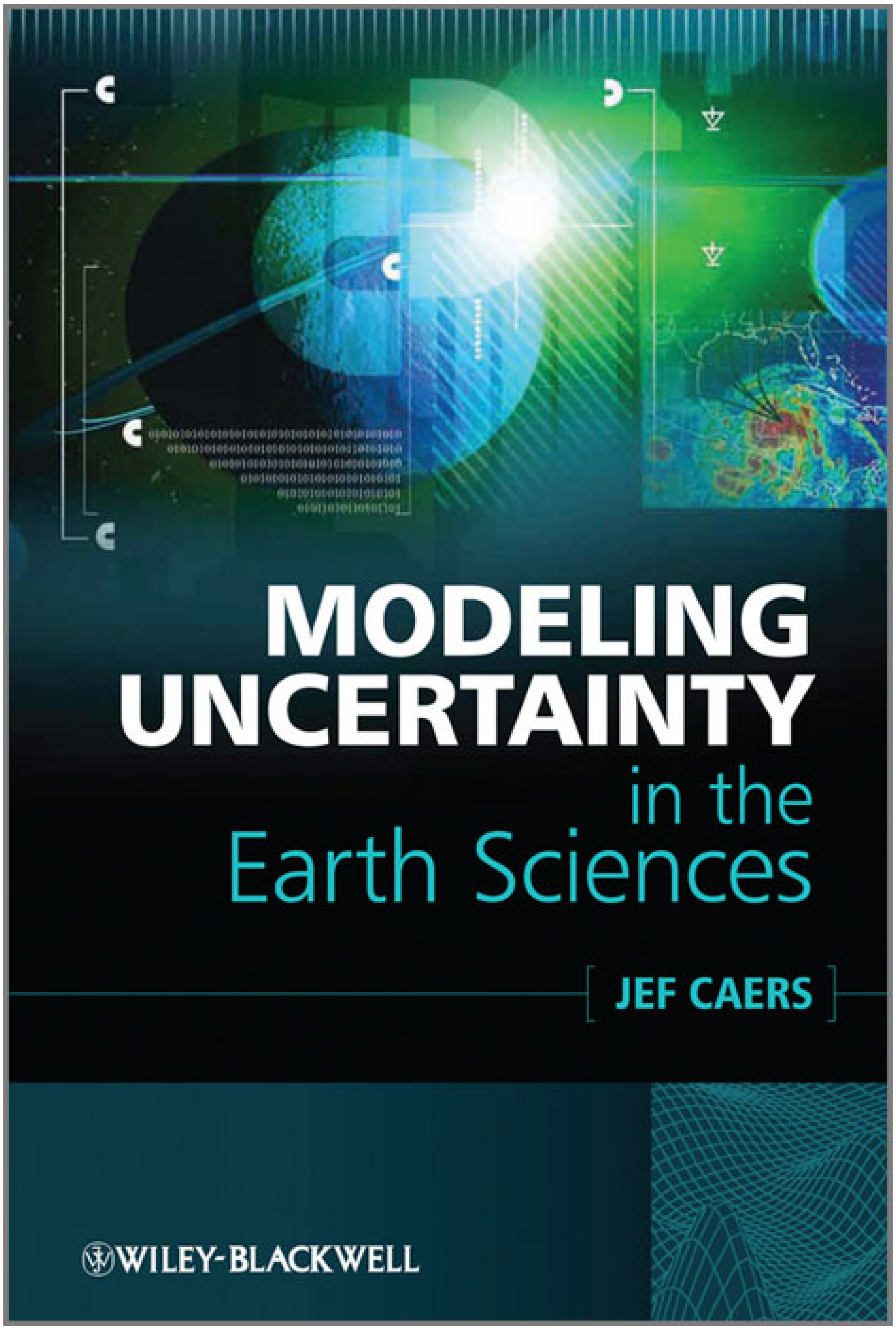
MODELING UNCERTAINTY in the Earth Sciences

JEF CAERS

WILEY-BLACKWELL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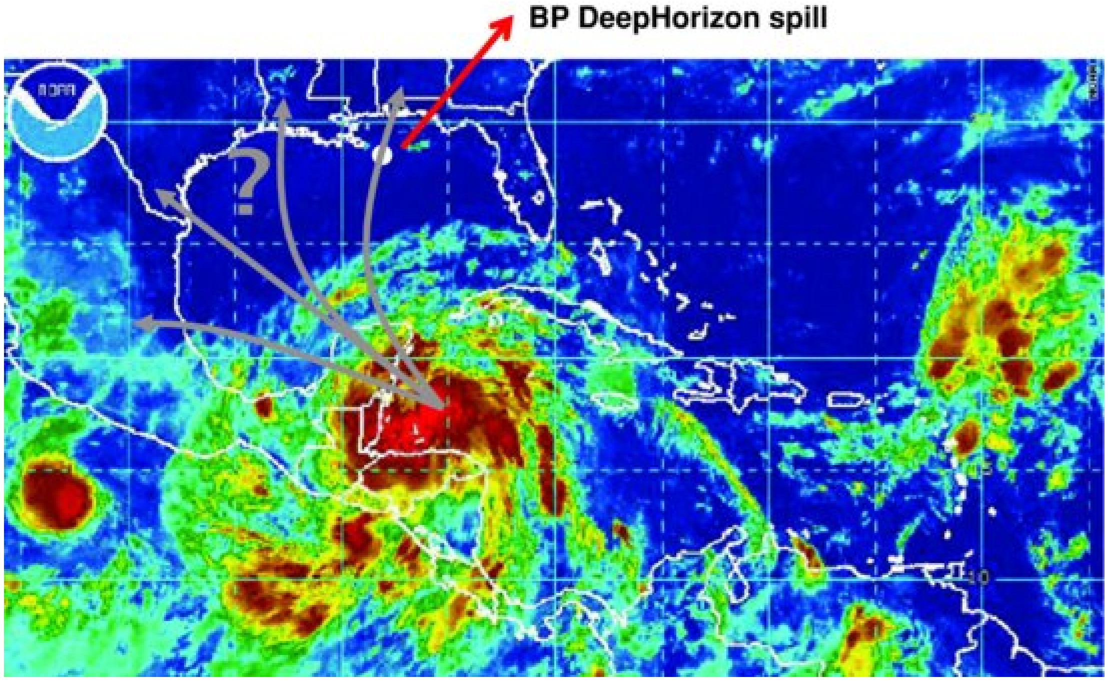
Preface

26 June 2010: CNN headlines

Tropical storm plus oil slick equal uncertainty



Decision question: “Will BP evacuate the clean-up crew knowing that evacuation requires at least three days, with the consequence of more oil spilling in the Gulf from the deep-water well, or, will BP leave the crew, possibly exposing them to tropical storm Alex, which may or may not become a hurricane?” A simple question: what is the best decision in this case?

Whether Earth Science modeling is performed on a local, regional or global scale, for scientific or engineering purposes, uncertainty is inherently present due to lack of data and lack of understanding of the underlying phenomena and processes taking place. This book highlights the various issues, techniques and practical modeling tools available for modeling uncertainty of complex Earth systems, as well as the impact it has on practical geo-engineering decision problems.

Modeling has become a standard tool in the Earth Sciences. Atmospheric scientists build climate models, seismologists build models of the deep Earth's structure, and hydrogeologists build models of aquifers. Many books and papers have been written on modeling, spread over many subdisciplines of mathematics and the Earth Sciences. Often, one or at most a few models are built to test certain hypothesis and assumptions, to validate or test certain engineering actions taken in the real world, or to attempt to describe physical processes as realistic as possible. The issue of uncertainty (historic, present or future) is often mentioned, but more as a side note; it is still rarely used for quantitative and predictive purposes. Very few books have uncertainty in Earth Sciences modeling as a primary topic; to date, no book to my knowledge discusses this at the level an undergraduate student in the Earth Sciences can actually comprehend and master. Professionals that are not academics often get lost in the myriad of technical details, limitations and assumptions of models of uncertainty in highly technical journal publications or books.

Therefore, in 2009, I decided to teach an entirely new class at Stanford University termed “Modeling Uncertainty in the Earth Sciences,” as part of the curriculum for Earth Science senior undergraduate and first year graduate students (geology, geophysics and reservoir engineers) as well as related fields (such as civil and environmental engineering and Earth systems studies). The focus of this class is not to build a single model of the Earth or of its physical processes for whatever purpose and then “add on” something related to uncertainty, but to build directly a model of uncertainty for practical decision purposes. The idea is not to start from a single estimate of a certain phenomenon and then “jiggle” the numbers a bit to get some confidence statement about that estimate. The idea is to have students think in terms of uncertainty directly, not in terms of a single climate, seismological or hydrological model or any single guess, from the beginning. The quest for a new syllabus was on.

In many discussions I had with various colleagues from various disciplines in the Earth Sciences, as well as from my decade-long experience as Director of the Stanford Center for Reservoir Forecasting, I had come to the conclusion that any modeling of uncertainty is only relevant if made dependent on the particular decision question or practical application for which such modeling is called for. This, I understand, is a rather strong statement. I strongly believe there is no “value” (certainly not in dollar terms) in spending time or resources in building models of uncertainty without focusing on what impact this uncertainty will have on the decision question at hand: do we change climate-related policies? Do we tax CO_2? Do we clean a contaminated site? Where do we drill the next well? and so on.

Let's consider this more closely: if uncertainty on some phenomenon would be “infinite”, that is, everything imaginable is possible, but that uncertainty has no impact on a certain decision question posed, then why bother building any model of uncertainty in the first place, it would be a waste of time and resources! While this is an extreme example, any model approach that first builds a model of uncertainty about an Earth phenomenon and then only considers the decision question is likely to be highly inefficient and possibly also ineffective. It should be stressed that there is a clear difference between building a model of the Earth and building a model of uncertainty of the Earth. For example, building a single model of the inner Earth from earthquake data has value in terms of increasing our knowledge about the planet we live on and getting a better insight into how our planet has evolved over geological time, or will evolve in the short and long term. A model of uncertainty would require the seismologist to consider all possibilities or scenarios of the Earth structure, possibly to its finest detail, which may yield a large set of possibilities because the earthquake data cannot resolve meter or kilometer-scale details at large depths. Constructing all these possibilities is too difficult given the large~computation times involved in even getting a single model. However, should the focus be on how a seismological study can determine future ground motion in a particular region and the impact on building structures, then many prior geological scenarios or subsurface possibilities may not need to be considered. This would make the task of building a model of uncertainty efficient computationally and effective in terms of the application envisioned. Knowing what matters is therefore critical to building models of uncertainty and an important topic in this book.

Thinking about uncertainty correctly or at least in a consistent fashion is tricky. This has been my experience with students and advanced researchers alike. In fact, the matter of uncertainty quantification borders the intersection of science and philosophy. Since uncertainty is related to "lack of knowledge" about what is being modeled, the immediate rather philosophical question of "what is knowledge?" arises. Even with a large amount of data, our knowledge about the universe is, by definition, limited because we are limited human beings who can only observe that which we are able to observe; we can only comprehend that which we are able to comprehend. Our "knowledge" is in constant evolution: just consider Newtonian physics, which was considered a certainty until Einstein discovered relativity resulting in the collapse of traditional mathematics and physics at that time. While this may seem a rather esoteric discussion, it does have practical consequence on how we think about uncertainty and how we approach uncertainty, even for daily practical situations. Often, uncertainty is modeled by including all those possibilities that cannot be excluded from the observations we have. I would call this the “inclusion” approach to modeling uncertainty: a list or set of alternative events or outcomes that are consistent with the information available is compiled. That list/set is a perfectly valid model of uncertainty. In this book, however, I will often argue for an “exclusion” approach to thinking about uncertainty, namely to start from all possibilities that can be imagined and then exclude those possibilities that can be rejected by any information available to us. Although the inclusion and exclusion approaches may lead to the same quantification of uncertainty, it is more likely that the exclusion approach will provide a more realistic statement of uncertainty in practice. It is a more conservative approach, for it is typical human behavior to tend to agree on including less than the remainder of possibilities after exclusion. In a group of peers we tend to agree quicker on what to include, but tend to disagree on what to exclude. In the exclusion approach one focuses primordially on all imaginable possibilities, without being too much biased from the beginning by information, data or other experts. In this way we tend to end up with having less (unpleasant) surprises ultimately. Nevertheless, at the same time, we need to recognize that both approaches are limited by the set of solutions that can be imagined, and hence by our own human knowledge of the universe, no matter what part of the universe (earth or atmosphere, for example) is being studied.

My personal practical experience with modeling uncertainty lies in the subsurface arena. The illustration example and case studies in this book contain a heavy bias towards this area. It is a difficult area for modeling uncertainty, since the subsurface is complex, the data are sparse or at best indirect, a medium exists that can be porous and/or fractured. Many applications of modeling uncertainty in the subsurface are very practical in nature and relevant to society: the exploration and extraction of natural resources, including groundwater; the storage of nuclear material and gasses such as natural gas or carbon dioxide to give a few examples. Nevertheless, this book need not be read as a manual for modeling uncertainty in the subsurface; rather, I see modeling of the subsurface as an example case study as well as illustration for modeling uncertainty in many applications with similar characteristics: complex medium, complex physics and chemistry, highly computationally complex, multidisciplinary and, most importantly, subjective in nature, but requiring a consistent repeatable approach that can be understood and communicated among the various fields of science involved. Many of the tools, workflows and methodologies presented in this book could apply to other modeling areas that have elements in common with subsurface modeling: the modeling of topology and geometry of surfaces and the modeling of spatial variation of properties (whether discrete or continuous), the assessment of response functions and physical simulation models, such as provided through physical laws. As such, the main focus of application of this book is in the area of “geo-engineering”. Nevertheless, many of the modeling tools can be used for domains such as understanding fault geometries, sedimentary systems, carbonate growth systems, ecosystems, environmental sciences, seismology, soil sciences and so on.

The main aim of this book is therefore twofold: to provide an accessible, introductory overview of modeling uncertainty for the senior undergraduate or first year graduate student with interest in Earth Sciences, Environmental Sciences or Mineral and Energy Resources, and to provide a primer reading for professionals interested in the practical aspects of modeling uncertainty. As a primer, I will provide a broad rather than deep overview. The book is therefore not meant to provide an exhaustive list of all available tools for modeling uncertainty. Such book would be encyclopedic in nature and would distract the student and the first reader from the main message and most critical issues. Conceptual thinking is emphasized over theoretical understanding or encyclopedic knowledge.

Many theoretical details of the inner workings of certain methodologies are left for other, more specialized books. In colleges or universities one is used to emphasizing learning on *how* things work exactly (for example, how to solve a matrix with Gaussian elimination); as a result, often, *why* a certain tool is applied to solve a certain problem in practice is lost in the myriad of technical details and theoretical underpinnings. The aim, therefore, is to provide an overview of modeling uncertainty, not some limited aspect of it in great detail, and to understand *what* is done, why it is done that way and not necessarily *how* exactly it works (similarly, one needs to know about Gaussian elimination and what this does, but one doesn't need to remember exactly how it works unless one is looking to improve its performance). A professional will rarely have time to know exactly the inner working of all modeling techniques or rarely be involved in the detailed development of these methods. This is a book for the user, the designer of solutions to engineering problems, to create an intelligence of understanding around such design; the book is not for the advanced developer, the person who needs to design or further enhance a particular limited component in the larger workflow of solving issues related to uncertainty.

Therefore, in summary: what this book does not provide:

- An encyclopedic overview of modeling uncertainty.
- A textbook with exercises.

- A detailed mathematical manifest explaining the inner workings of each technique.
- A cook-book with recipes on how to build models of uncertainty.
- Exhaustive reference lists on every relevant paper in this area.

What this book does attempt to provide:

- A personal view on decision-driven uncertainty by the author.
- An intuitive, conceptual and illustrative overview on this important topic that cuts through the mathematical forest with the aim of illuminating the essential philosophies and components in such modeling.
- Methods, workflows and techniques that have withstood the test in the real world and are implemented in high quality commercial or open source software.
- A focus on the subsurface but with a qualification in various sections towards other applications.
- Some further suggest reading, mostly at the same level of this book.
- Teaching materials, such as slides in PDF, homework, software, and data, as well as additional material, are provided on http://uncertaintyES.stanford.edu

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1

Introduction

1.1 Example Application

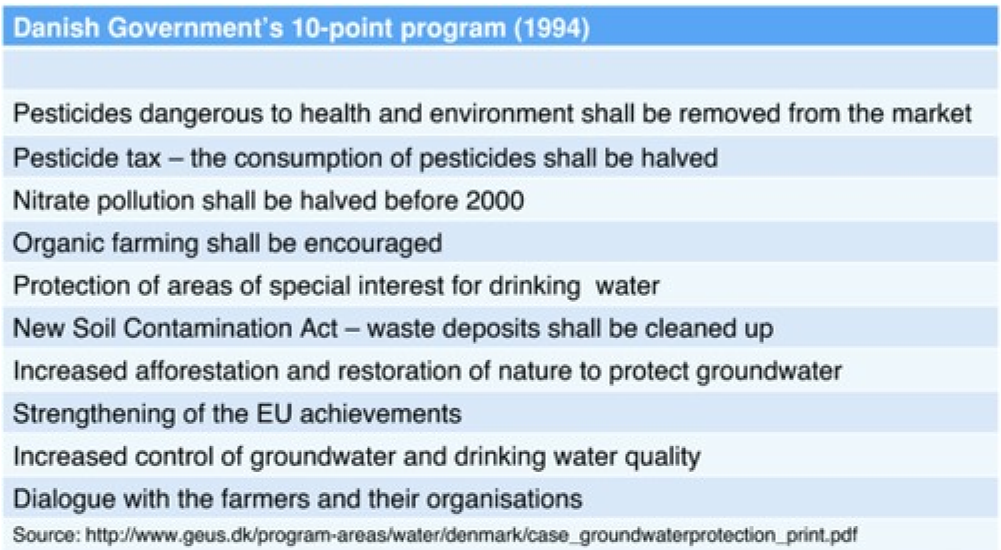
1.1.1 Description

To illustrate the need for modeling uncertainty and the concepts, as well as tools, covered in this book, we start off with a virtual case study. "Virtual" meaning that the study concerns an actual situation in an actual area of the world; however, the data, geological studies and, most importantly, the practical outcomes of this example should not be taken as "truth," which is understandably so after reading the application case.

Much of the world's drinking water is supplied from groundwater sources. Over the past several decades, many aquifers have been compromised by surface-borne contaminants due to urban growth and farming activities. Further contamination will continue to be a threat until critical surface recharge locations are zoned as groundwater protection areas. This can only be successfully achieved if the hydraulically complex connections between the contaminant sources at the surface and the underlying aquifers are understood.

Denmark is one example of this type of scenario. Since 1999, in an effort to identify crucial recharge zones (zones where water enters the groundwater system to replenish the system), extensive geophysical data sets were collected over the Danish countryside – the areas designated as particularly valuable due to their high rate of water extraction. The data were collected with the intention of making more informed decisions regarding the designation of recharge protection zones. The magnitude of these decisions is considerable, as it could involve the relocation of farms, industry, city development and waterworks together with related large compensations. Consequently, incorrectly identifying a vulnerable area can lead to a costly error. In fact, the Danish Government set out a 10-point program (Figure 1.1) that sets certain objectives and formulates certain desired preferences, some of which may be in conflict with keeping the farming industry alive and ensuring economic health next to ecological health for this area.

Figure 1.1 Objectives of the Danish Government.



Danish Government's 10-point program (1994)
Pesticides dangerous to health and environment shall be removed from the market
Pesticide tax – the consumption of pesticides shall be halved
Nitrate pollution shall be halved before 2000
Organic farming shall be encouraged
Protection of areas of special interest for drinking water
New Soil Contamination Act – waste deposits shall be cleaned up
Increased afforestation and restoration of nature to protect groundwater
Strengthening of the EU achievements
Increased control of groundwater and drinking water quality
Dialogue with the farmers and their organisations
Source: http://www.geus.dk/program-areas/water/denmark/case_groundwaterprotection_print.pdf

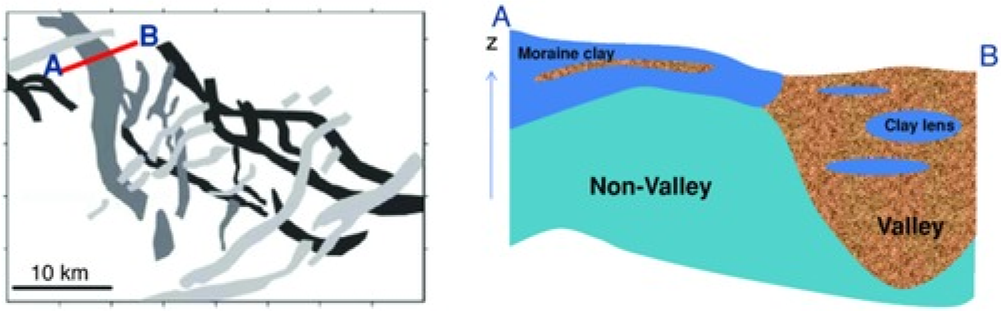
The subsurface in Denmark consists of so-called buried valleys, which are considered the informal term for Pleistocene (Quaternary) subglacial channels. They have also been described as the result of waxing and waning of Pleistocene ice sheets. The primary method by which these valleys are formed is subglacial meltwater erosion under the ice or in front of the ice margin. Thus, the valley formation is directly related to the morphology and erodability of the geological strata. The secondary method is through direct glacial erosion by ice sheets.

Several of the processes that created and filled buried valleys are important for understanding the complexity of the Danish aquifer systems and their vulnerability to surface-borne pollutants. In Denmark, the superposition of three different generations of glaciations has been observed. Thus, multigeneration glacial valleys cross-cut each other and can also appear to abruptly end (as seen in Figure 1.2). The existence and location of these glacial valleys can be thought of as the primary level of Denmark's aquifer system structure. If largely filled with sand, the buried valley has potential for being a high volume aquifer (reservoir). However, these buried valleys can be “re-used,” as revealed by the observed cut-and-fill structures. This describes the secondary level of uncertainty of heterogeneity in Danish aquifer systems.

> Most cut-and-fill structures are narrower than the overall buried valley, but in some places very wide structures that span the entire valley width can be seen. The complex internal structure can be observed in seismic surveys, electromagnetic surveys and occasionally in borehole data.
>
> *–Sandersen and Jorgensen (2006)*

Figure 1.2 shows a few different possible internal heterogeneities and varying extent of overlying strata, which deems the valley as actually “buried.”

Figure 1.2 Geological interpretation of subsurface glacial channels cross-cutting each other (left). Conceptual view of the inner structure of the glacial channels (right).



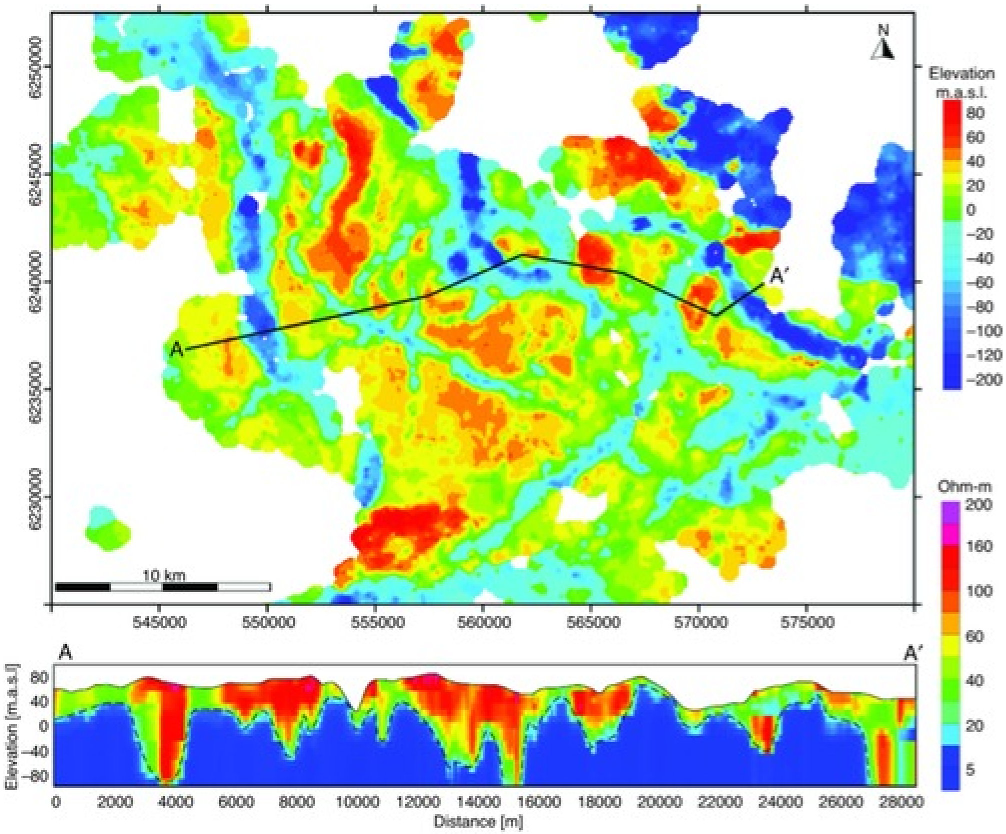
Due to the generally complex internal structure of the valleys, potentially protective clay layers above the aquifers are likely to be discontinuous. The aquifers inside the valley will thus have a varying degree of natural protection. Even if laterally extensive clay layers are present, the protective effect will only have local importance if the surrounding sediments are sand-dominated. The valleys may therefore create short-circuits between the aquifers in the valley and the aquifers in the surrounding strata.

1.1.2 3D Modeling

In this case study, the incompleteness of the information about the subsurface strata makes making specific decisions such as relocating farms difficult. A geologist may be tempted to study in great detail the process by which these glacial valleys were created and come up with a (deterministic) description of these systems based on such understanding, possibly a computer program to simulate the process that created these systems according the physical understanding of what is understood to occur. However, such description alone will fall short in addressing the uncertainty issue that has considerable impact on the decisions made. Indeed, even if full insight into the glaciation process exists (a considerable assumption), then that would not necessarily provide a deterministic rendering of the exact location of these valleys, let alone the detailed spatial distribution of the lithologies (shale, sand, gravel, clay) inside such valleys. This does not mean that the study of the geological processes is useless. On the contrary, such study provides additional information about the possible spatial variation of such channels next to the data gathered (drilling, geophysical surveys). Therefore, additional tools are needed that allow the building of a model of the subsurface glaciations as well as quantifying the uncertainty about the spatial distribution of valley/non-valley and the various lithologies within a valley. Such a model would ideally include the physical understanding as well as reflecting the lack of knowledge, either through limited data or limited geological understanding.

Data play a crucial role in building models and constraining any model of uncertainty, whether simple or complex. In the Danish case, two types of data are present: data obtained through drilling and data obtained through a geophysical method termed time-domain electromagnetic surveys (TEM surveys). Figure 1.3 shows the interpretation of the thickness of the valleys from such surveys, which are basically a collection of 1D (vertical) soundings. The data collected are typical of many Earth modeling situations: some detailed small scale information is gathered through sampling (in this case drilling a well) and some larger scale indirect measurement(s) collected either through geophysical or remote sensing methodologies. In the Danish study, the TEM data provide a reasonably good constraint on the location of the valleys but do not inform the internal valley structure (small scale variation), while the drilling data provide the exact opposite.

Figure 1.3 Thickness of the valley complex as processed and interpreted from TEM data. Thicker strata reflect the existence of valleys (with permission from Elsevier Science).



1.2 Modeling Uncertainty

From this case study of modeling the subsurface, several elements in modeling uncertainty that are typical to many similar applications can be identified:

1. **Decision making**: modeling uncertainty is not a goal on its own, it is usually needed because a particular decision question is raised. In fact, this decision question is usually framed in a larger context, such as done by the 10-point program, specifying objectives and preferences. Two example decisions are in this case: (1) in which areas do we relocate pollution sources and (2) do we consider taking more geophysical data to narrow the uncertainty on locating vulnerable areas, hence increasing the probability of a good decision? This latter question is termed a "Value of Information" question. Clearly, we need to make decisions without perfect information. These narrower

decision questions should not be considered as independent of the larger objective outlined in Figure 1.1.

2. Importance of the geological setting: a critical parameter influencing the decision is the heterogeneity of the subsurface medium (fluids and soils/rocks). Rarely do we have perfect information to deterministically model the geological variability of the subsurface. Hence there is a need to model all aspects of uncertainty as related to the subsurface heterogeneity. While Figures 1.2 and 1.3 may provide one such interpretation of the system, often many alternative and competing interpretations are formed.

3. Data: several sources of data are available to constrain the models of uncertainty built. These data sources can be very diverse, from wells (driller's logs, well-log, cores, etc.) to geophysical (TEM data in the Danish case) or remote sensing measurements. Tying all this data into a single model of uncertainty without making too many assumptions about the relationships between various data sources is challenging.

From this case study, it is clear that some of the tools for modeling random phenomena through traditional probability models are too rigid to handle all these complexities. The nature of modeling uncertainty in the Earth Science has various challenge and issues that need to be addressed.

1. Modeling uncertainty is often application tailored. If the application changes then the type of modeling and the approach to modeling uncertainty will be different, hence the model of uncertainty will be different. Building a model of uncertainty that includes all possible aspects of what is uncertain is too difficult and often not needed in the first place. Modeling uncertainty for the sake of uncertainty is basically irrelevant as well as an impossible task. For example, if one is looking to quantify the global reserves of an oil reservoir, then the focus should be on the structural model and global parameters such as net-to-gross, while if the question is about drilling the next well, than the analysis should focus on local reservoir heterogeneity and connectivity of flow units.

2. Several sources of uncertainty exist for this case study:

a. Uncertainty related to the measurement errors and processing of the raw measurements.

b. Uncertainty related to the fact that processed data can be interpreted in many ways and, in fact, that data interpretation and processing require a model on their own.

c. Uncertainty related to the type of geological setting used, which is interpreted from data or based on physical models which themselves are uncertain.

d. Spatial uncertainty: even if data were perfectly measured, they are still sparse with respect to the resolution at which we want to build models. This means that various models with different spatial distributions of properties or layering structures can be generated matching equally well the same data.

e. Response uncertainty: this includes uncertainty related to how geological uncertainty translates into modeling of processes such as flow, transport, wave, heat equations or even decisions made based on such models. There may be uncertainty related to the physics of these processes or other parameters that need to be specified to specify these processes. For example, solving partial differential equations requires boundary and initial conditions that may be uncertain.

3. Uncertainty assessment is subjective: while a “true” Earth exists with all of its true, but unknown properties, there is no “true uncertainty.” The existence of a true uncertainty would call for knowing the truth, which would erase the need for uncertainty assessment. Uncertainty can never be objectively measured. Any assessment of uncertainty will need to be based on a model. Any model, whether statistically or physically defined, based on probability theory or fuzzy logic, requires implicit or explicit model assumptions (because of lack of knowledge or data), hence is necessarily subjective. There is no true uncertainty; there are only models of uncertainty, hence the title of this book.

4. High dimensional/spatial aspect: we are dealing with complex Earth systems that require a large amount of variables to describe them. Typically, we will work with gridded models to represent all aspects of the natural system. If each grid cell in a model contains a few variables, then easily we have millions of variables for even relatively small models. Standard approaches of probability become difficult to apply, since probability theory and statistical techniques common to most introductory text books has not been developed with these complex situations in mind. Often, it is necessary to perform some sensitivity analysis to determine which factors impact our decision most. Traditional statistical methods for sensitivity analysis are difficult to apply in this high dimensional and spatial context.

5. Several data sources informing various scales of variability: we will need to deal with a variety of data or information to constrain models of uncertainty. Without any data, there would be no modeling. Such data can be detailed information obtained from wells or more indirect information obtained from geophysical or remote sensing surveys. Each data source (such as wells) informs what we are modeling at a certain “volume support” (such as the size of a soil sample) and measures what we are targeting directly or indirectly, for example, electromagnetic (EM) waves for measuring water saturation.

Following this introductory chapter, this book covers many of these issues in the following chapters:

Chapter 2 Probability, Statistics and Exploratory Data Analysis: basically an overview of basic statistics and probability theory that is required to understand the material in subsequent chapters. The aim is not to provide a thorough review of these fields, but to provide a summary of what is relevant to the kind of modeling in this book.

Chapter 3 Modeling Uncertainty: Concepts and Philosophies: uncertainty is a misunderstood concept in many areas of science, so the various pitfalls in assessing uncertainty are discussed; also, a more conceptual discussion on how to think about uncertainty is provided. Uncertainty is not a mere mathematical concept, it deals with our state of knowledge, or lack thereof, as the world can be perceived by human beings. Therefore, it also has some interesting links with philosophy.

Chapter 4 Engineering the Earth, Making Decisions Under Uncertainty: the basic ideas of decision analysis are covered without going too much into detail. The language of decision analysis is introduced, structuring decision problems is discussed and some basic tools such as decision trees are introduced. The concept of sensitivity analysis is introduced; this will play an important role through many chapters in the book.

Chapter 5 Modeling Spatial Continuity: the chapter covers the various techniques for modeling spatial variability, whether dealing with modeling a rock type in the subsurface, the porosity of these rocks, soil types, clay content, thickness variations and so on. The models most used in practice for capturing spatial continuity are covered; these models are (i) the variogram/covariance model, (ii) the Boolean or object model and (iii) the 3D training image model.

Chapter 6 Modeling Spatial Uncertainty: once a model of spatial continuity is established, we can "simulate the