FUNDAMENTALS

OF

NUMERICAL ANALYSIS

The Equivalence Theorem

- Consider a linear partial differential equation

$$\mathcal{L}(\tilde{u}) = 0.$$

- Let L be the discrete version of the operator $\mathcal{L}$.

- Let $\widehat{u_j}$ be the exact solution of the difference equation

$$L(\hat{u}_j) = 0.$$

- The actual numerical solution of the difference equation is $u_j \neq \hat{u}_j$.

The Equivalence Theorem

- Under which conditions the exact solution of the difference equation $\widehat{u_j}$ is a good approximation of the exact solution of the PDE, $\tilde{u}$?
  If $\widehat{u_j} \to \tilde{u}$ as $\Delta t,\ \Delta x \to 0 \Rightarrow$ Approximation is *consistent*.

- Under which conditions the actual solution of the difference equation u_j is a good approximation of $\widehat{u_j}$?
  $||u_j - \widehat{u_j}|| < \infty$ as $\Delta t,\ \Delta x \to 0 \Rightarrow$ Approximation is *stable*.

- Under which conditions u_j is a good approximation of $\tilde{u}$?
  $u_j \to \tilde{u}$ as $\Delta t,\ \Delta x \to 0 \Rightarrow$ Approximation is *convergent*.

- How many grid points are required for the error to be small?
  $\Rightarrow$ Approximation is *accurate*.

Lax's Equivalence Theorem

If a numerical approximation of a well-posed linear initial value problem is both *consistent* and *stable*, its solution is also *convergent* to that of the initial value problem.

- To prove convergence of a numerical scheme applied to the solution of a given initial value problem, it is only necessary to prove the *consistency* and *stability*.

Model equations

- *Model equations* are linear equations that contain the important physical features of the governing equations of fluid flows.

- The hyperbolic model equation represents wave-like phenomena.

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0; \qquad u(x,0) = g(x) \quad u(0,t) = u_o(t)$$

- The parabolic model equation represents dissipative phenomena.

$$\frac{\partial u}{\partial t} = \nu\frac{\partial^2 u}{\partial x^2}; \qquad u(x,0) = g(x), \quad u(0,t) = u(L,t) = 0$$

- The elliptic model equation

$$A\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$

Consistency of finite difference schemes

- Consider the generic partial differential equation $\mathcal{L}(\tilde{u}) = 0$.

- Consider its finite-difference approximation $L(u) = 0$.

- One can write

$$L(u) = \mathcal{L}(\tilde{u}) + \text{Truncation error}.$$

- A finite difference scheme is said to be *consistent* if the truncation error approaches zero as Δt and Δx approach zero.

Consistency of finite difference schemes

- Consider the following finite difference approximation of the hyperbolic model equation:

$$L(u) = \frac{u_j^{n+1} - u_j^n}{\Delta t} + c\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0. \qquad (1)$$

- The truncation error can be found by Taylor series expansion:

$$\begin{cases} u_j^{n+1} &= u_j^n &+\Delta t\frac{\partial u_j^n}{\partial t} &+\frac{\Delta t^2}{2!}\frac{\partial^2 u_j^n}{\partial t^2} &+\frac{\Delta t^3}{3!}\frac{\partial^3 u_j^n}{\partial t^3} &+o(\Delta t^4) \\ u_{j+1}^n &= u_j^n &+\Delta x\frac{\partial u_j^n}{\partial x} &+\frac{\Delta x^2}{2!}\frac{\partial^2 u_j^n}{\partial x^2} &+\frac{\Delta x^3}{3!}\frac{\partial^3 u_j^n}{\partial x^3} &+o(\Delta x^4) \\ u_{j-1}^n &= u_j^n &-\Delta x\frac{\partial u_j^n}{\partial x} &+\frac{\Delta x^2}{2!}\frac{\partial^2 u_j^n}{\partial x^2} &-\frac{\Delta x^3}{3!}\frac{\partial^3 u_j^n}{\partial x^3} &+o(\Delta x^4). \end{cases}$$

Consistency of finite difference schemes

- Substituting into (1) yields

$$\begin{aligned} L(u_j^n) &= \frac{\partial u_j^n}{\partial t} + c\frac{\partial u_j^n}{\partial x} + \frac{\Delta t}{2!}\frac{\partial^2 u_j^n}{\partial t^2} + c\frac{\Delta x^2}{3}\frac{\partial^3 u_j^n}{\partial x^3} + o(\Delta t^2, \Delta x^4) \\ &= \mathcal{L}(\tilde{u}_j^n) + \frac{\Delta t}{2!}\frac{\partial^2 u_j^n}{\partial t^2} + c\frac{\Delta x^2}{3}\frac{\partial^3 u_j^n}{\partial x^3} + o(\Delta t^2, \Delta x^4). \end{aligned}$$

- The truncation error is, therefore:

$$TE = \frac{\Delta t}{2!}\frac{\partial^2 u_j^n}{\partial t^2} + c\frac{\Delta x^2}{3}\frac{\partial^3 u_j^n}{\partial x^3} + o(\Delta t^2, \Delta x^4).$$

and approaches zero as Δt and Δx approach zero. The approximation (1) is, therefore, consistent with the hyperbolic model equation.

Consistency of finite difference schemes

- Consider the Dufort-Frankel scheme applied to the parabolic model equation.

- Write $\partial^2 u/\partial x^2 = (u^n_{j+1} - 2u^n_j + u^n_{j-1})/\Delta x^2$ and then apply the approximation $u^n_j = (u^{n+1}_j + u^{n-1}_j)/2$:

$$L(u^n_j) = \frac{u^{n+1}_j - u^{n-1}_j}{2\Delta t} - \nu \frac{u^n_{j+1} - u^{n+1}_j - u^{n-1}_j + u^n_{j-1}}{\Delta x^2}. \qquad (2)$$

- Taylor series expansions give

$$\begin{aligned}
u^n_{j+1} + u^n_{j-1} &= 2u^n_j + 2\frac{\Delta x^2}{2!}\frac{\partial^2 u^n_j}{\partial x^2} + 2\frac{\Delta x^4}{4!}\frac{\partial^4 u^n_j}{\partial x^4} + o(\Delta x^6), \\
u^{n+1}_j + u^{n-1}_j &= 2u^n_j + 2\frac{\Delta t^2}{2!}\frac{\partial^2 u^n_j}{\partial t^2} + 2\frac{\Delta t^4}{4!}\frac{\partial^4 u^n_j}{\partial t^4} + o(\Delta t^6), \\
u^{n+1}_j - u^{n-1}_j &= 2\Delta t\frac{\partial u^n_j}{\partial t} + \frac{\Delta t^3}{3!}\frac{\partial^3 u^n_j}{\partial t^3} + o(\Delta t^5).
\end{aligned}$$

Consistency of finite difference schemes

- These can be substituted into (2) yields

$$L(u_j^n) = \mathcal{L}(\tilde{u}_j^n) + \frac{\Delta t^2}{6}\frac{\partial^3 u_j^n}{\partial t^3} - \nu \frac{\Delta t^2}{\Delta x^2}\frac{\partial^2 u_j^n}{\partial t^2} + o(\Delta t^4/\Delta x^2, \Delta x^2, \ldots).$$

- If Δt and Δx approach zero in such a way that their ratio remains constant, the truncation error does not vanish.

- The Dufort-Frankel scheme, therefore, is inconsistent with the parabolic model equation.

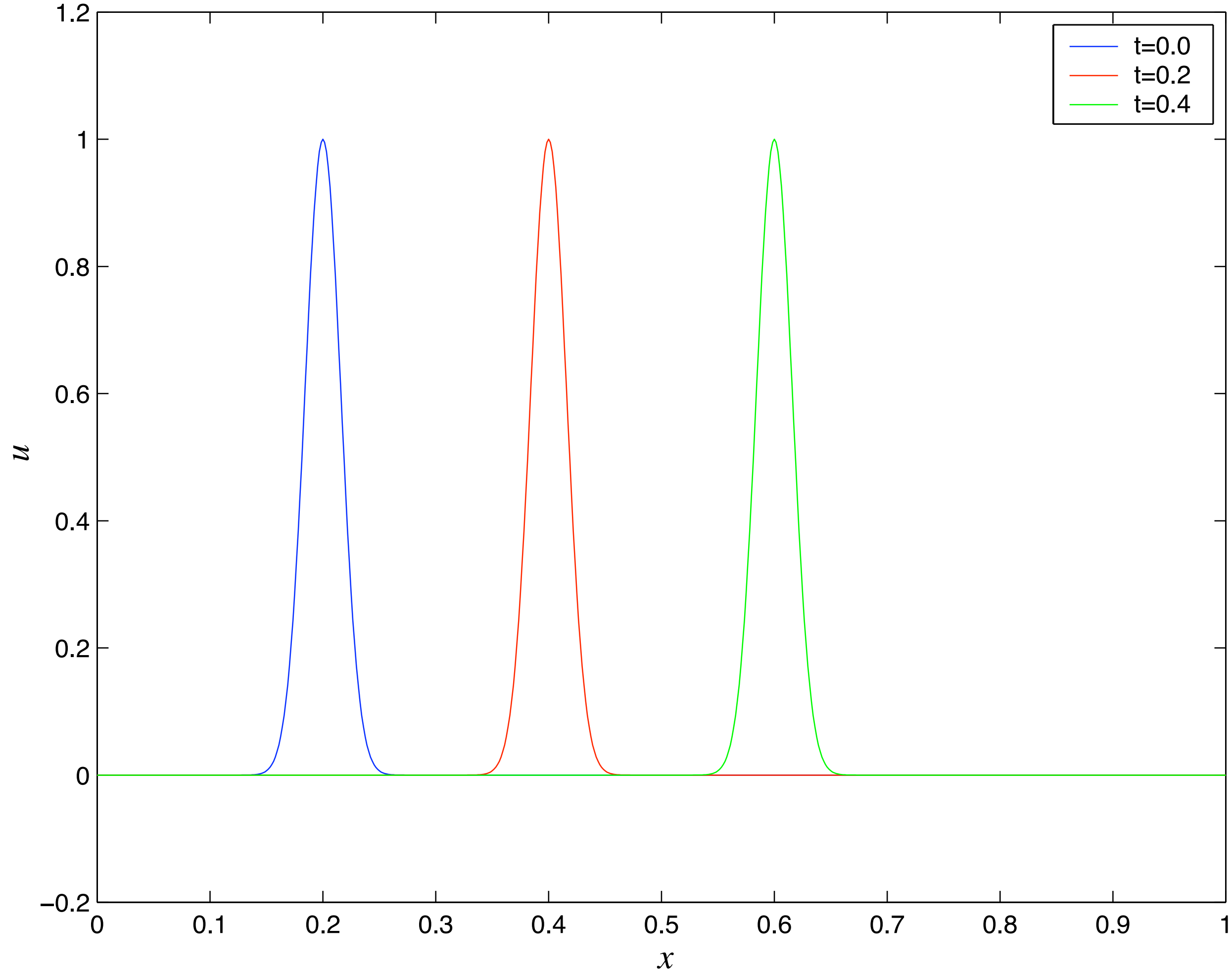
Equations in wave space

- Consider the inhomogeneous hyperbolic model equation

$$\frac{\partial \tilde{u}}{\partial t} + c\frac{\partial \tilde{u}}{\partial x} = f,$$

where $\tilde{u} = \tilde{u}(x,t)$, with homogeneous boundary conditions $\tilde{u}(0,t) = \tilde{u}(L,t) = 0$.

Equations in wave space



Solution of the hyperbolic model equation, $c > 0$.

Equations in wave space

- Define now a new dependent variable, $u_j(t)$, continuous in time but discrete in space [*i.e.*, $u_j(t) = \tilde{u}(x_j, t) = \tilde{u}(j\Delta x, t)$, and $\Delta x = L/(M+1)$. $j = 1, \ldots, M$ correspond to the inner points only].

Equations in wave space

- Replace then the spatial derivative with a finite-difference approximation

$$\frac{du_j}{dt} = -\frac{c}{2\Delta x}\Big(u_{j+1} - u_{j-1}\Big) + f_j \qquad \text{for} \quad j = 1, 2, \ldots, M.$$

- Inhomogeneous boundary conditions for the form $u(0,t) = a$, $u(L,t) = b$ can easily be cast in this form by modifying the right-hand side vector $\mathbf{f}$.

Equations in wave space

- This coupled set of ordinary differential equations (ODEs) can be expressed in matrix form as

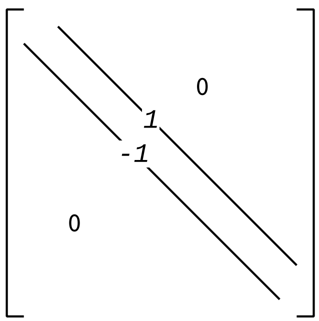
$$\frac{d\mathbf{u}}{dt} = A\mathbf{u} + \mathbf{f}, \tag{3}$$

where

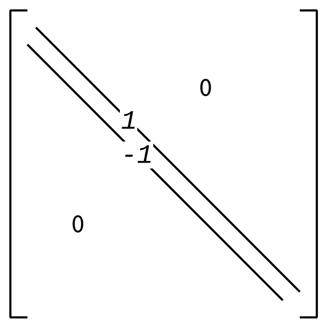
$$\begin{aligned}
\mathbf{u} &= (u_1, u_2, \ldots, u_m, \ldots, u_M)^T \\
A &= -\frac{c}{2\Delta x}\begin{pmatrix} 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -1 & 0 & 1 & \\ & & & \ddots & \ddots & \ddots \\ & & & & -1 & 0 \end{pmatrix} \\
\mathbf{f} &= (f_1, f_2, \ldots, f_m, \ldots, f_M)^T .
\end{aligned}$$

Equations in wave space

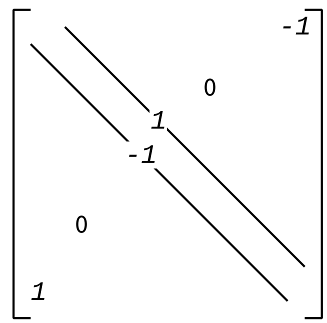
- Such a procedure can be applied to any model equation, set of boundary conditions, differencing scheme.
- For the hyperbolic model equation:

$A = -\frac{c}{2\Delta x}$ 

Central, Dirichlet

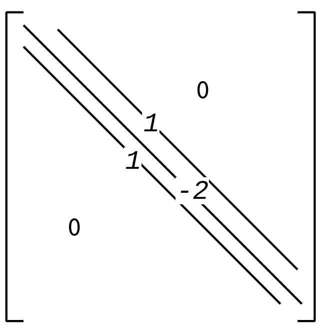
$A = -\frac{c}{\Delta x}$ 

Backwards, Dirichlet

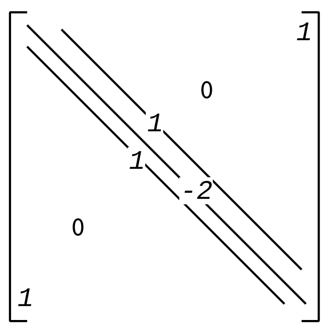
$A = -\frac{c}{2\Delta x}$ 

Central, Periodic

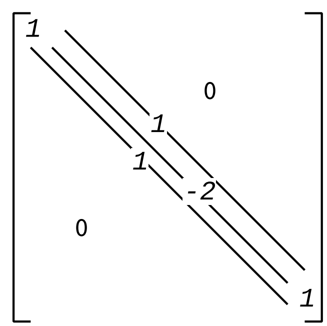
- For the parabolic model equation:

$A = \frac{\nu}{\Delta x^2}$ 

Central, Dirichlet

$A = \frac{\nu}{\Delta x^2}$ 

Central, Periodic

$A = \frac{\nu}{\Delta x^2}$ 

Central, Neuman

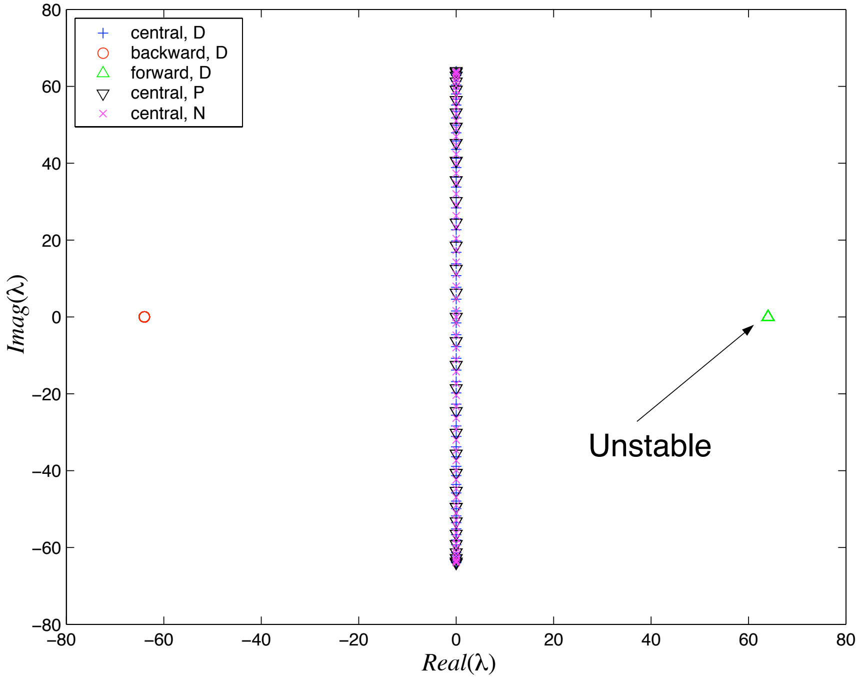
Equations in wave space

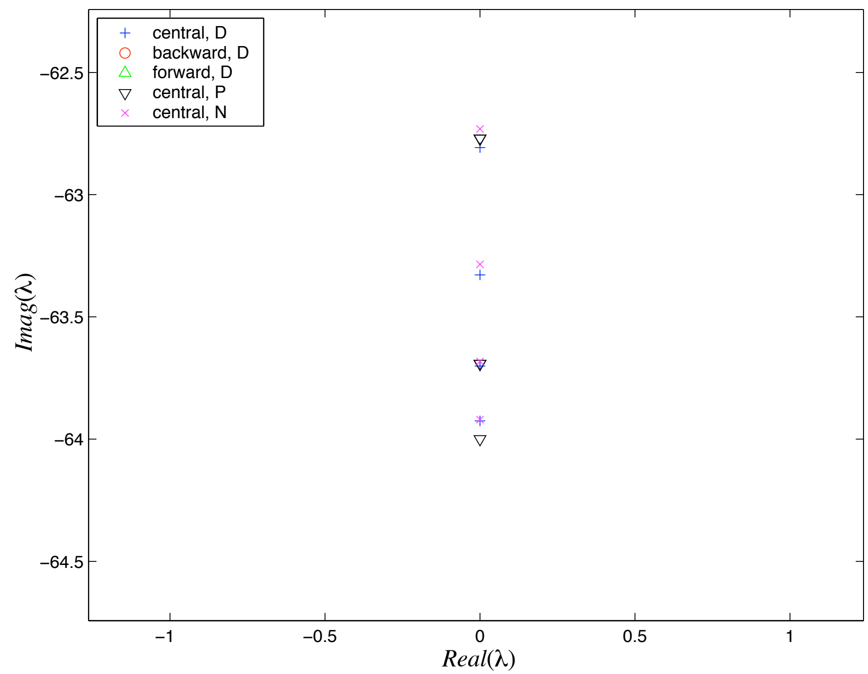
- Assuming that A is non-singular with a set of distinct eigenvalues and linearly independent eigenvectors, let $\mathbf{x_m}$ be the eigenvector associated with the m-th eigenvalue of the matrix A, λ_m:

$$A\mathbf{x_m} = \lambda_m \mathbf{x_m}.$$

- The system (3) is said to be *stable* if $Re(\lambda_m) \leq 0$ for all m.
  $\Rightarrow$ the model ODE has non-singular solutions.

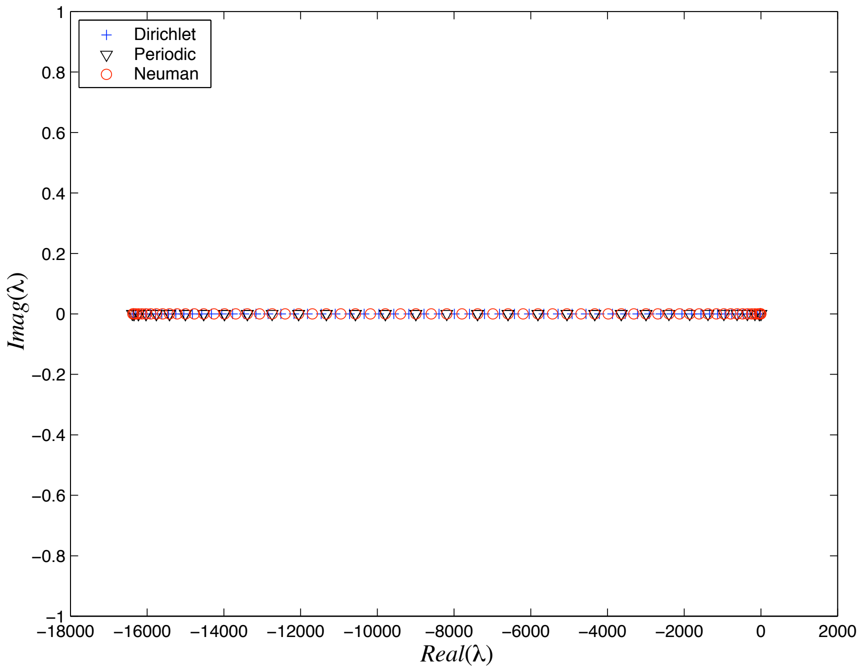
Equations in wave space

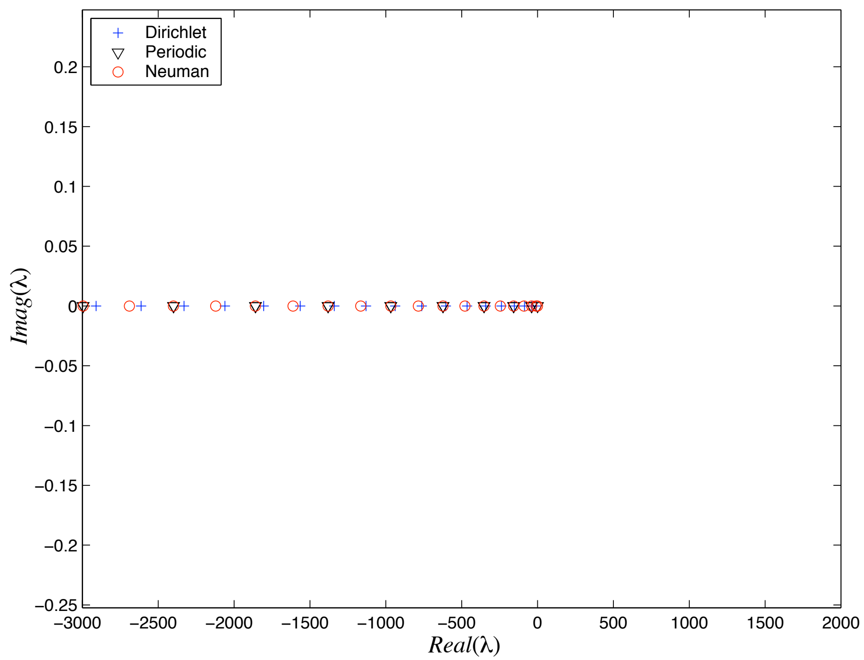




Eigenvalues of matrix A. Hyperbolic model equation.

Equations in wave space





Eigenvalues of matrix A. Parabolic model equation.

Equations in wave space

- Let X be the right-handed eigenvector matrix:

$$X = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{x_1} & \mathbf{x_2} & \ldots & \mathbf{x_m} & \ldots & \mathbf{x_M} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

- By definition, $X^{-1}AX = \Lambda$, where Λ is a matrix whose diagonal elements are the eigenvalues and the off-diagonal elements are zero.

Equations in wave space

- Multiplying(3) by X^{-1} we obtain

$$
\begin{aligned}
X^{-1}\frac{d\mathbf{u}}{dt} &= X^{-1}A\mathbf{u} + X^{-1}\mathbf{f}, \\
\frac{d}{dt}(X^{-1}\mathbf{u}) &= X^{-1}AX(X^{-1}\mathbf{u}) + X^{-1}\mathbf{f}, \\
\frac{d\mathbf{w}}{dt} &= \Lambda\mathbf{w} + \mathbf{g}, \qquad (4)
\end{aligned}
$$

  with $\mathbf{w} = X^{-1}\mathbf{u}$ and $\mathbf{g} = X^{-1}\mathbf{f}$.

- The two systems (3) and (4) are equivalent, but the latter is completely decoupled.

Equations in wave space

- The equation

$$\frac{d\mathbf{w}}{dt} = \Lambda\mathbf{w} + \mathrm{g}$$

can be written as a set of ODEs

$$\left\{ \begin{array}{rcl} dw_1/dt & = & \lambda_1 w_1 + g_1 \\ dw_2/dt & = & \lambda_2 w_2 + g_2 \\ \vdots & & \vdots \\ dw_m/dt & = & \lambda_m w_m + g_3 \\ \vdots & & \vdots \\ dw_M/dt & = & \lambda_M w_M + g_M, \end{array} \right.$$

each of which can be solved separately to yield

$$w_j = C_j e^{\lambda_j t} + PS_j,$$

where PS is a particular solution that depends on $\mathbf{g}$.

Equations in wave space

- The solution for u_i can then be reconstructed:

$$u_i = \sum_{j=1}^{M} x_{ij} w_j = \sum_{j=1}^{M} x_{ij} \left(C_j e^{\lambda_j t} + PS_j \right).$$

- If the ODEs are stable ($\lambda_j \leq 0$), the first term corresponds to a transient that vanishes with time, while the particular solution represents the steady-state condition of the system.

- The system of equations above is referred to as the *system of ODEs in wave space*.

The isolation theorem

- Applying any standard numerical scheme to each equation in a coupled set of ODEs with constant coefficients is mathematically equivalent to:

  1. Uncoupling the set (including the forcing term).
  2. Integrating each equation in the uncoupled set.
  3. Recoupling the result to form the final solution.

- Studying a time advancement method for any model equation can be reduced to studying the same time advancement method for a single ODE:

$$\frac{du}{dt} = \lambda u + a e^{\mu t}$$

  (λ, μ are complex scalars).

The isolation theorem

- Equation

$$\frac{du}{dt} = \lambda u + a e^{\mu t}$$

has an exact solution of the form

$$u(t) = \underbrace{C_1 e^{\lambda t}}_{\text{Homogeneous soln}} + \underbrace{\frac{a e^{\mu t}}{\mu - \lambda}}_{\text{Particular soln}} .$$

- Since

$$\begin{aligned} e^{\lambda t} &= e^{\lambda n \Delta t} = \left(e^{\lambda \Delta t}\right)^n \\ &= \left[1 + \lambda \Delta t + \frac{1}{2}(\lambda \Delta t)^2 + \frac{1}{6}(\lambda \Delta t)^3 + \ldots\right]^n, \end{aligned}$$

the solution can be recast in the form

$$u(t) = C_1 \left[1 + \lambda \Delta t + \frac{1}{2}(\lambda \Delta t)^2 + \frac{1}{6}(\lambda \Delta t)^3 + \ldots\right]^n + \frac{a e^{\mu t}}{\mu - \lambda}.$$

Accuracy of time-advancement schemes

The σ roots

- Applying a time-advancement scheme to

$$\frac{du}{dt} = \lambda u$$

results in a homogeneous difference equation:

$$\sum_{k=P}^{Q} A_{n+k} u^{n+k} = A_{n+P} u^{n+P} + \ldots + A_{n+Q} u^{n+Q} = 0.$$

where $u^n = u(n\Delta t)$ (n is the time-index).

- Introduce the operator E such that $E^k u^n = u^{n+k}$.

- The difference equation can then be rewritten as

$$\sum_{k=P}^{Q} A_{n+k} E^k u^n = \left[A_{n+P} E^P + \ldots + A_{n+Q} E^Q \right] u^n = 0$$

$$\Rightarrow P(E) u^n = 0$$

The σ roots

- The exact solution of $\sum_{k=P}^{Q} A_{n+k} E^k u^n = 0$ is

$$u^n = \sum_{k=1}^{Q-P} C_k \, (\sigma_k)^n,$$

where σ_k are the roots of the characteristic polynomial $P(\sigma) = 0$.

- The roots of the characteristic equation are called the *σ-roots*; For every eigenvalue λ there will be *at least* one σ-root.

- The σ-root that forms the approximation

$$\begin{aligned} \sigma \simeq e^{\lambda \Delta t} \; &= \; 1 + \lambda\Delta t + (\lambda\Delta t)^2/2! + (\lambda\Delta t)^3/3! + \ldots \\ &\quad + (\lambda\Delta t)^k/k! + \Delta t \; o\left(\Delta t^k\right) \end{aligned}$$

is called the principal root; the others are the spurious roots.

The σ roots

$$\frac{du}{dt} = \lambda u + a e^{\mu t} \quad \rightarrow \quad P(E)u^n = Q(E)ab^n,$$

$$\underbrace{u(t) = C_1 e^{\lambda t} + \frac{a e^{\mu t}}{\mu - \lambda};}_{\text{Exact solution}} \quad \rightarrow \quad \underbrace{u^n = \sum_{k=1}^{Q-P} C_k \left(\sigma_k\right)^n + ab^n \frac{Q(b)}{P(b)}.}_{\text{Numerical solution}}$$

- The error in the evaluation of the homogeneous and particular solutions is

$$\epsilon_\lambda = e^{\lambda \Delta t} - \sigma_1. \qquad \epsilon_\mu = \Delta t(\mu - \lambda)\left[\frac{PS_{num}}{PS_{ex}} - 1\right].$$

- The order of accuracy of a given time-advancement method is equal to the smallest order of the two errors defined above.

The σ roots – Explicit Euler example, part 1

- Apply the explicit Euler scheme to solve the homogeneous ODE

$$u' = \frac{du}{dt} = \lambda u.$$

- The explicit Euler scheme approximates the time derivative by a forward difference: $u'^n = (u^{n+1} - u^n)/\Delta t$.

- This gives

$$u^{n+1} = u^n + \lambda \Delta t u^n.$$

- Introduce the displacement operator E,

$$\underbrace{(E - 1 - \lambda \Delta t)}_{P(E)} u^n = 0.$$

The σ roots – Explicit Euler example, part 2

- Setting

$$P(\sigma) = \sigma - 1 - \lambda\Delta t = 0$$

we obtain the single root $\sigma = 1 + \lambda\Delta t$.

- Since

$$e^{\lambda\Delta t} = 1 + \lambda\Delta t + \Delta t \; o(\Delta t),$$

the error in the transient solution, ϵ_λ, is

$$\epsilon_\lambda = e^{\lambda\Delta t} - \sigma = \Delta t \; o(\Delta t).$$

The σ roots – MacCormack scheme (1)

- Consider a two-step scheme, MacCormack's predictor-corrector scheme:

$$\begin{cases} u^{n+1^*} &= u^n + \Delta t u'^n \\ u^{n+1} &= \frac{1}{2}\left[u^n + u^{n+1^*} + \Delta t \ (u^{n+1^*})'\right]. \end{cases}$$

- Introduce the representative equation:

$$\begin{cases} u^{n+1^*} &= u^n + \lambda \Delta t \ u^n + \Delta t \ a e^{\mu n \Delta t} \\ u^{n+1} &= \frac{1}{2}\left[u^n + u^{n+1^*} + \lambda \Delta t \ u^{n+1^*} + \Delta t \ a e^{\mu (n+1) \Delta t}\right]; \end{cases}$$

- Use the displacement operator E and collect terms

$$\begin{cases} E u^{n*} & -(1+\lambda\Delta t) u^n &= \Delta t \ a e^{\mu n \Delta t} \\ -\frac{1}{2}(1+\lambda \Delta t) E u^{n*} & + \left(E - \frac{1}{2}\right) u^n &= \frac{1}{2} E \Delta t \ a e^{\mu n \Delta t}. \end{cases}$$

The σ roots – MacCormack scheme (2)

- The characteristic polynomial is

$$
\begin{aligned}
P(E) &= \det \begin{bmatrix} E & -(1+\lambda\Delta t) \\ -(1+\lambda\Delta t)E/2 & E-1/2 \end{bmatrix} \\
&= E\left[E - 1 - \lambda\Delta t - (\lambda\Delta t)^2/2\right].
\end{aligned}
$$

- $Q(E)$ is given by

$$
\begin{aligned}
Q(E) &= \det \begin{bmatrix} E & \Delta t \\ -(1+\lambda\Delta t)E/2 & \frac{1}{2}\Delta t E \end{bmatrix} \\
&= E\left[E + 1 + \lambda\Delta t\right]\Delta t/2.
\end{aligned}
$$

- The σ-roots are:

$$
\sigma_1 = 1 + \lambda\Delta t + (\lambda\Delta t)^2/2 \quad ; \qquad \sigma_2 = 0.
$$

- The first root is the principal one, while the second one is trivial.

The σ roots – MacCormack scheme (3)

- The particular solution is

$$PS = ae^{\mu n \Delta t} \frac{\Delta t \left(e^{\mu \Delta t} + 1 + \lambda \Delta t \right) / 2}{e^{\mu \Delta t} - 1 - \lambda \Delta t - (\lambda \Delta t)^2 / 2}$$

- The errors are respectively

$$\epsilon_\lambda = (\lambda \Delta t)^3 / 6 = \Delta t \, o(\Delta t^2); \qquad \epsilon_\mu = (\mu - \lambda) \mu^2 \Delta t^3 = \Delta t \, o(\Delta t^2).$$

- The scheme is a one-root method of order Δt^2.

The σ roots – Leapfrog scheme (1)

- The leapfrog scheme is:

$$u^{n+1} = u^{n-1} + 2\Delta t \; u'^{n}.$$

- Introduce the displacement operator and the representative equation:

$$\left(E - \frac{1}{E} - 2\lambda\Delta t\right) u^n = 2\Delta t a \left(e^{\mu \Delta t}\right)^n,$$
$$P(E) = E^2 - 2\lambda\Delta t E - 1; \qquad Q(E) = 2\Delta t E.$$

- The roots of the characteristic polynomial are

$$\sigma = \lambda\Delta t \pm \sqrt{1 + (\lambda\Delta t)^2}.$$

- The principal and spurious roots can be found by expanding $[1 + (\lambda\Delta t)^2]^{1/2}$ in Taylor series:

$$\sigma = \lambda\Delta t \pm \left[1 + (\lambda\Delta t)^2/2 - (\lambda\Delta t)^4/8 + \ldots\right].$$

The σ roots – Leapfrog scheme (2)

- The σ-roots of the leapfrog scheme are given by

$$\begin{aligned}\sigma_1 &= 1 + \lambda\Delta t + (\lambda\Delta t)^2/2 - (\lambda\Delta t)^4/8 + \ldots,\\ \sigma_2 &= -1 + \lambda\Delta t - (\lambda\Delta t)^2/2 + (\lambda\Delta t)^4/8 + \ldots.\end{aligned}$$

- The leapfrog scheme is a two-root method.

- The principal root, σ_1, determines the order of accuracy of the scheme (second order).

- The spurious root does not affect the accuracy of the method, but only its stability.

- Schemes with multiple roots are not self-starting, and a different scheme is required to advance the solution for the first m steps, where m is the number of spurious roots.

Stability of time-advancement schemes

- Definitions:
  - An ODE is stable if $Re(\lambda_m) \leq 0$ for all m.
  - A numerical approximation is stable if the solution of the difference equations remains finite with time (i.e., if the error norm $||u(t) - u^n|| < \infty$).
- This requirement is satisfied if $|\sigma| \leq 1$ for all σ.
- σ depends on the eigenvalues of the spatial discretization matrix λ.
- To determine the stability of a numerical scheme one must consider the spatial discretization, the time advancement and the boundary condiions.

Stability of time-advancement schemes

Explicit Euler scheme

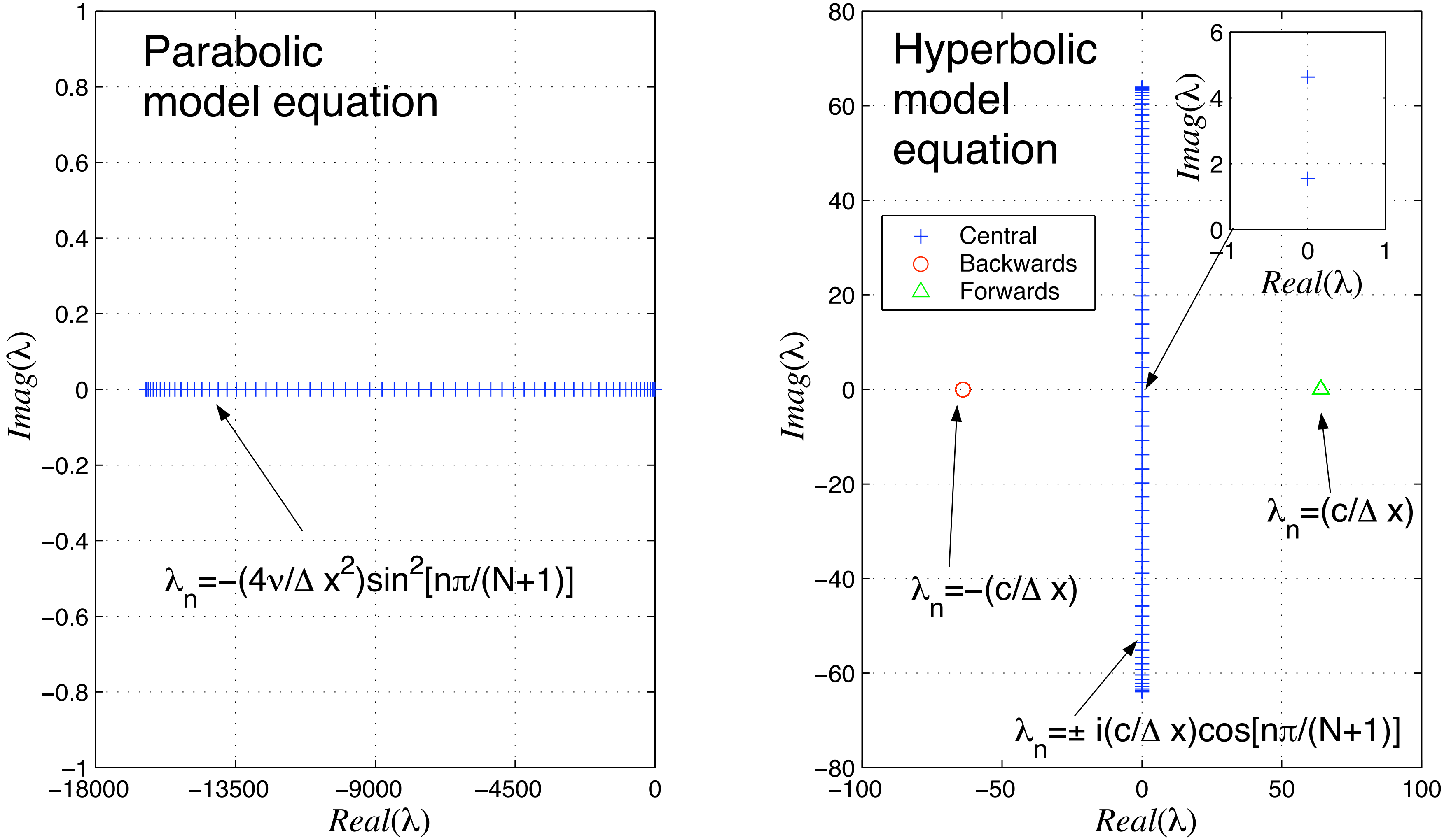
- The explicit Euler scheme is

$$\frac{u^{n+1} - u^n}{\Delta t} = \lambda u^n.$$

- Assume Homogeneous Dirichlet bcs.
- The σ root is $\sigma = 1 + \lambda \Delta t$.
- The scheme is stable if $|1 + \lambda \Delta t| \leq 1 \Rightarrow -1 \leq |1 + \lambda \Delta t| \leq 1$

Stability of time-advancement schemes

Explicit Euler scheme



Stability of time-advancement schemes

Explicit Euler scheme

- Parabolic model equation:
  - For central differences the eigenvalues are all real and negative. They are given by

$$\lambda_m = -\frac{4\nu}{\Delta x^2} \sin^2 \left[\frac{m\pi}{2(M+1)} \right].$$

  - $|1 + \lambda \Delta t| \leq 1$implies

$$-1 \leq 1 + \lambda_m \Delta t \leq 1 \qquad \text{for } m = 1, 2, \ldots, M.$$

  - The inequality on the right is satisfied trivially; the one on the left is satisfied if $|\lambda \Delta t| \leq 2$.
  - Since $\max(\sin x) \simeq 1$,

$$\Rightarrow \text{the scheme is stable if } \frac{\nu \Delta t}{\Delta x^2} \leq \frac{1}{2}.$$

Stability of time-advancement schemes
Explicit Euler scheme

- Hyperbolic model equation:
  - For central differences the eigenvalues are pure imaginary. They are given by
    $$\lambda_m = \pm i \frac{c}{\Delta x} \cos\left[\frac{m\pi}{M+1}\right].$$
    The σ-root becomes
    $$|\sigma| = |1 + \lambda \Delta t| = |1 + \lambda \Delta t = 1 + i\omega \Delta t| = \left[1 + (\omega \Delta t)^2\right]^{1/2} > 1.$$
    The scheme is unstable.
  - For forward differences, the eigenvalues are real and positive: $\lambda_m = c/\Delta x \Rightarrow |1 + \lambda \Delta t| > 1$. The scheme is unstable.
  - For backward differences, the eigenvalues are real and negative: $\lambda_m = -c/\Delta x \Rightarrow |1 + \lambda \Delta t| = |1 - c\Delta t/\Delta x|$. The scheme is stable if $\underbrace{c\Delta t/\Delta x}_{\text{CFL No.}} \leq 2$.

Explicit Euler scheme – Parabolic equation

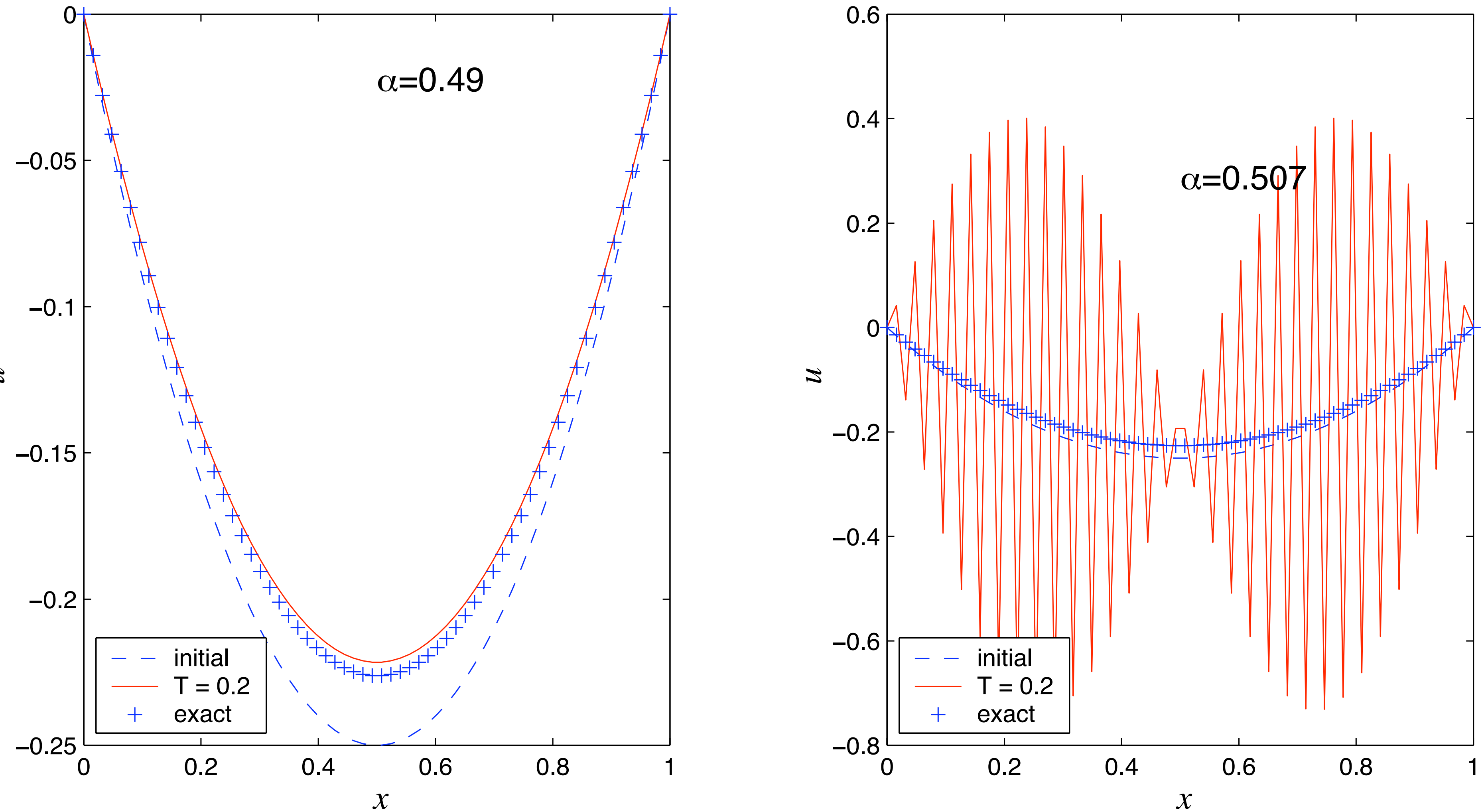
$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} + (-x^2 + x - 2)$$
$$u(0,t) = u(1,t) = 0; \qquad u(x,0) = x(1-x).$$

- Exact solution: $u_{ex}(x,t) = x(1-x)e^{-t}$.
- Choose $\nu = 0.001$, $J = 100$, $\Delta x = 1./J$.
- Discretized equation:

$$u_j^{n+1} \;=\; u_j^n - \nu \Delta t \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} + (-x_j^2 + x_j - 2)$$

- Choose $\nu \Delta t / \Delta x^2 = \alpha$, with $\alpha = 0.49$ (stable) and 0.507 (unstable).

Explicit Euler scheme – Parabolic equation



Explicit Euler scheme – Hyperbolic equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

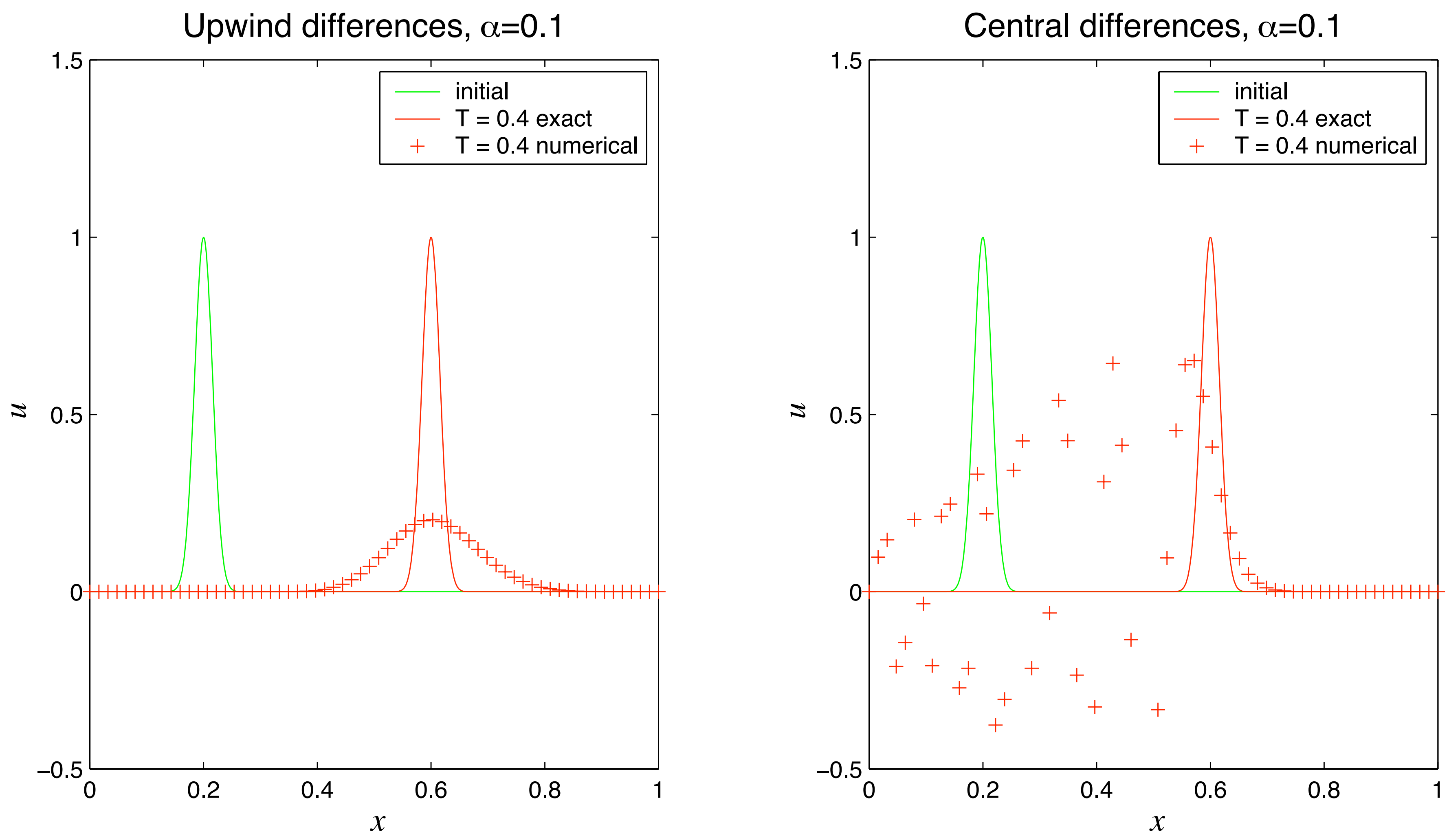
$$u(0,t) = e^{-A(-x_o-ct)^2}; \qquad u(x,0) = e^{-A(x-x_o)^2}.$$

- Exact solution: $u_{ex}(x,t) = e^{-A(x-x_o-ct)^2}$.
- Choose $x_o = 0.2$, $A = 2000$, $c = 1$.
- Discretized equation:

$$\begin{aligned} u_j^{n+1} &= u_j^n - \Delta t \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} \qquad \text{central} \\ u_j^{n+1} &= u_j^n - \Delta t \frac{u_j^n - u_{j-1}^n}{\Delta x} \qquad \text{upwind} \end{aligned}$$

- Choose $\Delta t = \alpha \Delta x$ (since $cu = 1$), with $\alpha = 1$.

Explicit Euler scheme – Hyperbolic equation



Stability of time-advancement schemes

- The same analysis can be applied to any numerical scheme, for any discretization and set of boundary conditions.

Stability of time-advancement schemes

Explicit and implicit schemes

- Explicit schemes are those in which the right-hand-side of the model equation is evaluated at previous times only (n, $n-1$ etc.)

- It can be shown that explicit schemes can at most be conditionally stable.

- In implicit schemes the RHS is also a function of u^{n+1}, and some form of matrix must be inverted to obtain the new solution.

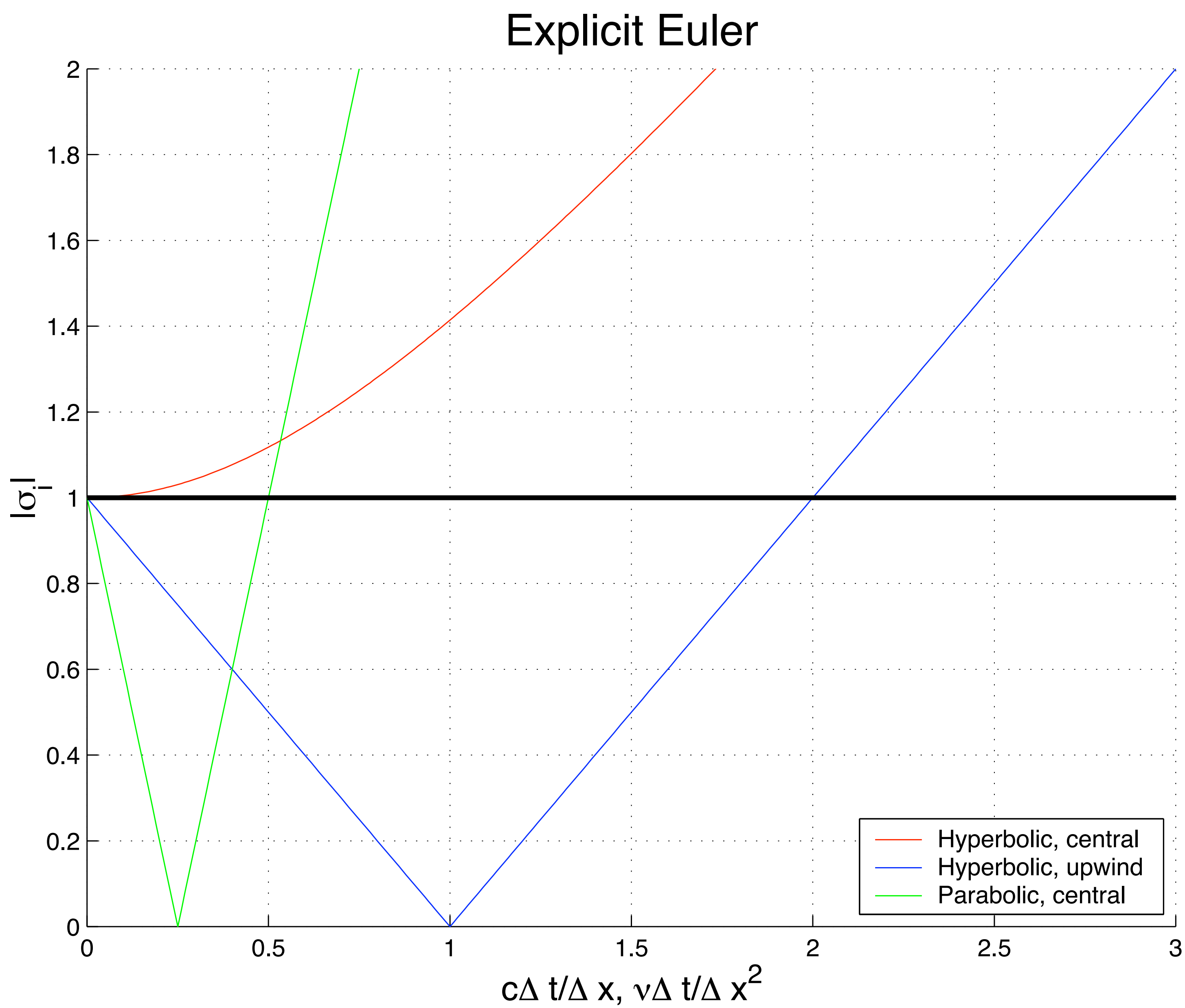
- Implicit schemes of second-order accuracy or less can be unconditionally stable.

Explicit Euler

- Explicit scheme given by

$$u^{n+1} = u^n + \Delta t u'^n, \qquad \text{where } u' = \lambda u$$

- The σ-root is $\sigma = 1 + \lambda \Delta t$.
- First-order accurate.
- Parabolic equation: stable for $\nu \Delta t / \Delta x^2 = 1/2$.
- Hyperbolic, central: unstable.
- Hyperbolic, upwind: stable for $c \Delta t / \Delta x \leq 2$.



Explicit Euler
$|\sigma_i|$
$c\Delta\, t/\Delta\, x,\ \nu\Delta\, t/\Delta\, x^2$
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.5
1
1.5
2
2.5
3
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central

McCormack scheme

- Explicit predictor-corrector scheme given by

$$\left\{ \begin{array}{ccl} u^* & = & u^n + \Delta t u'^n \\ u^{n+1} & = & u^n + \frac{\Delta t}{2}\left[u'^* + u'^n\right]. \end{array} \right.$$

  where again $u' = \lambda u$.

- The σ-root is

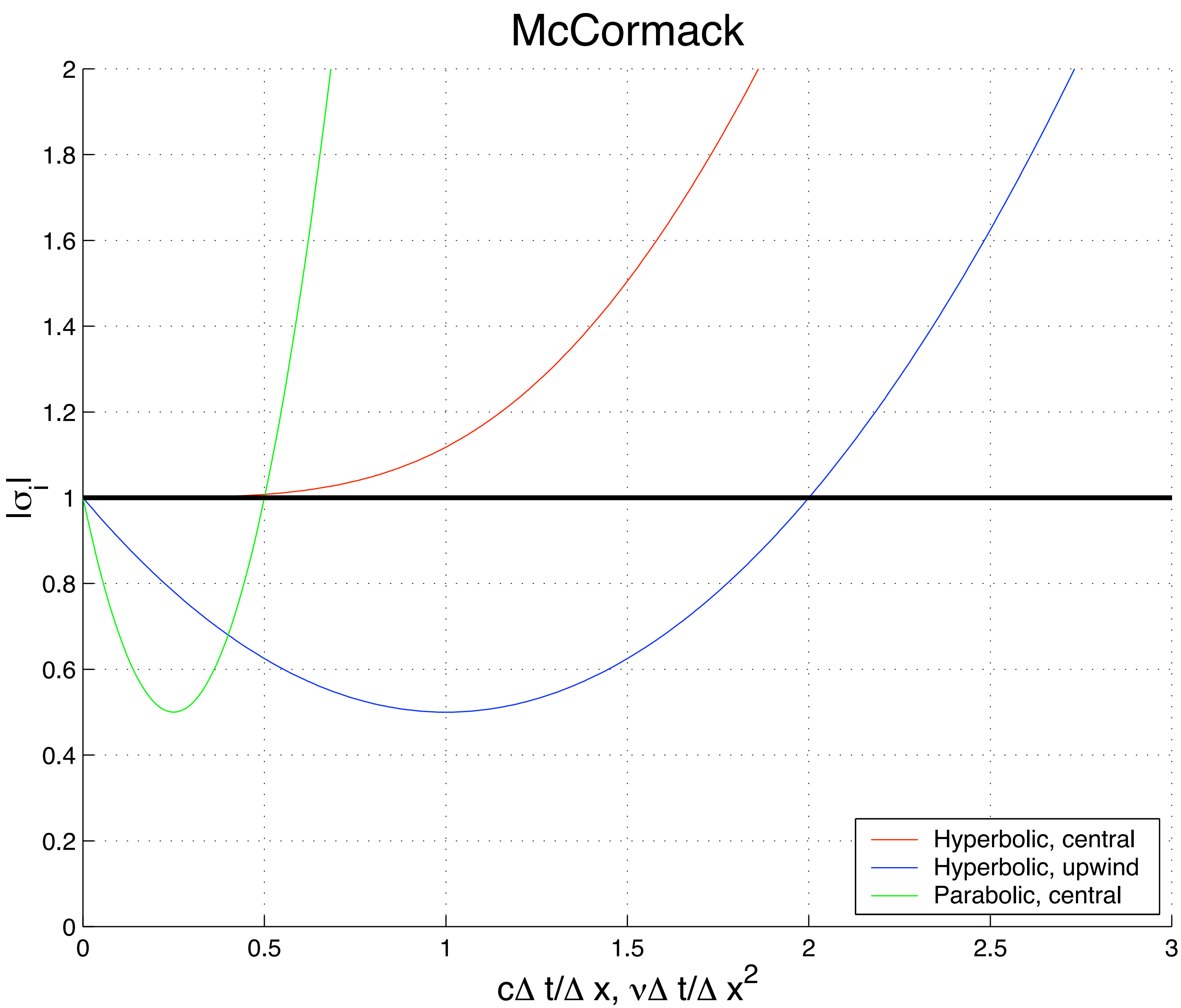
$$\sigma = 1 + \lambda \Delta t + \frac{(\lambda \Delta t)^2}{2}.$$

- Second-order accurate.

- Parabolic equation: stable for $\nu \Delta t / \Delta x^2 = 1/2$.

- Hyperbolic, central: weakly unstable for $c\Delta t/\Delta x \leq 0.6$.

- Hyperbolic, upwind: stable for $c\Delta t/\Delta x \leq 2$.


McCormack
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
|σ_i|
0
0.5
1
1.5
2
2.5
3
cΔ t/Δ x, νΔ t/Δ x^2
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central

Adams-Bashforth scheme

- Explicit scheme given by

$$u^{n+1} = u^n + \frac{\Delta t}{2}\left(3u'^n - u'^{n-1}\right). \qquad \text{where } u' = \lambda u$$

- The σ-roots are

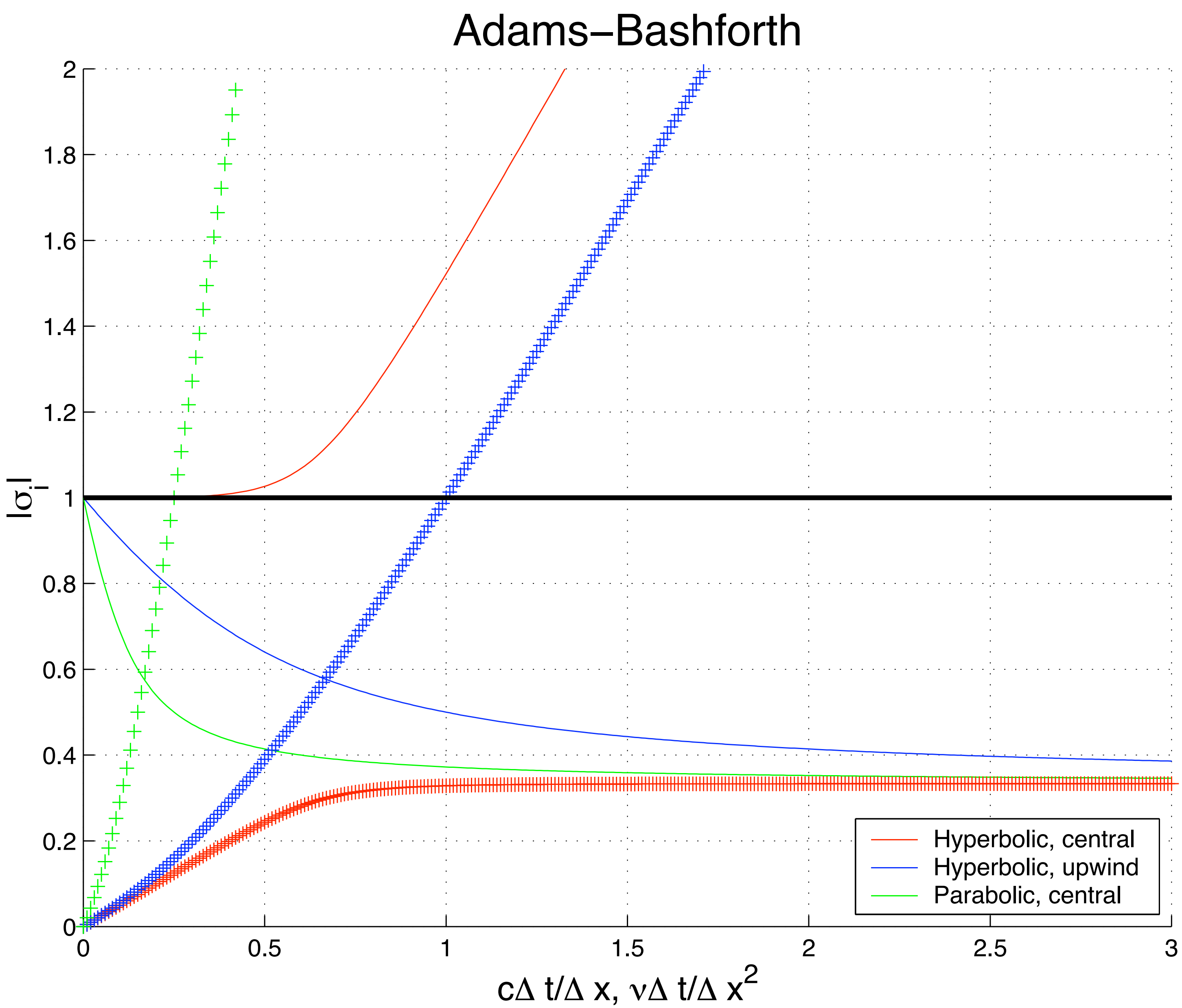
$$\sigma_{1,2} = \frac{1}{2}\left[1 + \frac{3}{2}\lambda\Delta t \pm \sqrt{1 + \lambda\Delta t + \frac{9}{4}(\lambda\Delta t)^2}\right].$$

- Second-order accurate; requires special starting procedure (Euler expicit).

- Parabolic equation: stable for $\nu\Delta t/\Delta x^2 = 1/4$.

- Hyperbolic, central: weakly unstable for $c\Delta t/\Delta x \leq 0.5$.

- Hyperbolic, upwind: stable for $c\Delta t/\Delta x \leq 1$.



Adams−Bashforth
|σi|
cΔ t/Δ x, νΔ t/Δ x^2
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.5
1
1.5
2
2.5
3
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central

Runge-Kutta schemes

- Runge-Kutta (RK) schemes are a class of multi-step methods.
- They are one-root schemes whose σ-root is given by a truncation of Taylor's expansion of $\exp(\lambda\Delta t)$ to the order of the scheme.
- The explicit Euler scheme is the first-order Runge-Kutta scheme (RK1) and $\sigma = 1 + \lambda\Delta t$.
- MacCormack's predictor-corrector is RK2 and $\sigma = 1 + \lambda\Delta t + (\lambda\Delta t)^2/2$.

RK4 scheme

- The fourth-order accurate RK for an ODE of the form $du/dt = F(u,t)$ can be written as

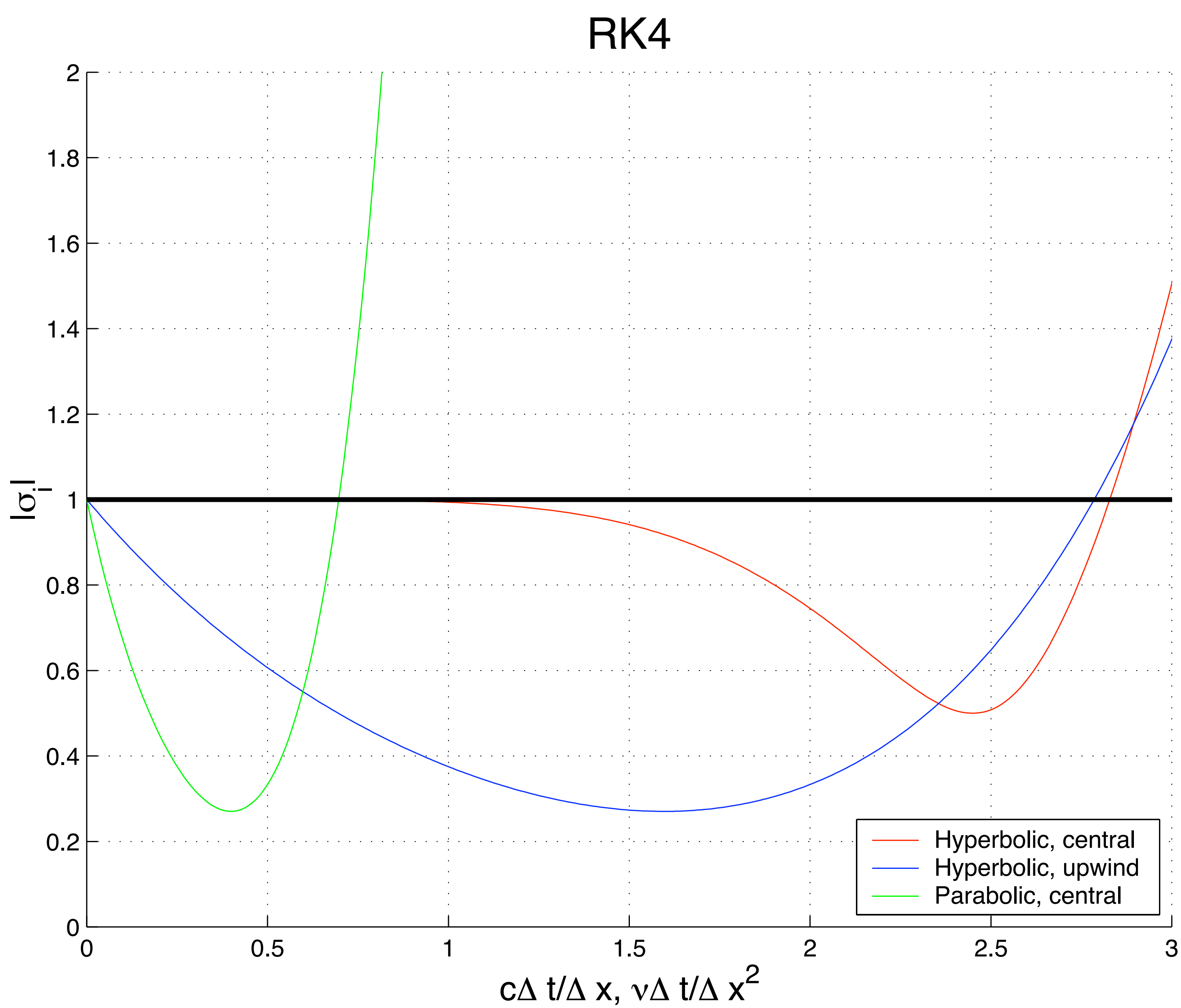
$$\left\{ \begin{array}{rcl} u^* & = & u^n + \frac{\Delta t}{2} F(u^n, t_n) \\ u^{**} & = & u^n + \frac{\Delta t}{2} F(u^*, t_n + \Delta t/2) \\ u^{***} & = & u^n + \Delta t F(u^{**}, t_n + \Delta t) \\ u^{n+1} & = & u^n + \frac{\Delta t}{6} \left[F(u^{***}, t_n + \Delta t) + 2F(u^{**}, t_n + \Delta t) \right. \\ & & \left. +2F(u^*, t_n + \Delta t/2) + F(u_n, t_n) \right], \end{array} \right.$$

- Fourth-order accurate.

- Parabolic equation: stable for $\nu \Delta t / \Delta x^2 = 0.69$.

- Hyperbolic, central: weakly unstable for $c\Delta t/\Delta x \leq 2.83$.

- Hyperbolic, upwind: stable for $c\Delta t/\Delta x \leq 2.8$.



RK4
$|\sigma_i|$
$c\Delta t/\Delta x$, $\nu\Delta t/\Delta x^2$
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.5
1
1.5
2
2.5
3

RK4 scheme

- The RK4 scheme written above requires 4 variables per point $(u^n,\ u^*,\ u^{**},\ u^{***})$.
- An alternative formulation requires only 3 variables per point:

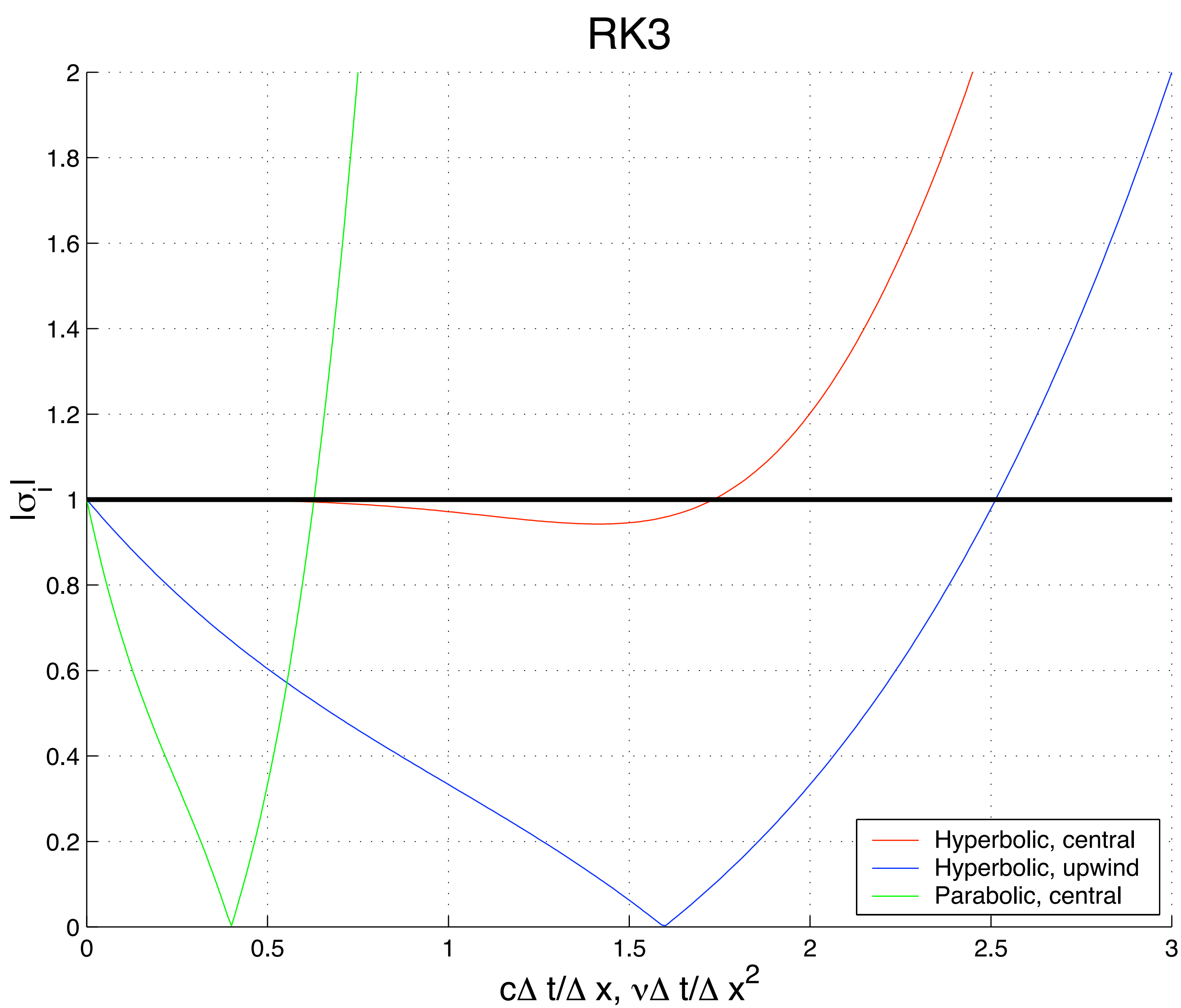
$$
\begin{cases}
U = u^n; & G = U; & P = F(U, t_n) \\
U = U + \frac{\Delta t}{2} P; & G = P; & P = F(U, t_n + \Delta t/2) \\
U = U + \frac{\Delta t}{2}(P - G); & G = G/6; & P = F(U, t_n + \Delta t/2) \\
U = U + \Delta t P; & G = G - P; & P = F(U, t_n + \Delta t) \\
 & & \qquad +2P \\
u^{n+1} = U + \Delta t(G + P/6). & &
\end{cases}
$$

RK3 scheme

- The low-storage, third-order accurate RK scheme can be written as

$$\begin{cases} U = u_n; & G = F(U, t_n) \\ U = U + \frac{\Delta t}{3} G; & G = -\frac{5}{9} G + F(U, t_n + \Delta t/3) \\ U = U + \frac{15\Delta t}{16} G; & G = -\frac{153}{128} G + F(U, t_n + 3\Delta t/4) \\ u_{n+1} = U + \frac{8\Delta t}{15} G. & \end{cases}$$

- Third-order accurate.
- Parabolic equation: stable for $\nu \Delta t/\Delta x^2 \leq 0.62$.
- Hyperbolic, central: stable for $c\Delta t/\Delta x \leq 1.73$.
- Hyperbolic, upwind: stable for $c\Delta t/\Delta x \leq 2.51$.

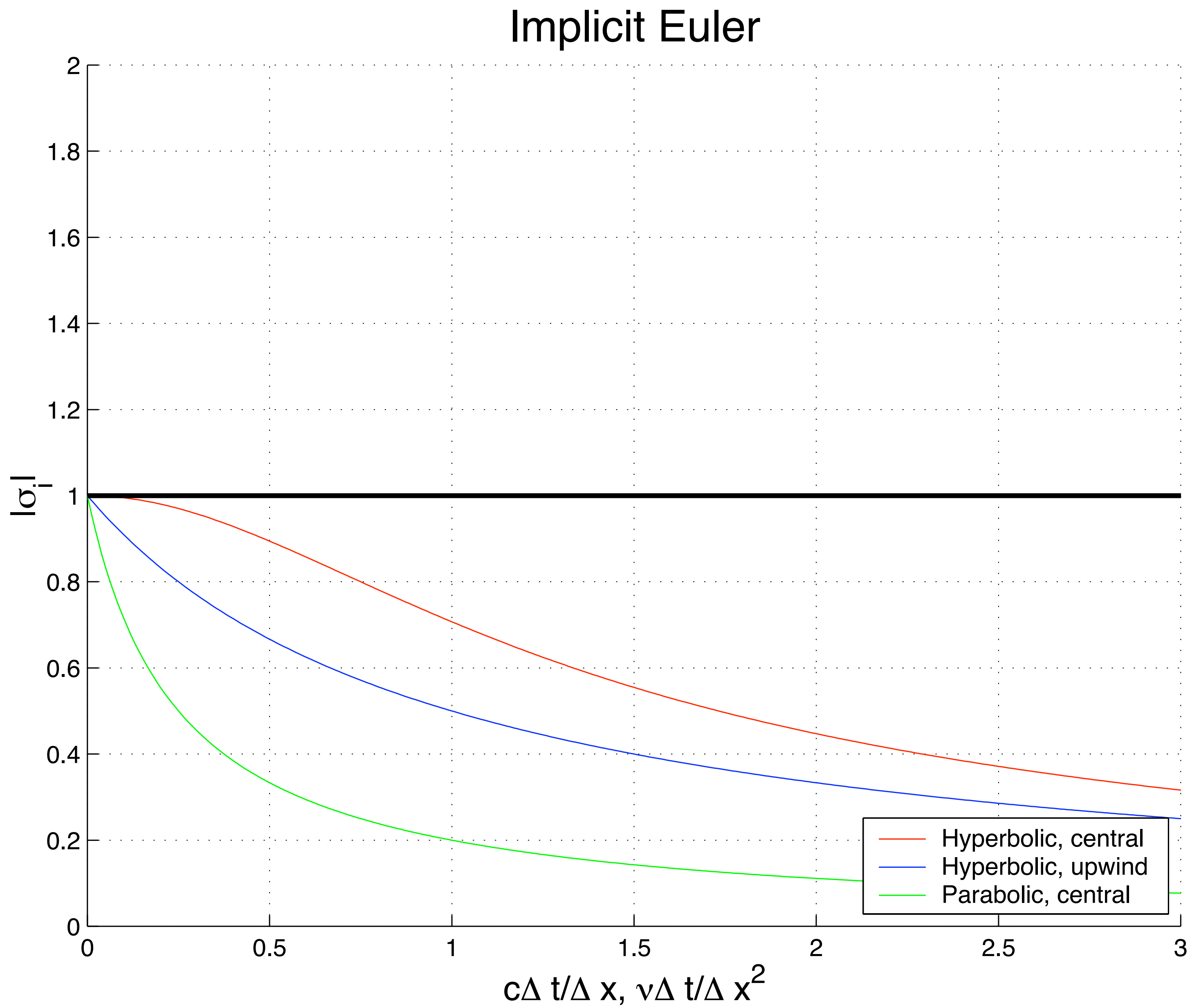

RK3
$|\sigma_i|$
$c\Delta t/\Delta x$, $\nu\Delta t/\Delta x^2$
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.5
1
1.5
2
2.5
3

Implicit Euler scheme

- Implicit schemes evaluate the derivative (the RHS of the equation) at $n+1$.
- The simplest is the implicit Euler scheme, which uses a backwards difference (rather than the forwards difference used by the explicit Euler).

$$u^{n+1} = u^n + \Delta t {u'}^{n+1}.$$

- The σ-root is $1/(1-\lambda\Delta t) \simeq 1 + \lambda\Delta t + (\lambda\Delta t)^2$.
- First-order accurate.
- Stable if $Re(\lambda\Delta t) \leq 0$.



Implicit Euler
|σ_i|
cΔ t/Δ x, νΔ t/Δ x^2
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.5
1
1.5
2
2.5
3
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central

Crank-Nicolson scheme

- Implicit scheme that evaluates the derivative (the RHS of the equation) at $n+1/2$ as the average of the values at n and $n+1$:

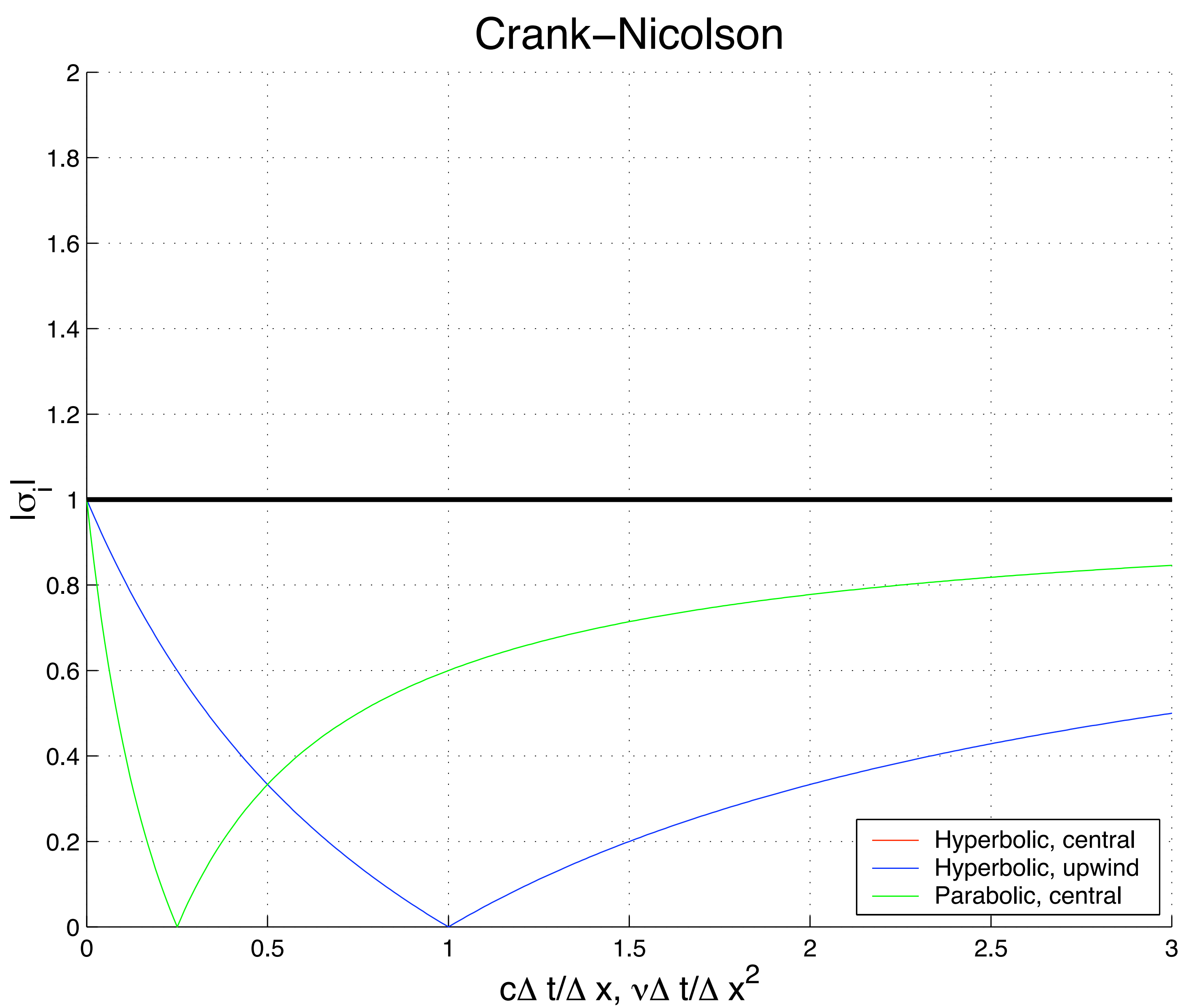
$$u^{n+1} = u^n + \frac{\Delta t}{2}\left(u'^{n+1} + u'^{n}\right).$$

- The σ-root is

$$\sigma = \frac{1+\lambda\Delta t/2}{1-\lambda\Delta t/2} \simeq 1 + \lambda\Delta t + \frac{1}{2}(\lambda\Delta t)^2 + \frac{1}{4}(\lambda\Delta t)^3.$$

- Second-order accurate.

- Stable if $Re(\lambda\Delta t) \leq 0$.



Crank–Nicolson
$|\sigma_i|$
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.5
1
1.5
2
2.5
3
$c\Delta t/\Delta x$, $\nu\Delta t/\Delta x^2$
Hyperbolic, central
Hyperbolic, upwind
Parabolic, central

Stability of time-advancement schemes

Summary

Method	Parabolic Central	Hyperbolic Central	Hyperbolic Upwind
Explicit Euler	$\frac{\nu\Delta t}{\Delta x^2} \leq 0.5$	Unstable	$\frac{c\Delta t}{\Delta x} \leq 2$
MacCormack	$\frac{\nu\Delta t}{\Delta x^2} \leq 0.5$	Weakly unstable	$\frac{c\Delta t}{\Delta x} \leq 2$
Adams-Bashforth	$\frac{\nu\Delta t}{\Delta x^2} \leq 0.25$	Weakly unstable	$\frac{c\Delta t}{\Delta x} \leq 1$
RK3	$\frac{\nu\Delta t}{\Delta x^2} \leq 0.62$	$\frac{c\Delta t}{\Delta x} \leq 1.73$	$\frac{c\Delta t}{\Delta x} \leq 2.51$
RK4	$\frac{\nu\Delta t}{\Delta x^2} \leq 0.69$	$\frac{c\Delta t}{\Delta x} \leq 2.82$	$\frac{c\Delta t}{\Delta x} \leq 2.80$
Implicit Euler	Stable	Stable	Stable
Crank-Nicolson	Stable	Stable	Stable