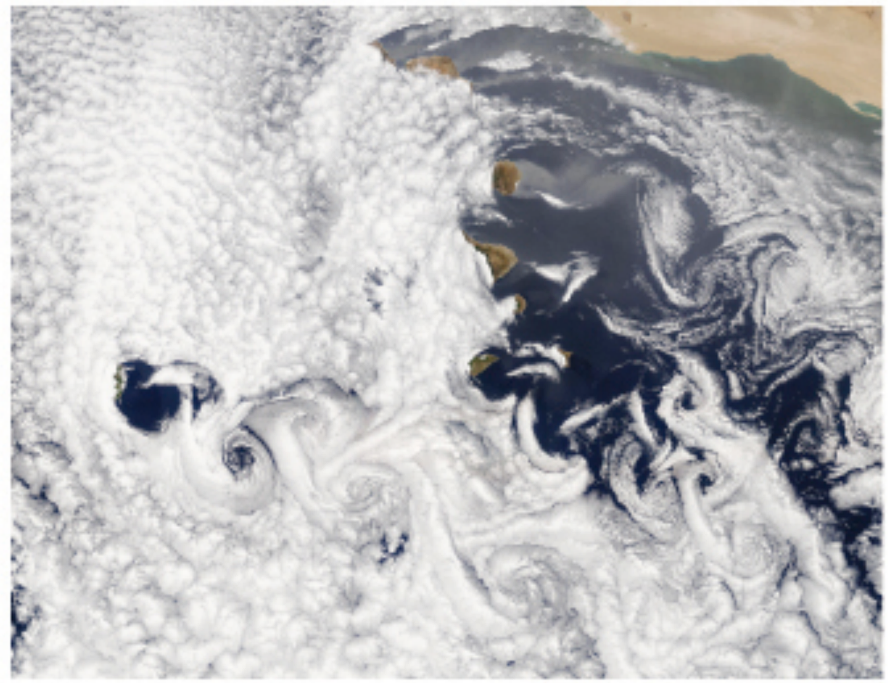
Ocean Modeling - EAS 8803

- Solving dynamical equations on a computer requires knowledge of numerical analysis and methods
- Scale Analysis
- Estimating derivatives with finite differencing
- Accuracy and higher order methods
- Convergence and Stability

Introduction to
Geophysical Fluid Dynamics
Physical and Numerical Aspects



Benoit Cushman-Roisin and Jean-Marie Beckers

Academic Press

Material is found at the end of Chap. 1 and 2

Modeling the Ocean and the Atmosphere

example of an early computation (1928)

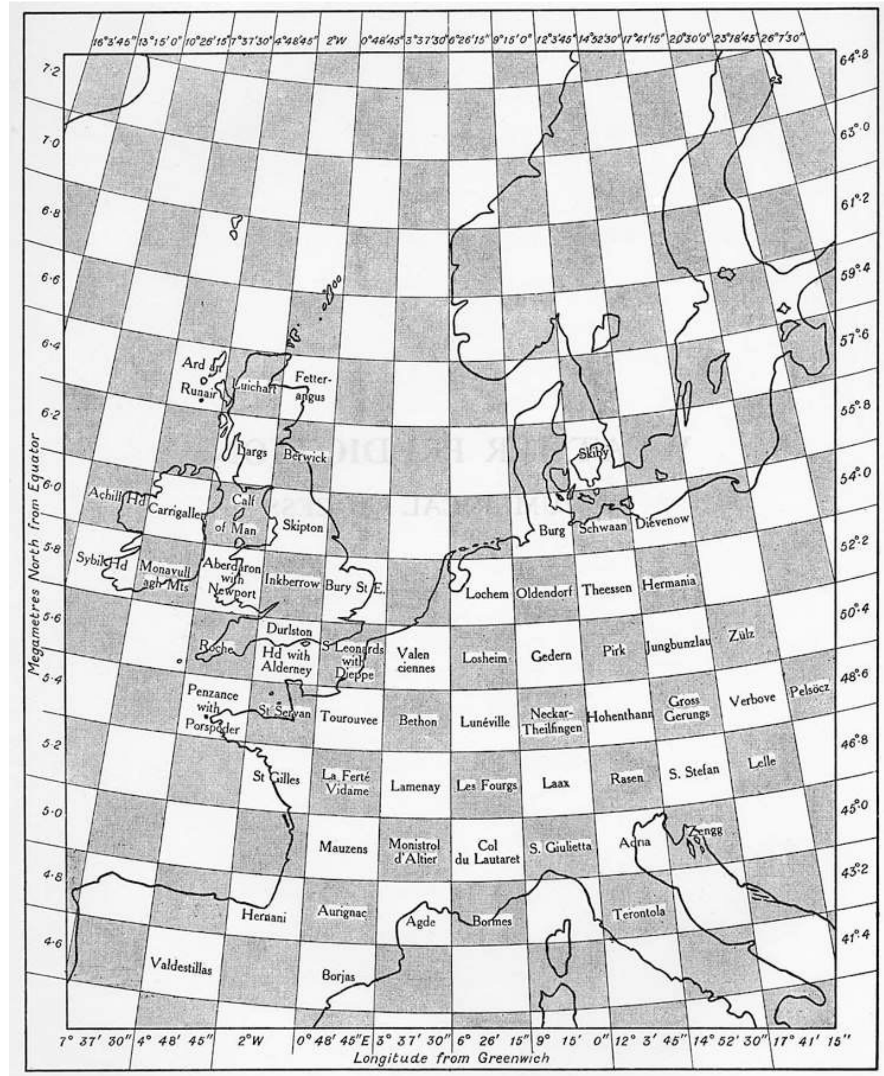
Complex differential equations

↓

Set of arithmetic operations

↓

step by step method of solution
(*model time-stepping*)
at selected points in space
(*model spatial grid*)



Model grid used by Lewis Fry Richardson

CAVEAT ! The concept of numerical stability was not known until 1928 when it was elucidated by Richard Courant, Karl Friedrichs and Hans Lewy.

Scale Analysis basis for estimating the relative importance of different terms in time-marching equations

$$\frac{du}{dt} \sim \frac{U}{T}.$$

$$\frac{d^2u}{dt^2} = \frac{d}{dt}\left(\frac{du}{dt}\right) \sim \frac{U/T}{T} = \frac{U}{T^2}$$

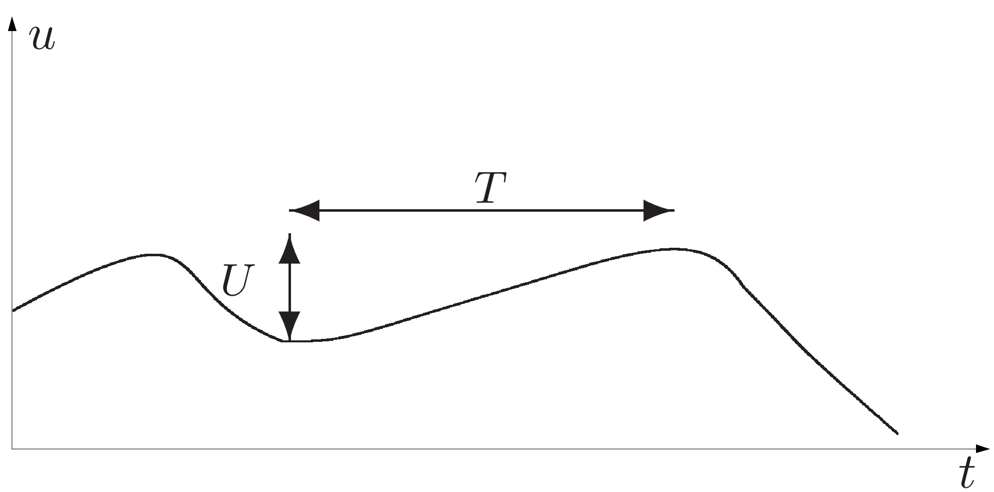


Figure 1-11 Time-scale analysis of a variable u. The time scale T is the time interval over which the variable u exhibits variations comparable to its standard deviation U.

Estimating Derivative with accuracy using a discretized version of the equations

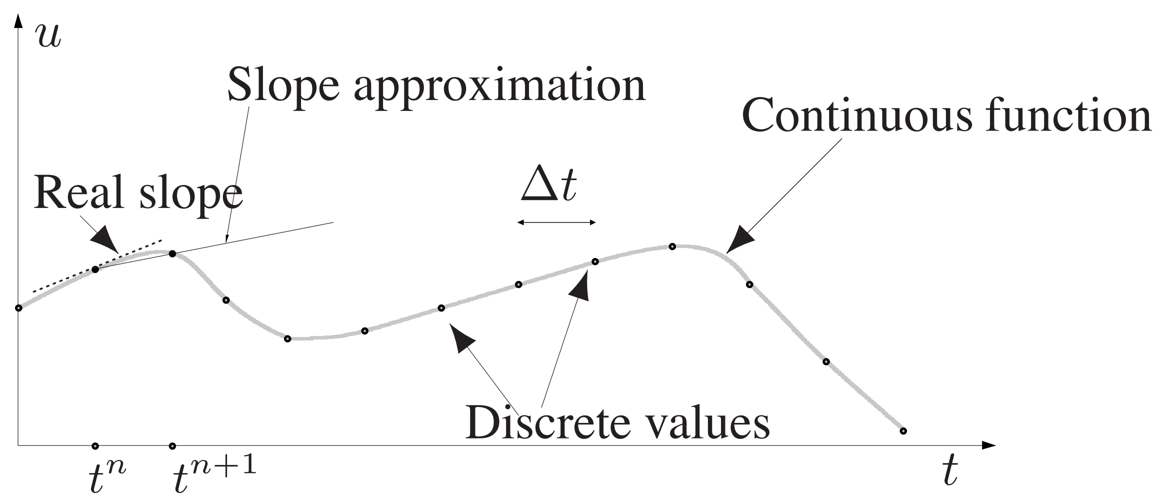


Figure 1-12 Representation of a function by a finite number of sampled values and approximation of a first derivative by a finite difference over Δt.

discretize the independent variable time *t* with a constant *time step Δt*

Having stored only a few values of the function, how can we retrieve the value of the function's derivatives that appear in the equations?

$$t^n = t^0 + n\,\Delta t, \quad n = 1, 2, \ldots.$$

Estimating Derivative with accuracy using a discretized version of the equations --> *finite differencing*

$$\frac{du}{dt} = \lim_{\Delta t \to 0} \frac{u(t+\Delta t) - u(t)}{\Delta t}, \tag{1.10}$$

we could directly deduce an approximation by allowing Δt to remain the finite time step

$$\frac{du}{dt} \simeq \frac{u(t+\Delta t) - u(t)}{\Delta t} \rightarrow \left.\frac{du}{dt}\right|_{t^n} \simeq \frac{u^{n+1} - u^n}{\Delta t}. \tag{1.11}$$

The accuracy of this approximation can be determined with the help of a Taylor series:

$$u(t+\Delta t) = u(t) + \Delta t \left.\frac{du}{dt}\right|_t + \underbrace{\frac{\Delta t^2}{2}\left.\frac{d^2u}{dt^2}\right|_t}_{\Delta t^2 \frac{U}{T^2}} + \underbrace{\frac{\Delta t^3}{6}\left.\frac{d^3u}{dt^3}\right|_t}_{\Delta t^3 \frac{U}{T^3}} + \underbrace{\mathcal{O}(\Delta t^4)}_{\Delta t^4 \frac{U}{T^4}}. \tag{1.12}$$

To the leading order for small Δt, we obtain the following estimate

$$\frac{du}{dt} = \frac{u(t+\Delta t) - u(t)}{\Delta t} + \mathcal{O}\left(\frac{\Delta t}{T}\frac{U}{T}\right). \tag{1.13}$$

Estimating Derivative

$$\frac{du}{dt} = \frac{u(t+\Delta t) - u(t)}{\Delta t} + \mathcal{O}\left(\frac{\Delta t}{T}\frac{U}{T}\right).$$

error term or ***truncation error*** need to be smaller than 1 so that Δt ≪ T

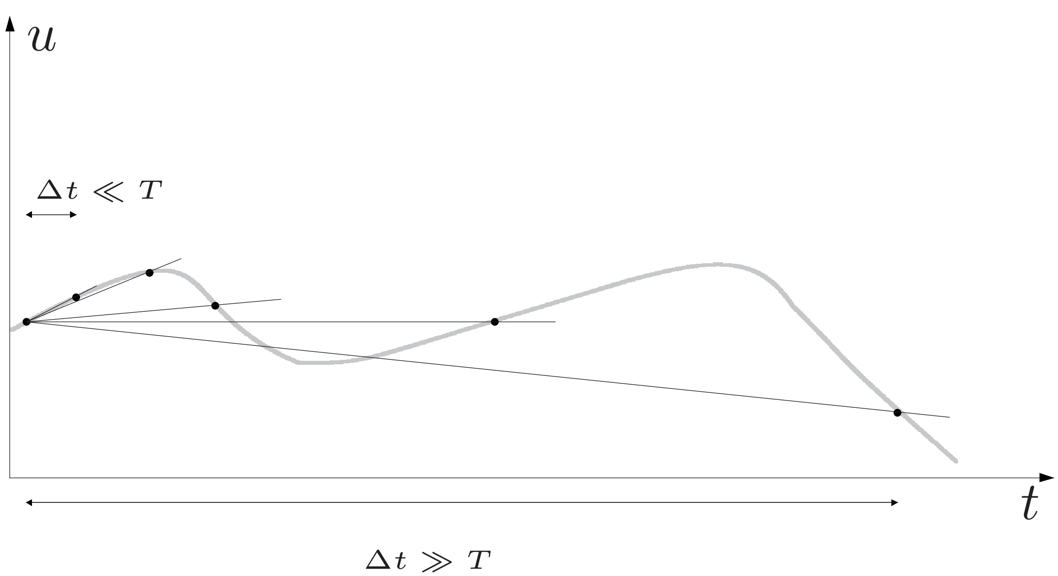
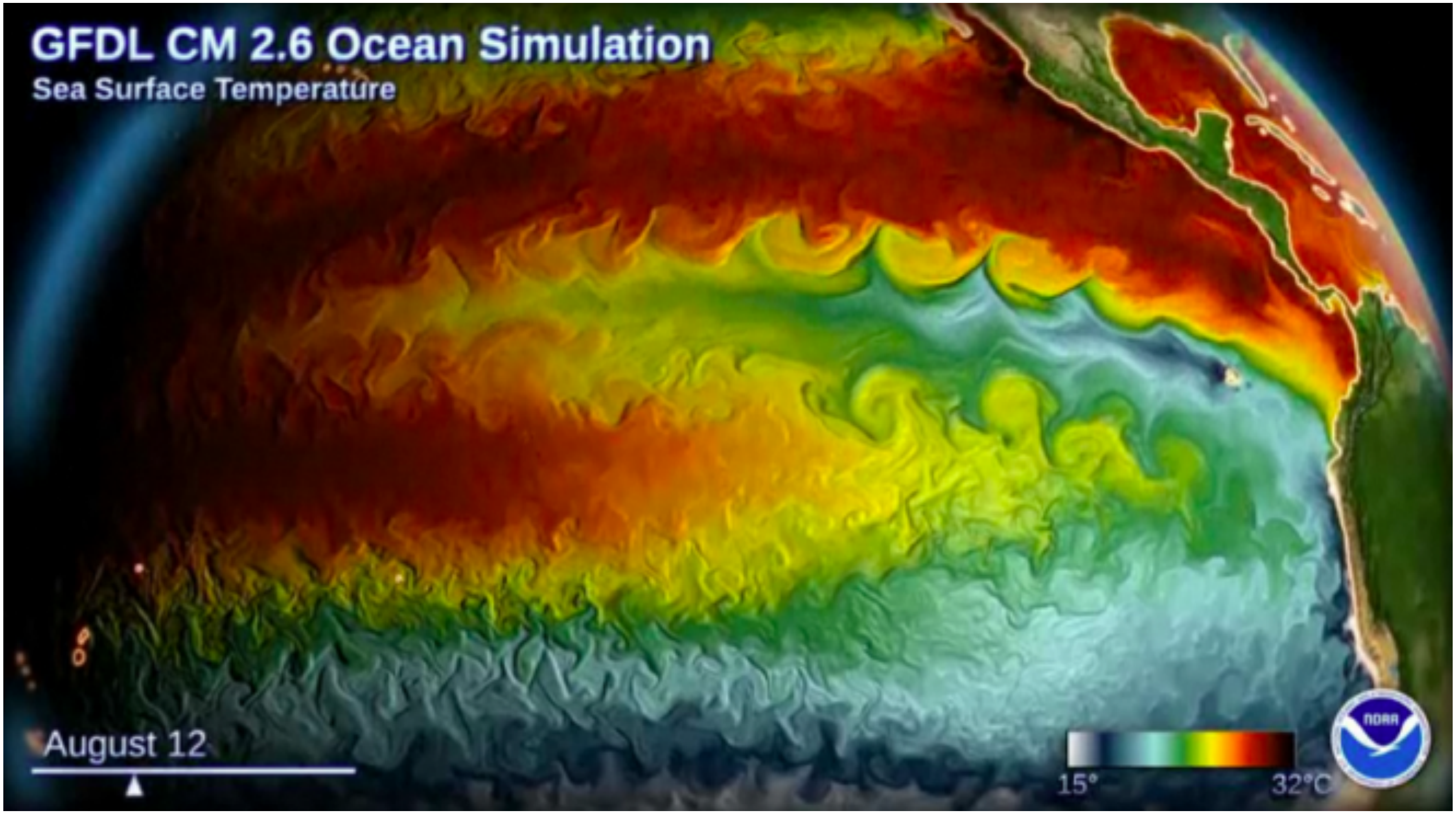


Figure 1-13 Finite differencing with various Δt values. Only when the time step is sufficiently short compared to the time scale, $\Delta t \ll T$, is the finite-difference slope close to the derivative, *i.e.*, the true slope.

Total Number of Operations grows fast when we consider both space and time



1 Teraflops = 10^{12} floating operations per second

Higher-order methods

rather than to increase resolution use other approximations for derivatives in the finite differencing

$$u^{n+1} = u^n + \Delta t \left.\frac{du}{dt}\right|_{t^n} + \frac{\Delta t^2}{2} \left.\frac{d^2u}{dt^2}\right|_{t^n} + \frac{\Delta t^3}{6} \left.\frac{d^3u}{dt^3}\right|_{t^n} + \mathcal{O}(\Delta t^4) \tag{1.19}$$

$$u^{n-1} = u^n - \Delta t \left.\frac{du}{dt}\right|_{t^n} + \frac{\Delta t^2}{2} \left.\frac{d^2u}{dt^2}\right|_{t^n} - \frac{\Delta t^3}{6} \left.\frac{d^3u}{dt^3}\right|_{t^n} + \mathcal{O}(\Delta t^4), \tag{1.20}$$

we can imagine that instead of using a *forward difference* approximation of the time derivative (1.11) we try a backward Taylor series (1.20) to design a *backward difference* approximation. This approximation is obviously still of first order because of its truncation error:

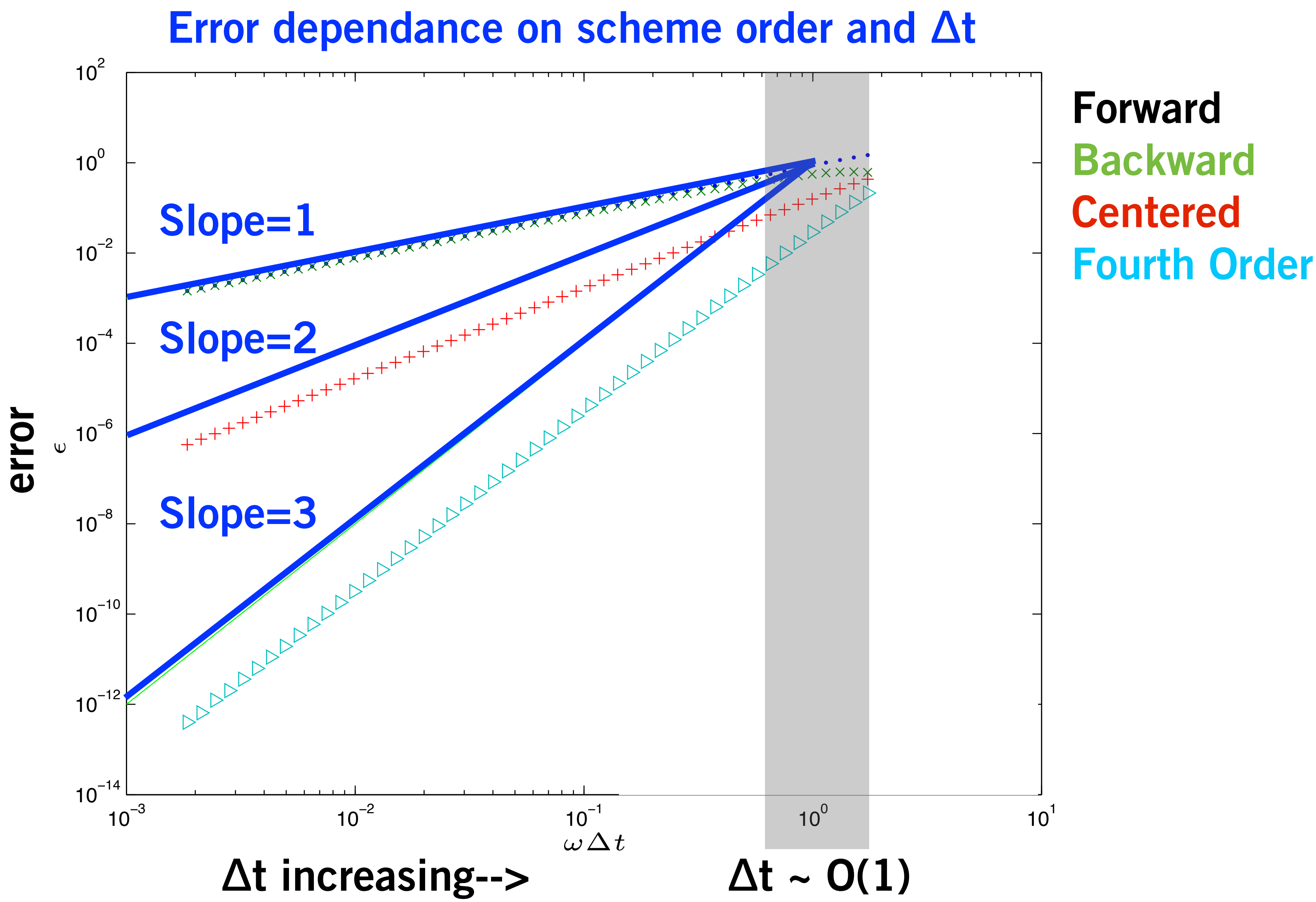
$$\left.\frac{du}{dt}\right|_{t^n} = \frac{u^n - u^{n-1}}{\Delta t} + \mathcal{O}(\Delta t). \tag{1.21}$$

Comparing (1.19) with (1.20), we observe that the truncation errors of the first-order forward and backward finite differences are the same but have opposite signs, so that by averaging both, we obtain a second-order truncation error (you can verify this statement by taking the difference between (1.19) and (1.20)):

$$\left.\frac{du}{dt}\right|_{t^n} = \frac{u^{n+1} - u^{n-1}}{2\Delta t} + \mathcal{O}(\Delta t^2). \tag{1.22}$$

Higher-order methods

rather than to increase resolution use other approximations for derivatives in the finite differencing



Higher-order methods
Taylor series is not useful to derive higher order schemes
(e.g. ***4th order centered finite-difference*** approximation of the first derivative)

$$\left.\frac{du}{dt}\right|_{t^n} \simeq a_{-2}u^{n-2} + a_{-1}u^{n-1} + a_0u^n + a_1u^{n+1} + a_2u^{n+2}.$$

higher order approximation need more information
about a function (*e.g. at multiple time levels*)

Higher-order methods

Taylor series is not useful to derive higher order schemes
(e.g. ***4th order centered finite-difference*** approximation of the first derivative)

Expanding u^{n+2} and the other values around t^n by Taylor series, we can write

$$
\begin{aligned}
\left.\frac{du}{dt}\right|_{t^n} = &\underbrace{(a_{-2} + a_{-1} + a_0 + a_1 + a_2)}_{=0} u^n \\
&+ \underbrace{(-2a_{-2} - a_{-1} + a_1 + 2a_2)}_{=1} \Delta t \left.\frac{du}{dt}\right|_{t^n} \\
&+ \underbrace{(4a_{-2} + a_{-1} + a_1 + 4a_2)}_{=0} \frac{\Delta t^2}{2} \left.\frac{d^2u}{dt^2}\right|_{t^n} \\
&+ \underbrace{(-8a_{-2} - a_{-1} + a_1 + 8a_2)}_{=0} \frac{\Delta t^3}{6} \left.\frac{d^3u}{dt^3}\right|_{t^n} \\
&+ \underbrace{(16a_{-2} + a_{-1} + a_1 + 16a_2)}_{=0} \frac{\Delta t^4}{24} \left.\frac{d^4u}{dt^4}\right|_{t^n} \\
&+ (-32a_{-2} - a_{-1} + a_1 + 32a_2) \frac{\Delta t^5}{120} \left.\frac{d^5u}{dt^5}\right|_{t^n} \\
&+ \mathcal{O}(\Delta t^6).
\end{aligned}
$$

Higher-order methods

Taylor series is not useful to derive higher order schemes
(e.g. ***4th order centered finite-difference*** approximation of the first derivative)

$$a_{-2} + a_{-1} + a_0 + a_1 + a_2 = 0,$$
$$(-2a_{-2} - a_{-1} + a_1 + 2a_2)\,\Delta t = 1.$$

$$\begin{aligned} 4a_{-2} + a_{-1} + a_1 + 4a_2 &= 0 \\ -8a_{-2} - a_{-1} + a_1 + 8a_2 &= 0 \\ 16a_{-2} + a_{-1} + a_1 + 16a_2 &= 0. \end{aligned}$$

$$-a_{-1} = a_1 = \frac{8}{12\Delta t}\,,\ a_0 = 0,\ -a_{-2} = a_2 = -\frac{1}{12\Delta t}$$

Solution

$$\left.\frac{du}{dt}\right|_{t^n} \simeq \frac{4}{3}\left(\frac{u^{n+1} - u^{n-1}}{2\Delta t}\right) - \frac{1}{3}\left(\frac{u^{n+2} - u^{n-2}}{4\Delta t}\right)$$

4th order centered finite-difference

Higher-order methods

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(e.g. ***4th order centered finite-difference*** approximation of the first derivative)

$$\left.\frac{du}{dt}\right|_{t^n} \simeq a_{-2}u^{n-2} + a_{-1}u^{n-1} + a_0 u^n + a_1 u^{n+1} + a_2 u^{n+2}.$$

$$\left.\frac{du}{dt}\right|_{t^n} \simeq \frac{4}{3}\left(\frac{u^{n+1} - u^{n-1}}{2\Delta t}\right) - \frac{1}{3}\left(\frac{u^{n+2} - u^{n-2}}{4\Delta t}\right)$$

4th order centered finite-difference

$$-a_{-1} = a_1 = \frac{8}{12\Delta t},\ a_0 = 0,\ -a_{-2} = a_2 = -\frac{1}{12\Delta t}$$

Solution

Higher-order methods

Taylor series is not useful to derive higher order schemes
(e.g. ***4th order centered finite-difference*** approximation of the first derivative)

$$\left.\frac{du}{dt}\right|_{t^n} \simeq a_{-2}u^{n-2} + a_{-1}u^{n-1} + a_0 u^n + a_1 u^{n+1} + a_2 u^{n+2}.$$

Generalize this approach to derive any order scheme

$$\left.\frac{d^p u}{dt^p}\right|_{t_n} = a_{-m}u^{n-m} + ... + a_{-1}u^{n-1} + a_0 u^n + a_1 u^{n+1} + ... + a_m u^{n+m}$$

Higher-order methods
(e.g. ***2nd order centered finite-difference*** approximation of the **2nd derivative**)

... again from Taylor Series

$$u^{n+1} = u^n + \Delta t \left.\frac{du}{dt}\right|_{t^n} + \frac{\Delta t^2}{2} \left.\frac{d^2u}{dt^2}\right|_{t^n} + \frac{\Delta t^3}{6} \left.\frac{d^3u}{dt^3}\right|_{t^n} + \mathcal{O}(\Delta t^4)$$
$$u^{n-1} = u^n - \Delta t \left.\frac{du}{dt}\right|_{t^n} + \frac{\Delta t^2}{2} \left.\frac{d^2u}{dt^2}\right|_{t^n} - \frac{\Delta t^3}{6} \left.\frac{d^3u}{dt^3}\right|_{t^n} + \mathcal{O}(\Delta t^4),$$

2nd order centered finite-difference

$$\left.\frac{d^2u}{dt^2}\right|_{t_n} \simeq \left(\frac{u^{n-1} - 2u^n + u^{n+1}}{\Delta t^2}\right)$$

Understanding ALIASING

To sample a wave of frequency ω the time step Δt may not exceed

$\Delta t_{max} = \pi/\omega = T/2$

which implies that at least two samples of the signal must be taken per period. This minimum required sampling frequency is called the ***Nyquist frequency***

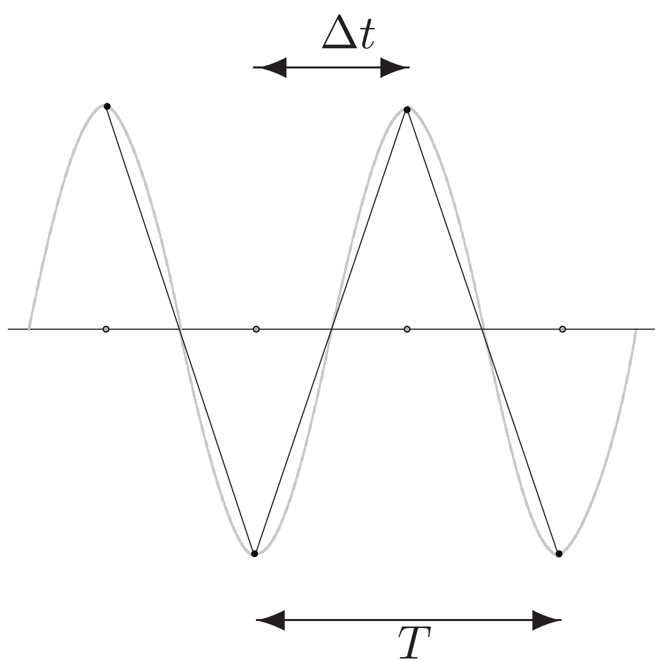
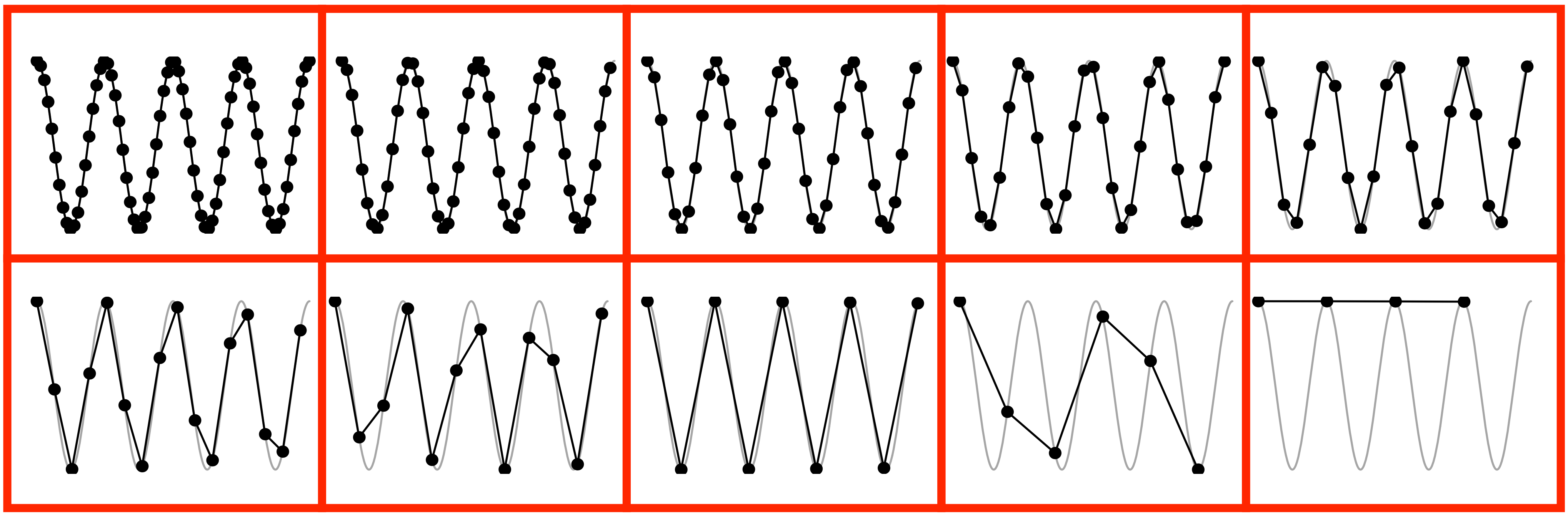


Figure 1-16 Shortest wave (at *cut-off frequency* $\pi/\Delta t$ or period $2\Delta t$) resolved by uniform grid in time.

Δt *increases* →



signal amplitude becomes irregular

N Frequency

signal appears lower frequency

Δt *increases* →

Numerical convergence and stability

Consistency

discretized equation for increasing resolution is the exact equation.

Numerical convergence and stability

Consistency
discretized equation for increasing resolution is the exact equation.

Convergence
difference between the exact and discrete solutions tends to zero as Δt vanishes.

Lax-Richtmyer equivalence theorem [lax and Richtmyer, 1956]
A consistent finite-difference scheme for a linear partial differential equation for which the initial value problem is well posed is convergent if and only if it is stable.

Numerical convergence and stability

Consistency
discretized equation for increasing resolution is the exact equation.

Convergence
difference between the exact and discrete solutions tends to zero as Δt vanishes.

Lax-Richtmyer equivalence theorem [lax and Richtmyer, 1956]
A consistent finite-difference scheme for a linear partial differential equation for which the initial value problem is well posed is convergent if and only if it is stable.

Stability (a concept that has different definition in numerical methods)
An algorithm for solving a linear evolutionary partial differential equation is stable if the total variation of the numerical solution at a fixed time remains bounded as the step size goes to zero.
(e.g. the energy of the system does not increase with every time step).

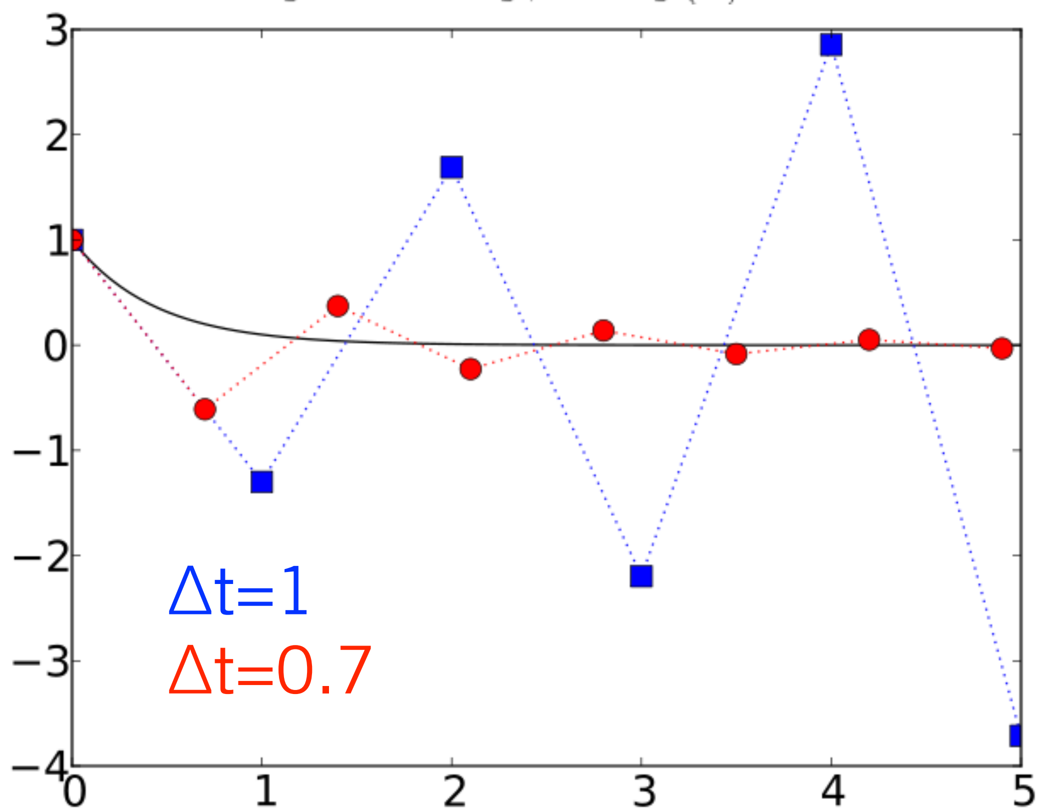
Numerical stability

*An example with the **Euler Method***

$$\tilde{u}^{n+1} = \tilde{u}^n + \Delta t \left[\frac{d\tilde{u}}{dt}\right]_{t=t^n} + \frac{\Delta t^2}{2}\left[\frac{d^2\tilde{u}}{dt^2}\right]_{t=t^n} + \mathcal{O}(\Delta t^3)$$

***stiff equation** is a differential equation for which certain numerical methods for solving the equation are numerically unstable,*

$$y' = -2.3y, \qquad y(0) = 1.$$



http://en.wikipedia.org/wiki/Euler_method

8.12: Stability behavior of Euler's method

We consider the so-called linear test equation

$$\dot{y}(t) = \lambda y(t)$$

where $\lambda \in \mathbb{C}$ is a system parameter which mimics the eigenvalues of linear systems of differential equations.

The equation is stable if $\mathrm{Real}(\lambda) \leq 0$. In this case the solution is exponentially decaying. ($\lim_{t\to\infty} y(t) = 0$).

When is the numerically solution u_i also decaying, $\lim_{i\to\infty} u_i = 0$?

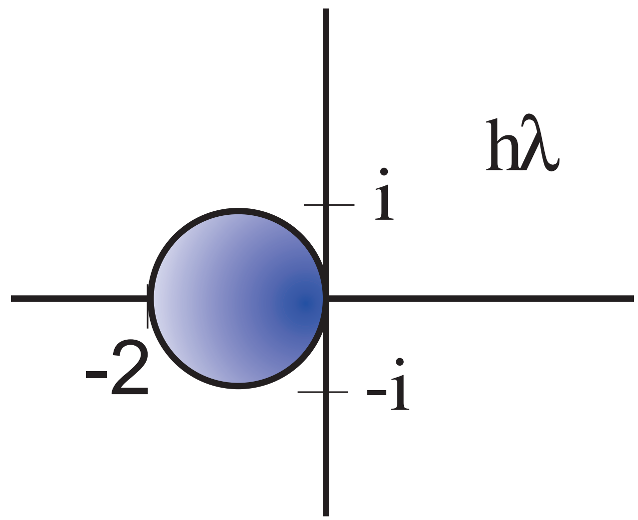
8.12: Stability behavior of Euler's method (Cont.)

Explicit Euler discretization of linear test equation:

$$u_{i+1} = u_i + h\lambda u_i$$

This gives $u_{i+1} = (1 + h\lambda)^{i+1} u_0$.

The solution is decaying (stable)
if $|1 + h\lambda| \leq 1$

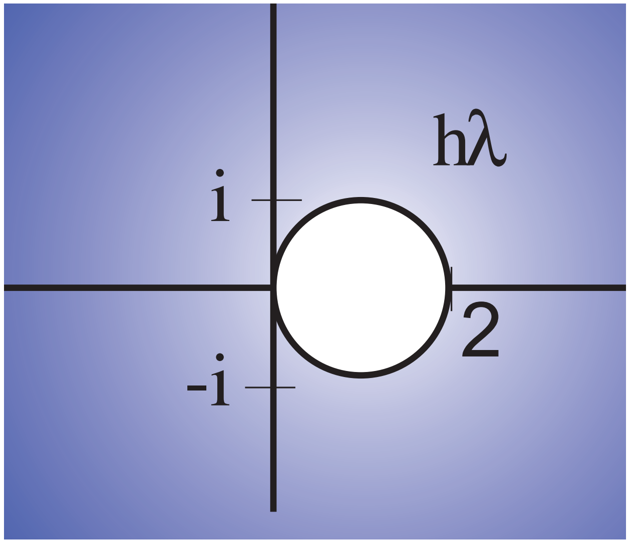


8.13: Stability behavior of Euler's method (Cont.)

Implicit Euler discretization of linear test equation:

$$u_{i+1} = u_i + h\lambda u_{i+1}$$

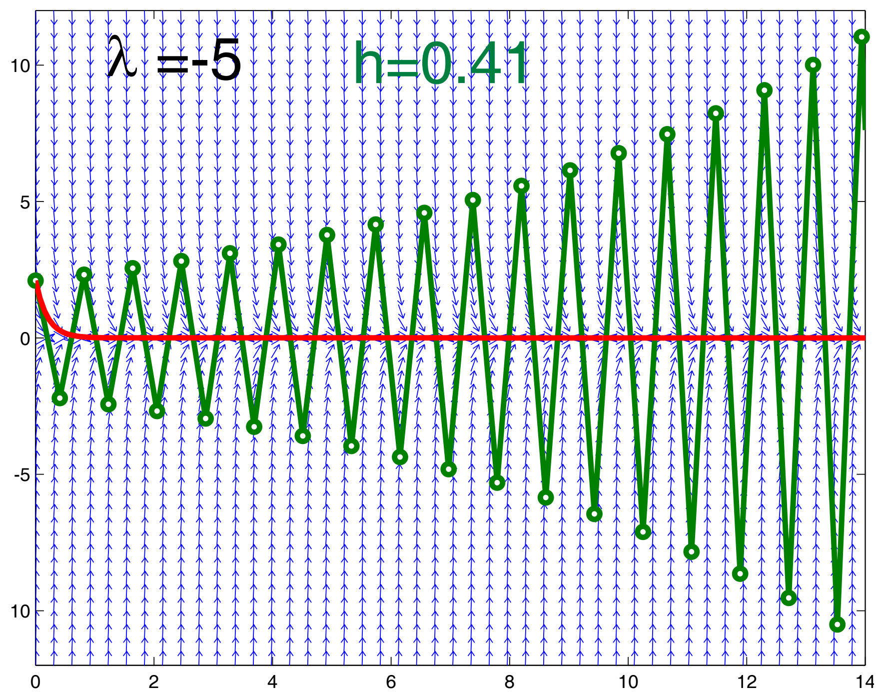
This gives $u_{i+1} = \left(\frac{1}{1-h\lambda}\right)^{i+1} u_0$.



The solution is decaying (stable)
if $|1 - h\lambda| \geq 1$

8.14: Stability behavior of Euler's method (Cont.)

Explicit Euler's instability for fast decaying equations:



8.15: Stability behavior of Euler's method (Cont.)

Facit:
For stable ODEs with a fast decaying solution ($\mathrm{Real}(\lambda) << -1$)
or highly oscillatory modes ($\mathrm{Im}(\lambda) >> 1$)
the explicit Euler method demands small step sizes.

This makes the method inefficient for these so-called stiff systems.

Alternative: implicit Euler method.

8.16: Implementation of implicit methods

Implicit Euler method $u_{i+1} = u_i + h_i f(t_{i+1}, u_{i+1})$

Two ways to solve for u_{i+1}:

k is the iteration counter, i the integration step counter

- Fixed point iteration: $u_{i+1}^{(k+1)} = \underbrace{u_i + h_i f(t_{i+1}, u_{i+1}^{(k)})}_{=\varphi(u_{i+1}^{(k)})}$

- Newton iteration:

$$u_{i+1} = u_i + h_i f(t_{i+1}, u_{i+1}) \Leftrightarrow \underbrace{u_{i+1} - u_i - h_i f(t_{i+1}, u_{i+1})}_{=F(u_{i+1})} = 0$$

$$F'(u_{i+1}^{(k)})\Delta u_{i+1} = -F(u_{i+1}^{(k)}) \qquad u_{i+1}^{(k+1)} = u_{i+1}^{(k)} + \Delta u_{i+1}$$

8.17: Implementation of implicit methods (Cont.)

These iterations are performed at every integration step!
They are started with explicit Euler method as so-called predictor:

$$u_{i+1}^{(0)} = u_i + h_i f(t_i, u_i)$$

When should fixed points iteration and when Newton iteration be used?

The key is contractivity!

Let's check the linear test equation again: $\dot{y} = \lambda y$.

Contractivity: $|\varphi'(u)| = |h\lambda| < 1$.

8.18: Implementation of implicit methods (Cont.)

If the differential equation is

- nonstiff: explicit Euler or
- nonstiff: implicit Euler with fixed point iteration
- stiff: implicit Euler with Newton iteration

Numerical stability

$$\| \mathbf{x}^n \| \leq C \| \mathbf{x}^0 \|$$

Stability

$$\| \mathbf{x}^n \| \leq \| \mathbf{x}^0 \|$$

Strict Stability Condition