16.920J/SMA 5212

Numerical Methods for Partial Differential Equations

Lecture 5

Finite Differences: Parabolic Problems

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OUTLINE

- Governing Equation
- Stability Analysis
- 3 Examples
- Relationship between σ and λh
- Implicit Time-Marching Scheme
- Summary

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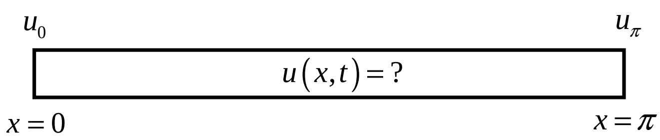
GOVERNING EQUATION

Consider the Parabolic PDE in 1-D

$$\frac{\partial u}{\partial t} = \upsilon \frac{\partial^2 u}{\partial x^2} \qquad x \in [0, \pi]$$

subject to $u = u_0$ at $x = 0$, $u = u_\pi$ at $x = \pi$



- If $\upsilon \equiv$ **viscosity** $\rightarrow$ Diffusion Equation
- If $\upsilon \equiv$ **thermal conductivity** $\rightarrow$ Heat Conduction Equation

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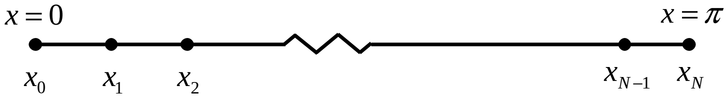
STABILITY ANALYSIS
Discretization

Keeping time continuous, we carry out a spatial discretization of the RHS of

$$\frac{\partial u}{\partial t} = \upsilon \frac{\partial^2 u}{\partial x^2}$$



There is a total of $N+1$ grid points such that $x_j = j\Delta x$,
$j = 0,1,2,....,N$

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STABILITY ANALYSIS
Discretization

Use the Central Difference Scheme for $\dfrac{\partial^2 u}{\partial x^2}$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} + O(\Delta x^2)$$

which is second-order accurate.

- Schemes of other orders of accuracy may be constructed.

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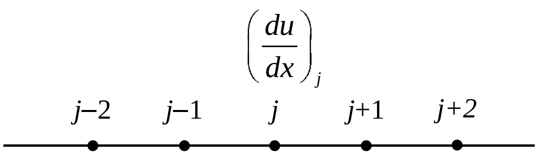
Construction of Spatial Difference Scheme of Any Order *p*

The idea of constructing a spatial difference operator is to represent the spatial differential operator at a location by the neighboring nodal points, each with its own weightage.

The order of accuracy, *p* of a spatial difference scheme is represented as $O\left(\Delta x^p\right)$. Generally, to represent the spatial operator to a higher order of accuracy, more nodal points must be used.



Consider the following procedure of determining the spatial operator $\left(\dfrac{du}{dx}\right)_j$ up to the order of accuracy $O\left(\Delta x^2\right)$:

1. Let $\left(\frac{du}{dx}\right)_j$ be represented by u at the nodes j–1, j, and j+1 with α_{-1}, α_0 and α_1 being the coefficients to be determined, i.e.

$$\left(\frac{du}{dx}\right)_j + \alpha_{-1}u_{j-1} + \alpha_0 u_j + \alpha_1 u_{j+1} = O\left(\Delta x^p\right) \tag{1}$$

2. Seek Taylor Expansions for u_{j-1}, u_j and u_{j+1} about u_j and present them in a table as shown below.

(Note that p is not known *a priori* but is determined at the end of the analysis when the α's are made known.)

This column consists of all the terms on the LHS of (1).

	u_j	u_j'	u_j''	u_j'''
u_j'	0	1	0	0
$\alpha_{-1}u_{j-1}$	α_{-1}	$-\Delta x \cdot \alpha_{-1}$	$\frac{1}{2}\Delta x^2 \cdot \alpha_{-1}$	$-\frac{1}{6}\Delta x^3 \cdot \alpha_{-1}$
$\alpha_0 u_j$	α_0	0	0	0
$\alpha_1 u_{j+1}$	α_1	$\Delta x \cdot \alpha_1$	$\frac{1}{2}\Delta x^2 \cdot \alpha_1$	$\frac{1}{6}\Delta x^3 \cdot \alpha_1$
⋮	⋮	⋮	⋮	⋮
↓	↓	↓	↓	↓
$u_j' + \sum_{k=-1}^{k=1} \alpha_k u_{j+k}$	S_1	S_2	S_3	S_4

Each cell in this row comprises the sum of its corresponding column.

where
$$S_1 = \left(\alpha_{-1} + \alpha_0 + \alpha_1\right) u_j$$
$$S_2 = \left(1 - \Delta x \cdot \alpha_{-1} + \Delta x \cdot \alpha_1\right) u_j'$$
$$S_3 = \left(\frac{1}{2}\Delta x^2 \cdot \alpha_{-1} + \frac{1}{2}\Delta x^2 \cdot \alpha_1\right) u_j''$$
$$S_4 = \left(-\frac{1}{6}\Delta x^3 \cdot \alpha_{-1} + \frac{1}{6}\Delta x^3 \cdot \alpha_1\right) u_j'''$$

$$\therefore \; u_j' + \sum_{k=-1}^{k=1} \alpha_k u_{j+k} = S_1 + S_2 + S_3 + S_4 + \ldots.$$

3. Make as many S_i's as possible vanish by choosing appropriate α_k's.

In this instance, since we have three unknowns α_{-1}, α_0 and α_1, we can therefore set:

$$S_1 = 0$$
$$S_2 = 0$$
$$S_3 = 0$$

(Note that in the Taylor Series expansion, one starts off with the lower-order terms and progressively obtain the higher-order terms. We have deliberately set the S_i pertaining to the lower-order terms to zero, thereafter followed by increasingly higher-order terms.)

Hence,

$$\begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_{-1} \\ \alpha_0 \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} 0 \\ -\dfrac{1}{\Delta x} \\ 0 \end{bmatrix}$$

Solving the system of equations, we obtain

$$\alpha_{-1} = \frac{1}{2\Delta x}$$
$$\alpha_0 = 0$$
$$\alpha_1 = -\frac{1}{2\Delta x}$$

4. Substituting the α_k 's into $u_j' + \sum_{k=-1}^{k=1} \alpha_k u_{j+k} = S_1 + S_2 + S_3 + S_4 + \ldots.$ yields

$$u_j' - \frac{1}{2\Delta x}\left(u_{j+1} - u_{j-1}\right) = \frac{1}{6}\Delta x^2 \cdot u_j''' + \text{ higher-order terms}$$

In other words,

$$u_j' = \left(\frac{du}{dx}\right)_j = \frac{u_{j+1} - u_{j-1}}{2\Delta x} + \underset{\substack{\updownarrow \\ O\left(\Delta x^p\right),\ p=2}}{O\left(\Delta x^2\right)} + \ldots.$$

i.e. the above representation is accurate up to $O\left(\Delta x^2\right)$.

Some useful points to note:

1. These 4 steps are the general procedure used to obtain the representation of the spatial operator up to the order of accuracy $O\left(\Delta x^p\right)$.

2. For other spatial operators, say $\left(\frac{d^2u}{dx^2}\right)_j$, we simply replace $\left(\frac{du}{dx}\right)_j$ in (1) with the said spatial operator.

3. For one-sided representations, one can choose nodal points $u_{j+k}, k \geq 0$. This may be important especially for representations on a boundary. For example

$$\left(\frac{du}{dx}\right)_j + \alpha_0 u_j + \alpha_1 u_{j+1} + \alpha_2 u_{j+2} + \ldots. = O\left(\Delta x^p\right)$$

One possibility is

$$\left(\frac{du}{dx}\right)_j + \frac{3u_j - 4u_{j+1} + u_{j+2}}{2\Delta x} = O\left(\Delta x^2\right)$$

which is also second-order accurate.

(We can also use a similar procedure to construct the finite difference scheme of Hermitian type for a spatial operator. This is not covered here).

STABILITY ANALYSIS
Discretization

We obtain at
$$x_1 : \frac{du_1}{dt} = \frac{\upsilon}{\Delta x^2}(u_o - 2u_1 + u_2)$$
$$x_2 : \frac{du_2}{dt} = \frac{\upsilon}{\Delta x^2}(u_1 - 2u_2 + u_3)$$
$$\vdots \qquad\qquad \vdots$$
$$x_j : \frac{du_j}{dt} = \frac{\upsilon}{\Delta x^2}(u_{j-1} - 2u_j + u_{j+1})$$
$$\vdots \qquad\qquad \vdots$$
$$x_{N-1} : \frac{du_{N-1}}{dt} = \frac{\upsilon}{\Delta x^2}(u_{N-2} - 2u_{N-1} + u_N)$$

Note that we need not evaluate u at $x = x_0$ and $x = x_N$ since u_0 and u_N are given as boundary conditions.

STABILITY ANALYSIS
Matrix Formulation

Assembling the system of equations, we obtain

$$\begin{bmatrix} \frac{du_1}{dt} \\ \frac{du_2}{dt} \\ \vdots \\ \frac{du_j}{dt} \\ \vdots \\ \frac{du_{N-1}}{dt} \end{bmatrix} = \frac{\upsilon}{\Delta x^2} \underbrace{\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & \mathbf{0} & \\ & \ddots & \ddots & \ddots & & \\ & & 1 & -2 & 1 & \\ & \mathbf{0} & & \ddots & \ddots & 1 \\ & & & & 1 & -2 \end{bmatrix}}_{A} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_j \\ \vdots \\ u_{N-1} \end{bmatrix} + \begin{bmatrix} \frac{\upsilon u_o}{\Delta x^2} \\ 0 \\ 0 \\ \vdots \\ 0 \\ \frac{\upsilon u_N}{\Delta x^2} \end{bmatrix}$$

STABILITY ANALYSIS
PDE to Coupled ODEs

Or in compact form

$$\frac{d\vec{u}}{dt} = A\vec{u} + \vec{b}$$

where $\vec{u} = [\, u_1 \quad u_2 \quad \cdots\cdots \quad u_{N-1} \,]^T$

$$\vec{b} = \left[\frac{\upsilon u_o}{\Delta x^2} \quad 0 \quad 0 \quad \cdots\cdots \quad 0 \quad \frac{\upsilon u_N}{\Delta x^2} \right]^T$$

We have reduced the 1-D PDE to a set of **Coupled ODEs**!

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STABILITY ANALYSIS
Eigenvalue and Eigenvector of Matrix A

If A is a nonsingular matrix, as in this case, it is then possible to find a set of eigenvalues

$$\lambda = \left\{ \lambda_1, \lambda_2, \ldots., \lambda_j, \ldots., \lambda_{N-1} \right\}$$

from $\det\left(A - \lambda I \right) = 0$.

For each eigenvalue λ_j, we can evaluate the eigenvector V^j consisting of a set of mesh point values v_i^j, i.e.

$$V^{j^T} = \left[v_1^j \quad v_2^j \quad \cdots\cdots \quad v_{N-1}^j \right]$$

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STABILITY ANALYSIS
Eigenvalue and Eigenvector of Matrix A

The $(N-1)\times(N-1)$ matrix E formed by the $(N-1)$ columns V^j diagonalizes the matrix A by

$$E^{-1}AE = \Lambda$$

where $\Lambda = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & 0 \\ & & \ddots & \\ 0 & & & \lambda_{N-1} \end{bmatrix}$

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STABILITY ANALYSIS
Coupled ODEs to Uncoupled ODEs

Starting from $\frac{d\vec{u}}{dt} = A\vec{u} + \vec{b}$

Premultiplication by E^{-1} yields

$$E^{-1}\frac{d\vec{u}}{dt} = E^{-1}A\vec{u} + E^{-1}\vec{b}$$

$$E^{-1}\frac{d\vec{u}}{dt} = E^{-1}A\underbrace{\left(EE^{-1}\right)}_{I}\vec{u} + E^{-1}\vec{b}$$

$$E^{-1}\frac{d\vec{u}}{dt} = \underbrace{\left(E^{-1}AE\right)}_{\Lambda}E^{-1}\vec{u} + E^{-1}\vec{b}$$

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STABILITY ANALYSIS
Coupled ODEs to Uncoupled ODEs

Continuing from

$$E^{-1}\frac{d\vec{u}}{dt} = \Lambda E^{-1}\vec{u} + E^{-1}\vec{b}$$

Let $\vec{U} = E^{-1}\vec{u}$ and $\vec{F} = E^{-1}\vec{b}$, we have

$$\frac{d}{dt}\vec{U} = \Lambda\vec{U} + \vec{F}$$

which is a set of **Uncoupled ODEs**!

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STABILITY ANALYSIS
Coupled ODEs to Uncoupled ODEs

Expanding yields

$$\frac{dU_1}{dt} = \lambda_1 U_1 + F_1$$

$$\frac{dU_2}{dt} = \lambda_2 U_2 + F_2$$

$$\vdots$$

$$\frac{dU_j}{dt} = \lambda_j U_j + F_j$$

$$\vdots$$

$$\frac{dU_{N-1}}{dt} = \lambda_{N-1} U_{N-1} + F_{N-1}$$

Since the equations are independent of one another, they can be solved separately.

The idea then is to solve for $\vec{U}$ and determine $\vec{u} = E\vec{U}$

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STABILITY ANALYSIS
Coupled ODEs to Uncoupled ODEs

Considering the case of $\vec{b}$ independent of time, for the general j^{th} equation,

$$U_j = c_j e^{\lambda_j t} - \frac{1}{\lambda_j} F_j$$

is the solution for j = 1,2,….,N–1.

Evaluating, $\vec{u} = E\vec{U} = \underbrace{\boxed{E\left(\overrightarrow{ce^{\lambda t}}\right)}}_{\text{Complementary (transient) solution}} - \underbrace{\boxed{E\Lambda^{-1}E^{-1}\vec{b}}}_{\text{Particular (steady-state) solution}}$

where $\left(\overrightarrow{ce^{\lambda t}}\right) = \left[c_1 e^{\lambda_1 t} \quad c_2 e^{\lambda_2 t} \cdots\cdots\cdots c_j e^{\lambda_j t} \cdots\cdots\cdots c_{N-1} e^{\lambda_{N-1} t}\right]^T$

The stability analysis of the space discretization, keeping time continuous, is based on the eigenvalue structure of A. The exact solution of the system of equations is determined by the eigenvalues and eigenvectors of A.

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STABILITY ANALYSIS
Coupled ODEs to Uncoupled ODEs

We can think of the solution to the semi-discretized problem

$$\vec{u} = E\left(\overrightarrow{ce^{\lambda t}}\right) - E\Lambda^{-1}E^{-1}\vec{b}$$

as a superposition of eigenmodes of the matrix operator A.

Each mode j contributes a (transient) time behaviour of the form $e^{\lambda_j t}$ to the time-dependent part of the solution.

Since the transient solution must decay with time,

$$\text{Real}\left(\lambda_j\right) \leq 0 \qquad \text{for all } j$$

This is the criterion for stability of the space discretization (of a parabolic PDE) keeping time continuous.

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STABILITY ANALYSIS
Use of Modal (Scalar) Equation

It may be noted that since the solution $\vec{u}$ is expressed as a contribution from all the modes of the initial solution, which have propagated or (and) diffused with the eigenvalue λ_j, and a contribution from the source term b_j, all the properties of the time integration (and their stability properties) can be analysed separately for each mode with the scalar equation

$$\left(\frac{dU}{dt} = \lambda U + F\right)_j$$

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STABILITY ANALYSIS
Use of Modal (Scalar) Equation

The spatial operator A is replaced by an eigenvalue λ, and the above modal equation will serve as the basic equation for analysis of the stability of a time-integration scheme (yet to be introduced) as a function of the eigenvalues λ of the space-discretization operators.

This analysis provides a general technique for the determination of time integration methods which lead to stable algorithms for a given space discretization.

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EXAMPLE 1
Continuous Time Operator

Consider a set of coupled ODEs (2 equations only):

$$\frac{du_1}{dt} = a_{11}u_1 + a_{12}u_2$$
$$\frac{du_2}{dt} = a_{21}u_1 + a_{22}u_2$$

Let $\vec{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$, $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ $\Rightarrow$ $\frac{d\vec{u}}{dt} = A\vec{u}$

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EXAMPLE 1
Continuous Time Operator

Proceeding as before, or otherwise (solving the ODEs directly), we can obtain the solution

$$u_1 = c_1\xi_{11}e^{\lambda_1 t} + c_2\xi_{12}e^{\lambda_2 t}$$
$$u_2 = c_1\xi_{21}e^{\lambda_1 t} + c_2\xi_{22}e^{\lambda_2 t}$$

where λ_1 and λ_2 are eigenvalues of A and $\begin{bmatrix}\xi_{11}\\ \xi_{21}\end{bmatrix}$ and $\begin{bmatrix}\xi_{21}\\ \xi_{22}\end{bmatrix}$ are eigenvectors pertaining to λ_1 and λ_2 respectively.

As the transient solution must decay with time, it is imperative that $\text{Real}\left(\lambda_{\text{j}}\right) \le 0$ for $j = 1, 2$.

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EXAMPLE 1
Discrete Time Operator

Suppose we have somehow discretized the time operator on the LHS to obtain

$$u_1^{\,n} = a_{11}u_1^{\,n-1} + a_{12}u_2^{\,n-1}$$
$$u_2^{\,n} = a_{21}u_1^{\,n-1} + a_{22}u_2^{\,n-1}$$

where the subscript n stands for the n^{th} time level, then

$$\vec{u}^{\,n} = A\vec{u}^{\,n-1} \qquad \text{where } \vec{u}^{\,n} = \begin{bmatrix}u_1^{\,n} & u_2^{\,n}\end{bmatrix}^T \text{ and } A = \begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix}$$

Since A is independent of time,

$$\vec{u}^{\,n} = A\vec{u}^{\,n-1} = AA\vec{u}^{\,n-2} = ... = A^n\vec{u}^{\,0}$$

In later examples, we shall apply specific time discretization schemes such as the "leapfrog" and Euler-forward time discretization schemes.

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EXAMPLE 1
Discrete Time Operator

As $A = E\Lambda E^{-1}$,

$$\vec{u}^n = \underbrace{E\Lambda E^{-1}}_{A} \cdot \underbrace{E\Lambda E^{-1}}_{A} \cdot \ldots \cdot \underbrace{E\Lambda E^{-1}}_{A} \cdot \overrightarrow{u^0}$$

$$\vec{u}^n = E\Lambda^n E^{-1}\overrightarrow{u^0} \quad \text{where } \Lambda^n = \begin{bmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{bmatrix}$$

$$\begin{aligned} u_1^n &= \lambda_1^n \xi_{11} c_1' + \lambda_2^n \xi_{12} c_2' \\ u_2^n &= \lambda_1^n \xi_{21} c_1' + \lambda_2^n \xi_{22} c_2' \end{aligned} \qquad \text{where } \begin{bmatrix} c_1' \\ c_2' \end{bmatrix} = E^{-1}\overrightarrow{u^0} \text{ are constants.}$$

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Alternative View

Alternatively, one can view the solution as:

$$\begin{bmatrix} U_1^n \\ U_2^n \end{bmatrix} = \begin{bmatrix} \lambda_1^n & \lambda_2^n \end{bmatrix} \begin{bmatrix} U_1^0 \\ U_2^0 \end{bmatrix}$$

$$\vec{U}^n = \Lambda^n \vec{U}^0 \qquad \text{where } \vec{U} = E^{-1}\vec{u}$$

EXAMPLE 1
Comparison

Comparing the solution of the semi-discretized problem where time is kept continuous

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} c_1 & c_2 \end{bmatrix} \begin{bmatrix} \xi_{11} & \xi_{12} \\ \xi_{21} & \xi_{22} \end{bmatrix} \begin{bmatrix} e^{\lambda_1 t} \\ e^{\lambda_2 t} \end{bmatrix}$$

to the solution where time is discretized

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}^n = \begin{bmatrix} c_1' & c_2' \end{bmatrix} \begin{bmatrix} \xi_{11} & \xi_{12} \\ \xi_{21} & \xi_{22} \end{bmatrix} \begin{bmatrix} \lambda_1^n \\ \lambda_2^n \end{bmatrix}$$

The difference equation where time is continuous has exponential solution $e^{\lambda t}$.

The difference equation where time is discretized has power solution λ^n.

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EXAMPLE 1
Comparison

In equivalence, the transient solution of the difference equation must decay with time, i.e.

$$\left|\lambda^n\right| < 1$$

for this particular form of time discretization.

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EXAMPLE 2
Leapfrog Time Discretization

Consider a typical modal equation of the form

$$\left(\frac{du}{dt} = \lambda u + ae^{\mu t}\right)_j$$

where λ_j is the eigenvalue of the associated matrix A.

(For simplicity, we shall henceforth drop the subscript j).

We shall apply the "leapfrog" time discretization scheme given as

$$\frac{du}{dt} = \frac{u^{n+1} - u^{n-1}}{2h} \qquad \text{where } h = \Delta t$$

Substituting into the modal equation yields

$$\begin{aligned}\frac{u^{n+1} - u^{n-1}}{2h} &= \left(\lambda u + ae^{\mu t}\right)_{t=nh} \\ &= \lambda u^n + ae^{\mu hn}\end{aligned}$$

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Reminder

Recall that we are considering a typical modal equation which had been obtained from the original equation

$$\frac{d\vec{u}}{dt} = A\vec{u} + \vec{b}$$

EXAMPLE 2
Leapfrog Time Discretization: Time Shift Operator

$$\frac{u^{n+1} - u^{n-1}}{2h} = \lambda u^n + ae^{\mu hn} \quad \Rightarrow \quad u^{n+1} - 2h\lambda u^n - u^{n-1} = 2ha\left(e^{\mu hn}\right)$$

Solution of u consists of the complementary solution c^n, and the particular solution p^n, i.e.

$$u^n = c^n + p^n$$

There are several ways of solving for the complementary and particular solutions. One way is through use of the shift operator S and characteristic polynomial.

The time shift operator S operates on c^n such that

$$Sc^n = c^{n+1}$$

$$S^2c^n = S\left(Sc^n\right) = Sc^{n+1} = c^{n+2}$$

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EXAMPLE 2
Leapfrog Time Discretization: Time Shift Operator

The complementary solution c^n satisfies the homogenous equation

$$c^{n+1} - 2h\lambda c^n - c^{n-1} = 0$$

$$Sc^n - 2h\lambda c^n - \frac{c^n}{S} = 0$$

$$(S^2c^n - 2h\lambda Sc^n - c^n)\frac{1}{S} = 0$$

$$\underbrace{(S^2 - 2h\lambda S - 1)}_{\text{characteristic polynomial}}\frac{c^n}{S} = 0$$

$$p(S) = (S^2 - 2h\lambda S - 1) = 0$$

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EXAMPLE 2
Leapfrog Time Discretization: Time Shift Operator

The solution to the characteristic polynomial is

$$\sigma(\lambda h) = S = \lambda h \pm \sqrt{1+\lambda^2 h^2}$$

σ_1 and σ_2 are the two roots

The complementary solution to the modal equation would then be

$$c^n = \beta_1 \sigma_1{}^n + \beta_2 \sigma_2{}^n$$

The particular solution to the modal equation is $p^n = \dfrac{2ahe^{\mu hn}e^{\mu h}}{e^{2\mu h} - 2h\lambda e^{\mu h} - 1}$.

Combining the two components of the solution together,

$$\begin{aligned} u^n &= \left(c^n\right) + \left(p^n\right) \\ &= \left(\beta_1\left(\lambda h + \sqrt{1+h^2\lambda^2}\right)^n + \beta_2\left(\lambda h - \sqrt{1+h^2\lambda^2}\right)^n\right) + \left(\frac{2ahe^{\mu hn}e^{\mu h}}{e^{2\mu h} - 2h\lambda e^{\mu h} - 1}\right) \end{aligned}$$

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EXAMPLE 2
Leapfrog Time Discretization: Stability Criterion

For the solution to be stable, the transient (complementary) solution must not be allowed to grow indefinitely with time, thus implying that

$$\left|\sigma_1 = \left(\lambda h + \sqrt{1+h^2\lambda^2}\right)\right| < 1$$

$$\left|\sigma_2 = \left(\lambda h - \sqrt{1+h^2\lambda^2}\right)\right| < 1$$

is the stability criterion for the leapfrog time discretization scheme used above.

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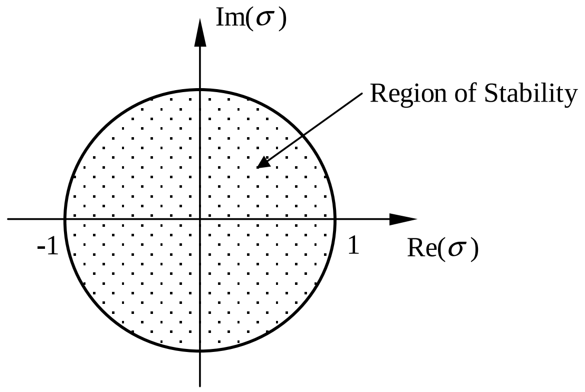
EXAMPLE 2
Leapfrog Time Discretization: Stability Diagram

The stability diagram for the leapfrog (or any general) time discretization scheme in the σ-plane is



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Stability Diagram in the λh-plane

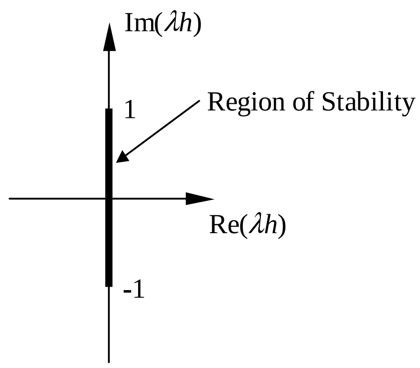
Alternatively, we can express the stability criterion for the leapfrog time discretization scheme as

$$\lambda h = \frac{1}{2}\left(\sigma - \frac{1}{\sigma}\right) \qquad \text{s.t. } |\sigma| < 1$$

Since $|\sigma| < 1$ and $\sigma = \exp(i\theta)$,

$$\lambda h = i \sin\theta \ \text{ for stability.}$$

The stability diagram for the leapfrog time discretization scheme in the λh-plane would therefore be as shown:



EXAMPLE 2
Leapfrog Time Discretization

In particular, by applying to the 1-D Parabolic PDE

$$\frac{\partial u}{\partial t} = \upsilon \frac{\partial^2 u}{\partial x^2}$$

the central difference scheme for spatial discretization, we obtain

$$A = \frac{\upsilon}{\Delta x^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \mathbf{0} \\ & \ddots & \ddots & \ddots & \\ & & & & 1 \\ \mathbf{0} & & & 1 & -2 \end{bmatrix}$$

which is the tridiagonal matrix

EXAMPLE 2
Leapfrog Time Discretization

According to analysis of a general triadiagonal matrix $B(a,b,c)$, the eigenvalues of B are

$$\lambda_j = b + 2\sqrt{ac}\cos\left(\frac{j\pi}{N}\right), \qquad j = 1,\ldots,N-1$$

$$\lambda_j = \left[-2 + 2\cos\left(\frac{j\pi}{N}\right)\right]\frac{\upsilon}{\Delta x^2}$$

The most "dangerous" mode is that associated with the eigenvalue of largest magnitude

$$\lambda_{\max} = -\frac{4\upsilon}{\Delta x^2}$$

i.e.

$$\sigma_1\left(\lambda_{\max}h\right) = \lambda_{\max}h + \sqrt{\lambda^2{}_{\max}h^2 + 1}$$
$$\sigma_2\left(\lambda_{\max}h\right) = \lambda_{\max}h - \sqrt{\lambda^2{}_{\max}h^2 + 1}$$

which can be plotted in the absolute stability diagram.

One may note that λ_j is always real and negative, thereby satisfying the criterion for stability of the space discretization of a parabolic PDE, keeping time continuous.

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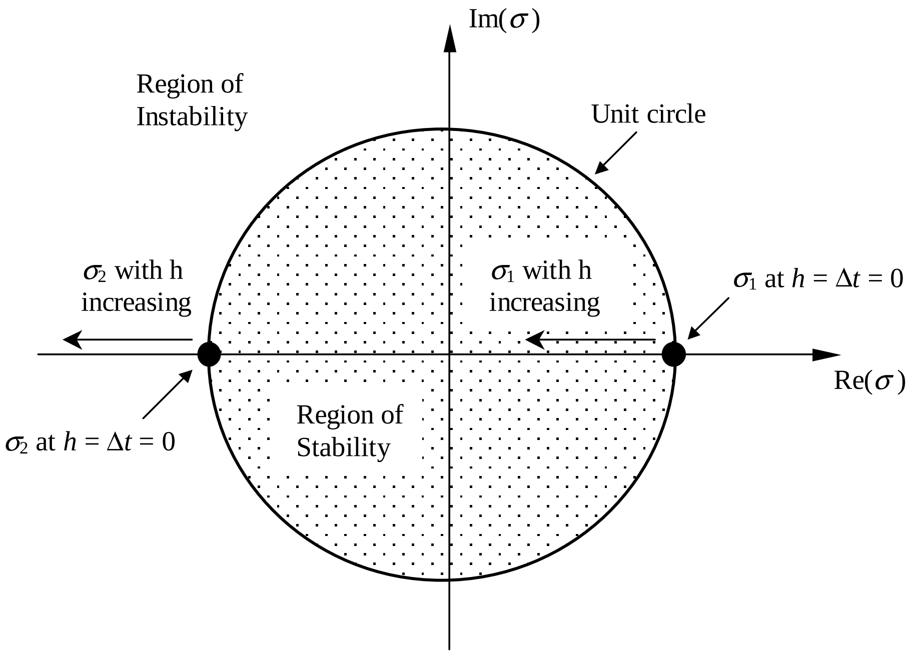
EXAMPLE 2

Leapfrog Time Discretization: Absolute Stability Diagram for σ

As applied to the 1-D Parabolic PDE, the absolute stability diagram for σ is



*In this case, σ_1 and σ_2 start out being on the unit circle (h = Δt = 0). However, the spurious root (refer to following slide) leaves the unit circle as h starts increasing. Therefore, the spurious root causes the leapfrog time discretization scheme to be unstable, irrespective of how small h = Δt is, although it does not affect the accuracy. The leapfrog time discretization for the 1-D Diffusion Equation is **unstable**.*

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STABILITY ANALYSIS
Some Important Characteristics Deduced

A few features worth considering:

1. Stability analysis of time discretization scheme can be carried out for all the different modes λ_j.
2. If the stability criterion for the time discretization scheme is valid for all modes, then the overall solution is stable (since it is a linear combination of all the modes).
3. When there is more than one root σ, then one of them is the principal root which represents an approximation to the physical behaviour. The principal root is recognized by the fact that it tends towards one as $\lambda h \to 0$, i.e. $\lim_{\lambda h \to 0} \sigma(\lambda h) = 1$. (The other roots are spurious, which affect the stability but not the accuracy of the scheme.)

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STABILITY ANALYSIS
Some Important Characteristics Deduced

4. By comparing the power series solution of the principal root to $e^{\lambda h}$, one can determine the order of accuracy of the time discretization scheme. In this example of leapfrog time discretization,

$$\sigma_1 = \lambda h + \left(1 + h^2\lambda^2\right)^{\frac{1}{2}} = \lambda h + 1 + \frac{1}{2}\left(h^2\lambda^2\right) + \frac{\frac{1}{2} . -\frac{1}{2}}{2!} . h^4\lambda^4$$

$$\sigma_1 = 1 + h\lambda + \frac{h^2\lambda^2}{2} + \ldots$$

and compared to

$$e^{\lambda h} = 1 + h\lambda + \frac{h^2\lambda^2}{2!} + \ldots$$

is identical up to the second order of $h\lambda$. Hence, the above scheme is said to be second-order accurate.

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EXAMPLE 3
Euler-Forward Time Discretization: Stability Analysis

Analyze the stability of the explicit Euler-forward time discretization

$$\frac{du}{dt} = \frac{u^{n+1} - u^n}{\Delta t}$$

as applied to the modal equation

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

Substituting $u^{n+1} = u^n + h\dfrac{du}{dt}$ where $h = \Delta t$

into the modal equation, we obtain $u^{n+1} - (1+\lambda h)u^n = 0$

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EXAMPLE 3
Euler-Forward Time Discretization: Stability Analysis

Making use of the shift operator S

$$c^{n+1} - (1+\lambda h)c^n = Sc^n - (1+\lambda h)c^n = \underbrace{[S - (1+\lambda h)]}_{\text{characteristic polynomial}}c^n = 0$$

Therefore $\sigma(\lambda h) = 1 + \lambda h$
and $c^n = \beta\sigma^n$

The Euler-forward time discretization scheme is stable if

$$|\sigma \equiv 1 + \lambda h| < 1$$

or bounded by $\lambda h = \sigma - 1$ s.t. $|\sigma| < 1$ in the λh-plane.

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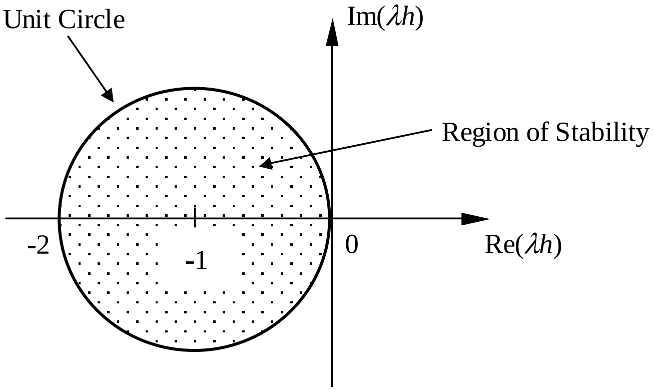
EXAMPLE 3
Euler-Forward Time Discretization: Stability Diagram

The stability diagram for the Euler-forward time discretization in the λh-plane is



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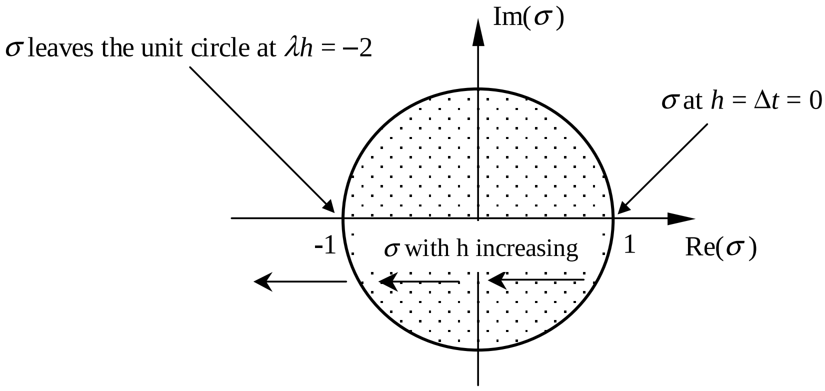
EXAMPLE 3
Euler-Forward Time Discretization: Absolute Stability Diagram

As applied to the 1-D Parabolic PDE, $\lambda = \lambda_{\max} = \dfrac{-4\upsilon}{\Delta x^2}$



The stability limit for largest $h \equiv \Delta t = \dfrac{-2}{\lambda_{\max}}$

σ leaves the unit circle at $\sigma = -1$, i.e. $\sigma = 1 + \lambda h = -1$

$\lambda h = -2 \qquad \Rightarrow \qquad h = \dfrac{-2}{\lambda_{max}}$ *since it is the extreme.*

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Predictor-Corrector Time Discretization

Consider the numerical stability of the following predictor-corrector time discretization scheme

$$\hat{u}^{n+1} = u^n + h\frac{du^n}{dt^n}$$
$$u^{n+1} = \frac{1}{2}\left(u^n + \hat{u}^{n+1} + h\frac{d\hat{u}^{n+1}}{dt^{n+1}}\right)$$

as applied to the typical modal equation

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

of the parabolic PDE. Substituting $\frac{du}{dt}$ and $\frac{d\hat{u}}{dt}$ into the predictor-corrector scheme yields

$$\hat{u}^{n+1} = u^n + h\left(\lambda u^n + ae^{\mu hn}\right) \qquad \text{where } t = n\Delta t = nh$$
$$u^{n+1} = \frac{1}{2}\left[u^n + \hat{u}^{n+1} + h\left(\lambda\hat{u}^{n+1} + ae^{\mu h(n+1)}\right)\right]$$

Utilizing the shift operator

$$Su^n = u^{n+1}$$
$$S\hat{u}^n = \hat{u}^{n+1}$$

and rearranging the equations into matrix form, we obtain

$$\begin{bmatrix} S & -(1+\lambda h) \\ -\frac{1}{2}(1+\lambda h)S & S-\frac{1}{2} \end{bmatrix}\begin{bmatrix} \hat{u}^n \\ u^n \end{bmatrix} = \begin{bmatrix} h \\ \frac{1}{2}hS \end{bmatrix} ae^{\mu hn}$$

To determine the characteristic polynomial, set

$$\mathrm{P}(\sigma) = \mathrm{P}(S) = \begin{vmatrix} S & -(1+\lambda h) \\ -\frac{1}{2}(1+\lambda h)S & S-\frac{1}{2} \end{vmatrix} = 0$$

$$\mathrm{P}(\sigma) = \mathrm{P}(S) = S\left(S - 1 - \lambda h - \frac{1}{2}\lambda^2 h^2\right) = 0$$

$$\Rightarrow \qquad \sigma = 0 \quad \text{(trivial root)}$$

$$\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2$$

i.e. the scheme is a one-root method. Compared to

$$e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + ...$$

the scheme is second-order accurate.

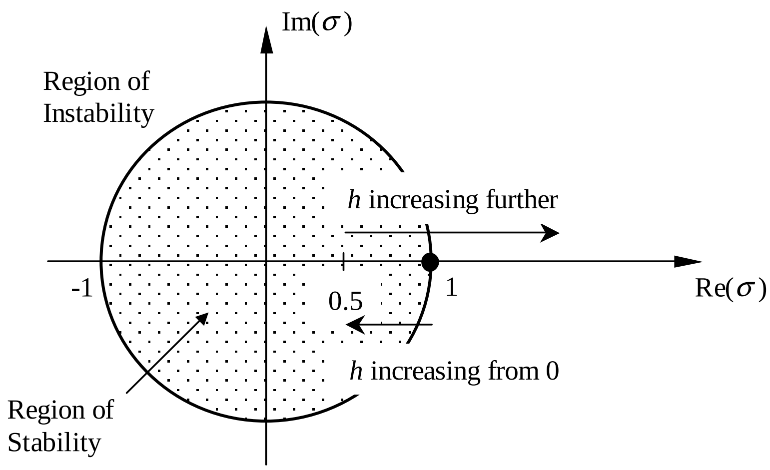
To obtain the particular solution, one can perform a matrix inversion and obtain

$$p^n = \frac{\frac{1}{2} a h e^{\mu h n}\left(e^{\mu h} + 1 + \lambda h\right)}{e^{\mu h} - 1 - \lambda h - \frac{1}{2}\lambda^2 h^2}$$

with the complementary solution being

$$c^n = \beta \sigma^n = \beta\left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2\right)^n$$

The absolute stability diagram (showing $\lambda = -\frac{4\upsilon}{\Delta x^2}$) for the 1-D Parabolic PDE is



When h increases from zero, σ decreases from 1.0. As h continues to increase, σ reaches a minimum of 0.5 with $\lambda h = -1$ and then increases. As h increases further, σ returns to 1.0 with $\lambda h = -2$. Prior to this point, the scheme is stable. Increasing h and thus σ beyond this point renders the scheme unstable.

Hence, this predictor-corrector scheme is stable for small h's and unstable for large h's; the limit for stability is $\lambda h = -2$ (from above).

In general, we can analyze the absolute stability diagram for the predictor-corrector time discretization method in terms of

$$\sigma: \qquad \sigma(\lambda h) = 1 + \lambda h + \frac{(\lambda h)^2}{2}$$

or

$$\lambda h: \qquad \lambda h = -1 \pm \sqrt{2\sigma - 1}$$

λ, the eigenvalue(s) of the A matrix can take on complex forms depending on the governing equation (as opposed to negative real values for the 1-D parabolic PDE with central differencing for the spatial derivative).

RELATIONSHIP BETWEEN σ AND λh
σ = σ(λh)

Thus far, we have obtained the stability criterion of the time discretization scheme using a typical modal equation. We can generalize the relationship between σ and λh as follows:

- Starting from the set of coupled ODEs

$$\frac{d\vec{u}}{dt} = A\vec{u} + \vec{b}$$

- Apply a specific time discretization scheme like the leapfrog time discretization as in Example 2

$$\frac{du}{dt} = \frac{u^{n+1} - u^{n-1}}{2h}$$

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RELATIONSHIP BETWEEN σ AND λh
σ = σ(λh)

- The above set of ODEs becomes

$$\frac{\vec{u}^{n+1}-\vec{u}^{n-1}}{2h}=A\vec{u}^{n}+\vec{b}^{n}$$

- Introducing the time shift operator S

$$S\vec{u}^{n}=\frac{\vec{u}^{n}}{S}+2hA\vec{u}^{n}+2h\vec{b}^{n}$$

$$\left[A-\frac{S-S^{-1}}{2h}I\right]\vec{u}^{n}=-\vec{b}^{n}$$

- Premultiplying E^{-1} on the LHS and RHS and introducing $I=EE^{-1}$ operating on $\vec{u}^{n}$

$$\left[\underbrace{E^{-1}AE}_{\Lambda}-E^{-1}\frac{S-S^{-1}}{2h}E\right]E^{-1}\vec{u}=-E^{-1}\vec{b}^{n}$$

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RELATIONSHIP BETWEEN σ AND λh
σ = σ(λh)

- Putting $\vec{U}^{n}=E^{-1}\vec{u}^{n}$, $\quad \vec{F}^{n}=E^{-1}\vec{b}^{n}$

we obtain $\left[\Lambda-\underbrace{E^{-1}\frac{S-S^{-1}}{2h}E}_{\frac{S-S^{-1}}{2h}}\right]\vec{U}^{n}=-\vec{F}^{n}$

i.e. $\left[\Lambda-\frac{S-S^{-1}}{2h}\right]\vec{U}^{n}=-\vec{F}^{n}$

which is a set of **uncoupled** equations.

Hence for each j, $j = 1,2,\ldots,N-1$,

$$\left[\lambda_j - \frac{S - S^{-1}}{2h}\right] U_j = -F_j$$

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RELATIONSHIP BETWEEN σ AND λh
σ = σ(λh)

Note that the analysis performed above is **identical** to the analysis carried out using the modal equation

$$\left(\frac{dU}{dt} = \lambda U + F\right)_j$$

All the analysis carried out earlier for a single modal equation is applicable to the matrix after the appropriate manipulation to obtain an uncoupled set of ODEs.

Each j^{th} equation can be solved independently for U_j^n and the U_j^n's can then be coupled through $\vec{u}^n = E\vec{U}^n$.

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RELATIONSHIP BETWEEN σ AND λh
σ = σ(λh)

Hence, applying any "consistent" numerical technique to each equation in the set of coupled linear ODEs is mathematically equivalent to

1. Uncoupling the set,

2. Integrating each equation in the uncoupled set,

3. Re-coupling the results to form the final solution.

These 3 steps are commonly referred to as the

ISOLATION THEOREM

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IMPLICIT TIME-MARCHING SCHEME

Thus far, we have presented examples of explicit time-marching methods and these may be used to integrate weakly stiff equations.

Implicit methods are usually employed to integrate very stiff ODEs efficiently. However, use of implicit schemes requires solution of a set of simultaneous algebraic equations at each time-step (i.e. **matrix inversion**), whilst updating the variables at the same time.

Implicit schemes applied to ODEs that are inherently stable will be **unconditionally stable** or **A-stable**.

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IMPLICIT TIME-MARCHING SCHEME
Euler-Backward

Consider the Euler-backward scheme for time discretization

$$\left(\frac{du}{dt}\right)^{n+1} = \frac{u^{n+1} - u^n}{h}$$

Applying the above to the modal equation for parabolic PDE

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

yields

$$\frac{u^{n+1} - u^n}{h} = \left[\lambda u^{n+1} + ae^{\mu(n+1)h}\right]$$
$$(1 - h\lambda)u^{n+1} - u^n = ahe^{\mu(n+1)h}$$

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IMPLICIT TIME-MARCHING SCHEME
Euler-Backward

Applying the *S* operator,

$$\left[(1 - h\lambda)S - 1\right]u^n = ahe^{\mu(n+1)h}$$

the characteristic polynomial becomes

$$\mathrm{P}(\sigma) = \mathrm{P}(S) = \left[(1 - h\lambda)S - 1\right] = 0$$

The principal root is therefore

$$\sigma = \frac{1}{1 - \lambda h} = 1 + \lambda h + \lambda^2 h^2 + ...$$

which, upon comparison with $e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + ...$, is only first-order accurate.

The solution is

$$U^n = \beta \left(\frac{1}{1 - \lambda h} \right)^n + \frac{ahe^{\mu(u+1)h}}{(1 - \lambda h)e^{\mu h} - 1}$$

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IMPLICIT TIME-MARCHING SCHEME
Euler-Backward

For the Parabolic PDE, λ is always real and < 0. Therefore, the transient component will always tend towards zero for large *n* irregardless of *h* ($\equiv \Delta t$).

The time-marching scheme is always numerically stable.

In this way, the implicit Euler/Euler-backward time discretization scheme will allow us to resolve different time-scaled events with the use of different time-step sizes. A small time-step size is used for the short time-scaled events, and then a large time-step size used for the longer time-scaled events. There is no constraint on h_{max}.

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IMPLICIT TIME-MARCHING SCHEME
Euler-Backward

However, numerical solution of *u* requires the solution of a set of simultaneous algebraic equations or matrix inversion, which is computationally much more

intensive/expensive compared to the multiplication/
addition operations of explicit schemes.

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SUMMARY

- Stability Analysis of Parabolic PDE
    - Uncoupling the set.
    - Integrating each equation in the uncoupled set $\rightarrow$ modal equation.
    - Re-coupling the results to form final solution.
- Use of modal equation to analyze the stability $|\sigma(\lambda h)| < 1$.
- Explicit time discretization versus Implicit time discretization.

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Reference:

Numerical Computation of Internal and External Flows, Vol I & II by C. Hirsch, 1992, Wiley Series.