

Numerics: The analysis and implementation of numerical methods for solving differential equations

Dr Hilary Weller, <h.weller@reading.ac.uk>

November 6, 2017

Timetable

| Week | Chapters to read before class | Videos to watch before class | Class Date | Assignment | Deadline | Prop- ortion |
|------|---|---------------------------------|---------------|------------------------------|----------|-----------------|
| 1 | 1-3 | 1-4 | Wed 4 Oct | Code review | 25 Oct | 5% |
| | Introduction and linear advection schemes | | | | | |
| 3 | 4-5 | 5.0-5.4, 6.0-6.1 | Wed 18 Oct | Draft report for feedback | 15 Nov | 5% |
| | Analysis of Linear Advection Schemes and dispersion | | | | | |
| 6 | 6-7 | 7.0-7.5, 8.0-8.5 | Wed 8 Nov | Final code | 29 Nov | 15% |
| | More Advection Schemes and Wave equations | | | | | |
| | | | | Final report | 6 Dec | 25% |

Further Resources (Not essential reading)

Python

- “A Hands-On Introduction to Using Python in the Atmospheric and Oceanic Sciences” by Johnny Wei-Bing Lin. <http://www.johnny-lin.com/pyintro>
- “Think Python. How to Think Like a Computer Scientist” by Allen B. Downey. <http://www.greenteapress.com/thinkpython/thinkpython.html>
- “Numerical Methods in Engineering with Python” by Jaan Kiusalaas
- www.southampton.ac.uk/sesg3020/textbook/SciPyIntro.pdf
- <http://www.python.org>
- <http://docs.python.org/tutorial/>
- <http://matplotlib.sourceforge.net/users/index.html>
- <http://matplotlib.sourceforge.net/users/pyplotutorial.html>
- <http://software-carpentry.org/>
- <http://www.diveintopython.net/>
- <http://learnpythononthehardway.org/>
- <http://www.ibiblio.org/g2swap/byteofpython/read/>
- “Making Use of Python” by Rashi Gupta
- “Python Essential Reference” by David M. Beazley (Addison Wesley)
- “Learning Python” Mark Lutz (O’Reilly Media)

Numerical Methods

- Weller, H. Draft of chapter for “Mathematics for Planet Earth, a Primer”
<http://www.met.reading.ac.uk/~sws02hs/teaching/>
3

PDEsNumerics/WellerPrimer.pdf

- Wikipedia <http://en.wikipedia.org>
- Durran, D. R. Numerical methods for fluid dynamics (Springer).
- LeVeque, R. Numerical Methods for Conservation Laws (Springer)
- Ortega, J.M. and Poole, W.G. An Introduction to Numerical Methods for Differential Equations. 1981 (Pitman Publishing Inc)
- Ferziger, J. H. and Peric, M. Computational Methods for Fluid Dynamics (Springer).
- Numerical Recipes: The Art of Scientific Computing, Third Edition (2007), (Cambridge University Press). <http://www.nr.com/>
- Lloyd N. Trefethen. Finite Difference and Spectral Methods for Ordinary and Partial Differential Equations.
<https://people.maths.ox.ac.uk/trefethen/pdetext.html>

Other People’s lecture notes for similar courses

- <https://people.maths.ox.ac.uk/trefethen/pdetext.html>
- http://www.aei.mpg.de/~rezzolla/lnotes/Evolution_Pdes/
[evolution_pdes_lnotes.pdf](http://www.aei.mpg.de/~rezzolla/lnotes/Evolution_Pdes_lnotes.pdf)

Websites for this course:

<http://mpecdt.bitbucket.org/>

It contains notes, example programs and solutions to problems and practicals.

<https://share.imperial.ac.uk/fons/mathematics/mpecdt/students/Lists/TeamDiscussion/>

For discussion cite to asking and answering questions about the module

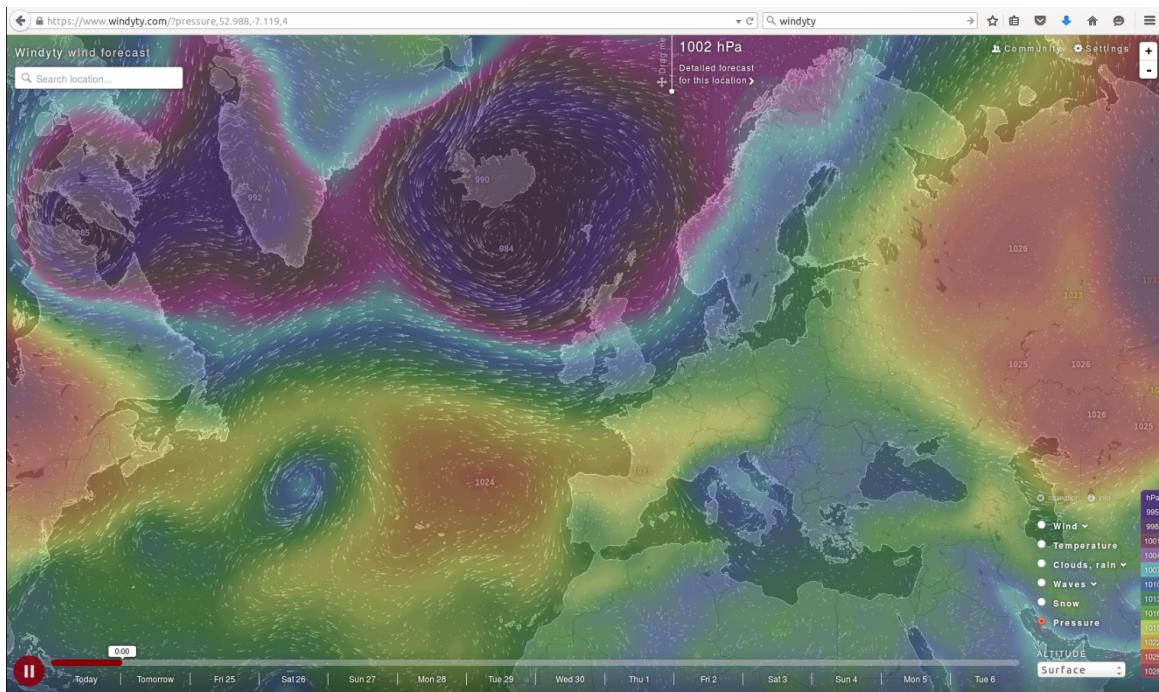
Contents

| | |
|--|-----------|
| 1 The Navier Stokes Equations | 10 |
| 1.1 The Potential Temperature Equation | 11 |
| 1.2 Advection of Pollution | 12 |
| 1.2.1 Pure Linear Advection | 12 |
| 1.2.2 Advection/Diffusion with Sources and Sinks | 13 |
| 1.3 The Momentum Equation | 14 |
| 1.3.1 Coriolis | 14 |
| 1.3.2 The Pressure Gradient Force | 15 |
| 1.3.3 Gravitational Acceleration: A simulation of a dam break | 19 |
| 1.3.4 Diffusion | 21 |
| 1.3.5 The Complete Navier Stokes Equations | 22 |
| 2 Linear Finite Difference Schemes for Advection | 23 |
| 2.1 Forward in Time, Backward in Space (FTBS) | 24 |
| 2.1.1 Order of Accuracy of FTBS | 26 |
| 2.2 Centred in Time, Centred in Space (CTCS) and FTCS | 27 |
| 2.2.1 Order of Accuracy of CTCS | 28 |
| 2.3 Implicit and Explicit Schemes | 29 |
| 2.4 Backward in Time, Centred in Space (BTCS) | 30 |
| 3 Fourier Analysis | 32 |
| 3.1 Fourier Series | 32 |
| 3.2 Fourier Transform | 36 |
| 3.3 Discrete Fourier Transform | 36 |
| 3.4 Differentiation and Interpolation | 38 |
| 3.5 Spectral Models | 38 |
| 3.6 Wave Power and Frequency | 38 |
| 3.7 Recap Questions | 39 |
| 3.8 Analysing Power Spectra | 40 |
| 4 Numerical Analysis of Advection Schemes | 43 |
| 4.1 Introduction: What is Numerical Analysis and why is it done | 43 |
| 4.2 Some Definitions | 44 |
| 4.3 Convergence and errors | 47 |
| 4.4 Lax-Equivalence Theorem | 48 |
| 4.5 Domain of Dependence | 49 |
| 4.5.1 Courant-Friedrichs-Lowy (CFL) criterion: | 50 |
| 4.5.2 Domain of Dependence of FTBS | 50 |
| 4.5.3 The Domain of Dependence of the CTCS Scheme | 51 |
| 4.6 Von-Neumann Stability Analysis | 52 |
| 4.6.1 Von-Neumann Stability Analysis of FTBS | 53 |
| 4.6.2 What should A be for real linear advection? | 54 |
| 4.6.3 Von Neumann Stability Analysis of CTCS | 55 |
| 4.7 Conservation | 56 |
| 4.7.1 Conservation of higher moments | 57 |
| 4.8 Exercises: Analysis of Advection Schemes (answers on blackboard) | 58 |
| 5 Waves, Dispersion and Dispersion Errors | 59 |
| 5.1 Some Background on Waves | 59 |
| 5.2 Dispersion | 62 |

| | | |
|----------|---|-----------|
| 5.3 | Some Excellent Animations and Videos which demonstrate Dispersion | 67 |
| 5.4 | Phase speed of linear advection | 68 |
| 5.5 | Phase speed and dispersion errors of CTCS | 69 |
| 5.6 | Exercise | 71 |
| 6 | Alternative Advection Schemes | 73 |
| 6.1 | Semi-Lagrangian Advection | 74 |
| 6.1.1 | Semi-Lagrangian Advection in One Dimension | 75 |
| 6.2 | Artificial Diffusion to Remove Spurious Oscillations | 76 |
| 6.3 | The Finite Volume Method | 77 |
| 6.3.1 | The Finite Volume Method in one dimension, for constant u | 78 |
| 6.4 | Lax-Wendroff | 79 |
| 6.5 | Total Variation | 81 |
| 6.6 | Total Variation Diminishing (TVD) schemes | 82 |
| 6.6.1 | Limiter functions | 83 |
| 6.6.1.1 | Exercise | 83 |
| 6.6.2 | The Sweby Diagram | 84 |
| 6.6.3 | The Van Leer Limiter | 84 |
| 7 | Modelling Wave Equations | 85 |
| 7.1 | Simulations of the SWE on the surface of a sphere | 86 |
| 7.2 | Processes Represented by the SWE | 87 |
| 7.2.1 | Linearised SWE | 89 |
| 7.3 | Analytic Solution | 89 |
| 7.4 | Unstaggered Forward-Backward (1d A-grid FB) | 90 |
| 7.4.1 | Von-Neumann Stability Analysis | 91 |
| 7.4.2 | Dispersion of Unstaggered Forward-Backward (1d A-grid FB) | 92 |
| 7.5 | Problems with Co-location of h and u | 93 |
| 7.6 | Staggered Forward-Backward (1d C-grid FB) | 94 |
| 7.7 | Arakawa Grids | 95 |
| 7.8 | Linearised Shallow-Water Equations on Arakawa Grids | 96 |
| 7.9 | Discussion Question | 96 |

Numerical Modelling of the Atmosphere and Ocean

Weather, ocean and climate forecasts predict the winds, temperature and pressure from the Navier-Stokes equations:



9

Chapter 1: The Navier Stokes Equations

The Navier-Stokes Equations for a compressible, rotating atmosphere

$$\text{The Lagrangian derivative: } \frac{D\Psi}{Dt} = \frac{\partial\Psi}{\partial t} + \mathbf{u} \cdot \nabla\Psi$$

$$\text{Momentum } \frac{D\mathbf{u}}{Dt} = -2\boldsymbol{\Omega} \times \mathbf{u} - \frac{\nabla p}{\rho} + \mathbf{g} + \mu_u \left(\nabla^2 \mathbf{u} + \frac{1}{3} \nabla(\nabla \cdot \mathbf{u}) \right)$$

$$\text{Continuity } \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0$$

$$\text{Energy } \frac{D\theta}{Dt} = Q + \mu_\theta \nabla^2 \theta$$

An equation of state, eg perfect gas law, $p = \rho RT$

| | | | |
|-----------------------|-------------------------|---------------------|---|
| u | Wind vector | g | Gravity vector (downwards) |
| <i>t</i> | Time | θ | Potential temperature, $T (p_0/p)^\kappa$ |
| $\boldsymbol{\Omega}$ | Rotation rate of planet | κ | heat capacity ratio ≈ 1.4 |
| ρ | Density of air | Q | Source of heat |
| p | Atmospheric pressure | μ_u, μ_θ | Diffusion coefficients |

We will learn how to solve simplified versions numerically.

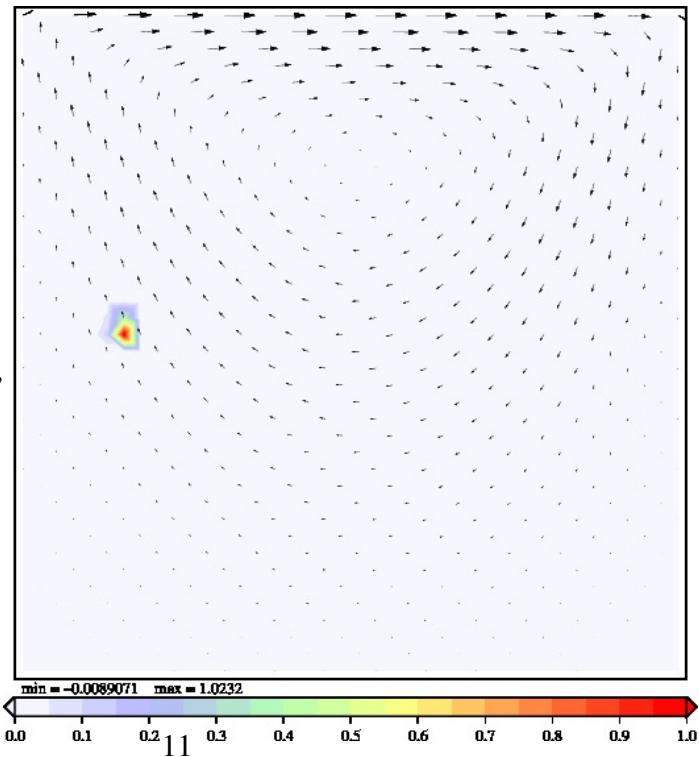
You do not need to memorise the equations but you should be able to describe the meaning and behaviour of the terms ...

1.1 The Potential Temperature Equation

$$\frac{D\theta}{Dt} = \frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = Q + \mu_\theta \nabla^2 \theta$$

Lagrangian derivative Rate of change at fixed point Advection of θ Heat source Diffusion of θ

θ will be created and destroyed by the heat source, Q , it will be moved around by the wind field, \mathbf{u} , and θ will be diffused by a diffusion coefficient, μ_θ



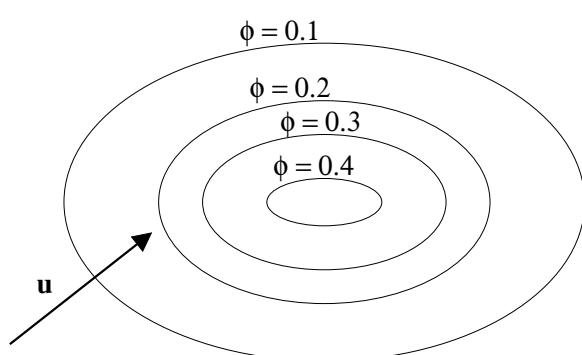
1.2 Advection of Pollution

1.2.1 Pure Linear Advection

Advection of concentration ϕ without diffusion or sources or sinks:

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \quad (1.1)$$

Changes of ϕ are produced by the component of the wind in the same direction as gradients of ϕ . In order to understand why the $\mathbf{u} \cdot \nabla \phi$ term leads to changes in ϕ , consider a region of polluted atmosphere where the pollutant has the concentration contours shown below:



Exercise: Draw on the figure the directions of the gradients of ϕ and thus mark with a +, - or 0 locations where $\mathbf{u} \cdot \nabla \phi$ is positive, negative and zero. Thus deduce where ϕ is increasing, decreasing or staying the same based on equation 1.1. Hence overlay contours of ϕ at a later time.

1.2.2 Advection/Diffusion with Sources and Sinks

$$\frac{D\Psi}{Dt} = \frac{\partial\Psi}{\partial t} + \mathbf{u} \cdot \nabla\Psi = S + \mu\Psi\nabla^2\Psi$$

Lagrangian derivative Rate of change at fixed point Advection of Ψ Sources and sinks Diffusion of Ψ



13

1.3 The Momentum Equation

$$\frac{D\mathbf{u}}{Dt} = -2\boldsymbol{\Omega} \times \mathbf{u} - \frac{\nabla p}{\rho} + \mathbf{g} + \mu_u \left(\nabla^2 \mathbf{u} + \frac{1}{3} \nabla(\nabla \cdot \mathbf{u}) \right)$$

Lagrangian derivative Coriolis Pressure gradient Gravitational acceleration Diffusion

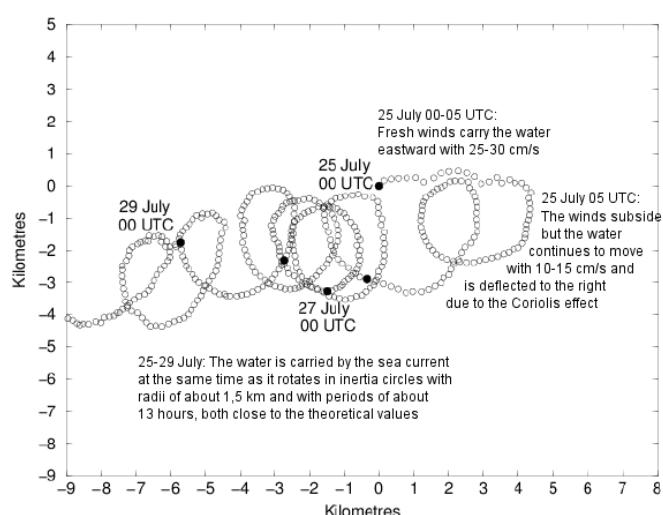
1.3.1 Coriolis

Inertial Oscillations governed by part of the momentum equation:

$$\frac{\partial \mathbf{u}}{\partial t} = -2\boldsymbol{\Omega} \times \mathbf{u}$$

- A drifting buoy set in motion by strong westerly winds in the Baltic Sea in July 1969.
- Once the wind subsides, the upper ocean follows inertia circles

Image copyright: Anders Persson.
Source of scientific data: Barry Broman.
Reproduced with kind permission from Anders Persson and Barry Broman.



14

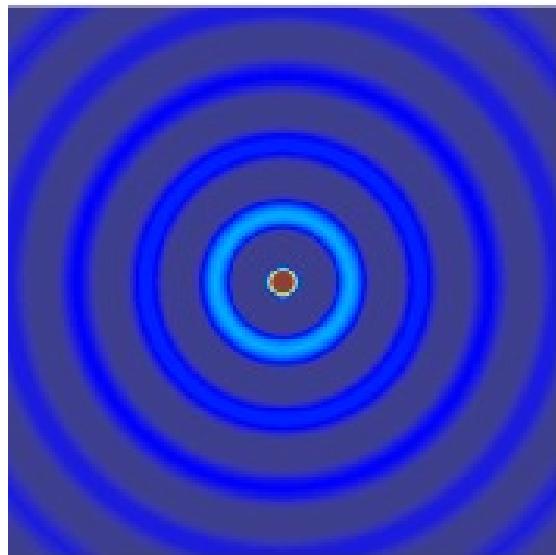
1.3.2 The Pressure Gradient Force

If the pressure gradient force is the only large term in the momentum equation, then together with the continuity equation and perfect gas law, we get equations for acoustic waves:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\rho_0} \nabla p = 0$$

$$\frac{\partial p}{\partial t} + \rho_0 c^2 \nabla \cdot \mathbf{u} = 0$$

where ρ_0 is a reference density and c is the speed of sound.



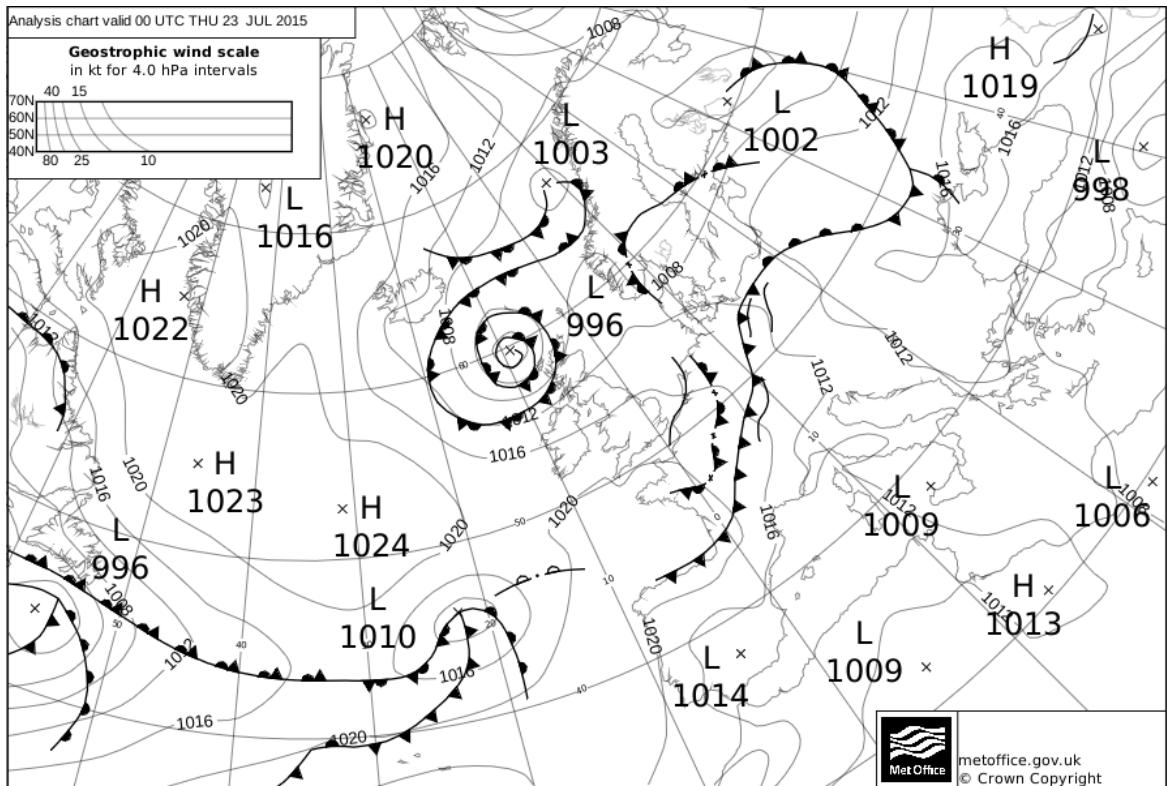
15

Pressure Gradients lead to very fast acceleration - Acoustic Waves



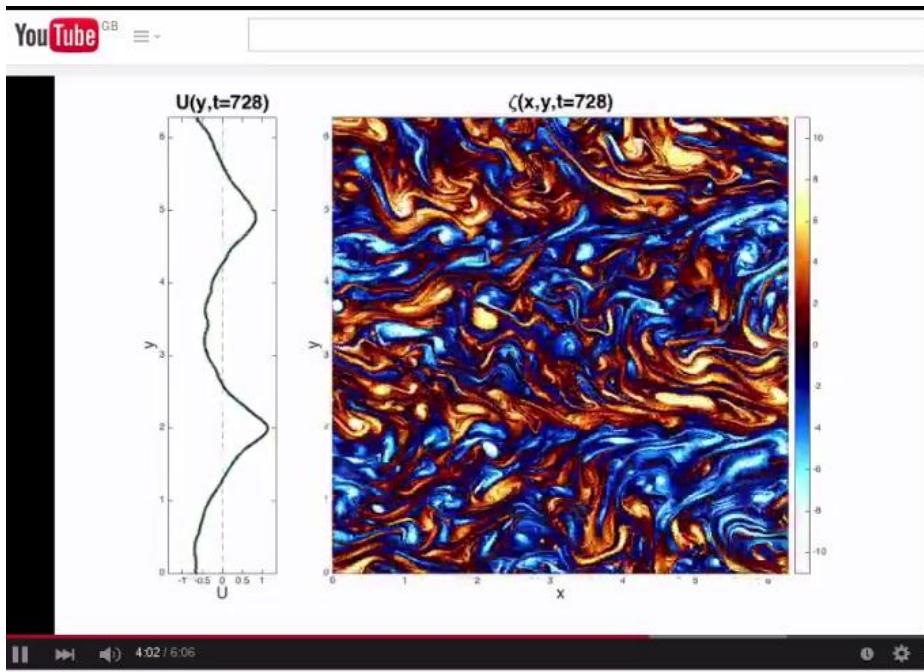
16

Geostrophic Balance: Pressure Gradients versus Coriolis

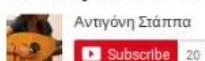


17

Geostrophic turbulence: pressure gradients, Coriolis and the (non-linear) advection of velocity by velocity

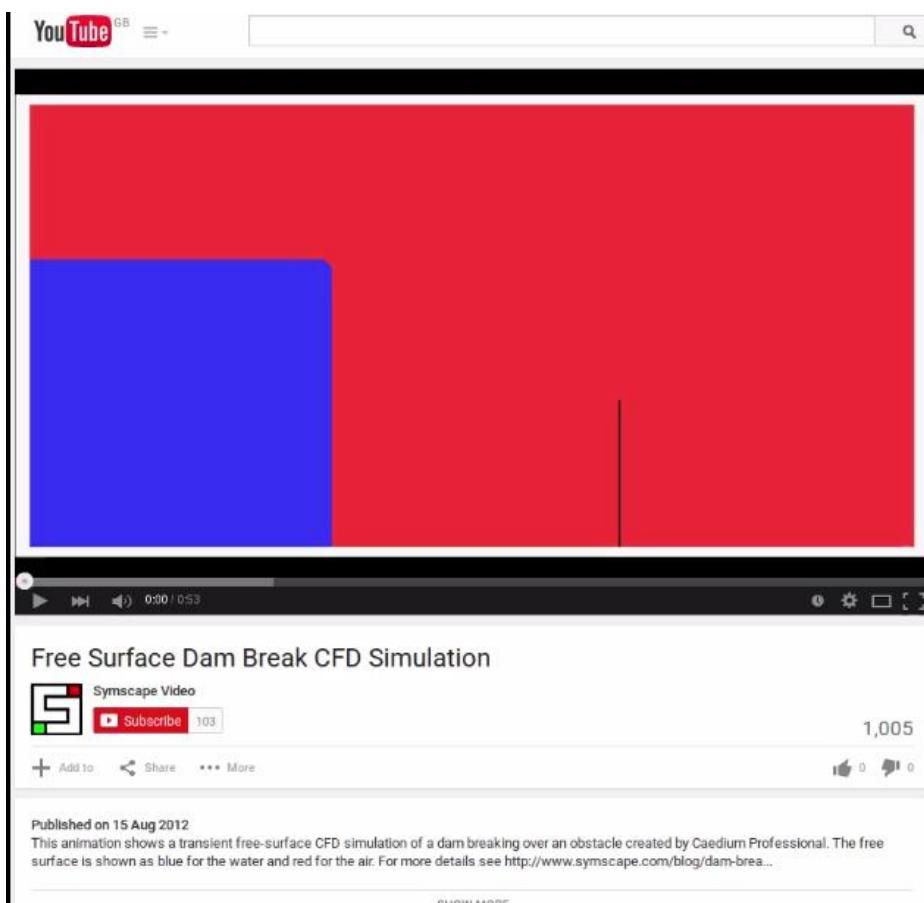


Zonal jet formation in beta-plane turbulence



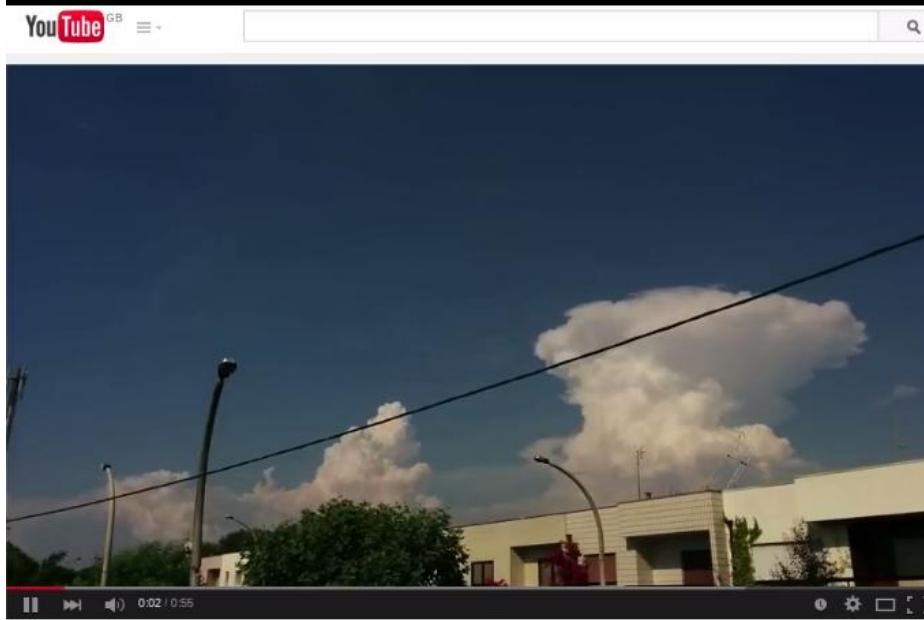
244 vi

1.3.3 Gravitational Acceleration: A simulation of a dam break



19

Gravitational Acceleration: Explosive Cumulonimbus



20

1.3.4 Diffusion

Diffusion of quantity ϕ with diffusion coefficient μ_ϕ in arbitrary spatial dimensions

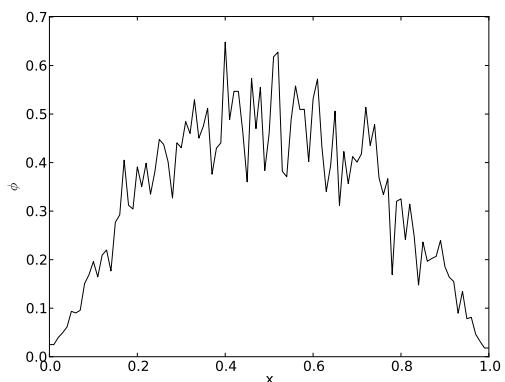
$$\frac{\partial \phi}{\partial t} = \mu_\phi \nabla^2 \phi$$

And in 1d:

$$\frac{\partial \phi}{\partial t} = \mu_\phi \frac{\partial^2 \phi}{\partial x^2}$$

The second derivative of ϕ is high at troughs and low in peaks of ϕ . Therefore diffusion tends to remove peaks and troughs and make a profile more smooth:

Diffusion of a noisy profile
(zero gradient boundary conditions)



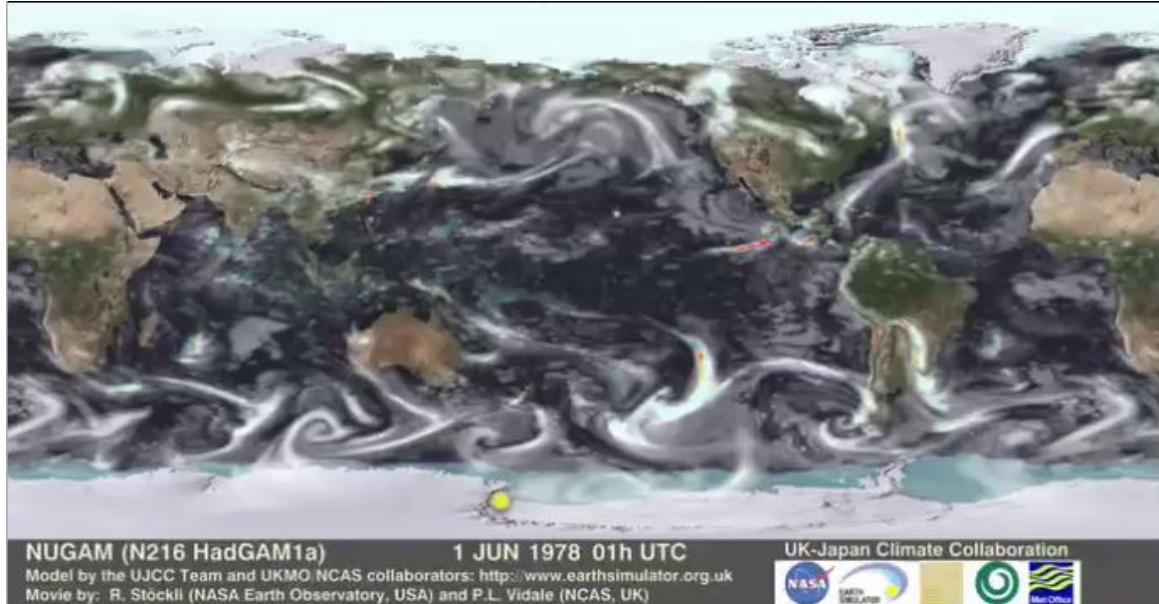
Discussion Questions:

- Which equations have a diffusion coefficient?
- What causes diffusion?
- Is diffusion a large term of the equations of atmospheric motion?

21

1.3.5 The Complete Navier Stokes Equations

With moisture, phase changes, radiation, ... from NUGAM (courtesy of Pier Luigi Vidale)



22

Chapter 2: Linear Finite Difference Schemes for Advection

In one spatial dimension, x , with constant wind, u , no diffusion and no sources or sinks, the linear advection equation (eqn 1.1) for ϕ reduces to:

$$\frac{\partial \phi}{\partial t} + \quad \text{or} \quad \phi_t + \quad (2.1)$$

This equation has an analytic solution. If the initial condition is $\phi(x, 0)$ then the solution at time t is $\phi(x, t) = \phi(x - ut, 0)$.

Exercise:

Check that this is the analytic solution.

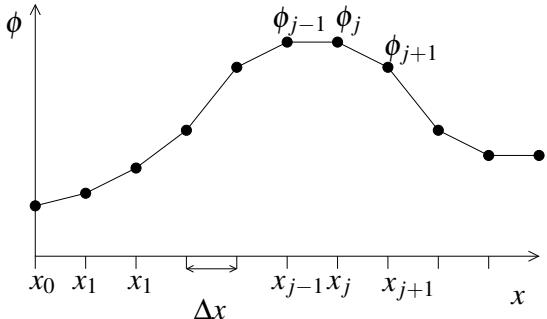
(Hint: define $X = x - ut$, calculate $\frac{\partial X}{\partial x}$ and $\frac{\partial X}{\partial t}$ and use the chain rule, $\frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial X} \frac{\partial X}{\partial x}$)

23

2.1 Forward in Time, Backward in Space (FTBS)

To solve $\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0$ numerically:

- divide space into N equal intervals of size Δx so that $x_j = j\Delta x$ for $j = 0, 1, \dots, n_x$



- Divide time into time steps Δt (so that $t_n = n\Delta t$, $n = 0, 1, 2, \dots$)
- Define $\phi_j^{(n)} = \phi(x_j, t_n)$.

- Approximate $\partial \phi / \partial t$ at x_j, t_n by a forward difference: $\frac{\partial \phi_j^{(n)}}{\partial t} = \frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t}$

- Approximate $\partial \phi / \partial x$ at x_j, t_n by a backward difference: $\frac{\partial \phi_j^{(n)}}{\partial x} =$

- Substituting these into eqn (2.1) gives FTBS:

(2.2)

- This can be re-arranged to get $\phi_j^{(n+1)}$ on the LHS and all other terms on the RHS so that we can calculate ϕ at the new time step at all locations based on values at previous time steps. Also in this equation, remove $u, \Delta t$ and Δx by substituting in the Courant number, $c = u\Delta t / \Delta x$:

$$\phi_j^{(n+1)} = \quad (2.3)$$

24

Questions

- Why did we go forwards in time?
- Why did we go backwards in space? We will come back to this
- What order accuracy is FTBS in space and time? (ie, what is the order, n , such that the error of the approximation is proportional to Δx^n or Δt^n)
- What influence will the errors have on the solution?...

25

2.1.1 Order of Accuracy of FTBS

We will use a Taylor series to derive the backward in space approximation in FTBS, find its order of accuracy and describe how the errors will affect the solution. The Taylor series for ϕ_{j-1} about ϕ_j is:

$$\phi_{j-1} = \phi_j - + O(\Delta x^3).$$

We can rearrange this to find the backward in space approximation for $\partial\phi/\partial x = \phi'_j$:

$$\phi'_j =$$

- The leading error term is $\frac{\Delta x}{2}\phi''$. This tells us two things:
 - The error is proportional to Δx^1 so the spatial derivative approximation is first-order accurate.
 - The error behaves like ϕ'' which is the spatial term from the diffusion equation. Adding this error to the advection equation makes the equation diffusive.

You will be writing code to solve the linear advection equation using FTBS in the assignment. Is the solution diffusive in comparison to the analytic solution? Is the error proportional to Δx ?

26

2.2 Centred in Time, Centred in Space (CTCS) and FTCS

To solve $\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0$ numerically:

- Approximate $\partial \phi / \partial t$ at x_j, t_n by a centred difference, using $\phi_j^{(n-1)}$ and $\phi_j^{(n+1)}$:

$$\frac{\partial \phi_j^{(n)}}{\partial t} =$$

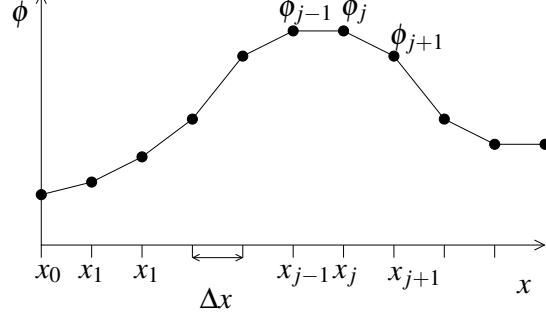
- Approximate $\partial \phi / \partial x$ at x_j, t_n by a centred difference: $\frac{\partial \phi_j^{(n)}}{\partial x} =$

- Substituting these into eqn (2.1) and re-arrange to get $\phi_j^{(n+1)}$ on the LHS and all other terms on the RHS and substituting in the Courant number, $c = u\Delta t / \Delta x$ gives CTCS:

$$\phi_j^{(n+1)} = \quad (2.4)$$

- This is a three-time-level formula (it involves values of ϕ at times t_{n-1} , t_n and t_{n+1}). To start the simulation, values of ϕ are needed at times t_0 and t_1 . However, only $\phi(x, t_0)$ is available. So another scheme (such as FTCS) must be used to obtain $\phi^{(1)} = \phi(x, t_1)$:

$$\text{FTCS: } \phi_j^{(n+1)} = \quad (2.5)$$



27

2.2.1 Order of Accuracy of CTCS

Use Taylor series approximations for ϕ_{j-1} and ϕ_{j+1} about ϕ_j to find a second-order approximation for ϕ'_j and show that it is second-order accurate:

$$\phi_{j-1} = \phi_j$$

$$\phi_{j+1} =$$

Subtract these to eliminate ϕ''_j and rearrange to find ϕ'_j and find its order of accuracy:

Question to consider during the assignment:

Does CTCS do better than FTBS? Why or why not?

2.3 Implicit and Explicit Schemes

Explicit Values at the next time-step are determined from values at the current (and previous) time-steps. Straightforward.

Implicit Values at the next time-step are determined from values at the next time step!

- This leads to a set of simultaneous equations
- How do we solve a set of linear simultaneous equations?
- How do we solve a set of non-linear simultaneous equations?
- Easier to solve a linear equation implicitly rather than a non-linear equations
- Why would we want to use an implicit method at all?...

29

2.4 Backward in Time, Centred in Space (BTCS)

Derive an equation for BTCS

(2.6)

Is this an implicit or explicit scheme?

Exercise: Assume that all of the j values, $\phi_j^{(n)}$ (for a particular n) can be represented as a vector: $\underline{\phi}^{(n)} = (\phi_0^{(n)}, \phi_1^{(n)}, \dots, \phi_j^{(n)}, \dots, \phi_{N-1}^{(n)})^T$. Find a matrix M such that BTCS is defined as $M\underline{\phi}^{(n+1)} = \underline{\phi}^{(n)}$ given $x : 0 \rightarrow 1$ and periodic boundary conditions so that $\phi_0 = \phi_N$.

30

- Will these advection schemes approximate the continuous PDE given sufficient resolution?
- Will we be able to take large time-steps?

In order to answer these questions, we will need von-Neumann stability analysis.

von-Neumann stability analysis relied on Fourier analysis. Some revision of Fourier analysis will be presented for 3 reasons:

1. It is needed for stability analysis
2. Some weather forecasting models use spectral decompositions (eg ECMWF) which are a spherical version of Fourier decompositions
3. Fourier analysis is used to analyse climate data

This is revision material and so is not directly examinable

31

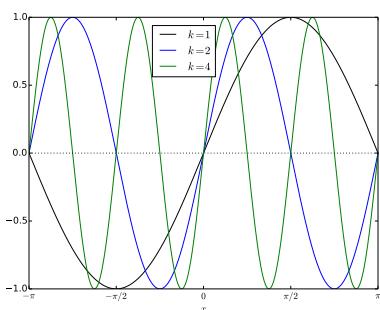
Chapter 3: Fourier Analysis

3.1 Fourier Series

Any periodic, integrable function, $f(x)$ (defined on $[-\pi, \pi]$), can be expressed as a Fourier series; an infinite sum of sines and cosines:

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos kx + \sum_{k=1}^{\infty} b_k \sin kx \quad (3.1)$$

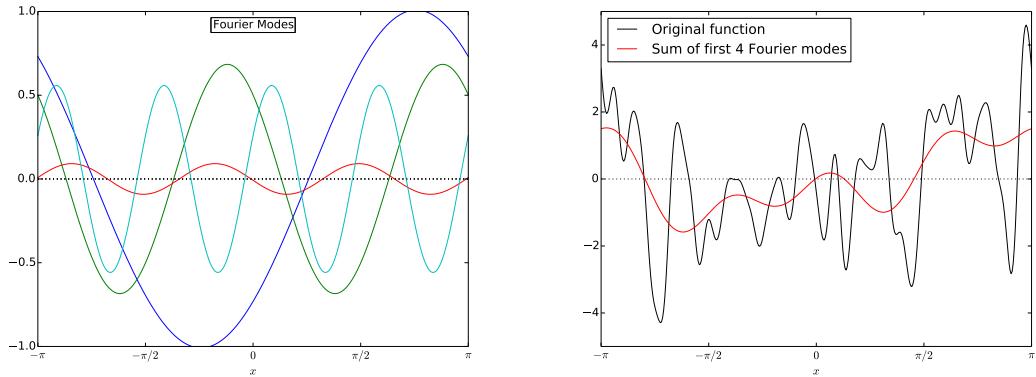
- The a_k and b_k are the Fourier coefficients.
- The sines and cosines are the Fourier modes.
- k is the wavenumber - number of complete waves that fit in the interval $[-\pi, \pi]$ $\sin kx$ for different values of k



- The wavelength is $\lambda =$
- The more Fourier modes that are included, the closer their sum will get to the function.

32

Sum of First 4 Fourier Modes of a Periodic Function

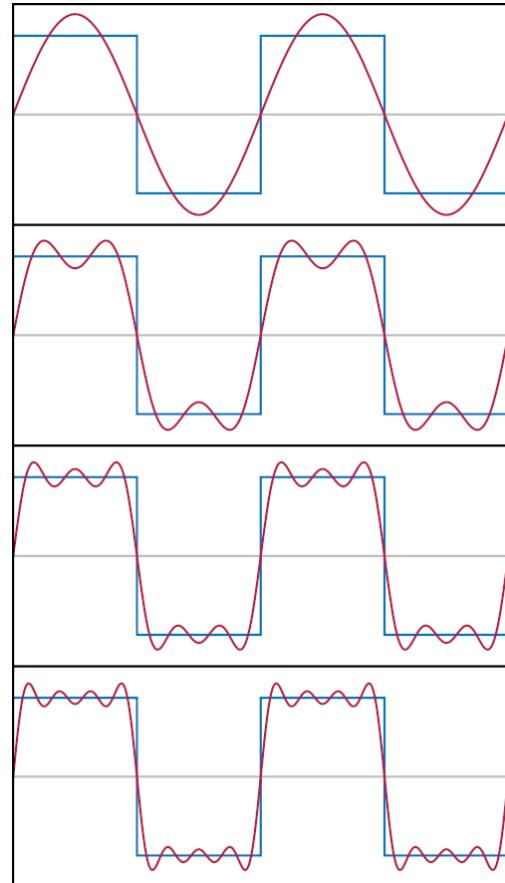
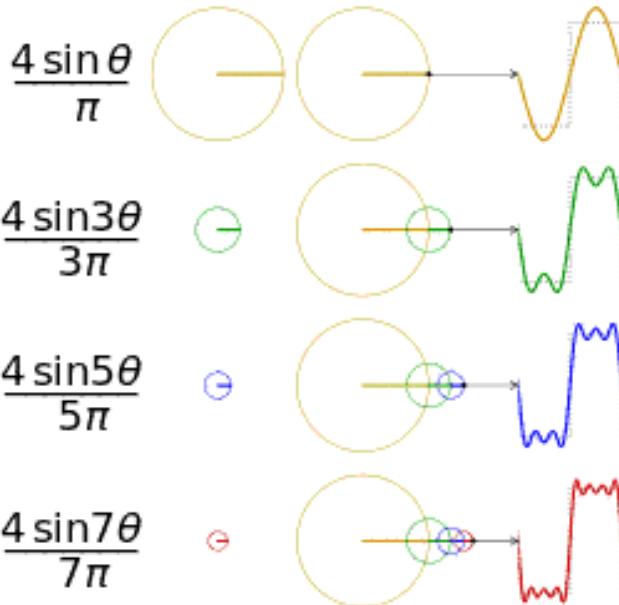


33

The first four Fourier modes of a square wave.
The additional oscillations are “spectral ringing”

Each mode can be represented by motion around a circle. ↓

The motion around each circle has a speed and a radius. These represent the wavenumber and the Fourier coefficients. Which is which?



34

Equivalently, equation (3.1) can be expressed as an infinite sum of exponentials using the relation $e^{i\theta} = \cos \theta + i \sin \theta$ where $i = \sqrt{-1}$:

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos kx + \sum_{k=1}^{\infty} b_k \sin kx = \sum_{k=-\infty}^{\infty} A_k e^{ikx}. \quad (3.2)$$

Exercise

Evaluate the A_k s in terms of the a_k s and b_k s.

3.2 Fourier Transform

- The Fourier Transform transforms a function f which is defined over space (or time) into the frequency domain, so that it is defined in terms of Fourier coefficients.
- The Fourier transform calculates the Fourier coefficients as:

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx) dx, \quad b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx) dx$$

3.3 Discrete Fourier Transform

A discrete Fourier Transform converts a list of N equally spaced samples in $[0, 2\pi)$ of a complex valued, periodic function, f_n , to the list of the first N complex valued Fourier coefficients:

$$A_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n e^{-2i\pi nk/N}. \quad (3.3)$$

The truncated Fourier series:

$$f(x) \approx \sum_{k=0}^{N-1} A_k e^{ikx} \quad (3.4)$$

is an approximation to the function f which fits the sampled points, f_n , exactly.

On a computer this is done with a **Fast Fourier Transform** (or `fft`). The inverse Fourier transform (sometimes called `ifft`) transforms the Fourier coefficients back to the f values (transforming from spectral back to real space):

$$\begin{array}{ccc} f_0, f_1, f_2, \dots, f_{N-1} & \xrightarrow{\text{fft}} & A_0, A_1, \dots, A_{N-1} \\ A_0, A_1, \dots, A_{N-1} & \xrightarrow{\text{ifft}} & f_0, f_1, f_2, \dots, f_{N-1} \end{array}$$

Exercise

Check the formulae in equations (3.3) and (3.4) by defining your own function, f , at $2N + 1$ equally space points in $[0, 2\pi]$. Use these function values to calculate the Fourier coefficients from equation (3.3) then plug them back into equation (3.4) to check that you retrieve the same function values at the original points. Please contact me if you have problems as there could be errors in equations (3.3) and (3.4).

3.4 Differentiation and Interpolation

If we know the Fourier coefficients, A_k , of a function f then we can calculate the gradient of f at any point, x : If

$$f(x) = \sum_{k=0}^{\infty} a_k \cos kx + \sum_{k=0}^{\infty} b_k \sin kx = \sum_{k=-\infty}^{\infty} A_k e^{ikx} \quad (3.5)$$

then

$$f'(x) = \quad (3.6)$$

and the second derivative:

$$f''(x) = \quad (3.7)$$

These have spectral accuracy; the order of accuracy is as high as the number of points.

Similarly equation 3.1 or 3.2 can be used directly to interpolate f onto an undefined point, x . Again, the order of accuracy is spectral.

3.5 Spectral Models

- ECMWF use a spectral model.
- The prognostic variables are transformed between physical and spectral space using `ffts` and `iffts`.
- Gradients are calculated very accurately in spectral space

3.6 Wave Power and Frequency

- If a function, f , has Fourier coefficients, a_k and b_k , then wavenumber k has power $a_k^2 + b_k^2$.
- A plot of wave frequency versus power is referred to as the power spectrum. Before we learn how power spectra are used, we will have some revision questions...

3.7 Recap Questions

1. In the Fourier decomposition

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos kx + \sum_{k=1}^{\infty} b_k \sin kx$$

what are:

- (a) the Fourier coefficients
- (b) the Fourier modes
- (c) the wavenumbers (or frequencies)
- (d) the power of a given wavenumber

2. How would you describe the operation:

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx) dx, \quad b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx) dx$$

3. Given a list of $2N + 1$ equally spaced samples of a real valued, periodic function, f_n , how would you describe the following operation to convert this into a list of $N + 1$ values:

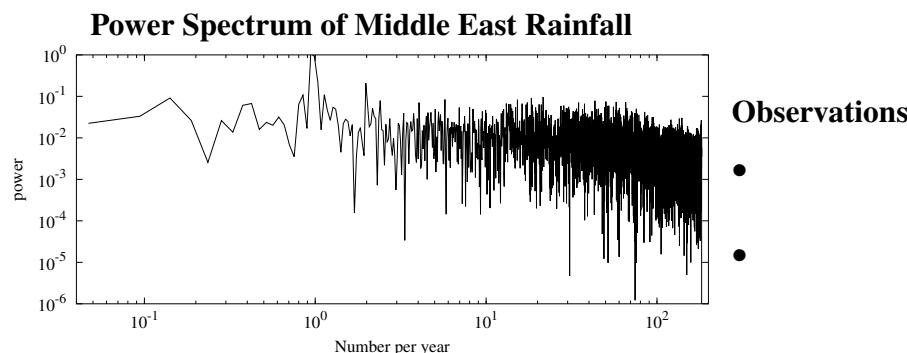
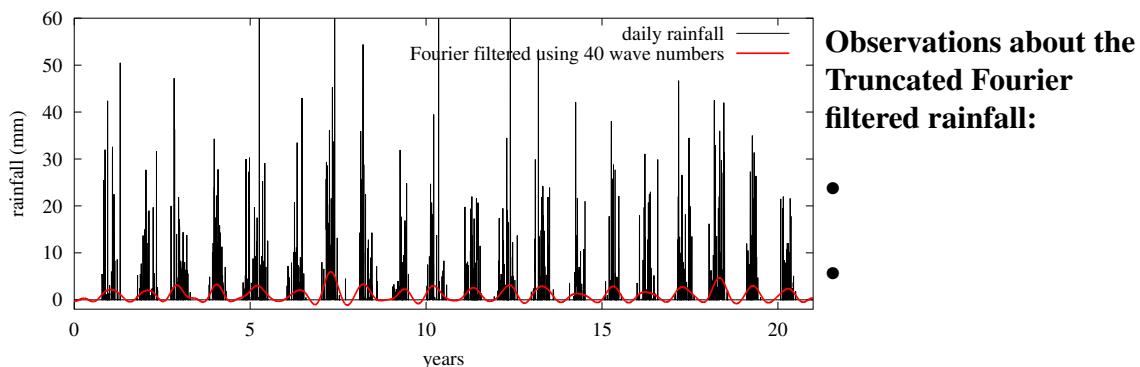
$$A_k = \frac{1}{N} \sum_{n=-N}^{N} f_n e^{-i\pi knx/N}$$

4. What is the wavelength of a wave described by $\sin 4x$

39

3.8 Analysing Power Spectra

Daily rainfall at a station in the Middle East for 21 years

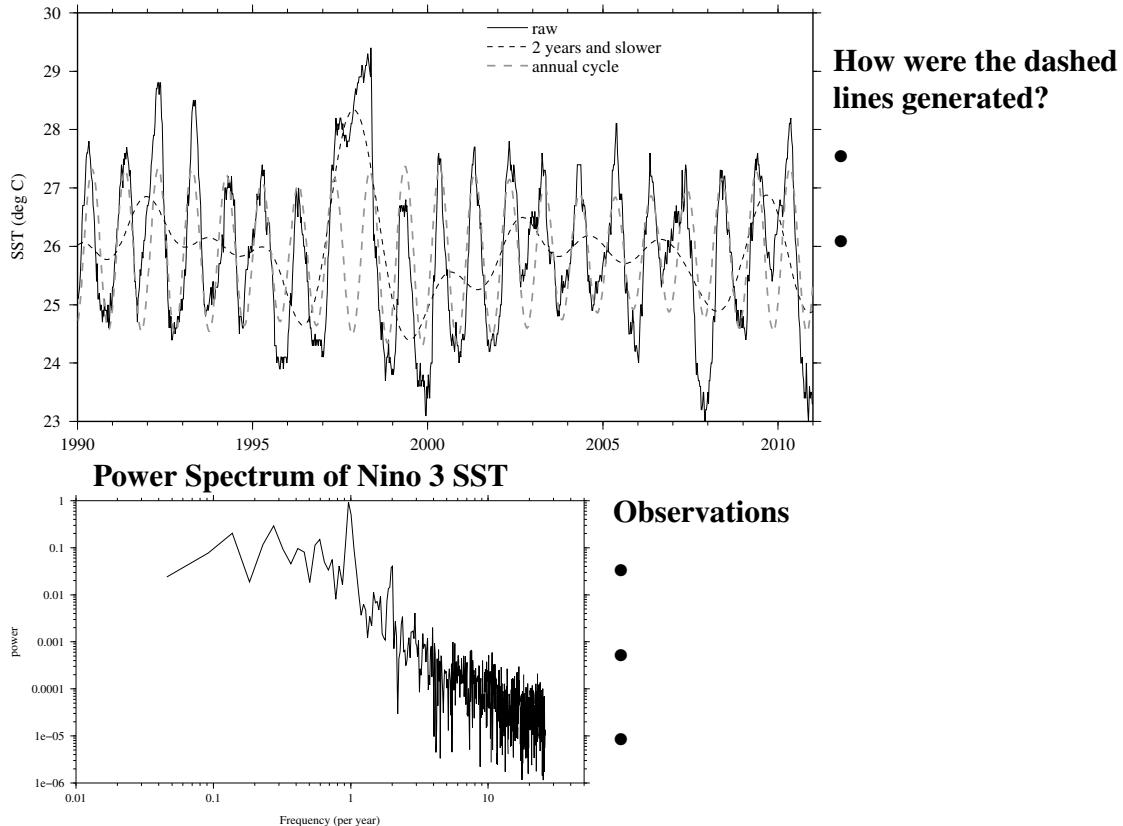


number per year = wavenumber $\times 365/\text{total number of days}$

40

Time Series of the Nino 3 sea surface temperature (SST)

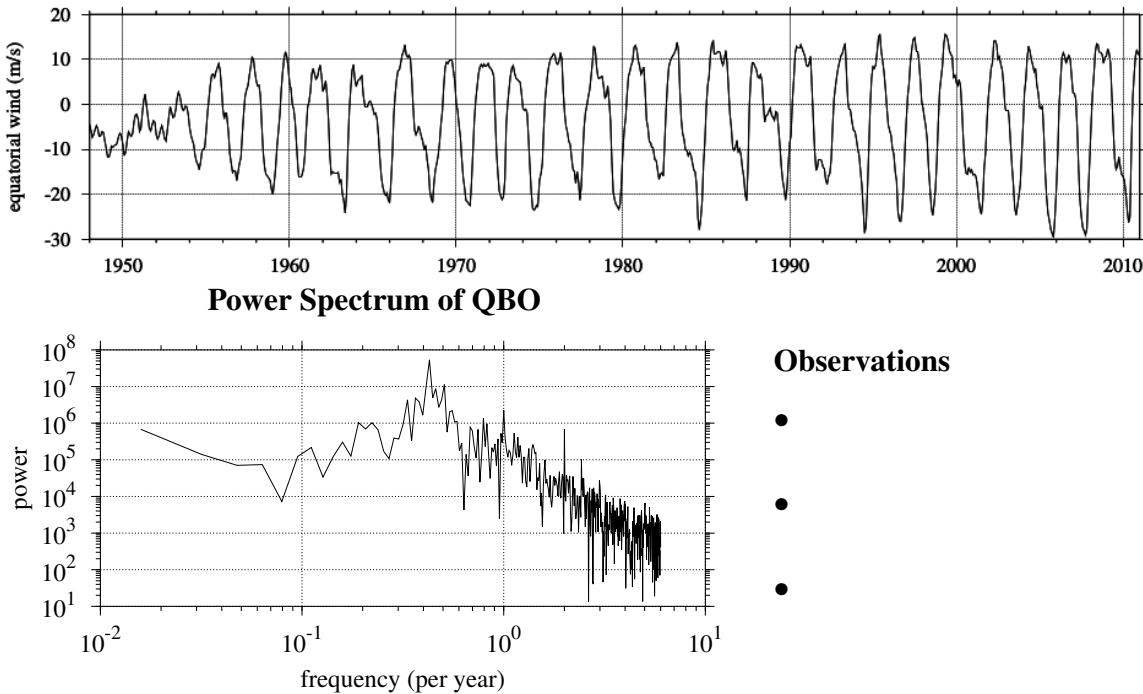
The SST in the Nino 3 region of the equatorial Pacific is a diagnostic of El Nino



41

Time Series of the Quasi-Biennial Oscillation (QBO)

The QBO is an oscillation of the equatorial zonal wind between easterlies and westerlies in the tropical stratosphere which has a mean period of 28 to 29 months:



... Fourier decompositions will be used to mathematically analyse the behaviour of the numerical schemes...

42

Chapter 4: Numerical Analysis of Advection Schemes

4.1 Introduction: What is Numerical Analysis and why is it done

- Numerical analysis involves mathematically analysing numerical methods in order to predict how they will behave when they are used.
- Numerical analysis is important because
 - Model development by trial and error is very time consuming
 - We cannot test our models for every possible situation. We need evidence that they will work for all situations
 - We gain insight into how numerical methods work and so how to design better ones
- This chapter describes various types of analysis that are done for advection schemes for atmospheric models

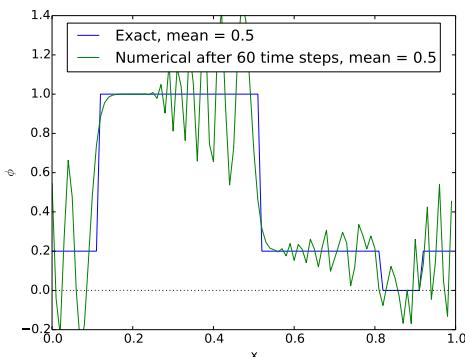
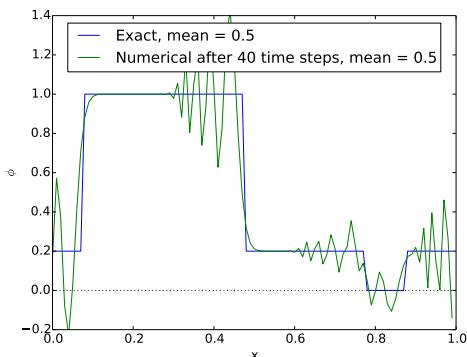
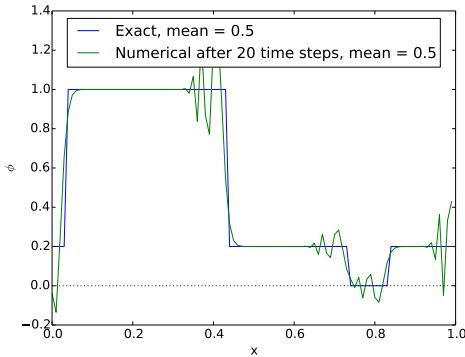
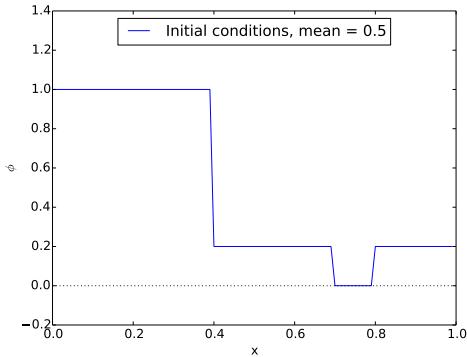
43

4.2 Some Definitions

1. **Convergence:** A finite difference scheme is convergent if the solutions of the scheme converge to the solutions of the PDE as Δx and Δt tend to zero.
2. **Consistency:** A finite difference scheme is consistent with a PDE if the errors in approximating *all of the terms* tend to zero as Δx and/or Δt tend to zero. (Terms of the finite difference scheme are typically analysed using Taylor series.)
3. **Order of accuracy:** Error $\propto \Delta x^n$ (error is $O(\Delta x^n)$) means scheme is n^{th} order accurate. Errors of an n^{th} order scheme converge to zero with order n .
4. **Stability:** Errors do not tend to infinity for any number of time steps. Stability is typically proved using von-Neumann stability analysis.
 - (a) Conditionally stable - if stable only for a sufficiently small time-step
 - (b) Unconditionally stable - if stable for any time-step
 - (c) Unconditionally unstable - if unstable for any time-step
5. **Conservation:** If, eg mass, energy, potential vorticity are conserved by the PDEs, are they conserved by the numerical scheme?
6. **Boundedness:** If the initial conditions are bounded between values a and b then a bounded solution will remain bounded between a and b for all time.
7. **Monotonicity:** Monotone schemes do not generate new extrema or amplify existing extrema. If the initial conditions are monotonic then they will remain monotonic after the action of a monotonic numerical scheme.

44

Based on your knowledge of FTCS and based on the numerical solutions below, which of properties 2-7 apply to the numerical solution of the linear advection equation using FTCS?



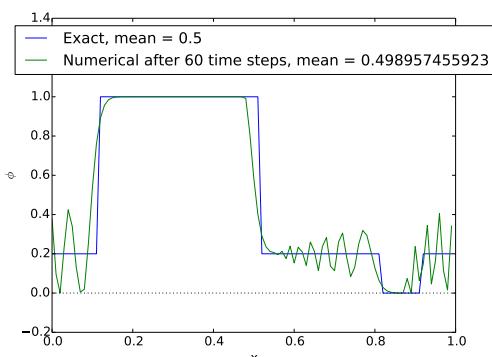
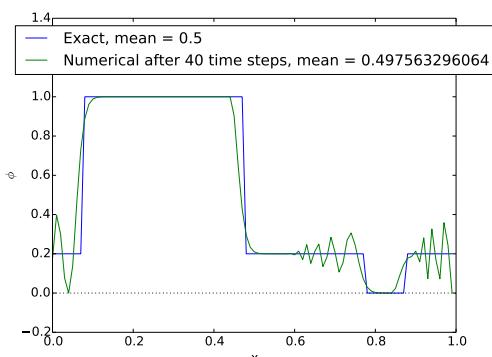
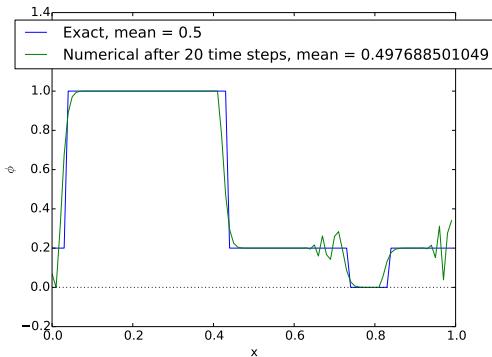
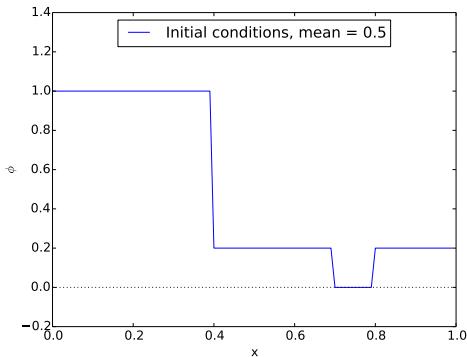
Consistent
Conservative

Order of Accuracy
Bounded

Stable
Monotone

45

How about when modifying all out of range values to be one or zero at every time-step?



Consistent
Conservative

Order of Accuracy
Bounded

Stable
Monotone

46

4.3 Convergence and errors

If an analytic solution, $f(x, t)$, to a PDE is known, then errors of a numerical solution, $\phi(x, t)$, can be calculated as functions of space and time. Errors over space can be summarised by integrating over space to calculate error norms:

$$\begin{aligned}\ell_1(\phi) &= \frac{\sum_j \Delta x |\phi_j - f(x_j)|}{\sum_j \Delta x |f(x_j)|} \\ \ell_2(\phi) &= \sqrt{\frac{\sum_j \Delta x (\phi_j - f(x_j))^2}{\sum_j \Delta x f(x_j)^2}} \\ \ell_\infty(\phi) &= \frac{\max |\phi_j - f(x_j)|}{\max |f(x_j)|}.\end{aligned}$$

If a numerical scheme is described as n^{th} order accurate, then these error metrics should converge to zero at a rate proportional to Δx^n :

$$\ell_i \propto \Delta x^n.$$

4.4 Lax-Equivalence Theorem

The Lax equivalence theorem is the fundamental theorem in the analysis of finite difference methods for the numerical solution of partial differential equations. It states that for a consistent finite difference method for a well-posed linear initial value problem, the method is convergent if and only if it is stable:

$$\text{consistency} + \text{stability} \iff \text{convergence}$$

So if you can show that the finite difference approximations for each of the terms is at least first-order accurate and you can show that the scheme is stable, then you know that solutions to the finite difference scheme will converge to solutions of the PDE.

This is why we study order of accuracy and stability.

4.5 Domain of Dependence

The domain of dependence of the solution of a PDE at position \mathbf{x} and at time t is the set of points at a previous time that influence the solution at position \mathbf{x} and at time t .

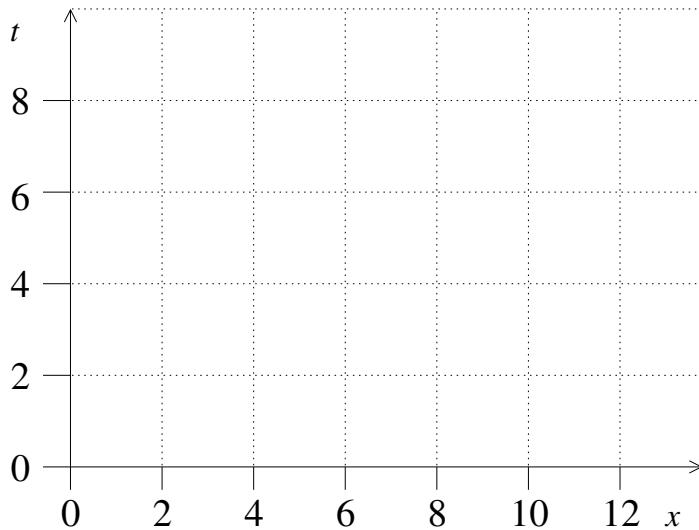
Let us consider the 1D linear advection equation for dependent variable ϕ and advecting velocity u :

$$\phi_t + u\phi_x = 0$$

Remember the analytic solution:

$$\phi(x, t) =$$

Draw the domain of dependence of $x = 12\text{m}$, $t = 8\text{s}$ on the graph, assuming $u = 1.5\text{m/s}$:



49

4.5.1 Courant-Friedrichs-Lowy (CFL) criterion:

The domain of dependence of the numerical solution should include the domain of dependence of the original PDE.

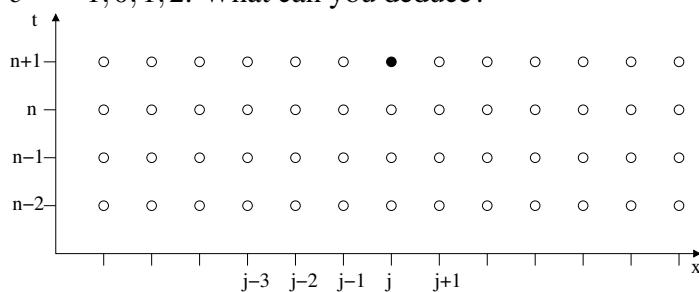
- The CFL criterion is necessary but not sufficient
- For linear advection, the domain of dependence of the differential equation at $(j\Delta x, n\Delta t)$ is the straight line of slope $1/u$ through $(j\Delta x, n\Delta t)$ for $t \leq n\Delta t$ in the (x, t) plane.

4.5.2 Domain of Dependence of FTBS

$$\text{FTBS: } \phi_j^{(n+1)} = \phi_j^{(n)} - c(\phi_j^{(n)} - \phi_{j-1}^{(n)})$$

$\phi_j^{(n)}$ depends on $\phi_j^{(n-1)}$ and $\phi_{j-1}^{(n-1)}$. In turn, these depend on $\phi_j^{(n-2)}$, $\phi_{j-1}^{(n-2)}$ and $\phi_{j-2}^{(n-2)}$.

Exercise: Mark the dots that make up the domain of dependence of $\phi_j^{(n+1)}$ for FTBS. Draw lines corresponding to the real (physical) domain of dependence for cases when $c = -1, 0, 1, 2$. What can you deduce?

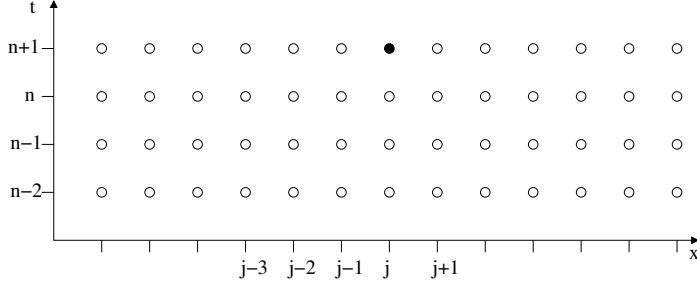


50

4.5.3 The Domain of Dependence of the CTCS Scheme

$$\text{CTCS: } \phi_j^{(n+1)} = \phi_j^{(n-1)} - c(\phi_{j+1}^{(n)} - \phi_{j-1}^{(n)})$$

Draw the domain of dependence of $\phi_j^{(n+1)}$ for CTCS.



For what values of c will CTCS be unstable?

Except at the initial time, the solution is found on two sets of points that are not coupled. The solution can oscillate between two unrelated solutions. This is a manifestation of the **computational mode** of CTCS.

The domain of dependence and the CFL criterion can tell us when some schemes are unstable. How about proving stability? ...

51

4.6 Von-Neumann Stability Analysis

- Assume that the solution at time level $n + 1$ can be represented as an amplification factor, A , multiplied by the solution at time-level n :

$$\phi^{(n+1)} = A\phi^{(n)}$$

- The amplification factor will tell us the following about the numerical method:

$$|A| < 1 \quad \forall k, \Delta x$$

$$|A| = 1 \quad \forall k, \Delta x$$

$$|A| > 1 \quad \text{for any } k, \Delta x$$

Where $|A|^2 = AA^*$ (A multiplied by its complex conjugate).

- For linear advection A should be complex since the solution changes location every time-step. So how are we going to find A ? ...
- The solution of a PDE in one spatial dimension can be expressed as a sum of Fourier modes:

$$\phi = \sum_{k=-\infty}^{\infty} A_k e^{ikx} \tag{4.1}$$

each with wavenumber k .

- Consider the stability of a solution for individual wavenumbers
- For a uniform grid, $x = j\Delta x$
- Substitute $\phi_j^{(n)} = A^n e^{ikj\Delta x}$ into the equation for a linear numerical scheme.
- Rearrange to give an equation for the amplification factor, $A(k, \Delta x, \Delta t)$

52

4.6.1 Von-Neumann Stability Analysis of FTBS

FTBS for linear advection is:

$$\phi_j^{(n+1)} = \phi_j^{(n)} - c(\phi_j^{(n)} - \phi_{j-1}^{(n)}) \quad (4.2)$$

Substitute in $\phi_j^{(n)} = A^n e^{ikj\Delta x}$:

$$(4.3)$$

Cancel powers of $A^n e^{ikj\Delta x}$ and rearrange to find A in terms of c and $k\Delta x$:

$$A = \dots \quad (4.4)$$

We need to find the magnitude of A so we need to write it down in real and imaginary form.
So substitute $e^{-ik\Delta x} = \cos k\Delta x - i \sin k\Delta x$:

$$A = \dots \quad (4.5)$$

and calculate $|A|^2 = AA^*$ (A multiplied by its complex conjugate):

$$\begin{aligned} |A|^2 &= 1 - 2c(1 - \cos k\Delta x) + c^2(1 - 2\cos k\Delta x + \cos^2 k\Delta x) + c^2 \sin^2 k\Delta x \\ \implies |A|^2 &= 1 - 2c(1 - c)(1 - \cos k\Delta x) \end{aligned}$$

We need to find for what value of Δt or c is $|A| \leq 1$ in order to find when FTBS is stable:

$$\begin{aligned} |A| \leq 1 &\iff |A|^2 - 1 \leq 0 \\ &\iff -2c(1 - c)(1 - \cos k\Delta x) \leq 0 \\ &\iff c(1 - c)(1 - \cos k\Delta x) \geq 0 \end{aligned}$$

53

We know that $1 - \cos k\Delta x \geq 0$ for all $k\Delta x$ so FTBS is stable when $c(1 - c) \geq 0 \iff 0 \leq c \leq 1$.

We have proved that FTBS is unstable if $u < 0$ or if $\frac{u\Delta t}{\Delta x} > 1$. We will now define:

| | |
|----------------------|---|
| Upwind scheme | $\text{FTBS} \quad \text{when } u \geq 0$ $\text{FTFS} \quad \text{when } u < 0$ |
|----------------------|---|

The upwind scheme is first order accurate in space and time, conditionally stable and damping.

4.6.2 What should A be for real linear advection?

For initial conditions consisting of a single Fourier mode: $\phi(x, 0) = A_k e^{ikx}$, the solution at time t is:

$$\phi(x, t) =$$

This can be represented as a factor times e^{ikx} :

$$\phi(x, t) = e^{ikx}$$

So if $t = n\Delta t$ we have $A^n = e^{-ikut} = e^{-ikun\Delta t}$. Therefore $A = e^{-iku\Delta t}$ which has $|A| = 1$ and so, under the influence of the linear advection equation, waves should not amplify or decay.

4.6.3 Von Neumann Stability Analysis of CTCS

The amplification factor, A , is found by substituting $\phi_j^{(n)} = A^n e^{ikj\Delta x}$ into the equation for CTCS:

$$\phi_j^{(n+1)} = \phi_j^{(n-1)} - c(\phi_{j+1}^{(n)} - \phi_{j-1}^{(n)}). \quad (4.6)$$

This gives:

\implies

$\implies A =$

There are two cases to consider:

$$\begin{aligned} \text{(i)} |c| \leq 1 &\implies c^2 \sin^2 k\Delta x \leq 1 \\ &\implies |A|^2 = 1 - c^2 \sin^2 k\Delta x + c^2 \sin^2 k\Delta x = 1 \end{aligned}$$

\implies The solution is stable and not damping

$$\begin{aligned} \text{(ii)} |c| > 1 &\implies c^2 \sin^2 k\Delta x > 1 \text{ for some } k\Delta x \\ &\implies |A|^2 = (c \sin k\Delta x \pm \sqrt{c^2 \sin^2 k\Delta x - 1})^2 \end{aligned}$$

\implies At least one of the roots has $|A| > 1$. The solution is unstable

So CTCS is conditionally stable: it is stable for $|c| \leq 1$

Regardless of c , there are always two possible values of A . This means that there will always be two possible solutions; a realistic solution (the physical mode) and the un-realistic, oscillating solution; the **spurious computational mode**. This will contaminate the solution and behave in an un-realistic way.

55

4.7 Conservation

For a property, ϕ , advected with velocity, u : ($\phi_t + u\phi_x = 0$) we can show that the total mass of ϕ is conserved. Define the total mass to be

$$M = \int_0^1 \phi \, dx$$

and assume that ϕ has periodic boundary conditions so that $\phi(0, t) = \phi(1, t) \forall t$. Then:

$$\frac{dM}{dt} = \frac{d}{dt} \left(\int_0^1 \phi \, dx \right) = \int_0^1 \frac{d\phi}{dt} \, dx = - \int_0^1 u \frac{d\phi}{dx} \, dx = -u \int_0^1 d\phi = -u[\phi]_0^1 = 0.$$

since $\phi(0, t) = \phi(1, t)$. Therefore M is conserved.

Is M conserved by a numerical scheme? Consider FTBS advection:

$$\phi_j^{(n+1)} = \phi_j^{(n)} - c(\phi_j^{(n)} - \phi_{j-1}^{(n)}).$$

From this we can calculate $M^{(n+1)}$ as a function of $M^{(n)}$:

$$\begin{aligned} M^{(n+1)} &= \sum_{j=1}^{n_x} \Delta x \phi_j^{(n+1)} = \Delta x \sum_{j=1}^{n_x} (\phi_j^{(n)} - c(\phi_j^{(n)} - \phi_{j-1}^{(n)})) = M^{(n)} - c\Delta x \left(\sum_{j=1}^{n_x} \phi_j^{(n)} - \sum_{j=1}^{n_x} \phi_{j-1}^{(n)} \right) \\ &= M^{(n)} - c\Delta x \left(\sum_{j=1}^{n_x} \phi_j^{(n)} - \sum_{j=0}^{n_x-1} \phi_j^{(n)} \right) = M^{(n)} - c\Delta x (\phi_{n_x}^{(n)} - \phi_0^{(n)}) = M^{(n)} \end{aligned}$$

due to the periodic boundaries since $\phi_{n_x}^{(n)} = \phi_0^{(n)}$. Therefore $M^{(n+1)} = M^{(n)}$ which means that mass is conserved.

56

4.7.1 Conservation of higher moments

We can show that the variance of ϕ is also conserved under linear advection. The variance is:

$$V = \int_0^1 \phi^2 dx - M^2.$$

Then we can calculate the rate of change of variance under linear advection, assuming that $M_t = 0$:

$$\frac{dV}{dt} = \int_0^1 \frac{d\phi^2}{dt} dx = \int_0^1 2\phi \frac{d\phi}{dt} dx = - \int_0^1 2\phi u \frac{d\phi}{dx} dx = -2u \int_0^1 \phi d\phi = -u [\phi^2]_0^1 = 0.$$

Is V conserved by a numerical scheme? Consider FTBS advection:

$$\phi_j^{(n+1)} = \phi_j^{(n)} - c(\phi_j^{(n)} - \phi_{j-1}^{(n)}).$$

From this we can calculate $V^{(n+1)}$ as a function of $V^{(n)}$ (ignoring M for brevity):

$$\begin{aligned} V^{(n+1)} &= \sum_{j=1}^{n_x} \Delta x \left(\phi_j^{(n+1)} \right)^2 = \Delta x \sum_{j=1}^{n_x} \left(\phi_j^{(n)} - c(\phi_j^{(n)} - \phi_{j-1}^{(n)}) \right)^2 \\ &= \Delta x \sum_{j=1}^{n_x} \left(\phi_j^{(n)} \right)^2 - 2c\Delta x \sum_{j=1}^{n_x} \phi_j^{(n)} \phi_{j-1}^{(n)} + 2c\Delta x \sum_{j=1}^{n_x} \phi_j^{(n)} \phi_{j-1}^{(n)} + c^2 \Delta x \sum_{j=1}^{n_x} \left(\phi_j^{(n)} - \phi_{j-1}^{(n)} \right)^2 \\ &= V^{(n)} - 2c(1-c) \left(V^{(n)} - \Delta x \sum_{j=1}^{n_x} \phi_j^{(n)} \phi_{j-1}^{(n)} \right) \end{aligned}$$

The term multiplying $2c(1-c)$ is always greater than zero and so the variance always decreases when using FTBS.

4.8 Exercises: Analysis of Advection Schemes (answers on blackboard)

1. Derive expressions for the amplification factors for the following advection schemes:
 - (a) FTCS
 - (b) BTCS
 - (c) CTBS
2. Which of the above schemes suffer from a spurious computational mode?
3. Sketch of the domain of dependence for these schemes
4. For FTCS and BTCS
 - (a) Find for what Courant numbers the schemes are stable.
 - (b) Are the schemes damping, amplifying or neutral?
5. Determine if mass is conserved by CTCS

Chapter 5: Waves, Dispersion and Dispersion Errors

Inaccurate dispersion of numerical methods is a common source of errors. Therefore we will learn about dispersion and dispersion errors of numerical methods.

5.1 Some Background on Waves

A travelling wave can be described by the equation

$$y = a \sin(kx - \omega t) \quad (5.1)$$

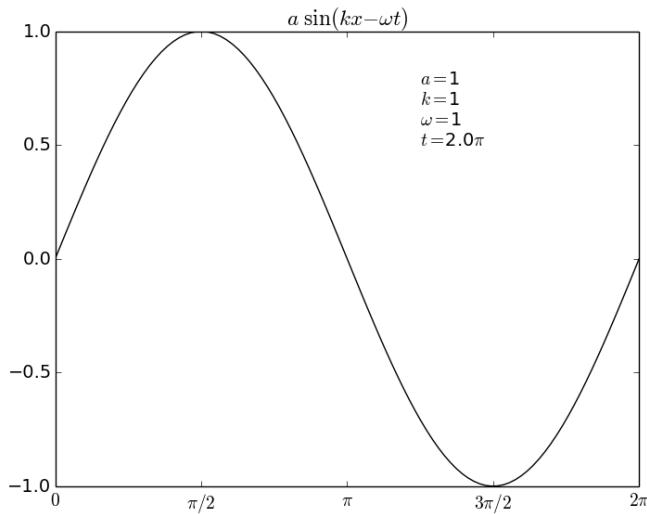
where $y(x, t)$ is the height of the wave at position x , time t

a is the amplitude of the wave

k is the wavenumber (number of whole waves between 0 and 2π)

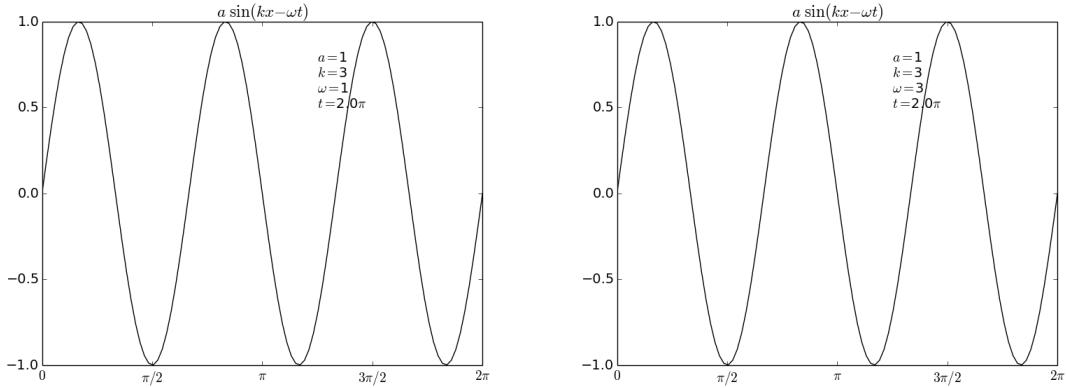
ω is the angular wave frequency – the number of complete oscillations in time 2π at a fixed point

59



How do variations in k and ω influence the wave and its propagation according to the equation

$$y = a \sin(kx - \omega t)$$



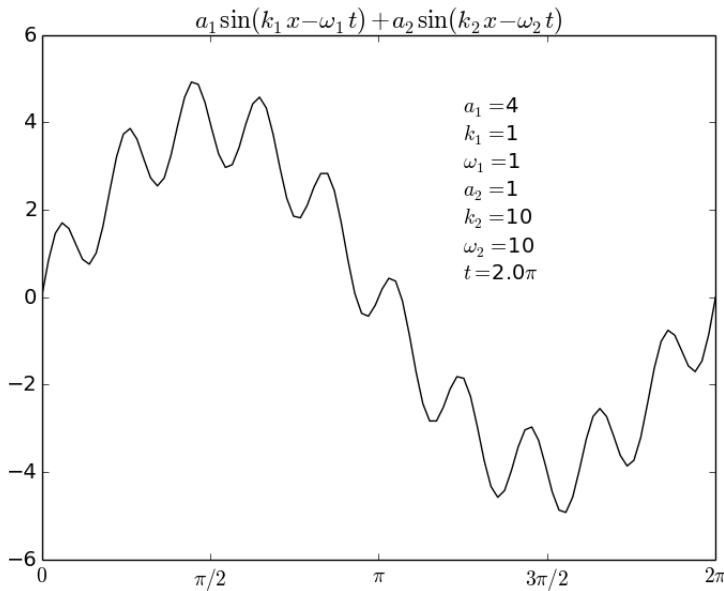
Exercise:

Write down an expression for the wave length, λ , and the wave speed, u in terms of k and ω

61

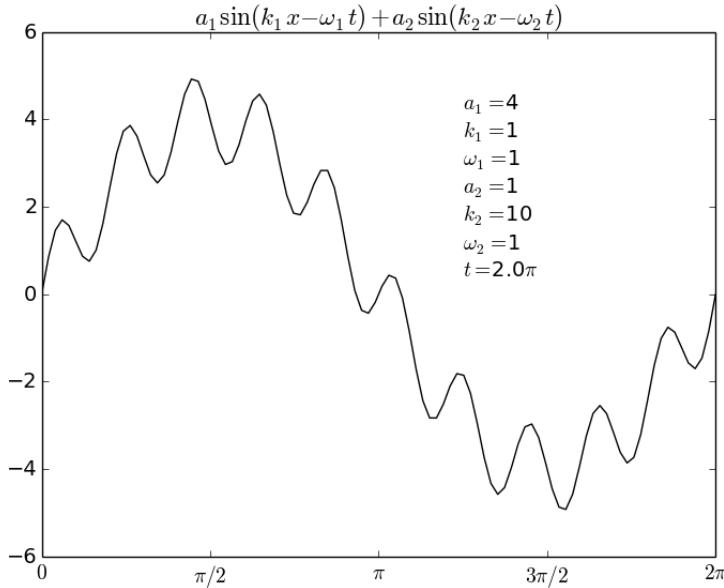
5.2 Dispersion

Dispersion occurs when waves of different frequencies propagate at different speeds.



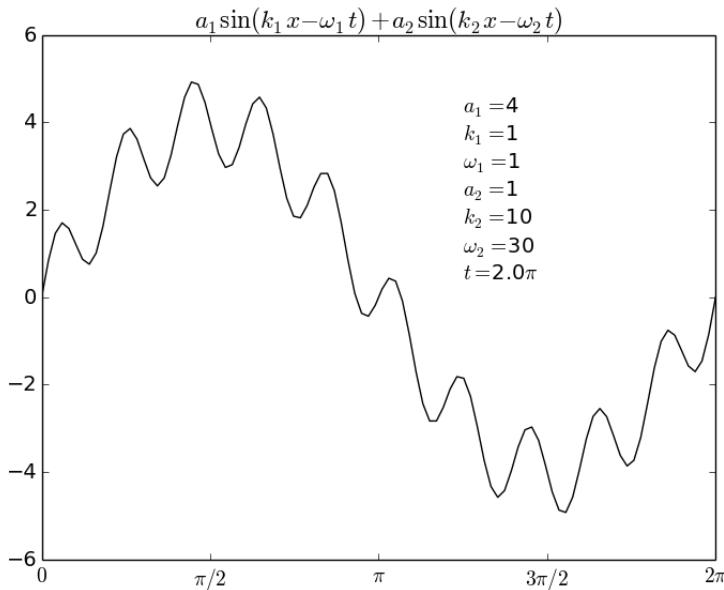
- $u = \frac{\omega_1}{k_1} = \frac{\omega_2}{k_2}$ so wave of both wavelengths propagate at the same speed
- No dispersion occurs – the function does not change shape

62



- $u_1 = \frac{\omega_1}{k_1} = 10 \frac{\omega_2}{k_2}$ so the short wavelength waves are much slower than the long waves
- Dispersion occurs – the function changes shape

63

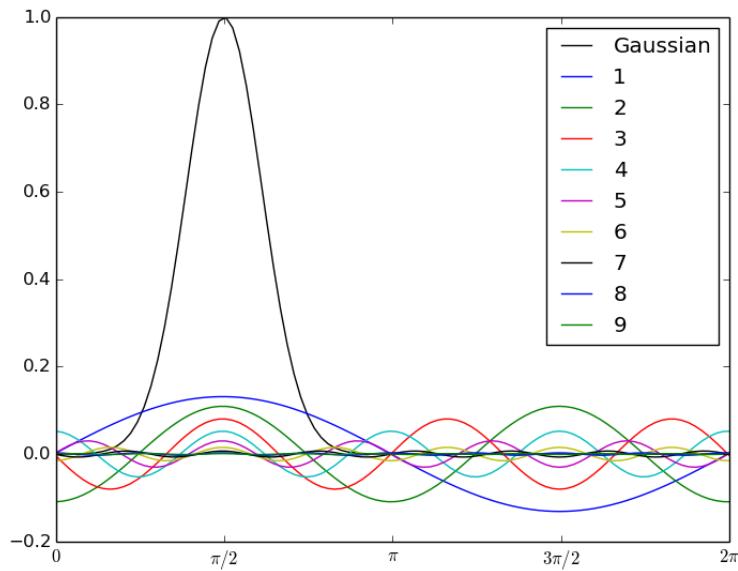


- $u_1 = \frac{\omega_1}{k_1} = \frac{1}{3} \frac{\omega_2}{k_2}$ so the short wavelength waves travel more quickly
- Dispersion occurs – the function changes shape

64

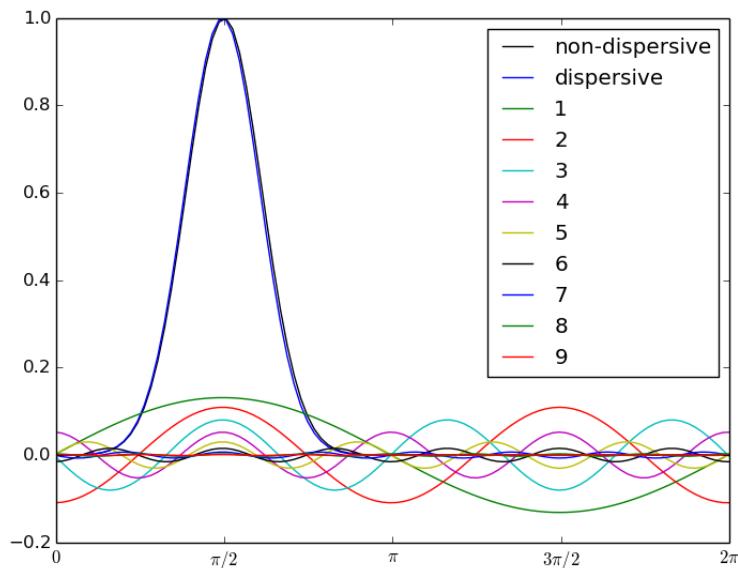
For a function to propagate without changing shape, all of the Fourier modes must propagate at the same speed:

This shows the propagation of a Gaussian and propagation of the first 9 Fourier modes.



65

Propagation of a Gaussian with high wavenumber waves propagating more slowly



The original Gaussian function changes shape

66

5.3 Some Excellent Animations and Videos which demonstrate Dispersion

- Some description and animations from Dr. Dan Russell, Grad. Prog. Acoustics, Penn State:
http://www.acs.psu.edu/drussell/Demos/Dispersion/dispersion.html
- A video of the wake of a motor-boat from JNHeyman (41 seconds):
https://www.youtube.com/watch?v=lWi_KpBy8kU
- A video of ripples in a pond with descriptions of the dispersion (2:28)
<https://www.youtube.com/watch?v=dESm6VjfSNs>

67

5.4 Phase speed of linear advection

We know:

- the one-dimensional linear advection equation:

- its analytic solution:

$$\phi(x, t) =$$

- under the action of the linear advection equation, waves propagate with phase speed u . (linear advection is non-dispersive since u does not depend on k)
- If we multiply a single Fourier mode, e^{ikx} , by $e^{-iku\Delta t}$ then that mode will move a distance ... around the x -axis
- The amplification factor for exact linear advection is $A =$
- Therefore if a numerical method has amplification factor $re^{-i\theta}$ for wavenumber k then the phase speed of the numerical waves of wavenumber k will be ...
- If the phase speed is dependent on k then we will get numerical dispersion

68

5.5 Phase speed and dispersion errors of CTCS

The amplification factor of CTCS is

$$A =$$

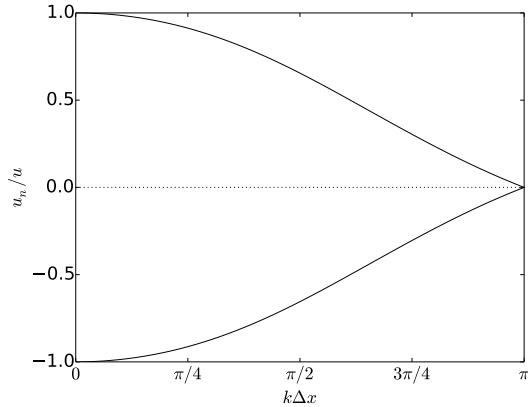
where $c = \dots$. Therefore we can find the phase-speeds of the numerical waves relative to the analytic waves:

$$\frac{u_n}{u} =$$

This can be simplified by substituting in $u\Delta t = c\Delta x$ and $\sin \alpha = c \sin k\Delta x$:

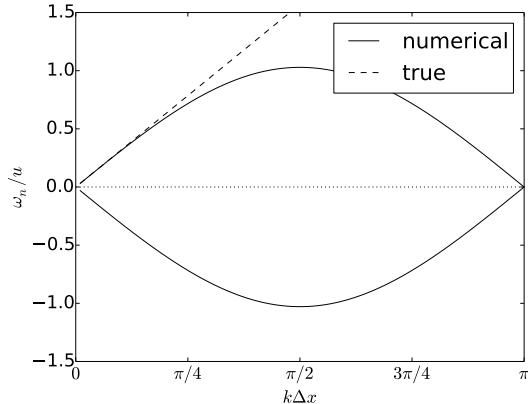
$$\frac{u_n}{u} =$$

There are two possible phase-speeds for each mode. These can be plotted against $k\Delta x$ to find out how waves propagate when advected by CTCS. A plot of u_n/u against $k\Delta x$ (or $\omega = ku$ against k) is called a dispersion relation. The dispersion relation for CTCS for $c = 0.4$:



69

The dispersion relation for CTCS for $c = 0.4$ plotted as ω against $k\Delta x$



What does this tell us about CTCS?

- There are two possible solutions:
 - the physical mode ($u_p/u \geq 0$)
 - the computational mode ($u_p/u < 0$)
- The computational mode propagates in the wrong direction
- All waves propagate too slowly
- For the physical mode, when waves are well resolved (small k or small Δx), they propagate at nearly the correct speed (this is why it is called the physical mode)
- Grid-scale waves ($k\Delta x = \pi$) do not propagate

70

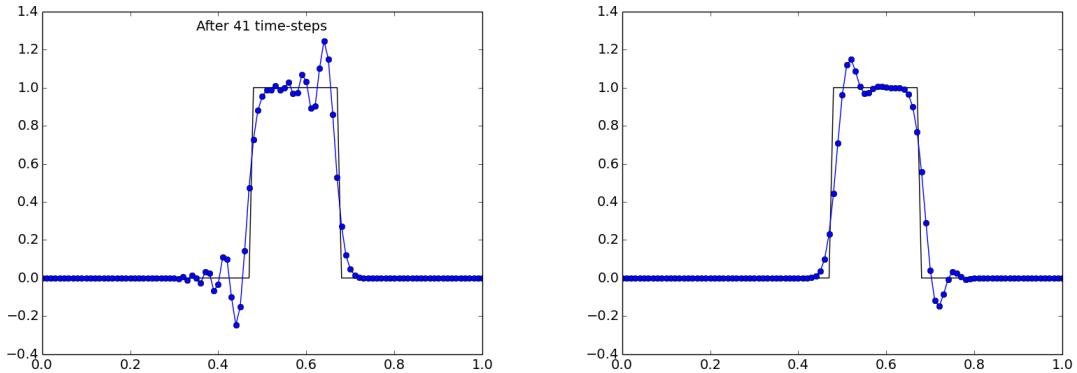
5.6 Exercise

What can dispersion relations tell us about the behaviour of numerical methods? These are the results of solving the linear advection equation using two finite volume methods. The generic finite-volume method for linear advection in 1d for a uniform grid is define as:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t} = -u \frac{\phi_{j+1/2} - \phi_{j-1/2}}{\Delta x}$$

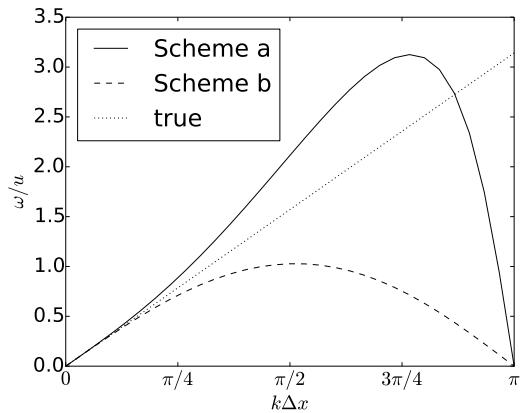
The two finite-volume methods are:

| | |
|--|--|
| Lax-Wendroff $\phi_{j+1/2} = \frac{1}{2}(1+c)\phi_j + \frac{1}{2}(1-c)\phi_{j+1}$ Advection of a top-hat profile to the right using $c = 0.2$, 100 points | Warming and Beam $\phi_{j+1/2} = \frac{1}{2}(3-c)\phi_j - \frac{1}{2}(1-c)\phi_{j-1}$ |
|--|--|



71

These are the dispersion relations for the two schemes. Which dispersion relation is related to which scheme and why?



72

Chapter 6: Alternative Advection Schemes

Some problems we have encountered with advection schemes:

-

These are consistent with **Godunov's theorem**:

Linear numerical schemes for solving partial differential equations, having the property of not generating new extrema (monotone scheme), can be at most first-order accurate.

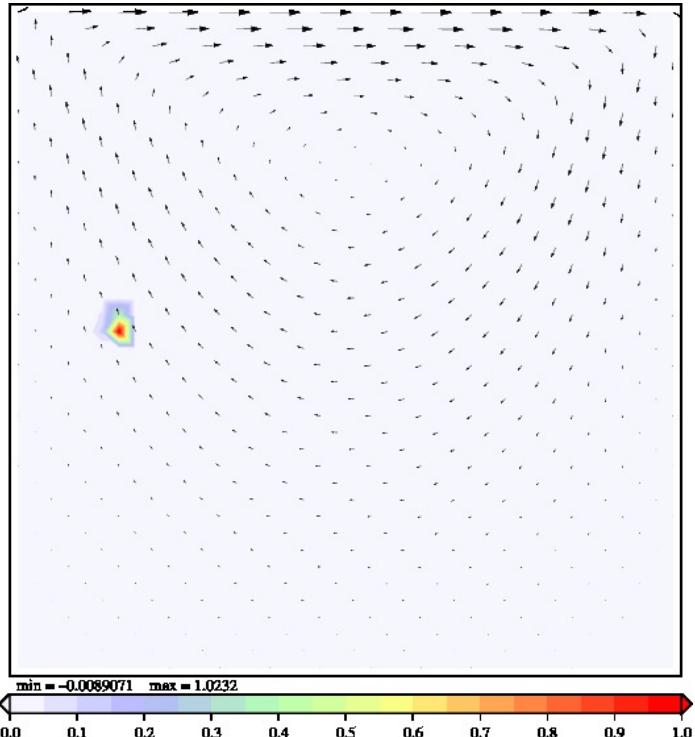
We will therefore present some alternatives:

1. Semi-Lagrangian advection
2. Artificial diffusion to remove spurious oscillations
3. The Finite Volume Method
4. Lax-Wendroff and Warming and Beam
5. Total variation diminishing (TVD) schemes

73

6.1 Semi-Lagrangian Advection

- Explicit without time-step restrictions associated with $c = u\Delta t / \Delta x$
- Used by the UK Met Office and ECMWF
- To calculate a new value of a dependent variable, look upwind to where it has come from

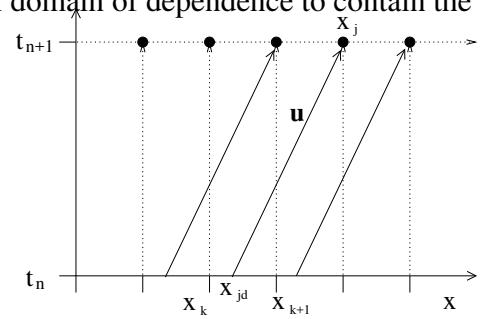


74

6.1.1 Semi-Lagrangian Advection in One Dimension

CFL criterion: The domain of dependence of the numerical solution must contain the domain of dependence of the original PDE.

- So to allow long time-steps, construct the numerical domain of dependence to contain the physical domain of dependence.
- Recall the linear advection equation: $\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0$
- and its analytic solution: $\phi(x, t) = \phi(x - ut, 0)$
- Semi-Lagrangian advection is defined from this:
 $\phi(x_j, t_{n+1}) = \phi(x_j - u\Delta t, t_n) = \phi(x_{jd}, t_n)$
 $x_{jd} = x_j - u\Delta t$ is the departure point of point x_j .
- So interpolate ϕ from known points onto x_{jd} .
- First find k such that $x_k \leq x_{jd} \leq x_{k+1}$: (Use $\text{floor}(x)$ meaning the integer below or at x)
 $k =$
- Interpolate from $x_{k-1}, x_k, x_{k+1}, \dots$ onto x_{jd} (for example using cubic-Lagrange interpolation)



Exercise: Find $\beta = (x_{jd} - x_k)/\Delta x$ as a function of only j, k and c given $x_j = j\Delta x$ and $c = u\Delta t/\Delta x$.

Advantage: Explicit scheme without Courant number restriction

Problem: The advected quantity is not conserved

Order of Accuracy: Ignoring errors in calculating the departure point, semi-Lagrangian should achieve an order of accuracy of $O[(\Delta x)^{p+1}/\Delta t]$ where p is the order of the interpolation [1].

75

6.2 Artificial Diffusion to Remove Spurious Oscillations

Numerical schemes are designed not to produce spurious oscillations. However, once a forecasting model is put together, often spurious oscillations are still generated. These can be removed by adding an artificial diffusion term to the equations. For example, the linear advection equation with diffusion:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi - K \nabla^2 \phi = 0 \quad (6.1)$$

or in one dimension:

$$\frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial x^2} = 0 \quad (6.2)$$

- This is dampens spurious oscillations and real features
- It is only (but frequently) used as a last resort.
- More scale-selective filtering can be achieved using ∇^4 rather than ∇^2 :

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi + K \nabla^4 \phi = 0 \quad (6.3)$$

Stability limits of the advection-diffusion scheme

The advection diffusion scheme:

$$\phi_j^{(n+1)} - \phi_j^{(n-1)} + c(\phi_{j+1}^{(n)} - \phi_{j-1}^{(n)}) - 2d(\phi_{j+1}^{(n-1)} - 2\phi_j^{(n-1)} + \phi_{j-1}^{(n-1)}) = 0 \quad (6.4)$$

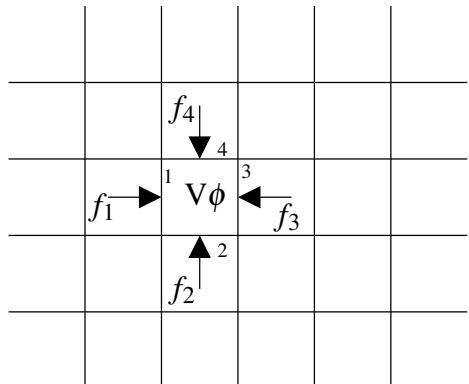
where $c = u\Delta t/\Delta x$ and the diffusion number, $d = K\Delta t/\Delta x^2$ has the stability constraint $c^2 + 4d \leq 1$. The algebra is complicated and does not need to be reproduced.

Questions: How much diffusion is needed to control oscillations? How much does this reduce accuracy?

76

6.3 The Finite Volume Method

The volume integrals of predicted variables (eg ϕ) are calculated on small volumes (cells with volume V) by calculating the quantities entering and leaving the cell:



$$\frac{d}{dt} (V\phi) = \sum_{i=1}^4 f_i$$

Where f_i is the flux of ϕ through edge i .

The finite volume method can also be derived by discretising the flux form of the advection equation. Constant density flow is divergence free ($\nabla \cdot \mathbf{u} = 0$) and so two forms of the linear advection equation are equivalent:

$$\begin{aligned} \partial \phi / \partial t + \mathbf{u} \cdot \nabla \phi &= 0 && \text{advective form} \\ \partial \phi / \partial t + \nabla \cdot (\mathbf{u} \phi) &= 0 && \text{flux form} \end{aligned}$$

The flux (or conservative) form can be discretised using Gauss's divergence theorem:

$$\nabla \cdot \mathbf{u}\phi \approx \frac{1}{V} \int_V \nabla \cdot \mathbf{u}\phi \, dV = \frac{1}{V} \int_S \phi \mathbf{u} \cdot \mathbf{dS} = \frac{1}{V} \sum_i f_i$$

where volume V has surface S , \mathbf{dS} is the outward pointing normal to surface S and $f_i = \phi \mathbf{u} \cdot \mathbf{dS}$ is the flux over edge i .

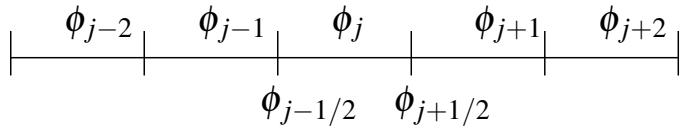
Conservation: the finite volume method is conservative: however f_i is calculated, the total mass of ϕ is conserved because exactly what leaves one cell will enter another.

Finite volume is a family of methods. There are numerous approximations for estimating f_i from surrounding ϕ and \mathbf{u} values.

77

6.3.1 The Finite Volume Method in one dimension, for constant u

For constant u : $f_{j+1/2} = u\phi_{j+1/2}$.
So to solve: $\phi_t = -u\phi_x$ we use

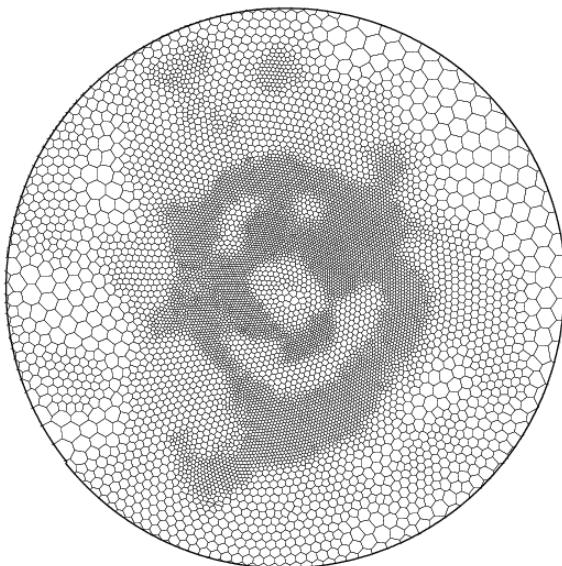


$$\frac{\partial \phi_j}{\partial t} = -u \frac{\phi_{j+1/2} - \phi_{j-1/2}}{\Delta x}$$

It remains to estimate $\phi_{j\pm 1/2}$ from surrounding values of ϕ_j .

Exercise Demonstrate the following:

- If we choose centred in time for $\frac{\partial \phi_j}{\partial t}$ and $\phi_{j+1/2} = \frac{1}{2}(\phi_j + \phi_{j+1})$ we recover the CTCS finite difference scheme
- If we choose forward in time for $\frac{\partial \phi_j}{\partial t}$ and $\phi_{j+1/2} = \phi_j$ we recover the FTBS finite difference scheme



Solution on notes on blackboard.

Using the finite volume method, we can solve equations on arbitrary meshes.

6.4 Lax-Wendroff

We start with the finite volume method:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t} = -u \frac{\phi_{j+1/2} - \phi_{j-1/2}}{\Delta x}.$$

For Lax-Wendroff, $\phi_{j+1/2}$ is calculated to be the average value that passes through position $x_{j+1/2}$ between time-steps n and $n + 1$. So you could call it $\phi_{j+1/2}^{(n+1/2)}$. Therefore we need to calculate the average value of ϕ between positions $x_{j+1/2}$ and a distance $u\Delta t$ upstream of $x_{j+1/2}$. In order to calculate the average, we assume that ϕ varies linearly between x_j and x_{j+1} . Then we can calculate ϕ at $x_{j+1/2} - 1/2u\Delta t$.

This could be written $\phi_{j+1/2}^{(n+1/2)} = \phi^{(n)}(x_{j+1/2} - 1/2u\Delta t)$.

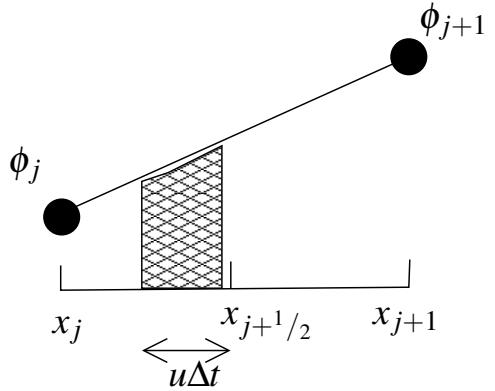
Exercise: Using the Courant number, $c = u\Delta t/\Delta x$, show that this gives:

$$\phi_{j+1/2}^{(n+1/2)} = 1/2(1+c)\phi_j^{(n)} + 1/2(1-c)\phi_{j+1}^{(n)}$$

(solution on blackboard notes)

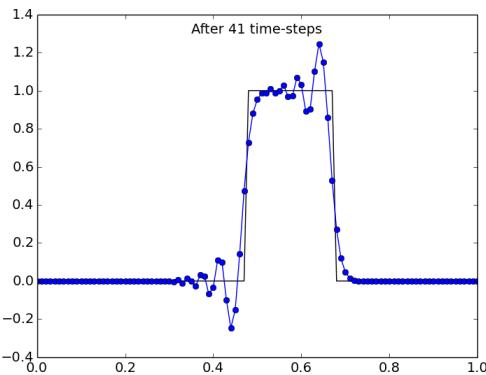
Notes:

- Lax-Wendroff is second-order accurate in space and time.
- Lax-Wendroff is not monotonic or bounded
- Stable for $|c| \leq 1$

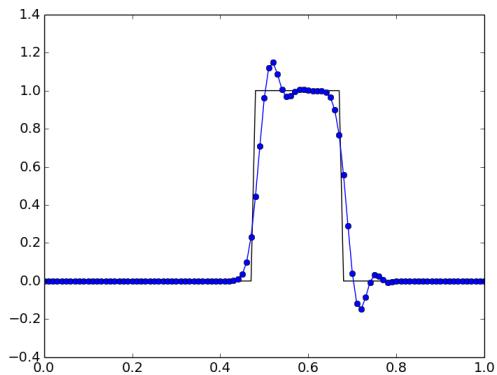


79

| | |
|---|---|
| Lax-Wendroff $\phi_{j+1/2} = 1/2(1+c)\phi_j + 1/2(1-c)\phi_{j+1}$ Advection of a top-hat profile to the right using $c = 0.2$, 100 points | Warming and Beam $\phi_{j+1/2} = 1/2(3-c)\phi_j - 1/2(1-c)\phi_{j-1}$ |
|---|---|



Smooth ahead of the discontinuity



Smooth behind the discontinuity

Remember **Godunov's theorem**:

Linear numerical schemes for solving partial differential equations, having the property of not generating new extrema (monotone scheme), can be at most first-order accurate.

- So if we want a monotone, second-order scheme it must be ...
- Warming and Beam is also second-order accurate in space and time
- So why not combine Lax-Wendroff and Warming and Beam based on local gradients?
- By making the scheme based on the gradient of ϕ , the scheme is non-linear.

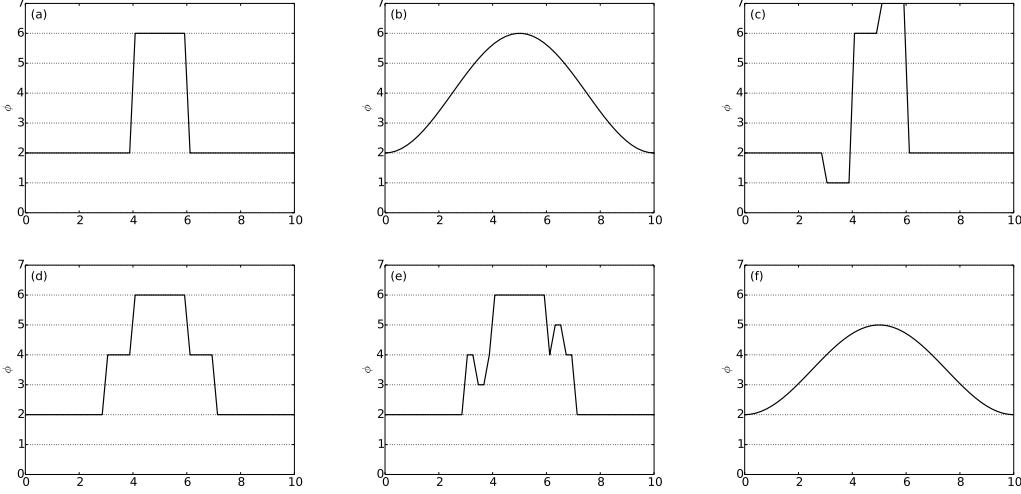
80

6.5 Total Variation

- Linear, second-order advection schemes produce unbounded, unrealistic, grid-scale oscillations. These can be measured by the total variation:

$$TV = \sum_{j=0}^{n_x-1} |\phi_{j+1} - \phi_j|$$

Exercise: Calculate the total variation of these functions:



- A total variation diminishing (TVD) scheme has $TV^{(n+1)} \leq TV^{(n)}$.

Question: Why is total variation used rather than boundedness to measure the generation of spurious oscillations? ...

81

6.6 Total Variation Diminishing (TVD) schemes

- A total variation diminishing (TVD) scheme has $TV^{(n+1)} \leq TV^{(n)}$
- First-order upwind is the only *linear* TVD scheme. Other TVD schemes are non-linear...
- We start with the linear advection equation discretised in conservative (flux) form:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t} = -u \frac{\phi_{j+1/2} - \phi_{j-1/2}}{\Delta x}. \quad (6.5)$$

- Each $\phi_{j+1/2}$, is calculated as a weighted average of a high order flux (ϕ_H) and a low order flux (ϕ_L):

$$\phi_{j+1/2} = \Psi_{j+1/2} \phi_H + (1 - \Psi_{j+1/2}) \phi_L$$

where Ψ is a limiter function.

- Use as much of ϕ_H as possible without introducing oscillations
- So Ψ should be close to one where the solution is smooth so that the solution is close to second-order accurate and Ψ close to zero where the solution changes rapidly so as to use the upwind flux which guarantees boundedness.
- The scheme is now non-linear since Ψ depends on ϕ .
- We can use:
 - Lax-Wendroff as the high-order flux: $\phi_H = \frac{1}{2}(1+c)\phi_j + \frac{1}{2}(1-c)\phi_{j+1}$
 - First-order upwind as the low-order flux: $\phi_L = \begin{cases} \phi_j & \text{if } u \geq 0 \\ \phi_{j+1} & \text{otherwise} \end{cases}$
- So what should Ψ be?

82

6.6.1 Limiter functions

The limiter function, Ψ , is based on the ratio of the upwind gradient to the local gradient:

$$r_{j+1/2} = \frac{\phi_j - \phi_{j-1}}{\phi_{j+1} - \phi_j}$$

for $u > 0$.

6.6.1.1 Exercise

Warming and Beam (WB) is not a TVD scheme but the flux,

$\phi_{j+1/2} = \frac{1}{2}(3-c)\phi_j - \frac{1}{2}(1-c)\phi_{j-1}$ can be expressed in the form:

$$\phi_{j+1/2} = \Psi_{j+1/2} \phi_H + (1 - \Psi_{j+1/2}) \phi_L$$

where ϕ_H is Lax-Wendroff ($\phi_H = \frac{1}{2}(1+c)\phi_j + \frac{1}{2}(1-c)\phi_{j+1}$) and ϕ_L is backward in space ($\phi_L = \phi_j$). If WB is expressed in this form, what is $\Psi_{j+1/2}$ as a function of $r_{j+1/2}$? (Hint, equate the two forms for $\phi_{j+1/2}$ and then equate coefficients of either c^0 or c^1)

$$\Rightarrow \Psi_{j+1/2} = \frac{\phi_j - \phi_{j-1}}{\phi_{j+1} - \phi_j} = r_{j+1/2}$$

83

6.6.2 The Sweby Diagram

The Sweby diagram shows the limiter function, Ψ , as a function of the upwind to local gradient, r . It is used to find limiter functions that give TVD advection schemes.

1. Draw lines of Ψ for Lax-Wendroff (LW) and Warming and Beam (WB):
2. Shade the region outside the two lines.
The unshaded region shows the convex combination of LW and WB. If Ψ takes a value in the unshaded region then the scheme will be 2nd-order accurate because LW and WB are 2nd-order
3. Draw lines of $\Psi = 2$ and $\Psi = 2r$. Sweby (SIAM J. Numer. Anal. 1984) showed that if $\Psi \leq 2$ and $\Psi \leq 2r$ then the scheme is TVD
4. Shade the region where $\Psi > 2$ and $\Psi > 2r$.

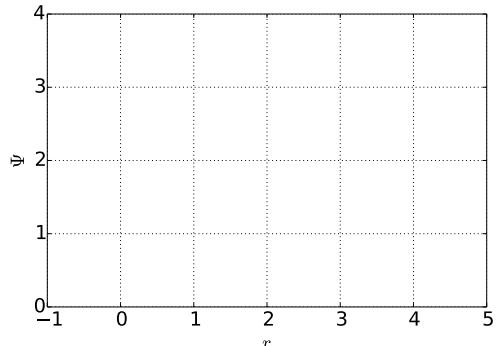
The unshaded region now is the 2nd-order TVD region. If Ψ lies in this region then the scheme will be 2nd-order TVD

6.6.3 The Van Leer Limiter

A popular limiter function is due to Van Leer: $\Psi(r) = (r + |r|) / (1 + |r|)$

Sketch this function on the Sweby diagram.

There are many other limiter functions that give TVD schemes. See, eg
https://en.wikipedia.org/wiki/Flux_limiter



Chapter 7: Modelling Wave Equations

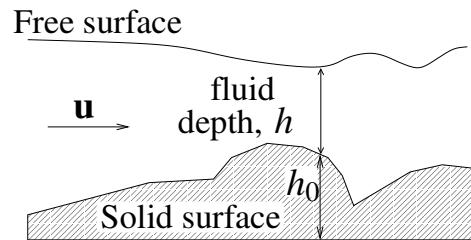
Many of the processes in the atmosphere are represented by the shallow water equations (SWE). The assumptions needed to derive the SWE are:

- Horizontal length scale \gg vertical length scale
- Very small vertical velocities

Depth integrate the Navier-Stokes equations over orography to give the SWE:

$$\frac{D\mathbf{u}}{Dt} = -2\Omega \times \mathbf{u} - g\nabla(h + h_0) + \mu_u \nabla^2 \mathbf{u} \quad (7.1)$$

$$\frac{Dh}{Dt} + h\nabla \cdot \mathbf{u} = 0 \quad (7.2)$$



where

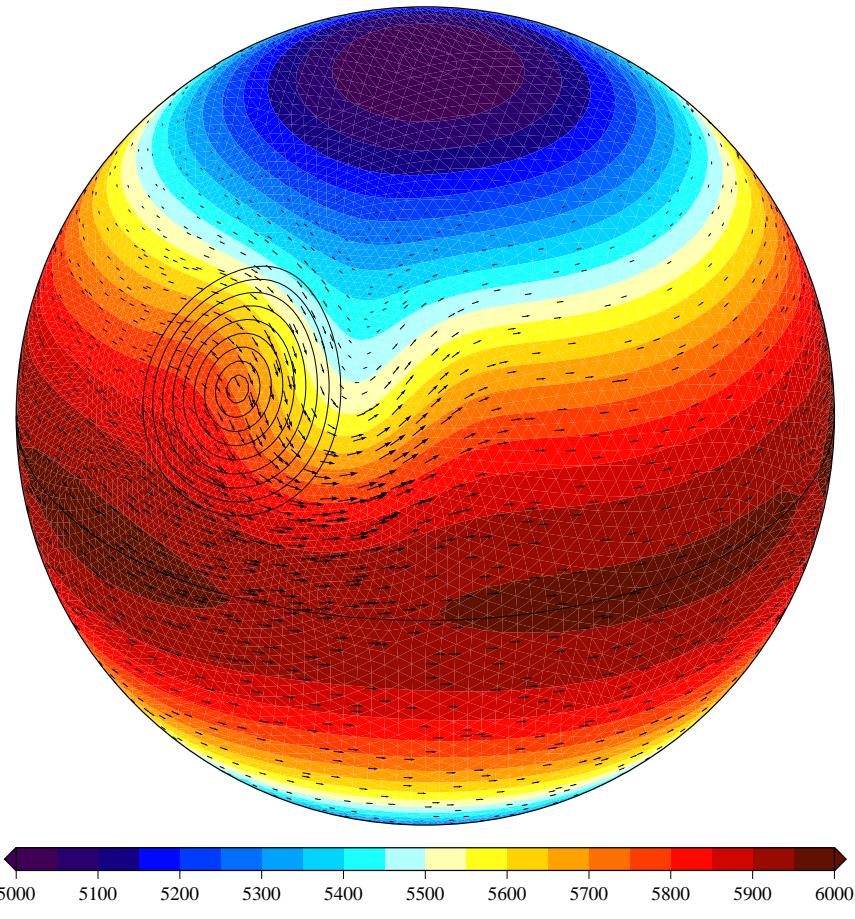
| | | | |
|--------------|------------------------------|----------|---------------------------------|
| \mathbf{u} | Depth integrated wind vector | g | Acceleration due to gravity |
| t | Time | ∇ | Gradients in the horizontal |
| Ω | Rotation rate of planet | h_0 | Height of the bottom topography |
| h | Fluid depth | μ_u | Diffusion of momentum |

Exercise: Considering the meaning of the terms in the momentum equation in section 1.3, what are the meaning of the terms of the momentum equation of the SWE?

85

7.1 Simulations of the SWE on the surface of a sphere

The shallow-water equations can be solved on the surface of a sphere with \mathbf{u} being the horizontal wind (ignoring updrafts and downdrafts) and h being the depth of a layer of atmosphere. The results look similar to large-scale atmospheric circulation. The vectors show \mathbf{u} , the black contours show a mountain (h_0) and colours show $h + h_0$.



86

7.2 Processes Represented by the SWE

Which of these processes are represented by the SWE and which are only represented by the full NS equations?

| | |
|----------------------|------------------------|
| Horizontal advection | Acoustic waves |
| Vertical advection | Coriolis |
| Gravity waves | Diffusion |
| Rossby waves | Heat transport |
| Adiabatic expansion | Atmospheric convection |
| Geostrophic balance | Geostrophic turbulence |

Component Form of the SWE

Assuming $\mathbf{u} = (u, v, 0)^T$ and $2\Omega = (0, 0, f)^T$, equations (7.1) and (7.2) written in component form are:

$$\begin{aligned}\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= fv - g \frac{\partial(h+h_0)}{\partial x} + \mu_u \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} &= -fu - g \frac{\partial(h+h_0)}{\partial y} + \mu_v \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \\ \frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} + h \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) &= 0 \quad \text{or} \quad \frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} + \frac{\partial hv}{\partial y} = 0\end{aligned}$$

7.2.1 Linearised SWE

In order to find analytic solutions and to analyse numerical methods, we linearise the SWE. Assume:

- $\mathbf{u} = (u, v, 0)^T$ is small
- $2\Omega = (0, 0, f)^T$
- $h = H + h'$ where H is uniform in space and time and h' is small
- the product of two small variables is ignored (even if one or both are inside a differential)
- h_0 and μ_u are ignored

This gives the following equations for u, v and h' expressed in terms of f (rather than Ω):

(7.3)

(7.4)

(7.5)

7.3 Analytic Solution

Ignoring Coriolis, the linearised SWE have wave-like solutions – *gravity waves*. In 1d these are:

$$h' = \mathbb{H} e^{ikx} e^{\pm ikt\sqrt{gH}} \quad (7.6)$$

$$u = \pm \sqrt{g/H} \mathbb{H} e^{ikx} e^{\pm ikt\sqrt{gH}} \quad (7.7)$$

for any constant \mathbb{H} . So waves with wavenumber k in space oscillate with frequency $k\sqrt{gH}$ and the wave speed is ... (so gravity waves are non-dispersive).

89

7.4 Unstaggered Forward-Backward (1d A-grid FB)

As there are two equations that depend on each other, it is quite natural to solve them using forward-backward time-stepping – forward for u and backward for h . We will also start by assuming that h and u are defined at the same spatial positions (this is called co-located, unstaggered or A-grid) and we will use centred spatial discretisation:

$$\frac{\partial u}{\partial t} = -g \frac{\partial h}{\partial x} \rightarrow = \quad (7.8)$$

$$\frac{\partial h}{\partial t} = -H \frac{\partial u}{\partial x} \rightarrow = \quad (7.9)$$

where $x_j = j\Delta x$, $t^{(n)} = n\Delta t$, $h_j^{(n)} = h(x_j, t^{(n)})$ and $u_j^{(n)} = u(x_j, t^{(n)})$.

7.4.1 Von-Neumann Stability Analysis

We can find the stability limits and dispersion relation for the numerical scheme given in section 7.4 (1d A-grid FB) using von-Neumann stability analysis.

To calculate an amplification factor, A , for each wavenumber, k , we assume wave-like solutions for h and u :

$$h_j^{(n)} = \mathbb{H} A^n e^{ikj\Delta x} \quad (7.10)$$

$$u_j^{(n)} = \mathbb{U} A^n e^{ikj\Delta x} \quad (7.11)$$

for some constants \mathbb{H} and \mathbb{U} . Substituting these into (7.8) and (7.9) and defining the Courant number $c = \frac{\sqrt{gH}\Delta t}{\Delta x}$ leads to:

$$A = 1 - \frac{c^2}{2} \sin^2 k\Delta x \pm \frac{ic}{2} \sin k\Delta x \sqrt{4 - c^2 \sin^2 k\Delta x} \quad (7.12)$$

There are two solutions for A but this is correct because there are also two analytic solutions to the equations (because of the \pm in the analytic solution). For $|c| \leq 2$ this gives $|A|^2 = 1$ so the scheme is stable and undamping for sufficiently small time steps. However for $|c| > 2$ we have:

$$|A|^2 = \left(1 - \frac{c^2}{2} \sin^2 k\Delta x \pm \frac{c}{2} \sin k\Delta x \sqrt{c^2 \sin^2 k\Delta x - 4} \right)^2$$

which can be greater than 1 and so the scheme is unstable for $|c| > 2$ where $c = \sqrt{gH}\Delta t/\Delta x$. So this scheme is conditionally stable. Stable for $c \leq 2$.

91

7.4.2 Dispersion of Unstaggered Forward-Backward (1d A-grid FB)

A reminder of the amplification factor for this method:

$$A = 1 - \frac{c^2}{2} \sin^2 k\Delta x \pm \frac{ic}{2} \sin k\Delta x \sqrt{4 - c^2 \sin^2 k\Delta x}.$$

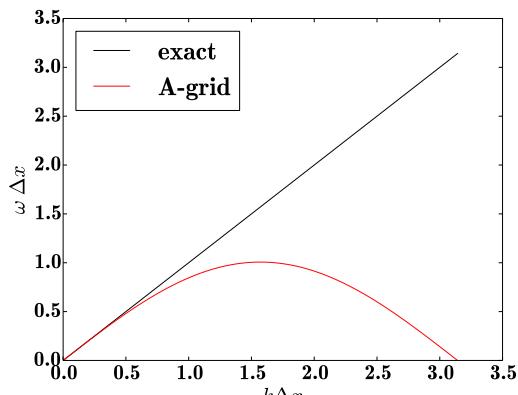
The argument of A gives us the wave frequency as a function of wavenumber:

$$\omega = \pm \frac{1}{\Delta t} \tan^{-1} \frac{\frac{c}{2} \sin k\Delta x \sqrt{4 - c^2 \sin^2 k\Delta x}}{1 - \frac{c^2}{2} \sin^2 k\Delta x} \quad (7.13)$$

This can be simplified by assuming that $\frac{c}{2} \sin k\Delta x = \sin \alpha$ to give:

$$\omega = \pm \frac{2\alpha}{\Delta t} = \pm \frac{2}{\Delta t} \sin^{-1} \left(\frac{c}{2} \sin k\Delta x \right) \quad (7.14)$$

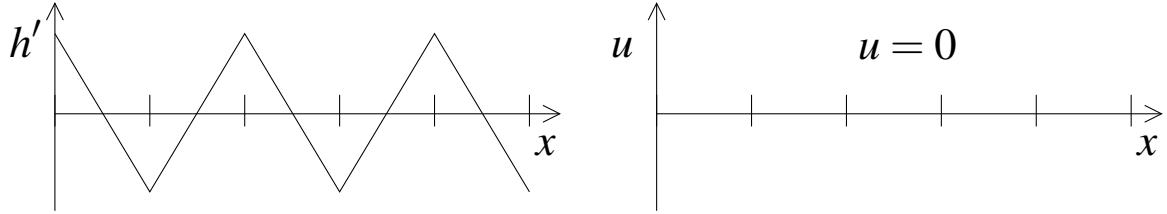
This is the A-grid dispersion relation:



Grid-scale gravity waves ($k\Delta x/\pi = 1$) have zero frequency! This is highly unrealistic.

7.5 Problems with Co-location of h and u

Consider the following initial conditions of the linearised non-rotating SWE:



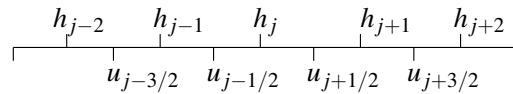
Questions:

1. How do you expect the real solution of the linearised SWE to evolve?
2. How will the solution of the 1d A-grid FB scheme evolve?

93

7.6 Staggered Forward-Backward (1d C-grid FB)

So that gradients of h can be calculated where u is located and gradients of u can be calculated where h is located, h and u can be staggered in space:



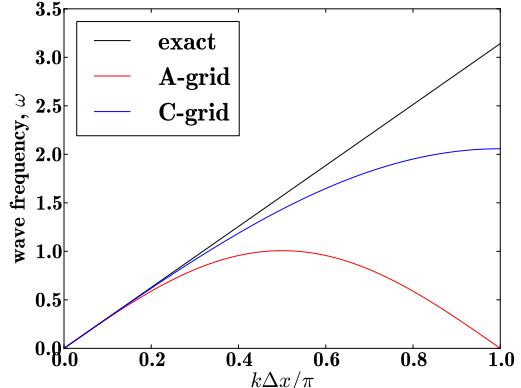
Using centered, 2-point spatial differences and forward-backward in time gives:

$$\frac{\partial u}{\partial t} = -g \frac{\partial h}{\partial x} \rightarrow = \quad (7.15)$$

$$\frac{\partial h}{\partial t} = -H \frac{\partial u}{\partial x} \rightarrow = \quad (7.16)$$

Von-Neumann stability analysis gives:

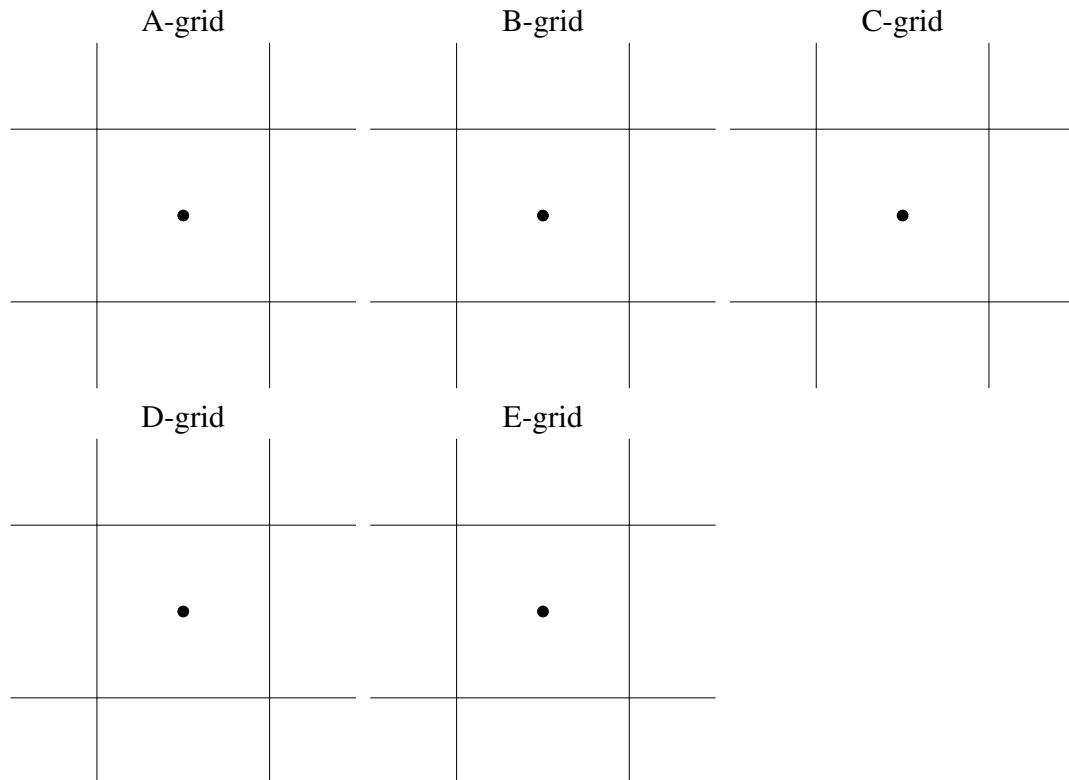
- $|A| = \begin{cases} 1 & \text{for } |c| \leq 1 \\ > 1 & \text{for } |c| > 1 \text{ for some } k\Delta x \end{cases}$
 \therefore neutrally stable for $|c| \leq 1$
- Dispersion relation:
 $\omega = \pm 2\alpha = \pm 2 \sin^{-1} \left(c \sin \frac{k\Delta x}{2} \right)$
- \therefore the C-grid is dispersive
- grid-scale waves propagate too slowly
- C-grid widely used in atmosphere and ocean models
- What about in 2d?



94

7.7 Arakawa Grids

In two dimensions, there are more possibilities for where the prognostic variables are located:



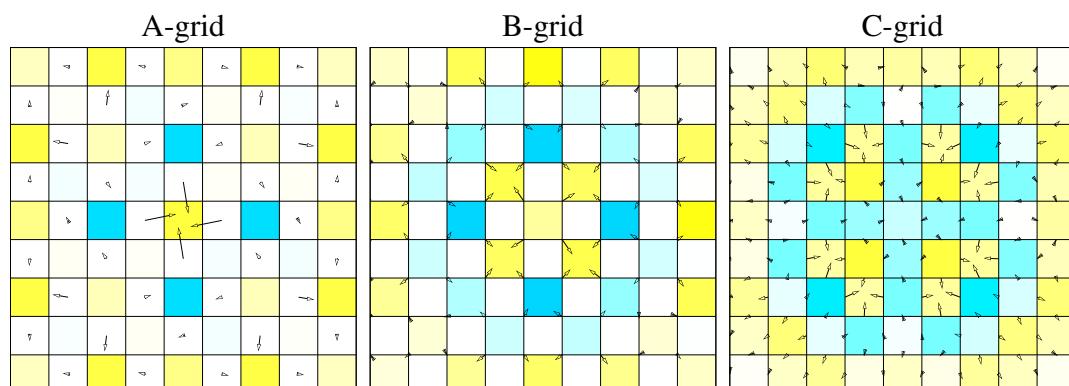
95

7.8 Linearised Shallow-Water Equations on Arakawa Grids

The linearised SWE with rotation are:

$$\begin{aligned}\partial \mathbf{u} / \partial t &= -2\Omega \times \mathbf{u} - g\nabla h \\ \partial h' / \partial t + H\nabla \cdot \mathbf{u} &= 0\end{aligned}$$

- The linearised SWE are solved numerically on Arakawa A, B and C grids, starting from initial conditions consisting of zero velocity and zero h' everywhere except a positive h' in one central grid-box
- The colours show h' in the grid boxes. Red/yellow positive, blue/negative, white zero



7.9 Discussion Question

For solving the 2d, linearised rotating SWE (eqns 7.3-7.5) what are the advantages and disadvantages of the different grids? Which terms or which balances between terms will be represented accurately by different grids?

96

Bibliography

- [1] D. Durran. *Numerical Methods for Fluid Dynamics With Applications to Geophysics*, volume 32 of *Texts in Applied Mathematics*. Springer, 2nd edition, 2010. ISBN 1441964118.