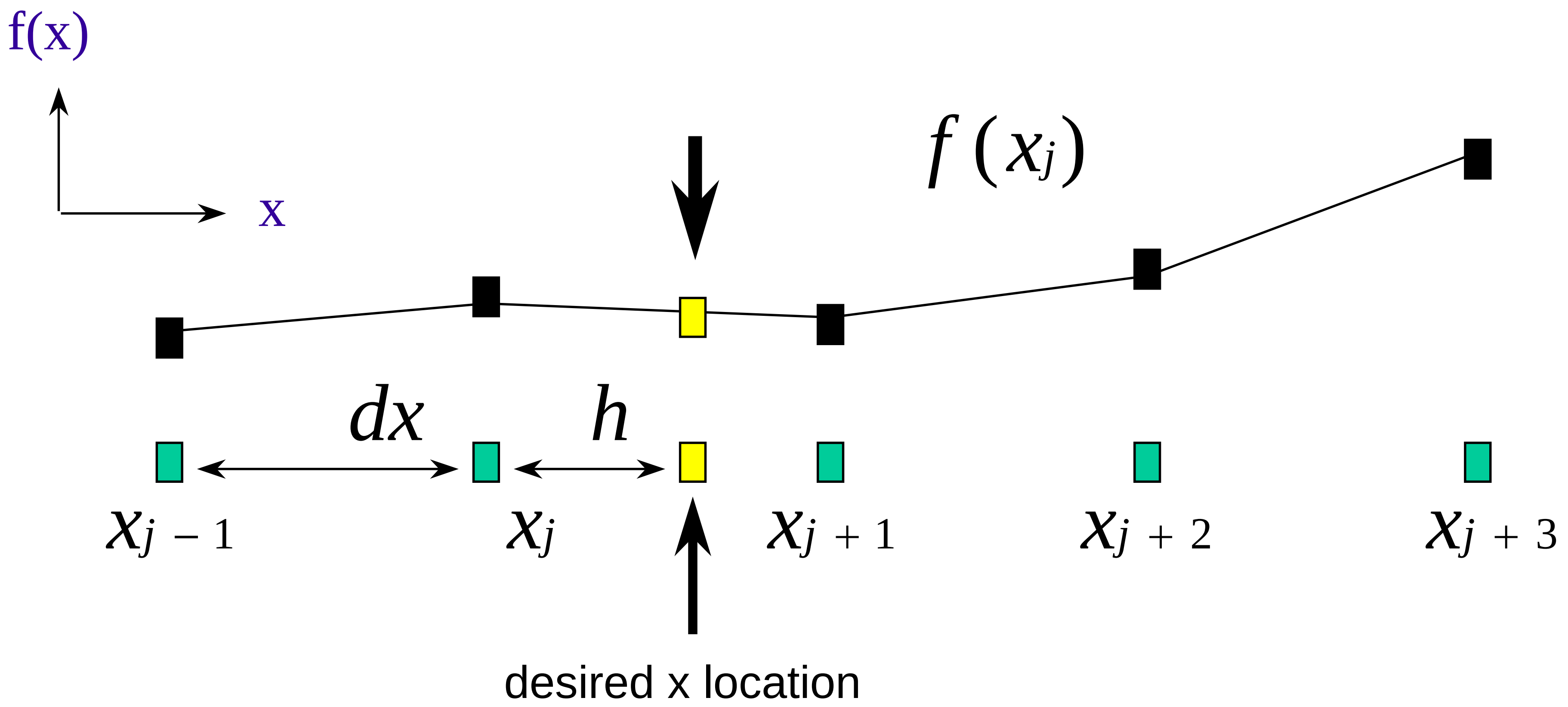
$$\frac{f(x+dx/2)-f(x-dx/2)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^3}{3!}f^{'''}(x)+\ldots\right]$$

$$=f^{'}(x)+O(dx^2)$$

The error of the first derivative using the centered approximation is *of order dx²*.

This is an **important** results: it DOES matter which formulation we use. The centered scheme is more accurate!

Alternative Derivation of FD

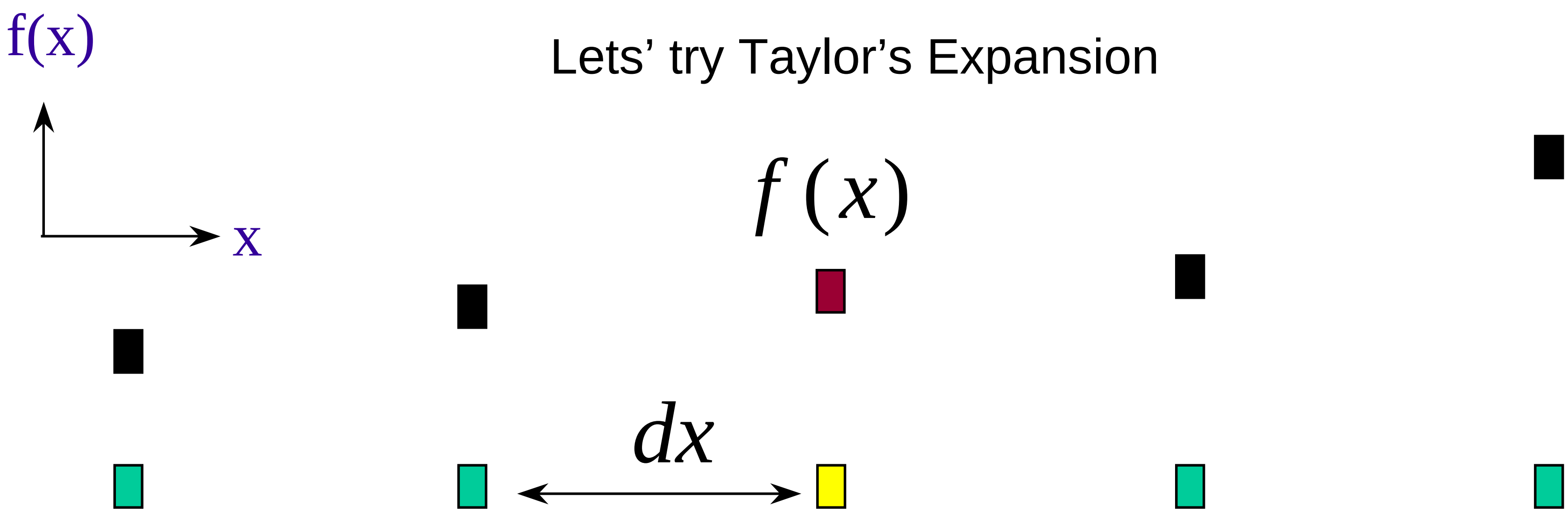


What is the (approximate) value of the function or its (first, second ..) derivative at the desired location ?

How can we calculate the weights for the neighboring points?

Alternative Derivation of FD

Lets' try Taylor's Expansion



$$f(x+dx) = f(x) + f'(x)dx \qquad (1)$$

$$f(x-dx) = f(x) - f'(x)dx \qquad (2)$$

we are looking for something like

$$f^{(i)}(x) \approx \sum_{j=1,L} w_j^{(i)} f(x_{index(j)})$$

Alternative Derivation of FD

$$af^{+} \approx af + af'dx \quad + \quad bf^{-} \approx bf - bf'dx$$

$$\Rightarrow af^{+} + bf^{-} \approx (a+b)f + (a-b)f'dx$$

Interpolation	Derivative
$a - b = 0$	$a + b = 0$
$\Downarrow$	$\Downarrow$
$f \approx \frac{1}{2}f^{-} + \frac{1}{2}f^{+}$	$f' \approx \frac{f^{+} - f^{-}}{2dx}$
$w_1 = 0.5, w_2 = 0.5$	$w_1 = -\frac{1}{2dx}, w_2 = \frac{1}{2dx}$
Interpolation weights	Derivative weights

Newtonian Cooling

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:

$$t_j = t_0 + j dt$$

and for Temperature T

$$T_j = T(t_j)$$

Newtonian Cooling

Let us try a forward difference:

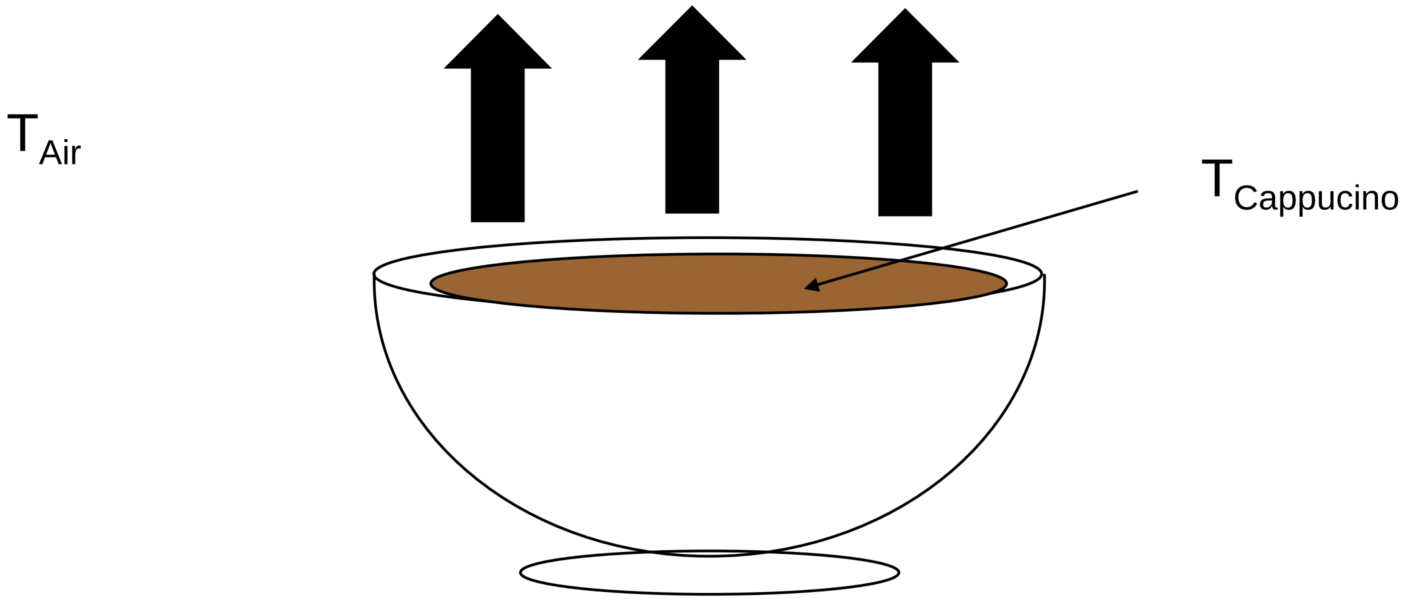
$$\left.\frac{dT}{dt}\right|_{t=t_j} = \frac{T_{j+1} - T_j}{dt} + O(dt)$$

... 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?

Newtonian Cooling

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 $f(T,t) = -T/\tau$ 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:

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

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

Newtonian Cooling

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

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

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

$$T_1 = T_0(1 - \frac{dt}{\tau})$$

$$T_2 = T_1(1 - \frac{dt}{\tau}) = T_0(1 - \frac{dt}{\tau})(1 - \frac{dt}{\tau})$$

leading to :

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

Newtonian Cooling

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

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*

$$T_j = T_0 \left[1^j + 1^{j-1} \left[-\frac{t}{j\tau} \right] \binom{j}{1} + 1^{j-2} \left[-\frac{t}{j\tau} \right]^2 \binom{j}{2} + \ldots \right]$$

Newtonian Cooling

... where

$$\begin{pmatrix} j \\ r \end{pmatrix} = \frac{j!}{(j-r)!r!}$$

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

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

as a result

$$\begin{pmatrix} j \\ r \end{pmatrix} \rightarrow \frac{j^r}{r!}$$

Newtonian Cooling

substituted into the series for T_j 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

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

Newtonian Cooling - *Convergence*

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 $T_{j+1} < T_j$?

Newtonian Cooling - *Convergence*

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

$T_{j+1} < T_j$ requires

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

or

$$0 \leq dt < \tau$$

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

Newtonian Cooling - *Convergence*

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

if $\tau < dt < 2\tau$ then $(1 - \frac{dt}{\tau}) < 0$

→ the solution oscillates but converges as |1-dt/τ|<1

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

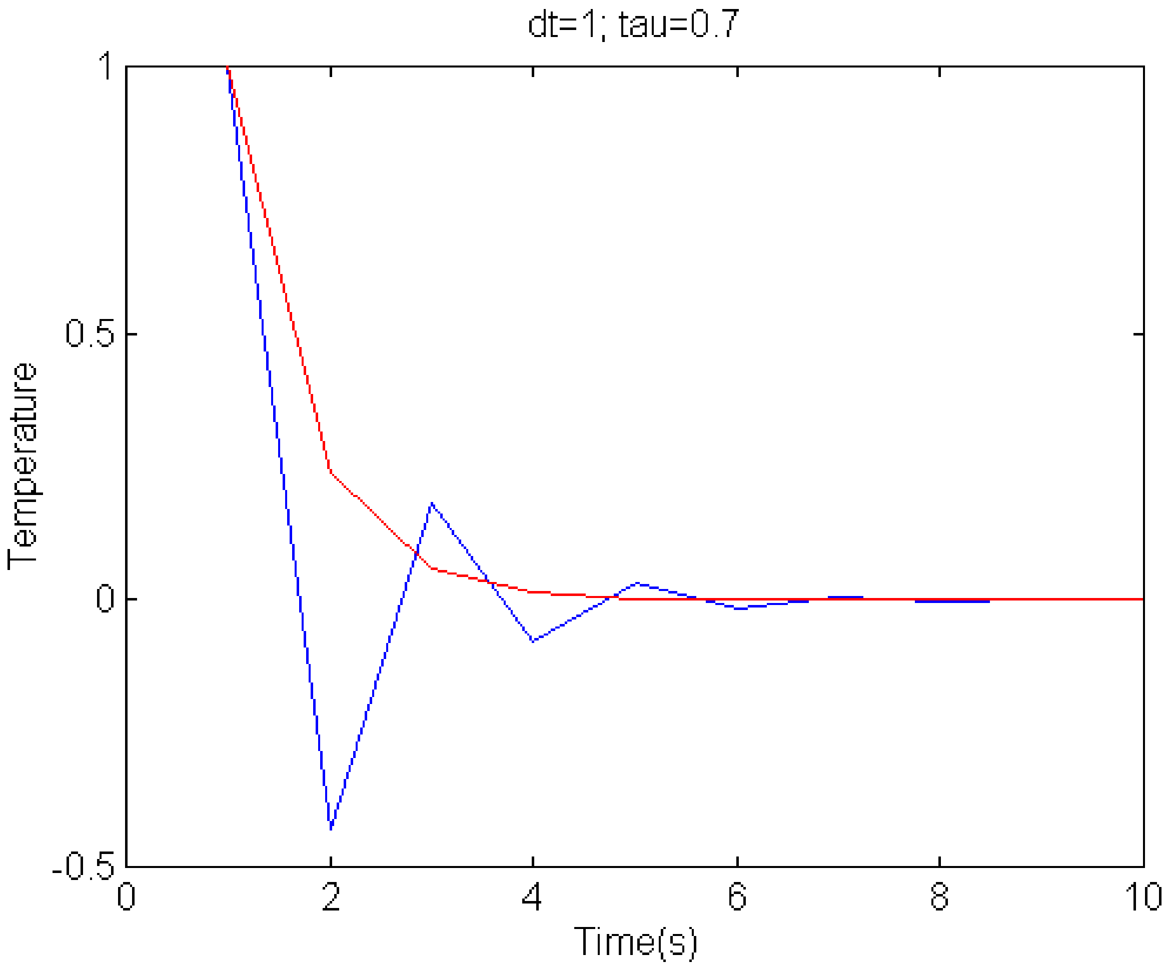
→ 1-dt/τ<-1 and the solution oscillates and diverges

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

Newtonian Cooling - *Convergence*

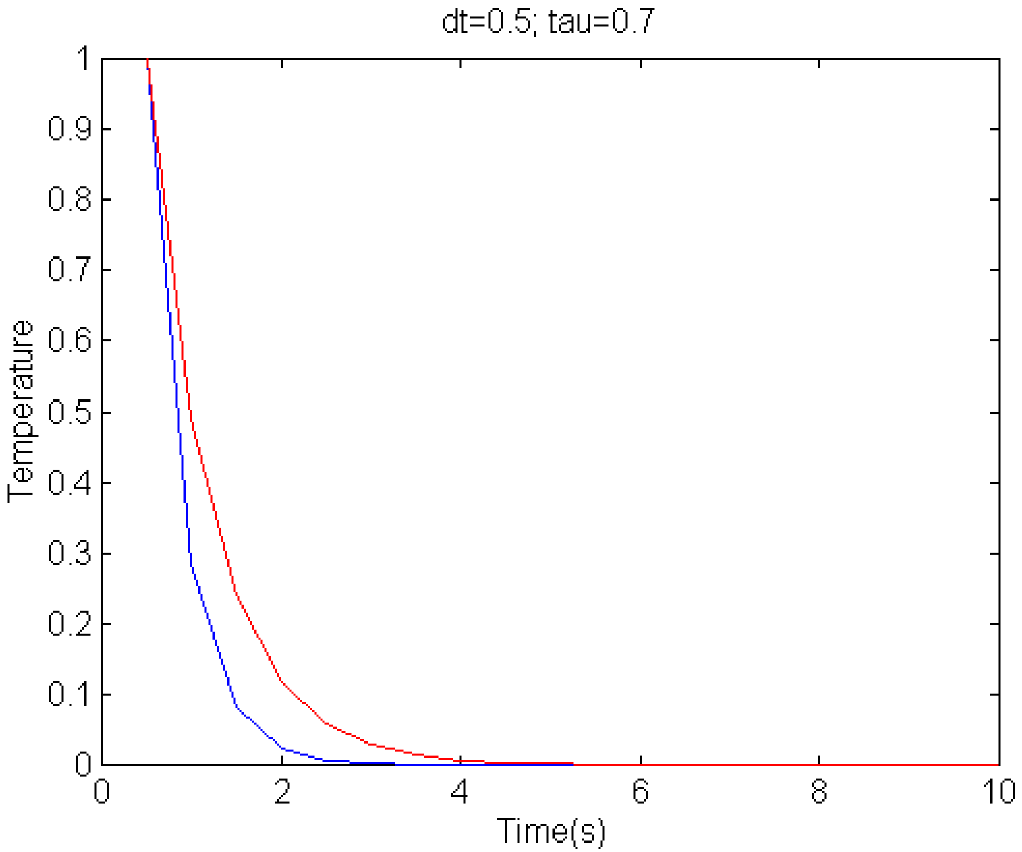
```
% Matlab Program - Newtonian Cooling

% 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)
```

Newtonian Cooling - *Convergence*



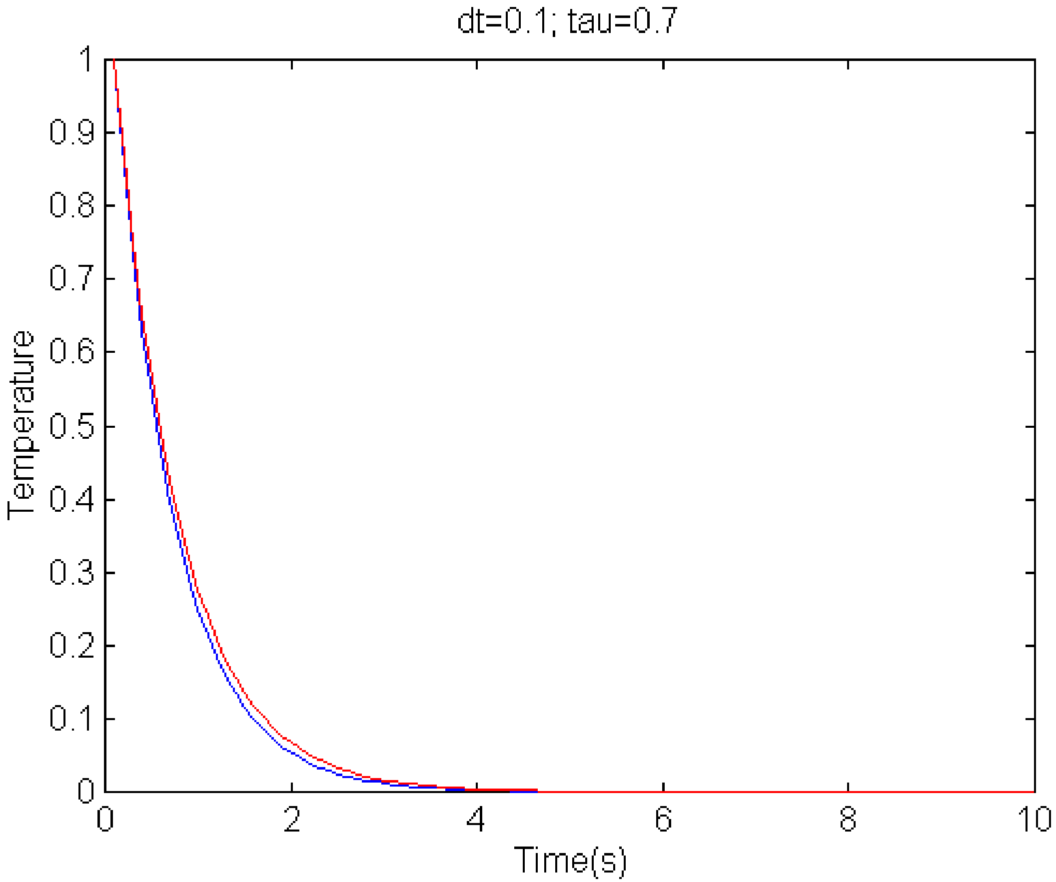
Newtonian Cooling - *Convergence*

Solution converges but does not have the right time-dependence



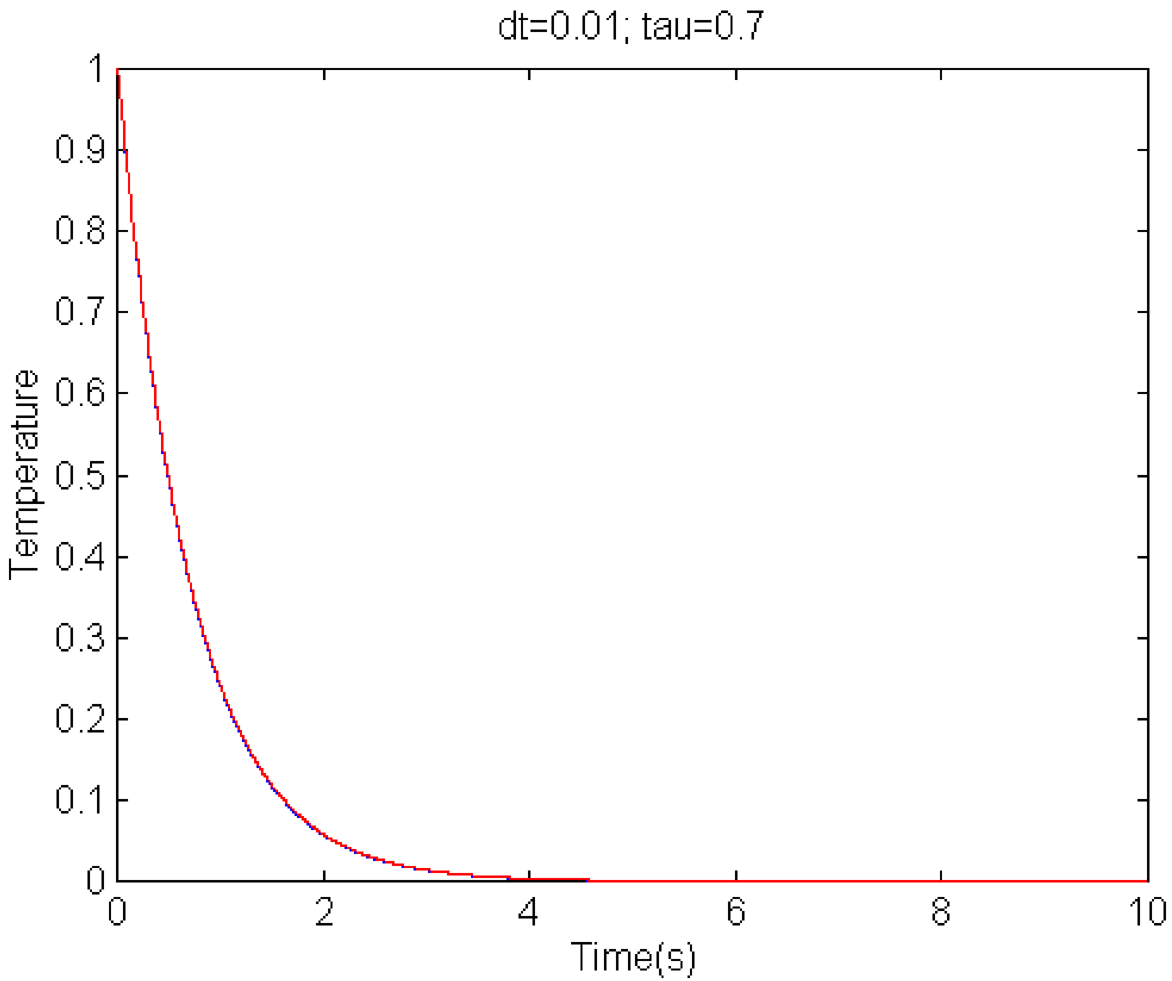
Newtonian Cooling - *Convergence*

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



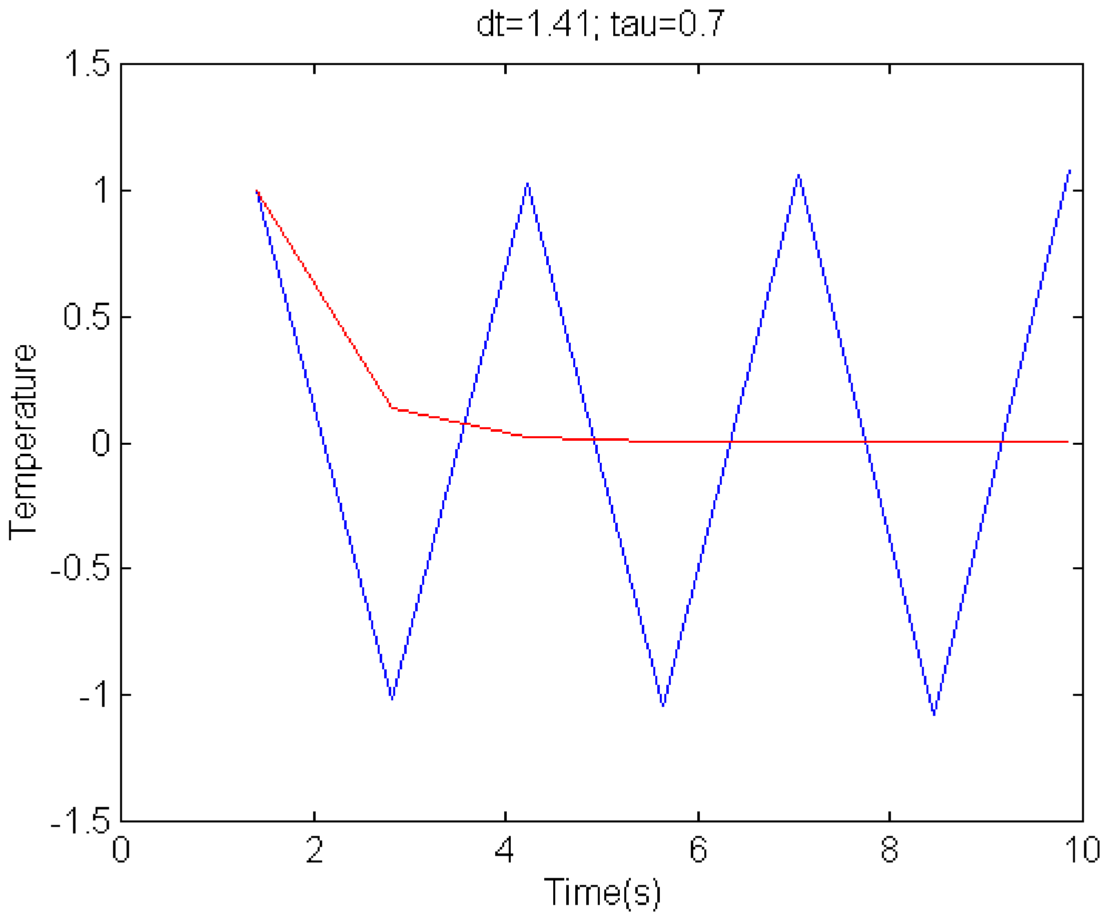
Newtonian Cooling - *Convergence*

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



Newtonian Cooling - *Convergence*

... this solution is wrong and unstable !



$$\rho(x)\partial_t^2 u(x,t) = \partial_x \left[E(x)\, \partial_x u(x,t) \right]$$

Elastic parameters E(x) vary only in one direction.

$$E(x) = \mu(x)$$ shear waves

$$E(x) = \lambda(x) + 2\mu(x)$$ P waves

with the corresponding velocities

$$v_S = \sqrt{\frac{\mu}{\rho}}$$ shear waves

$$v_P = \sqrt{\frac{\lambda + 2\mu}{\rho}}$$ P waves

The 1-D wave equation

We want to avoid having to take derivatives of the material parameters (why?). This can be achieved by using a *velocity-stress* formulation, which leads to the following simultaneous equations:

$$\partial_t \dot{u} = \frac{1}{\rho(x)} \partial_x \tau$$

$$\partial_t \tau = E(x) \partial_x \dot{u}$$

where

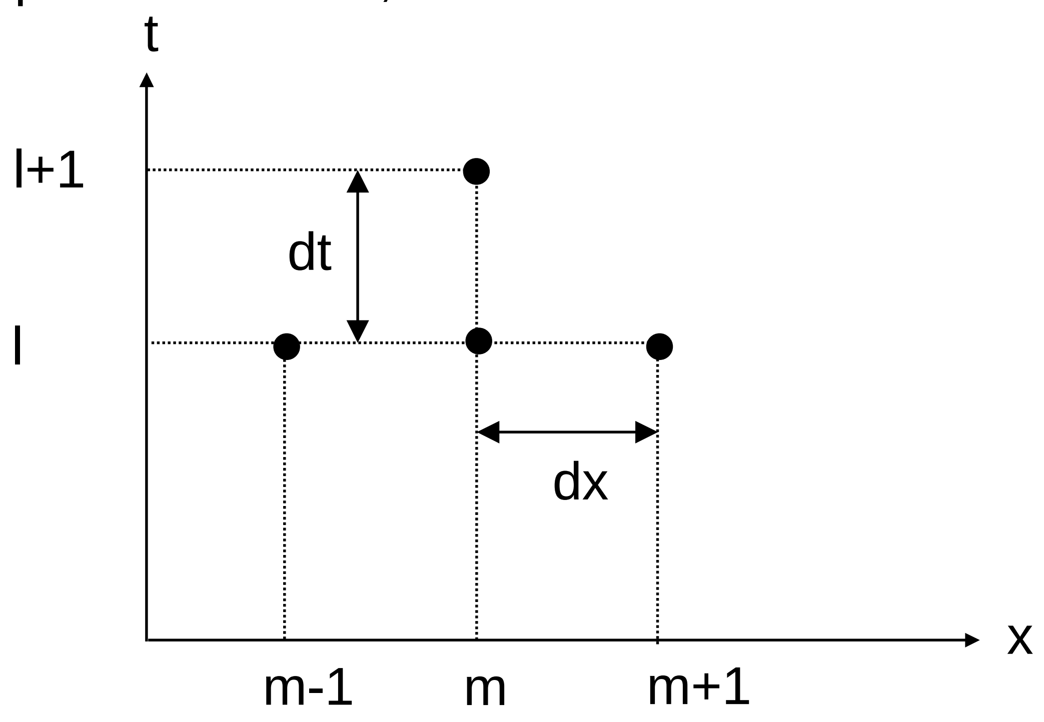
$$\tau = E(x) \partial_x u \qquad \text{stress}$$

The 1-D wave equation - FD scheme

Let us try to use one of the previously introduced FD schemes: central difference for space and forward difference for time

Discretization: $(l\mathrm{dt}, m\mathrm{dx})$

dx space increment, dt time increment



The 1-D wave equation - FD scheme

... leading to the following scheme:

forward

$$\frac{\dot{u}_m^{l+1} - \dot{u}_m^{l}}{dt} = \frac{1}{\rho_m} \frac{\tau_{m+1}^{l} - \tau_{m-1}^{l}}{2dx}$$

centered

forward

$$\frac{\tau_m^{l+1} - \tau_m^{l}}{dt} = E_m \frac{\dot{u}_{m+1}^{l} - \dot{u}_{m-1}^{l}}{2dx}$$

centered

like in the continuous case, we can make the following *Ansatz:*

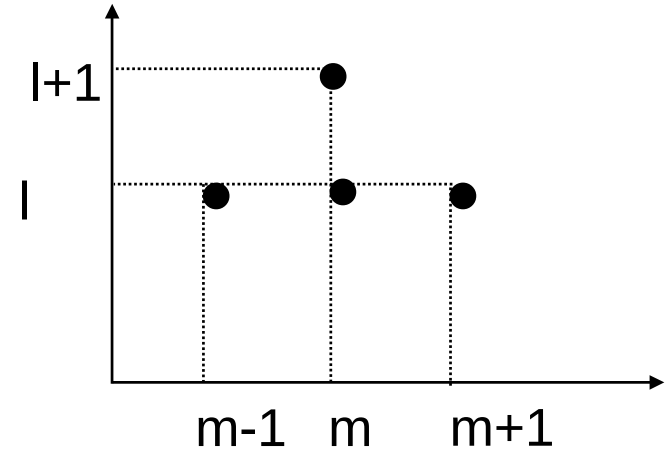
$$f(x,t) = A\exp(ikx - iwt)$$

which in the discrete world is :

$$f_{lm} = A\exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

The 1-D wave equation - FD scheme

... in practical terms: first solve



$$\dot{u}_m^{l+1} = dt\left[\frac{1}{\rho_m}\frac{\tau_{m+1}^{l} - \tau_{m-1}^{l}}{2dx}\right] + \dot{u}_m^{l}$$

then solve

$$\tau_m^{l+1} = dt\left[E_m\frac{\dot{u}_{m+1}^{l} - \dot{u}_{m-1}^{l}}{2dx}\right] + \tau_m^{l}$$

... let us assume a signal is propagating:

$$f(\tau_m^l) = A\exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

$$f(\dot{u}_m^l) = B\exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

we now put this *Ansatz* into the following equations ...

$$\frac{\dot{u}_m^{l+1} - \dot{u}_m^l}{dt} = \frac{1}{\rho_m}\frac{\tau_{m+1}^l - \tau_{m-1}^l}{2dx}$$

$$\frac{\tau_m^{l+1} - \tau_m^l}{dt} = E_m\frac{\dot{u}_{m+1}^l - \dot{u}_{m-1}^l}{2dx}$$

The 1-D wave equation - FD scheme

...after some algebra (hours later) ...

$$\exp(-iwdt) = 1 \pm i\sqrt{\frac{E_m}{\rho_m}}\left(\frac{dt}{dx}\right)\sin kdx$$

What does this result tell us about the numerical solution?

$$\left|\exp(-iwdt)\right| > 1$$

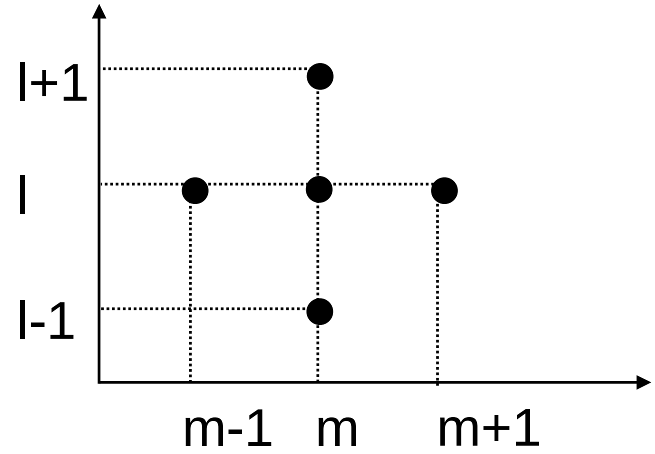
for any choice of dt and dx! So ω must be complex.
But then for example:

$$f(\tau_m^l) = A\exp(ikm\mathrm{dx} - iwl\mathrm{dt}) = A\exp(ikm)\exp(-w^* ldt)$$

will grow exponentially as, ω^* is real.

The 1-D wave equation - FD scheme

Can we find a scheme that works?
Let us use a centered scheme in time:



$$\frac{\dot{u}_m^{l+1} - \dot{u}_m^{l-1}}{2dt} = \frac{1}{\rho_m} \frac{\tau_{m+1}^{l} - \tau_{m-1}^{l}}{2dx}$$

$$\frac{\tau_m^{l+1} - \tau_m^{l-1}}{2dt} = E_m \frac{\dot{u}_{m+1}^{l} - \dot{u}_{m-1}^{l}}{2dx}$$

And again we use the following Ansatz to investigate the behavior of the numerical solution:

$$f(\tau_m^l) = A \exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

$$f(\dot{u}_m^l) = B \exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

...again after some algebra (minutes later) ...

$$\sin w dt = \pm \sqrt{\frac{E_m}{\rho_m}} \left(\frac{dt}{dx} \right) \sin k dx$$

... has real solutions as long as

$$\sqrt{\frac{E_m}{\rho_m}} \left(\frac{dt}{dx} \right) \leq 1$$

... knowing that for example ...

$$\sqrt{\frac{E_m}{\rho_m}} = v_p$$

P-wave velocity

The 1-D wave equation - FD scheme

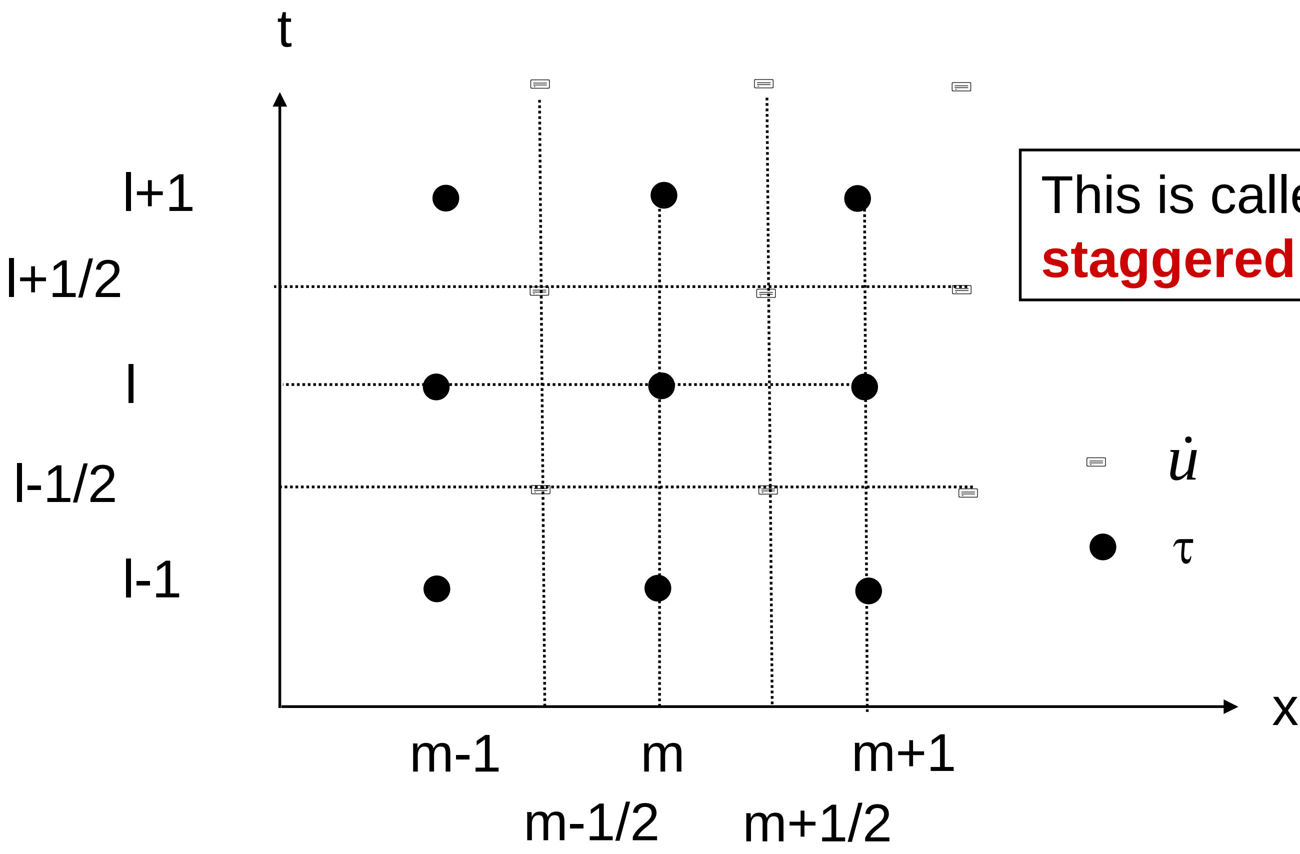
... we arrive at maybe the most important result for FD schemes applied to the wave equation:

$$v_{P,S}\left(\frac{dt}{dx}\right) \leq 1$$

$v_{P,S}$ is the locally homogeneous velocity. This is called a *conditionally stable* finite-difference scheme. Finding the right combination of dt and dx for a practical application, where the velocities vary in the medium is one of the most important tasks.

The 1-D wave equation - FD scheme

There is an even better scheme!



This is called a **staggered** scheme

... leading to the FD scheme:

$$\frac{\dot{u}_m^{l+1/2} - \dot{u}_m^{l-1/2}}{dt} = \frac{1}{\rho_m} \frac{\tau_{m+1/2}^{l} - \tau_{m-1/2}^{l}}{dx}$$

$$\frac{\tau_{m+1/2}^{l+1} - \tau_{m+1/2}^{l}}{dt} = E_{m+1/2} \frac{\dot{u}_{m+1}^{l+1/2} - \dot{u}_m^{l+1/2}}{dx}$$

And again we use the following *Ansatz* to investigate the behaviour of the numerical solution:

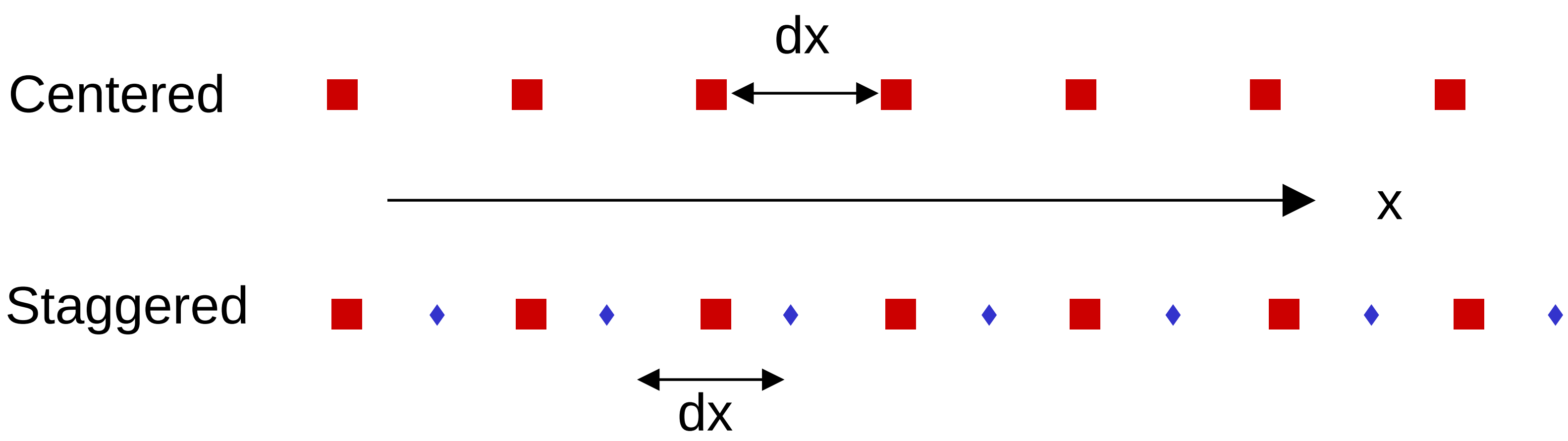
$$f(\tau_m^l) = A\exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

$$f(\dot{u}_m^l) = B\exp(ikm\mathrm{dx} - iwl\mathrm{dt})$$

Find the corresponding stability condition (Exercise)!

Staggered Grids

Which scheme is more accurate?



centered: $$\partial_x f \approx \frac{f(x+dx) - f(x-dx)}{2dx}$$

staggered: $$\partial_x f \approx \frac{f(x+dx/2) - f(x-dx/2)}{dx}$$

Because the error is $O(h^2)$, the error of the centered scheme is 4 times larger.

Numerical Dispersion

What does the stability criterion tell us about the quality of the numerical solution?

$$\sin\frac{\omega dt}{2} = \pm\sqrt{\frac{E_{m+1/2}}{\rho_m}}\left(\frac{dt}{dx}\right)\sin\frac{kdx}{2}$$

To answer this we need the concept of ***phase velocity*.**

Remember we assumed a harmonic oscillation with frequency ω and wavenumber k, for example

$$y(x,t) = \sin(kx - \omega t) = \sin(k(x - \frac{\omega}{k}t)) = \sin(\omega(\frac{k}{\omega}x - t))$$

where the phase velocity is

$$c_{phase} = \frac{\omega}{k}$$

Numerical Dispersion

$$\sin\frac{\omega dt}{2} = \pm\sqrt{\frac{E_{m+1/2}}{\rho_m}}\left(\frac{dt}{dx}\right)\sin\frac{kdx}{2}$$

we can first assume that dt and dx are very small, in this case :

$$\sin(x) \approx x$$ for small x

then

$$\frac{\omega}{k} = \sqrt{\frac{E_{m+1/2}}{\rho_m}} = c$$ wave speed

for small dt and dx we simulate the correct velocity:
The scheme is **convergent**.

Numerical Dispersion

How about the general case?

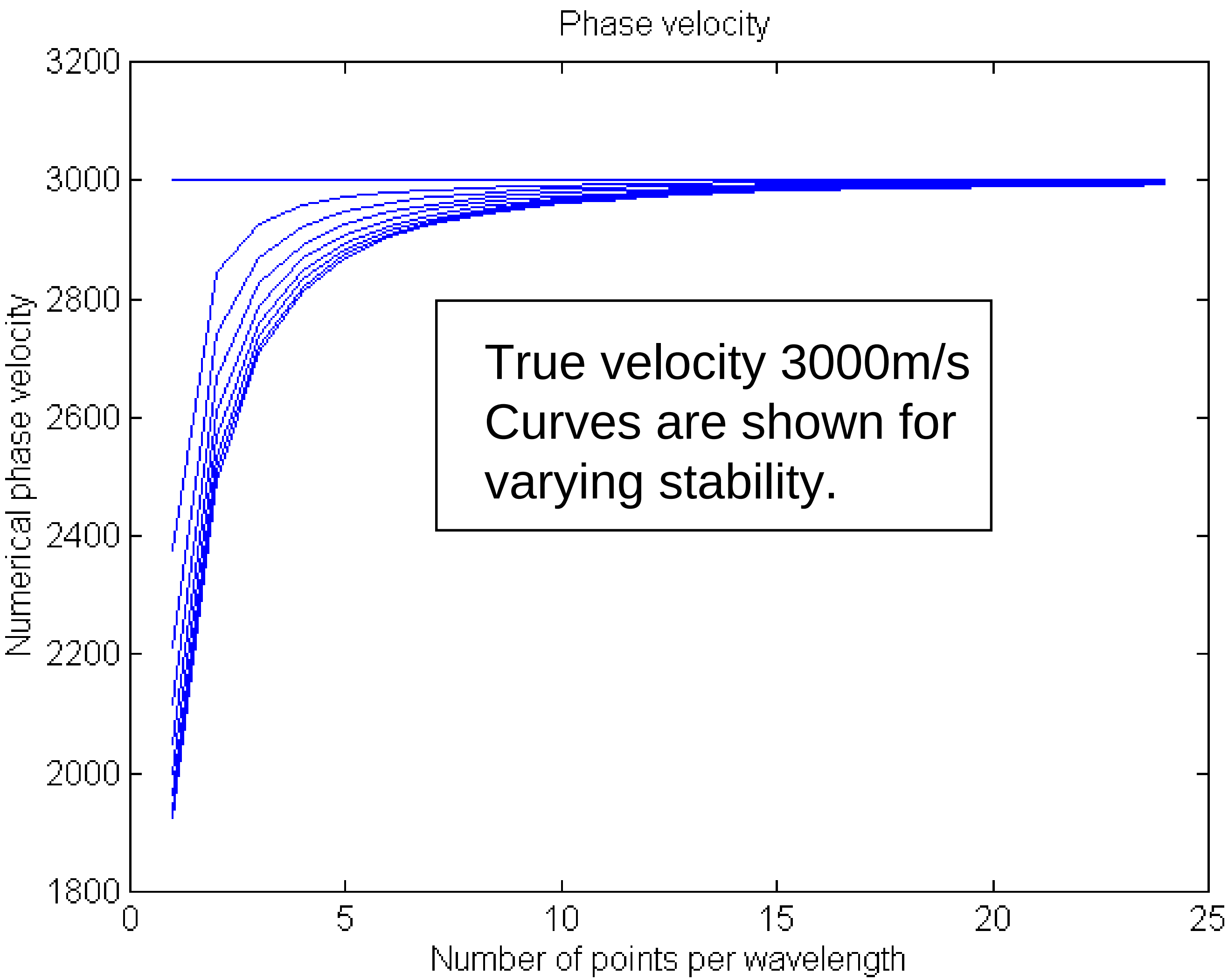
$$\sin\frac{\omega dt}{2} = \pm\sqrt{\frac{E_{m+1/2}}{\rho_m}}\left(\frac{dt}{dx}\right)\sin\frac{kdx}{2}$$

using $k = \frac{2\pi}{\lambda}$ we obtain

$$c(\lambda) = \frac{\omega}{k} = \frac{\lambda}{\pi dt}\sin^{-1}\left(c_0\frac{dt}{dx}\sin\frac{\pi dx}{\lambda}\right)$$

This formula expresses our *numerical* phase velocity as a function of the wave speed and the propagating wavelength.

Numerical Phase Velocity

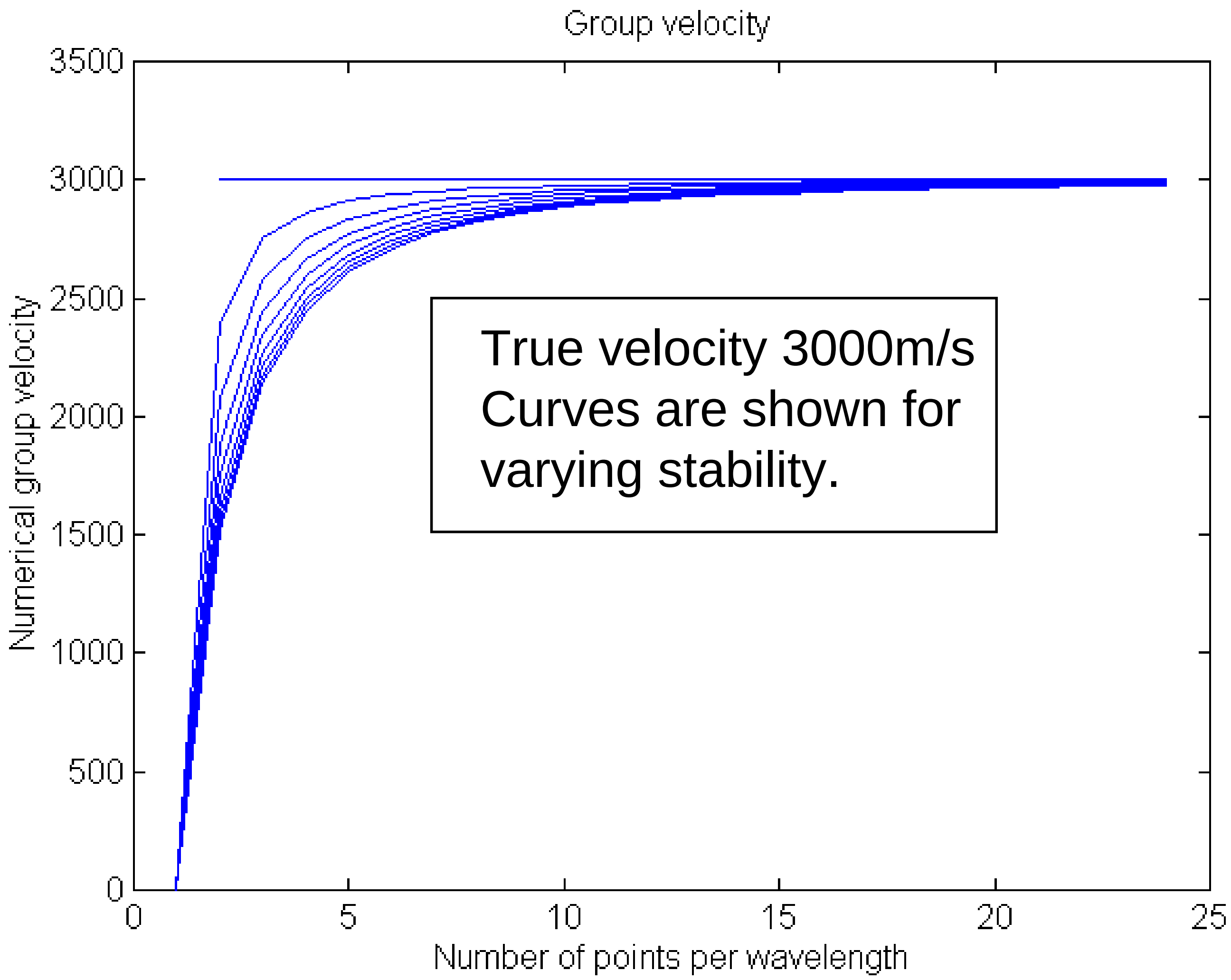


What we really measure in a seismogram is the group velocity:

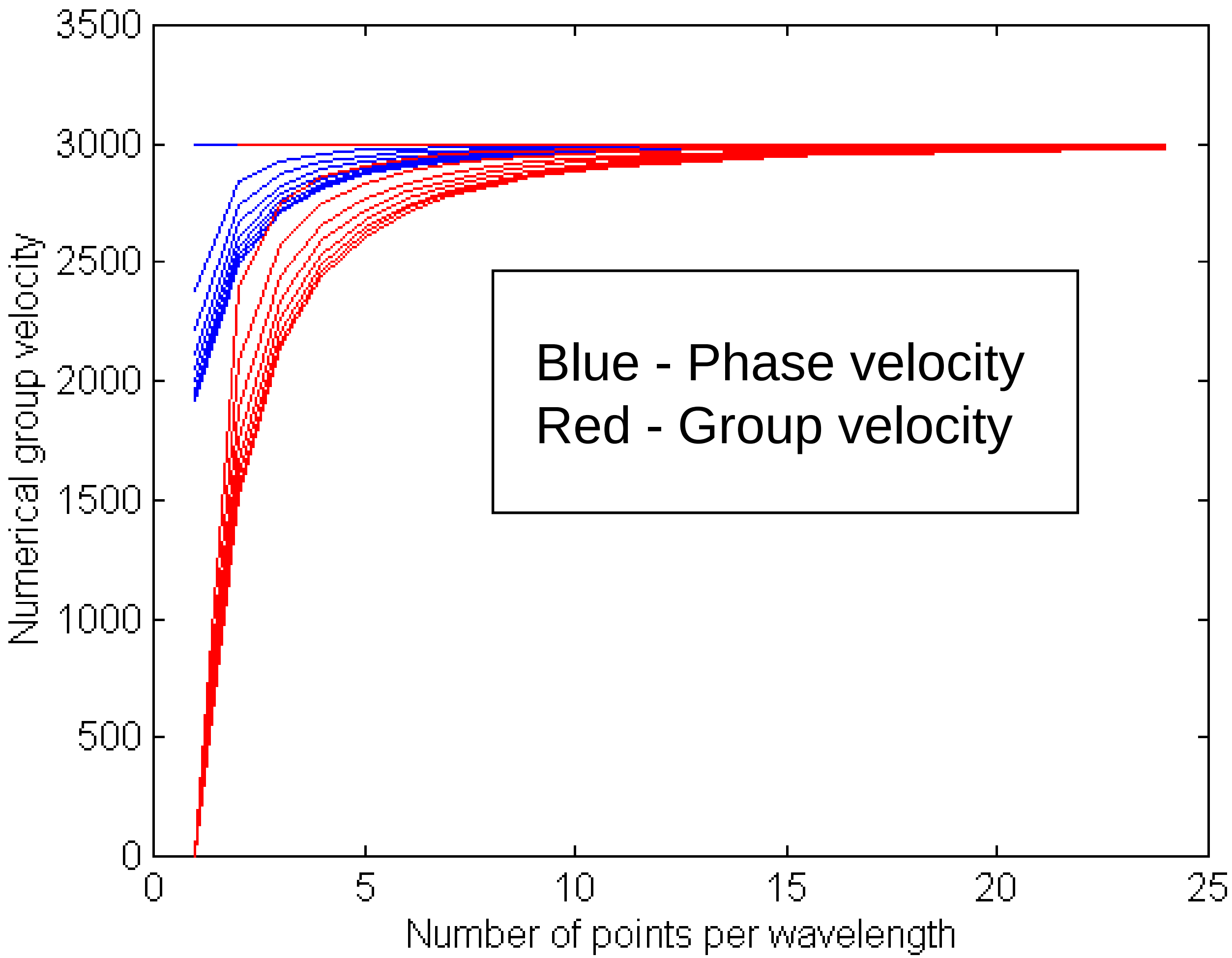
$$\frac{\partial \omega}{\partial k} = \frac{c \cos \frac{\pi dx}{\lambda}}{\left[1 - \left(c \frac{dt}{dx} \sin \frac{\pi dx}{\lambda}\right)^2\right]^{1/2}}$$

This formula expresses our *numerical* group velocity as a function of the wave speed and the propagating wavelength.

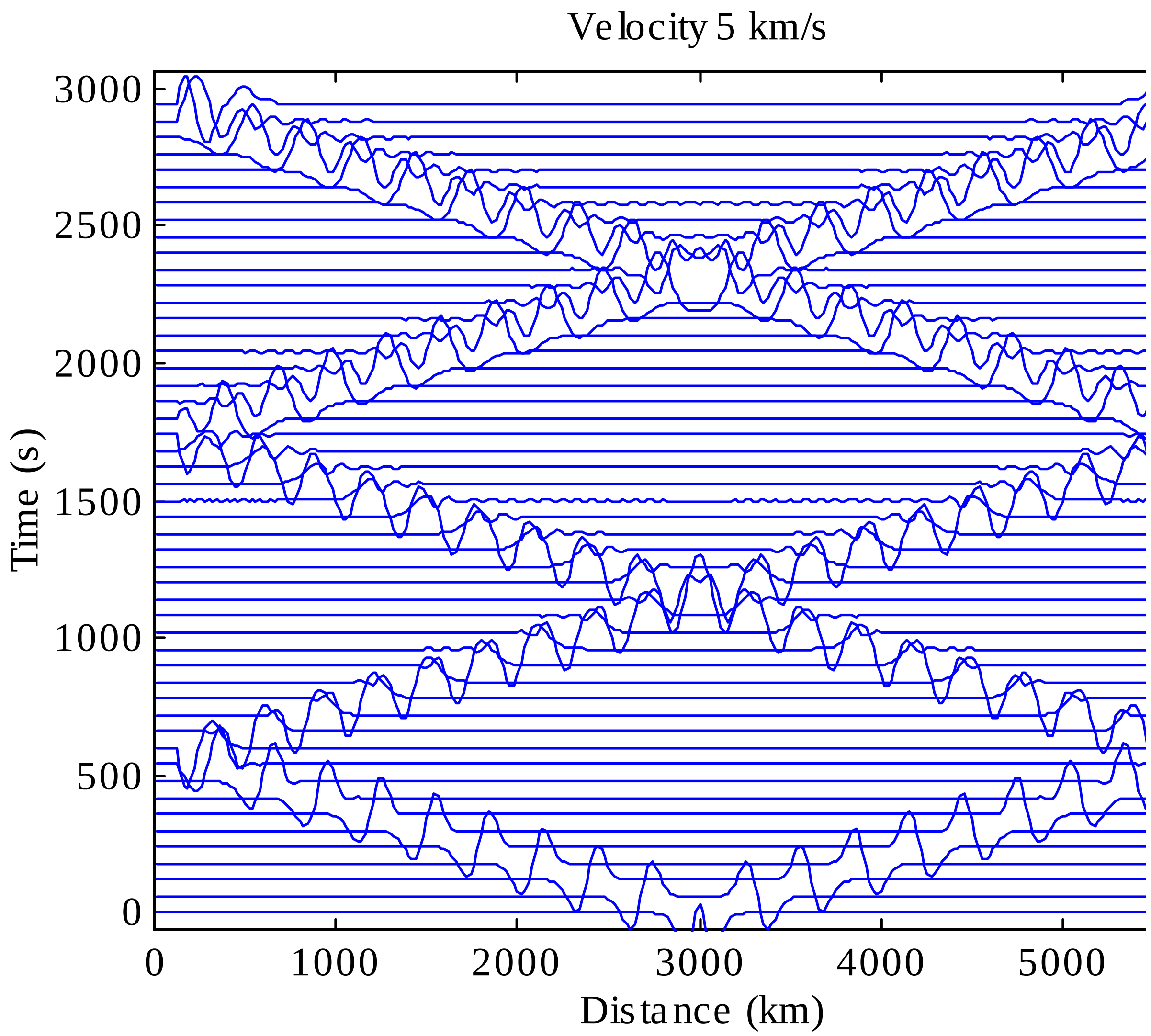
Numerical Group Velocity



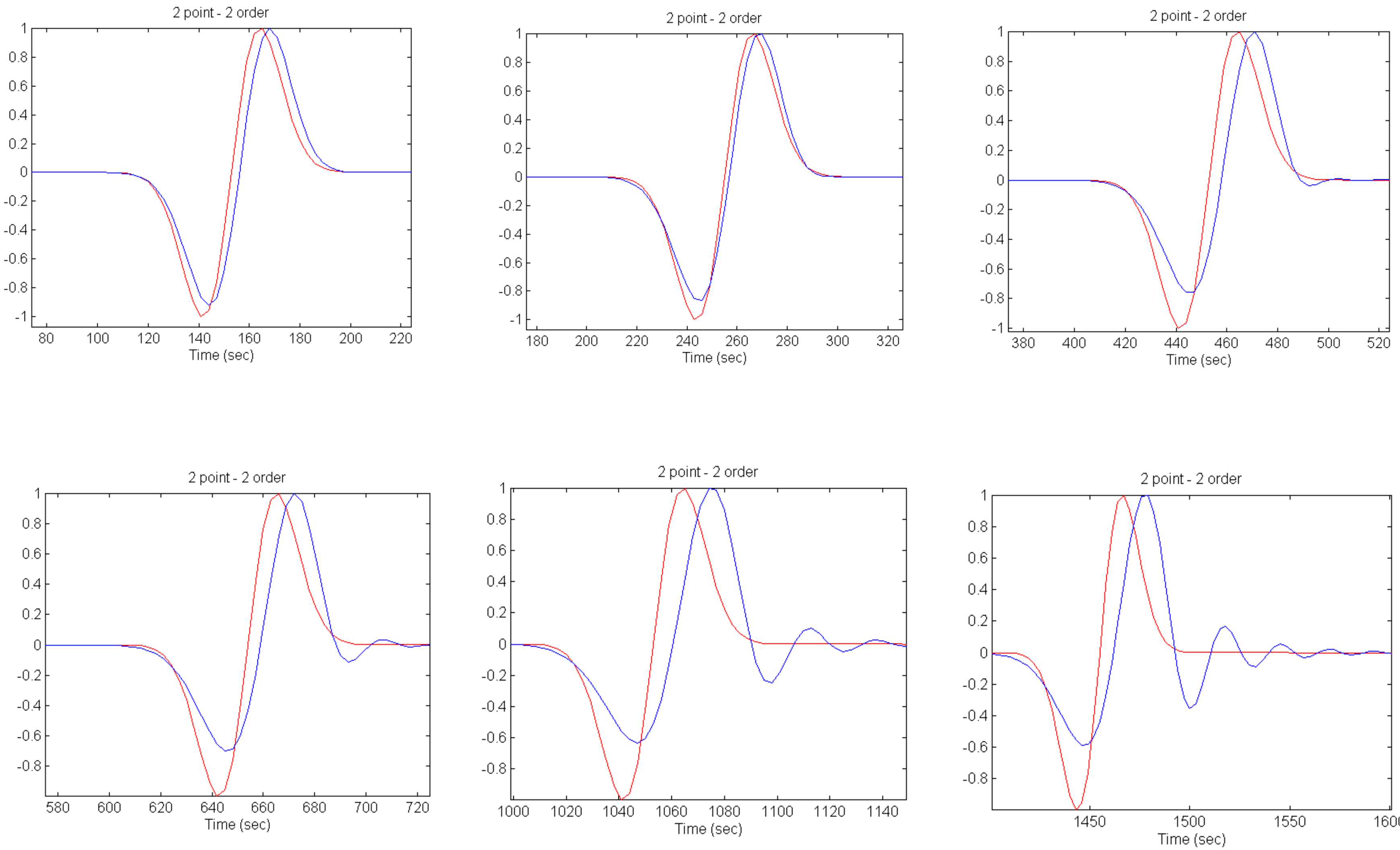
Numerical Group Velocity



Snapshot Example



Seismogram Dispersion



Finite Differences - Summary

Depending on the choice of the FD scheme (e.g. forward, backward, centered) a numerical solution may be more or less accurate.

Explicit finite difference solutions to differential equations are often *conditionally stable*. The correct choice of the space or time increment is crucial to enable accurate solutions.

Sometimes it is useful to employ so-called *staggered grids* where the fields are defined on seperate grids which may improve the overall accuracy of the scheme.