Computational and Numerical Challenges in Environmental Modelling

Zahari Zlatev

National Environmental Research Institute

Frederiksborgvej 399, P. O. Box 358

DK-4000 Roskilde

e-mail: zz@dmu.dk

http://www.dmu.dk/AtmosphericEnvironment/staff/zlatev.htm

http://www.dmu.dk/AtmosphericEnvironment/DEM

Contents of the course

- General discussion of the **systems of PDEs** arising in environmental modelling and the justification of the need of high-speed computers
- Use of **splitting** techniques in the numerical treatment of the models
- Treatment of the **advection (the horizontal transport) part** in an environmental model
- Treatment of the **chemical part**: general ideas and major numerical methods used in this sub-model
- **Partitioning** the ODE systems describing the chemical reactions

Contents of the course: continuation

- Optimizing the **matrix computations** (types of the matrices arising in different parts of an environmental model)
- **Parallel computations**: need for parallel computations and major requirements (standard tools + portability). Use of templates
- Discussion of some typical **applications** related to different environmental studies
- Impact of **future climate changes** on **high pollution levels**
- **Open problems** and plans for future research efforts

General discussion of the models

1. ***Why** environmental modelling?*
2. ***Major** physical and chemical processes*
3. ***Mathematical** description of the processes*
4. ***Need** for splitting*
5. ***Computational** difficulties*
6. ***Need for faster and accurate algorithms***
7. ***Different matrix computations***
8. ***Inverse and optimization** problems*
9. ***Unresolved** problems*

Great environmental challenges in the 21st century

1. *More detailed information about the pollution levels and the possible damaging effects*
2. *More reliable information (especially about worst cases)*

How to resolve these two tasks?

Models vs measurements

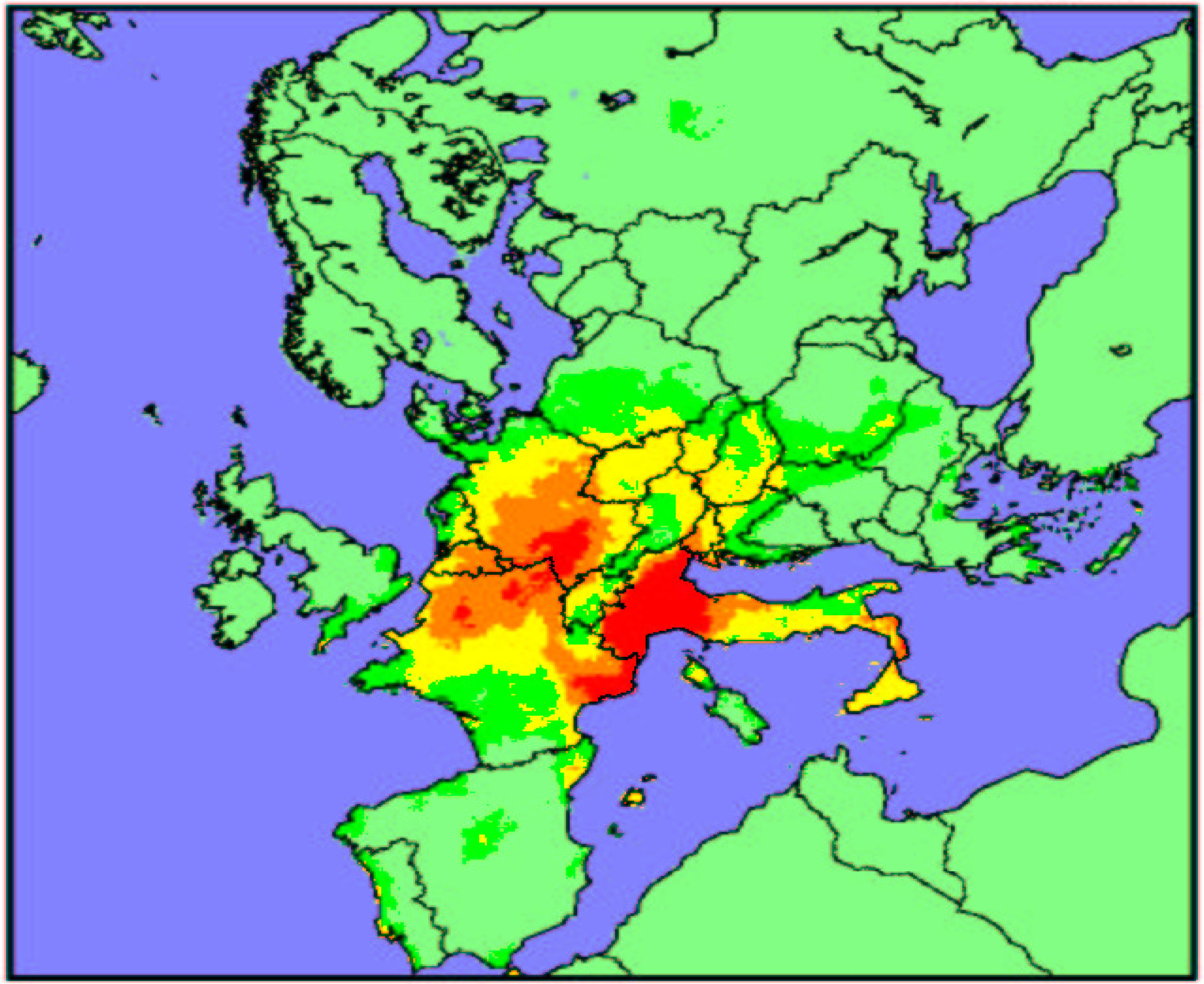
1. Why environmental models?

- **Distribution** of the pollution levels
- **Trends** in the development of pollution levels
- Establishment of **relationships** between pollution levels and key parameters (emissions, meteorological conditions, boundary conditions, etc.).
- **Predicting** appearance of high levels

EXPOSURE TO HIGH OZONE CONCENTRATIONS

Numbers of days in which 8–hour rolling averages
of ozone concentrations exceeded 60 ppb.
The fine resolution version of DEM (480x480).
Anthropogenic emissions for 1995 are used.
Maximum value in the domain: 72

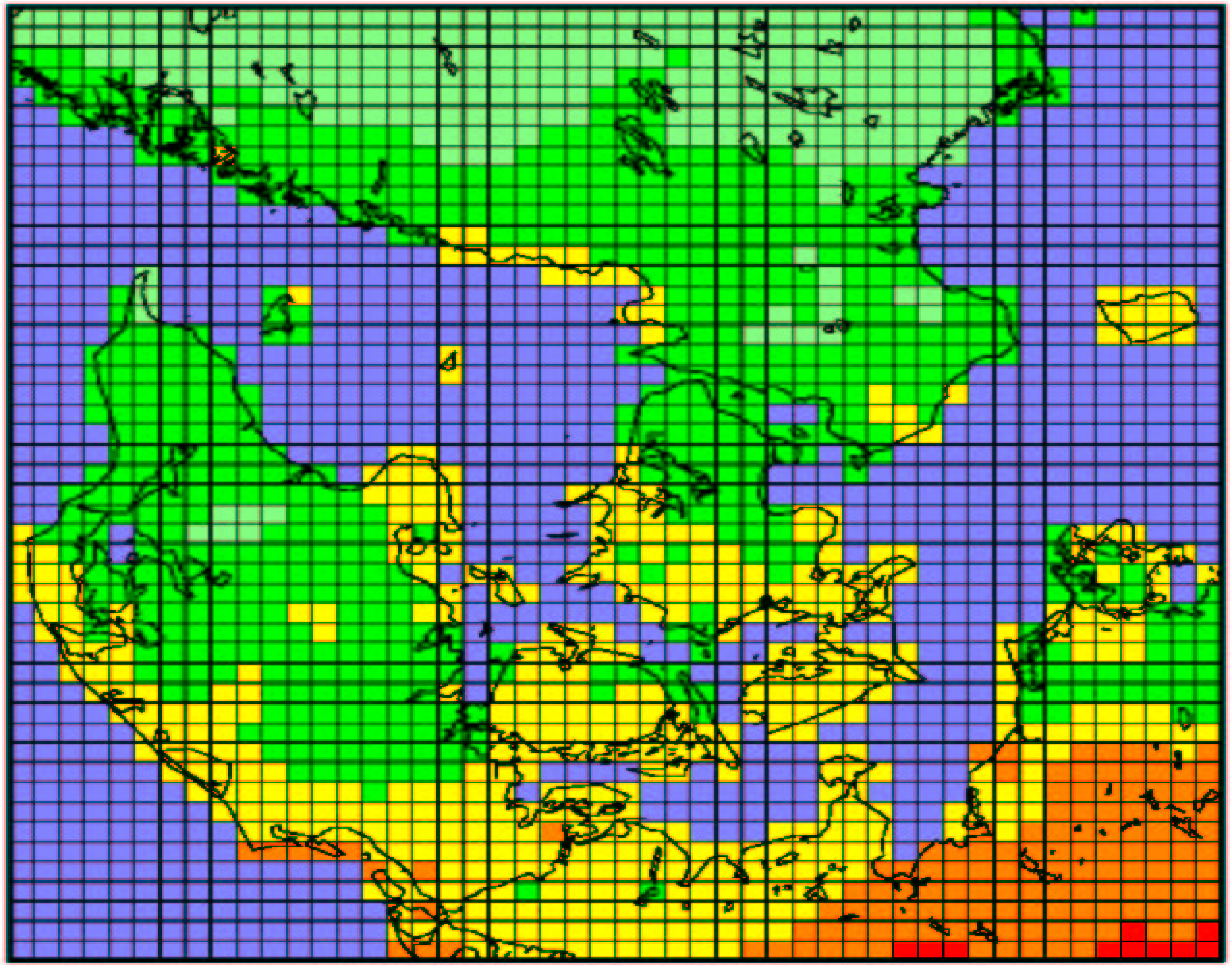
Above 40
31 – 40
21 – 30
11 – 20
0 – 10
Water areas

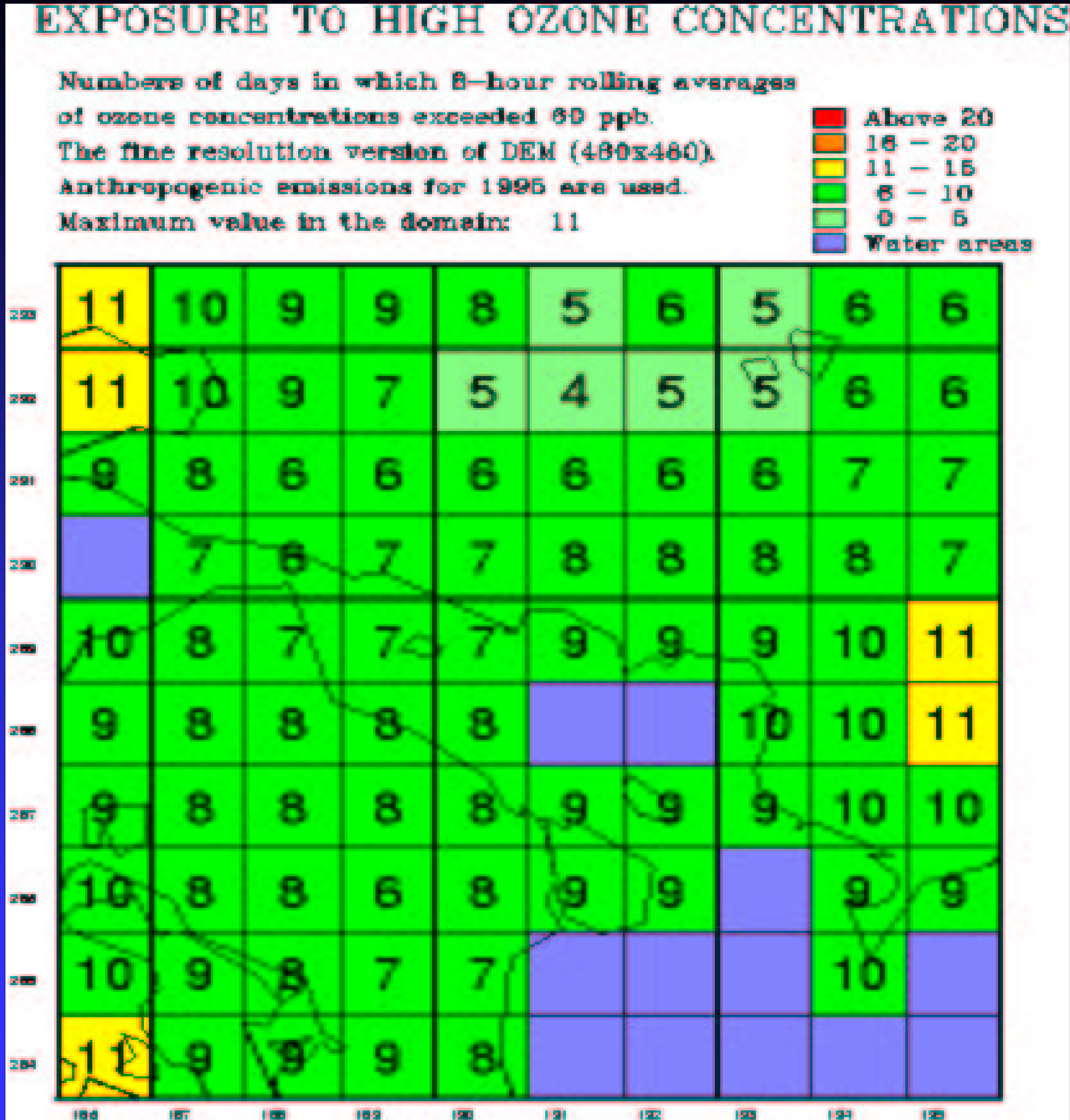


EXPOSURE TO HIGH OZONE CONCENTRATIONS

Numbers of days in which 8-hour rolling averages
of ozone concentrations exceeded 60 ppb.
The fine resolution version of DEM (480x480).
Anthropogenic emissions for 1995 are used.
Maximum value in the domain: 23

- Above 20
- 16 – 20
- 11 – 15
- 6 – 10
- 0 – 5
- Water areas




EXPOSURE TO HIGH OZONE CONCENTRATIONS
Numbers of days in which 8-hour rolling averages
of ozone concentrations exceeded 80 ppb.
The fine resolution version of DEM (480x480).
Anthropogenic emissions for 1995 are used.
Maximum value in the domain: 11
Above 20
16 – 20
11 – 15
6 – 10
0 – 5
Water areas
11 10 9 9 8 5 6 5 6 6
11 10 9 7 5 4 5 5 6 6
9 8 6 6 6 6 6 6 7 7
7 6 7 7 8 8 8 8 7
10 8 7 7 7 9 9 9 10 11
9 8 8 8 8 10 10 11
9 8 8 8 8 9 9 9 10 10
10 8 8 6 8 9 9 9 9
10 9 8 7 7 10
11 9 9 9 8

2. Major physical processes

- **Horizontal transport** (advection)
- Horizontal diffusion
- Deposition (dry and wet)
- **Chemical reactions** + emissions
- **Vertical transport and diffusion**

Major task: Describe these processes mathematically and unite the resulting mathematical terms in a model

3. Mathematical Models

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y}$$ hor. transport

$$+\frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right)$$ hor. diffusion

$$-(k_{1s} + k_{2s})c_s$$ deposition

$$+E_s + Q_s(c_1, c_2, \ldots, c_q)$$ chem. + emis.

$$-\frac{\partial (wc_s)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s}{\partial z}\right)$$ vert. transport

$$s = 1, 2, \ldots, q$$

4. Need for splitting

- Bagrinowskii and Godunov 1957
- Strang 1968
- Marchuk 1968, 1982
- McRay, Goodin and Seinfeld 1982
- Lancer and Verwer 1999
- Dimov, Farago and Zlatev 1999

- Zlatev 1995

4. Criteria for choosing the splitting procedure

- **Accuracy**
- **Efficiency**
- **Preservation of the properties of the involved operators**

5. Resulting ODE systems

$$\frac{d g^{[i]}}{dt} = f^{[i]}\left(t, g^{[i]}\right) \qquad 1 \le i \le m,$$

$$g^{[i]} \in \Re^{N}, \qquad m > 1,$$

$$f^{[i]} \in \Re^{N},$$

$$N = \left(NX \times NY \times NZ\right) \times NC.$$

6. Size of the ODE systems

- (480x480x10) grid and 35 species results in ODE systems with more than 80 mill. equations (8 mill. in the 2-D case).
- More than 20000 time-steps are to be carried out for a run with meteorological data covering one month.
- Sometimes the model has to be run over a time period of up to 10 years.
- Different scenarios have to be tested.

7. Matrix Computations

- Fast Fourier Transforms
- Banded matrices
- Tri-diagonal matrices
- General sparse matrices
- Dense matrices

Typical feature: The matrices are not large, but these are to be handled many times in every sub-module during every time-step

8. Major requirements

- Efficient performance on a single processor
- Reordering of the operations

What about parallel tasks?

"Parallel computation actually reflects the concurrent character of many applications"

D. J. Evans (1990)

9. Why is a good performance needed?

Non-optimized code, one month simulation: about 5.4 hours
Ten-year run, one scenario : about 27 days
24 scenarios with biogenic emissions : about 22 months

Grid	Comp. Time
(96x96)	about 14.4 days (speed-up: 45.8)
(288x288)	about 196 days (one scenario 8.2 days)

IBM *"Night Hawk"* (2 nodes); NSIZE=48

10. Other challenges

- Need for optimal solutions
- Treatment of inverse problems

Open questions