Today’s topics

- Time-dependent problems
    - Heat equation
    - Wave equation
- Explicit & implicit methods
- Stability & accuracy

Time-Dependent Problems

- Problems in the time domain:
  - Diffusion / Heat: $\frac{\partial u}{\partial t} = \Delta u$ ➡ $\frac{\partial u_h}{\partial t} = A u_h$
  - Wave: $\frac{\partial^2 u}{\partial t^2} = \Delta u$ ➡ $\frac{\partial^2 u_h}{\partial t^2} = A u_h$

The matrix *A* is from the FD / FEM / analytic basis discretization that includes the boundary conditions

- Differerent in character:
  - Diffusion / Heat: Solution is flattened out
  - Wave: Inital shape preserved

Discuss: Differnces between heat and wave equation?

Time-Dependent Problems: Key Concepts

- Stepping in the time domain from *a* to *b*: $a = t_0 < t_1 < t_2 < \cdots < t_{N-1} < t_N = b$

  $k_i = t_{i+1} - t_i$

- Approximation at every time step: $w_i \approx u_h(t_i) \qquad w_0 = u_h(t_0)$
- Method to go from *j=0,1,..,i → i+1*
  - One-step method: $w_{i+1} = \phi(A, t_i, w_i, w_{i+1}, k_i)$
    - Explicit: $w_{i+1} = \phi(A, t_i, w_i, k_i)$
    - Otherwise implicit
  - Multistep method:

$$w_{i+1} = \phi(A, t_{i+1-m}, \ldots, t_i, w_{i+1-m}, \ldots, w_{i+1}, k_i)$$

Heat Equation: First Steps

- Take first the heat equation. Write

$$u_h(t_{i+1}) = u_h(t_i) + k_i u_h'(t_i) + \frac{1}{2}k_i^2 u_h''(t_i) + \cdots = u_h(t_i) + k_i A u_h(t_i) + \frac{1}{2}k_i^2 u_h''(t_i) + \cdots$$

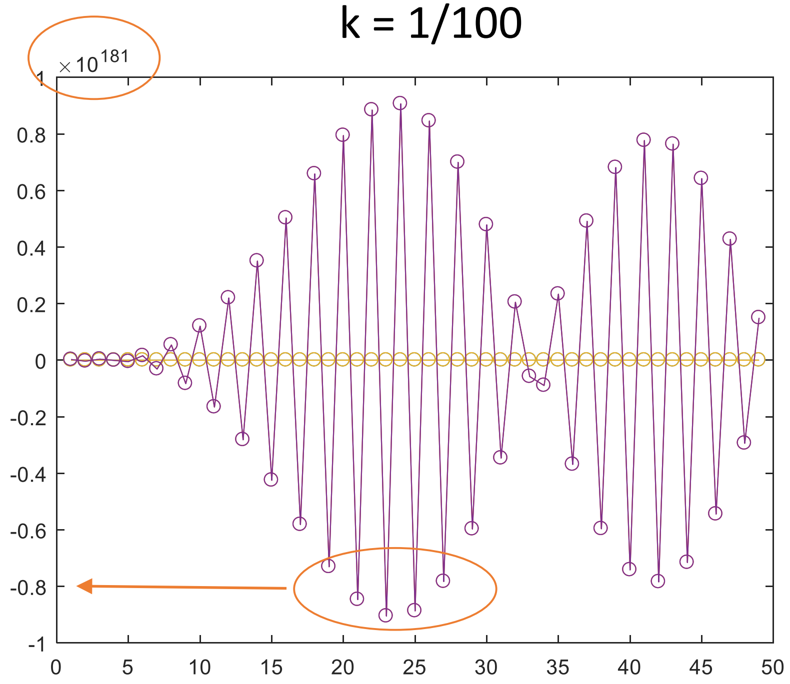
$$w_{i+1} = w_i + k_i A w_i = (I + k_i A) w_i$$

Explicit Euler method – the simplest of them all

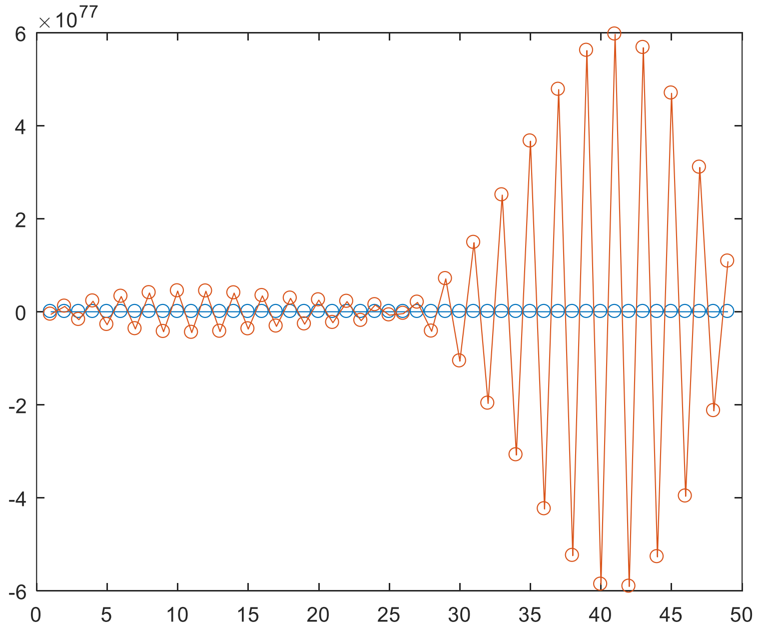
One-dimensional problem h = 1/50

Looks terribly unstable

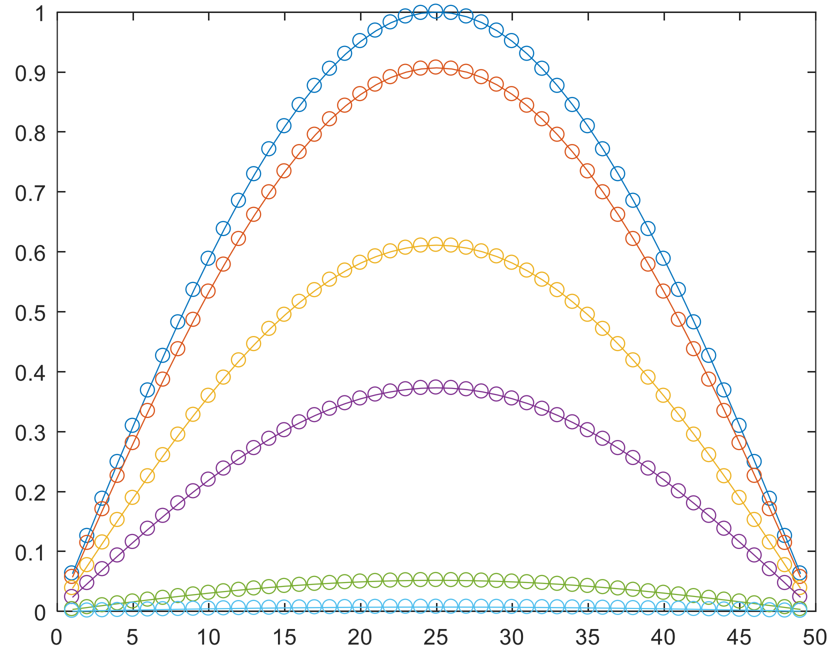
k = 1/100



k = 1/1000



k = 1/10000



Heat Equation: First Steps

- Explicit Euler $w_{i+1} = w_i + k_i A w_i = (I + k_i A) w_i$

The method is actually $w_{i+1} = (I + kA)^i w_0$

A has full set of eigenvectors, write $w_0 = \sum_j \alpha_j v_j$ ➡ $w_{i+1} = \sum_j \alpha_j (1 + k\lambda_j)^i v_j$

Gets unstable unless $|1 + k\lambda_j| < 1 \quad \forall j$ Doable, but maximal |λ| grows as $O(h^{-2})$ → impractical

Heat Equation: Next Steps

- Explicit Euler was rather bad
- Will higher order methods help?

$$u_h(t_{i+1}) = u_h(t_i) + k_i u_h'(t_i) + \frac{1}{2}k_i^2 u_h''(t_i) + \cdots + \frac{1}{n!}k_i^n u_h^{(n)}(t_i) + \cdots$$

$$\Rightarrow \quad w_{i+1} = (I + k_i A + \frac{1}{2}k_i^2 A^2 + \cdots + \frac{1}{n!}k_i^n A^{(n)})w_i$$

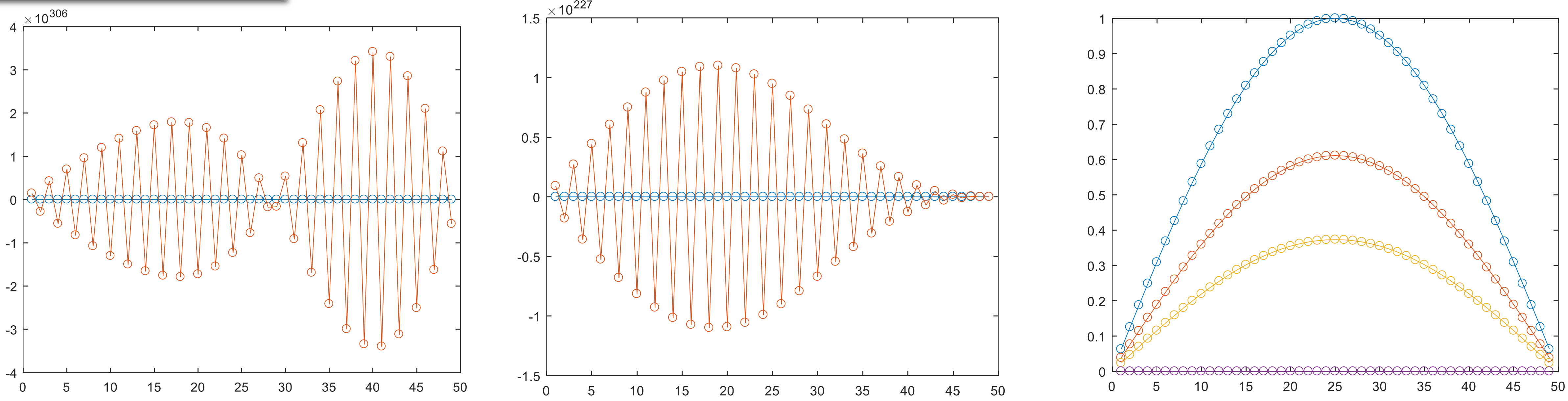
Taylor method of order *n*

Story remains the same

k = 1/100

k = 1/1000

k = 1/10000



Heat Equation: Taylor Methods

- Stability analysis leads to

$$w_{i+1} = (I + k_i A + \frac{1}{2}k_i^2 A^2 + \cdots + \frac{1}{n!}k_i^n A^{(n)})w_i$$

$$w_0 = \sum_j \alpha_j v_j \quad \Rightarrow \quad w_{j+1} = \sum_j \alpha_j (1 + k\lambda_j + \frac{1}{2}k^2\lambda_j^2 + \cdots + \frac{1}{n!}k^n\lambda_j^n)^i v_j$$

This would require $|1 + k\lambda_j + \frac{1}{2}k^2\lambda_j^2 + \cdots + \frac{1}{n!}k^n\lambda_j^n| < 1$

Not going to happen any more easily than for explicit Euler

$\boxed{\text{Hence, it is not a question of accuracy but a question of stability}}$

Side-step: Runge-Kutta Methods

This is a side-step since none of these methods solves the stability problem

- If the problem is not linear: $\frac{\partial u}{\partial t} = f(t,u)$
  - ➢ the higher-order derivates are not known in

$$u_h(t_{i+1}) = u_h(t_i) + k_i u_h'(t_i) + \frac{1}{2}k_i^2 u_h''(t_i) + \cdots + \frac{1}{n!}k_i^n u_h^{(n)}(t_i) + \cdots$$

Try to get w at $t + \delta_2$

$$\Rightarrow \frac{w_{i+1} - w_i}{k_i} = u_h'(t_i) + \frac{1}{2}k_i u_h''(t_i) + \cdots + \frac{1}{n!}k_i^{n-1} u_h^{(n)}(t_i) \approx \boxed{a_1 f(t, w_i) + a_2 f(t + \alpha_2, w_i + \delta_2 f(t, w_i))}$$

Approximating the Taylor expansion with two evaluations of *f*

For consistency $\alpha_2 = \delta_2 \quad a_1 + a_2 = 1$

Modified Euler method (a_1=0, a_2=1, α_2=δ_2 = $k/2$)

$$\begin{cases} \tilde{w} = w_i + \frac{k}{2} f(t_i, w_i) \\ w_{i+1} = w_i + k f(t_i + k/2, \tilde{w}) \end{cases}$$

Heun method (a_1=a_2=½, α_2=δ_2 = k)

$$\begin{cases} \tilde{w} = w_i + k f(t_i, w_i) \\ w_{i+1} = w_i + \frac{k}{2}\left(f(t_i, w_i) + f(t_i + k, \tilde{w})\right) \end{cases}$$

$$\begin{cases} d_1 = k f(t_i, w_i) \\ d_2 = k f(t_i + k/2, w_i + d_1/2) \\ d_3 = k f(t_i + k/2, w_i + d_2/2) \\ d_4 = k f(t_i + k, w_i + d_3) \end{cases}$$

Using more terms in the expansion: Fourth-Order Runge-Kutta: $w_{i+1} = w_i + \frac{1}{6}(d_1 + 2d_2 + 2d_3 + d_4)$

Back to Heat Equation

- So far: Good methods but not for the heat equation
- Must try something else: Switch to integration

$$u_h'(t) = Au_h(t) \quad \Rightarrow \quad u_h(t_{i+1}) - u_h(t_i) = \int_{t_i}^{t_{i+1}} Au_h(t)\,dt = A\int_{t_i}^{t_{i+1}} u_h(t)\,dt$$

Multistep methods: Interpolate $u_h(t)$ in the interval using values

- Up-to t_i → Adams-Bashforth methods
- Up-to t_{i+1} → Adams-Moulton methods

Two-step Adams-Bashforth
$$u_h(t) \approx \frac{t-t_{i-1}}{t_i-t_{i-1}}w_i + \frac{t-t_i}{t_{i-1}-t_i}w_{i-1} \quad \Rightarrow \quad \frac{w_{i+1}-w_i}{k_i} = A\left(\frac{3}{2}w_i - \frac{1}{2}w_{i-1}\right)$$

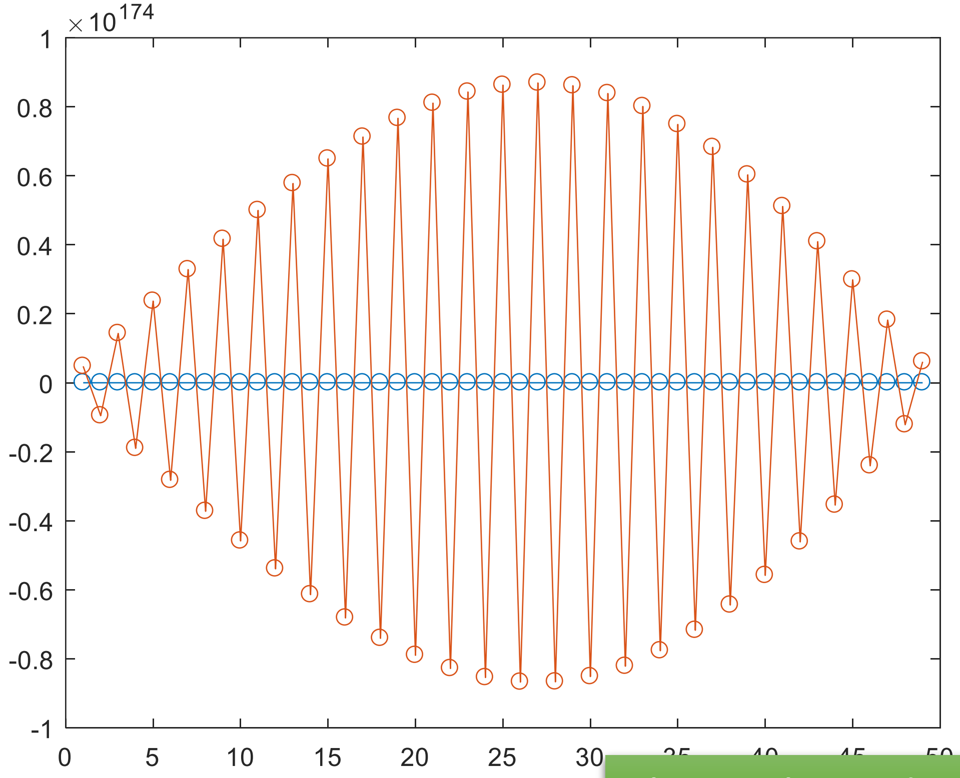
Two-step Adams-Moulton
$$u_h(t) \approx \frac{(t-t_i)(t-t_{i-1})}{(t_{i+1}-t_i)(t_{i+1}-t_{i-1})}w_{i+1} + \frac{(t-t_{i+1})(t-t_{i-1})}{(t_i-t_{i+1})(t_i-t_{i-1})}w_i + \frac{(t-t_{i+1})(t-t_i)}{(t_{i-1}-t_{i+1})(t_{i-1}-t_i)}w_{i-1}$$

$$\Rightarrow \quad \frac{w_{i+1}-w_i}{k_i} = A\left(\frac{5}{12}w_{i+1} + \frac{2}{3}w_i - \frac{1}{12}w_{i-1}\right)$$

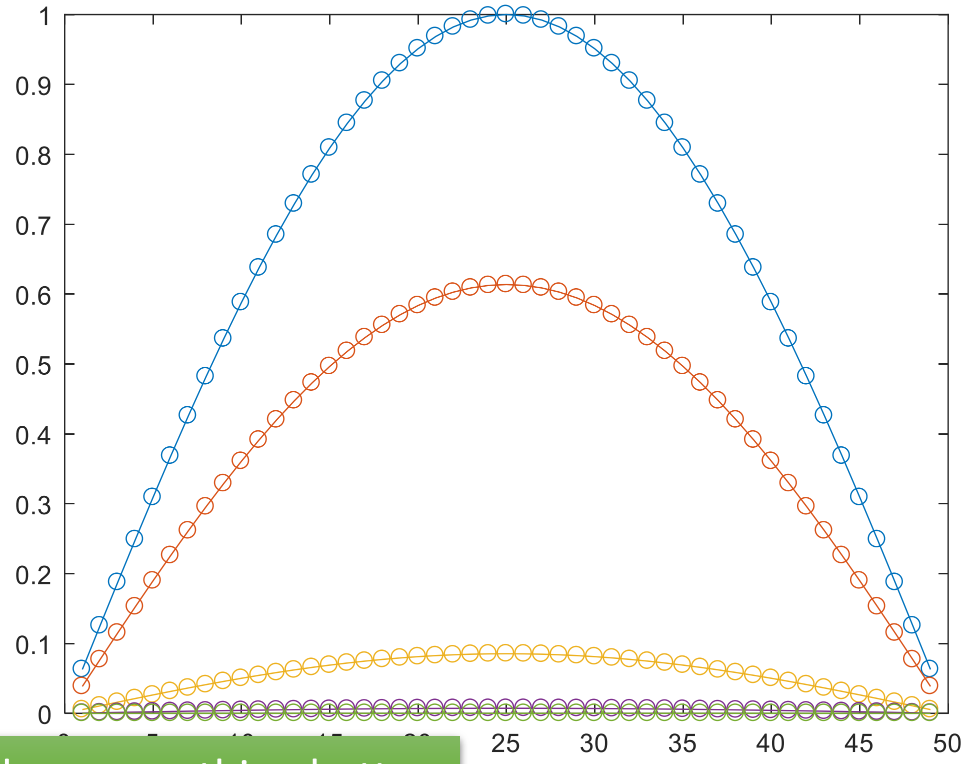
Need initial values from some other method

Heat Equation: Multistep methods

Adams-Bashforth, k = 1/5000



Adams-Moulton, k = 1/2000



The implicit Adams-Moulton clearly does something better

Discuss: Why would implicit method be better for heat equation?

Heat Equation: The Magic of Being Implicit

- Let's rewind a bit. The Euler method was: $w_{i+1} = w_i + k_i A w_i = (I + k_i A) w_i$
- This could be written also as $w_{i+1} = w_i + k_i A w_{i+1} \Rightarrow w_{i+1} = (I - k_i A)^{-1} w_i$

Implicit Euler method

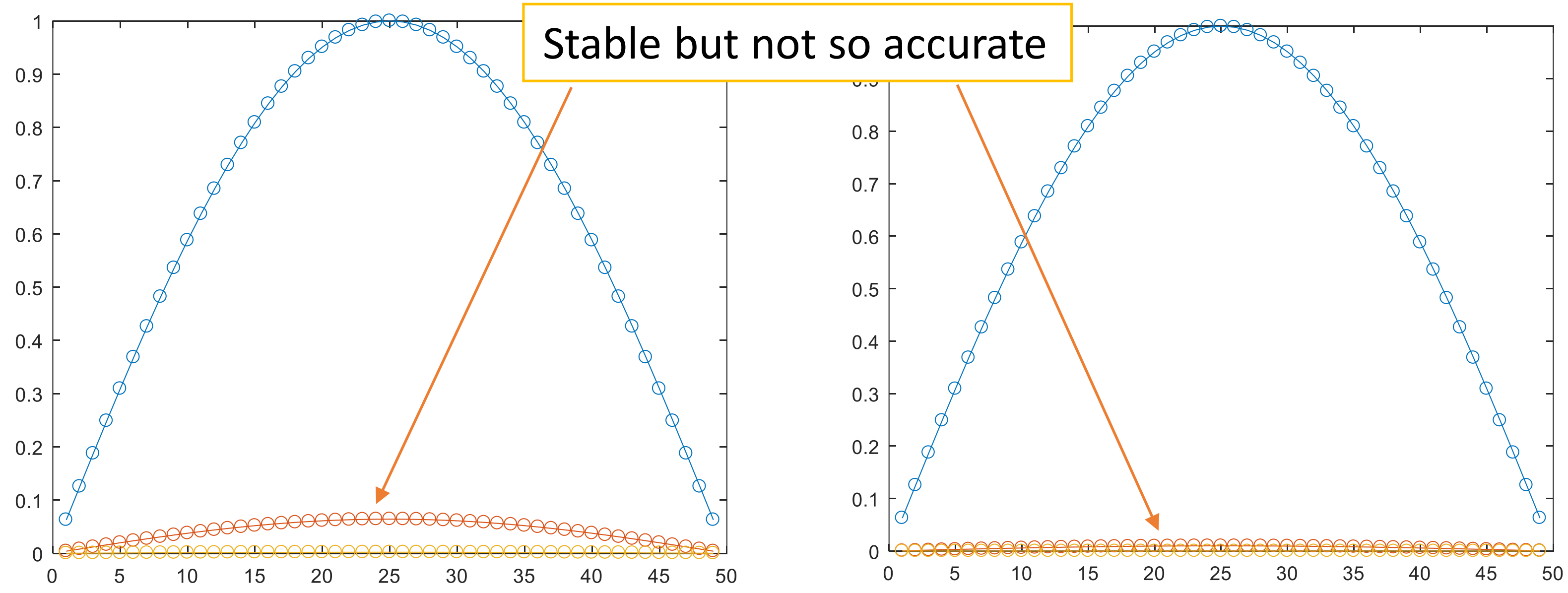
$$\begin{cases} w_{i+1} = (I - kA)^{-i} w_0 \\ w_{i+1} = \sum_j \alpha_j \frac{1}{(1 - k\lambda_j)^i} v_j \end{cases}$$

Stable if $\frac{1}{|1 - k\lambda_j|} < 1$

Since $\lambda_j < 0$, this is the case always

k = 1/10

k = 1/100



Heat Equation: Higher-Order and Implicit?

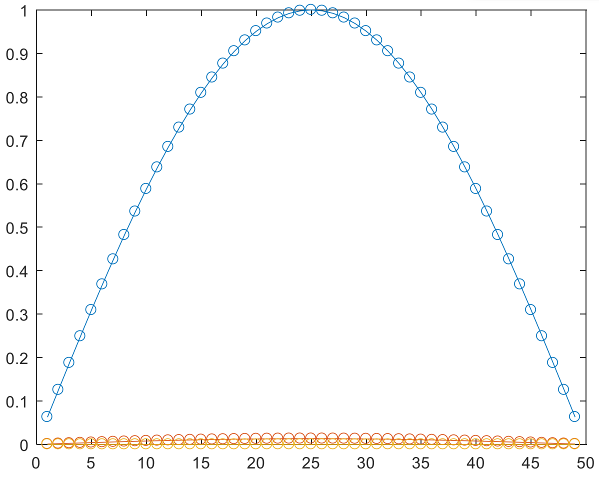
- Implict Euler is stable but its accuracy leaves room for improvement
- Let's rethink $u_h(t_{i+1}) - u_h(t_i) = A \int_{t_i}^{t_{i+1}} u_h(t)\,dt \approx A\frac{1}{2}\left(u_h(t_i) + u_h(t_{i+1})\right)$

$$\rightarrow \quad w_{i+1} = \left(I - \frac{1}{2}kA\right)^{-1}\left(I + \frac{1}{2}kA\right) w_i$$

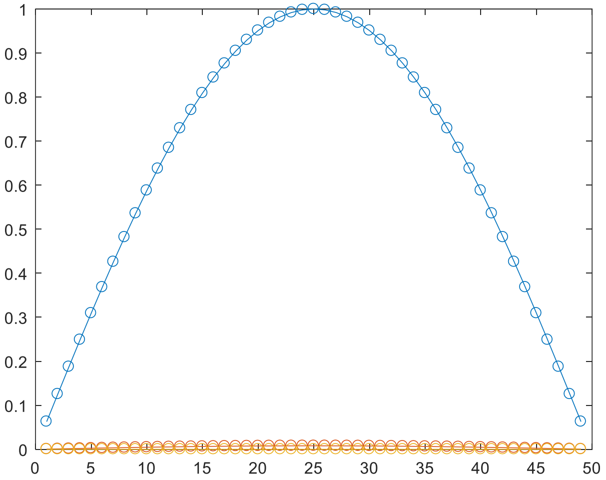
Crank-Nicolson method

k = 1/10

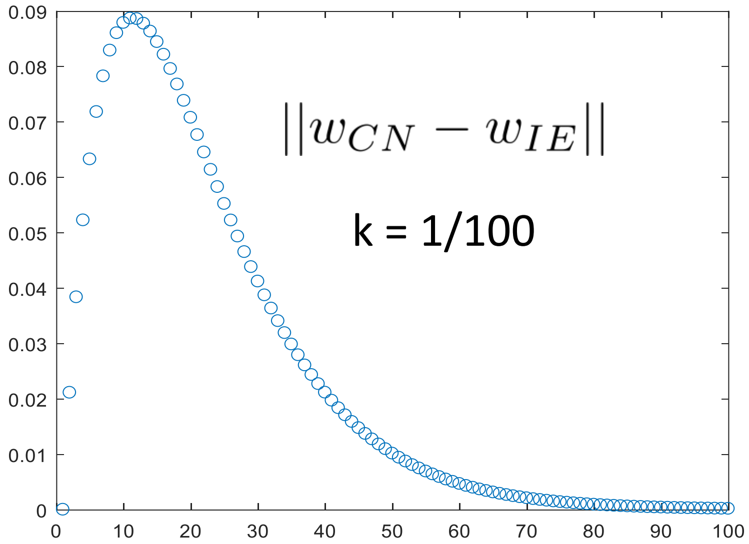
..is stable



k = 1/100



..and differs from implicit Euler



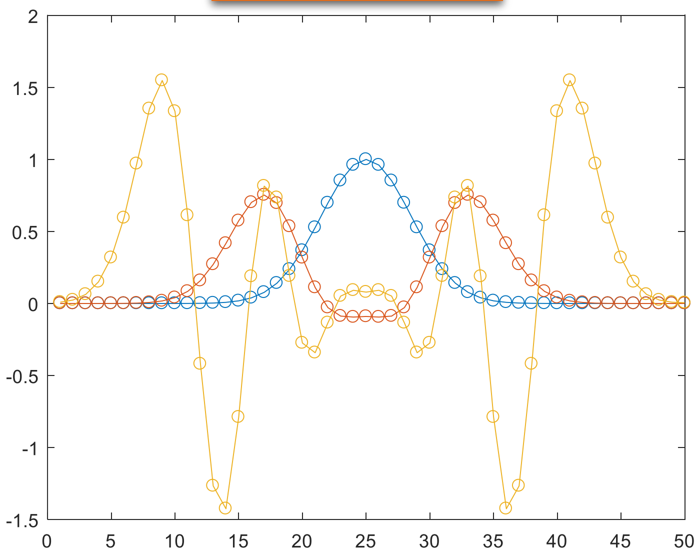
Another Case: Wave Equation

- First deal with $\frac{\partial^2 u_h}{\partial t^2} = A u_h$
- Set $v_h = \frac{\partial u_h}{\partial t}$ $\Rightarrow$ $\begin{pmatrix} \frac{\partial u_h}{\partial t} \\ \frac{\partial v_h}{\partial t} \end{pmatrix} = \begin{pmatrix} v_h \\ A u_h \end{pmatrix} = \begin{pmatrix} 0 & I \\ A & 0 \end{pmatrix} \begin{pmatrix} u_h \\ v_h \end{pmatrix}$

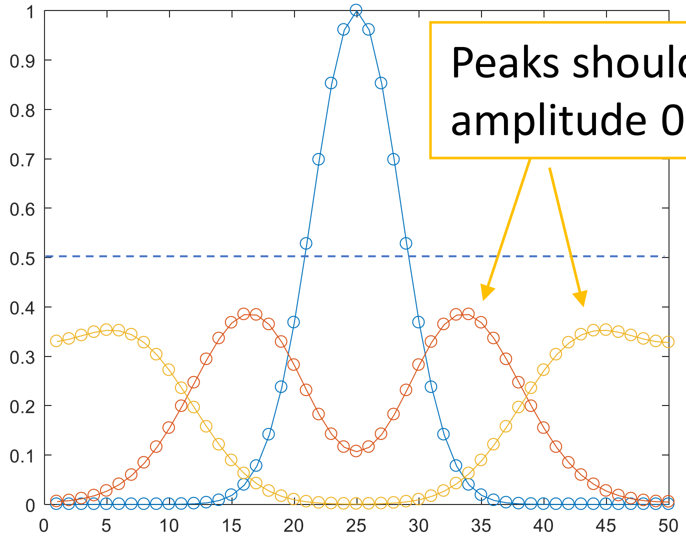
All algorithms for the heat equation are available for testing but now eigenvalues are complex $\mu_j = \pm i\sqrt{-\lambda_j}$

Test with periodic boundary conditions, $u_0(x) = \exp\left(-100(x - L/2)^2\right)$ $v_0(x) = 0$

Explicit Euler

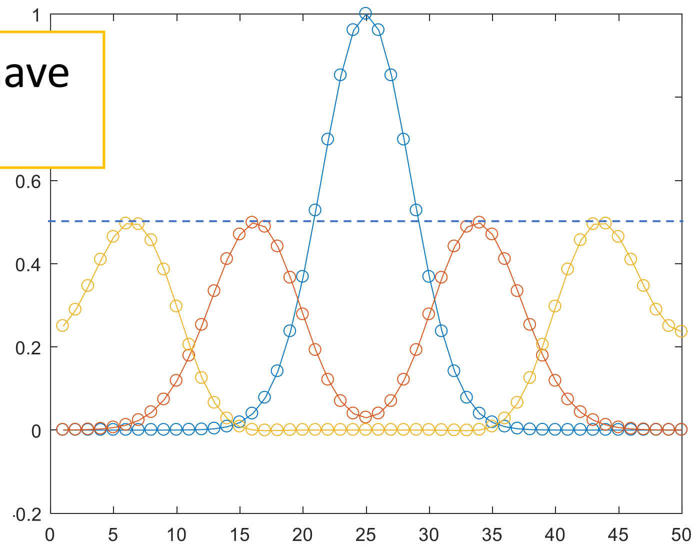


Implicit Euler



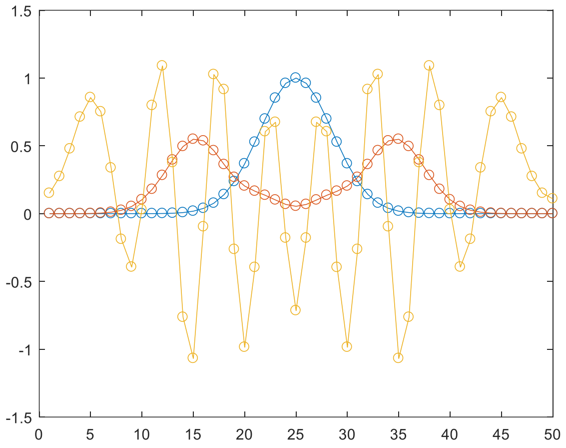
Peaks should have amplitude 0.5

Crank-Nicolson

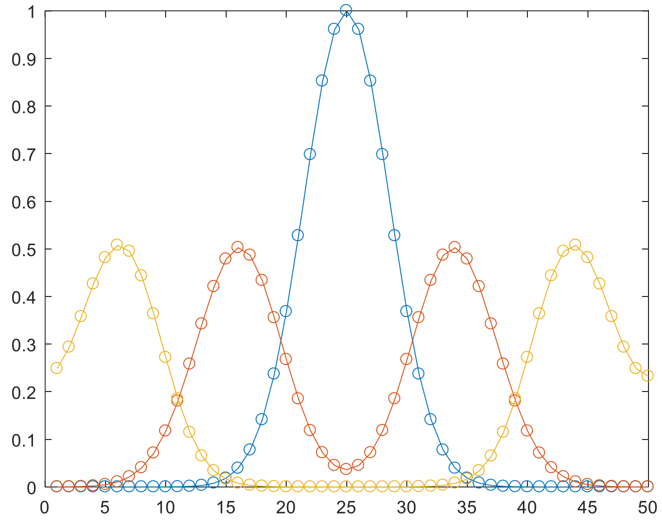


Wave Equation

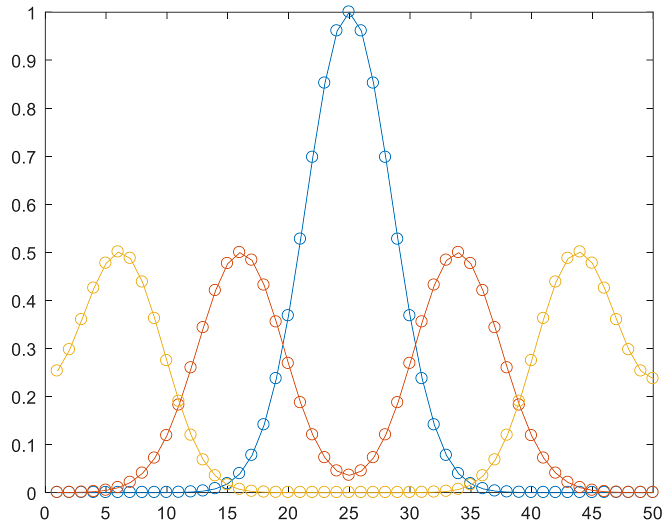
Adams-Bashforth



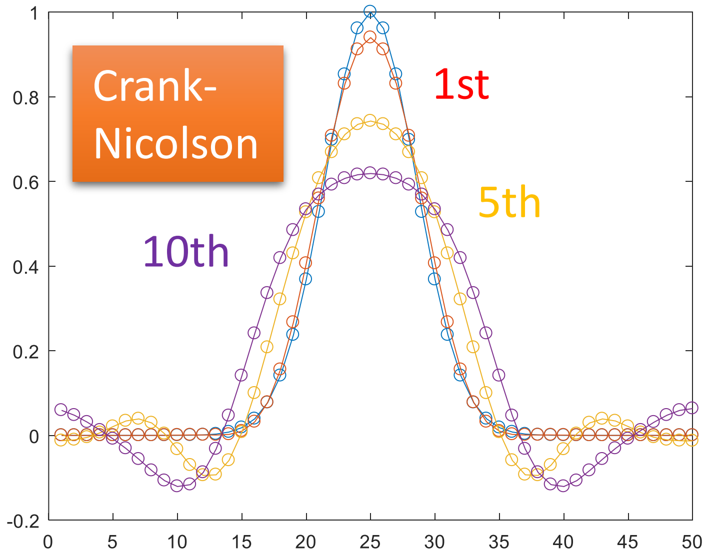
Adams-Moulton

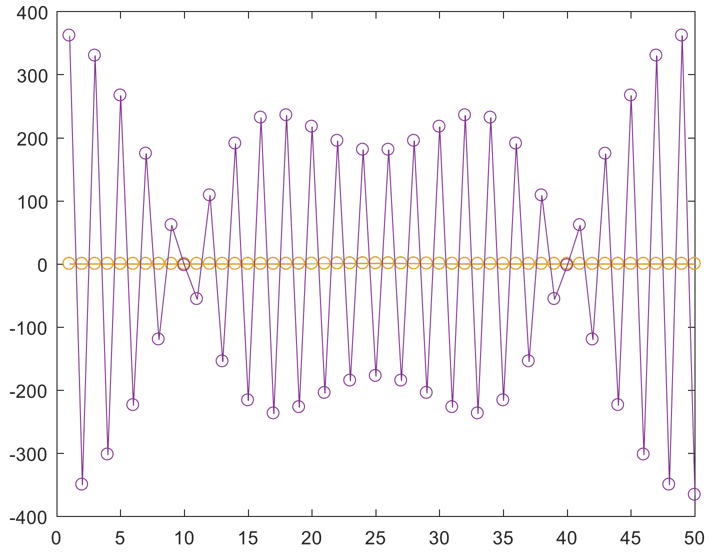


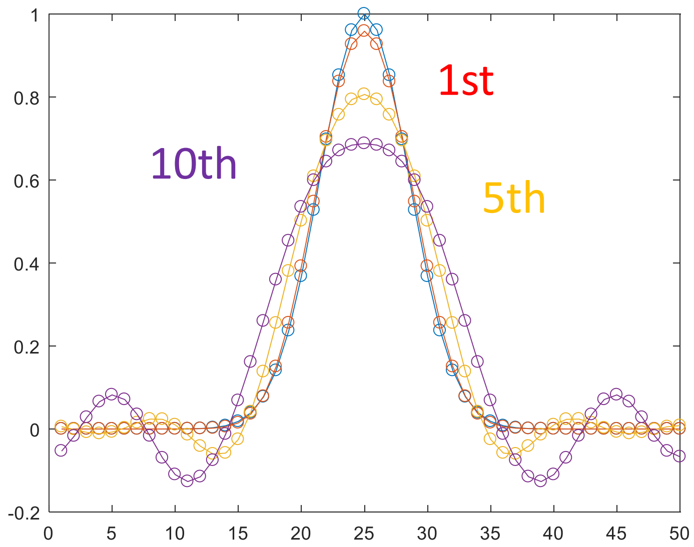
Taylor of order 4



Over a longer period of time







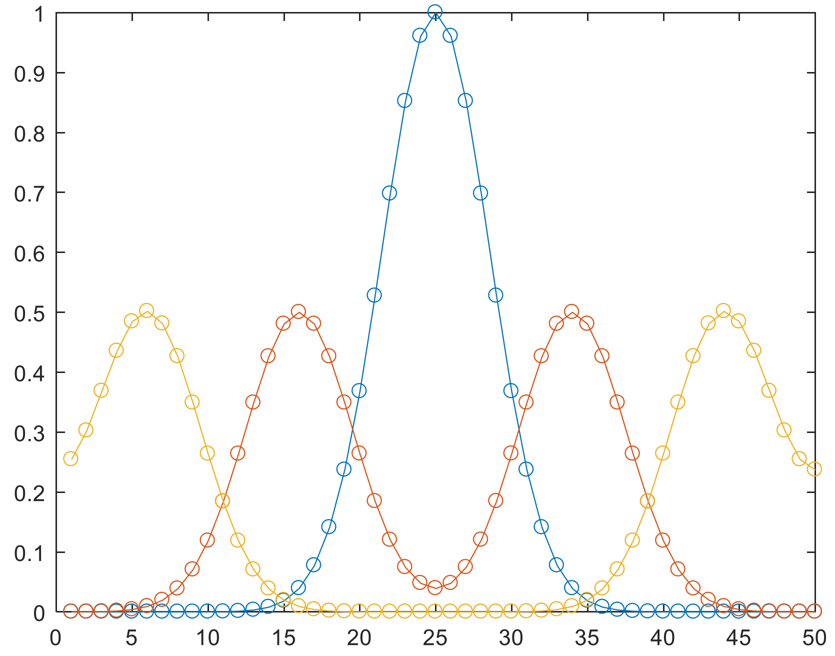
Wave Equation: Symmetric Discretization

- Since the time derivative is also of order 2 in the wave equation we can try:

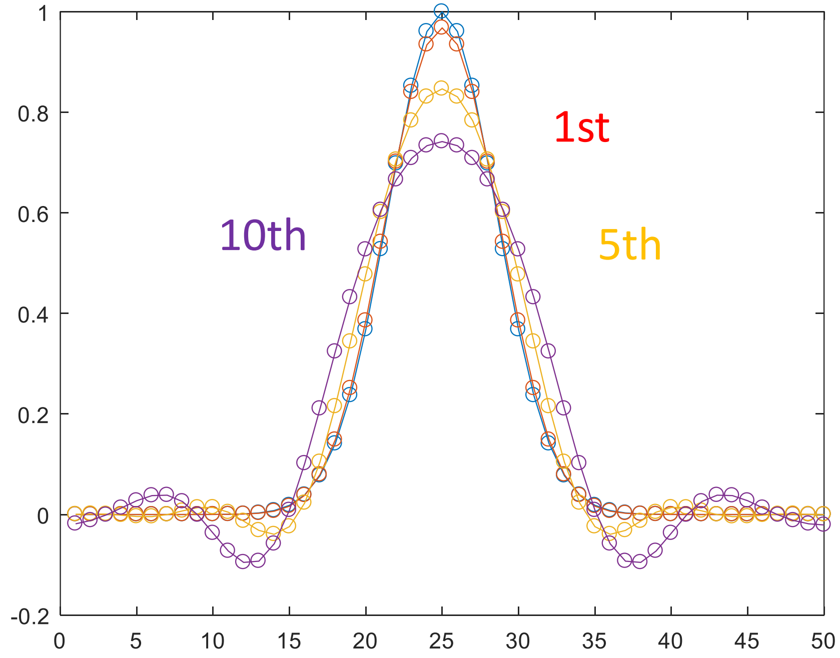
$$\frac{\partial^2 u_h}{\partial t^2} \approx \frac{w_{j+1} - 2w_j + w_{j-1}}{k^2} \quad \Rightarrow \quad w_{j+1} = 2w_j + k^2 A w_j - w_{j-1}$$

(need also w_{-1} from the initial condition)

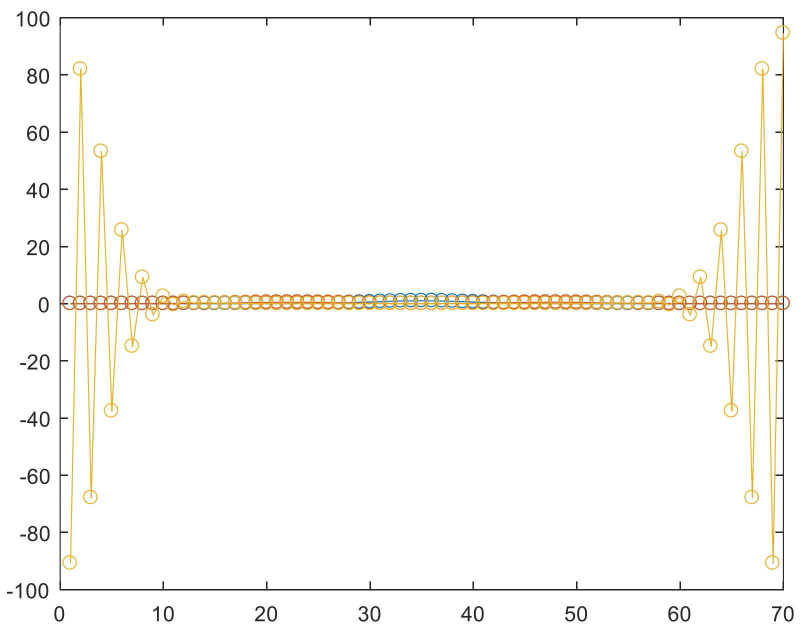
Peak splits nicely



Dispersion is manageable

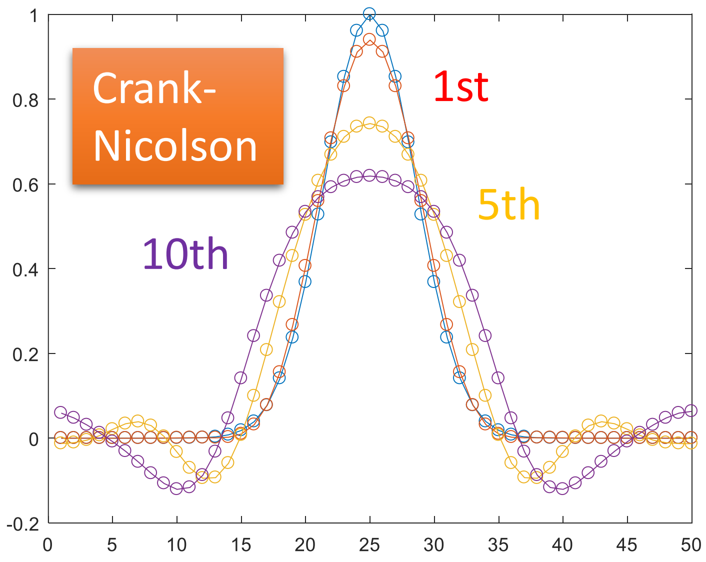


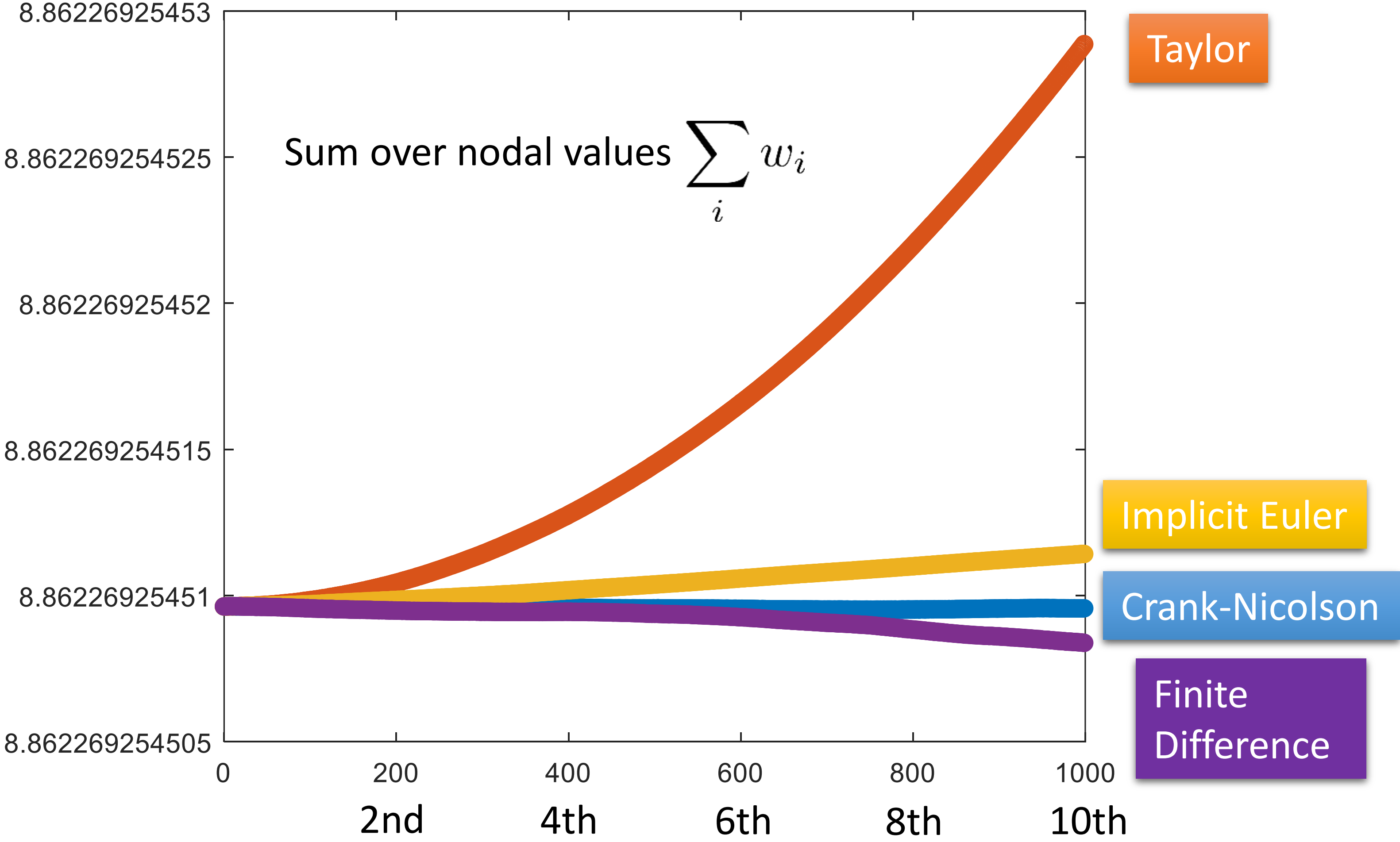
But stability is a risk, here h = 1/70, k = 1/50



Wave Equation: Dispersion

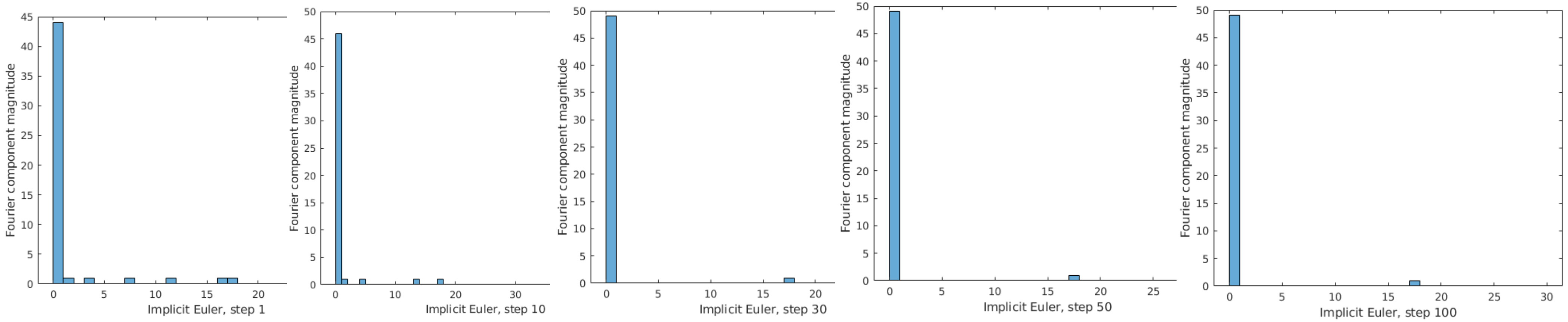
- Change in the shape of the peak is actually dispersion, not so much inaccuracy



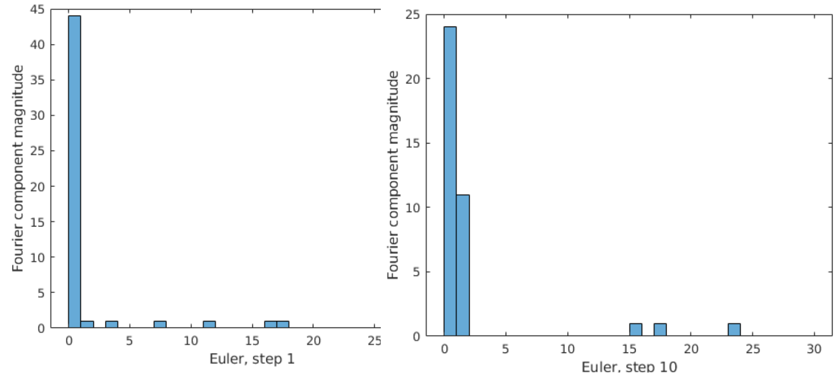


Discuss: What are the sources of dispersion?

Wave Equation: Dispersion via Fourier Analysis

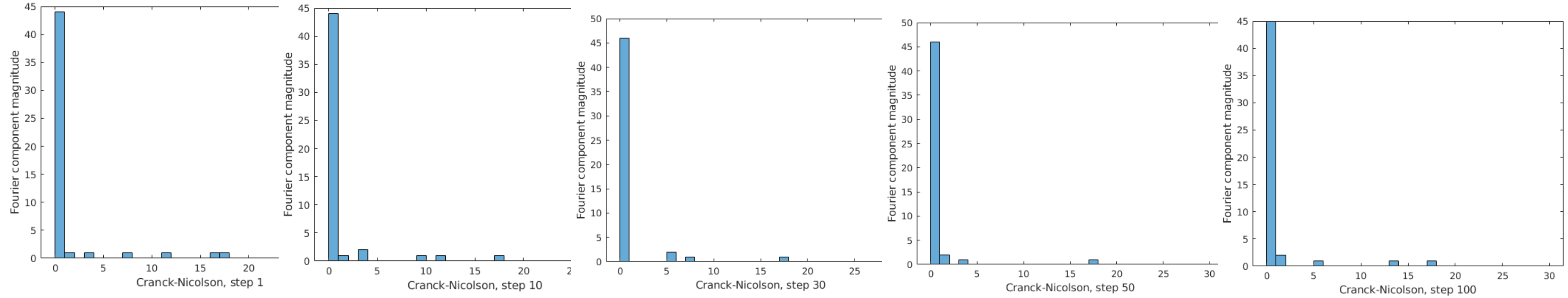


Implicit Euler



Euler

Discrete Fourier transforms of the waveforms



Crank-Nicolson

Homework 11

Can You Turn Back Time?

a) Consider first the one-dimensional heat equation with Dirichlet boundary conditions:

$$\begin{cases} \frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}u(x,t), \quad x \in [0,1],\, t > 0 \\ u(0,t) = u(1,t) = 0,\; u(x,0) = u_0(x) = 1.831\exp\left(-10(x-0.5)^2\right) \end{cases}$$

Choose a suitable discretization for the spatial part (FD or FEM will do fine) and implement implicit Euler and Crank-Nicolson time-integration schemes. Integrate up-to the time $t_f = 0.1$. Then reverse the flow of time and integrate back to $t_0 = 0$. Does either of the methods return to $u_0(x)$?

b) Consider next the one-dimensional wave equation with periodic boundary conditions

$$\begin{cases} \frac{\partial^2}{\partial t^2}u(x,t) = \frac{\partial^2}{\partial x^2}u(x,t), \quad x \in [0,1],\, t > 0 \\ u(0,t) = u(1,t),\; u(x,0) = u_0(x) = 1.831\exp\left(-10(x-0.5)^2\right) \end{cases}$$

Using suitable spatial discretization integrate up-to $t_f = 0.2$ using both implicit Euler and Crank-Nicolson methods. Then reverse the flow of time. What do you get at $t_0 = 0$? (2 p.)

A Slide on Convergence

- Suppose our method is ϕ: $w_i = \phi(A, k, w_{i-1}, w_{i-2}, \ldots)$
- The exact solution to this interval is $u(t_i) = e^{kA} u(t_{i-1})$
- The error is then $e_i = w_i - u(t_i) = \phi(A, k, w_{i-1}, w_{i-2}, \ldots) - e^{kA} u(t_{i-1})$

$$= \phi(A, k, w_{i-1}, w_{i-2}, \ldots) - e^{kA} w_{i-1} + e^{kA} w_{i-1} - e^{kA} u(t_{i-1})$$

$$= \phi(A, k, w_{i-1}, w_{i-2}, \ldots) - e^{kA} w_{i-1} + e^{kA} e_{i-1}$$

$$= \tau_i + e^{kA} e_{i-1}$$

Local truncation error

Error that propagates through the equation

The method has actually only effect on τ_i, the propagation of the error is done by the equation

- Heat equation dampens everything and masks all the previous errors
- Wave equation forgets nothing

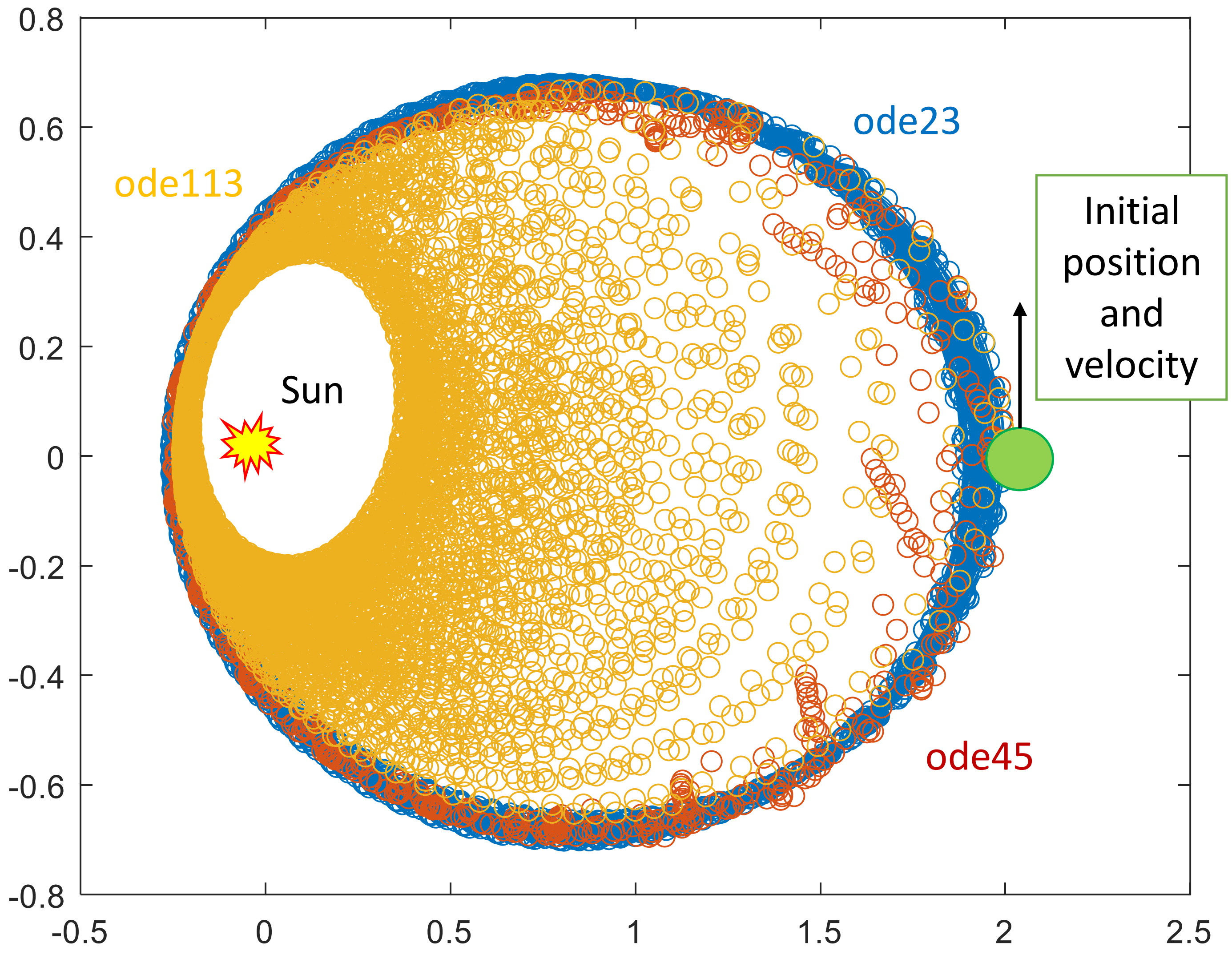
One More Thing: Planetary Motion

Newton's law of motion

$$m\ddot{\vec{r}} = -\gamma \frac{Mm}{r^2}\hat{r}$$

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} u \\ v \\ -\gamma \frac{M}{(x^2+y^2)^{3/2}} x \\ -\gamma \frac{M}{(x^2+y^2)^{3/2}} y \end{pmatrix}$$

Something is not right. The solution is
- ✓ Stable
- ✓ Locally accurate
- ❖ But useless in the long term



This is because none of the methods conserve invariants of the planetary motion. Need special methods

Wrap-up: Solution of Time-Dependent Problems

- Lessons learned:
  - Opposed to ellipitic PDEs, no single solution available
  - Must consider at each case
    - ✓ Stability
    - ✓ Accuracy
    - ✓ Conservation of invariants

  - This reflects the fact that time-dependent equations have a large variety of characteristics (parabolic, hyperbolic,…)
- Still missing:
  - Adaptive time integration (can be done, benefits in some systems)
  - Basis functions in time (doable, no major gains)
  - Special cases, e.g. flow equations (need nonsymmetric methods also in space)