Development and Application of Computer Techniques to Environmental Studies VI

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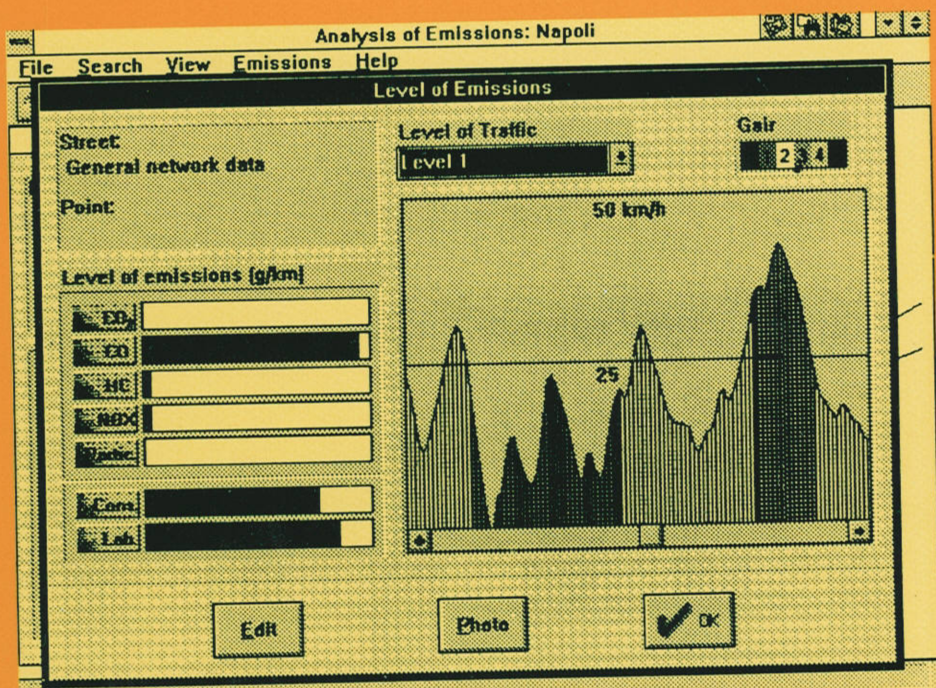

Computational Mechanics Publications

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Published by

Computational Mechanics Publications
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http://www.cmp.co.uk/

For USA, Canada and Mexico

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British Library Cataloguing-in-Publication Data

A Catalogue record for this book is available
from the British Library

ISBN: 1-85312-4117 Computational Mechanics Publications, Southampton

Library of Congress Catalog Card Number 96-083651

The texts of the various papers in this volume were set individually by the authors or under their supervision

Printed and bound in Great Britain by Antony Rowe Ltd, Chippenham.

KEYNOTE ADDRESS

Environmental modeling – the next generation

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Abstract

This chapter provides a brief introduction to that which will affect the next generation of computer systems for simulating environmental phenomena.

Keywords: Environmental modeling, pollution, computer simulation, numerical modeling, computer sciences, research and development, multimedia modeling, comprehensive modeling systems, virtual reality

1 Introduction

What should we call "environmental sciences"?

I recently proposed a definition of environmental sciences which seems to be acceptable to most of the scientists I interacted with (Zannetti, 1993).

> *Environmental sciences are defined as the sciences that cover, as their principal subject, anthropogenic pollution: its generation, its transport and fate in different environmental media (air, water, soil, groundwater, and biota), and its adverse effects.*

We could use a more general characterization, if you prefer, and define environmental sciences as that concerned with pollution, population control, and resource conservation. But I would resist the temptation of "contaminating" environmental sciences with the inclusion of controversial and ideological topics that better belong to the political and economic sciences and to the agendas of modern-day environmentalism.

One of the main challenges in environmental sciences today is to simulate environmental flows and the behavior of anthropogenic pollutants injected into them. This process is called "environmental modeling" and is performed today mostly by using computer simulation techniques.

Today environmental modeling software is still divided into two major fields. On one side we have relatively simple commercial products, mostly for regulatory applications, i.e., to help the industry in complying with environmental laws and regulations. On the other side, we have complex "research codes," developed at universities and research centers. Research codes are (in theory) more advanced but remain difficult to use. This dichotomy is expected to persist for a while, even though we should expect that within 5 to 10 years computers will become so user-friendly that even the codes developed for research and development (R&D) goals will be available to a larger segment of users.

Environmental phenomena remain a formidable scientific challenge. The simulation of environmental flows and the behavior of pollutants injected into them will remain a difficult task plagued by uncertainties in input parameters and always requiring some form of simplification of the "primitive" equations.

Soon the new generation of computer tools will provide models that will actually quantify the uncertainties of their own calculations. These models will not only supply forecasts and simulations, but they will provide the full probability density function of their outputs. People who use these simulations will receive "uncertainty intervals" that will allow them to better interpret the results.

2 To Model or Not to Model?

As a modeler, my interactions with the rest of the world have been complex and sometimes frustrating. In most cases, I have received gratifying and competent appreciation from my work with models and a fair understanding of what models can do. But in other cases things have been complicated. Often, in certain circles, I have found it difficult to explain what computer modeling is. This is because computer illiteracy in certain segments of the population, including mid-level and high-level business management, is still not uncommon today, despite the clear progress made during the last decade through the personal-computer revolution. In many cases, I faced a profound skepticism for the capabilities of environmental models.

Environmental modeling, like most things on earth, can be done perfectly or can be an example of "garbage in, garbage out." Most applications, of course, lie somewhere between these two extremes. It is difficult to define how a modeling application can be done perfectly, but I have tried to make a list of 10 conditions for what we can call "excellence in modeling":

1. The computer code must be fully tested, both as a whole and in its individual modules.

2. The code should be used by other groups, besides the developers, to assure external peer-review and approval.

3. The code should be fully documented. All equations and assumptions should come from formulations and methods published in peer-reviewed publications.

4. The input data should be reliable and pertinent to the specific application. The spatial and temporal resolution of the input data should be consistent with the time and space scales of the phenomenon that one wants to simulate.

5. The code should apply the best available science, e.g., by using full three-dimensional (3D) representations and avoiding the use of steady-state solutions to simulate time-varying phenomena.

6. The code should be numerically correct. That is, all iterative calculations should reach full convergence and results should not be affected by the size of the grid or the length of the integration time.

7. The code should be fully validated against reliable field data. This validation should include a careful evaluation of the physical significance of both the model outputs and the field measurements. For example, a comparison between model outputs on large spatial grids with point measurements can be phenomenologically incorrect.

8. Any calibration of the code should be done properly. Proper calibration means the tuning of some input parameters within their range of uncertainty in order to maximize the agreement between model outputs and field data. Calibration, however, is not proper when it ends up making the model work for the wrong reason!

   This has happened, unfortunately on several occasions in the past. A well-known example is the application of photochemical models to simulate ozone concentrations in urban areas. In the past, reaction rates in these photochemical models were "tuned" to allow the models to agree with the available measurements of ozone in the region. Later, it was discovered that the main model inputs, i.e., the emissions of VOC and NO_x in the region, were incorrect. That means that these models could be tuned to provide "correct" ozone concentrations with highly incorrect emission values of the ozone precursors. Therefore, what people called calibration in that case was just forcing the models to work for the wrong reason. Any practical application of these models, for example to calculate the emission reductions in VOC and NO_x required to achieve a certain predefined reduction of ozone concentrations in the region, was clearly incorrect.

9. The model application should be fully documented in a report presenting all assumptions and a description of all computer runs. The reader should be able to rerun the application on his computer and obtaining the same results in an independent manner.

10. In summary, use your brain, do it right, and do not cheat!

3 Environmental Modeling Tomorrow

This section presents a discussion of expected future developments in environmental modeling. Three factors are discussed: (1) the increasing use of multimedia models, (2) the current design and development efforts toward the creation of comprehensive modeling systems, and (3) the possible incorporation of virtual reality techniques into environmental models.

3.1 Multimedia Modeling

Traditionally, environmental models were designed to cover the dynamics of pollution in one particular medium, e.g., the atmosphere or a body of water. Recently, multimedia models have become necessary (Seigneur, 1993), since pollutants such as pesticides can migrate and be detected in different media. Conceptually, a multimedia model is not necessarily more complex than a model designed for a specific medium. However, multimedia simulations require a more extensive set of input parameters. They must include, for example, intermedia transport terms such as atmospheric deposition, sedimentation, volatilization, and erosion.

3.2 Comprehensive Modeling Systems

In the early 1990s, a few project teams, typically formed by environmental and computer scientists, explored the possibility of developing comprehensive modeling systems (CMS) for environmental sciences. In a nutshell, a CMS should include three major functions (Zannetti, 1993):

1. Education. The education section of a CMS should contain several modules designed for environmental education. These modules could typically cover six topics: the atmosphere, rivers and lakes, seas and oceans, soil and groundwater, human health, and environmental effects.

2. Simulation. The simulation section of a CMS should contain modules that simulate environmental phenomena and adverse effects of pollution. Results could be visualized by still images or animation. The simulation modules could cover ten topics: air, watershed, soil and groundwater, surface water, multimedia, indoor pollution, noise, human health, environmental damage, and environmental engineering.

3. Management. The management section of a CMS should contain several modules to assist the environmental manager and the environmental regulator. These modules could address eight topics: environmental information management, regulatory compliance, risk assessment, emergency response, pollution control, environmental remediation, litigation support, and literature search.

Much progress has been made recently toward the development of a CMS for air pollution (Hansen et al., 1994 and 1995; Dennis et al., 1996; Zannetti et al., 1996). These efforts are expected to be extended to other media in the near future. The air pollution CMS, as envisioned by its designers initially, should provide an infrastructure that helps its users do their jobs better and faster, whether those jobs be regulatory and policy analysis, source impact assessment, understanding atmospheric chemistry and physics, or performing atmospheric research studies. As such, this CMS should provide the following:

- A platform for modeling pollutant emissions, atmospheric physics and chemistry, and the impact of pollution in as scientifically sound a fashion as is desired or possible.

- A readily accessible interface, so that its use is a benefit, not a distraction.

- A powerful set of analysis and decision-support tools, including graphical, visual, economic, and scientific tools, and also including report preparation.

- A method to make maximum use of the available computational resources, including CPU power, disk storage, and communication systems.

The air pollution CMS is being designed in a way that facilitates its continuous evolution with science, computer capabilities, and user needs. This will require that it employ well-acknowledged standards (e.g., computer languages and data protocols).

Perhaps the best way to illustrate the CMS is to provide a realistic description of its future use:

> Palo Alto, 7 April 1999. A user sits in front of an Apple-IBM *Penta III* computer screen. The screen shows a stylish CMS logo and several other buttons. The user issues a voice command to the system, or clicks (with a foot mouse) the button *Beginners click here*, and a series of windows is displayed. These windows contain detailed information sections and an animated user's guide to describe the entire system. By clicking the button *Education,* the user brings up a new series of "windows" and "chapters." These sections are connected to CDs, laser disks, and multimedia devices and provide, on the *Penta III* screen, interactive education tools on the subjects of atmospheric sciences, air pollution, laws/regulations, simulation modeling, and databases. A special *Communication* button allows the user to communicate, via user-friendly interfaces, with library databases, meteorological/air quality databases, and other users.
>
> By clicking the *CMS Regulatory* button, the user accesses a subset of the CMS system in which only models and techniques that have received some regulatory approval are available. The use of these models is "locked," in the sense that they can only be used with computational options that are acceptable to the regulatory agencies. Regulations of different countries (USA, Canada, ECC, Japan, etc.) can be selected, thereby locking the execution of the simulations under different regulatory constraints. By clicking the *CMS full set* button, the user accesses the entire simulation system. Through a password and a voice recognition check, a user-developer is allowed access to the master version of CMS (in remote computer storage) and modify/add/update modules and functions.
>
> A typical CMS session consists of a CMS-guided computer simulation and "report" preparation. The user defines the computational domain, the simulation period, and other options. CMS assists the user in performing a sequence of simulations and making choices to calculate emission data, meteorological fields, transport and diffusion scenarios, chemical reactions, dry and wet deposition, and some adverse effects of air pollution, such as visibility impairment. Any step can be fully visualized by superimposing input/output data on geographical information using a

GIS and full 3D views (in a fly-through fashion). A special *Real-time* button allows real-time simulation for emergency response of accidental releases, if proper connections are made to access meteorological and other data on-line. At any time, the user can select input/output data and ask CMS to perform special calculations and analyses in different computational environments (such as new versions of *Mathematica*, *Spyglass*, *Systat*, etc.) on the *Penta III* screen.

What is described above illustrates the first and by far the most important goal of the CMS – to let the computer do the work. In the crudest sense, this means more complex and more sophisticated computations, but this is only the tip of the iceberg. Far more important is using the computer to compile, cross-reference, and comprehend intentions. The goal of the CMS is as much a manifesto as a plan; it is meant to be revolutionary, not incremental.

3.3 Virtual Reality

In the world of information sciences, two trends seem particularly relevant in the mid-1990s. The first trend is the increasing power of PCs (IBM-compatible and Macintosh-type machines). Internal PC clocks can now run at about 200 MHz providing very substantial computer power.

Many scientists have invested their time and resources heavily in Unix workstations in the last few years. This investment was certainly a smart move at the beginning of the decade, when it became clear that mainframe computers and supercomputers were not cost-effective in comparison with the new generation of Unix-based microcomputers. A similar phenomenon is occurring now. Scientists are discovering the increased power of the new generation of personal computers running under new, powerful operating systems such as IBM OS/2, Microsoft Win95/NT, and Apple OS. These new hardware/software platforms, and especially Microsoft NT, are expected to substantially erode the market for Unix workstations by providing high-speed, advanced features, user-friendliness, and inexpensive software for scientific calculations and simulations.

The second trend is virtual reality (VR). VR may appear frivolous in nature because of its close relation to interactive games and, therefore, its "arcade" connotation. But VR techniques appear to be the most interesting trend in computer software today.

VR has been defined as

> ". . . a computer-synthesized, three-dimensional environment in which a plurality of human participants, appropriately interfaced, may engage and

> manipulate simulated physical elements in the environment and, in some forms, may engage and interact with representations of other humans, past, present or fictional, or with invented creatures." (Nugent, 1991, quoted in Larijani, 1993)

and

> ". . . an interactive computer system so fast and intuitive that *the computer disappears from the mind of the user,* leaving the computer-generated environment as the reality." (Goldfarb, 1991, quoted in Larijani, 1993)

According to Goerbe (1992),

> ". . . virtual reality enables users to immerse themselves in computer-generated environments that include three-dimensionality through sound, sight, and touch."

Larijani (1994) simply describes VR as ". . . a cartoon world you can get into."

VR techniques cover two basic applications: (1) those in which the user puts on appropriate gadgets and enters an artificial world in which he or she manipulates objects in an interactive manner and (2) those in which the user observes and moves virtual humans operating in a virtual world.

VR techniques differ from multimedia tools. The reader should note that in this section the term "multimedia" has a different connotation. "Multimedia" here indicates the expansion of our communication capabilities and the inclusion of sounds, images, animations, and video. VR techniques employ multimedia tools and expand upon them. Thus, allowing an interaction between the user and "objects" in a virtual world. Examples of VR applications are some of the most sophisticated video games and some training techniques used by the military (for example, jet fighter simulations).

VR techniques are expanding rapidly. According to Martin (1994), the marketing firm Forst & Sullivan reported that the VR market is expected to exceed $1 billion in 1997, following a growth rate in which the market almost tripled from 1991 to 1993 (from $49.7 million to $130 million).

I expect VR techniques to become, within 10 years (and perhaps even 5), the *preferred* way in which any user interacts with any computer. To understand why, one must look at the history of the computer user interface. There we find a logical evolution: from primitive techniques such as punched cards and dumb terminals to today's microcomputer software, developed using object-oriented techniques and available to users through GUIs (graphical user interfaces). The next step is the use of 3D icons and, almost inevitably, the total immersion of the user in a 3D world – a VR world.

Clearly, the environmental modeling community will be affected, at least indirectly, by this trend. Certainly, the use and the development of environmental models will be influenced by the increasing availability of VR-based productivity tools. But the real question is how this trend will *directly* affect environmental scientists (Zannetti, 1995).

As discussed in Section 3.2, an important trend in environmental modeling today is the ongoing development effort directed toward "comprehensive" systems. These new air quality modeling systems are expected to be scientifically advanced, comprehensive (e.g., covering local, regional, and continental scales), easy to access and use, self-consistent, and computationally efficient. For example, a comprehensive modeling system (CMS), such as that described by Hansen et al. (1995), is expected to change the way people use air pollution models by allowing both scientists and nontechnical people to operate complex atmospheric simulations and run air pollution scenarios almost anywhere.

I would argue that the ultimate step in the development of environmental models – and probably the only step that can assure full user-friendliness and accessibility to nontechnical people – is the incorporation of VR techniques. After all, what is environmental modeling? Environmental modeling can be seen as an organized and interactive series of computational modules that transform one set of databases (emissions, human activities, meteorology, geography, etc.) into another set (concentrations, depositions, health damage, etc.) The more comprehensive environmental modeling systems become, the more users will be able to apply simulation techniques as black boxes, i.e., without necessarily understanding the details of the computations. Users, therefore, will be able to focus on exploring the relationships among the databases (inputs and outputs) and experimenting with changes without worrying about the computational details.

In less than 10 years, the use of environmental models may very well become a simple and entertaining VR exploration into databases. It may look like a video game, but it will incorporate the best of science. Manipulations of input databases (e.g., emissions) will automatically generate related changes in output databases (e.g., concentrations). Inverse calculations (e.g., the emission controls required to achieve predefined concentration standards) could be simply triggered by imposing a constraint on an object in the output database. It is not science fiction to envision a user wearing a VR device such as a helmet, entering a virtual database, walking through objects and their functional relationships, and performing direct and inverse simulations, analyses, and optimizations by simple manual operations on 3D objects. It will be like walking through a gigantic spreadsheet in which a single cell may contain the same number of calculations as one of today's air pollution models (e.g., 10^5 to 10^6 lines of FORTRAN code).

3.4 Conclusions

Clearly, at this point one can hardly guess to what extent CMSs and VR will figure into future environmental modeling studies. To forecast the evolution of computer systems and user needs is problematical, and one may easily be fooled by fashionable trends with no future. However, let me conclude this chapter with two pieces of advice to the reader. First, this is probably not the best time to make a big Unix investment – wait till 1997 if you can, and do consider NT as an alternative. Second, next time your kids go to the arcade and start playing with helmets and other gadgets, join them; you may develop very useful skills for the computer work that is awaiting you just a few years ahead.

Disclaimer

The opinions presented herein are those of the author alone and should not be interpreted as necessarily those of Failure Analysis Associates, Inc.

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