MTH2005 — Modelling: Theory & Practice
Group projects brief 2025

1 Summary

You will work in a small group to complete a short project applying numerical methods and/or optimisation to real-world problems, complementing the taught material in this module.

Each group are required to submit:

- via ELE, a paper in the style of those published in the SIAM Undergraduate Research Online journal (see the technical specifications below).
- via email to your project tutor, a zipfile containing the code required to replicate your findings.

The deadline for submission of the paper and zipfile is noon on Thursday 27th March 2025. Late submissions could be awarded a mark of zero unless mitigation is applied for and granted.

2 How to submit your choices

Submit *three choices* of project from the list below via the project preferences task on the module ELE page by **noon Monday 10th February 2025**.

3 Assessment criteria

This project will contribute 30% to your final module mark. Marks for your submissions will be awarded as follows:

Code (15 marks): You must submit the complete code you have used to produce the results in your paper. Your code should be modular to allow for testing of each component, efficient, readable, well commented, and you should ensure that variables are specified as inputs rather than hard-coded.

Your project tutor will provide further guidance as to what they expect to see in your code based on the specific requirements of your project.

Paper (15 marks): The paper will be assessed according to the following criteria:

- **Progress**
  - *Higher:* Substantial evidence of independent investigation of all the threshold elements, and at least one of the higher elements.
  - *Threshold:* All the threshold elements have been attempted and for the most part have been explored competently.
  - *Fail:* There are significant missing elements from the list of threshold tasks for the investigation and/or engagement is minimal with little independent investigation of the key ideas.
- **Analysis**
  - *Higher:* Substantial progress has been made in presenting and discussing comparative analysis of different methods for solving the problem.

  - *Threshold:* Some progress has been made in analysing different methods for solving the problem, but this is primarily descriptive or the conclusions are poorly supported by the data.
  - *Fail:* Little progress has been made to implement and compare different methods for solving the problem. The conclusions cannot be justified by the data selected.

- **Mathematical accuracy**
  - *Higher:* All statements made are correct, containing complete hypotheses and proofs where appropriate. Notation is correct and uniform. Assumptions made are clearly identified.
  - *Threshold:* Some general results identified and largely accurate, but occasionally containing some inaccuracies, imprecisions or omissions. Language and/or notation used is occasionally imprecise.
  - *Fail:* Significant and frequent inaccuracies in the statement of results, presentation of examples and use of notation. Language used is frequently imprecise.

- **Clarity and referencing**
  - *Higher:* No spelling, grammatical or editing errors. A coherent and logical narrative runs through the presentation, binding the material together. All statements are fully and correctly referenced.
  - *Threshold:* Occasional spelling, grammatical and/or editing errors. Occasional loss of flow when watching the presentation. Some material is not clearly referenced, or there are minor errors in the referencing.
  - *Fail:* Significant and frequent spelling, grammatical and/or editing errors. Little or no logical flow or narrative to the presentation. Little or no attempt to reference material appropriately, or significant and persistent errors in the referencing.

- **Quality**
  - *Higher:* The paper looks polished and professional — it is obvious that a great deal of care has been taken in the preparation and editing of the finished product.
  - *Threshold:* Some small errors, but not so significant as to seriously detract from what is otherwise a good paper.
  - *Fail:* Significant errors that render the paper difficult to read or does not meet the technical specifications.

The marker will first determine the level of the paper against each category and by means of a best-fit principle will determine the overall profile of the paper (higher, threshold, fail). At the marker's discretion, a mark will then be awarded within the corresponding level where: a mark of 0–5 corresponds to a fail; a mark of 6–10 corresponds to threshold level; and a mark of 11–15 corresponds to higher level.

4 Notes on the use of AI

Please note that whilst the use of AI (e.g. ChatGPT) as a tool to help you work on your project is not forbidden, it is strongly discouraged. ChatGPT gets some things in numerical methods correct, but it certainly gets other things very wrong. Please make sure that whatever you hand is in entirely your group's own work. Copying work from AI sources would constitute academic misconduct, as detailed in the University's policy (here). If the marker suspects misconduct then you may be required to attend a viva to demonstrate your understanding. Coursework is designed to help solidify your understanding of the material, and you cannot do that if you just copy what an AI produces.

5 Assessing individual contributions to the projects

By default, all members of the group will get the same project mark. However, we recognise that sometimes group members either contribute significantly more or less than their peers. To help diagnose this, we will be assessing individual contributions in two ways:

- We would like each project to have a final section describing 'contributions to the project', where you are asked to detail who contributed what to do the project. We ask you to do this using the following categories:
  - Formal Analysis: Application of statistical, mathematical, computational, or other formal techniques to analyze or synthesize study data.
  - Investigation: Conducting a research and investigation process, specifically performing the experiments, or data/evidence collection.
  - Methodology: Development or design of methodology; creation of models.
  - Software: Programming, software development; designing computer programs; implementation of the computer code and supporting algorithms; testing of existing code components.
  - Visualization: Preparation, creation and/or presentation of the published work, specifically visualization/data presentation.
  - Writing – Original Draft Preparation: Creation and/or presentation of the published work, specifically writing the initial draft (including substantive translation).
  - Writing – Review and Editing: Preparation, creation and/or presentation of the published work by those from the original research group, specifically critical review, commentary or revision – including pre- or post-publication stages.

  These categories are taken from the 'CRediT' taxonomy for defining roles when contributing to a research paper. An example of the type of statement we are expecting is given below:

  Student-1: writing - review and editing (equal), writing - original draft of question 2 (lead). Student-2: writing – original draft of question 3 (lead); formal analysis (lead); writing – review and editing (equal). Student-3: Software for question 4 (lead); writing – review and editing (equal).

- In addition to the contribution statement, we will also be conducting a 'peer assessment' as part of the project. This means that we will be asking the members of each group to anonymously score their fellow group members on their contributions to the projects. If (and only if) there is a clear indication from these scores that some members have contributed substantially more or less to the project, then the project marks of those individuals will be adjusted up or down.

6 Feedback

There will be plenty of opportunity for regular feedback throughout your project. In particular, you should seek advice from your project tutor each week in the specified hour slot.

7 Technical specifications

Please ensure that all your submitted outputs conform to the technical specifications detailed below — this is a critically important skill.

Paper: The technical specifications for the paper are adapted from those specified for submissions to the SIAM Undergraduate Research Online journal `http://www.siam.org/students/siuro/authors.php` and its sister publications e.g. `http://www.siam.org/journals/siopt/authors.php` (URLs correct on January 28, 2025). I have deliberately used the original wording for consistency where appropriate.

A large duplication of another author's or one's own work is a sign of poor scholarship. There is also a copyright issue if the source is not cited. Your manuscript should provide proper citations, use quotation marks or indentation (for quotations of five or more lines) to indicate borrowed wording, and minimize duplication.

Papers must be typeset using LaTeX and must be submitted in electronic form. Hard-copy submissions will not be considered. Each group should submit a .pdf copy of the correctly compiled paper. We recommend creating a shared LaTeX document using Overleaf `www.overleaf.com`, for which the University has a license.

Papers may not exceed the equivalent of **20 ordinary journal pages** (minimum 11pt font, 2 cm margins) and 3 megabytes and the zipfile must not exceed 10 megabytes. Figures and tables should be labelled consecutively throughout the paper.

The paper should contain each of the following parts:

Title: Titles should be brief and should specifically describe the content of the paper.

Authors: The name of the group and the candidate numbers of each member of the group should appear here.

Abstract: An abstract not exceeding 250 words that summarizes the principal techniques and conclusions of the manuscript in relation to known results must accompany the manuscript. Mathematical formulas and bibliographic references in the abstract should be avoided entirely.

Introduction: The paper must have a clearly written introduction in which the authors outline their new results, describe the motivation for the study, and explain why their work is of interest. The introduction should help the reader to decide whether to read the details in the paper.

Methodology: A description of the numerical modelling approach and underlying theory applied in the project.

Results/findings: Presentation and description of the findings of your study along with figures where appropriate. Main bulk of the report.

Discussion and conclusions: Summary of the major findings and discussion in the context of existing studies (these can be combined or separate sections).

References: References should be listed in either alphabetical order or order of citation at the end of the manuscript. The following reference styles should be used:

- Journal articles; when possible, titles of journals should be abbreviated in accordance with Mathematical Reviews; abbreviations are available at `http://www.ams.org/msnhtml/serials.pdf` (URL correct on January 28, 2025):

  [7] R. T. ROCKAFELLAR, Lagrange multipliers and optimality, SIAM Rev., 35(1993), pp. 183-238.

- Books, pamphlets, research reports:

  [2] B. MANDELBROT, Fractal: Form, Chance and Dimension, W. H. Freeman, San Francisco, CA, 1977.

- Paper in a bound collection:

  [4] A. NAGURNEY, Parallel computation of economic equilibria, in Applications on Advanced Architecture Computers, G. Astfalk, ed., SIAM, Philadelphia, PA, 1996, pp. 265-276.

  Acceptable variants on SIAM's references style are:

  [R] R. T. ROCKAFELLAR, Lagrange multipliers and optimality, SIAM Rev., 35 (1993), pp. 183-238.
  or
  R. T. ROCKAFELLAR (1993), Lagrange multipliers and optimality, SIAM Rev., 35, pp. 183-238.

- Citations within the text: A consistent style should be used, and the style of in-text citations should conform to the reference style chosen. To refer to a specific page or item in an article or book the following formats may be used: [2, p. 51]; [M, p. 51]; Mandelbrot [2, p. 51]; or Mandelbrot (1977, p. 51).

Any queries regarding this coursework brief should be raised with us at your earliest possible convenience. We hope you enjoy your project!

Will Seviour and Stephen Thomson, module leaders MTH2005 January 28, 2025

8 Projects

In the remaining pages is the list of seven projects being offered, along with the supervisors.

Hurricane vortex investigation

Bob Beare

December 2, 2024

1 Introduction

Hurricanes are low-pressure weather systems that develop mostly over the warm tropical oceans. They can cause catastrophic loss of life, as shown in 2005 with Huricane Katrina. The physics of the the full hurricane involves a complex mix of vortex dynamics and cloud physics. Despite this, some of the broad features of a hurricane can be understood with much simpler theory based on the fundamental balances in the vortex. The aim of this investigation will be to explore such a balanced vortex theory. This sheet summarises the theory and suggests directions for investigation.

2 Theory

The theory outlined here follows Smith (2006). It assumes an axi-symmetric vortex with tangential velocity, v, pressure, p, and cylindrical polar coordinates (r,z) where r is the radius and z height.

2.1 Thermal wind: compressible assumption

This section outlines the relationship between the density and the vortical wind (the so called thermal wind balance), assuming compressibility. The pressure gradient in the horizontal balances the sum of the centrifugal and Coriolis terms. In the vertical hydrostatic balance applies,

$$\left(\frac{\partial p}{\partial r}, \frac{\partial p}{\partial z}\right) = \rho(C, -g) \tag{1}$$

where:

$$C = \frac{v^2}{r} + fv \tag{2}$$

f is the Coriolis parameter, g gravitational acceleration. Eliminating pressure from (1) gives the thermal wind balance:

$$\frac{\partial}{\partial r} \ln \rho + \frac{C}{g} \frac{\partial}{\partial z} \ln \rho = -\frac{1}{g} \frac{\partial C}{\partial z} \tag{3}$$

Using characteristics this can be re-phrased as two ODEs:

$$\frac{dz}{dr} = \frac{C}{g} \tag{4}$$

Along these characterics the thermal wind is given by:

$$\frac{d}{dr} \ln \rho = -\frac{1}{g} \frac{\partial C}{\partial z} \tag{5}$$

Pressure is related to density and temperature via the ideal gas law.

2.2 Thermal wind: anelastic assumption

A useful simplification of (5) is to decompose the density into a sum of a reference state, which is a function of height ($\rho_0(z)$) and an anomaly ($\rho_a(r, z)$).

$$\rho = \rho_0(z) + \rho_a(r, z) \tag{6}$$

and approximate the vertical gradient of density as $\frac{\partial \rho_0}{\partial z}$, the anelastic assumption:

$$\frac{\partial \rho}{\partial r} = -\frac{1}{g} \frac{\partial (\rho_0 C)}{\partial z} \tag{7}$$

3 Initial investigation

An initial investigation could be to solve (7) for density, given a prescribed wind profile. An example vortex would be:

$$\begin{aligned} v(r, z) &= V_{max} exp\left(-\frac{z}{H_v}\right) sin\left(\frac{\pi r}{2R}\right) \quad r < 2R \\ &= 0 \quad otherwise \end{aligned} \tag{8}$$

and then solve (4) and (5) using the method of characteristics. In the far field you will need assume a density profile.

$$\rho(r >> R, z) = \rho_s exp(-\frac{z}{H_\rho}) \tag{9}$$

$H_v = 30km$, $V_{max} = 40ms^{-1}$, $R = 40km$, $H_\rho = 9km$, $\rho_s = 1kgm^{-3}$. Also, use $f = 0.5 \times 10^{-4}$ as a typical tropical value.

4 Further investigations

Here are some suggestions for further investigations:

- Solve for pressure in addition to density.
- How do the anelastic and compressible solutions compare?
- Calculate the inverse problem: prescribe density and calculate the wind.
- Use more realistic wind fields (see, for example Holland (1980)) for the hurricane vortex. The vortex given by (8) is symmetric about its maximum, but more realistic profiles have stronger winds towards the cyclone centre.
- How do the solutions change for an anti-cyclonic vortex ($v < 0$).
- Explore the relative contribution of the centrifugal ($\frac{v^2}{r}$) and geostrophic (fv) terms in C. Explore how changing the size and magnitude of the vortex, and the Coriolis parameter alter the balance of these terms. What is the relevant non-dimensional parameter for this?
- This is an approximate steady state vortex. Explore applying a time evolution of the density, for example a heating from the bottom boundary.
- Further reading on hurricanes can be found by googling: "Kerry Emanuel" or "Roger Smith hurricane publications".
- A good book on Dynamical Meteorology is Holton (1992).

References

Holland, G. J.: 1980, 'An analytic model of the wind and pressure profiles in hurricanes'. *Mon. Wea. Rev.* **108**, 1212–1218.

Holton, J. R.: 1992, 'An introduction to dynamic meteorology'. *Academic Press, New York, 507pp.*

Smith, R. K.: 2006, 'Accurate determination of a balanced axisymmetic vortex in a compressible atmosphere'. *Tellus* **58A**, 98–103.

Project 2

Time-dependent and stochastic dynamical systems

Frank Kwasniok

Many applied problems involve dynamical systems described by ordinary differential equations (ODEs). Here you will study two extensions of the usually considered setting which greatly enhance the richness of the modelled behaviour: ODEs with time-dependent parameters and stochastic differential equations (SDEs).

Dynamical systems with time-dependent parameters may undergo abrupt qualitative, possibly irreversible changes called bifurcations or tipping points. Equilibria may change stability or disappear completely; equilibria may turn into limit cycles or vice versa.

Stochastic noise terms enable the trajectory to explore regions of state space which are not accessible to the deterministic dynamics. We may, for example, observe random transitions between different metastable states. SDEs require special numerical integration schemes which are different from those for ODEs. A SDE is linked to a Fokker-Planck equation, a partial differential equation (PDE) governing the time evolution of the probability density function.

To receive a pass mark (threshold) for this investigation you must complete the following tasks:

Threshold

- Numerically generate trajectories of a bistable SDE.
- Study numerically simple examples of time-dependent ODEs and SDEs.
- Solve numerically the Fokker-Planck equation for an Ornstein-Uhlenbeck process and a bistable SDE and compare with the analytical solution.

To receive a first class mark (higher) for this investigation you must additionally complete one of the following extension tasks:

Higher

- Apply the Crank-Nicolson scheme to solve numerically the Fokker-Planck equation of a time-dependent SDE and compare the results with direct simulations of the SDE.
- Study the notions of weak and strong convergence of integration schemes for SDEs and explore them numerically on examples.

Numerically solving cloud droplet growth by condensation

Dan Partridge

In this assignment you will create your own simple model of the growth of a cloud droplet by condensation of water vapour in a vertically moving adiabatic parcel of air. Such models are traditionally known as adiabatic cloud parcel models in the atmospheric science literature. They form the basis for the calculation of the number of cloud droplets in global climate models.

You will focus on to creating a simple model in MATLAB that describes how the supersaturation and subsequently droplet size evolves in time within a cloud as air ascends from cloud base. This process can be modelled using a set of four first order ODEs, which will be provided to you with the necessary supporting literature.

You should apply numerical methods to solve the given set of ODEs and provide a comparison of the accuracy and efficiency of different methods. With your final model you will investigate how varying the initial conditions for different parameters affects the maximum supersaturation and droplet size attained within your simulated cloud.

To receive a pass mark (threshold) for this investigation you must complete the following tasks:

Threshold

- Question 1

a. Write a MATLAB code that will model the growth of a single droplet of initial size 1 μm radius assuming constant supersaturation, s (0.35 %) and temperature (280 K) over a period of 45 minutes. Use a forward Euler time stepping scheme. Repeat using a 4th order Runge Kutta time stepping scheme. Plot how the droplet radius varies with time for both schemes.

b. Demonstrate that you have checked the correctness of your numerical solution.

c. Repeat for a range of initial temperatures and droplet sizes and discuss the implications of your findings from this simple model of droplet diffusion growth on how the size of a distribution of droplets within a cloud growing by condensation would evolve over time.

d. Calculate how long it would take to form precipitation size drops from droplet growth via condensation alone and discuss your findings.

e. Consider an isothermal atmosphere in which the relative humidity is 75 %. The terminal fall speed (u) of a droplet of radius r (in m) can be approximated by $u = k_1 r^2$, where $k_1 = 1.19 \times 10^6$ $cm^{-1}s^{-1}$ is a constant.

   For a range of droplet sizes, calculate the distance fallen before complete evaporation. Discuss the implications for how cloud droplets and rain droplets are classified by size

PLEASE TURN OVER

- Question 2

a. Write a MATLAB code that will model and plot the evolution of supersaturation and droplet size with height from cloud base to cloud top for the case in which pressure and temperature are assumed constant. Use a forward Euler time stepping scheme.

b. Replace your forward Euler time stepping scheme with a higher order time stepping scheme (e.g. 4th order Runge Kutta). Compare the accuracy of the methods in calculating cloud maximum supersaturation for different model timesteps.

To receive a first-class mark (higher) for this investigation you must additionally complete additionally complete a minimum of: extension task 1, plus extension task 2 or 3.

Higher extension tasks

1. Extend the model you have created in question 2b to include the ODEs describing change of temperature and pressure with time to solve the full set of four ODEs provided numerically.
   Calculate the difference in simulated cloud top droplet size between your new model and your model from question 2b for two different cloud types: stratiform cloud (cloud depth: 300 m); convective cloud (cloud depth: 1000 m). Briefly discuss your findings.

   For your new model which considers the full set of ODEs, for a marine stratocumulus cloud (cloud depth: 300 m, cloud droplet number concentration: 100 cm^{-3}) analyse how the cloud top droplet size and cloud maximum supersaturation depend on the input parameter values chosen for: initial droplet radius, droplet number concentration and vertical velocity. Show your results and discuss your findings.

2. Using your model from higher extension task 1 for a marine stratocumulus cloud, extend one of your simulations to plot the evolution of supersaturation and droplet size during descent in a constant downdraft from cloud top to cloud base. Discuss the accuracy of your findings, taking into consideration that your model omits an important mechanism for the growth of large cloud droplets (radius > 10 microns).

3. Using your model from higher extension task 1 demonstrate the first aerosol indirect effect (also known as the Twomey effect), by calculating the change in cloud top albedo between two model simulations for the marine stratocumulus cloud.

   You should design the two simulations such that the parameters controlling the meteorology remain constant for each cloud, but the available cloud condensation nuclei (CCN) concentration (described by cloud droplet number concentration in your model) changes. Show your results and discuss your findings with references to the proposed solar radiation management technique: marine cloud brightening.

The quasi-biennial oscillation: Modelling the stratosphere's heartbeat

MTH2005 project; Supervisor: William Seviour

1 Background

The quasi-biennial oscillation (QBO) is phenomenon occurring in the stratosphere (the layer of the atmosphere from about 15-50 km in altitude), near the equator. The zonal (east-west) wind reverses direction with a strikingly regular frequency of about 28 months (a little over two years), as illustrated in figure 1. It is the most repeatable aspect of our atmospheric circulation that is not directly related to astronomical forcing, such as daily or annual cycles. After its discovery in the 1950s by scientists at the UK Met Office (now based in Exeter), there was much scientific interest in explaining this peculiarly regular feature.

2 This project

Plumb (1977) developed an idealised 1-D mathematical model of the QBO based on two upward propagating atmospheric gravity waves with equal and opposite phase speeds interacting with the background winds. In this model the time evolution of the zonal wind, U, satisfies

$$\frac{\partial U}{\partial t} = -\frac{\partial F_1}{\partial z} - \frac{\partial F_2}{\partial z} + \nu \frac{\partial^2 U}{\partial z^2}, \tag{1}$$

where z is altitude, ν represents viscosity, and F_1 and F_2 are forcing terms relating to the two atmospheric waves of equal and opposite phase speeds, given by

$$\begin{aligned} F_i(z) &= F_i(0) \exp\left(-\int_0^z g_i(z')\mathrm{d}z'\right), \\ g_i(z) &= \frac{\alpha}{k(U - c_i)^2}. \end{aligned} \tag{2}$$

Here α and k are constants representing the amplitude and wavenumber of the waves respectively, $c_1 = +1$ and $c_2 = -1$ are the wave phase speeds.

This model is able to reproduce many of the observed features of the QBO, and remains a vital tool in understanding its properties. In this project you will develop your own numerical model of the QBO following Plumb (1977), test its properties, and compare it to the observed QBO. Specifically, the project may involve the following tasks:

Threshold

- Evaluate relevant literature (scientific papers and textbooks) to gain an understanding of the Plumb QBO model.
- Implement time-stepping scheme (3rd-order Adams-Bashforth is recommended) to integrate (1) forward in time.
- Plot time-height evolution of the model output and compare to observational results as in figure 1, noting any deficiencies in the model.
- Investigate sensitivity of QBO amplitude and period to the nature of the forcing (e.g. amplitude, phase speeds, wavelengths).

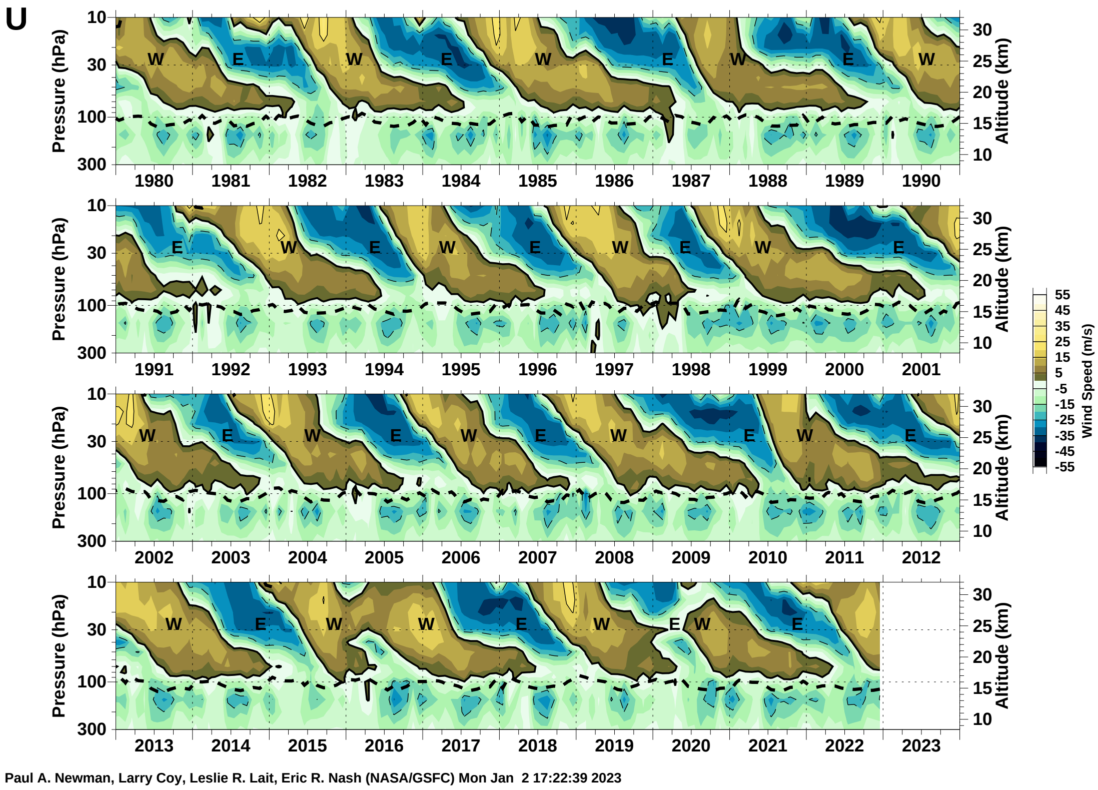

Figure 1: Time-altitude plot of the zonal wind as measured at Singapore. The QBO can be seen as the bands of descending easterly and westerly winds with a period close to two years.

Higher

- Replace one of the gravity wave forcing terms (F_2) with a different expression for a Rossby wave (another type of atmospheric wave). Integrate the model again and discuss any new features and whether it is more or less realistic.
- Add a time-dependent perturbation to the forcing. See if you can reproduce something that looks like a QBO disturbance. These are the interruptions to the usual cycle of the QBO that can be seen in 2016 and 2020 in figure 1, and are currently a topic of much scientific interest.

References

Plumb, R. A., 1977: The interaction of two internal waves with the mean flow: Implications for the theory of the quasi-biennial oscillation. *Journal of Atmospheric Sciences*, **34**, 1847–1858.

Many-particle system in the plane (Jan Sieber)

This project performs computer experiments with a large number of particles in a box, mimicking a simple gas. We treat the particles as small elastic balls that follow Newton's Laws of motion, travelling freely until they collide with each other or the wall. Quantities such as density, temperature and pressure at any location can be measured as averages over particles near this location and one can check if this confirms what theories predict, for example, about pressure or temperature in the atmosphere. Figure 1 shows a typical situation and the two types of collisions the particles can encounter.

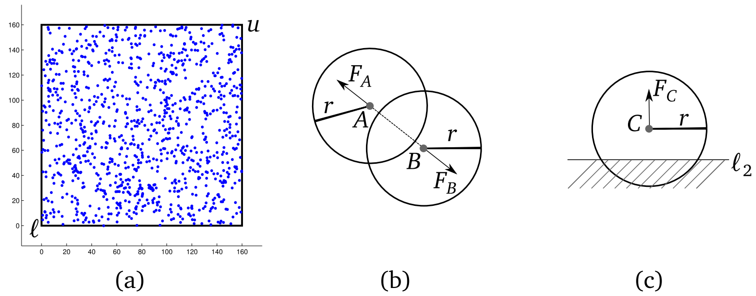

Figure 1: Sketches illustrating box and forces. (a): a typical situation with 1024 particles in a box, (b) illustration of forces F_A and F_B when two particles collide, (c) illustration of force F_C when particle collides with bottom wall

Implement and test a time-stepping simulation that takes a set of $2 \times N$ initial positions and $2 \times N$ initial velocities and updates them according to Newton's Laws of motion in small time steps h using the Verlet updating formula (an alternativ to Runge-Kutta methods, specifically suited for second-order systems).
Once implemented and tested, use the simulation to perform a sequence of experiments:

1. Observe the law of large numbers by measuring how temperature fluctuations depend on the number of particles.
2. Find the typical distribution of particle speeds in steady state.
3. See how pressure and temperature change as you compress the box by moving a wall inside and compare to theoretical predictions.
4. Check how gravity affects vertical temperature and pressure distribution.

Threshold

- **Correct implementation** All forces are taken into account on all particles and the simulation of particles follows Newton's Laws of motion, as tested on small numbers of particles.
- **Experiments** Simulations with several particle numbers have been demonstrated, measuring temperature, density, and pressure.
- **Presentation** Time series, and distributions as found ion the computations are presented in appropriate form and discrepancies to expectations from theory (if present) are described.

Higher

- **Linear complexity** For a large number N of particles it becomes computationally inefficient to compute the collision force for all pairs of particles, because there are $N(N-1)/2$ pairs and most of them are far apart. To enable larger particle numbers one may put a grid of smaller boxes over the entire box and only check for collisions between particles that are in the same box or in boxes neighbouring each other. One criterion for "higher level" is if the simulation avoids computations that require computational effort of order N^2.
- **Code structure** The code is well structured, broken up into functions that are easily testable on their own for correctness. The computational core is universal for all experiments, containing no code duplication. Scripting of the experiments (which may be computationally expensive) and data analysis of the results are separate and well structured, making the experiments repeatable.
- **Statistics** Statistical quantities such as temperature, density and pressure have to be averaged over space (and possibly time), and their distributions have to be fitted with appropriate methods to appropriate models.
- **Theory** For each result a comparison to theoretically expected results is made, with a good explanation of possible differences in observations, all integrated well into the report.

A simple model of radiative transfer applied to Earth's climate

Dr Stephen I. Thomson

Climate change is one of the defining issues of our time. At the heart of climate change is the physics of radiative transfer, specifically how the various gases in Earth's atmosphere interact with the incoming radiation from the sun and the outgoing infrared radiation from the warm surface and atmosphere. The physics of radiative transfer is highly complex - molecules absorb and re-emit radiation differently as a function of the wavelength of the radiation. In this project we will simplify this system down using grey radiation, where we treat radiative transfer as being divided into two-wavelength bands, the 'short-wave' band, encompassing visible wavelengths as emitted by the sun, and the 'long-wave', encompassing infrared wavelengths.

If we assume that the atmosphere is completely transparent in the short-wave, we can model the temperature in the atmosphere using the Schwarzchild equations:

$$\frac{dD}{d\tau} = B - D \tag{1}$$

$$\frac{dU}{d\tau} = U - B, \tag{2}$$

where $U(\tau)$ is the upward flux of long-wave radiation in Wm^{-2}, $D(\tau)$ is the downward flux of long-wave radiation, $B(\tau) = \sigma T(\tau)^4$ is the Plank function. We further identify $\sigma = 5.67 \times 10^{-8}\mathrm{Wm}^{-2}\mathrm{K}^{-4}$ as the Stefan-Boltzmann constant, $T(\tau)$ as the atmospheric temperature profile, and $\tau(z)$ as the dimensionless optical depth profile. The optical depth profile is a measure of how much radiation can pass through a medium at a given height above the surface (z). The net radiation passing through the atmosphere is denoted $N = U - D$. The heating of the atmosphere caused by this net flux of radiation is governed by the equation

$$\rho c_p \frac{\partial T}{\partial t} = -\frac{\partial N}{\partial z} \tag{3}$$

where $\rho(z)$ is the atmospheric density at a given height, c_p is the specific heat capacity of dry air, t is time and z is geometric height above the surface of the Earth.

There are many climate-relevant problems to look at with these equations. During this project you'll develop numerical methods to solve them, and investigate how the solutions change with parameters.

The simplest setup for an Earth-like atmosphere is to assume that the upward flux of longwave radiation at the top of the atmosphere is equal to the amount of sunlight received from the sun, i.e. $U(\tau = 0) = S_0$, $D(\tau = 0) = 0$, where $S_0 = 1360(1-\alpha)/4$. Here $1360Wm^{-2}$ is the so-called solar-constant, which is a measure of the sun's radiative power at the top of our atmosphere, and α is the Earth's albedo, which is a measure of how much of the sun's radiation is reflected back into space. For Earth a commonly-taken value for $\alpha = 0.3$.

To gain the pass mark for this investigation, you must complete the following threshold tasks:

1 Threshold

1. Radiative equilibrium happens when the system reaches a steady-state such that the temperature is constant in time. Under the assumption of radiative equilibrium, you must solve equations 1, 2 and 3 above to find a temperature profile as a function of z. To do this, you should use the prescription for the optical depth $\tau = \tau_0 e^{-z/H_a}$ where $\tau_0 = 2.20$ is optical depth at $z = 0$, and H_a is a height scale associated with the absorbing gasses, which on Earth can be taken as roughly $2km$. You should find the temperature profile as a function of z analytically and plot the results over a range from $z = 0$ to $z = 20km$.

2. Use the same analytical process as in part 1 to find and plot vertical profiles of U and D as functions of z.

3. Having solved the equations analytically in radiative equilibrium, we now want to solve them numerically. This will be useful, as we can then compare our numerical and analytical solutions under the assumption of radiative equilibrium, and they should match. Use your analytical solution to calculate a temperature profile. Then, by converting this to a B profile, integrate equations 1 and 2 between τ_i and τ_{i+1} using integrating factors, where i denotes the index of your vertical grid. You should then end up with a recursion relation for U and

D. Solve this numerically, finding an appropriate approximation for the integral part of the recursion relation. (Remember to account for the boundary conditions!). Compare your numerically-generated profiles of U and D to your analytic solutions for U and D. Do they match over a range between $z = 0$ and $z = 20$km? If not, try and adjust the numerical parameters of your integration to get a closer match.

4. To solve equation 3 under non-equilibrium conditions, we need to find the unknown density ρ. To do this, combine equation 3 with the hydrostatic equilibrium equation $\partial p/\partial z = -g\rho$ to eliminate ρ. You should find we now need to know the pressure in order to solve the resulting equation. In order to find the pressure, combine hydrostatic equilibrium with the ideal-gas equation $p = \rho R_d T$, and integrate numerically using a recursion relation between the levels, as you did for U and D, to find a profile of pressure as a function of z. You should use the boundary condition that $p(z = 0) = 1 \times 10^5$Pa, and take T to be your analytical solution. Here $R_d = 287.04\text{Jkg}^{-1}\text{K}^{-1}$ is the specific gas constant, and is related to the specific heat capacity $C_p = 7R_d/2$. You should should test your pressure profile code by calculating $p(z)$ analytically by taking $T = 270(K)$, and solving this case numerically for comparison.

5. Using your of equation 3 where you have eliminated ρ, and your profile of pressure, we now want to evolve the temperature in time. Note that this means we can no longer use our analytical profile of T in any of our calculations, as this only applies under radiative equilibrium. Begin with a constant-temperature initial condition of $T(z) = 175$K and solve your modified equation 3 as a function of time using a forward-Euler timestepper to evolve the temperature. You should find that your profiles eventually reach radiative equilibrium. How well do they compare to your calculations in part 1? Which part of the profile reaches radiative equilibrium first?

6. Instead of solving these equations for a single vertical column of the atmosphere, we'd now like to try and solve them for a temperature profile that varies as a function of latitude (θ) and height z. By making efficient modifications of your code, first modify the incoming short-wave radiation $S(\theta)$ to vary in latitude according to

$$S(\theta) = S_0(1 + 0.25 * \Delta(1 - 3\sin^2(\theta))) \tag{4}$$

where $\Delta = 1.4$ and $-\pi/2 \leq \theta \leq \pi/2$. Then find the temperature distribution $T(\theta, z)$ after running your timestepping to equilibrium. Comment on the temperature distribution you find - how well does it compare with the real Earth? If the profiles are very different, why might this be?

To receive a first-class mark, you must complete the two following extension tasks:

2 Higher

1. Re-formulate your optical depth parameter τ_0 using $\tau_0 = \tau_1 + 0.2023\ln(CO_2/360)$, where $\tau_1 = 2.20$ and CO_2 is a measure of the concentration of carbon dioxide in the Earth's atmosphere, measured in ppmv, or parts per million by volume. Use a temperature profile in radiative equilibrium with $CO_2 = 360$ppmv as your initial condition, and run the calculation with $CO_2 = 720$ppmv. This is an instantaneous doubling of CO_2. How much does the temperature at $z = 0$ increase when CO_2 is doubled from 360ppmv to 720ppmv (you may remove any cycle in S_0 if you have implemented this in Higher part 2)? This value is sometimes referred to as the 'equilibrium climate sensitivity', or the equilibrium temperature increase in response to a doubling of CO_2. How does your value compare to those from realistic climate models (bear in mind though that our model here is missing a huge number of relevant processes, including convection, horizontal wind, variation with latitude, clouds, aerosols, etc)? After doubling CO_2, how long does the atmosphere take to come into equilibrium? How does the time to reach equilibrium compare with realistic climate models?

2. Using your code from question 6, add a horizontal diffusion to your temperatures, such that your temperature equation is now of the form

$$\rho c_p \frac{\partial T}{\partial t} = -\frac{\partial N}{\partial z} + \frac{\kappa}{a^2\cos(\theta)}\frac{\partial}{\partial \theta}\left(\cos(\theta)\frac{\partial T}{\partial \theta}\right), \tag{5}$$

where κ is a thermal diffusivity and a is the radius of the Earth. Does this increase the realism of your temperature profiles in latitude? What processes can you think of that are represented by this thermal diffusion? Can you find a value of κ that gives a reasonable value of Earth's equator to pole temperature gradient?

Analysing and fitting a mathematical model of ecological interactions.

MTH2005 project; Supervisor: Margaritis Voliotis

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Background

The Lotka-Volterra (LV) model, also known as the predator-prey model, is a mathematical model used to describe the dynamics of biological systems in which two species interact: a predator and its prey. The model was proposed independently by A. Lotka [1] and V. Volterra [2] and serves as a foundational concept in ecology, helping to understand predator-prey relationships and their impact on ecosystem stability.

The project

The LV model consists of a pair of differential equations that represent changes in the population sizes of prey (x) and predator (y) species over time:

$$\begin{aligned}\frac{dx}{dt} &= \alpha x - xy \\ \frac{dy}{dt} &= \beta xy - y\end{aligned} \tag{1}$$

where a, b are positive constants (model parameters). In this project, you will use a numerical stepping scheme to solve the model and study its dynamics, and then develop a numerical recipe to infer model parameters from data.

Threshold To receive a pass mark for this project, you must complete the following tasks:

- Review the literature to gain an understanding of the LV model.
- Implement a time-stepping scheme to integrate the model (1) forward in time (e.g., a 4th-order Runge-Kutta scheme).
- Study the behaviour of the model for different values of $\mathbf{p} = (a, b)$ and different initial conditions (x_0, y_0). Plot the behaviour and critically discuss your observations.
- Implement code to fit the model to time-series data $\{t_i, \hat{x}_i, \hat{y}_i\}, i = 1, \ldots, N$, by using gradient descent to minimise the function (Least Squares Fitting)

$$F(\mathbf{p}) \quad = \quad \sum_1^N (\hat{x}_i - x(t_i; \mathbf{p}))^2 + \sum_1^N (\hat{y}_i - y(t_i; \mathbf{p}))^2 . \tag{2}$$

  where $x(t; \mathbf{p})$, $y(t; \mathbf{p})$ are the solutions of the model at time t given model parameters $\mathbf{p}$.

- Generate 'synthetic' data by solving the model for parameter values of your choice, and using these data validate your fitting code.
- Use your code to fit the model to time-series data that will be provided to you.

Higher To receive a first class mark for this project, you must additionally complete the following extension tasks:

- Study the behaviour of your fitting results as a function of the initial estimate. How would you ensure that your fitting procedure does not get stuck in local optima.
- Evaluate the computational cost of your fitting procedure. Can you improve it?

References

[1] A J Lotka. “Analytical note on certain rhythmic relations in organic systems”. In: *Proceedings of the National Academy of Sciences* 6.7 (1920), pp. 410–415.

[2] V Volterra. *Variazioni e fluttuazioni del numero d’individui in specie animali conviventi*. Società anonima tipografica” Leonardo da Vinci”, 1926.