

# Chapter 1

## Introduction

As a text book to the lecture, the following book is recommended:

Durran, D. R., Numerical Methods for Wave Equations in Geophysical Fluid Dynamics, Springer-Verlag, New York - Berlin - Heidelberg, 1999, see also *Durran* [1999].

### 1.1 Motivation

Based on physical laws such as the Navier-Stokes Equations and a number of empirical relations, complex numerical simulations of the oceans and the atmospheres are carried out these days in various institutions. Global Ocean models are already down to fine resolutions as much as 1/16 of a degree in the horizontal and around 100 layers in the vertical. This has only been possible due to the amazing increase of computer resources in recent years. Some examples for such simulations are shown in figures 1.1, 1.2, 1.3 and 1.4.

However, apart from huge computer resources, numerical tools are needed in order to discretise the continuous partial differential physical equations such that they can be sufficiently approximated by computers in a finite number of algebraic computational steps. The science which is dealing with such tools is called numerical mathematics.

Let us consider a basic flow situation and try to discretise it with a simple (but consistent) approach. Let us assume a one-dimensional flow in the  $x$ -direction with a constant flow speed  $u$ , and a substance  $s$  (like salinity) which is transported by this flow. All other processes like mixing will be ignored. Then, the following partial differential equation is describing this flow situation:

$$\partial_t s + u \partial_x s = 0, \tag{1.1}$$

which has the analytical solution

$$s(x, t) = s_0(x - ut) \tag{1.2}$$

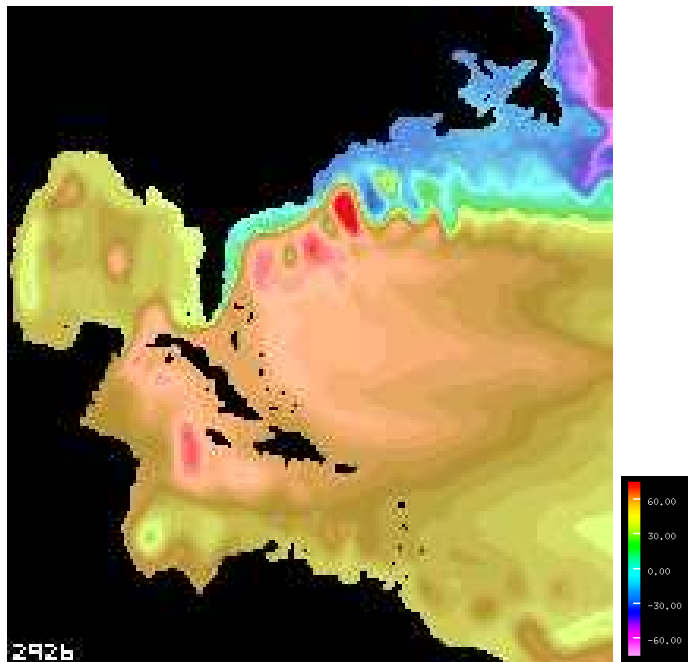


Figure 1.1: Sea surface elevation simulated by a high-resolution global ocean model with  $1/8$  degree resolution. Shown is the sea surface elevation (see colour code) at the east coast of North America where the Gulf Stream separates from the coast. Simulations have been carried out within the OCCAM project, see <http://www.soc.soton.ac.uk/JRD/OCCAM/>.

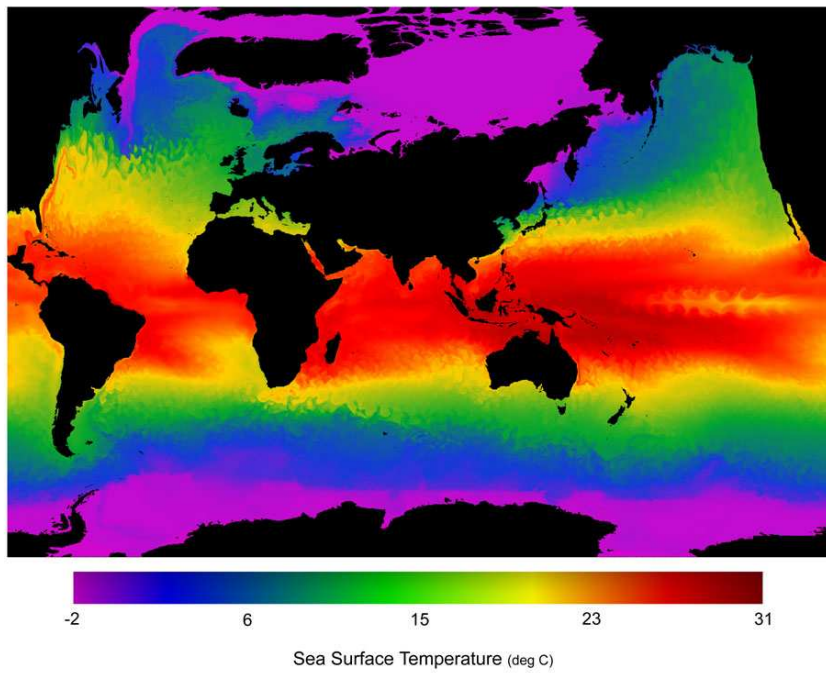


Figure 1.2: Global Sea Surface Temperature on January 1st, 1983, simulated with a 1/10 degree model of the US Navy, see <http://www.oc.nps.navy.mil/navypop/>.

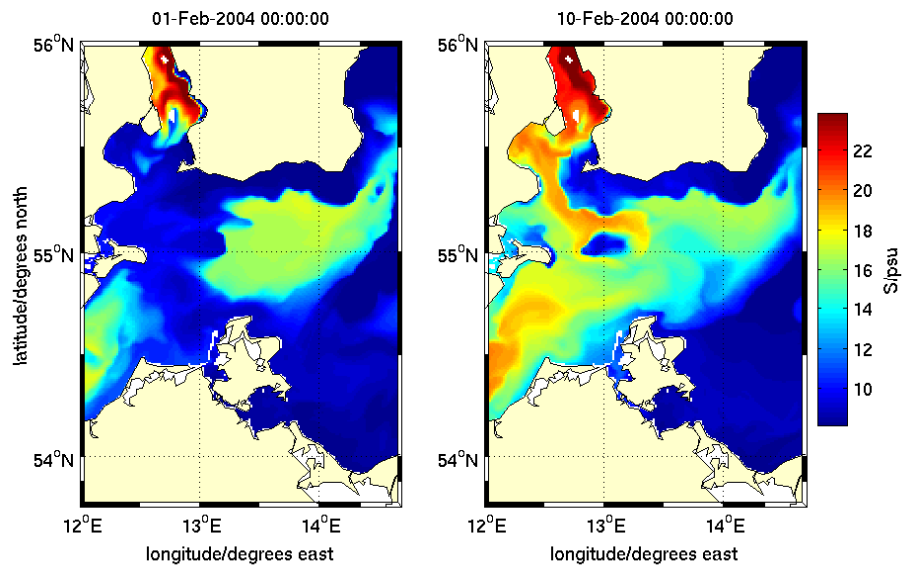


Figure 1.3: Simulated bottom salinity in the Arkona Basin (Western Baltic Sea) before a medium inflow event (February 1, left panel) and after a medium inflow event (February 10, right panel) the February medium intensity inflow over Drogden Sill, see *Burchard et al.* [2009]. For this simulation, the parallel version of the General Estuarine Transport Model (GETM, see *Burchard and Bolding* [2002]) has been used.

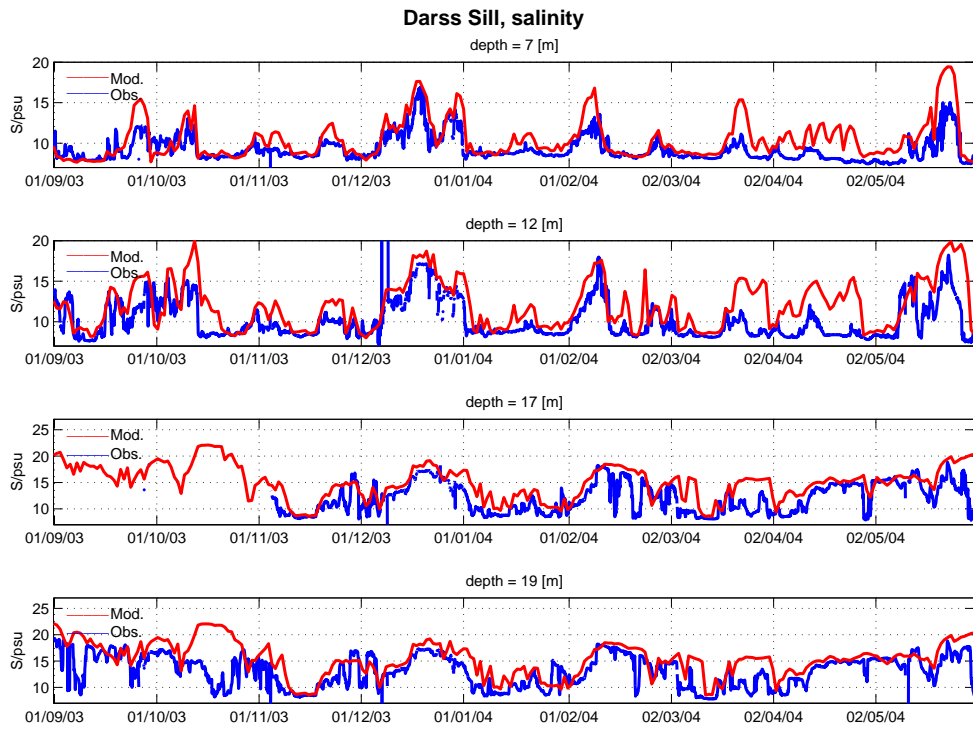


Figure 1.4: Time series of salinity at the Darss Sill mast. Blue: observations, red: model results. Shown are data at 7 m, 12 m, 17 m and 19 m below the mean sea level. For this simulation, the parallel version of the General Estuarine Transport Model (GETM, see *Burchard and Bolding* [2002]) has been used, see *Burchard et al.* [2009] for details.

for an initial condition  $s(x, 0) = s_0(x)$ . For  $s(-\infty) = s(\infty) = 0$  we can clearly see that the total amount of  $S$  remains constant:

$$\partial_t \left( \int_{-\infty}^{\infty} s \, dx \right) + u(s(\infty) - s(-\infty)) = 0. \quad (1.3)$$

If we discretise the space in  $x$ -direction with equidistant increments of length  $\Delta x$  and the time with equidistant time intervals with length  $\Delta t$  and denote the approximate solution for  $s(i\Delta x, j\Delta t)$  by  $s_i^j$ , then the so-called upstream (for some obvious reasons called upwind in meteorology) discretisation approximation gives

$$\frac{s_i^{j+1} - s_i^j}{\Delta t} + \frac{u}{\Delta x} (s_i^j - s_{i-1}^j) = 0, \quad (1.4)$$

which may be transformed to

$$s_i^{j+1} = s_i^j - u \frac{\Delta t}{\Delta x} (s_i^j - s_{i-1}^j). \quad (1.5)$$

With a step-like initial condition for  $s$  with  $s_0(x) = 10$  for  $0 \leq x \leq 100$  and  $s_0(x) = 0$  for  $x > 100$ , a time step of  $\Delta t = 10$  s, a spatial increment of  $\Delta x = 1$  m, a current velocity of  $u = 1$  m s<sup>-1</sup>, we obtain for the first time step an approximation at  $x = 0$  which is as follows:

$$s_i^{j+1} = s_i^j - u \frac{\Delta t}{\Delta x} (s_i^j - s_{i-1}^j) = 10 - 1 \cdot \frac{10}{1} \cdot (10 - 0) = -90, \quad (1.6)$$

which is far away from any reasonable approximation to the solution, which should be in any case between 0 and 10 (the analytical solution is zero, of course). What we have done with this naive approach is to use a numerically stable method (explicit two-step scheme with upstream discretisation of the spatial gradient) at a too large time step (with explicit schemes the flow should not transport material for more than one increment per time step).

It should be noted that the scheme (1.7) is still conservative, i.e. the total amount of  $s$  is conserved:

$$\begin{aligned} & \Delta x \sum_{i=-\infty}^{\infty} s_i^{j+1} - \Delta x \sum_{i=-\infty}^{\infty} s_i^j + u \Delta t \left( \sum_{i=-\infty}^{\infty} (s_i^j - s_{i-1}^j) \right) \\ &= \Delta x \sum_{i=-\infty}^{\infty} s_i^{j+1} - \Delta x \sum_{i=-\infty}^{\infty} s_i^j \\ &= 0. \end{aligned} \quad (1.7)$$

Another numerical problem is also easy to understand. Let us multiply equation (1.1) by  $2s$ , such that we obtain

$$\partial_t s^2 + u \partial_x (s^2) = 0, \quad (1.8)$$

showing that (1.1) does also include an advection equation for  $s^2$ .

The explicit in time and first-order upstream in space scheme (see eq. (1.7)) provides a numerically stable solution to (1.1), if the time step is sufficiently small (the Courant number  $c = u\Delta t/\Delta x$  must be between 0 and 1). However, when (1.7) is multiplied by  $(s_i^{j+1} + s_i^j)$ , we will get a discrete equation for  $s^2$  which is of the following form:

$$\begin{aligned} \frac{(s_i^{j+1})^2 - (s_i^j)^2}{\Delta t} + \frac{u}{\Delta x} \left( (s_i^j)^2 - (s_{i-1}^j)^2 \right) = \\ -2 \frac{u\Delta x}{2} (1-c) \frac{(s_i^j - s_{i-1}^j)^2}{(\Delta x)^2}, \end{aligned} \quad (1.9)$$

where the left hand side of (1.9) is an explicit upstream discretisation of the left hand side of (1.8), but the right hand side provides a loss term to  $s^2$ . Thus, the first-order upstream scheme is stable, but strongly dissipative. Equation (1.9) actually motivated *Burchard and Rennau* [2008] to define the numerical variance loss as a measure for numerical mixing.

It will be the major aim of this lecture to understand some basic principles of numerical approximation for conservation laws (conservation of mass, energy) from which the dynamic equations in marine and atmospheric models are derived. In hands-on exercises some numerical techniques will be coded and applied by the students.

## 1.2 Historical remarks

In 1922, *Richardson* [1922] had the following vision of a human-computed weather forecast system:

It took me the best part of six weeks to draw up the computing forms and to work out the new distribution in two vertical columns for the first time. My office was a heap of hay in a cold rest billet. With practice the work of an average computer might go perhaps ten times faster. If the time-step were 3 hours, then 32 individuals could just compute two points so as to keep pace with the weather, if we allow nothing for the very great gain in speed which is invariably noticed when a complicated operation is divided up into simpler parts, upon which individuals specialise. If the co-ordinate chequer were 200 km square in plan, there would be 3200 columns on the complete map of the globe. In the tropics the weather is often foreknown, so that we may say 2000 active columns. So that  $32 \times 2000 = 64,000$  computers would be needed to race the weather for

the whole globe. That is a staggering figure. Perhaps in some years' time it may be possible to report a simplification of the process. But in any case, the organisation indicated is a central forecast-factory for the whole globe, or for portions extending to boundaries where the weather is steady, with individual computers specialising on the separate equations. Let us hope for their sakes that they are moved on from time to time to new operations.

After so much hard reasoning, may one play with a fantasy? Imagine a large hall like a theatre, except that the circles and galleries go right round through the space usually occupied by the stage. The walls of this chamber are painted to form a map of the globe. The ceiling represents the north polar regions, England is in the gallery, the tropics in the upper circle, Australia on the dress circle and the antarctic in the pit. A myriad computers are at work upon the weather of the part of the map where each sits, but each computer attends only to one equation or part of an equation. The work of each region is coordinated by an official of higher rank. Numerous little "night signs" display the instantaneous values so that neighbouring computers can read them. Each number is thus displayed in three adjacent zones so as to maintain communication to the North and South on the map. From the floor of the pit a tall pillar rises to half the height of the hall. It carries a large pulpit on its top. In this sits the man in charge of the whole theatre; he is surrounded by several assistants and messengers. One of his duties is to maintain a uniform speed of progress in all parts of the globe. In this respect he is like the conductor of an orchestra in which the instruments are slide-rules and calculating machines. But instead of waving a baton he turns a beam of rosy light upon any region that is running ahead of the rest, and a beam of blue light upon those who are behindhand.

Four senior clerks in the central pulpit are collecting the future weather as fast as it is being computed, and despatching it by pneumatic carrier to a quiet room. There it will be coded and telephoned to the radio transmitting station.

Messengers carry piles of used computing forms down to a storehouse in the cellar.

In a neighbouring building there is a research department, where they invent improvements. But these is much experimenting on a small scale before any change is made in the complex routine of the computing theatre. In a basement an enthusiast is observing eddies in the liquid lining of a huge spinning bowl, but so far the arithmetic proves the better way. In another building are all the usual financial, correspondence and administrative offices. Outside are playing fields, houses, mountains and lakes, for it was thought that those who compute the weather should breathe of it freely.

These phantastic thoughts by Richardson did of course never come true as far as human computers are concerned. However, the first computer ENIAC (Electronic Numerator Integrator Analyser and Computer) with 500 Flops (Floating point operations per second) came out in 1946 and was later used for first numerical weather predictions. In 1949 Charney developed a barotropic model (density is only a function of pressure), which was doing the weather prediction until 1962, in 1955, he developed a fully baroclinic model (density also function of temperature). Three-dimensional primitive equation models (with equations for velocity vector) for the atmosphere exist since 1963.

In oceanography, Bryan developed a barotropic model for the global ocean in 1963 and a baroclinic model in 1969 (*Bryan* [1969], the basic concept of which is still in use, see the Modular Ocean Model still maintained by the Geophysical Fluid Dynamic Laboratory in Princeton, which is also used at IOW for Baltic Sea modelling).

It is worth mentioning that the first multi-layer, baroclinic model for the North Atlantic has been implemented by Hans Friedrich, a physical oceanographer from Hamburg, see *Friedrich* [1970]. Although the model resolution of  $3^\circ$  was very coarse (measured by today's standards), some of the basic features of the North Atlantic circulation could be reproduced, see figure 1.5.

An interesting fairly early example for numerical modelling is given by *Sündermann and Vollmers* [1972] who simulated large scale laboratory experiments for the Jade Bay (Germany). They showed that they in principle could reproduce the currents observed in the lab. However, when it came to the investigation of the Earth rotation effect on the currents near slack tide, then it was easy to switch this effect on in the model simulations, but impossible to do this in the large scale lab model, see figure 1.6.

Improvements for ocean models since those early models are related to model architecture (generalised coordinates), better parameterisations (e.g. for turbulence), higher order numerical schemes (monotonicity, conservation) and data assimilation techniques.

The increase of computer resources is best described by Moores law, which is here defined according to [www.webopedia.com](http://www.webopedia.com):

The observation made in 1965 by Gordon Moore, co-founder of Intel, that the number of transistors per square inch on integrated circuits had doubled every year since the integrated circuit was invented. Moore predicted that this trend would continue for the foreseeable future. In subsequent years, the pace slowed down a bit, but data density has doubled approximately every 18 months, and this is the current definition of Moore's Law, which Moore himself has blessed. Most experts, including Moore himself, expect Moore's Law to hold for at least another two decades.

A closer view shows that the doubling actually occurs roughly every two years, see figure 1.7.

Despite all innovations in the last four decades, the major programming language in oceanography is still FORTRAN (FORMula TRANslation language).

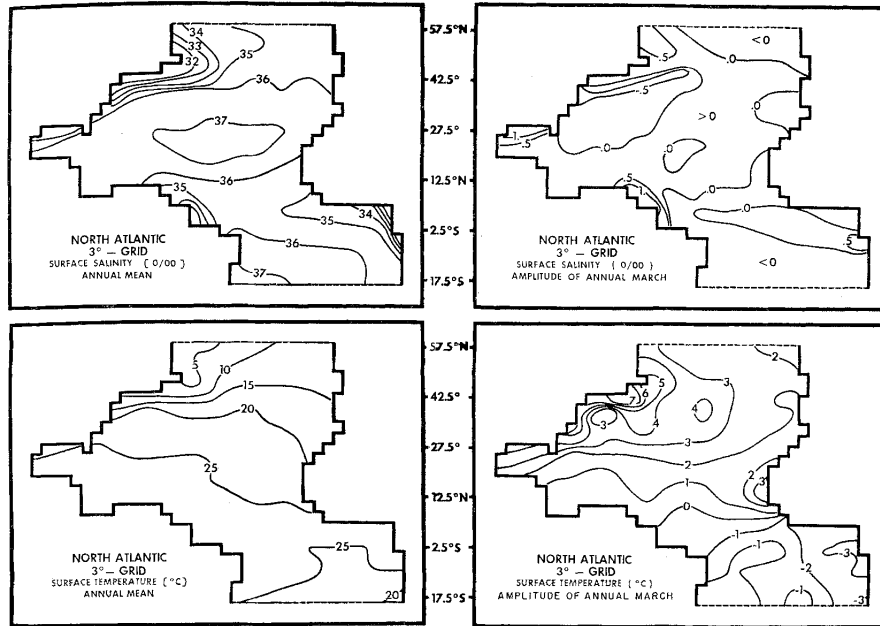
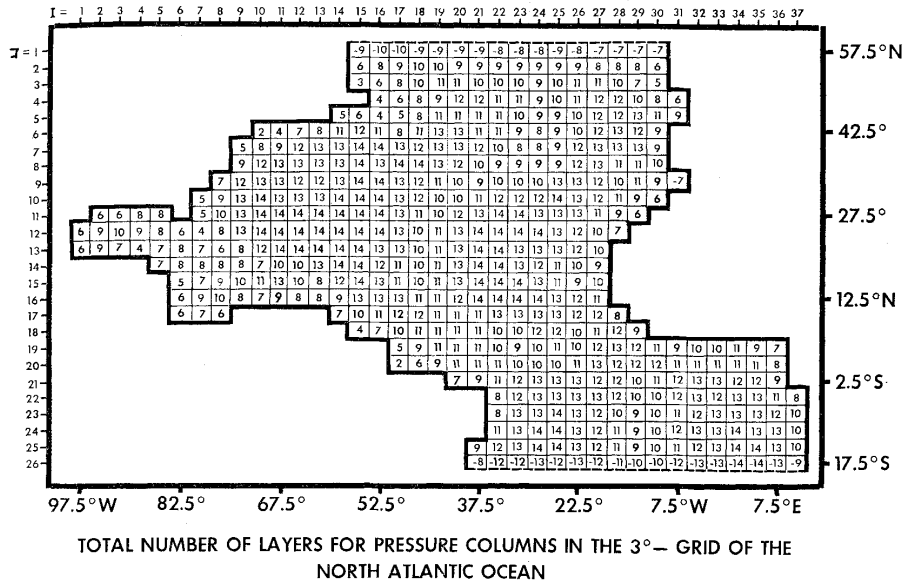


Figure 1.5: Results of the first multi-layer, baroclinic North Atlantic numerical model by *Friedrich* [1970]. Upper panel: Number of layers for each grid box. Lower panels: Mean values and mean amplitude of surface salinity and temperature.

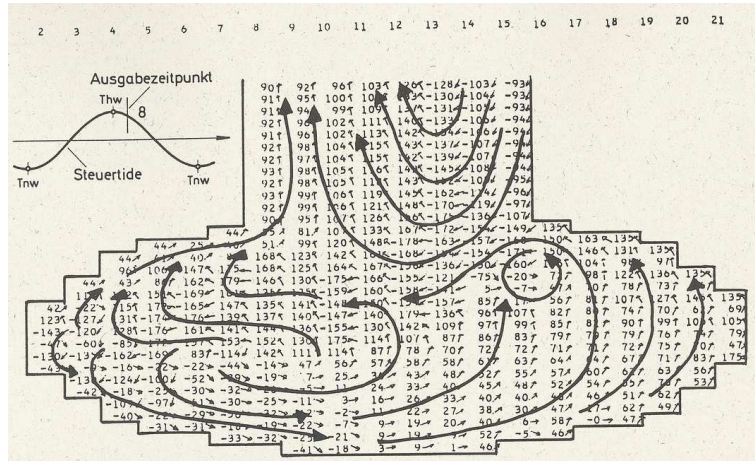


Figure 1.6: Simulated surface currents in Jade Bay short time after slack tide flood, see *Sündermann and Vollmers* [1972].

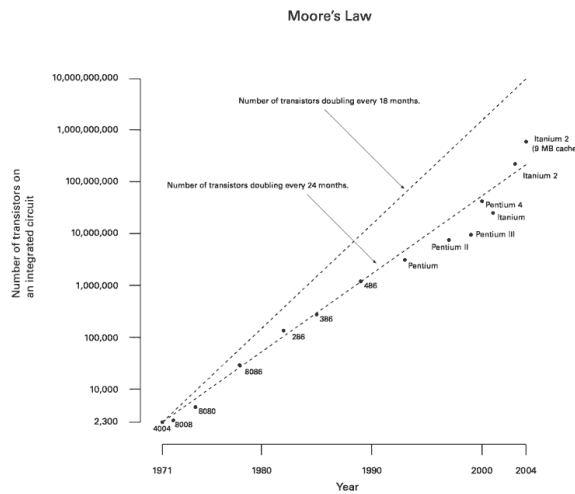


Figure 1.7: Moore's Law graphically displayed (from [http://en.wikipedia.org/wiki/Moore's\\_law](http://en.wikipedia.org/wiki/Moore's_law)).

### 1.3 Differential operators

For one-dimensional sufficiently smooth functions  $f(x)$ , the one-sided derivative is defined as

$$\frac{d}{dx}f(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}. \quad (1.10)$$

For multidimensional functions with the independent variable vector  $\vec{x} = (x_1, x_2, \dots, x_n)$ , the partial derivative with respect to the coordinate  $x_i$  is defined as

$$\frac{\partial}{\partial x_i}f(\vec{x}) = \lim_{\Delta x \rightarrow 0} \frac{f(x_1, \dots, x_i + \Delta x, \dots, x_n) - f(x_1, \dots, x_i, \dots, x_n)}{\Delta x}. \quad (1.11)$$

Let  $\vec{x}(t)$  be the position of a fluid particle passively drifting with the fluid velocity  $\vec{v} = (v_1, v_2, v_3)$ . Then,

$$\frac{d}{dt}\vec{x}(t) = \vec{v}(\vec{x}(t)). \quad (1.12)$$

Thus, the substantial derivative of a function  $f(\vec{x}(t), t)$  with respect to time reads as

$$\frac{D}{Dt}f(\vec{x}(t), t) = v_i \frac{\partial}{\partial x_i}f(\vec{x}(t), t) + \frac{\partial}{\partial t}f(\vec{x}(t), t). \quad (1.13)$$

If convenient and misunderstandings are excluded, then arguments are often dropped.

Since many complex partial differential equations are contained in this lecture, a compact way of denoting partial derivatives has been chosen here:

$$\partial_t = \frac{\partial}{\partial t}, \quad \partial_x = \frac{\partial}{\partial x}, \quad (1.14)$$

and

$$\partial_i = \frac{\partial}{\partial x_i}. \quad (1.15)$$

For simplicity, the summation convention of Einstein is extensively used in this manuscript. This means that summation from 1 to 3 is applied to repeated indices:

$$a_j b_j = a_1 b_1 + a_2 b_2 + a_3 b_3 \quad (1.16)$$

### 1.4 Ordinary differential equations

The general form of an Ordinary Differential Equation (ODE), in which only functions and their derivatives of one independent variable occur is:

$$F\left(t, c, c', \dots, c^{(n)}\right) = 0, \quad (1.17)$$

where  $t$  is the independent variable (typically time),  $c$  a function of  $t$  which is  $n$  times derivable and  $F$  is a function of  $n + 2$  variables which gives real scalars or vectors.  $c$  may be a scalar or a vector.  $n$  is called the order of the ODE. A first order explicit ODE is of the following form:

$$c' = F(t, c), \quad (1.18)$$

where  $c$  and  $F$  may again be vectors. Such explicit first order ODE's are so-called initial value problems in which the specification of an initial value  $c(t_0) = c_0$  at a given  $t_0$  is sufficient for obtaining a unique solution. In population models, the independent variable is the time  $t$ , and  $F$  is representing fluxes between the different components of the vector  $c$ :

$$\partial_t c_i = \sum_{j=1}^I (p_{ij}(\vec{c}) - d_{ij}(\vec{c})), \quad (1.19)$$

with  $I$  denoting the number of state variables and the non-negative production and destruction terms

$$p_{ij}(\vec{c}) = d_{ji}(\vec{c}), \text{ for } i \neq j. \quad (1.20)$$

It can be easily seen that the system is conservative for  $p_{ii} = d_{ii} = 0$ :

$$\partial_t \sum_{i=1}^I c_i = \sum_{i=1}^I \sum_{j=1}^I (p_{ij}(\vec{c}) - d_{ij}(\vec{c})) = \sum_{i=1}^I (p_{ii}(\vec{c}) - d_{ii}(\vec{c})). \quad (1.21)$$

Often the  $c_i$  describe positive definite quantities (such as concentrations), such that the equations must be formulated such that

$$d_{ij}(\vec{c}) \rightarrow 0 \text{ for } c_i \rightarrow 0. \quad (1.22)$$

For typical ecosystem models, the concentrations  $c_i$  represent nutrients and other chemical compounds, phytoplankton, zooplankton, and dead organic material, such that the dimension of the problem can easily extend to  $\mathcal{O}(10) - \mathcal{O}(100)$  variables.

An example for a simple ecosystem model is the NPZD (nutrient-phytoplankton-zooplankton-detritus) model, where detritus is dead organic matter:

$$\begin{aligned} \dot{n} &= d_{dn} - d_{np} + d_{pn} + d_{zn} \\ \dot{p} &= +d_{np} - d_{pn} - d_{pz} - d_{pd} \\ \dot{z} &= -d_{zn} + d_{pz} - d_{zd} \\ \dot{d} &= -d_{dn} + d_{zd} + d_{pd}, \end{aligned} \quad (1.23)$$

where  $d_{dn}$  is the remineralisation of dead organic matter,  $d_{np}$  is the primary production (nutrient take-up),  $d_{pn}$  is the respiration of phytoplankton,  $d_{zn}$  is the

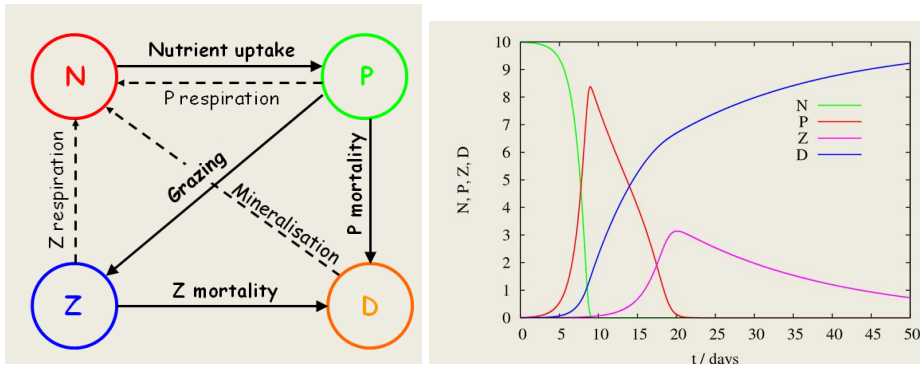


Figure 1.8: Structure (left) and typical result (right) for the zero-dimensional NPZD model. Note that detritus mineralisation has been neglected ( $d_{dn}$ ).

exudation of zooplankton,  $d_{pz}$  is the grazing of zooplankton on phytoplankton,  $d_{zd}$  is the mortality of zooplankton, and  $d_{pd}$  is the mortality of phytoplankton. The state variables  $n$ ,  $p$ ,  $z$  and  $d$  are given in units of their nitrogen content. Figure 1.8 shows structure and typical result for the NPZD model. The total nitrogen conservation of this NPZD model is obvious from (1.23). For further details, see e.g. *Oschlies and Kähler* [2004] or *Burchard et al.* [2005].

Complete ecosystem models do also contain transport terms due to the ocean currents, due to settling or rising, and due to mixing such that are partial differential equations (they depend not only on the independent variable time, but also on the space vector), see section 1.5.

## 1.5 Partial differential equations

Typical Partial Differential Equations (PDE's) in one spatial dimension are the (parabolic) diffusion equation (with the diffusivity  $\nu$ )

$$\partial_t s - \nu \partial_{xx} s = 0, \quad (1.24)$$

the (hyperbolic) wave equation (with the phase speed  $c$ )

$$\partial_{tt} s - c^2 \partial_{xx} s = 0, \quad (1.25)$$

or the (hyperbolic) first-order advection equation (with the phase speed  $c$ )

$$\partial_t s + c \partial_x s = 0, \quad (1.26)$$

and the (elliptic) potential equation

$$\partial_{xx} s + \partial_{yy} s = 0. \quad (1.27)$$

It can be easily shown that the wave equation (1.25) can be derived from the advection equation (1.26), if the function  $s$  is smooth enough.

In oceanography and meteorology, the advection-diffusion equation

$$\partial_t s + c \partial_x s - \nu \partial_{xx} s = 0, \quad (1.28)$$

is the most important PDE. In the three-dimensional space, the advection-diffusion equation for scalars may be formulated in vector notation as

$$\partial_t s + \vec{c} \cdot \nabla s - \nu \nabla^2 s = 0 \quad (1.29)$$

or in component notation as

$$\partial_t s + c_j \partial_j s - \nu \partial_{jj} s = 0, \quad (1.30)$$

where the summation convention by Einstein (see eq. (1.16)) has been used.

The first-order one-dimensional linear shallow water equations may be denoted as

$$\partial_t \eta = -H \partial_x u, \quad \partial_t u = -g \partial_x \eta, \quad (1.31)$$

with the sea surface elevation  $\eta$ , the horizontal velocity  $u$ , the constant water depth  $H$  and the gravitational acceleration  $g$ . Combining these two equations and eliminating  $u$  leads to the second-order wave equation

$$\partial_{tt} \eta - gH \partial_{xx} \eta = 0, \quad (1.32)$$

such that  $c = \sqrt{gH}$  is the phase speed of the waves.