Report
on the Dagstuhl Seminar on
Modelling and Simulation of Complex Environmental Problems
October 2 - 6, 1995

The Dagstuhl Seminar on Modelling and Simulation of Complex Environmental Problems was organized by Greg R. Carmichael (University of Iowa), Granino A. Korn (Korn Industrial Consultants, USA) and Achim Sydow (GMD FIRST Berlin).

14 detailed lectures (some with included video demonstrations) and 3 short presentations were given by 24 participants from 9 countries. 10 participants came from Germany, 3 from the USA, 3 from Austria, 2 from Russia, 2 from Bulgaria and 1 from the Netherlands, Norway, Poland and Romania.

The participants appreciated the outstanding local organization and the beautiful environment including all Dagstuhl facilities which contributed not least to the success of the seminar.

REPORTED BY THOMAS LUX

Abstracts

The Current State and Future Directions in Simulating Tropospheric Chemistry and Transport

BY GREGORY R. CARMICHAEL

One of the challenges facing societies of the world during the next several decades is the effect of human activities on the environment. It now seems evident that global environmental change will be one of the more pressing international issues in the remainder of this century and the beginning of the next. Numerous environmental problems are linked to human-induced chemical perturbations on the atmosphere. Atmospheric phenomena such as acid deposition, increasing greenhouse gas concentrations, stratospheric ozone depletion, increasing incidences of urban and regional smog, are just a few examples. Over the next few decades difficult decisions will be made by policy-makers world-wide to deal with these issues.

Air quality models are an essential tool in studying and managing the environment. In this paper the limitations and challenges for future air quality models are discussed. A number of central improvements for the science modules are discussed, along with issues related to computational framework and computer resources.

The issue of sensitivity analysis is discussed in some detail. Comprehensive sensitivity analysis of air quality models remains the exception rather than the rule. However, the further improvement and use of such models requires that sensitivity and uncertainty analysis become an integral part of air quality modeling. New techniques associated with automatic differentiation offer many possibilities for realizing this goal. We discus the use of ADIFOR (Automatic Differentiation for FORTRAN) in the sensitivity analysis of comprehensive air quality models. ADIFOR performs differentiation by use of pre-compilers that analyze the code which augments the original code with derivative statements. The resulting derivatives are calculated accurately, optimally and requires no run-time support. results demonstrating the use of ADIFOR are presented and discussed.

Computer Aided Air Quality Control on Regional Scale

BY PIOTR HOLNICKI

In the paper an implementation of air pollution control strategy on regional scale is considered. Formulation presented is sulfur-oriented, and the approach relates to optimal funds allocation for emission reduction in a given set of major

power/heating plants located in the region. The formal problem statement is based on minimization of certain environmental cost function by the optimal choice of desulfurization technologies available. The total cost of emission abatement is considered a global constraint.

Linearity of air pollution dispersion process is assumed and the unit emission → deposition transfer matrices (averaged over the season) are preprocessed by a regional-scale transport model. Integral-type environmental cost index to be minimized, depends on the current deposition field and the area sensitivity function. Desulfurization cost of the technology applied is a sum of the investment and the maintenance components in all the controlled sources. Decision variable is an integer-type matrix that indicates the optimal assignment of reduction technologies to emission sources considered.

An heuristic, iterative optimization algorithm has been developed to solve the problem. It is based on the most effective allocation of funds to one of the sources in each iteration. The algorithm has been implemented for the optimal selection of (8) desulfurization technologies in the set of 20 major power plants located in Upper-Silesia Region in Poland. Selected computational results of this case-study are presented.

Parallelism, a key issue in future system modelling

BY LEN DEKKER

Parallel digital computing and simulation will have a great impact on the human society at large. It makes possible to realize simulation for much more complex systems and for large-scale applications in much more details, e.g. arising in ecology.

As a consequence a great change will happen in system modelling. Analysis and modelling of systems will be done in a very different way. Tracing the intrinsic parallelism of a system in the analysis phase and preservation of parallelism in all steps of the modelling phase as well as conservation of parallelism in the implementation phase will become a normal design rule. As a consequence for many types of systems the mode of description will change.

In the presentation some existing modes of system description have been analysed with regard to preservation of parallelism. A brief comparison was made between parallel analogue and parallel digital computation. Some simple examples of analysis and exploration of parallelism were presented like a given function of one variable and the solution of a 2nd order boundary problem formulated as a function of one variable by means of the function of Green. In both cases the execution of the functions evaluations can be done in parallel by means of the Single Program Multiple Data Programming model.

As a quite different example is considered the evaluation of an analytic function f(x,y) formulated as a four-point expansion of the partial derivatives of even order in the corner points of a rectangle. This explicit formulation opens the way to efficient parallel evaluation by means of the SPMD programming model. This 4-point expansion allows to solve linear distributed-parameter systems in a quite different way with much exploitable parallelism. A great advantage is that there is no need to discretize the independent variables.

To solve sets of linear equations two methods were presented: a direct method, called Minimal Norm method and a continuous iterative method. In the last method a set of linear equations is transformed in a set of unconditionally stable 2nd order systems having the required solution as steady-state. This set can be solved numerically in an efficient parallel and scalable way.

Modelling and Simulation of Pathophysiological Changes in the Human Lung Caused by Air Pollution

BY BERNHARD QUATEMBER

It is necessary to investigate the health effects of air pollution. Population studies of the damage caused by air pollution have to be carried out. In these studies, the initial stages in the development of chronic bronchitis play a decisive role. However, the initial stages cannot be assessed appropriately by using parameters obtained by performing classical lung function tests. We developed a simulation model that allows us to perform thorough investigations of the effects of the pathophysiological changes in these initial stages on breathing mechanics. Particular attention has to be given to the lining of the small airways with an excessive layer of secretion (mucus). The simulation results attained with our simulation model demonstrate the consequences of this pathophysiological manifestation. By carrying out a parameter identification procedure we are able to assess the severity of these pathophysiological changes. The method can be used in population studies and will allow a better evaluation of the health effects of airborne contaminants.

Self-Organizing Modelling - State and Further Development

BY J.-A.MÜLLER

Problems of complex object modelling can be solved by deductive logical-mathematical or by inductive sorting-out methods. Common used deductive methods have advantages in the cases of rather simple modelling problems, but there are several methodological problems. Efforts in using the known tools of artificial intelligence to solve these problems were in many cases not successful. That is why model-building is a subjective and creative domain. In this case

knowledge extraction from data, i.e. to derive a model from experimental measurements, has advantages in cases of rather complex objects. One development direction that takes account of practical demand represents the self-organization of mathematical models which is based on further development of statistical learning networks. Self-organizing modelling is based on statistical learning networks, which uses the black-box concept and the connectionism. Additionally there are used the inductive approach and the principle of external complement.

In the presentation there is given a comparison with the neural network approach in connection with their application to data analysis. In contrast to neural networks, the results of self-organizing modelling are explicit mathematical models, obtained in a relatively short time on the basis of extremely short samples. The well-known problems of an optimal (subjective) choice of the neural networks architecture are solved by means of an adaptive synthesis (objective choice) of the architecture. A priori information can be used directly to select the reference functions (which are derived from the systems theory) and criteria. In neural networks the a priori information must be transformed in the world of neural networks, but the rules of translation are not known. For ill-defined objects, with very large noise, better results should be obtained by selection of data sample clusterizations and analog complexing, particularly in the case, when the basic function of the object is not a polynomial one.

The GMDH type algorithm "SelfOrganize!" of DeltaDesign Software Berlin is a powerful software tool which makes use of the GMDH technique for modelling and prediction of complex linear or nonlinear multi input/multi output systems. The application field is decision support in economics (analysis and prediction of economical systems as well as for market, sales, financial predictions, balance analysis) and in ecology (analysis and prediction of ecological processes such as temperature of air and soil, air and water pollution, water quality, growth of wheat etc, drainage flow, Cl- and NO_3 - settlement, influence of natural position factors on harvest) but also in other fields with small a priori knowledge about the systems. As examples are represented

- analysis and prediction model for the distribution of COD concentration in the OSAKA BAY
- modelling the dependence of CL-discharge of seeping water and drainage outflow of selected parameters of the meteorological regime as well as the upper soil horizon, soil properties a.o.

The latest special issue of "Systems analysis modelling simulation" {SAMS vol. 20, No 1-2 (1995)} is dedicated to "Automatic model selection by means of self-organizing modelling", in which are published the scientific results of scientists from the USA, Germany, Ukraine, China, Japan and Russia.

Simulation of Complex Ecological Systems Using a Mathematical-Heuristic Model. Application to Danube Delta System

BY FLORIN STANCIULESCU

The mathematical - heuristic model of an environmental system is a hybrid model composed of several mathematical models, and heuristic models (derived from expert knowledge). An algorithm for simulation and control of environmental systems is presented, where the simulation is based on the mathematical model, while the heuristic model helps evaluate the new control variables (actings), able to reset the state variables into the suboptimality intervals. The architecture of the simulation and control system of environmental systems is also presented, using the simulation language Mathcad under Windows, and an expert system shell (TurboProlog). An application has been made in the case of a large scale hydrological complex of the Danube Delta, composed of 10 great lakes, interconnected by canals and channels. Each lake is characterized by means of 14 state equations: 4 describe the hydrological processes, 2 describe the hydro- chemical processes, and 8 describe the biological processes. A knowledge-base including 510 behavioral, control, and decision rules was set-up, based on the expert knowledge. Simulation and control experiments have been carried out using the mathematical-heuristic model, the simulation algorithm and program, and a 386 PC computer (IBM compatible). The simulation results show a good conformity with the measurements; it has been necessary in several cases to resimulate the system using new control variables (evaluated by the control module), in view to improve the evolution of some state variables.

The Bearing of Wiener's Cybernetics on the Ecological Problem

BY P. R. MASANI

The year 1994 was the birth centenary of Norbert Wiener, the father of cybernetics, and now is a propitious moment to recall its deep roots and its widespread ramifications.

A conception of the world in which time is reversible, and every event occurring now was determined at the time when the universe began is unrealistic in that it rules out the very concepts of purpose and purposive activity on which human life depends. The modern conception of the cosmos, emanating from scientific advances during the late 19th and early 20th centuries, is one in which time-reversibility and strict determinism are the exceptions rather than the rule. The cosmos is governed by strict laws, but these laws pertain not to individual events, but to the probabilities governing different classes of these events (stochastic cosmos or contingent universe).

Very briefly, cybernetics provides the scientific methodology with the new principles called for by the realization that universal time is irreversible and the cosmos is stochastic in its organization. The new principles pertain to the new concepts that temporal anisotropy and stochasticity allow, such as communication, control, self-regulation, teleology, self-organization and reproduction, and the absorption of mind into nature. An instance of the latter is the concept of the noosphere (or cerebral envelope) of the earth, due to Fr. Pierre Teilhard de Chardin.

The ecological thrust of cybernetics is the proposition that the noosphere, as a part of the earth, needs equal ecological concern and protection as the other terrestrial spheres. Among the pollutants of the noosphere have been the exploitative political economies that have controlled human society during the last 5000 years. Today, the pollution consists in the systematic misuse of the channels of communication by vested interests, the substandard schooling and entertainment, and the incumbent decline in intellectual, cultural and moral values.

Interactive Simulation of Neural Networks and Fuzzy Control Systems

BY GRANINO A. KORN

We describe true hands-on computer simulation of neural networks and fuzzy-logic controllers on small digital computers. Real experiments let you relate to neural-network models like no ordinary course of instruction. You can try classical learning algorithms or invent your own entirely new models. It is possible to interconnect several neural networks, and to simulate neural networks together with other dynamic systems like robots. DESIRE/NEUNET simulations represent neuron layers and connection-weight matrices by arrays of numbers which stand for neuron activations. Then statements like

VECTOR layer1 =3D input + bias
VECTOR layer2 =3D sigmoid(Weight * layer1)

define and manipulate models involving possibly thousands of neurons. The simple vector/matrix language handles nonlinear as well as linear neuron operations. Fuzzy-logic membership functions and rule tables are similarly created and manipulated for convenient simulation of fuzzy-logic control systems, which can be combined with neural networks and models of physical plants.

DESIRE admits scalar and/or vector differential equations entered in ordinary mathematical form, e.g.

d/dt x =3D k * sin(x) - r * xdot

and are automatically solved as model time proceeds. Once defined, complete neural networks can be invoked as submodels in larger simulations. You can combine different networks, and you can simulate neural networks together with models of control systems or physiological systems defined by differential equations or difference equations.

Our readable matrix notation is equally readable for your computer. The resulting simulations are dramatically more useful for research or teaching than conventional neural-network programs which only control a few canned algorithms with menus. What is more, execution is very substantially faster. Our simulation language is embedded in a complete, user-friendly environment for programming, display, and report preparation. Instructors can easily write their own neural-network courseware: new help screens and also "live", context-sensitive menus are simply user-written text files.

DESIRE stands for Direct Executing Simulation in Real time. An extra-fast run-time compiler translates screen-edited simulation-run programs so quickly that they appear to execute directly on a typed run command.

Parallel Computation and Simulation of Groundwater Flow

BY PETER-WOLFGANG GRÄBER

The simulation of processes in the soil and groundwater zone is one of the prerequisites for controlling and monitoring of such applications like pumping wells in water works or drainage systems in mines and building pits. The physical, chemical and biological processes proceeded in this connection are described mathematically by a system of partial differential equations (PDE). To solve the PDE it is necessary to solve equation systems of the form Ax =3D b. This is one "bottleneck" of fast and efficient simulation systems in the field of groundwater streams, too. Therefore we restrict to treat this part of simulation specially without neglect of general problem. In the last years among other the cg-method (conjugate gradients) including preconditioning became important to find fast and robust solving algorithms. So it arose algorithms that is suitable also for parallel treatment. The purpose of this work was to implement and test such an algorithm at the PARSYTEC-PowerXplorer. Apart from the numerical side of algorithm particularly the problems of parallelism were attended. This means the question of parallel model, communication and synchronisation. Moreover it was to clarify, if the application of the parallel computer is worth for the concrete problems of users. In the first section we will treat with some basics both hydrogeological and numerical natures. The second section is devoted to the parallel work and in the third section we will present our results as well as an outlook for points of contact on this project.

Aeroantigens and their Potential Usefulness in Ecological Analysis

BY V.P. CHEKHONIN (joint work with S.V. Lebedev, I.Ye. Gribova, O.I. Gurina, Yu.A. Zhirkov, Yo.V. Klinsky, R.V. Kudryavtsev, M.M. Ushakova and T.Yu. Dorodnydh)

Aeroantigens are permanently present in atmospheric air. They play a certain positive role in forming immune mechanisms of human ecological adaption in course of ontogenesis. Accumulation of aeroantigens in ventilation and air-conditioning systems (VACS) of inhabited industrial and municipal buildings may be used for a development of a real-life based model of antigenous influence on human health. From natural pollutant mixtures condensed in those systems we isolated a high-molecular component which proved to be able to provoke the formation of antibodies in experimental animals and in humans. This immunogenic substance is detectable in samples obtained from VACS located in various regions of Russia, and in aerosol samples of ground-level air in Moscow. This items of evidence suggested an idea of a new methodological approach to the problem of assessment of antigenous influence. This approach implies a quantitative determination of aeroantigens correlated with the observed sensitization levels in population and with morbidity rates in particular regions. With adequate mathematical methods, it would be possible to perform an ecological analysis, as well as to make a prognosis for the status of intrinsic ecological defense of inhabitants in regions with different urbanization degrees.

The Application of the Real-Time Dispersion Model SNAP to the European Tracer Experiment

BY JORGEN SALTBONES (joint work with Anstein Foss and Jercy Bartnicki)

The presentation consisted of three parts: 1. SNAP (Severe Nuclear Accident Program - a real-time dispersion model), 2. ETEX (the European Tracer EXperiment - DNMI's participation in an international programme for evaluation of real-time dispersion models), 3. a video presentation of the first ETEX release as simulated using SNAP.

1. SNAP

SNAP is a dispersion model with real-time capability, developed at DNMI. This model is a central tool for the decision makers in the Norwegian Preparedness Organization against Nuclear Accidents. The development of the model is part of the Norwegian application of MEMbrain (Major Emergency Management brain), an EUREKA project no. 507 (or 904). It started out of a cooperation between UK Meteorological Office and DNMI. Basic properties of SNAP are:

- type: Lagrangian particle model.
- advection: horizontal and vertical; 14 layers in the vertical, 50 km grid size in the horizontal.
- diffusion: random walk approach, vertical entrainment zone.
- dry deposition: selected particles in the Atmospheric Boundary Layer.
- wet deposition: all particles affected by rain.
- meteorological input: from DNMI's operational Numerical Weather Prediction Model (LAM50S and HIRLAM).
- hardware: Silicon Graphics platform.

The model is "tailor-made" for the situation of radioactive releases from a nuclear power plant anywhere in Europe. The model aims to answer the question: "Will our area of responsibility be affected ? When-where-and to what extent ?" The model is fully operational, which means that it can at any time be run (on request) by the meteorologist on duty. Output consists of concentration fields and deposition fields for chosen time intervals during the simulation period. The model can be run in both forecast-, hindcast (near past)- and mixed mode. During the presentation a selection of output examples were presented.

2. ETEX

ETEX is jointly managed and sponsored by CEC (Commission of the European Community), IAEA (International Atomic Energy Agency), and WMO (World Meteorological Organization). Most countries in Europe participated. The motivation for running this large-scale tracer experiment came from: Testing the dispersion models used in forecasting when the releases from nuclear accident might be transported. The objectives were:

- conduct an atmospheric tracer experiment (releases under well-defined conditions, coordinate atmospheric sampling up to 2000 km).
- notify institutes producing forecasts (test the capability of these institutes, evaluate their forecasts).
- assemble a database (source term data, meteorological data, measurement of concentrations).

DNMI participated using SNAP. Results from this simulations were shown, and also some preliminary results from comparison with measurements. A more fully evaluation will be presented at a workshop in Prague (21 - 23 October, 1995). Some concluding remarks: ETEX has been a success; both for the management side (fulfilled its aims) and from the participants (inspiration, competition, showcase, symbiosis from models and measurements).

3. Video

A video was presented for the first ETEX release with simulations using SNAP. Such a video presentation is very instructive to see the complex interactions of transport processes on different scales interact. It also shows a more complete picture of the transport and also the limitation of e.g. trajectory analysis. But for quantitative measures print out of fields is more useful.

Modelling and Simulation of Air Pollution

BY ACHIM SYDOW (joint work with Thomas Lux)

The author presented results of scenario analyses by means of an air pollution simulation system developed at GMD FIRST in order to support users in governmental administrations and industry in operative decision making (smog management) as well as short to long-term regional planning. The components of the simulation system are parallelly implemented simulation models for meteorology, transport, and air chemistry, data bases for model input and simulation results, as well as a graphic user interface for data visualization in spatial relations. By means of this system end-users can carry out scenario analyses for winter smog, summer smog, and antigenous air pollution. The influence of emission reduction measures such as the use of other fuels for power plants and heating, the building of new roads, the closure of parts of a city for groups of vehicles, speed limits, etc can be studied. Results were presented from two recent applications. On behalf of the environmental department of the state government of Berlin and the ministry for environment of the state Brandenburg summer smog analyses were performed concerning the duration of the measuring campaign FLUMOB in July 1994. On behalf of Greenpeace the influence of emissions caused by traffic in Munich on the ozone concentration in the Munich area was analyzed for a typical midsummer day in 1994. The performed scenario analysis were based on statistical input data of traffic emissions. To improve the quality of simulation results and to allow a more detailed assessment of the consequences of traffic control measures and general urban planning issues the traffic emission data should be calculated dynamically. To this aim a new complex model system for the simulation of traffic flow, traffic emissions and air pollution dispersion is under development at GMD FIRST basing on the air pollution simulation system already in use.

A video was presented showing visualized simulation results of the last summer smog analysis for the region of Berlin/Brandenburg.

Integrated Assessment of Strategies to Reduce Air Pollution

BY MARKUS AMANN

The RAINS model has been developed as a tool to enable the integrated assessment of strategies to reduce air pollution. Originally focussing on acid deposition, the model follows the pathways of emissions of sulfur dioxide, nitrogen oxides and ammonia from their sources, their options for controlling them and the associated costs over the atmospheric dispersion processes to the impacts emissions have on the environment. The model can be operated in the 'scenario analysis' mode to explore costs and regional environmental benefits of user-specified emission control strategies, and in the 'optimization mode' to

identify the cost-minimal allocation of measures in order to achieve specified environmental targets. The RAINS model has been used in the negotiation process leading to the Second Sulfur Protocol under the Convention on Long-range Transboundary Air Pollution.

The model is being further developed to assess strategies to reduce tropospheric ozone in Europe. For this purpose, modules are developed to describe emissions and control costs of VOC emissions and to represent source-receptor relationships between the precursor emissions and regional ozone levels. Based on numerous runs of the EMEP ozone model developed at the Norwegian Meteorological Institute, a statistical analysis has identified a polynomial function which describes changes of long-term ozone concentrations in response to changes of the precursor emissions. To generate the comprehensive data sample of EMEP model results, the EMEP model has been transformed to parallel computing at GMD-FIRST.

Work has succeeded in developing a non-linear optimization scheme for the ozone model, which enables the design of cost-effective solution to reduce tropospheric ozone in Europe.

Environmental Modeling and Simulation - Some Features of Experiments

BY ROLF GRÜTZNER

Up to now the state of the environment has been changed by human activities ina dramatic and dangerous way. This situation must be stopped as soon as possible. Therefore we need innovative theoretical and practical scientific approaches.Consequently, there are to solve many research tasks in different fields to overcome these problems. We have to strengthen activities in:

- investigation of environmental systems
- in getting better system models (structure adequate models)
- in developing better simulation software
- and we have to strengthen the effort in developing and using of experiment descriptions to execute complex simulation experiments for planning and decision.

In the paper only the last task has been considered. It is proposed an experiment description language based on the separation of model and experiment description. An experiment description means a description of an algorithm which uses the model to realize the experimentation goal. The experiment description has been developed to describe complex experiments in a simulation system environment. That means multi model use, parallel and distributed experiment description.

The experiment may be defined either by a language form or interactive. Architectures of simulation systems which control runs of such experiments are

represented. Important is the introduction of an experiment protocol to record all the activities of a user during the experiment runs.

This is a report of some results of the research project SAMEC, granted by the German Research Society (DFG).