“Open” problems and plans for future research work

1. *Data assimilation*
2. *Optimization problems in environmental studies*
3. *Inverse problems*
4. *Local refinement*
5. *Object oriented codes*
6. *Final comments about this course*
7. *References*

General discussion of the data assimilation approach

- The use of data assimilation can be considered as applying a sequence of corrections of the results (or some part of the results), which is performed at successive times during the treatment of the model
- Each correction combines an appropriate field of model results with the available set of measurements (in most of the cases)
- Different applications: (a) to improve the initial conditions, (b) to improve the deposition rates, (c) to improve the emission rates and (d) to improve the output concentrations
- This approach has successfully been used in the meteorology, but it is relatively new in the environmental modelling
- The EURAD group in Cologne (Germany) is a leading group in this field

The method used before the data assimilation approach

- Optimal analysis or optimal interpolation
- Provides a simple and internally consistent procedure for treating a large number of observations with different distributions, nature and accuracy
- Takes into account the dynamics of the meteorological processes only indirectly
- The method of optimal control (J. L. Lions, 1971) is taken into account in the data assimilation approach
- The theory of optimal control deals with the problem of finding how the output parameters of a given mathematical model can be controlled by acting on the input parameters of the model

Major implementation principles

- Assume that the initial value field is to be improved
- The initial values are considered as control parameters
- A special function, the distance function, is defined. This function provides weighted and accumulated distances between available measurements and the corresponding state variables calculated by the model during a predefined data assimilation window
- Important: An optimization procedure has to be applied to minimize the distance function
- Adjoint equations are to be derived and used in order to calculate some local gradients of the distance function, which are needed in the optimization procedure
- Four-dimensional variational data assimilation

Definition of the distance function

$$\frac{dx}{dt} = M(x), \quad x \in \aleph,$$

x – some state variable,

$\aleph$ – some Hilbert space,

M – some non – linear operator

$$Z(x(t)) \stackrel{def}{=} \frac{1}{2}\left(x_{meas}(t) - x(t)\right) O^{-1} \left(x_{meas}(t) - x(t)\right)$$

$$\Im(x(t)) \stackrel{def}{=} \int_{t_0}^{t_N} \left[Z(x(t)) + \left\langle \lambda(t), \frac{dx(t)}{dt} - M(x(t)) \right\rangle \right] dt$$

Calculating the gradient of the distance function

$$\frac{d(\delta x)}{dt} = M'(\delta x) \quad \text{perturbation (variational) equation}$$

δx some "small" deviation of x

M' the tangential (linear) operator of x

$$g_1 = \left\langle \lambda(t), \frac{dx(t)}{dt} - M(x(t)) \right\rangle$$

$$g_2 = \left\langle \delta\lambda(t), \frac{d(\delta x(t))}{dt} - M'(\delta x(t)) \right\rangle$$

$$\delta \Im \overset{def}{=} \int_{t_0}^{t_N} \left[\langle \delta Z, \delta x(t) \rangle + g_1 + g_2 \right] dt \quad \text{variation of } \Im$$

$$-\frac{d\lambda(t)}{dt} - M'^{*}\lambda(t) = O^{-1}\left[x_{meas}(t) - x(t) \right] \quad \text{adjoint equation}$$

Calculating approximations of the distance function and its gradient at certain grids

Forward step :

Calculate approximations of x and $\ddot{a}x$

at $t = t_1, t_2, ..., t_N$ by solving numerically

$\frac{dx}{dt} = M(x)$ and $\frac{d(\delta x)}{dt} = M'(\delta x)$

Backward step :

Use the adjoint equation to obtain approximations

of $\lambda(t)$ at $t = t_{n-1}, t_{N-2}, ..., t_0$ starting with $\lambda(t_N) = 0$

The values of x are used to calculate approximations

of $\Im$, while the values of δx and λ are used to

calculate approximations of $\delta\Im$

Minimization procedure in the data assimilation approach

- The values of the distance function and the values of the gradient of the distance function are used in the minimization procedure
- The Broyden-Fletcher-Goldfarb-Shanno algorithm is often used
- Constraints are needed in order to ensure non-negative solutions (Bertsekas, 1982)

Advantages and disadvantages of the data assimilation approach

Adavantages

- The model results might be improved when the data assimilation approach is used

Disadvantages

- The application of the data assimilation approach leads to a very considerable increase of the computer time
- There are difficulties with missing observations
- The selection of representative measurements might be a problem

Keeping the concentrations in a given sensitive area under some prescribed level

- The problem can be considered as an optimal planning in the efforts to achieve sustainable development.
- An example:

$c(x, y, t) \leq C$ when $(x, y) \in \Omega$

An emission source $E(t)$

must be located somewhere in Ω

Find $\omega \subset \Omega$ where $E(t)$ can be

can be located so that $c(x, y, t) \leq C$

is still satisfied

The problem can be solved by introduction of adjoint equations. Only rather simple cases have been studied until now.

Inverse problems

1. Reduction of the emissions in order to keep pollution levels under prescribed critical levels
2. Where to reduce the emissions and by how much to reduce them?
3. One should be very careful when the inverse problem is defined mathematically (it is not easy to ensure existense of the solution)
4. The problems have not been formulated and treated for the general case

Local refinement

Dynamical local refinement:

- A. Tomlin and M. Berzins (Leeds)
- Applied in sub-areas where large gradients of some concentrations are observed

Static local refinement:

- One way nesting (Cologne, Germany)
- Two-way nesting (CWI, Amsterdam)
- Non-equidistant meshes combined by finite element approximation (Antonov in an object-oriented code)

Object oriented codes

- The structure of the code is in general improved during the preparation of an object oriented code
- More advanced programming tools can be used
- Flexibility (one can easily change numerical methods, physical mechanisms, etc.)
- Based mainly on c++
- It is easy to introduce local refinement

A. Antonov (2002)

General on Environmental Modelling

Multidisciplinary field:

- Physics
- Meteorology
- Chemistry
- Numerical Mathematics
- Scientific Computing
- Statistics
- Data handling
- Advanced graphical tools are absolutely necessary

Typical feature: the problems are very big when all relevant physical processes are adequately described in the models

Numerical algorithms

- Solution of systems of linear algebraic equations
- Solution of non-linear system of algebtraic equation
- Solution of systems of ODEs (stiff and non-stiff)
- Solution of systems of PDEs
- Optimization problems
- Monte Carlo methods
- Inverse problems

Most fascinating features

- Improvements are needed in many parts of the models
- There are a lot of open problems
- The requirements to the models are permanently increased

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Istvan Farago has some new investigations in this field

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