ME469A

Numerical Methods for Fluid Mechanics

Handout #2

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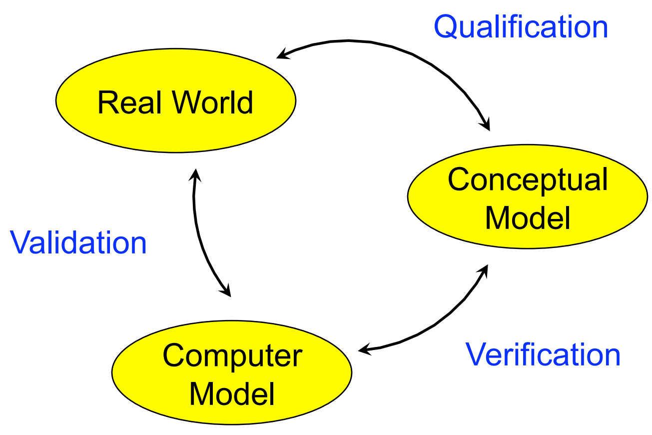


Qualification

Real World

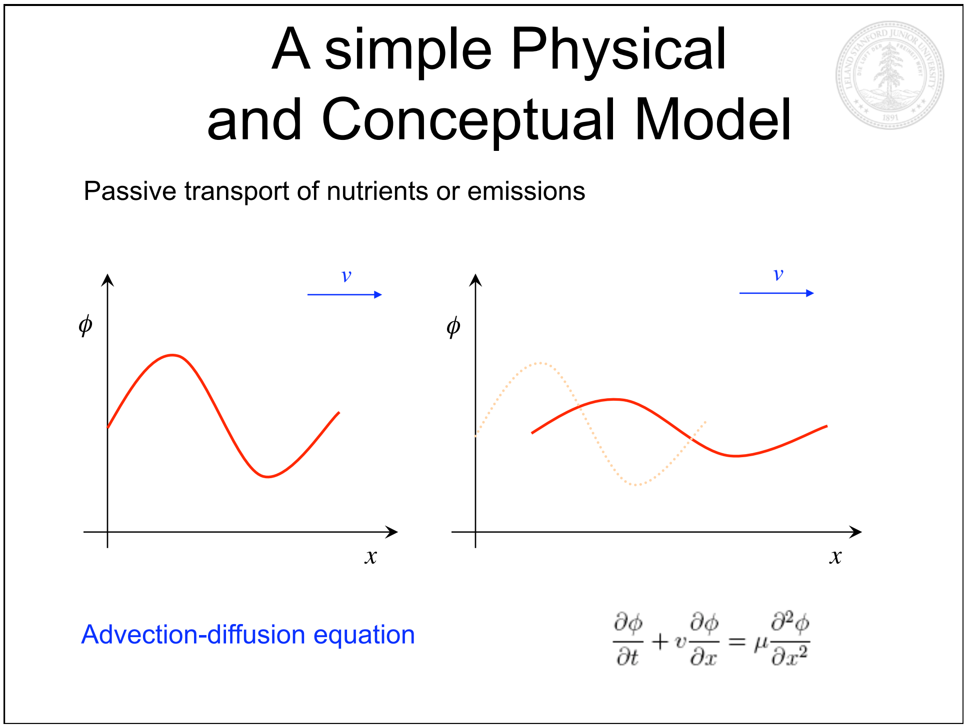
Conceptual Model

Validation

Computer Model

Verification

ME469A: study the connection between the conceptual model and a computer model for simulating incompressible fluid flows



A simple Physical and Conceptual Model

Passive transport of nutrients or emissions

Advection-diffusion equation

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \mu\frac{\partial^2 \phi}{\partial x^2}$$

A simple Physical and Conceptual Model

Qualification Step

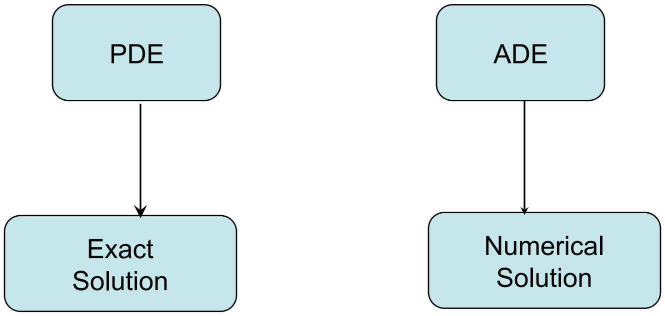
Advection-diffusion equation

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \mu\frac{\partial^2 \phi}{\partial x^2}$$

Convection is passive: velocity not a function of ϕ

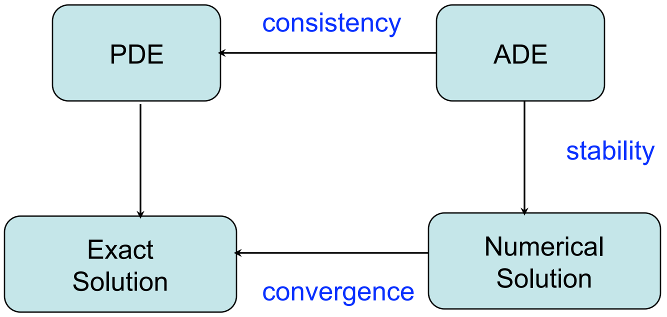
Diffusion is characterized by a constant diffusion coefficient μ

Numerical Simulations



What we would like… What we will get!

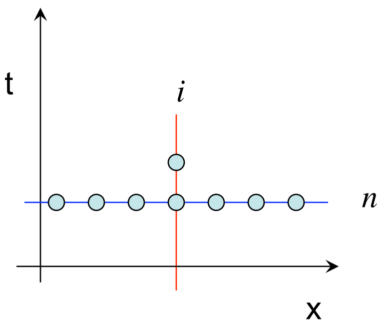
Properties of Numerical Methods



What we would like… What we will get!

Discretization Step

- The region of interest is transformed in a “discrete” tessellation: the grid.
- The solution to the original PDE is only sought at specific locations on this grid



Solution

$$\phi_i^n = \phi(x_i, t^n)$$

Simplest case: uniform spacing (Δx, Δt)

Discretization Step

- The continuous derivatives are transformed in discrete algebraic relationships between the grid point values (finite difference method)

- Using the definition of derivative:

$$\frac{\partial \phi(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x}$$

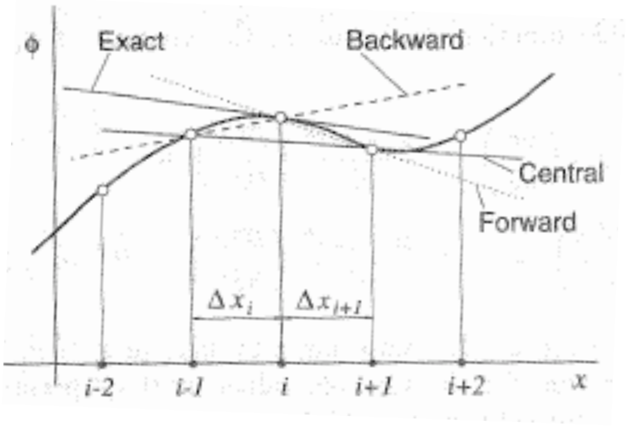
- But not evaluating to the limit *Δx*

$$\frac{\partial \phi(x,t)}{\partial x} \approx \frac{\phi(x + \Delta x, t) - \phi(x,t)}{\Delta x} = \frac{\phi_{i+1}^n - \phi_i^n}{\Delta x}$$

The approximate sign is the effect of the discretization error

Discretization Step

- Geometrical interpretation of discrete derivative



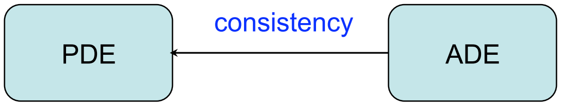
$$\left(\frac{\partial \phi}{\partial x}\right)_i \approx \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_i \approx \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_i \approx \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}}$$

Properties of Numerical Methods

Consistency: property of the discretization. The discretization of a PDE should asymptote to the PDE itself as the mesh/ timestep size tends to zero



PDE

consistency

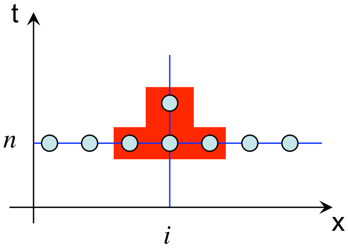
ADE

Consistency

Truncation error should vanish as the mesh size and time-step tend to zero

Pure convection: $\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = 0$

Discretized using a simple finite difference method:
forward (Euler) in time and central in space



$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + v\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = \mathcal{O}\left[(\Delta x)^p, (\Delta t)^q\right]$$

Consistency

Using Taylor series expansion:

$$\phi_i^{n+1} = \phi_i^n + \Delta t \left(\frac{\partial \phi}{\partial t}\right)_i^n + \frac{\Delta t^2}{2}\left(\frac{\partial^2 \phi}{\partial t^2}\right)_i^n \cdots$$

$$\phi_{i\pm 1}^n = \phi_i^n \pm \Delta x \left(\frac{\partial \phi}{\partial x}\right)_i^n + \frac{\Delta x^2}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i^n \pm \Delta x^3 6 \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i^n \cdots$$

We define the truncation error as:

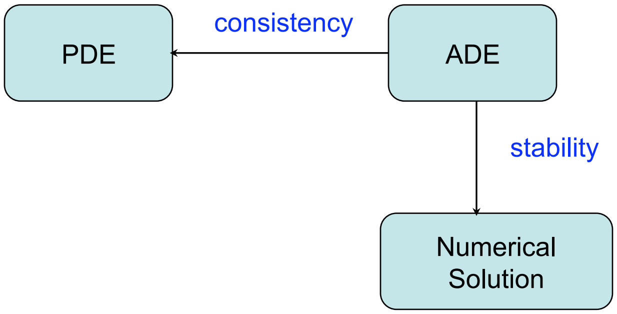
$$\underbrace{\left(\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x}\right)}_{conceptual\ model} - \underbrace{\left(\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + v\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}\right)}_{computational\ model} \equiv \epsilon_\tau$$

And therefore:

$$\epsilon_\tau = -\frac{\Delta t}{2}\left(\frac{\partial^2 \phi}{\partial t^2}\right)_i^n - v\frac{\Delta x^2}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i^n + \mathcal{O}\left[(\Delta x)^4, (\Delta t)^2\right]$$

Properties of Numerical Methods

Stability: Numerical errors (e.g. round-off due to the precision in the computer representation) are not allowed to grow unbounded



Stability

Stability is difficult to check. It can be verified for linear PDEs with constant coefficients and no-boundary conditions.

Define the error: $\epsilon_i^n = \phi_i^n - \bar{\phi}_i^n$

$\bar{\phi}_i^n$ Is the exact solution of the discretized equations

For example for the previous problem

$$\frac{\bar{\phi}_i^{n+1} - \bar{\phi}_i^n}{\Delta t} + v\frac{\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n}{2\Delta x} = 0$$

For linear problems, the error evolves in the same way as the numerical solution

Stability

Von Neumann analysis is one way to check stability

For linear problems and in the absence of boundary condition consider the error to be represented as a Fourier series

$$\epsilon_j^0 = \sum_{k=-N}^{N} E_j^0 e^{i\theta_k j}$$

Initial error

$$\epsilon_j^n = \sum_{k=-N}^{N} E_j^n e^{i\theta_k j}$$

After *n* steps, where $E_j^n = E_j^0 \lambda_j^n$

Amplification factor $G_j = \frac{E_j^{n+1}}{E_j^n} = \lambda_j$

Stability condition $|G_j| \leq 1 \quad \forall j$

Stability

Going back to the discretization considered before

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

And inserting the expression for the error

$$\left(E^{n+1} - E^n\right) e^{i\theta j} + v\frac{\Delta t}{\Delta x}\left(e^{i\theta(j+1)} - e^{i\theta(j+1)}\right) E^n \ = 0$$

Manipulating with $\alpha = v\frac{\Delta t}{\Delta x}$

$$E^{n+1} = E^n - \frac{\alpha}{2}E^n\left(e^{i\theta} - e^{-i\theta}\right)$$

We prove that the scheme is unstable

$$G = \frac{E^{n+1}}{E^n} = 1 - i\alpha sin\theta \qquad |G|^2 = 1 + \alpha^2 sin^2\theta \geq 1$$

Consistency & Stability

Recall the truncation error analysis

$$\epsilon_\tau = -\frac{\Delta t}{2}\left(\frac{\partial^2\phi}{\partial t^2}\right)_i^n - v\frac{\Delta x^2}{6}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i^n + \mathcal{O}\left[(\Delta x)^4, (\Delta t)^2\right]$$

Can be written in an equivalent form, noting:

$$\left(\frac{\partial\phi}{\partial t}\right)_i^n = -v\left(\frac{\partial\phi}{\partial x}\right)_i^n + \mathcal{O}\left[(\Delta x)^2, (\Delta t)\right]$$

$$\left(\frac{\partial^2\phi}{\partial t^2}\right)_i^n = -v\left(\frac{\partial^2\phi}{\partial t\partial x}\right)_i^n + \mathcal{O}\left[(\Delta x)^2, (\Delta t)\right] = v^2\left(\frac{\partial^2\phi}{\partial x^2}\right)_i^n + \mathcal{O}\left[(\Delta x)^2, (\Delta t)\right]$$

Consistency & Stability

We obtain

$$\epsilon_\tau = -\frac{\Delta t}{2}v^2\left(\frac{\partial^2\phi}{\partial x^2}\right)_i^n - v\frac{\Delta x^2}{6}\left(\frac{\partial^3\phi}{\partial x^3}\right)_i^n + \mathcal{O}\left[(\Delta x)^2, (\Delta t)^2\right]$$

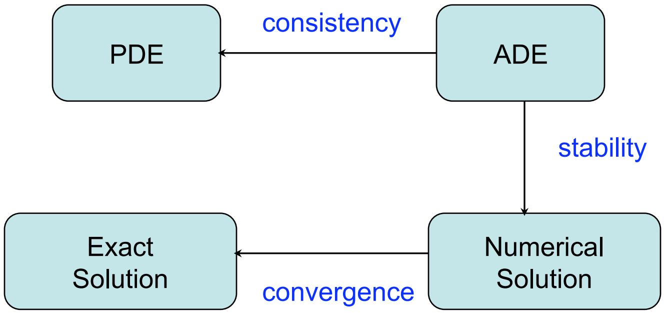
We can consider the effect of the truncation error as continuous terms in a modified differential equation

$$\frac{\partial\phi}{\partial t} + v\frac{\partial\phi}{\partial x} = -\frac{\Delta t}{2}v^2\frac{\partial^2\phi}{\partial x^2} + \mathcal{O}\left[(\Delta x)^2, (\Delta t)^2\right]$$

The nature of the discretization error is dissipative with a negative coefficient. Positive dissipation has the effect of reducing/damping the oscillations; negative viscosity has the effect of increasing oscillation, thus an unstable behavior.

Properties of Numerical Methods

Convergence: property of the solution. The numerical solution tend to the exact solution as the grid & timestep size decrease.



PDE

consistency

ADE

stability

Exact Solution

convergence

Numerical Solution

Convergence

Convergence can formally be checked only if the exact solution to the mathematical model is known!

$$\epsilon_i^n = \phi_i^n - \phi^e(i\Delta x, n\Delta t)$$

In practical terms one can investigate convergence numerically, by comparing numerical solution obtained on successively refined grids.

$$\phi^e = \phi_{\Delta x} + \epsilon(\Delta x)^p + \cdots = \phi_{2\Delta x} + \epsilon(2\Delta x)^p + \cdots = \cdots$$

Given three grids, we can compute the convergence order of the scheme

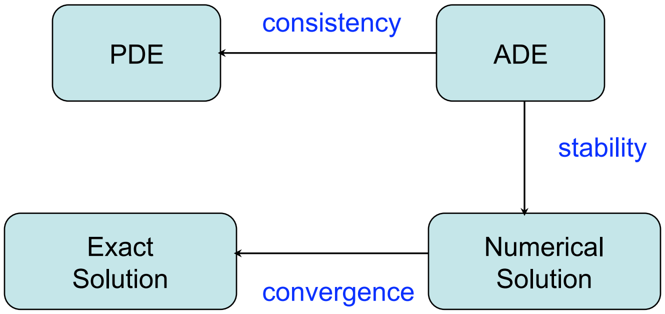
$$\phi_{2\Delta x} - \phi_{\Delta x} \approx \epsilon(\Delta x)^p \left(1 - 2^p\right)$$

$$\phi_{4\Delta x} - \phi_{2\Delta x} \approx \epsilon(\Delta x)^p \left(1 - 2^p\right) 2^p$$

$$p \approx log\left(\frac{\phi_{4\Delta x} - \phi_{2\Delta x}}{\phi_{2\Delta x} - \phi_{\Delta x}}\right)/log2$$

Lax Equivalence Theorem

For a well-posed linear problem discretized using a consistent method, stability is the necessary and sufficient condition for convergence



PDE

consistency

ADE

stability

Exact Solution

convergence

Numerical Solution

Convergence - Remarks

Grid convergence is an important step in solution verification

Given 3 nested grids the expected reduction of the error is:

$$p \approx log\left(\frac{\phi_{4\Delta x} - \phi_{2\Delta x}}{\phi_{2\Delta x} - \phi_{\Delta x}}\right)/log2$$

above formula require that ε is constant $\quad \phi^e = \phi_{\Delta x} + \epsilon(\Delta x)^p + \cdots$

The expression can be generalized for grids that are not nested but characterized by a non-integer grid space ratio *r*

$$p \approx log\left(\frac{\phi_{coarse} - \phi_{medium}}{\phi_{medium} - \phi_{fine}}\right)/log(r)$$

Grid space ratio is typically chosen as $1.1 > r > 2$

Richardson Extrapolation

The form of the grid convergence error allows to evaluate a high-order estimation of the solution

Solution on different grids differ only by the truncation error

$$f_1 = f_{\Delta x=0} + C\Delta x_1^p$$

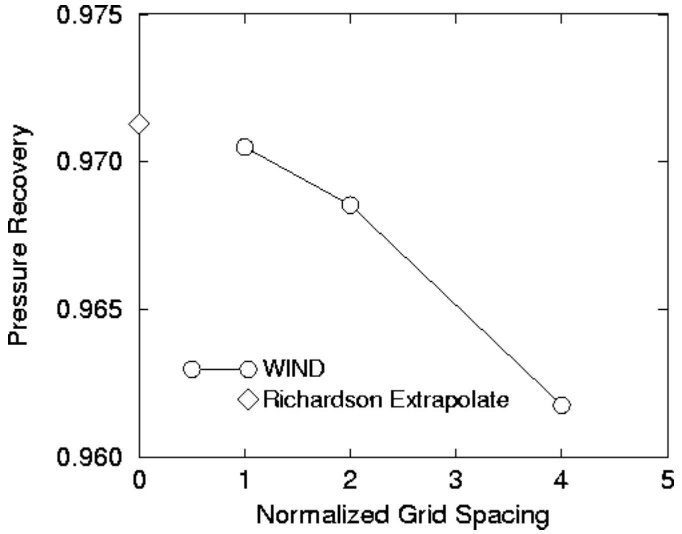
$$f_2 = f_{\Delta x=0} + C\Delta x_2^p$$

The estimate of the solution on an infinitely fine grid (continuous solution) is then

$$f_{\Delta x=0} \approx f_1 + \frac{f_1 - f_2}{r^p - 1}$$

The caveat is that the factor *C* in front of the truncation error is a constant – asymptotic rate of convergence.

Richardson Extrapolation



Convergence - Issues

How do you know if you are within the asymptotic range of convergence?

In spite of the numerical algorithm being p-order accurate, other aspect of the computational procedure introduce errors: floating numbers, iterative solvers, boundary condition treatment, etc. These error can become dominant once the discretization errors are reduced.

How do you evaluate convergence for non uniform meshes?

The simple expansion might not be representative of the true discretization error if the grid sequence is not chosen carefully

$$r_{effective} = \left(\frac{N_1}{N_2}\right)^{(1/D)}$$

Non-Linear Stability

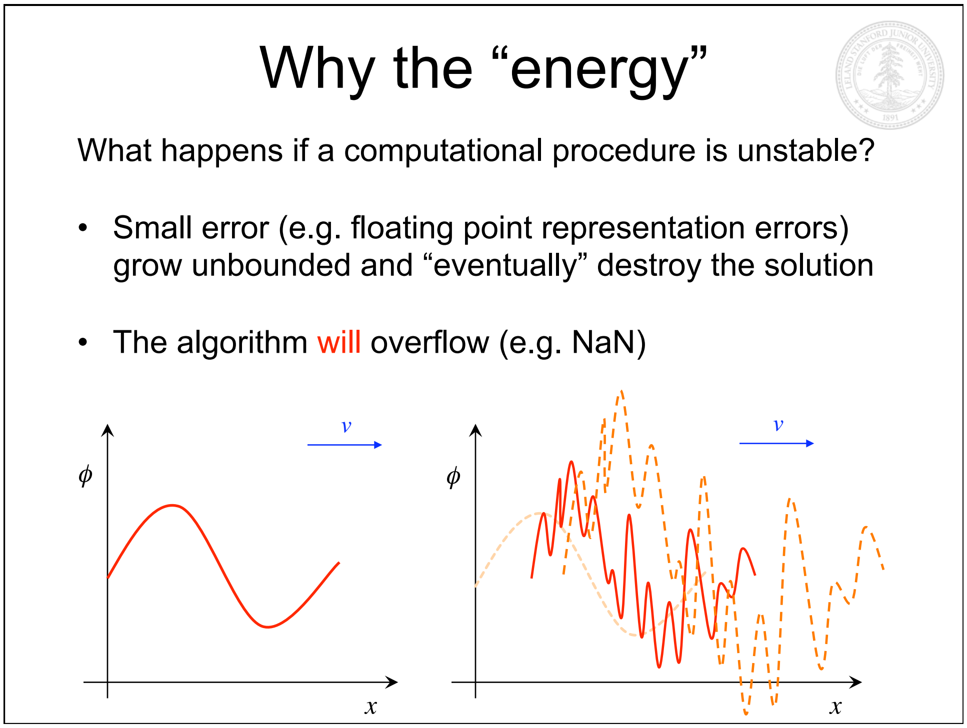
- Need to study non-linear stability for fluid flow applications
- One possibility is the “energy method”

As usual for the advection equation $\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$

Define a norm $||\phi|| = \phi^2/2$

The objective is to determine what is the behavior of the “energy”. Note that in the continuous space, the PDE for ϕ implies the same equation for $\phi^2/2$

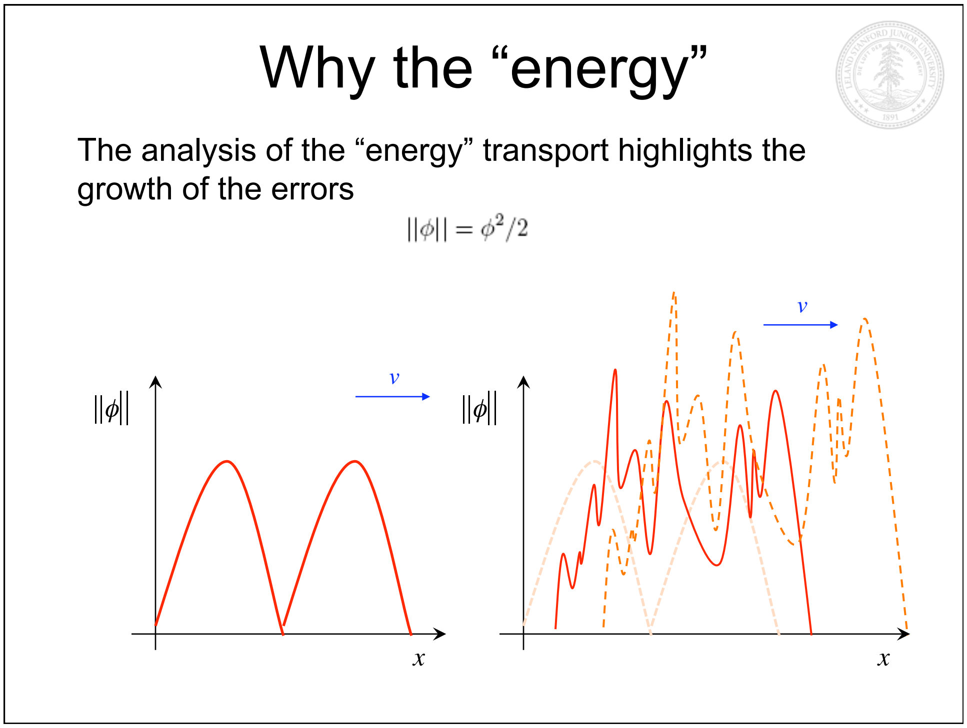
$$\phi\left[\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial x}\right] = 0 \longrightarrow \frac{\partial||\phi||}{\partial x} + v\frac{\partial||\phi||}{\partial x} = 0$$



Why the “energy”

What happens if a computational procedure is unstable?

- Small error (e.g. floating point representation errors) grow unbounded and “eventually” destroy the solution
- The algorithm will overflow (e.g. NaN)



Why the “energy”

The analysis of the “energy” transport highlights the growth of the errors

$$||\phi|| = \phi^2/2$$

Non-Linear Stability

Discretely:

$$\phi_j^{n+1}\frac{\phi_j^{n+1}-\phi_j^n}{\Delta t}+v\phi_j^{n+1}\frac{\phi_{j+1}^n-\phi_{j-1}^n}{2\Delta x}=0$$

$$\phi_j^n\frac{\phi_j^{n+1}-\phi_j^n}{\Delta t}+v\phi_j^n\frac{\phi_{j+1}^n-\phi_{j-1}^n}{2\Delta x}=0$$

Add

$$\frac{(\phi^2)_j^{n+1}-(\phi^2)_j^n}{\Delta t}+v\frac{1}{2\Delta x}\left(\phi_{j+1}^n-\phi_{j-1}^n\right)\left(\phi_j^{n+1}+\phi_j^n\right)=0$$

Manipulate

$$\frac{(\phi^2)_j^{n+1}-(\phi^2)_j^n}{\Delta t}+v\frac{1}{2\Delta x}\left(\phi_{j+1}^n-\phi_{j-1}^n\right)\left[\left(\phi_j^{n+1}-\phi_j^n\right)+2\phi_j^n\right]=0$$

Non-Linear Stability

Discretely:

$$\frac{(\phi^2)_j^{n+1}-(\phi^2)_j^n}{\Delta t}+v\frac{1}{2\Delta x}\left(\phi_{j+1}^n-\phi_{j-1}^n\right)\left(\phi_j^{n+1}-\phi_j^n\right)+2v\frac{1}{2\Delta x}\phi_j^n\left(\phi_{j+1}^n-\phi_{j-1}^n\right)=0$$

First term

$$v\frac{1}{2\Delta x}\left(\phi_{j+1}^n-\phi_{j-1}^n\right)\left(\phi_j^{n+1}-\phi_j^n\right)\approx v\frac{1}{2\Delta x}\left(\phi_{j+1}^n-\phi_{j-1}^n\right)\Delta t\frac{\partial\phi}{\partial t}$$

$$\approx -v^2\frac{\Delta t}{4\Delta x^2}\left(\phi_{j+1}^n-\phi_{j-1}^n\right)^2=\Delta t v^2\left(\frac{\partial\phi}{\partial x}\right)^2$$

Second term

$$2v\frac{1}{2\Delta x}\phi_j^n\left(\phi_{j+1}^n-\phi_{j-1}^n\right)\approx 2v\phi\frac{\partial\phi}{\partial x}=v\frac{\partial\phi^2}{\partial x}$$

Non-Linear Stability

We obtain a modified equation for the energy:

$$\frac{\partial(\phi^2)}{\partial t} + v\frac{\partial(\phi^2)}{\partial x} = \Delta t v^2 \left(\frac{\partial \phi}{\partial x}\right)^2$$

The modified equation for the "energy" includes a positive source term. Again, another proof of instability!

Dissipation vs. Dispersion

Consider again the pure convection equation

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = 0$$

Consider two discretization techniques and two different resulting modified equations

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} - \alpha\frac{\partial^2 \phi}{\partial x^2} = 0$$
$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} + \beta\frac{\partial^3 \phi}{\partial x^3} = 0$$

How to gain a physical understanding of the type of discretization error?

Dissipation vs. Dispersion

Model 1

$$\frac{\partial\phi}{\partial t}+v\frac{\partial\phi}{\partial x}-\alpha\frac{\partial^2\phi}{\partial x^2}=0$$

Postulate an expression for the solut $\phi=e^{pt}e^{ikx}$

Plug in the equation $pe^{pt}e^{ikx}+ivke^{pt}e^{ikx}+\alpha k^2e^{pt}e^{ikx}=0$

$$p=-ivk-\alpha k^2$$

Obtain : $\phi=e^{(-ivk-\alpha k^2)t}e^{ikx}=e^{ik(x-vt)}e^{-\alpha k^2 t}$

Dissipation vs. Dispersion

Model 2

$$\frac{\partial\phi}{\partial t}+v\frac{\partial\phi}{\partial x}+\beta\frac{\partial^3\phi}{\partial x^3}=0$$

Postulate an expression for the solution

Plug in the equation $pe^{pt}e^{ikx}+ivke^{pt}e^{ikx}-\beta ik^3e^{pt}e^{ikx}=0$

$$p=-ivk+\beta ik^3$$

Obtain : $\phi=e^{(-ivk+\beta ik^3)t}e^{ikx}=e^{ik\left[(x-vt)+\beta k^2 t\right]}=$

$$=e^{ik\left[x-(v-\beta k^2)\right]t}=e^{ik(x-\bar{v}t)}$$

Dissipation vs. Dispersion

Model 1

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} - \alpha\frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\phi = e^{ik(x-vt)}e^{-\alpha k^2 t}$$

Model 2

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} + \beta\frac{\partial^3 \phi}{\partial x^3} = 0$$

$$\phi = e^{ik(x-\tilde{v}t)}$$

Assuming that the initial condition is: $\phi(x, t=0) = e^{ikx}$

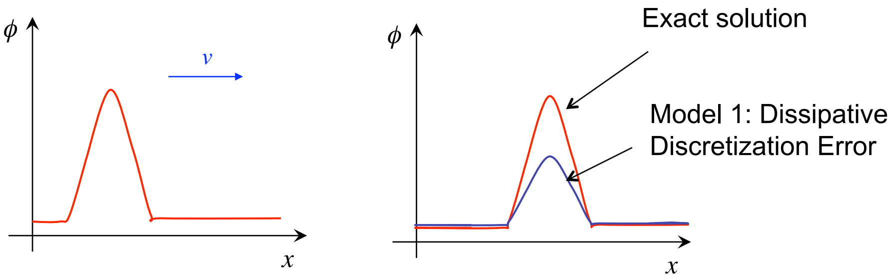
The exact solution is: $\phi_{exact} = e^{ik(x-vt)}$

Dissipation vs. Dispersion

Model 1

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} - \alpha\frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\phi = e^{ik(x-vt)}e^{-\alpha k^2 t}$$



Exact solution

Model 1: Dissipative Discretization Error

Initial condition

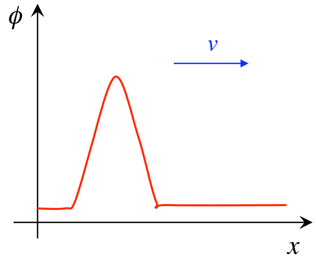
Later time

Dissipation vs. Dispersion

Model 2

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} + \beta\frac{\partial^3 \phi}{\partial x^3} = 0$$

$$\phi = e^{ik\left[x-(v-\beta k^2)\right]t} = e^{ik(x-\tilde{v}t)}$$

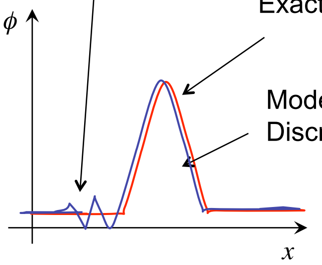


Initial condition

High frequency components propagate at slower speed

Exact solution

Model 2: Dispersive Discretization Error



Later time

Other properties

- Conservation
- Boundedness
- Symmetry
- …

We will consider them for the Navier-Stokes equations