1 Goal

The goal of this Lecture is to provide practical examples of PDE discretizations and discuss them in view of the general criteria exposed in the previous lecture.
2 Von Neumann analysis and discrete dispersion relation

A powerful way of analyzing the stability and accuracy of discrete equations is to derive their dispersion relation, discrete dispersion relation (DDR). This amounts to Fourier transforming the equation, i.e. expanding the discrete solution in plane waves of the form:

$$e^{i(kx_j - \omega t^n)}$$

and inspect the functional relation

$$f(\omega h, kd) = 0$$

Consistency requirement impose that this relation reduces to the continuum one in the limit $kd \rightarrow 0$ and $\omega h \rightarrow 0$. However, many sources of inaccuracy may arise due to the discretization. These errors split into two main categories: amplitude errors and phase errors. Amplitude errors may either show in the form of uncontrolled growth (instability) or excessive damping (numerical diffusion). Phase errors usually associate with defective propagation, i.e. correction to the exact propagation speed and deformation of the propagating profile (dispersion errors).

3 Diffusion equation in d=1

Consider the Diffusion Equation (DE) in d=1 spatial dimensions:

$$\partial_t \phi = D \partial_{xx} \phi \quad (1)$$

The exact solution in infinite space with initial condition $\phi(x, t = 0) = \delta(x)$ is a gaussian function centered about $x = 0$ with spread $\delta(t) = \sqrt{Dt}$. This is inherently stable. We next compute the Dispersion Relation (DR), which amounts to Fourier-transforming the above. With the operational correspondence $\partial_t = -i\omega$ and $\partial_x = ik$, we obtain

$$-i\omega = -Dk^2$$

namely, separating real and imaginary parts:

$$\omega_R = 0, \quad \gamma = -Dk^2$$

The physical meaning is that a wavelength $\lambda = 2\pi/k$ is exponentially damped at a rate $\gamma = Dk^2$, small wavelengths are much more damped than large ones. Everything is nicely stable (so long as $D > 0$).
4 Euler + centered space differences

This amounts to

\[ \phi^{n+1}_j - \phi^n_j = \frac{Dh}{d^2} (\phi^n_{j+1} - 2\phi^n_j + \phi^n_{j-1}) \]

Upon FT:

\[ e^{-i\omega h} - 1 = C_D (e^{ikd} - 2 + e^{-ikd}) \]

where \( C_D \equiv \frac{Dh}{d^2} \) is the diffusive CFL.

Separating the real-imaginary parts

\[ e^{\gamma h} \cos(\omega_R h) = 1 + 2C_D (\cos(kd) - 1) \]
\[ e^{\gamma h} \sin(\omega_R h) = 0 \]

The second immediately delivers \( \omega_R = 0 \), which is exact, no approximation. The first is less immediate; let us square both and sum up, to obtain

\[ e^{2\gamma h} = [1 + 2C_D (\cos(kd) - 1)]^2 = 1 + 4C_D X + 4C_D^2 X^2 \]

where we have set \( X \equiv \cos(kd) - 1 \).

Stability implies \( \gamma < 0 \), hence \( X + C_D X^2 < 0 \). For \( X < 0 \), the regime relevant to the continuum limit \( kd \to 0 \), this yields \( 1 - C_D |X| > 0 \) and since \( 0 < |X| < 2 \), this implies

\[ C_D < 1/2 \]

This is the CFL condition introduced in the previous lecture.

4.0.1 Continuum limit and order of accuracy

In the continuum limit \( kd \to 0 \) and \( \omega h \to 0 \), the discrete dispersion relation (DDR) reduces to

\[ 1 + 2\gamma h \sim 1 - 2C_D k^2 d^2 \]

namely

\[ \gamma \sim -k^2 D \]

which is precisely the continuum DR. Of course, this is approximateto first order in \( h \) and second order in \( d \): i.e. the scheme is first order in time and second in space.

4.1 Stability from realizability

Rearrange the scheme in 3-diagonal form:

\[ \phi^{n+1}_j = a\phi^n_{j-1} + c\phi^n_j + b\phi^n_{j+1} \]

where a simple calculation shows that:

\[ a = b = C_D, \ c = 1 - 2C_D \]
The above eq. lends itself to a transparent interpretation: the future state at a given location \( j \) is a weighted sum of the past state in a close neighborhood, in fact just the same site and its left/right neighbors. This is typical of local-explicit schemes, the simplest brand in town. One notes that the coefficients \( a, b, c \) sum to 1, which configures them as a sort of probability of transferring information from site to site in time. In this respect, a realizability constraint imposes that they are all non-negative, which implies indeed \( C_D < 1/2 \), i.e., the stability condition we found before by more elaborate calculations.

Realizability often offers a shortest path to assess stability; however the two conditions are not one-to-one related.

5 Advection equation

Let us now consider the advection equation

\[
\partial_t \phi = -U \partial_x \phi \tag{5}
\]

where \( U = \text{const} \) for simplicity.

Upon FT, the continuum DR reads as

\[
\omega_R = kU, \; \gamma = 0
\]

Let us now consider a first-order Euler in time as combined with centered differences in space

\[
\phi_j^{n+1} - \phi_j^n = -\frac{Uh}{2d} (\phi_{j+1}^n - \phi_{j-1}^n)
\]

After some elementary algebra, the tridiagonal form delivers the following coefficients

\[
a = C_A/2, \; b = -C_A/2, \; c = 1
\]

where

\[
C_A = \frac{Uh}{d}
\]

is the advective CFL number.

Simple calculations deliver the DDR in implicit form:

\[
e^{\gamma h} \cos(\omega_R h) = 1 \tag{6}
\]

\[
e^{\gamma h} \sin(\omega_R h) = C_A \sin(kd) \tag{7}
\]

By squaring and summing:

\[
e^{2\gamma h} = 1 + C_A^2 \sin^2(kd)
\]

This shows, that regardless of the value of \( C_A \), the rhs cannot be smaller than 1, which indicates unconditional instability.
The same conclusion would follow by inspecting the realizability of the tridiagonal formulation: one of the two side coefficients \(a\) and \(b\) is bound to be negative regardless of the value of \(C_A\).

How come such a simple scheme can be such a disaster? The reason is that it breaks a basic continuum symmetry between space and time. In the continuum, space and time derivatives come on the same footing, both first order, in fact \(x/U\) is an equivalent time.

5.1 Remedy: the upwind scheme

Having recognized the cause of the instability, a simple remedy comes by immediately: take finite-differences from one side only too. In particular, if \(U > 0\), one would difference the side the wind blows from, i.e. from left: 

\[-U(\phi_j - \phi_{j-1})/d.

Elementary algebra delivers the following coefficients

\[a = C_A, b = 0, c = 1 - C_A\]

This shows that stability is expected whenever \(C_A < 1\), again the CFL condition. But, how about accuracy?

By carrying on the detailed calculations, the upwind DDR reads as follows:

\[\gamma \sim (C_A - 1)Udk^2\]

This shows that under stable conditions, the upwind scheme introduces a substantial artificial damping, known as numerical diffusion.

Better solutions consist of adding some extra-diffusion term with negative diffusivity so as to compensate the artificial upwind diffusivity. This is known as Lax-Wendroff scheme, and it is tantamount to a centered difference of the original advection problem plus an artificial diffusion term of the form \((\delta + U^2h/2)\partial_{xx}\), with \(0 < \delta < 1\).

6 Advection-Diffusion-Reaction

\[\partial_t\phi = -U\partial_x\phi + D\partial_{xx}\phi + R(\phi)\]  

\(8\)
where the reaction term is local and non-linear. A very popular expression is the logistic growth \( R(\phi) = \alpha \phi(1 - \phi) \).

7 Other equations

The above notions are fairly powerful and general, they permit to analyse virtually any linear equation with constant coefficients. When non-linearity and/or inhomogeneity come into play, Fourier analysis formally fades away. However, it is still useful if these effects are sufficiently weak.

8 Boundary conditions

For the simple time-marching schemes discussed so far, it’s pretty simple. Consider the case of Dirichlet b.c.

\[ \phi^n_{j=1} = L, \phi^n_{j=N} = R, \]

Once this are set once and for all, one simply updates the bulk sites \( j = 2, N - 1 \) according to the usual scheme:

\[ \phi^{n+1}_j = a\phi^n_{j-1} + c\phi^n_j + b\phi^{n+1}_{j+1}, \ j = 2, N_1 \]

where boundary values are taken from the Dirichlet condition. The boundary nodes, on the other hand, require no update, since the Dirichlet conditions hold at all times.

![Boundary conditions diagram](image)

9 Multiple dimensions

The principles remain the same but new sources of error become relevant, a primary one being breaking of isotropy. Consider for instance the two-dimensional diffusion equation

\[ \partial_t \phi = D(\partial_{xx} + \partial_{yy})\phi(x, y; t) \]

With \( x_j = jd_x \) and \( y_l = ld_y \), a straightforward discrete Laplacian reads

\[ \Delta \phi \sim \frac{\phi_{j+1,l} - 2\phi_{j,l} + \phi_{j-1,l}}{d_x^2} + \frac{\phi_{j,l+1} - 2\phi_{j,l} + \phi_{j,l-1}}{d_y^2} \]

For the case \( d_x = d_y = d \), this leads to the well-known stencil
which is second order accurate and second order isotropic. To fourth order, anisotropic terms appear due to lack of connections along the diagonal, which introduce spurious terms proportional to the mixed derivatives $\partial_{xxyy}$. Powerful ways of obtaining accurate and isotropic stencils in $d=2$ and $d=3$ maybe discussed in a lecture apart, if desired.

10 Exercises

1. Write a computer program to solve the diffusion equation, test the accuracy and stability upon changing the mesh spacing

2. Same with the advection-diffusion equation

3. Show that the lax-Wendroff coefficients read as follows: $a = C_3 + C_A(1 + C_A)/2$, $b = C_3 + C_A(-1 + C_A)/2$, $c = 1 - a - b$, and analyze its stability and accuracy.
PDE’s for transport phenomena

**Diffusion Equation**

\[ \partial_t \varphi = D \partial_{xx} \varphi \]

**Advection-Diffusion Equation**

\[ \partial_t \varphi = -U \partial_x \varphi + D \partial_{xx} \varphi \]

**Advection-Diffusion-Reaction Equation**

\[ \partial_t \varphi = -U \partial_x \varphi + D \partial_{xx} \varphi + R \varphi \]

\[ \partial_t \varphi = \partial_x [(-U + D \partial_x) \varphi] + R \varphi \]
**PDE’s for transport phenomena**

**Linear homogeneous: similarity group**

\[ \varphi(x,0) \rightarrow \varphi(x,t) = \varphi(x - Ut) \quad \text{Translation} \]

\[ \varphi(x,0) \rightarrow \varphi(x,t) = \varphi(x^2 / Dt) \quad \text{Dilatation} \]

\[ \varphi(x,0) \rightarrow \varphi(x,t) = e^{Rt} \varphi(x,0) \quad \text{Growth/Decay} \]

**Inhomogenous, non-linear: broken symms**

\[ U = U(\varphi) \quad D(\varphi) \quad R = R(\varphi) \]

**DE: Dispersion Relation**

\[ \varphi(x, t) = Ae^{i(kx - \omega t)} = Ae^{i\gamma t} e^{ikx} \]

\[ \omega = \omega_r + i\gamma \]

\[ \omega_r = \omega_r(k) \quad \gamma = \gamma(k) \]

\[ V_{phys} = \frac{d\omega_r}{dk} \]

\[ \gamma < 0 \quad \text{Stable} \]

\[ \gamma > 0 \quad \text{Unstable} \]
Dispersion Relation: general

Propagation/Dispersion:

\[ \omega_r = c_1 k - c_3 k^3 + \ldots \]

Dispersion: different wavelengths
Propagate at different speed: shape changes

Diffusion/Hyperdiffusion

\[ \gamma = \gamma_0 - D k^2 + D_4 k^4 + \ldots \]

Hyperdiffusion: selective growth decay

\[ \gamma > 0 \quad \text{Unstable} \]

Numerical Diffusion: positive = overdamping
**Numerical dispersion:**

**Gibbs phenomena**

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**PDE’s in 1d: Tridiagonal form**

Using local (nearest-neighbor) stencils and simple fwd Euler in time:

\[
\varphi_j^{n+1} = a_j \varphi_{j-1}^n + c_j \varphi_j^n + b_j \varphi_{j+1}^n
\]

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**Computational Molecule:**

\[
\begin{array}{c}
n+1 \\
 n \\
 j-1 \\
 j \\
 j+1 \\
\end{array}
\]

---

11
**Discrete Dispersion Relation**

\[ \varphi_j^n = A e^{i(kx_j - \omega t_j)} \]

\[
\begin{align*}
    e^{\gamma_h} \cos(\omega, \hbar) &= 1 + (a + b)[\cos(kd) - 1] \\
    e^{\gamma_h} \sin(\omega, \hbar) &= (a - b)\sin(kd)
\end{align*}
\]

Direct observations, without even solving the DDR

- \( a = b \quad \omega_r = 0 \) **No Propagation**
- \( a, b > 0 \quad \gamma < 0 \) Stable in the continuum limit \( k \to 0 \)

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**Stability analysis: general**

\[ A_z = a \pm b \]

\[ C \equiv \cos(kd) - 1 \]

\[ S \equiv \sin(kd) \]

\[
\begin{align*}
    e^{2\gamma_h} &= (1 + A_z C)^2 + (A_z S)^2 \\
    \tan(\omega, \hbar) &= \frac{A_z S}{1 + A_z C}
\end{align*}
\]
Stability analysis: continuum limit

\[ A_i \equiv a \pm b \quad C \equiv \cos(kd) - 1 = -k^2d^2/2 \quad S = \sin(kd) = kd \]

\[ e^{2ik} = (1 - A_k k^2 d^2/2) + (A_k kd) = 1 - (A_k - A_k^2)k^2d^2 \]

\[ \tan(\omega, h) = A^{-1}kd \]

\[ \gamma = \frac{d^2}{2h}(A_k - A_k^2)k^2 \]

\[ \gamma > 0 \implies (a + b) > (a - b)^2 \]

\[ \omega = \frac{A_k d}{h} \implies V / V_{ad} = (a - b) \]

Now to actual PDE's
**Diffusion Equation d=1**

\[ \partial_t \varphi = D \partial_{xx} \varphi \]

\[ \varphi(x; 0) = \delta(x) \]

\[ \varphi(x; t) = \frac{1}{\sqrt{2Dt}} e^{-x^2/2Dt} \]

\[ \omega_r = 0 \]

\[ \gamma = -Dk^2 \]

**Diffusion Equation: Forward Euler**

\[ \partial_t \varphi \approx \frac{\varphi_{j}^{n+1} - \varphi_{j}^{n}}{h} \]

\[ n+1 \]

\[ n \]
\[ \frac{\varphi_j^{n+1} - \varphi_j^n}{h} = D \left[ \frac{\varphi_j^{n+1} - 2\varphi_j^n + \varphi_{j-1}^n}{d^2} \right] \]

\[ \delta \equiv \frac{Dh}{d^2} \equiv \frac{D}{D_{lat}} \]

\[ a = b = \delta \]

\[ c = 1 - 2\delta \]

\[ A_+ = 2\delta \quad A_- = 0 \text{ Surely stable in the continuum limit!} \]

No need to compute
Entry Exercise: Heat diffusion in 1d wire

\[ C \equiv \cos(k d) - 1 \]
\[ e^{2\delta k} = (1 + 2\delta C)^2 \]

\(-1 < 1 + 2\delta C < 1\)
\[ 2\delta C < 0 \Rightarrow \delta > 0 \quad (\text{Since } C < 0) \]
\[ 2\delta |C| < 2 \Rightarrow \delta < 1/2 \quad (\text{Since } |C| < 2) \]

This is the diffusive CFL.
**DE: Discrete DR**

Much swifter: **Realizability** (all coeffs must be non-negative):

\[ c > 0 \Rightarrow -1 < 1 - 4\delta < 1 \quad \delta < 1/2 \]

\[ \gamma = \frac{1}{2h} \log[1 + 4\delta C + 4\delta^2 C^2] = 2\delta C / h = -Dk^2 + O(kd)^3 \]

Stable and 2nd order accurate

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Entry Exercise: Heat diffusion in 1d wire
**Advection Equation**

\[ \partial_t \varphi + U \partial_x \varphi = 0 \]

\[ \varphi(x; t = 0) = \varphi_0(x) \]

\[ \varphi(x; t) = \varphi_0(x - Ut) \]

\[ \omega_r = U k \]

\[ \gamma = 0 \]

**AE: Centered-Euler**

\[ \frac{\varphi_j^{n+1} - \varphi_j^n}{h} = -U \left[ \frac{\varphi_{j+1}^n - \varphi_{j-1}^n}{2d} \right] \]

\[ \varphi_j^{n+1} = \frac{\alpha}{2} \varphi_{j-1}^n + \frac{1}{2} \varphi_j^n - \frac{\alpha}{2} \varphi_{j+1}^n \]

\[ a = \frac{\alpha}{2} \quad b = -\frac{\alpha}{2} \quad c = 1 \]

\[ \alpha \equiv \frac{U h}{d} = U / U_{lat} \]

Realizability: Never between [0,1] together >>> Always Unstable!
AE DDR

\[ e^{\nu h} \cos(\omega h) = 1 \]
\[ e^{\nu h} \sin(\omega h) = \alpha \sin(kd) \]

Stability:
\[ e^{2\nu h} = 1 + \alpha^2 \sin^2(kd) > 1 \]

Unconditionally unstable!

\[ A_+ = 0 \quad A_- = 2\alpha \]

AE: phase errors

\[ \tan(\omega_r h) = \alpha \sin(kd) \]

\[ \omega_r h = \alpha kd + O(kd^3) \]

\[ \omega_r = Uk + O(kd^3) \]

Dispersion errors: 3rd order
**Why centered FD is unstable?**

Broken space-time symmetry: time and space
Both first order in the continuum, broken by centered FD in space!

**AE: Stabilize centered FD**

Several families:

- Artificial Diffusion
- Lax-Wendroff
- Upwind (one-sided)
- Time Leapfrog
Artificial Diffusion: ADE

\[ \partial_t \varphi = -U \partial_x \varphi + \epsilon \partial_{xx} \varphi \]

\[ \frac{\varphi_{j}^{n+1} - \varphi_{j}^{n}}{h} = -U \left[ \frac{\varphi_{j+1}^{n} - \varphi_{j-1}^{n}}{2d} \right] + \epsilon \left[ \frac{\varphi_{j+1}^{n} - 2\varphi_{j}^{n} + \varphi_{j-1}^{n}}{d^2} \right] \]

\[ \varphi_{j}^{n+1} = a\varphi_{j-1}^{n} + c\varphi_{j}^{n} + b\varphi_{j+1}^{n} \]

ADE: Centered-Euler

\[ \varphi_{j}^{n+1} = a\varphi_{j-1}^{n} + c\varphi_{j}^{n} + b\varphi_{j+1}^{n} \]

\[ a = \delta - \alpha / 2 \]
\[ b = \delta + \alpha / 2 \]
\[ c = 1 - 2\delta \]

\[ \alpha = \frac{Uh}{d} \]
\[ \delta = \frac{\epsilon h}{d^2} \]
**Stability vs Realizability**

\[ a = \delta - \frac{\alpha}{2} > 0 \quad \alpha < 2\delta < 1 \]

\[ c = 1 - 2\delta > 0 \quad \delta < 1/2 \]

\[ \frac{\alpha}{\delta} = \frac{ud}{D} \equiv Pe_{\Delta} < 2 \]

\[ Pe_L = \frac{uL}{D} < 2L \]

**AE: Upwind**

\[ \frac{\varphi_{j+1} - \varphi_j}{h} = -U[\frac{\varphi_j - \varphi_{j-1}}{d}]; \quad U > 0 \]

\[ \frac{\varphi_{j+1} - \varphi_j}{h} = -U[\frac{\varphi_j - \varphi_{j+1}}{2d}]; \quad U < 0 \]

One sided: first order in BOTH space and time
**Upwind: DDR**

\[
e^{y_h} \cos(\omega, h) = 1 + \alpha(\cos(ka) - 1) \\
e^{y_h} \sin(\omega, h) = \alpha \sin(ka)
\]

\[
e^{y_h} = 1 + 2\alpha(\alpha - 1)[\cos(ka) - 1] < 0
\]

\[
\tan(\omega, h) = \frac{\alpha S}{1 + \alpha C}
\]

\[
\gamma = -(1 - \alpha)dU/k^2
\]

\[
D_{\text{num}} = Ud(1 - \alpha)
\]

---

**Lax-Wendroff**

Insert a velocity-dependent artificial diffusivity, to lower the strong numerical diffusivity of upwind

\[
L = -U \partial_x + (\epsilon + \frac{U^2 h}{2}) \partial_x^2
\]

\[
a = \frac{\alpha}{2}(1 + \alpha) \\
b = -\frac{\alpha}{2}(1 - \alpha) \\
c = (1 - \alpha^2)
\]
**Discrete ADE: Summary**

\[
\begin{array}{ccc}
\begin{array}{c}
a \\
\hline \\
\delta \\
\alpha / 2 \\
\delta + \alpha / 2 \\
\frac{\alpha}{2} + \frac{\alpha^2}{2} \\
1 - \alpha
\end{array} & b \\
\hline \\
\delta & \delta \\
-\alpha / 2 & \frac{\alpha}{2} - \alpha / 2 \\
\frac{\alpha}{2} + \frac{\alpha^2}{2} & \frac{\alpha}{2} + \frac{\alpha^2}{2} \\
0 & 0
\end{array}
\]

**ADR Equation**

\[
\partial_t \varphi + U \partial_x \varphi = D \partial_{xx} \varphi + R \varphi
\]

\[
\varphi(x; t = 0) = \varphi_0(x)
\]

\[
\varphi(x; t) = e^{Rt} \varphi_0[(x-Ut) / \sqrt{2Dt}]
\]

**Values**

\[
\begin{aligned}
\omega_r &= Uk \\
\gamma &= -Dk^2 + R
\end{aligned}
\]

*Large scale growth: k < sqrt(R/D)*
*Small scale decay: k > sqrt(R/D)*
**ADR: Centered-Euler**

\[ \Phi_{j}^{n+1} = a\Phi_{j-1}^{n} + c\Phi_{j}^{n} + b\Phi_{j+1}^{n} \]

\[ a = \delta - \alpha / 2 \]
\[ b = \delta + \alpha / 2 \]
\[ c = 1 - 2\delta + \kappa \]

\[ \alpha \equiv \frac{U\delta}{d} \quad \delta \equiv \frac{D\delta}{d^2} \quad \kappa \equiv Rh \]

**Boundary Conditions**

The DDR tells us about bulk behaviour, away from the boundaries. But boundaries MATTER!

The numerical eigenvalues of the transfer matrix must be computed. They are strongly affected by BC’s!

The numerical wavenumber is bounded between \( K_{\text{min}} = \frac{2\pi}{\text{size}} \) and \( K_{\text{max}} = \frac{2\pi}{d} \), with \( N=\text{size}/d \) there are \( N \) numerical eigenvalues. As \( N \) is sent to infinity they must recover the Continuum dispersion relation.
Boundary Conditions: Dirichlet

With explicit methods (present depends on past only) easy:

Dirichlet: \[ q_i^n = \Phi_i \quad q_{N}^n = \Phi_N \]

Bulk: \[ q_j^{n+1} = aq_{j-1}^n + cq_j^n + bq_{j+1}^n \]

Boundaries: \( j=1, j=N \) are taken by the BC specification:

The bulk gives a \((N-2)\times(N-2)\) matrix:

\[ q_2^{n+1} = a\Phi_1 + cq_3^n + bq_3^n \]

\[ q_{N-1}^{n+1} = aq_{N-2}^n + cq_{N-1}^n + b\Phi_N \]
Boundary Conditions: periodic

Periodic:

\[ q^{u}_{N+1} = q^{u}_1 \quad q^{u}_0 = \Phi_N \]

Spectra and 6 Fastest Growing Eigenfunctions of the Linearized ADR Spectra (2d random growth)

\[ \text{Im}(\lambda) \]

\[ \text{Re}(\lambda) \]

\[ F_i = 0.5 \]

\[ F_i = 1.5 \]
Assignments

1. Write a computer program to solve the 1d ADR with constant coefficients (with periodic boundaries).

2. Analyze the dispersion relation in the various parameter regimes (U,D,R) and associated CFL conditions.

3. Same, but computing the numerical spectrum of the transfer matrix $T$ (numerical propagator)

(Simple warm-up matlab programs available...)

End of Lecture