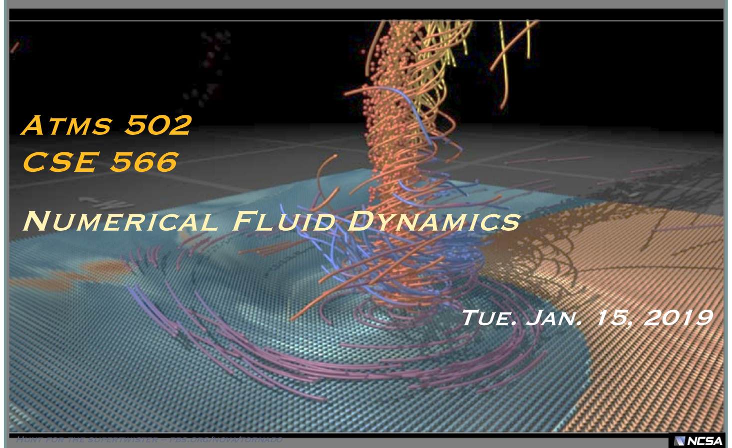

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Scientific computing

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A LOOK AHEAD, BY EXAMPLE.

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Characterize this phenomena

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- Scale
  - *spatial - wavenumber, wavelength*
  - *temporal: frequency, period*
- Dimensionality
  - *3-D but...*
  - *2-D form: XY slab, axisymmetric*
- Linearity
  - *is it or not?*
  - *one or the other...?*
- Limits
  - *on resolution*
  - *on duration, max V*
- Prognostic?
  - *steady state solutions?*
  - *form of equations*
- Solving it
  - *grid mesh*
  - *equation set, variables*
  - *types of waves in the solution*

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Welcome to ATMS 502, CSE 566

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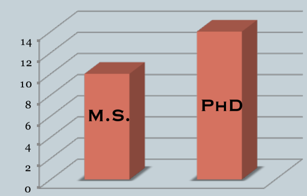
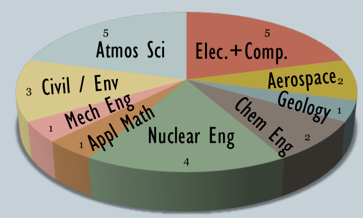
- Who are we here?
  - Me:
  - You:
    - As of today …
    - 24 enrolled
    - Mostly: Ph.D students





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Things to do *as soon as possible*

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1. Go to *xsede.org,* Make account
   1. Email me your *username* - not password!
2. Get remote login/transfer/X11* software on your PC
   - Windows:
     - Connect: Xshell/Xftp
     - X11 client: Xming
     - Editing: Notepad++ w/additions
   - Macintosh:
     - Connect: Terminal/iTerm2;
     - X11: built-in
     - Editing: Textwrangler/BBedit + additions

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Welcome to ATMS 502, CSE 566

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- Overview
  - What do we want to achieve?
- Course organization
  - Semester plan; grades; assignments
- Survey
- Computing accounts & assignments
- Scientific computing
- Our first computer problem

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Overview

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- What do we want to achieve?
  - The ability to:
    - develop, critique, improve, and apply numerical methods to multi-dimensional, nonlinear fluid flow problems.
  - One step at a time.
    - Develop: write the code. Debug. Run. View. Understand.
      - we will also address code efficiency and parallelism
    - Critique: What are the strengths/weaknesses of the approach? What caveats do we need to keep in mind for the solutions? How do we know we have a "good" solution?
    - Improve: Should the numerical approach be improved? How? And towards what objective?
    - Apply: With a numerical model ready: How do use it (wisely) to deliver the meaningful solutions we seek?

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Course organization

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- Introduction / schedule
  - *handout*
    - contact information
    - "books"
    - grade breakdown
    - planned exam/program due dates- next class
    - working with others; academic integrity
    - homework, readings
    - computer programs – test cases

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Three areas to cover.

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Fluid Flow	Coding, Data	Numerical Methods
This gives us context.	Nuts and bolts…	Finally, put it all together.
	Files.	
What are we solving?	Accounts etc.	Getting a solution you can believe in.
What solution(s) should we expect?	Dealing with data.	Quantifying "good" (or bad).

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Three areas to cover.

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Fluid Flow	Coding, Data	Numerical Methods
Concept	Old vs. new: IDEs	Classes
Kinematics	Languages	Dimensions
Equations	Compilers	Bound. conditions
Dimensions	Precision, accuracy	Symmetry
Units	(Super)computers	Linear, or not
Compressibility	Debugging	Stability
Stability, shear	Optimization basics	Systems of eqns
Simplifications	Data, 4^{th} paradigm	Discontinuities
Classic solutions	Visualization	Initialization

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Online tools/resources

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1. Compass
   a) Reading assignments will be here
   b) Computer problem submissions are here!
   c) Some data sets may be distributed from here.
2. Class content/home page - *ready by next class*
   https://www.atmos.illinois.edu/courses/atmos502-sp2019/
   a) Daily lecture notes
   b) Homework & computer program handouts
   c) Resources: textbook PDFs, links to presentations

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Program #1

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1-D linear and nonlinear transport ("advection")

- USING THE DEMONSTRATION CODE;
- WORKING ON & GETTING ANSWERS FOR OUR FIRST COMPUTER ASSIGNMENT

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Program 1 and **our three main topics -**

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1. Fluid Flow

This program concerns only *advection* (fluid transport)

2. Coding, Data

This is the main time sink here: *getting started!*

Computer accounts
Using linux
Modifying code
Compiling
Running
Making plots

3. Numerical Methods

We'll start with one simple method.

It is called *Lax-Wendroff*

We'll derive the method later.

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1. Fluid flow equations

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$$\frac{\partial u}{dt} = -\vec{V}\cdot\vec{\nabla}u - \frac{1}{\bar{\rho}}\frac{\partial p}{\partial x} + \nu\nabla^2 u$$

$$\frac{\partial v}{dt} = -\vec{V}\cdot\vec{\nabla}v - \frac{1}{\bar{\rho}}\frac{\partial p}{\partial y} + \nu\nabla^2 v$$

$$\frac{\partial w}{dt} = -\vec{V}\cdot\vec{\nabla}w - \frac{1}{\bar{\rho}}\frac{\partial p}{\partial z} + g\frac{\theta}{\bar{\theta}} + \nu\nabla^2 w$$

$$\frac{\partial \theta}{\partial t} = -\vec{V}\cdot\vec{\nabla}\theta + Q(x,y,z,t) + \nu\nabla^2\theta$$

$$\frac{\partial p}{\partial t} = -c_s^2\left[\bar{\rho}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \frac{\partial(\bar{\rho}z)}{\partial z}\right] + \nu\nabla^2 p$$

- Q: What are we solving?
- A: The time change + *advective* terms on right side.

Methods | Code, data | Fluid eqns

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Advection – linear and nonlinear

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- Program 1, *linear* (cases A and B)
  - Velocity field does not change
  - Such as: $\frac{\partial \theta}{\partial t} = -\vec{V}\cdot\vec{\nabla}\theta$
- Program 1, *nonlinear* (case C)
  - Field being advected is also the velocity!
  - Such as: $\frac{\partial u}{dt} = -\vec{V}\cdot\vec{\nabla}u$

Methods | Code, data | Fluid eqns

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2. Code and data

Demonstration code

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DEFAULT (GIVEN TO YOU)
BEHAVIOR: *DAMPING*

YOU WILL NEED TO
CHANGE THIS CODE
TO CORRECTLY SOLVE THE PROBLEM!

Methods | Code, data | Fluid eqns

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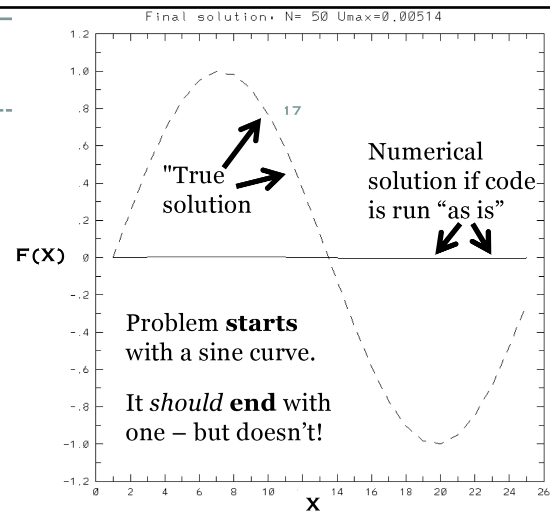


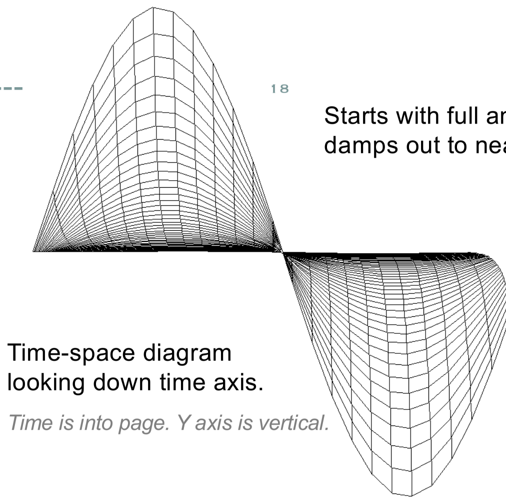
Problem **starts** with a sine curve.

It *should* **end** with one – but doesn't!

Methods | Code, data | Fluid eqns

DEMONSTRATION PROGRAM RESULTS

1/18/19



Starts with full amplitude damps out to near zero.

Time-space diagram looking down time axis.

Time is into page. Y axis is vertical.

Methods | Code, data | Fluid eqns

DEMONSTRATION PROGRAM RESULTS

1/18/19

Demonstration code

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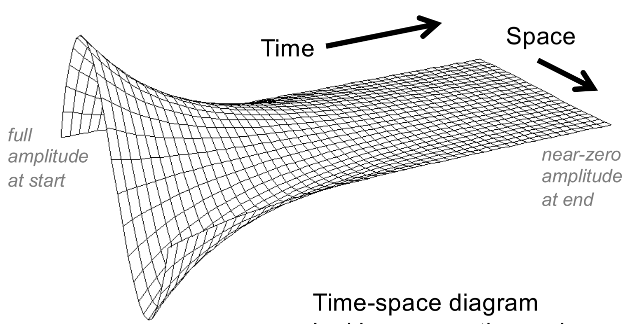

Time-space diagram looking across time axis.

This is the demo code run "as is", *not* the correct answer.

Methods | Code, data | Fluid eqns

DEMONSTRATION PROGRAM RESULTS

1/18/19

Code structure

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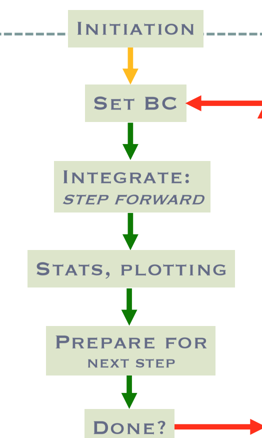
- Demonstration code has all the elements..
  - Initiation
  - Integration
  - Prepare for next step
  - Boundary conditions
  - Simple stats
  - Plotting



Methods | Code, data | Fluid eqns

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Review: cases A, B

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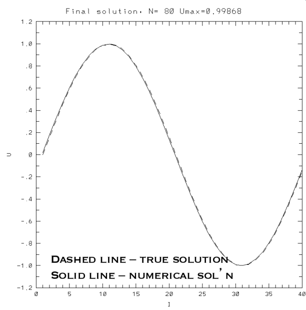

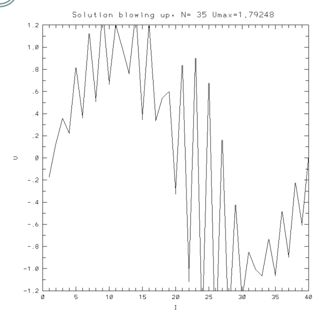

CASE A: STABLE

CASE B: UNSTABLE

SLIGHTLY DIFFERENT CODE CONFIGURATION FROM YOURS

Methods | Code, data | Fluid eqns

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Case "C"

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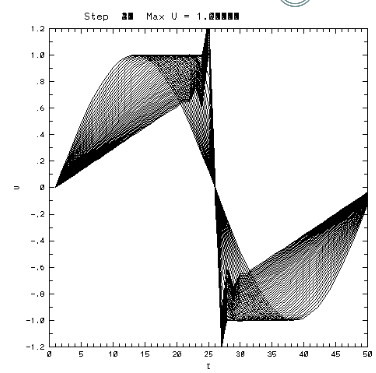

NONLINEAR (CASE "C")

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Time history: Case "C"

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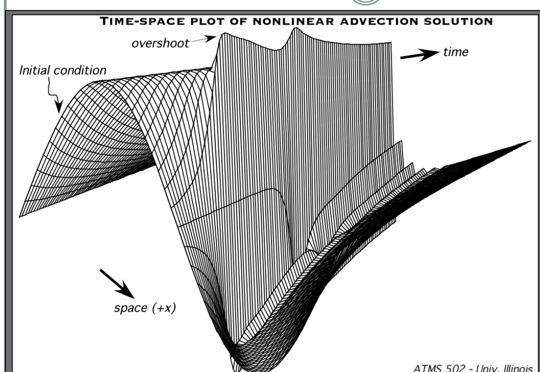

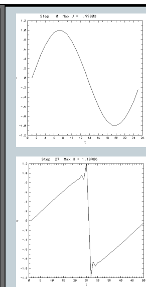

Methods | Code, data | Fluid eqns

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Lax-Wendroff *our first method*

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1. So what do we mean by this?

$$s_j^{n+1} = s_j^n - \frac{\nu}{2}\left(s_{j+1}^n - s_{j-1}^n\right) + \sigma\left(s_{j+1}^n - 2s_j^n + s_{j-1}^n\right)$$

2. S(j,n) is the value –
   - At grid point "j"; j = 1,nx
   - At time "level" n; n = 1, nstep
   - ν is a parameter, read in; σ = $\nu^2/2$.
   - We march forward; at each time level *n*, we compute values for *n+1* for all grid points *j*

Methods | Code, data | Fluid eqns

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