Long range air pollution transport over Europe, studied on the Grid

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- **Introduction**

- **Mathematical description of the problem**

- **Splitting into submodels**

- **Discretisation of the domain**

- **Numerical treatment of the submodels**

- **Experiments on the EGEE Grid**

- **Results and some important applications**

- **Conclusions**

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- **Subject: The concentrations of dangerous pollutants in the air, their transformations, transport and deposition**

- **Aims: To represent as close as possible to the reality the main physical and chemical processes as follows:**
  - horizontal and vertical wind,
  - diffusion,
  - chemical reactions,
  - emissions,
  - depositions, etc.

- **Application areas:**
  - Studies of environment status, trends and conditions
  - Human health protection
  - Economical impact of the pollution level to the crops production
  - Forestry and wild life protection
  - Global climate changes

$$\frac{\partial c_s}{\partial t} = -\frac{\partial(uc_s)}{\partial x} - \frac{\partial(vc_s)}{\partial y} - \frac{\partial(wc_s)}{\partial z}$$

$$+ \frac{\partial}{\partial x}\left(K_x\frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c_s}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c_s}{\partial z}\right)$$

$$+ E_s + Q_s(c_1, c_2, \ldots c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots q .$$

- c_s – **the concentrations**
- u, v, w – **the wind components along the coordinate axes**
- K_x, K_y, K_z – **diffusion coefficients**
- E_s – **the emissions**
- k_{1s}, k_{2s} – **dry / wet deposition coefficients**
- $Q_s(c_1, c_2, \cdots c_q)$ – **non-linear functions, describing the chemical reactions between the species**

- **Advection submodel:**

$$\frac{\partial c_s^{(1)}}{\partial t} = -\frac{\partial(u c_s^{(1)})}{\partial x} - \frac{\partial(v c_s^{(1)})}{\partial y}$$

- **Horizontal diffusion:**

$$\frac{\partial c_s^{(2)}}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial c_s^{(2)}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s^{(2)}}{\partial y}\right)$$

- **Chemistry & emissions:**

$$\frac{\partial c_s^{(3)}}{\partial t} = E_s + Q_s(c_1^{(3)}, c_2^{(3)}, \ldots c_q^{(3)})$$

- **Depositions:**

$$\frac{\partial c_s^{(4)}}{\partial t} = -(k_{1s} + k_{2s}) c_s^{(4)}$$

- **Vertical transport*:**

$$\frac{\partial c_s^{(5)}}{\partial t} = -\frac{\partial(w c_s^{(5)})}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s^{(5)}}{\partial z}\right)$$

Discretisation of the spatial domain

- **Size of the domain: 4800 x 4800 km. .**
- **Covers whole Europe, the Mediterranean, neighbouring parts of Asia, Africa and the surrounding waters.**
- **Uses the EMEP grid and subgrids compatible with it.**
- **Finer grid requires smaller time-step for stability reasons.**

Resolution	Step	Size	Number of cells	
			2D version	3D version
Coarse	150 km.	(32 x 32)	1024	10240
Medium	50 km.	(96 x 96)	9216	92160
Fine	16.5km.	(288 x 288)	82944	829440
Extra fine	10 km.	(480 x 480)	230400	2304000

- **Advection-diffusion part: Finite elements, followed by predictor-corrector schemes with several different correctors (Zlatev - 1984)**

- **Chemistry-deposition part: An improved version of the QSSA (Quazi Steady-State Approximation) (Hesstevedt et al. - 1978)**

- **Vertical transport: Finite elements, followed by Theta – methods**

For more details about the numerical methods, see (Alexandrov et al. – 1995)

- **A number of 1-year experiments with important applications has been carried out on the Grid.**

- **The 2D and 3D versions with medium resolution grid (96 x 96) are used in these experiments, and the chemical scheme with 35 species.**

- **The tasks for the same DEM version differ with respect to the following parameters:**

  § The year of calculation (different meteorology, emissions and calendar data)

  § Different emission data for one and the same year (for example, reduction in traffic emissions by some percent, etc.). Used in studies of different scenarios of emissions, subject to control.

  § Perturbation of some reaction coefficients (internal parameters of the model) for the same input data. This is to be used in sensitivity analysis of the model and possible improvement of the chemical scheme.

Grid site address	Run time of medium-size DEM [sec]	
	2D version	**3D version**
atlasce01.na.infn.it	11295	116284
cclcgceli01.in2p3.fr	33764	338923
ce.grid.tuke.sk	21011	212464
ce.hep.ntua.gr	20806	210355
ce.phy.bg.ac.yu	25932	260971
ce001.grid.bas.bg	20445	205847
ce01.ariagni.hellasgrid.gr	17589	178325
ce01.isabella.grnet.gr	25875	260107
ce01.kallisto.hellasgrid.gr	17602	178456
ce01.marie.hellasgrid.gr	17367	174922
ce02.marie.hellasgrid.gr	18205	183826
grid012.ct.infn.it	35874	360643

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Grid site address	Run time of medium-size DEM [sec]	
	2D version	3D version
grid10.lal.in2p3.fr	13922	141518
gridba2.ba.infn.it	23669	238795
gridgate.cs.tcd.ie	21135	212450
griditce01.na.infn.it	23320	235679
helmsley.dur.scotgrid.ac.uk	28712	288635
hudson.datagrid.jussieu.fr	31286	315094
lcgce01.gridpp.rl.ac.uk	19356	195224
mu6.matrix.sara.nl	18270	184827
polgrid1.in2p3.fr	18531	186448
prod-ce-01.pd.infn.it	19118	191793
tbn20.nikhef.nl	18224	184021
testbed001.grid.ici.ro	24990	251806

- **Several important application areas require a large number of experiments like those in the previous tables. Some of them will be shown in the next slides.**

- **Ozone is one of the most dangerous pollutants, harmful both to humans, animals and plants.**

- **It is not only the peak concentration valuable, but also several functions, related to the exposure should be calculated in order to evaluate its effect.**

- **Ozone participates in many reactions with other valuable pollutants, which should be also taken into account (nitrogen oxides, carbon monoxide, etc.)**

O_3 concentrations in ppb for July 1998 (basic)

> 60
50 - 60
40 - 50
30 - 40
< 30
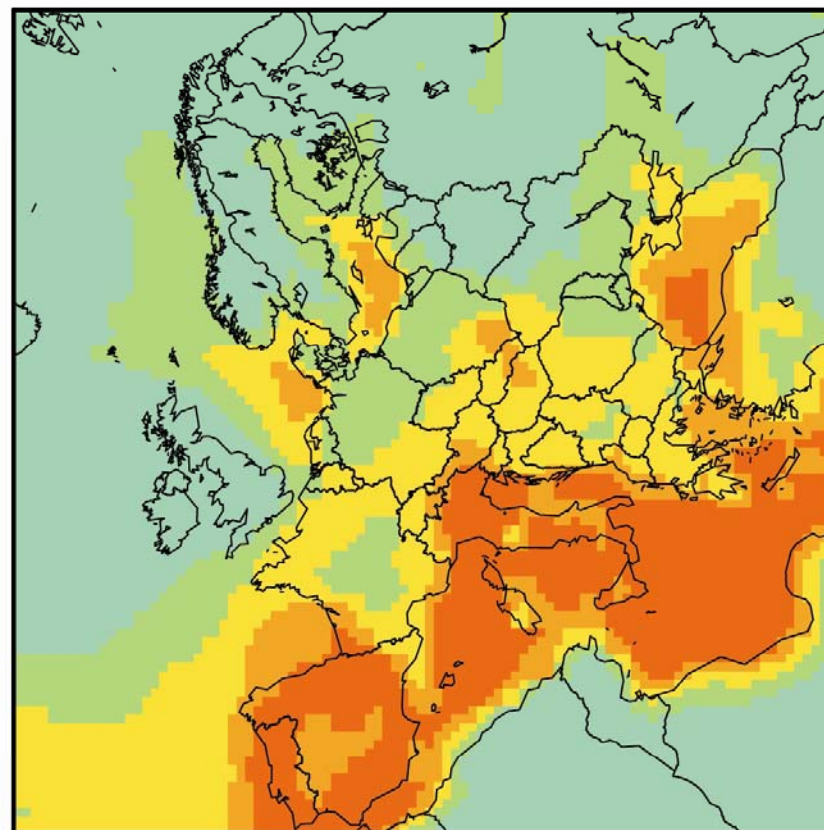
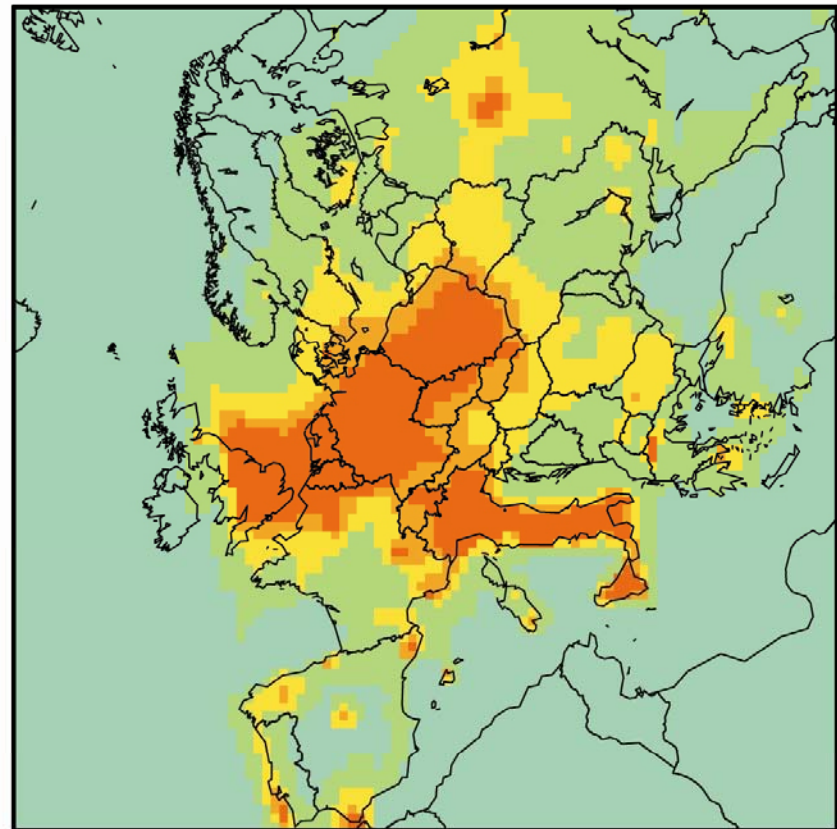NO concentrations in ppb for July 1998 (basic)

> 1.0
0.75 - 1.0
0.5 - 0.75
0.25 - 0.5
< 0.25
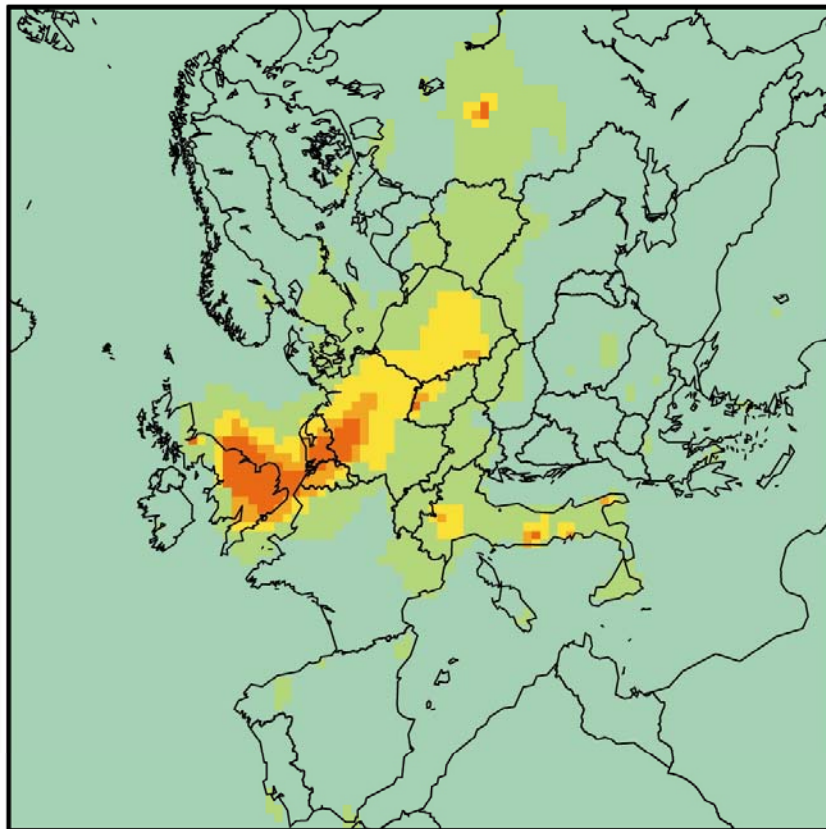
NO₂ concentrations in ppb for July 1998 (basic)

> 4
3 - 4
2 - 3
1 - 2
< 1

- **Long-term exposure to high ozone concentrations have harmful effect on the crops and reduces the yield. The crops are particularly sensitive to the ozone during the vegetation period (May – July).**

- **The exposures are measured in terms of AOT40 (Accumulated exposure Over Threshold of 40 ppb).**

- **As a result of many open-chamber experiments a critical level of 3000 ppb.hours has been established for the crops.**

- **Similarly the exposure to high ozone concentrations is harmful for the trees as well, with somewhat extended period of high sensitivity (April – September).**

- **The critical level for the trees (in this extended 6-month period) is respectively 10000 ppb.hours .**

AOT40C (for crops)
in % [100(AOT40C)/3000]
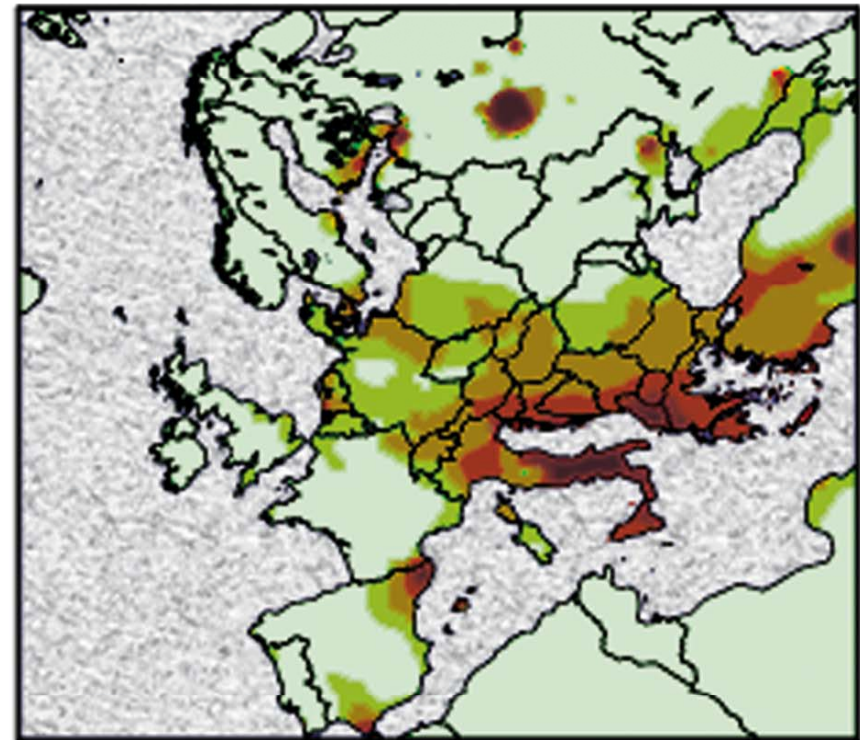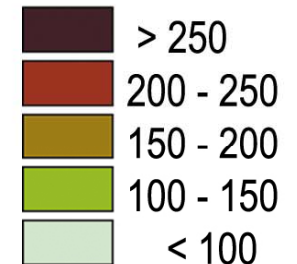May - July 2004

> 400
300 - 400
200 - 300
100 - 200
< 100
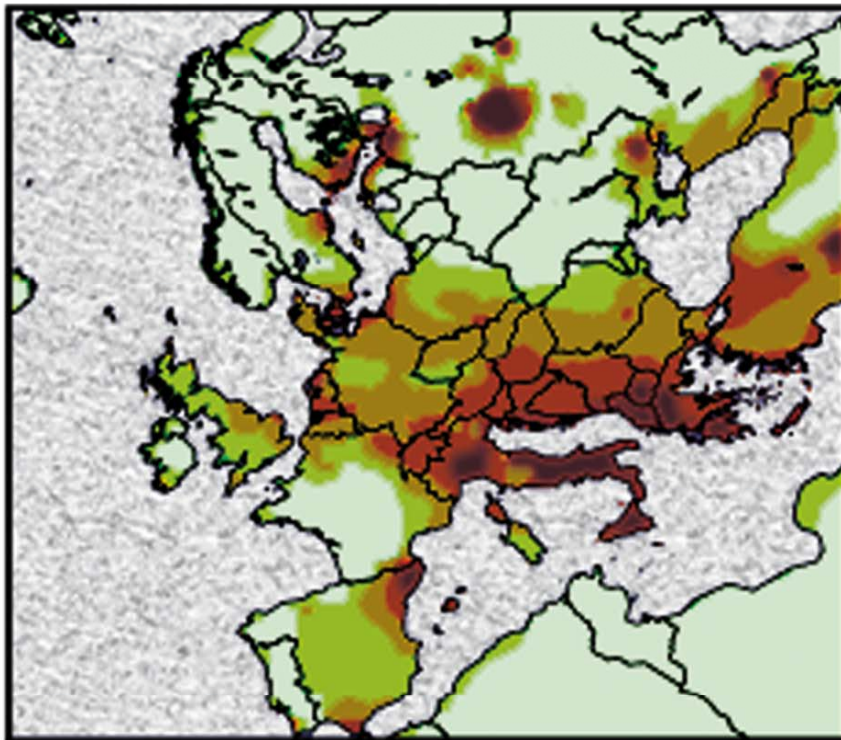
AOT40F (for forest trees)
in % [100(AOT40F)/10000]
April - September 2004

> 250
200 - 250
150 - 200
100 - 150
< 100
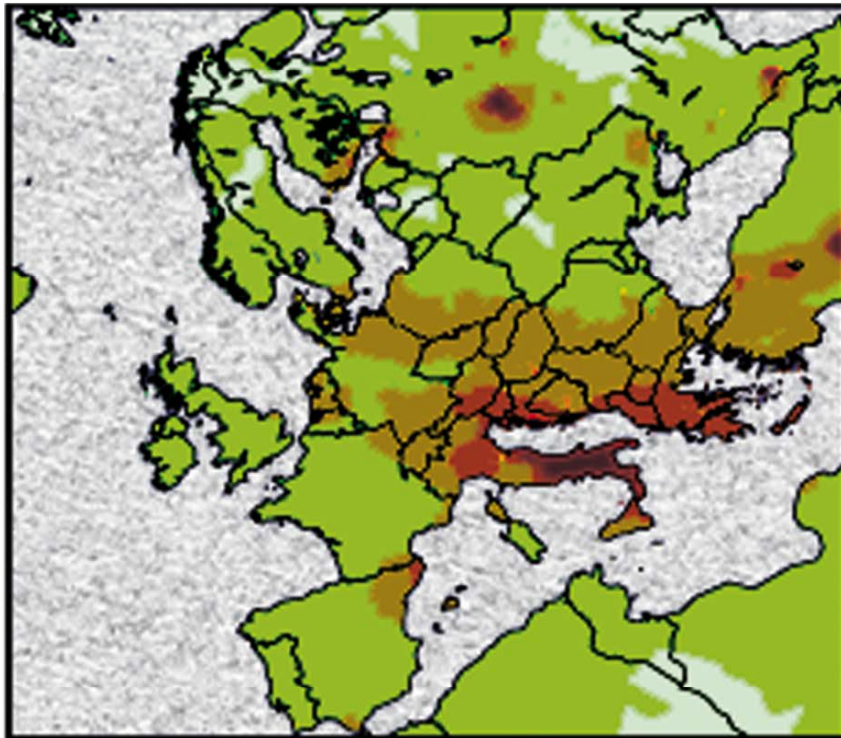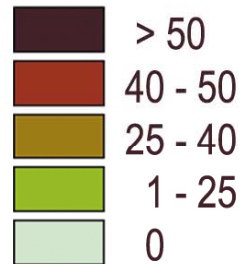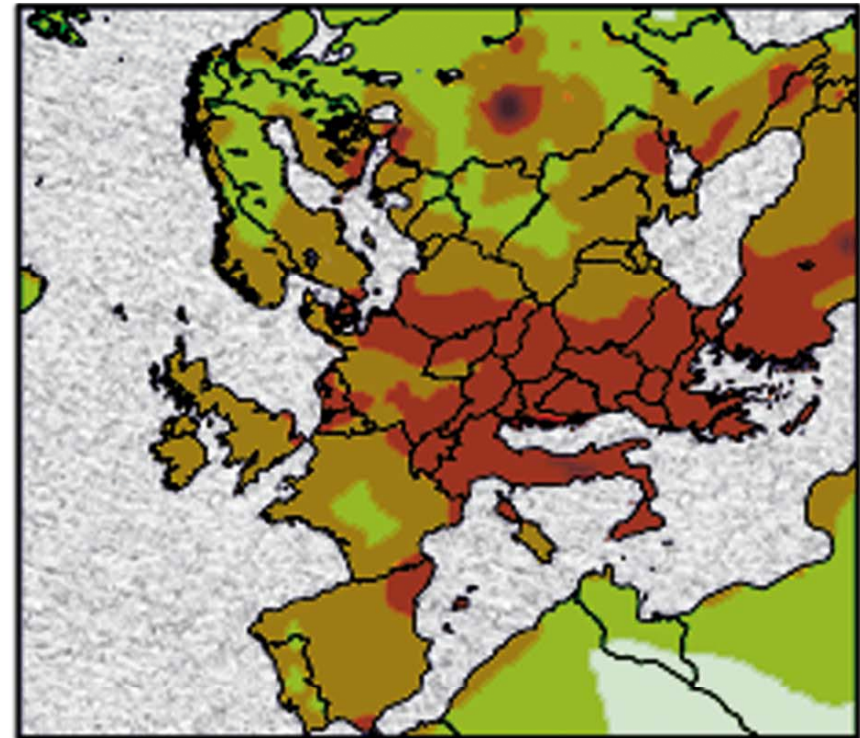
- **The people suffering from asthmatic deceases are sensitive to high ozone levels. If an 8-hour average of the ozone concentration exceeds the critical value of 60 ppb., the day is *bad* for these people as they have extra difficulties with breathing.**

- **The main suggestion of the EU health commission is to reduce the emissions so that the number of *bad* days in one year do not exceed 25.**

- **The hot summer days are usually those with ozone concentration exceeding the critical value.**

- **Long-term results (at least for 10 years) are needed in order to evaluate the situation and trends.**

Number of days with 8-hour average ozone concentrations > 60 ppb. April - September 2004

(dark)	> 50
(red)	40 - 50
(olive)	25 - 40
(green)	1 - 25
(light)	0

Averaged daily ozone maxima in Europe (in ppb) April - September 2004

(dark)	> 70
(red)	50 - 70
(olive)	30 - 50
(green)	10 - 30
(light)	< 10

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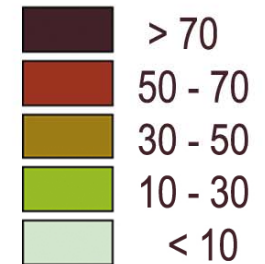
- **Grid proved to be a robust and efficient technology for large-scale air pollution modeling.**

- **On the Grid we are able to produce quickly a vast amount of results, which can be used in many applications in different areas.**

- **Some experimental results will be used for further improvements and faster new developments of the DEM code itself.**

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