RUNNING A LARGE SCALE AIR-POLLUTION MODEL ON THE EPCC SUPERCOMPUTERS

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Mathematical background of the air pollution modeling

A system of PDE for calculating the concentrations of a number of chemical species (pollutants*) in the atmosphere (3-D domain!).

The main physical and chemical processes should be adequately represented in the system:

1. horizontal wind *(advection)*;
2. *horizontal diffusion*;
3. *chemical reactions and emissions*;
4. *deposition (dry and wet)*;
5. *vertical transport* (convection and diffusion).

A huge computational task, because of the:

- size of the domain;
- dynamics of the processes – small time step;
- complexity of the equations – decomposition

*Some of these are natural components of the air.

The Danish Eulerian Model

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

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

$$+ E_s + Q_s(c_1, c_2, \dots c_q) - (k_{1s} + k_{2s})c_s$$

- q – the number of chemical species;
- c_s – the concentrations $(s = 1, \dots q)$;
- $u,\ v,\ w$ – 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;
- $Q_s(c_1, c_2, \dots c_q)$ – non-linear functions describing the chemical reactions between the species (the condensed CBM IV scheme, proposed by Gery et al. (1979) is used).

Splitting into submodels

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

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

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

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

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

Related work:

Strang - 1968

Marchuk - 1982

McRay, Goodin and Seinfeld - 1982

Lancer and Verwer - 1999

Dimov, Farago and Zlatev - 1999

Space discretization and numerical treatment of the five submodels

— Five large ODE systems*:

$$\frac{dg^{(i)}}{dt} = f^{(i)}(t, g^{(i)}) , \quad i = 1, 2, 3, 4, 5$$

$$g^{(i)} \in \mathcal{R}^{N_x \times N_y \times N_z \times q}$$
$$f^{(i)} \in \mathcal{R}^{N_x \times N_y \times N_z \times q}$$

- N_x, N_y, N_z – the number of grid-points along the coordinate axes (different versions);
- $q = 35$ – the number of chemical species considered in the model;
- the components of the $g^{(i)}$ – vector-functions, approximating the concentrations of the different species throughout the spatial domain.

* In general, these systems are simpler. For example, the chemical submodel system splits into $N_x \times N_y \times N_z$ independent ODE systems of size q.

Size of the different versions presented

- Coarse grid 2-D version (step 50 km.):
  $N_x = N_y = 96\ ,\ \ N_z = 1$
  — 4 ODE systems of order 322 560 each (no vertical exchange);

- Refined grid 2-D version (step 10 km.):
  $N_x = N_y = 480\ ,\ \ N_z = 1$
  — 4 ODE systems of more than 8 million equations;

- Coarse grid 3-D version (step 50 km.):
  $N_x = N_y = 96\ ,\ \ N_z = 10$
  — 5 ODE systems of order 3 225 600.

More than 20 000 primary time-steps are to be carried out to cover a time period of 1 month.

Smaller time-step must be used in the chemical submodel.

Numerical methods used in the chemical submodel

QSSA† (Hesstevedt et al. - 1978)

Backward Euler algorithm

Trapezoidal Rule

Runge-Kutta methods (Zlatev - 1981)

Rosenbrock methods (Verwer et al. - 1998)

Native parallel tasks: The calculations in a single grid-point.

†Quazi Steady-State Algorithm

Numerical methods used in the advection-diffusion part

Pseudo-spectral discretization (Zlatev - 1984)

Finite elements (Pepper et al. - 1979)

Finite differences (up-wind)

"Positive" methods (Bott - 1989, Holm - 1994)

Semi-Lagrangian methods (Neta - 1995)

Native parallel tasks: The calculations for a given pollutant.

Input data sets

Emission data: More or less constant over a long time period. Loaded at the begining, updated with internal constants if necessary.

$\leftarrow$ Antropogenic emissions: SO_2, NO_x,
Antr. hydro-carbons, NH_3;

$\leftarrow$ Natural hydro-carbons emissions

Geographical data: Constant. Loaded at the begining.

$\leftarrow$ Latutudes and longitudes

$\leftarrow$ Land and sea arreas

Meteorological data: Quickly changing, updated every 6 hours. New data must be read regularly after certain number of time steps.

$\Leftarrow$ Wind velocities (horizontal wind)

$\Leftarrow$ Precipitations

$\Leftarrow$ Mixing hights

$\Leftarrow$ Temperatures

$\Leftarrow$ Humidities

$\Leftarrow$ Cloud cover

$\Leftarrow$ Surface temperatures

$\Leftarrow$ Vertical wind

Numerical results

- Versions of the model, used in the experiments:
  - OpenMP and MPI codes for $(96 \times 96 \times 1)$ grid;
  - MPI code for $(480 \times 480 \times 1)$ grid;
  - OpenMP code for $(96 \times 96 \times 10)$ grid.

- All experiments are for a time period of 1 month.

- Machines at EPCC, used in the experiments:
  - SUN HPC cluster: HPC 3500 UltraSPARC, 400 MHz (shared memory)
  - CRAY T3E-900 (distributed memory)

- Compiler options:
  - On the SUN cluster: *"-fast -O4 -xarch=v8plusa -xparallel"*.
  - On the T3E: *"-O 3 "*.

- Some former results obtained on an IBM SP2 (distributed memory) and a SGI Origin-2000 (shared memory) computers at INI-C‡ are also given for comparison.

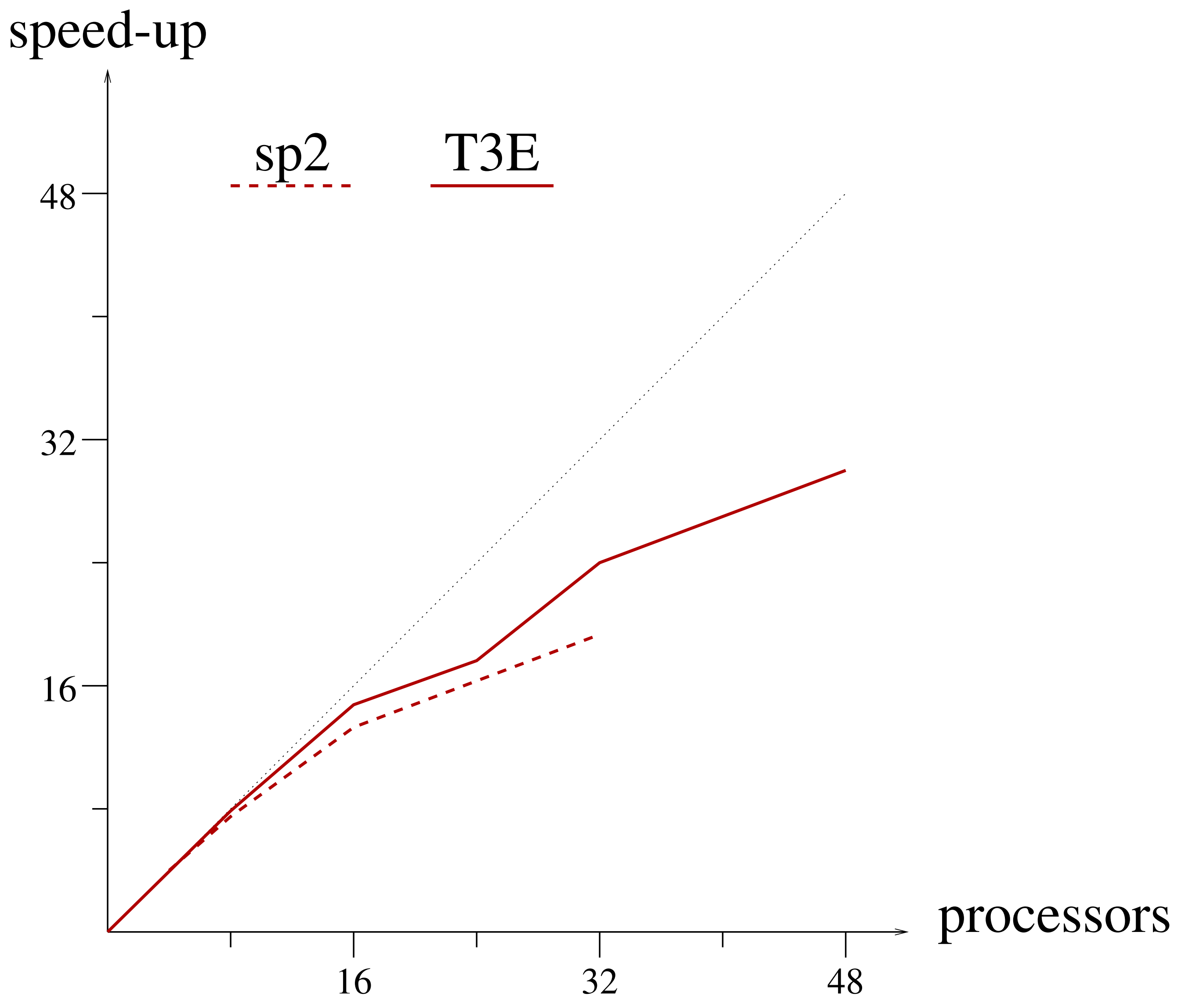
‡Danish Computing Centre for Research and Education

Times and performance of the 2-D coarse-grid codes on the SUN cluster

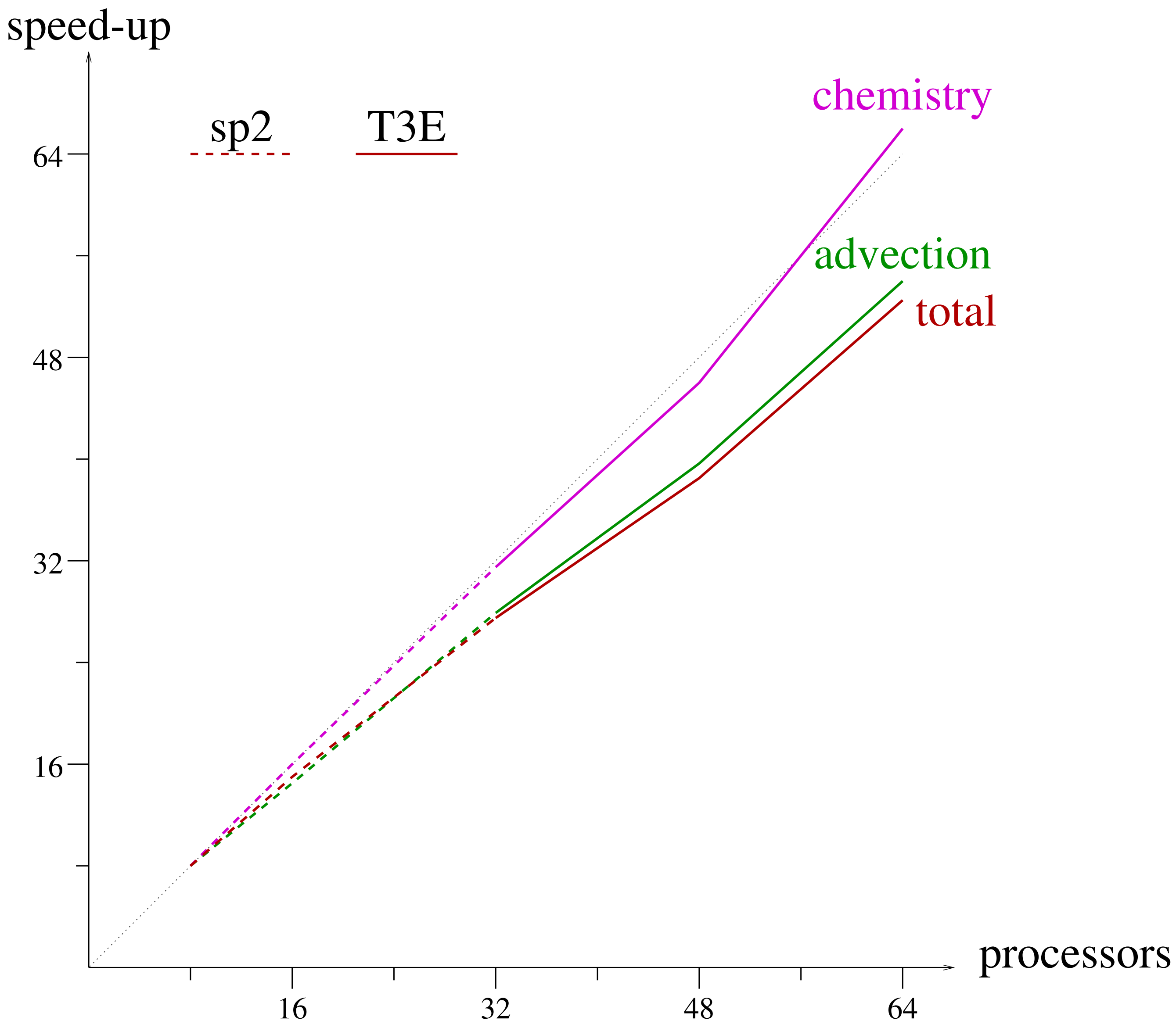
no. of proc.	OpenMP code		MPI code	
	Time [s]	Speed -up	Time [s]	Speed -up
1	4356		5067	
4	1199	3.6	1293	3.9
8	636	6.9	629	8.0
16	391	11.2	363	14.0

Time and speed-up of the OpenMP and the MPI versions of DEM for $(96 \times 96 \times 1)$ grid on the SUN HPC cluster at EPCC.

Scalability of the MPI code for the $(96 \times 96 \times 1)$ grid



Scalability of the MPI code for the $(480 \times 480 \times 1)$ grid



Times and performance of the 3-D code

Stage	SUN E3500		SGI Origin-2000	
	Time [s]	Part [%] of Total	Time [s]	Part [%] of Total
W+S (Input)	105	0.3 %	59	0.1 %
Adv.+Diff.	8602	22.9 %	10458	21.1 %
Chem.+Dep.	25381	67.6 %	35232	71.2 %
Vertical tr.	3307	8.8 %	3465	7.0 %
Output	202	0.5 %	277	0.6 %
Total	37565	100 %	49483	100 %

Time profile for sequential runs of the 3D version of DEM on two shared-memory supercomputers

Stage	Time [s]	% of Total	Speed-up
W+S (Input)	200	3.5 %	0.52
Adv.+Diff.	1244	22.0 %	6.91
Chem.+Dep.	3674	65.0 %	6.91
Vertical tr.	416	7.4 %	7.95
Output	219	3.9 %	0.92
Total	5656	100 %	6.64

Time profile of the 3D version of DEM, running on 8 proc. SUN E3500 at EPCC

Scalability of the 3-D OpenMP code

nu. of PE's	Speed-up			
	Total	Adv.+Diff.	Chem.+Dep.	Vert. tr.
2	1.96	1.91	1.98	2.09
4	3.71	3.62	3.81	4.23
8	6.64	6.91	6.91	7.95
16	10.27	10.71	11.53	18.90

Some applications

Calculating the excess ozone (AOT40) over Europe under different scenarios:

- basic_normal - the man-made (anthropogenic emissions are as in 1995 provided by EMEP (Oslo), while the biogenic (natural) emissions are as in Simpson et al., 1995
- basic_high - the man-made emissions are as in the previous scenario, while the natural emissions are as in Anastasi et al., 1991 (roughly speaking, about five times higher than in the previous scenario)
- s2010_normal - the expected man-made emissions in 2010 (which are considerably lower than the man made emissions for 1995) and the normal natural emissions (as in the first scenario)
- s2010_high - the man-made emissions as in the previous scenario, while the natural emissions are as in the second scenario.

SCALED AOT40 VALUES IN EUROPE

The period of time is May – July 1995.

AOT40 values in percentages: 100(AOT40/3000)

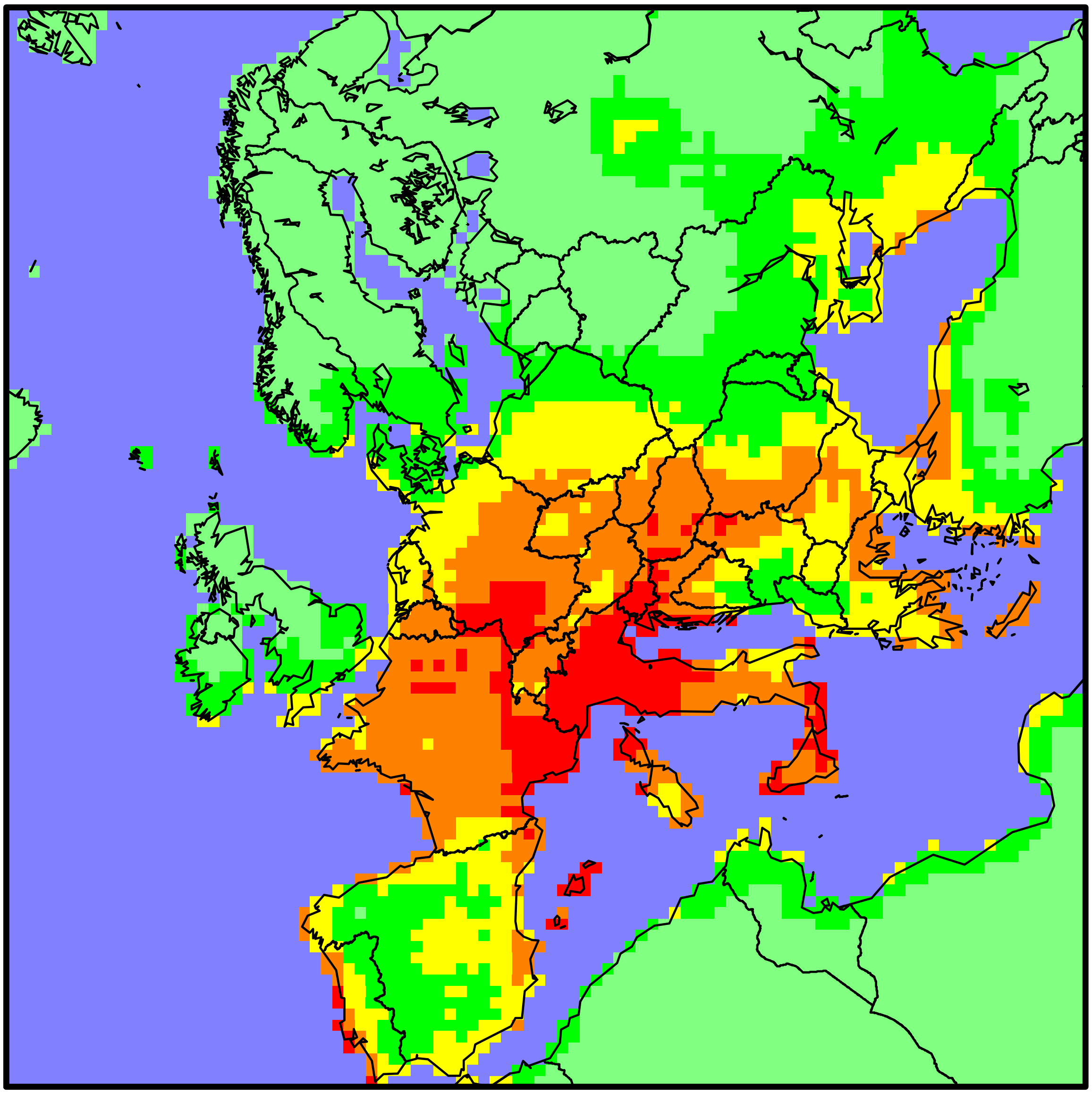
Run on a (96x96) grid / (50 km x 50 km) cells

Basic Scenario with Normal Biogenic emissions

Maximum value in the domain: 730

Minimal value in the domain: 2

Above 400
301 – 400
201 – 300
101 – 200
0 – 100
Water areas



SCALED AOT40 VALUES IN EUROPE

The period of time is May – July 1995.

AOT40 values in percentages: 100(AOT40/3000)

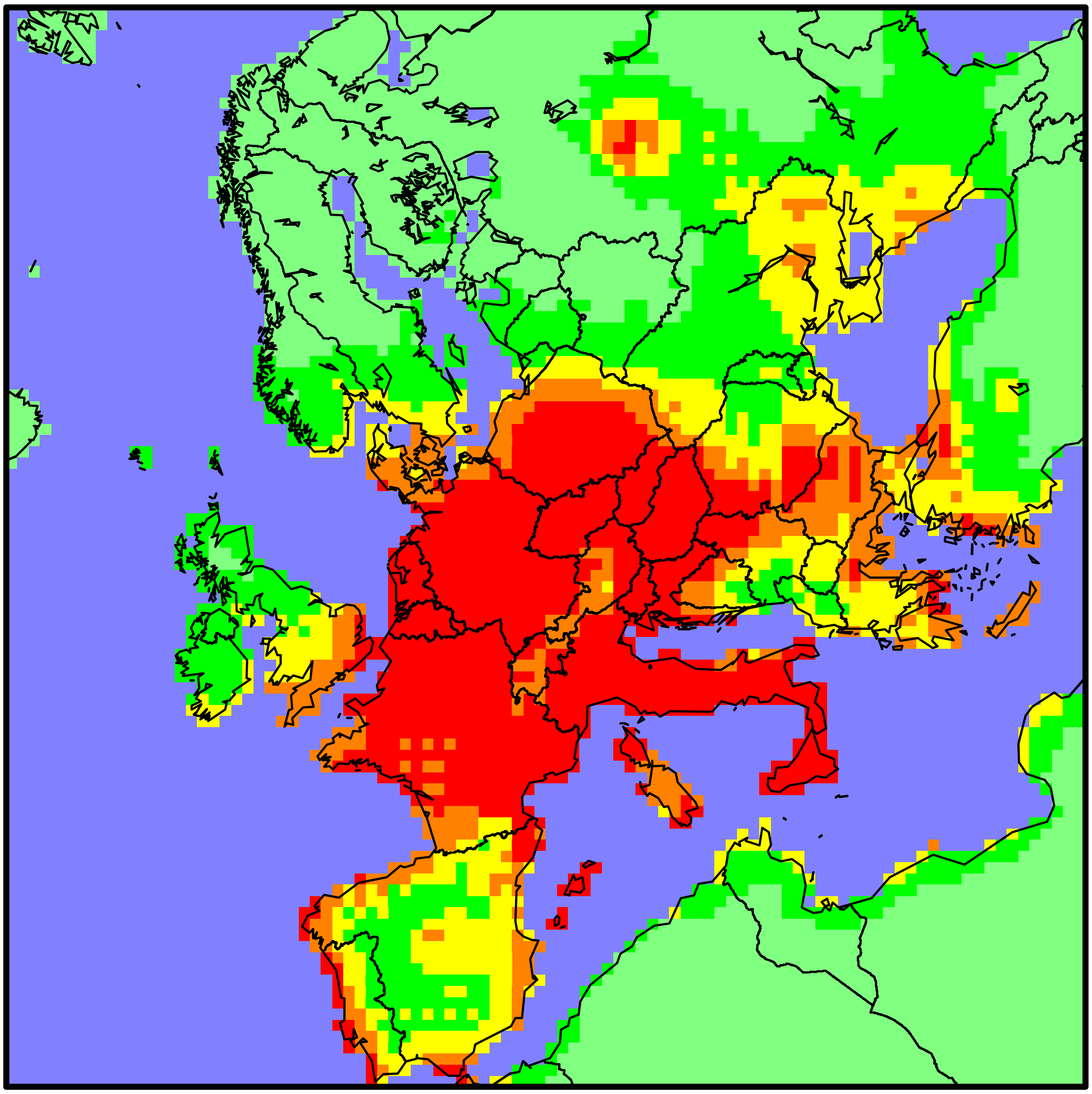
Run on a (96x96) grid / (50 km x 50 km) cells

Basic Scenario with High Biogenic emissions

Maximum value in the domain: 1105

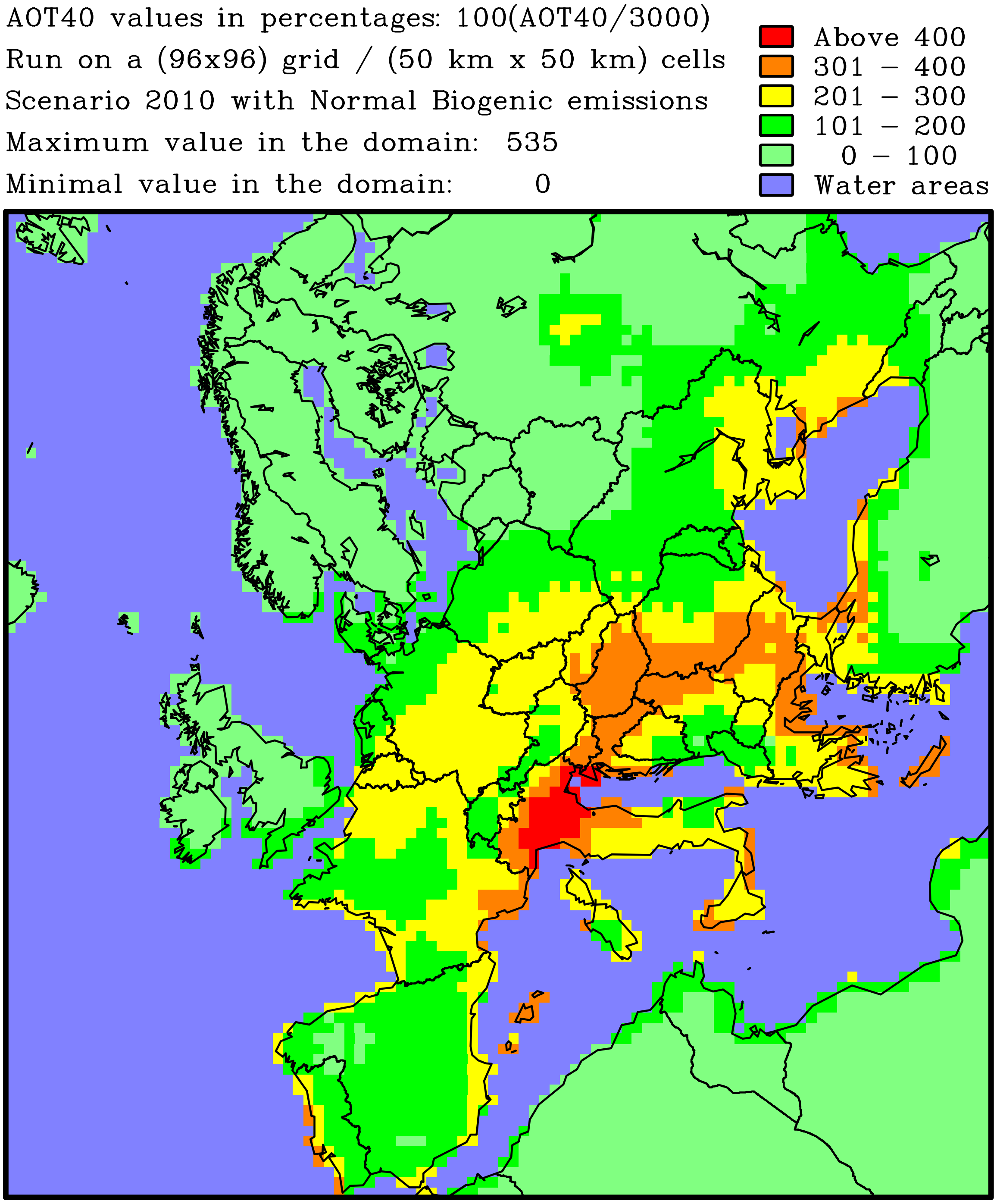
Minimal value in the domain: 3

Above 400
301 – 400
201 – 300
101 – 200
0 – 100
Water areas



SCALED AOT40 VALUES IN EUROPE

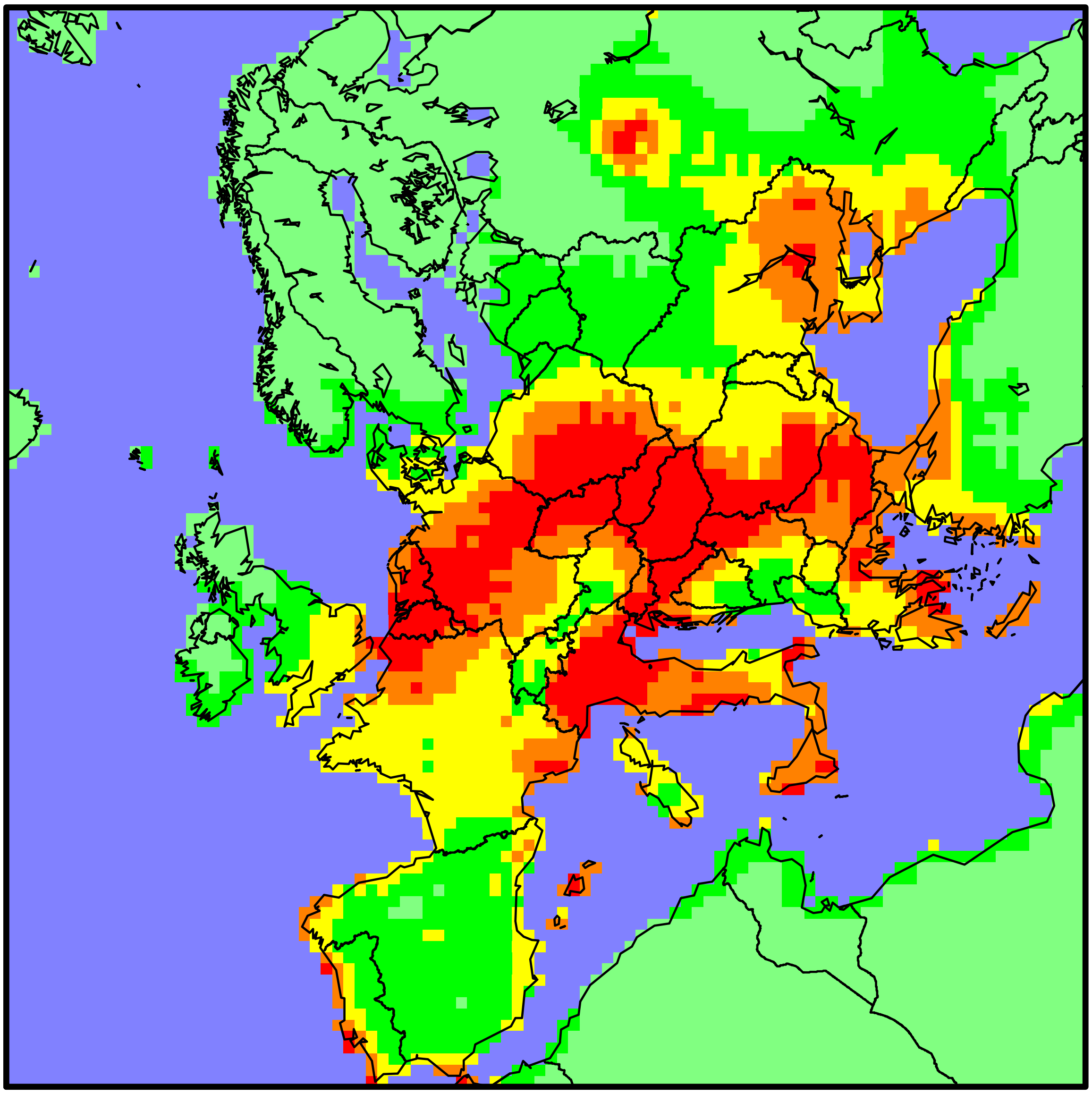
The period of time is May – July 1995.
AOT40 values in percentages: 100(AOT40/3000)
Run on a (96x96) grid / (50 km x 50 km) cells
Scenario 2010 with Normal Biogenic emissions
Maximum value in the domain: 535
Minimal value in the domain: 0



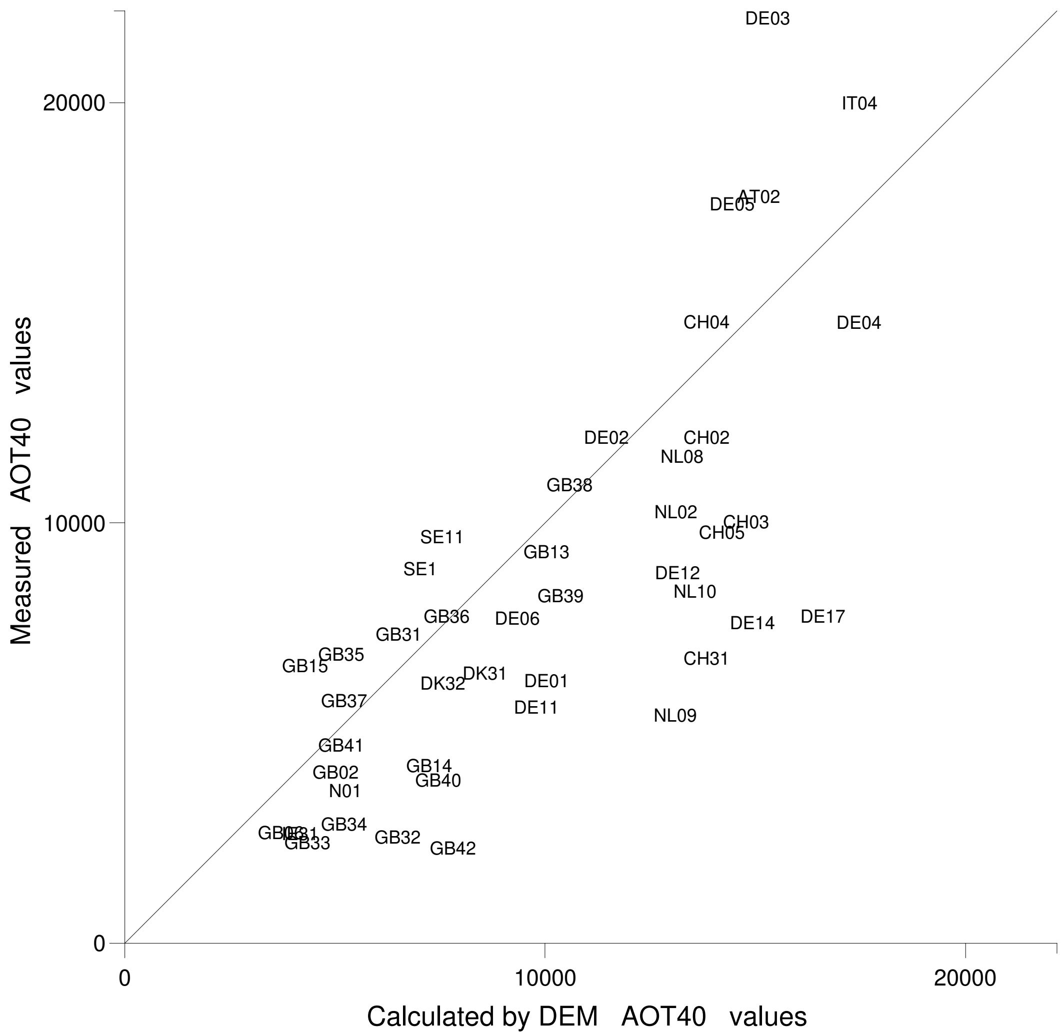
SCALED AOT40 VALUES IN EUROPE

The period of time is May – July 1995.
AOT40 values in percentages: 100(AOT40/3000)
Run on a (96x96) grid / (50 km x 50 km) cells
Scenario 2010 with High Biogenic emissions
Maximum value in the domain: 760
Minimal value in the domain: 0

Above 400	
301 – 400	
201 – 300	
101 – 200	
0 – 100	
Water areas	



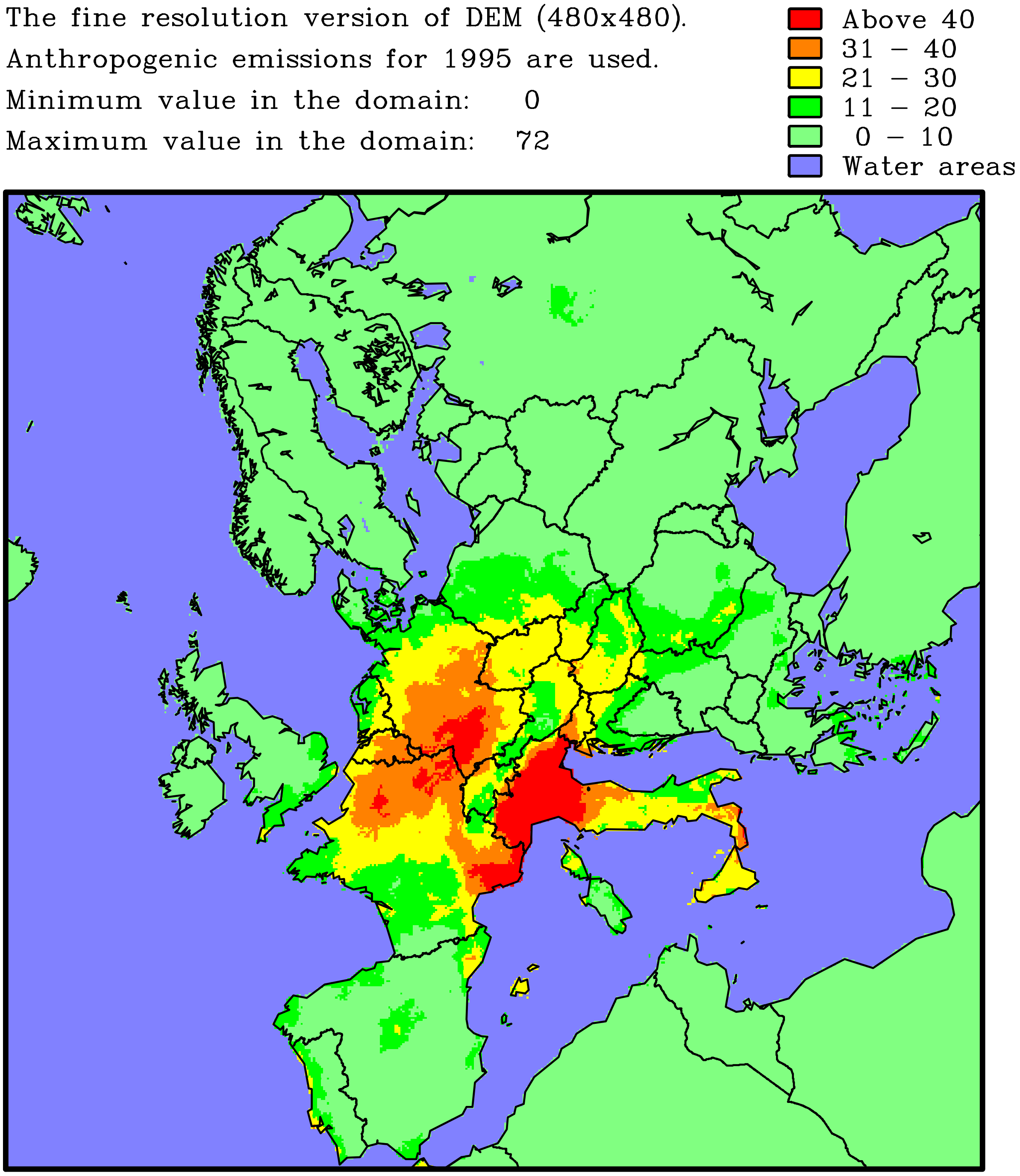
Measured vs calculated AOT40 values



COMPUTED MEAN, OBSERVED MEAN, CORRELATION FACTOR 10024.23 8496.89 0.75

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.
Minimum value in the domain: 0
Maximum value in the domain: 72



Plans for future work

- Optimization of the 3-D OpenMP code for $(96 \times 96 \times 10)$ grid .
- Development of a MPI version of the 3-D model.
- Obtaining results with new meteorological data sets and various emission scenarios.
- Development of a 3-D refined grid version of the model for $(480 \times 480 \times 10)$ grid for massively parallel computers (MPI).

Acknowledgments

This research was supported by EC via Access to Research Infrastructure action of the Improving Human Potential Programme (contract No. HPRI-1999-CT-00026). The results presented were obtained during a TRACS research visit at EPCC, the University of Edinburgh, where the author spent 3 months in the autumn 2000.

Special thanks to my EPCC contact Mario Antonioletti and to the whole TRACS team, who were always very kind and helped me a lot in this work.

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