MATHEMATICAL AND NUMERICAL GEOHYDRODYNAMIC MODELS

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Contents

Summary

The numerical methods that are used to solve the mathematical equations encountered in hydrodynamical models of ocean circulation are summarized. Special attention is paid to the specificities of ocean models compared to classical computational fluid

dynamics. Finite differences, finite elements, finite volumes, spectral methods are all of interest for ocean modeling and their basic properties, advantages and difficulties are highlighted. The problem of time-discretization, accuracy, stability as well as efficient algorithmic implementation is addressed and specific methods encountered in the present generation of models are outlined (mode-splitting, staggering, data assimilation). As for classical fluids dynamics, the equations governing the evolution of the hydrodynamics or ecosystem dynamics of the marine system have no general analytical solution, except in very simplified cases. Therefore, when even moderately complex systems are modeled, one rapidly has to resort to numerical methods to find approximate solutions to the governing equations. The present chapter describes some of the general methods that can be applied to the solution of partial differential equations similar to those encountered in ocean modeling. In particular, differences with methods of classical computational fluid dynamics are emphasized, explaining the reasons for developing dedicated numerical methods for ocean models. The presentation is limited to Eulerian methods since mot conservation laws are written in an Eulerian framework, the natural choice for the human observer. Presently, Lagrangian approaches are generally restricted to study of the dispersion of tracers in a given hydrodynamic field, which is itself modeled on an Eulerian grid.

1. Introduction

As for classical fluids dynamics, the equations governing the evolution of the hydrodynamics or ecosystem dynamics of the marine system have no general analytical solution, except in very simplified cases. Therefore, when even moderately complex systems are modeled, one rapidly has to resort to numerical methods to find approximate solutions to the governing equations. The present chapter describes some of the general methods that can be applied to the solution of partial differential equations similar to those encountered in ocean modeling. In particular, differences with methods of classical computational fluid dynamics are emphasized, explaining the reasons for developing dedicated numerical methods for ocean models. The presentation is limited to Eulerian methods since mot conservation laws are written in an Eulerian framework, the natural choice for the human observer. Presently, Lagrangian approaches are generally restricted to study of the dispersion of tracers in a given hydrodynamic field, which is itself modeled on an Eulerian grid.

2. Conservation Equations

Numerical methods in ocean modeling address the solution of equations of the type

$$\frac{\partial \phi}{\partial t} + \nabla_h \cdot (\boldsymbol{v}_h \phi) + \frac{\partial}{\partial z}(w\phi) = Q^{\phi} + \frac{\partial}{\partial z}\left(\tilde{\nu}\frac{\partial \phi}{\partial z}\right) + F_{\phi} \tag{1}$$

where ϕ is a state variable, $\boldsymbol{v}_h$ is the horizontal time-dependent velocity vector (defined at the scales of interest), Q^{ϕ} is the local source of $\phi, \tilde{\nu}$ the vertical turbulent diffusion

coefficient for ϕ and F_ϕ the parameterization of sub-grid scale processes not taken into account in the vertical turbulence; typically these sub-grid scale processes are modeled by a lateral diffusion.

This prototype of an evolution equation in oceanography is already reflecting the anisotropic nature of the flow in the sense that vertical turbulence is separated from lateral sub-grid scale parameterizations and that horizontal advection is separated from vertical advection, due to the strong anisotropy of the flow.

The form of the equation is however classical, in the sense that the evolution of the state variable is governed by a first order derivative in time (trend in time) related to the advection of the flow (first order spatial derivatives), its local source (non-linear local function) and its diffusion (typically second order derivatives). For such type of partial differential equations, several numerical methods exist. Here we mention only those relevant to oceanographic applications, where the topographic constraints and others are specific and different from classical fluid dynamic systems.

3. Preparation for Numerical Resolutions

The numerical solution of partial differential equations may be greatly simplified if appropriate preliminary mathematical transformations of the initial problem are made.

3.1. Coordinate Changes

One of such possibilities is an *a priori* coordinate change, with the general objective to obtain a "simple" computational domain (simplified logical structures) following "as close as possible" the physical structures (simplified representation of the physical solution in the new coordinates). Due to the anisotropic nature of the oceanographic flow, coordinate changes are performed independently for the vertical coordinate and the horizontal ones. Vertically, the logical, topological characteristics of the flow are set by the boundaries, which are the free surface (or the ice-sheet) and the ocean floor. Therefore, to simplify the computational domain, terrain-following coordinates are designed so that their lower coordinate line follows the bottom and the upper one the sea surface (Figure 1).

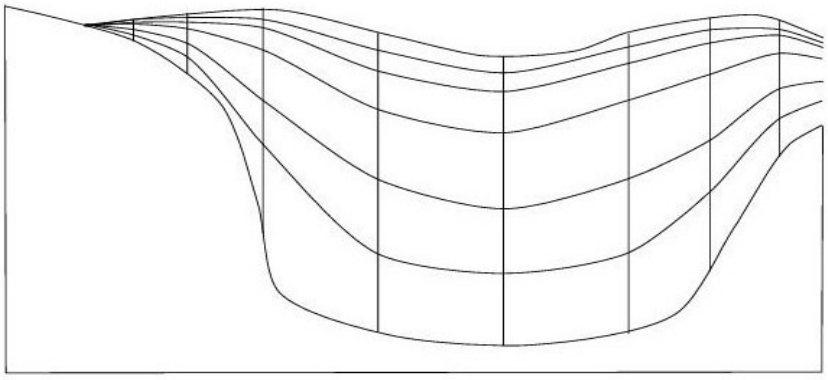

Figure 1: Terrain following vertical coordinates in a vertical plane

On the other hand, *z*-level coordinates (Figure 2) are interesting when the natural position of the density levels is almost horizontal.

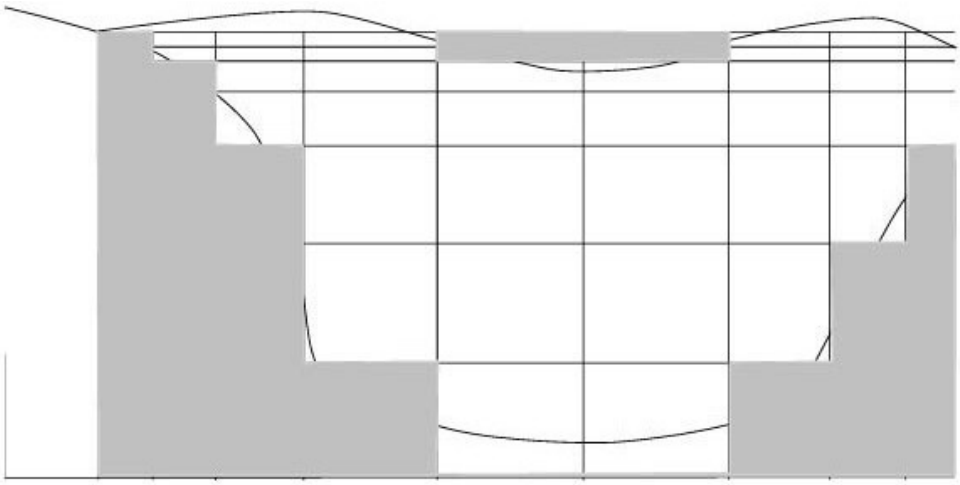

Figure 2: *z*-coordinate system in a vertical plane with masking of land points

Isopycnal coordinates are recommended when the flow is characterized by a few water-masses that are not mixing, so that the position of the interfaces between the water-masses is an easy and well defined characterization of the water masses.

Horizontally, model coordinates can be Cartesian, spherical or general curvilinear (orthogonal or non-orthogonal) (Figure 3).

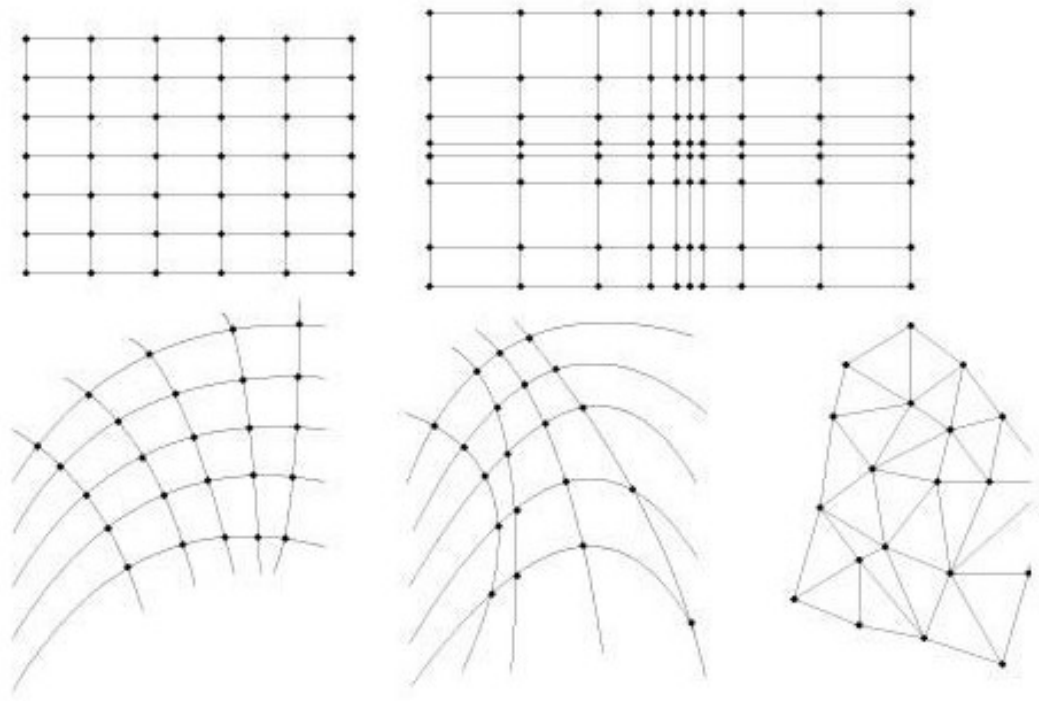

Figure 3: Cartesian grid, Stretched Cartesian grid, Orthogonal curvilinear grid, Non-Orthogonal curvilinear grid, Unstructured grid

Cartesian coordinates have the advantage of lending themselves to efficient numerical solvers at smaller scales, as do most spherical coordinate models on global scales. General curvilinear coordinates have the advantage of taking into account naturally the topological or topographic constraints, but on the other hand demand a preprocessing to generate the coordinate system as well as specific numeric treatments associated with the coordinate change. Once a coordinate system is chosen, the discretization of the equations that have been transformed into this new coordinate system can be tackled.

3.2. Elementary Notions for Numerical Analysis

When tuning towards such numerical approximations and discretizations, some basic characterizations of the scheme are related to their ability to represent correctly the mathematical solutions they are supposed to. A numerical approximation is therefore characterized by its truncation error, which measures the distance between the mathematical expression one tries to calculate numerically and the numerical representation. Using Taylor developments, this truncation error is generally expressed in terms of the grid spacing h and derivatives of the unknown function. If the grid spacing h appears as a power: h^n, the truncation error is said to be of nth order. For a given solution, decreasing the grid size by a factor 2 would decrease the truncation error by 2^n, justifying the interest of higher order schemes. A scheme is said to be *consistent* when the truncation error decreases to zero when the grid spacing tends towards zero. A solution is said to be *convergent* when decreasing the grid spacing to zero, one recovers the exact solution of the equation. The notion of consistency and convergence are not identical, since a consistent discretization could give rise to a solution which may not converge. In particular, a scheme may be unstable (i.e. amplify errors during the numerical iterations) and thus diverge, though it is consistent. A famous equivalence theorem shows that for linear equation, a consistent discretization converges if and only if the scheme is stable. This explains the large amount of theory dealing with the stability analysis of numerical schemes, mostly based on the so called Von Neumann method. This method analyzes the behavior of Fourier modes in linearized version of the equations. When unstable Fourier modes are allowed by the numerical discretization, the scheme is termed as unstable. In practice, convergence, consistency and stability are not easily verified, because of the non-linear nature of the ocean dynamics and the boundary effects. Therefore consistency and linear stability analysis are considered necessary preliminary steps, but numerical results should later be checked for slower non-linear instabilities or destabilizing boundary conditions. We should also mention here that the order of truncation is not necessarily a good measure of the actual precision of a given numerical solution. The truncation error analysis only allows us to tell how fast the solution tends to the correct one when one increases the grid resolution. For fixed grid sizes, low order methods can provide better solutions because of a lower coefficient multiplying the grid spacing power. Unfortunately, there is no general method to decide from which resolution on, a higher order method will outperform a lower order method in terms of real errors.

3.3. Grid and Resolution Choices

Once a coordinate change has been introduced and the mathematical equations reformulated in the new coordinate system, one has to choose a particular numerical

grid within this new coordinate system.

3.4. Parameterizations of Unresolved Features

At that point, one has to take into account any additional need for parameterizations introduced by the fact that the chosen grid has finite dimensions. Indeed, any process whose scale is smaller than the grid size is not resolved and if non-linear processes at these scales interact, this needs to be taken into account in the parameterization. The parameterization is often introduced before introducing the numerical coordinate choice and the discrete grid. In this case, the modeler implicitly assumes a subsequent discretization with a given scale; it also means that in ocean modeling, when refining the grid, one generally has to change the parameterizations, explaining why convergence studies (increasing resolution with fixed physical parameters) are seldom performed. The simplest and still most widely used parameterization of processes below the lateral scales of the numeric grid is the formulation based on the mixing hypothesis, assuming that sub-grid scale processes are essentially random and have an overall mixing effect. Then the Laplacian diffusion parameterization is commonly recommended. When larger scale or repetitive processes are filtered out, this may be more and more questionable, since the processes contain coherent signals not leading necessarily to a pure mixing. Then more elaborated parameterizations are needed, for example those aiming at representing baroclinic instabilities or tidal stirring. Once the parameterization for a given scale of the numerical grid is chosen, one can tackle the problem of finding a numerical approximation to the solution at these scales.

4. Spatial Discretizations

For the spatial discretization, several methods exist, each having its advantages and inherent problems, which we try to summarize in the following:

4.1. Finite Differences

Finite differences are the mathematically most straightforward to approximate a differential operator. By a local Taylor development of the yet unknown solution ϕ around a grid point, one can generate expressions for any spatial operator in terms of the values of the unknown at the surrounding grid points (Figure 4).

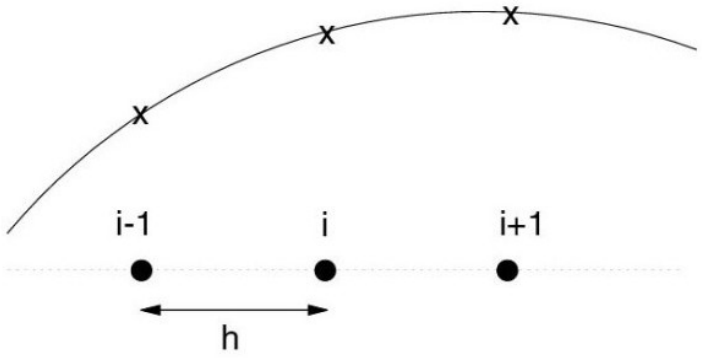

Figure 4: Nodal distribution of unknowns; *h* is the grid spacing and *i* denotes the discrete coordinate

At a given nodal point x_i , one can, for example, approximate a second derivative of the field ϕ on a uniformly spaced grid by

$$\left.\frac{\partial^2\phi}{\partial x^2}\right|_{x_i} \approx \frac{\phi(x_{i+1})-2\phi(x_i)+\phi(x_{i-1})}{h^2} \tag{2}$$

where h is the grid spacing. By using the Taylor development, one can also study the truncation error introduced by this finite differencing. In the present example one would write, with the notation $\phi_i = \phi(x_i)$

$$\left.\frac{\partial^2\phi}{\partial x^2}\right|_{x_i} \approx \frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{h^2} + O(h^2) \tag{3}$$

indicating that a second order approximation (quadratic in grid spacing) is used. Once each operator is approximated by such finite differences, one ends up with a series of algebraic relationships between the values at adjacent grid points and the time derivative at each point. In order to close such systems, boundary conditions must then be included in order to obtain in certain locations the values or gradients at the adjacent grid points. The advantage of such finite differencing is the facility of generation of schemes with arbitrary orders of truncation errors and hopefully more accurate methods for higher order approximations. Difficulties of classical finite differences are however rapidly encountered in ocean models: high order approximations are generally relying on a large number of adjacent points (one refers to this as a scheme having a large numerical stencil). Near complicated boundaries, this reduces drastically the precision, since at the boundaries, high order schemes implicitly need the knowledge of higher order derivates than those provided by the mathematical boundary conditions. It means that at the boundaries, the order of approximation is reduced in order to fit to the physical requirements for correctly imposed boundary conditions. In the case of complicated coastlines and inclusion of islands, it means that one loses in large parts of the domain the advantage of higher order approximations. Another disadvantage of classical finite differences is the difficulty of ensuring properties of global conservation or even local conservation. Typically a higher order scheme can have a lower truncation error but lead to non-conservation of a passive tracer. This could be a major problem for dispersion studies of pollutants, where one certainly would like to control the conservation property. Finally most finite differences are limited to numerical grids which are regular (Figure 3).

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Biographical Sketch

Jean-Marie Beckers was born in Eupen, Belgium, on May 13, 1965. He and his wife, an attorney at-law in Liège, are currently residing in Lontzen, Belgium. He received his Engineer diploma in 1988 at Liège University. In 1992 he obtained the Ph.D degree, for which he received the IBM Belgium award for the best Belgian thesis using high performance computing. He also was awarded the Prix Andre Leroux and the Belgian TYOP 1997 price. From 1988 to 1992 he was Research Assistant at the FNRS, 1993 Assistant at the University, 1993-95 Senior Research Assistant at the FNRS and since October 1995 he has a permanent position as Research Associate of the FNRS. From 1995-1996 he held an 18 month Alexander von Humboldt grant for a sabbatical stay at the Institut fuer Meereskunde in Hamburg, Germany. His main interest is the development of 3D models (including numerical aspects) and their application to the Mediterranean and Black Sea. He has written more than 60 publications in journals and books. He was coordinator of the European MEDMEX project and P.I. of several other E.U. projects. He has been guest editor of Journal of Marine Systems, acts as a member of the editorial board of the "Information" journal as well as editor for Ocean Dynamics. From October 2003 he will held the chair of Physical Oceanography at the Liège University.