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Numerical Methods

Edited by Jean-Michel Tanguy

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Numerical Methods

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Introduction

This environmental hydraulics treatise is made up of five volumes: Volume 1 describes the main physical processes and the physical domains where they can be observed and measured.

Volume 2 is dedicated to mathematical modeling in hydraulics and fluvial hydraulics.

In Volume 3, Chapters 1 to 7 constitute an introduction to numerical modeling, and more particularly on finite difference and finite element discretization. It in no way claims to constitute a treatise on the subject, but simply offers an overview of the discretization methods used in the domains covered by this work, which range from meteorology to shore morphodynamics. Chapters 8 to 13 deal with the finite volume discretization method, the spectral approach, numerical schemes and resolution methods.

Lastly, Volume 4 dealing with application examples completes Volume 3, along with a final volume (Volume 5) on operational software.

This volume is made up of three parts and comprises 13 chapters:

Part 1: general considerations concerning numerical tools;

Part 2: discretization methods;

Part 3: introduction to data assimilation.

Set out below is a brief summary of each chapter.

Introduction written by Jean-Michel TANGUY.

Part 1: General considerations concerning numerical tools

We will introduce a number of general concepts regarding models used in engineering and in the operational-forecast domain and detail the ways of constructing numerical models based on mathematical models.

Chapter outline

Part title	**Chapter no.**	**Chapter title**	**Problematic issue**
General Considerations Concerning Numerical Tools	1	Feedback on the Notion of a Model and the Need for Calibration	Placing perspective on the notion of a numerical model in the context of the study of physical phenomena. Importance of calibration
	2	Engineering Model and Real-Time Model	Transposing a model used in engineering into an operational forecast context requires significant computer-science and pairing work to be performed
	3	From Mathematical Model to Numerical Model	Switching from a mathematical model to a numerical model requires approximations to be performed; discretization methods suitable for the types of equations considered and suitable numerical schemes need to be used

What are the domain's perspectives?

– Operational forecast services such as the national meteorological services and flood forecasting services use real-time simulation tools based on numerical tools. *These tools need to be reliable, must not diverge and must be constantly recalibrated with respect to the reality in the field*, allowing civil security services and the general public to be warned of the imminence of a significant unforeseen event. Indeed, society's requirements are evolving towards a strong demand to be given preventative information as to risks, for there to be *greater risk-anticipation* and to be kept out of danger: we can cite as an example the mandatory preventive evacuation of the population of New Orleans when hurricane Gustav arrived in early September 2008, following the catastrophic events of Katrina in late August 2005.

– Significant progress has been made in recent years with respect to numerical modeling, underpinned by developments in computer science. This has enabled *complex geometries for very fine-scale studies* to be taken into account. Choosing appropriate discretization methods and efficient schemes is a major challenge in engineering today. The decision makers of today are demanding increasingly higher standards with regard to technical choices and the use of tried and tested simulation tools, and only the most effective tools will last.

Part two: Discretization methods

We will present the different numerical methods used within the domains covered by this book. Unlike a number of works dealing with these problems, we have opted not to remain focused on conceptual considerations, but to offer the reader a means of understanding the fundamentals of each method and their implementation. In particular, we explain the processing of boundary conditions, which are often overlooked. This lends something of a computational aspect to our presentations, but our aim is to provide the readers with the key principles, enabling them to follow the developments step by step.

Chapter outline

Part title	No.	Section title	Problematic issue
Discretization Methods	4	Problematic Issues Encountered	Highlighting of several difficulties relative to the behavior of computing codes to demonstrate the importance of having efficient numerical schemes
	5	General Presentation of Numerical Methods	Placing perspective on the main existing numerical methods
	6	Finite Differences	Succinct presentation of the method, illustrated using the equation for the diffusion of a pollutant
	7	Introduction to the Finite Element Method	Detailed presentation of the method, illustrated using the equation for swell propagation
	8	Presentation of the Finite Volume Method	Detailed presentation of the method, illustrated using the equation for the development of a water table
	9	Spectral methods in Meteorology	This method is widely used in meteorological computing codes
	10	Numerical-Scheme Study	Each discretization method requires a numerical scheme to be chosen, which must be studied to specify the behavior of the final model.
	11	Resolution Methods	A brief list of the resolution methods

What are the domain's perspectives?

– The recent developments of numerical methods are mainly led by industrial applications. All of these methods, each with different origins, ultimately translate into the resolution of matrix systems. There are numerous links between them, and current research appears to be oriented towards methods, such as discontinuous finite element methods, which present a combination of the advantages of each of them.

– As we have mentioned on a number of occasions in the course of this book, the numerical tools of tomorrow will need to be equipped with high-level processing functionalities to offer the user the possibility of performing a reverse action at any instant on the resolution cycle.

Part three: Introduction to data assimilation

This part presents the data assimilations methods that are most commonly used by forecast services.

The concepts on which these methods are based can appear somewhat abstruse, all the more so as the mathematical formulation is far from simple, but they represent powerful tools that are indispensable to forecasters to enable their models to adjust to the reality in the field.

We can expect these tools to undergo significant development in the coming years.

Chapter outline

Part title	Chapter no.	Chapter title	Problematic issue
Introduction to Data Assimilation	12	Data Assimilation	General presentation of the various applications of the method: meteorology, hydrology and hydraulics
	13	Data Assimilation Methodology	Detailed presentation of the different numerical methods used within the domains covered by this book

What are the domain's perspectives?

– Data assimilation is a method undergoing rapid expansion within our field of application. It is increasingly applied within the framework of computing-code calibration and problematic issues encountered in real time. Meteorology was one of the first disciplines to use these methods owing to the large quantity of measurements and observations resulting from work in the field. It has arrived at a level of maturity that means it can now *serve as a reference to other disciplines such as hydrology and hydraulics*.

– These methods will also be used to install measurement systems that are to be increasingly adapted to simulation models. In hydrology, for example, staff gauge stations were installed in areas presenting high stakes, without the entirety of the forecast chain being taken into account. The installation of new models will be accompanied by an approach aimed at optimizing the measurement systems to be assimilated. Likewise, it will be possible for gauging in rivers, very dangerous in the event of a flood, to be considered in relation to hydrodynamic-model usage in order to be able to optimize their installation and enable measurements at maximum reservoir level to be taken in less exposed locations.

Part 1

General Considerations Concerning Numerical Tools

Chapter 1

Feedback on the Notion of a Model and the Need for Calibration

In the previous volumes, numerous fields of physics were touched upon. The conventional scientific procedure used consists of understanding the observed phenomenon and then expressing it in the form of equations. These equations are programmed, and the numerical results are compared to the observations available.

With this perspective in mind, an interdisciplinary committee, the Technical Committee on Model Credibility, proposed a set of terminology reference guidelines [SCH 79]. This was based around a summary diagram presenting the different components of the simulation environment and the relationships connecting them:

– the reality (the studied phenomenon);

– the conceptual model (setting of corresponding equations);

– the computational model (the code).

This code is incorporated into a more or less ergonomic computer platform.

In the diagram below (Figure 1.1), the inner arrows describe the processes that make it possible to move from one component to another, and the outer arrows refer to the procedures assessing the credibility and reliability of each of these processes. These reference guidelines have been used in the hydrology field, notably by [REF 96].

Chapter written by Denis DARTUS.

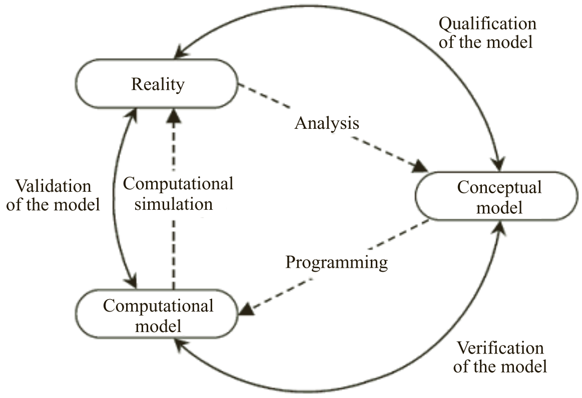

Figure 1.1. *Schlesinger diagram, modeling guidelines adapted from Schlesinger et al. (1979)*

In this chapter, our focus is not on the ergonomics of the product or of the computer platform, nor on notions of engineering software such as the V-cycle for information system development. We will assume that the model code is perfect and error free, and that all convergence, consistency and stability problems (see Chapter 10) have been resolved.

According to the guidelines mentioned above, it only remains to "validate the model" through "simulations" and, in the case of incorrect results, to return to the "analysis" that was performed on the "qualification of the model". We note that many difficulties are rejected during this stage. Indeed, during analysis, the modeler is confronted with many problems, which must be incorporated into their conceptual model. We can mention two categories of problems, illustrated using the problem of modeling flood propagation in a river:

– the model is only an approximation of the reality: the writing of the complete system of equations governing turbulent flow is not a closed problem. We can "make do" with Saint-Venant's equations, which consider the depth-averaged phenomena if we know the domain boundaries and the initial and boundary conditions;

– the model parameters are only approximately evaluated. During the depth-averaging process, or change of scale, or problem conceptualization, we obtain calibration parameters, for which it is possible to know the parameter range but impossible to obtain an exact value. The modeling of friction on a river bed using the Strickler coefficient is a "catchall" parameter, whereby the modeler recognizes his lack of knowledge in the field of physics.

These constants, added to the development of computing codes, demonstrate that the precedent guidelines have their limits because the notion of calibrating a code is difficult to introduce. The guidelines produced by Refsgaard and Henriksen within the framework of the European project, HARMONIQUA, offer a state-of-the-art report on quality assurance in digital modeling procedures related to river basin management [REF 02]. The authors propose a terminology which differentiates between computing code and numerical model and enables the notion of model calibration to be introduced (Figure 1.2).

The terms are defined as follows.

Term	Generic definition
Reality	Natural system type
Conceptual model	Description tending to describe the system considered in the form of functional relationship equations
Computing code	Computer program formalizing the system considered in a generic manner
Digital model	Computerized description of the specific system studied
Analysis	Set principles governing a physical system
Programming	Development of a computer code for the conceptual model
Construction of the model	Creating a model of the studied system
Simulation	Use of the numerical model in order to obtain predictions on the studied system
Confirmation of the theory	Matching of the reality and the conceptual model for the system studied
Verification of the code	Check of the conceptual model's computational representation
Calibration of the model	Adjustment of the digital model's parameters
Validation of the model	Matching of reality and modeling for the system studied

This distinction thus leads to the procedures for validating the model and for verifying the model defined by Schlesinger *et al.* being broken down into three new procedures:

– *verification of the code* controls the correctness of the computational implementation of the conceptual model;

– *calibration of the model* involves adjusting the parameters of the digital model with the purpose to reproduce the reality within the requested accuracy limits.

It should be noted that the model calibration may use itself a computing code, the aim of which being to automate the calibration procedure (optimization method);

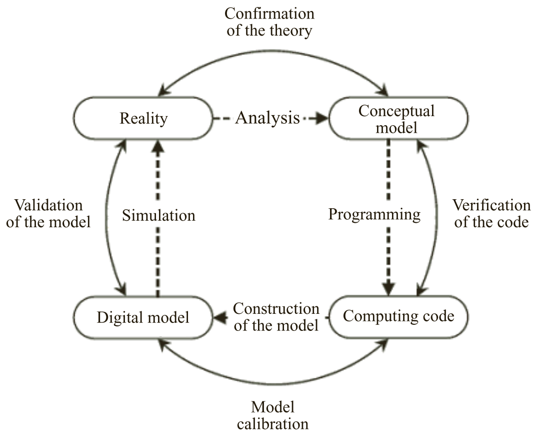

Figure 1.2. *Components of a modeling terminology incorporating the stage of model calibration. Adapted from [REF 04]*

– *validation of the model*, meanwhile, consists of ensuring that the digital model presents an accuracy level that is consistent with the requested application.

1.1. "Static" and "dynamic" calibrations of a model

1.1.1. *Static calibration*

As a result of the model's design or the nature of the problem to be solved, some parameters remain impossible to accurately measure or evaluate. However, we often have a range of variation for the parameter at our disposal when using "physical based" models. Moreover, it is often illusory to look for a parameter optimum value, and it seems more important to consider the model's sensitivity to this parameter.

1.1.1.1. *Static calibration methods*

The quality of the simulation is generally assessed using a "target function" or a "cost function" as a criterion, consisting of measuring the distance between the observation data and the simulation results. The choice of the cost function itself is not neutral: it may favor one particular part or another of the modeled curve.

Example – 3 cost functions are tested in the following example:

$$J = \sum \left(y_M^{\text{Power}} - y_O^{\text{Power}} \right)^2 .$$

The model used is simply $y_M = a.\sin(x) + b$ amongst the set of observations y_O. The results obtained are as follows (Figure 1.3).

	Power = 1	Power = 2	Power = 0.5
a	1.20	1.02	1.30
b	0.30	0.47	0.23

According to the power law used, the model will tend to approach *y* observations either less than 1 or greater than 1.

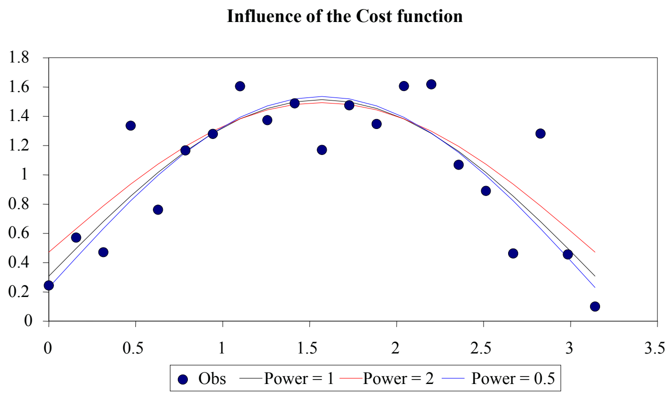

Figure 1.3. *Influence of the cost function for static calibration*

This illustrates the influence of the calibration method in an extremely simple example:

– least squares method, where the aim is to minimize the variance value between the results of the model and the measurements. In hydrology, the Nash criterion is often used as the reference indicator;

– the maximum likelihood, we can cite the GLUE method, which suggests randomly varying calibration parameters within likelihood intervals. The responses are still based upon a cost function, but the method offers validity ranges for the parameters and measures the likelihood of the value of these parameters. It also makes it possible to demonstrate that certain parameters within the range considered are not determinant in the results of the model;

– the "expert eye", where the cost function is a visual comparison favoring certain parts of the phenomenon studied. The adjustment method requires perfect knowledge of the field studied and of the model. Quantification of this cost function is quasi impossible, and comparison with a mathematical criterion can sometimes offer unexpected results.

Calibration thus requires an adjustment method:

– with the purpose to minimize a cost function automatically, we shall choose the category of inverse problems, with numerous "conjugated gradient" type descent methods;

– the maximum likelihood is based on a Monte-Carlo stochastic method for scanning the space for all parameters and Bayesian methods for analyzing the results;

– the manual method by trial and error procedure depends only on the expert. It is often worthwhile comparing it with another method because the expert can promote a solution he felt physical;

– methods without minimization may also be used, such as the moments method, which aims to adjust a parameter according to the set of data to which we have access; for example, a Gaussian method with its average and its standard deviation.

1.1.1.2. *Role of static calibration*

The explicit role of calibration is to estimate the model's parameters. If the model is physical, these are supposed to be completely known. We consider the example of the roughness coefficient in the calibration of the free surface flow location by solving Saint-Venant equations. In the literature, there is a plethora of tables enabling us to convert the river-bed typology into values of this coefficient. Nevertheless, modelers still persist in taking this parameter as a calibration parameter. In fact, in this straightforward example, the roughness coefficient is implicitly used to compensate for the imperfections of the model and the modeler's knowledge gaps with regard to friction at a river scale.

Example of calibration – What do we include in the Manning-Strickler coefficient: K?

Considering the 1D steady Saint-Venant model in a canal:

$$\frac{dH}{dx}=\frac{(I-J)}{\left(1-F^2\right)}, \text{ where } J=\frac{Q^2}{S^2}\frac{1}{K^2.R_h^{4/3}}, \; F^2=\frac{Q^2B}{gS^3}, \; R_h=\frac{S}{P_m}.$$

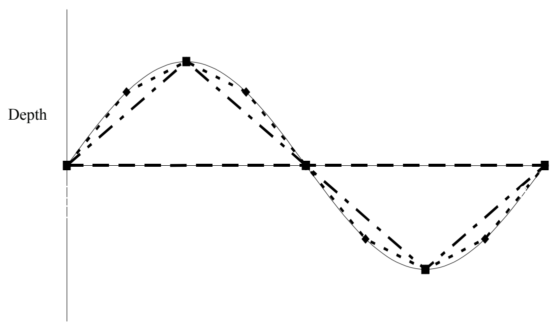

Figure 1.4. *Different shapes of the cross-section*

I is the slope of the river bottom, Q is the flow rate, S is the wetted cross-section, P_m is the wetted perimeter.

For a steady flow in a canal of constant slope I, we have

$$dH/dx = 0 \text{ and } I = J.$$

In this example (Figure 1.4), a sinusoidal-shaped bottom of spatial period B, with the chosen measurements (B; $B/2$; $B/4$; $B/8$, etc.), only P_m varies, but there is no variation in S, Q, B or H. As $K^2 * R_h^{4/3}$ must remain constant, it implies a value of K that depends on the number of measurements that have been taken in order to inspect the cross-section.

1.1.1.3. *Problems associated with static calibration*

Many problems can occur during the calibration of a model:

– the reference data contain errors and the model is not always able to detect them;

– the choice of the adjustment method and of the cost function influences the value of the calibrated parameters. It will then be preferable to define a validity range for this parameter. Most often, the adjustment method considers the measurement value as precise. If we add an uncertainty range to this, the approach to this optimization can be very different;

– the interdependency of the parameters or the non-linearities of the problem examined produces the response surface with numerous local minima. The extremum is then difficult to obtain;

– specialized models are often over-parameterized. Generally speaking, these models are physical, and their parameters may be determined by performing *in situ* measurements. Unfortunately, we do not always know the exact correspondence between the measurement and the parameter value (only a confidence interval is known), and the specialization of the measurement does not match the specialization of the model. We are thus led to apply values to parameters without any real objective criterion. This leads to the problem of non-uniqueness of the solution or an "equifinality problem". Several sets of parameters provide solutions presenting equivalent relevance for a given cost function. This difficulty may be partly removed using methods of studying the model sensitivity to these parameters. Only some of the parameters are optimized, others remain in their "physically acceptable" range due to their "lower influence" with respect to the response.

1.2. "Dynamic" calibration of a model or data assimilation

A starting point is that the direct model is imperfect and that it is difficult to know:

– all of the parameters;

– all initial conditions.

Using an external measurement, often in real time, we aim to recalculate parameters or initial conditions, in order to minimize a trajectory of the model with respect to a cost function that we have chosen, and the data assimilation methods.

1.3. Bibliography

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