The Modular Earth Submodel System (MESSy): Atmospheric Chemistry in Earth System Models

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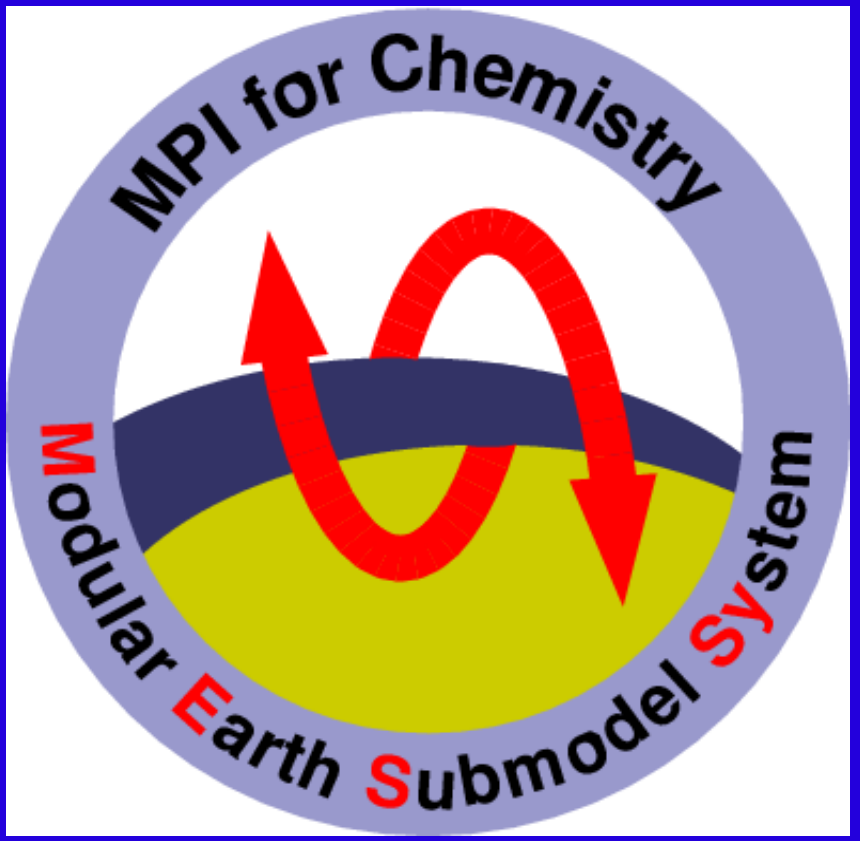
ScicomP13, July 16-20, 2007, Supercomputing Center Garching



http://www.messy-interface.org

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MESSy community

Max Planck Institute for Chemistry,
Air Chemistry Department, Mainz

DLR Institute for Physics of the Atmosphere,
Oberpfaffenhofen

Institute for Meteorology and Climate Research,
Karlsruhe Research Centre

Aristotle University of Thessaloniki

Institute for Meteorology, Free University Berlin

MPG Supercomputing Center Garching (RZG), Garching

Max Planck Institute for Meteorology,
Hamburg (ECHAM5)

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MESSy hall of fame

Developers, contributors, users, promoters:

Baumgärtner, Andreas; Brinkop, Sabine; Brühl, Christoph; Buchholz, Joachim; Burrows, Susannah; Butler, Tim; Dameris, Martin; Erhardt, Gabriele; Ganzeveld, Laurens; Giner, Bernhard; Giorgetta, Marco; Grewe, Volker; Gromov, Sergey; Jöckel, Patrick; Kerkweg, Astrid; Ketelsen, Klaus ;Kirner, Ole; Kubin, Anne; Kunze, Markus; Kurz, Christian; Lawrence, Mark; Langematz, Ulrike; Lauer, Axel; Lelieveld, Jos; Metzger, Swen; Nissen, Katrin; Ponater, Michael; Pozzer, Andrea; Rhodin, Andreas; Riede, Hella; Ruhnke, Roland; Sander, Rolf; Sausen, Robert; Schumann, Ulrich; Steil, Benedikt; Steinkamp, Jörg; Stier, Philip; Tanarhte, Meryem; Taraborrelli, Domenico; Tost, Holger; Tourpali, Kleareti; Traub, Michael; van Aalst, Maarten; van Aardenne, John; ...

... and much more data users ...

Outline

I. Motivation
II. Overview of the concept of MESSy
III. MESSy for atmospheric chemistry
IV. Evaluation of the AC-GCM ECHAM5/MESSy1 (E5/M1)
V. Some notes on the implementation and performance

I. Motivation

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Motivation

Atmospheric Chemistry:

- major player in the Earth Climate system
- provides link between different domains and processes:
  - radiative budget (CO_2, Ozone, clouds)
  - interaction with ocean and biosphere (C-,N-,S-,...-cycles)
  - human impact (pollution) and impact on humans (air quality)
- self-cleansing capacity of the atmosphere prevents runaway

Atmospheric Chemistry in Earth System Models (ESMs):

- a large number of processes involved ...
- ... which are “chemically” coupled
- highly non-linear processes:
  >>> avoid recompilation wherever possible
- wide range of time-scales (10^{-2} s ... 10^{6} years)
- large number of species (all relevant ?)

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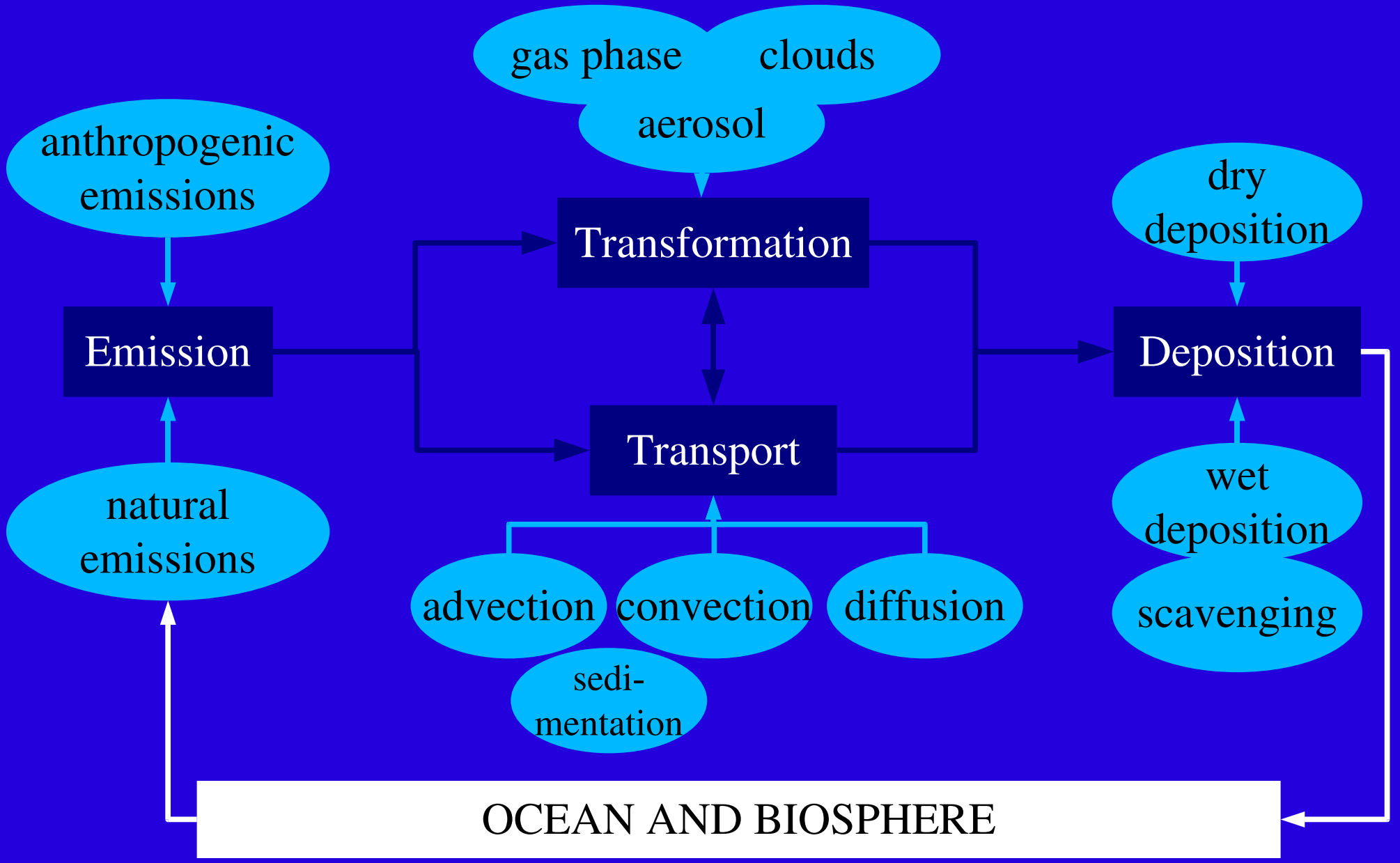
Motivation



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Motivation

Development aspects:

- always state-of-the-art
- prepared for the future

→ continuous further development

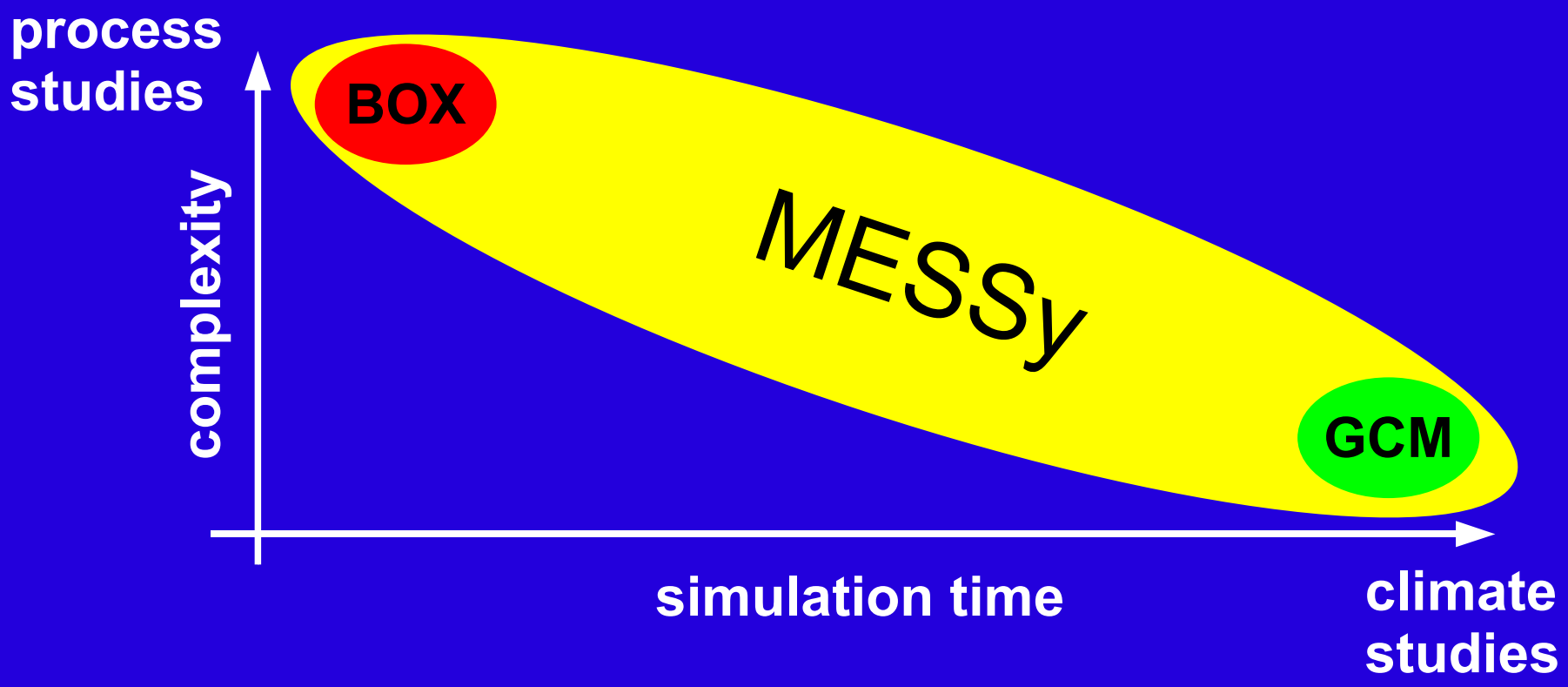
Scientific aspects:

- increasing **complexity** requires increasingly transparent **control**
- **variable** complexity depending on the scientific questions/demands -> high **flexibility**
- minimized effort for extension (**plug&play**, exchangeable code)
- **efficient** future developments (standardised interfaces)
- **feedback** mechanisms between processes (quantification)
- **process oriented**
- high degree of internal **consistency**
- **reproducibility**
- ...

Motivation

... consistency

many projects / ONE code



II. Overview of the concept of MESSy

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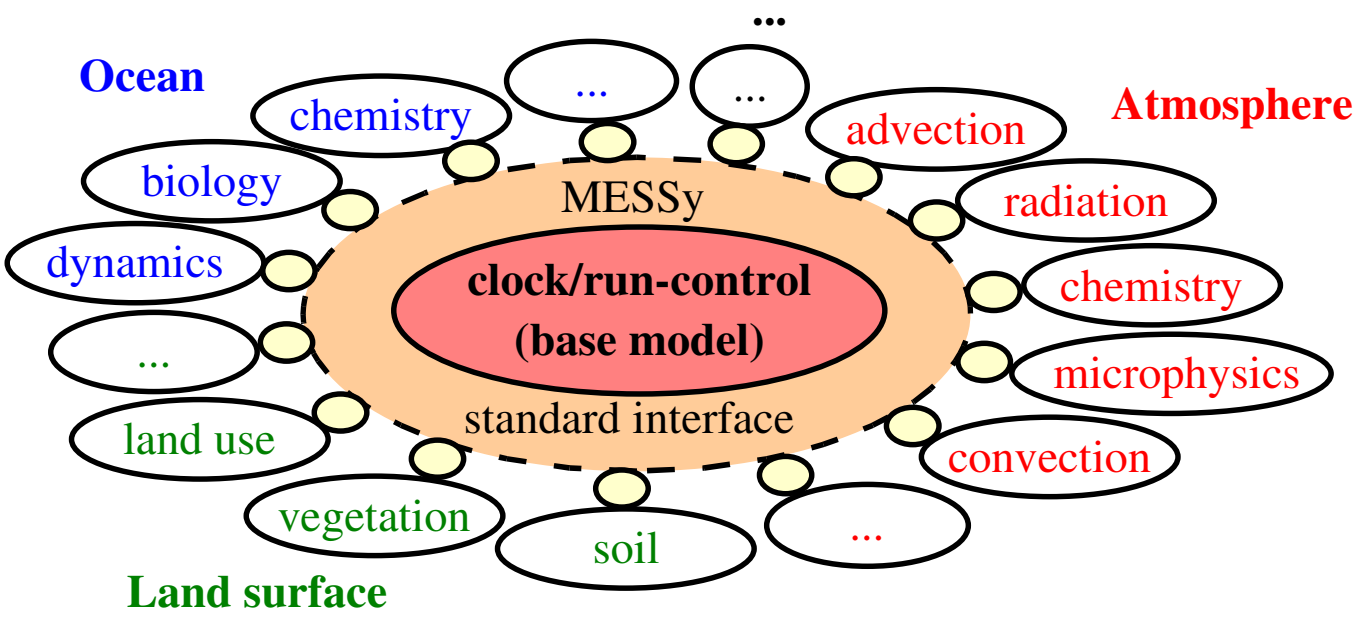
What is MESSy ?

MESSy is (a project providing) ...

Jöckel et al., ACP, 2005

- an interface with infrastructure to couple 'processes' (=submodels) to a GCM (= base model)
- a set of processes coded as switchable submodels
- a (simple) coding standard



process oriented approach of MESSy

The System is a coupled set of communicating processes.

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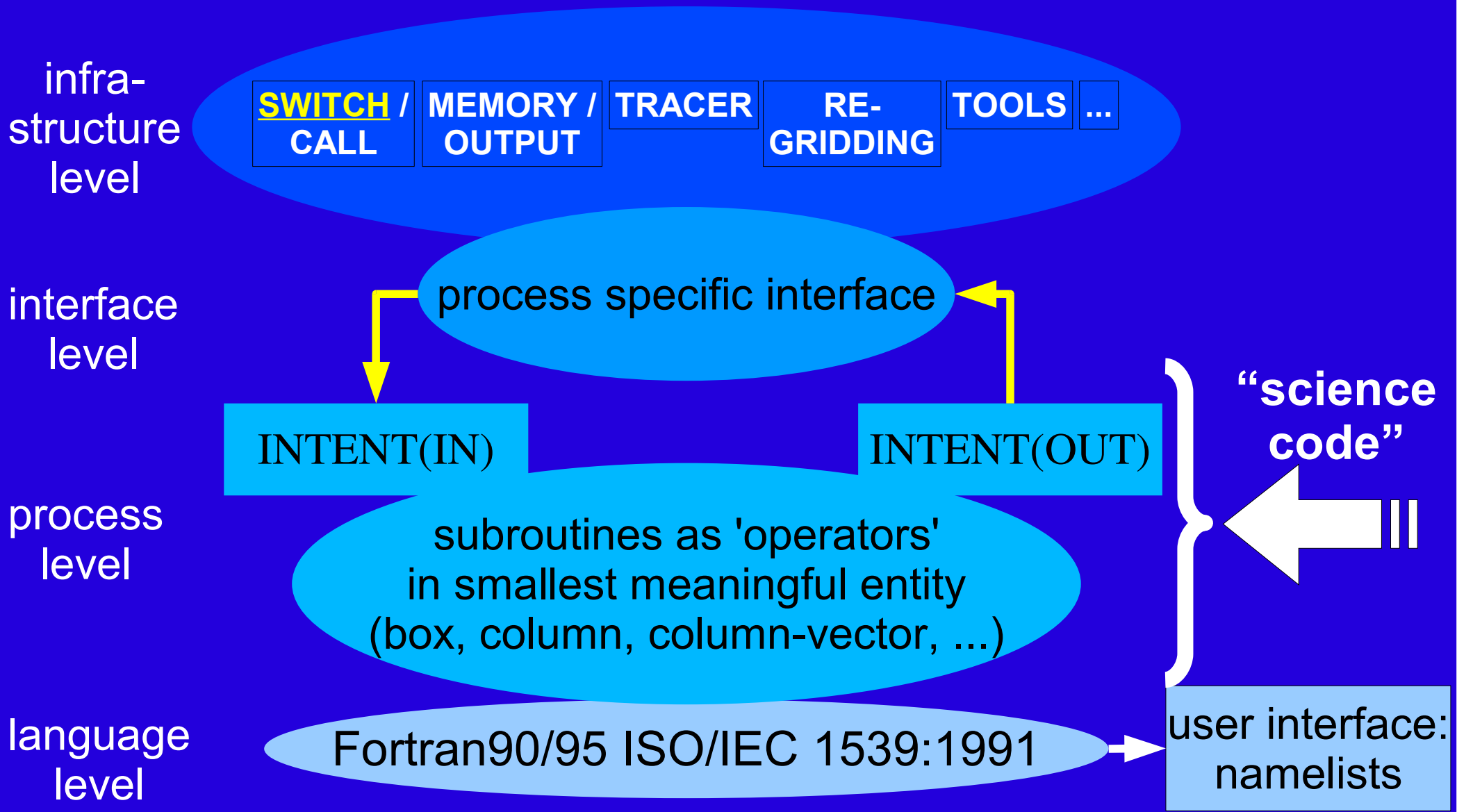
The key: Standardisation

Standardisation on the lowest possible level ...



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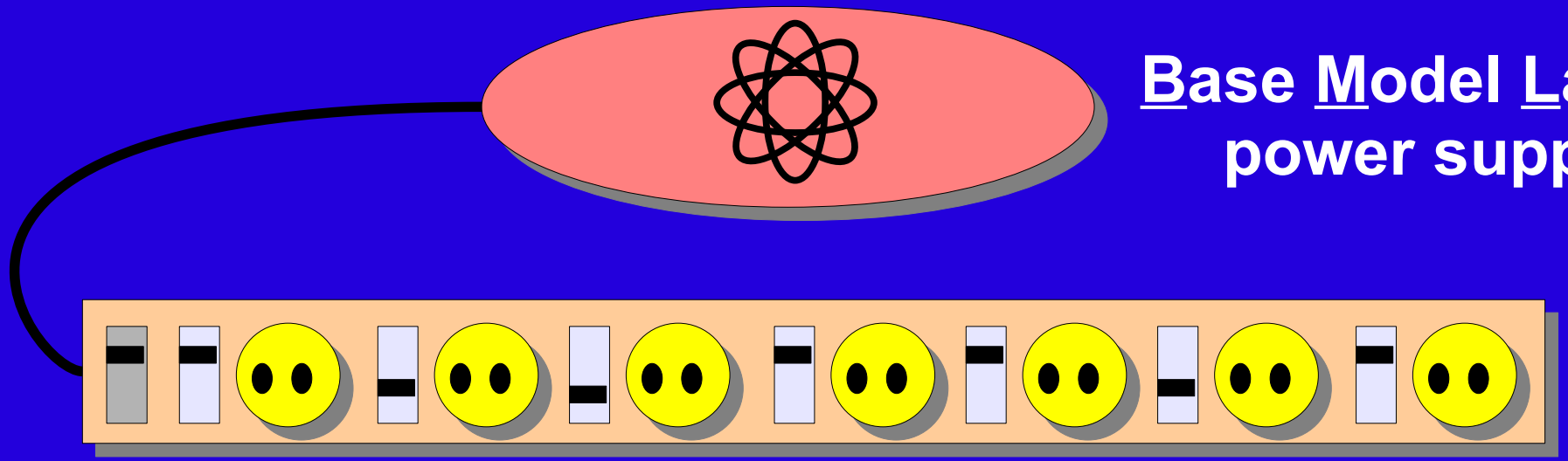
How does MESSy work ?



Base Model Layer: power supply

Base Model Interface Layer: multiple socket outlet

Submodel Interface Layer: connector

Submodel Core Layer: the machinery ...

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Basic flow chart

user friendly flexibility:
'model setup'

INPUT of boundary conditions

PERFORMANCE !!!

time loop, decomposition loop, ...

OUTPUT of results

III. MESSy for atmospheric chemistry

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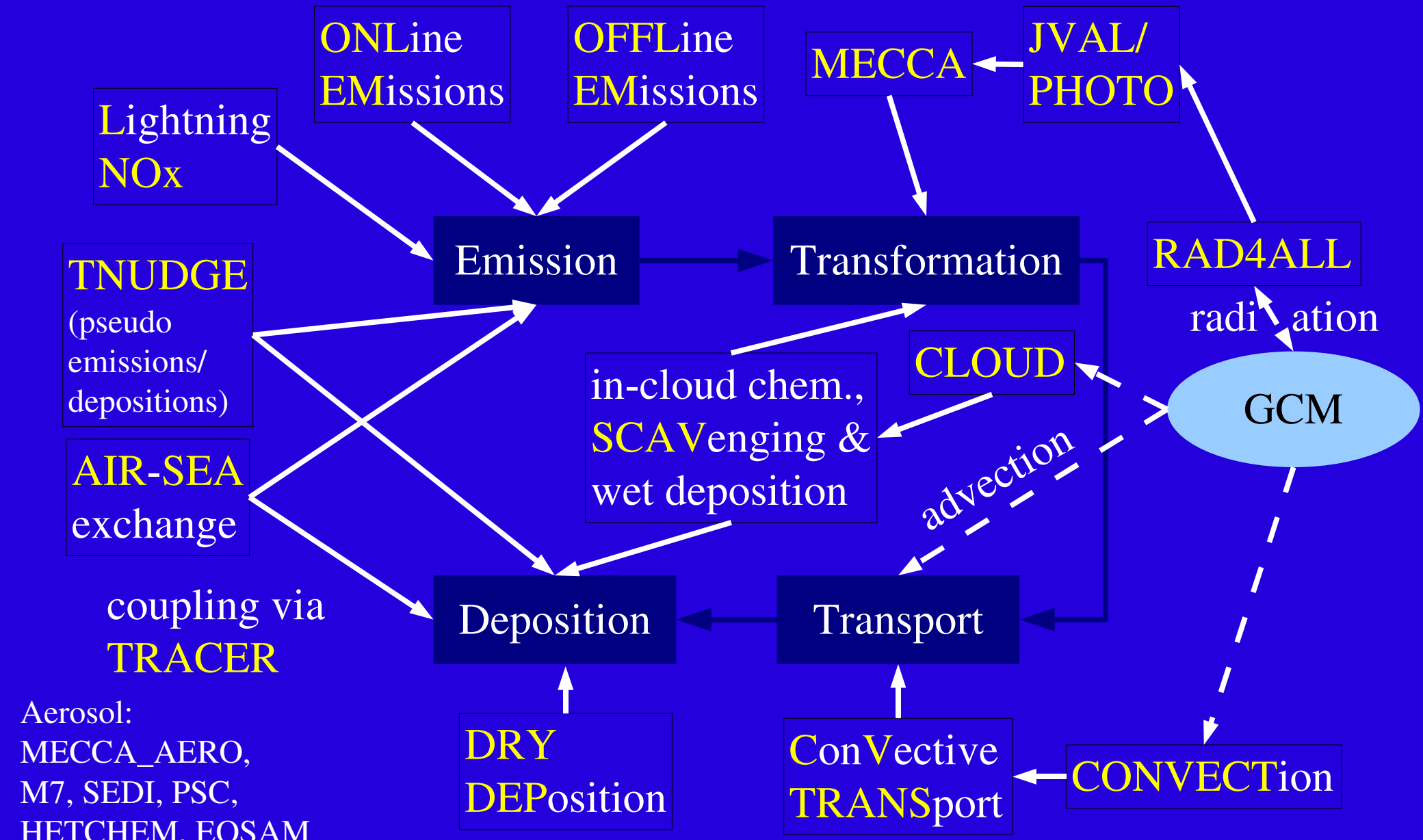
Atmospheric chemistry



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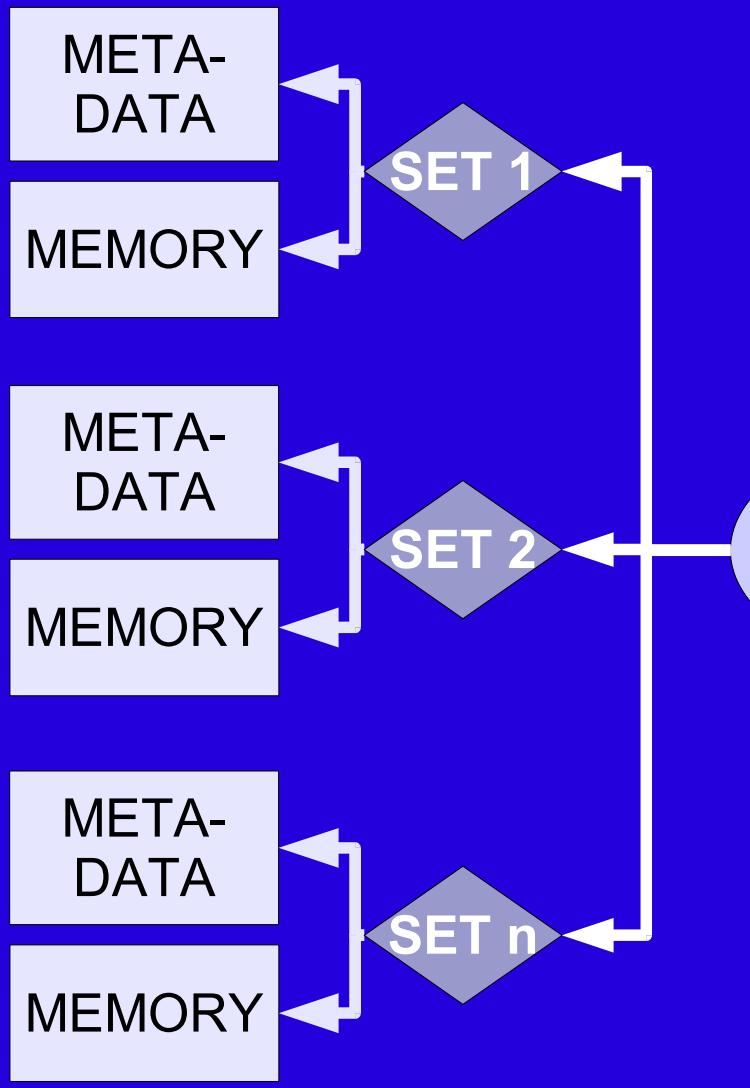
TRACER

- "generic" submodel (i.e., infrastructure coded as submodel)
- provides "chemical coupling" between different processes
  (e.g., emission -> chemical reaction -> advection -> deposition)



- transport families
- tagging (linearisation)

- keep positive
- track corrections
- global mass diagnostics

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TRACER

META-DATA: characteristics of tracers (= chemical species)
-> concatenated list of nested Fortran90-structures

```
TYPE t_trinfo_list
   TYPE(t_trinfo)                  :: info
   TYPE(t_trinfo_list), POINTER :: next
END TYPE t_trinfo_list
```

```
TYPE t_trinfo
   TYPE(t_ident)        :: ident        ! IDENTIFICATION
   TYPE(t_proc)         :: proc         ! PROCESS FLAGS
   TYPE(t_infra)        :: infra        ! INFRASTRUCTURE
   TYPE(t_typ_single)   :: typ_single   ! TYPE: SINGLE
   TYPE(t_typ_family)   :: typ_family   ! TYPE: FAMILY
   TYPE(t_typ_isotope)  :: typ_isotope  ! TYPE: ISOTOPE
   TYPE(t_med_aerosol)  :: med_aerosol  ! MEDIUM: AEROSOL
END TYPE t_trinfo
```

```
TYPE t_typ_single
   REAL(DP) :: molarmass  = 0.0_DP !
   REAL(DP) :: henry      = 0.0_DP ! henry coefficient [mol/L/atm]
   REAL(DP) :: dryreac_sf = 0.0_DP ! dry reaction coeff.
END TYPE t_typ_single
```

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MECCA(_AERO)

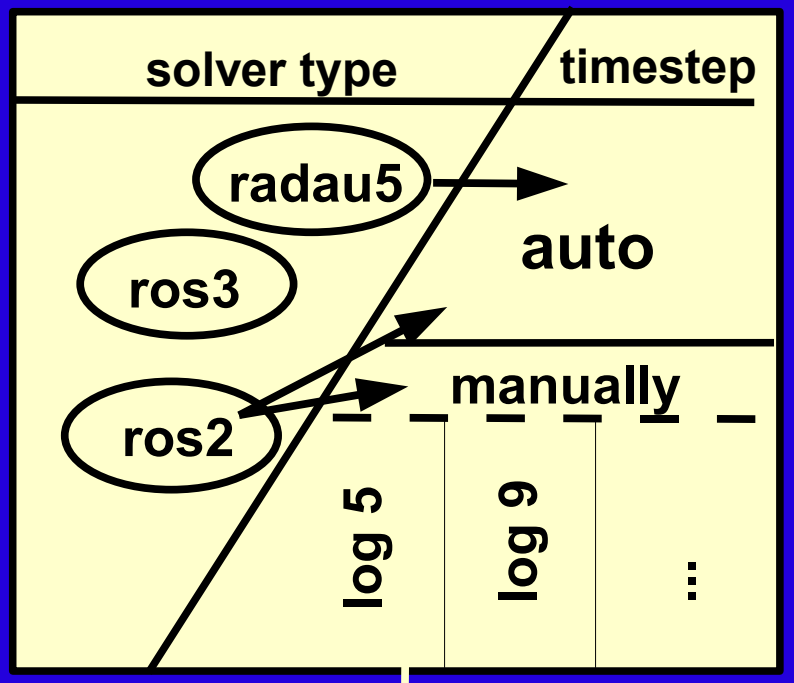
high flexibility >>> automatic code generation

chemical equation set

	basic	hydro-carbons	halogens	sulfur
troposph.	MBL[5]		MBL	MBL
	MATCH[1]		MISTRA[2]	
stratosph.	MA-ECHAM4/ CHEM[3]		MSBM[4]	
aqueous	MBL		MBL	MBL
	MISTRA		MISTRA	

1) v. Kuhlmann et al. 2003
2) v. Glasow et al. 2002
3) Steil et al. 1998
4) Meilinger, 2000
5) Kerkweg, 2005

kpp solver



chosen chemical setup:
e.g. basic gas phase

chosen solver:
e.g. ros3-auto

F90 code

Sander et al., ACP, 2005
Kerkweg et al., ACP, 2007

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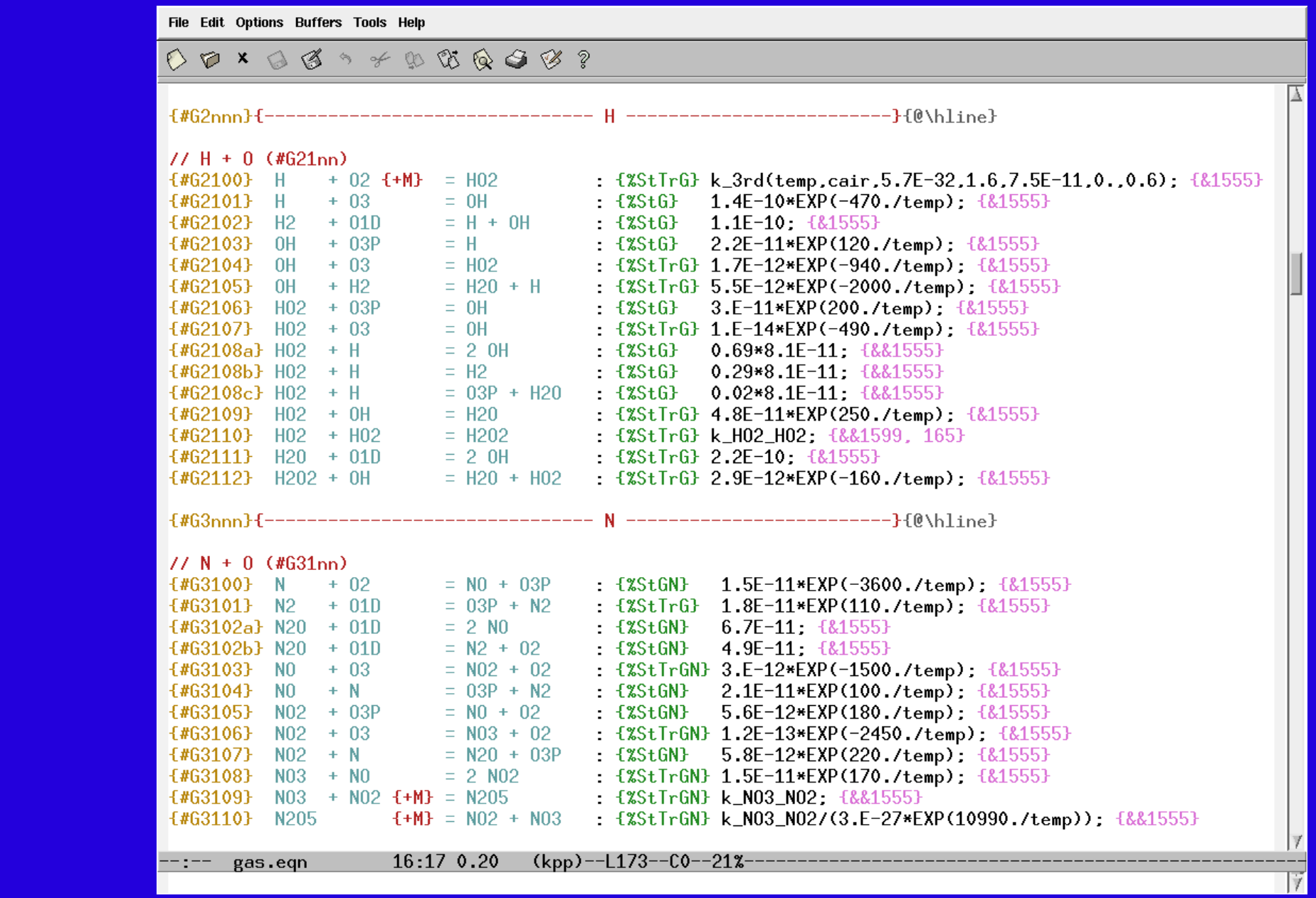
MECCA(_AERO) / KPP



```
File  Edit  Options  Buffers  Tools  Help

{#G2nnn}{------------------------------ H ------------------------}{@\hline}

// H + O (#G21nn)
{#G2100}  H     + O2 {+M}  = HO2          : {%StTrG} k_3rd(temp,cair,5.7E-32,1.6,7.5E-11,0.,0.6); {&1555}
{#G2101}  H     + O3       = OH           : {%StG}   1.4E-10*EXP(-470./temp); {&1555}
{#G2102}  H2    + O1D      = H + OH       : {%StG}   1.1E-10; {&1555}
{#G2103}  OH    + O3P      = H            : {%StG}   2.2E-11*EXP(120./temp); {&1555}
{#G2104}  OH    + O3       = HO2          : {%StTrG} 1.7E-12*EXP(-940./temp); {&1555}
{#G2105}  OH    + H2       = H2O + H      : {%StTrG} 5.5E-12*EXP(-2000./temp); {&1555}
{#G2106}  HO2   + O3P      = OH           : {%StG}   3.E-11*EXP(200./temp); {&1555}
{#G2107}  HO2   + O3       = OH           : {%StTrG} 1.E-14*EXP(-490./temp); {&1555}
{#G2108a} HO2   + H        = 2 OH         : {%StG}   0.69*8.1E-11; {&&1555}
{#G2108b} HO2   + H        = H2           : {%StG}   0.29*8.1E-11; {&&1555}
{#G2108c} HO2   + H        = O3P + H2O    : {%StG}   0.02*8.1E-11; {&&1555}
{#G2109}  HO2   + OH       = H2O          : {%StTrG} 4.8E-11*EXP(250./temp); {&1555}
{#G2110}  HO2   + HO2      = H2O2         : {%StTrG} k_HO2_HO2; {&&1599, 165}
{#G2111}  H2O   + O1D      = 2 OH         : {%StTrG} 2.2E-10; {&1555}
{#G2112}  H2O2  + OH       = H2O + HO2    : {%StTrG} 2.9E-12*EXP(-160./temp); {&1555}

{#G3nnn}{------------------------------ N ------------------------}{@\hline}

// N + O (#G31nn)
{#G3100}  N     + O2       = NO + O3P     : {%StGN}   1.5E-11*EXP(-3600./temp); {&1555}
{#G3101}  N2    + O1D      = O3P + N2     : {%StTrG}  1.8E-11*EXP(110./temp); {&1555}
{#G3102a} N2O   + O1D      = 2 NO         : {%StGN}   6.7E-11; {&1555}
{#G3102b} N2O   + O1D      = N2 + O2      : {%StGN}   4.9E-11; {&1555}
{#G3103}  NO    + O3       = NO2 + O2     : {%StTrGN} 3.E-12*EXP(-1500./temp); {&1555}
{#G3104}  NO    + N        = O3P + N2     : {%StGN}   2.1E-11*EXP(100./temp); {&1555}
{#G3105}  NO2   + O3P      = NO + O2      : {%StGN}   5.6E-12*EXP(180./temp); {&1555}
{#G3106}  NO2   + O3       = NO3 + O2     : {%StTrGN} 1.2E-13*EXP(-2450./temp); {&1555}
{#G3107}  NO2   + N        = N2O + O3P    : {%StGN}   5.8E-12*EXP(220./temp); {&1555}
{#G3108}  NO3   + NO       = 2 NO2        : {%StTrGN} 1.5E-11*EXP(170./temp); {&1555}
{#G3109}  NO3   + NO2 {+M} = N2O5         : {%StTrGN} k_NO3_NO2; {&&1555}
{#G3110}  N2O5      {+M}   = NO2 + NO3    : {%StTrGN} k_NO3_NO2/(3.E-27*EXP(10990./temp)); {&&1555}

--:--  gas.eqn        16:17 0.20   (kpp)--L173--C0--21%----------
```

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MECCA(_AERO) / KPP

File Edit Options Buffers Tools F90 Help

```
      X(46) = (X(46)-JVS(155)*X(95)-JVS(156)*X(99))/(JVS(154))
      X(45) = (X(45)-JVS(151)*X(83)-JVS(152)*X(95)-JVS(153)*X(100))/&
     &(JVS(150))
      X(44) = (X(44)-JVS(147)*X(97)-JVS(148)*X(99)-JVS(149)*X(100))/&
     &(JVS(146))
      X(43) = (X(43)-JVS(140)*X(48)-JVS(141)*X(66)-JVS(142)*X(71)&
     &-JVS(143)*X(75)-JVS(144)*X(92)-JVS(145)*X(95))/(JVS(139))
      X(42) = (X(42)-JVS(136)*X(78)-JVS(137)*X(95)-JVS(138)*X(96))/&
     &(JVS(135))
      X(41) = (X(41)-JVS(132)*X(67)-JVS(133)*X(95)-JVS(134)*X(96))/&
     &(JVS(131))
      X(40) = (X(40)-JVS(128)*X(80)-JVS(129)*X(95)-JVS(130)*X(96))/&
     &(JVS(127))
      X(39) = (X(39)-JVS(124)*X(62)-JVS(125)*X(87)-JVS(126)*X(95))/&
     &(JVS(123))
      X(38) = (X(38)-JVS(120)*X(79)-JVS(121)*X(95)-JVS(122)*X(100))/&
     &(JVS(119))
      X(37) = (X(37)-JVS(116)*X(69)-JVS(117)*X(95)-JVS(118)*X(96))/&
     &(JVS(115))
      X(36) = (X(36)-JVS(112)*X(62)-JVS(113)*X(95)-JVS(114)*X(96))/&
     &(JVS(111))
      X(35) = (X(35)-JVS(106)*X(80)-JVS(107)*X(83)-JVS(108)*X(85)&
     &-JVS(109)*X(95)-JVS(110)*X(96))/(JVS(105))
      X(34) = (X(34)-JVS(103)*X(91)-JVS(104)*X(95))/(JVS(102))
      X(33) = (X(33)-JVS(99)*X(83)-JVS(100)*X(95)-JVS(101)*X(96))/&
     &(JVS(98))
      X(32) = (X(32)-JVS(96)*X(87)-JVS(97)*X(100))/(JVS(95))
      X(31) = (X(31)-JVS(93)*X(46)-JVS(94)*X(95))/(JVS(92))
      X(30) = (X(30)-JVS(90)*X(91)-JVS(91)*X(95))/(JVS(89))
      X(29) = (X(29)-JVS(87)*X(87)-JVS(88)*X(95))/(JVS(86))
      X(28) = (X(28)-JVS(84)*X(61)-JVS(85)*X(95))/(JVS(83))
      X(27) = (X(27)-JVS(80)*X(32)-JVS(81)*X(91)-JVS(82)*X(100))/&
     &(JVS(79))
      X(26) = (X(26)-JVS(76)*X(31)-JVS(77)*X(47)-JVS(78)*X(95))/&
     &(JVS(75))
      X(25) = (X(25)-JVS(74)*X(95))/(JVS(73))
--:--  messy_mecca_kpp.f90   16:21 0.08   (F90)--L10592--C0--93%----------
```

IV. Evaluation of the AC-GCM ECHAM5/MESSy1 (E5/M1)

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Evaluated Setup

Evaluation simulation (S1):

- ECHAM5/MESSy
- T42 resolution (~2.8°x~2.8°)
- 90 vertical levels (up to 0.01 hPa)
- nudged in free-troposphere (200-700 hPa) towards analysis data from ECMWF operational model
- 245 reactions including hydrocarbons up to 4 carbon atoms
- feedback between chemistry and dynamics via radiation
- off-line anthropogenic emissions compiled for the year 2000
- 8 years of simulation (1998-2005)

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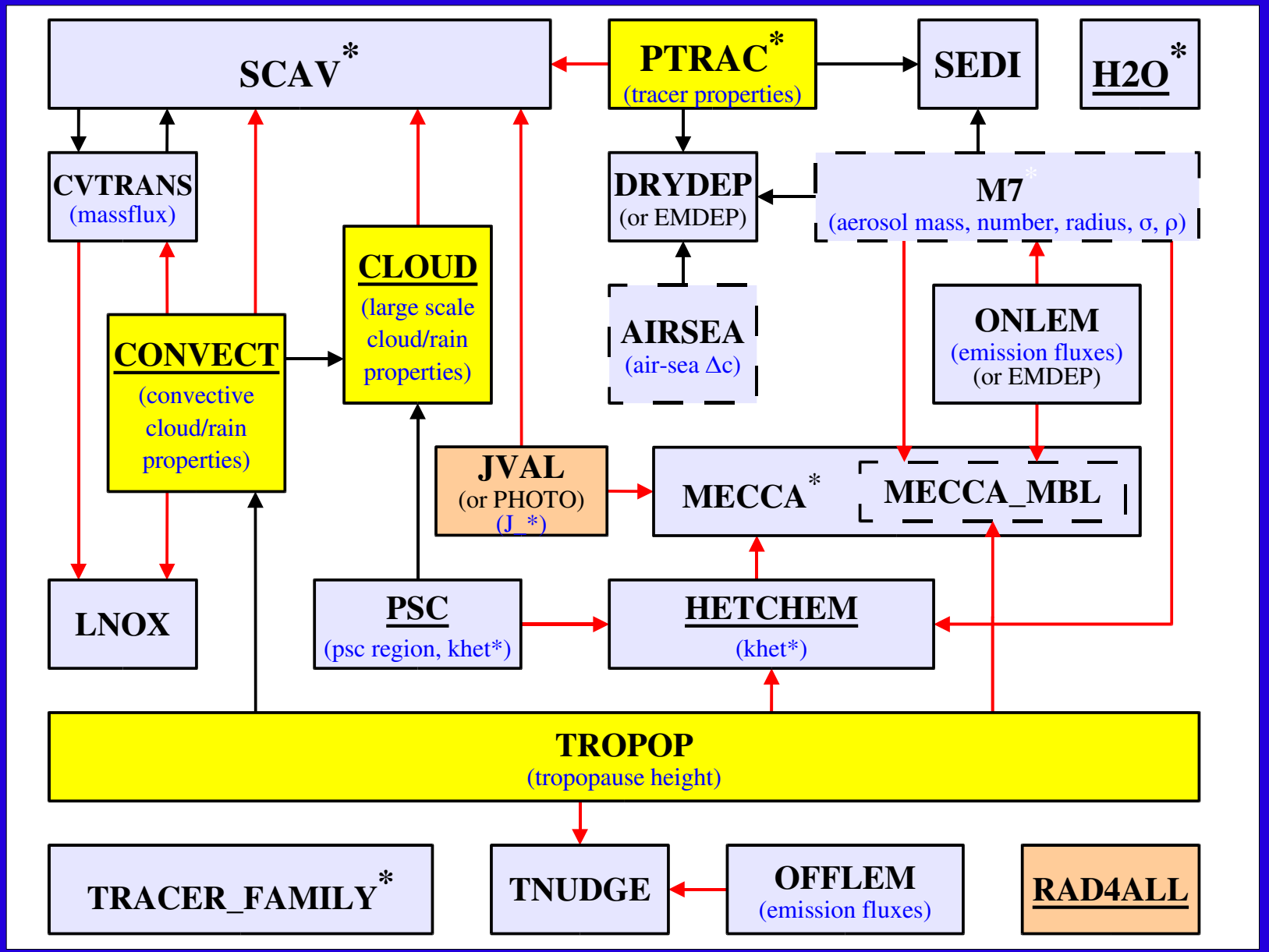
Complexity



coupling switchable

* define tracers

coupling to dynamics

modify tracers

use tracers

no tracer modific.

not used

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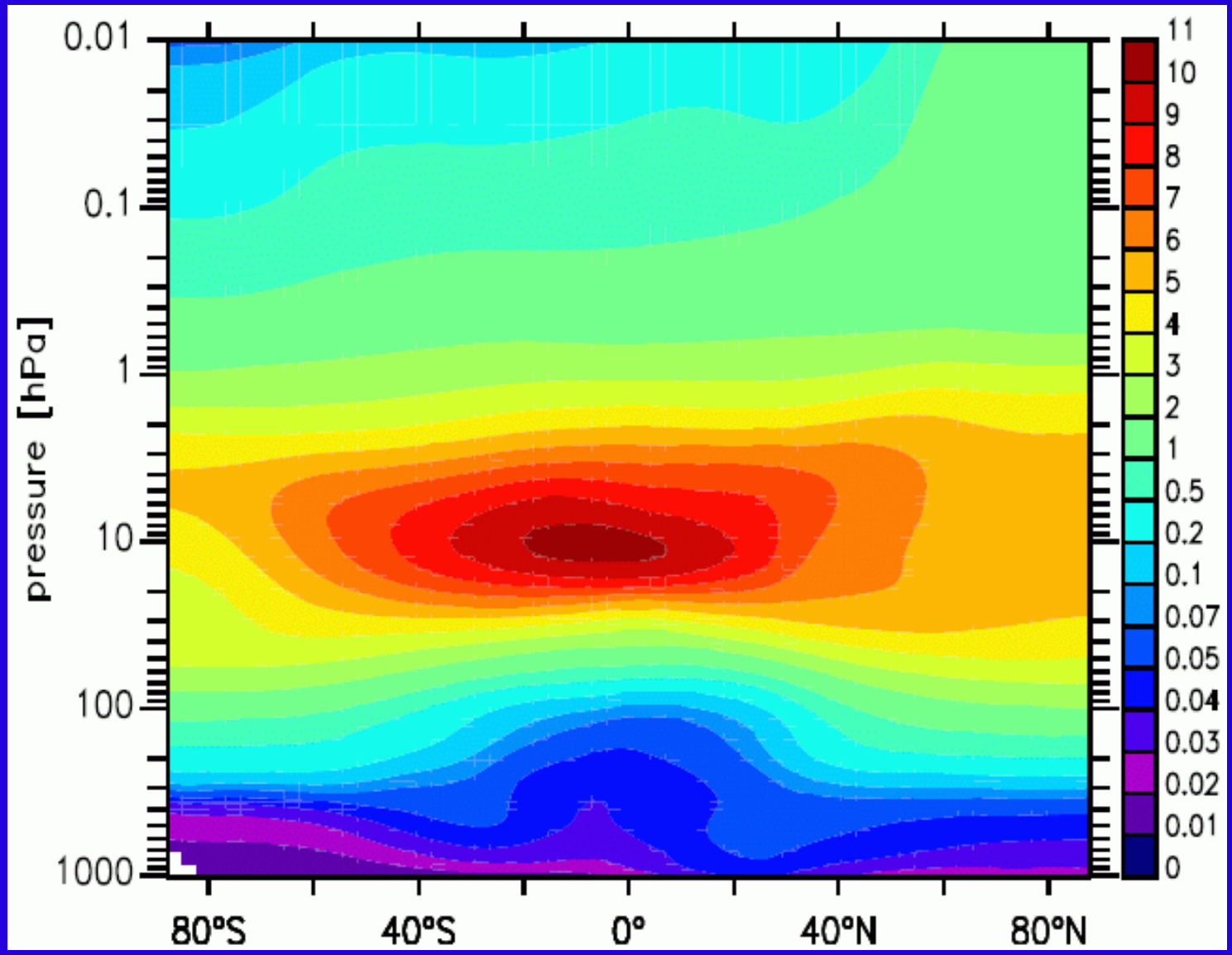
Ozone

Jöckel et al., ACP, 2006

consistent simulation of (dynamical and chemical) state of the atmosphere between surface and 0.01 hPa



4 year average (2000-2004, excl. 2002) of ozone (DJF) [µmol/mol]

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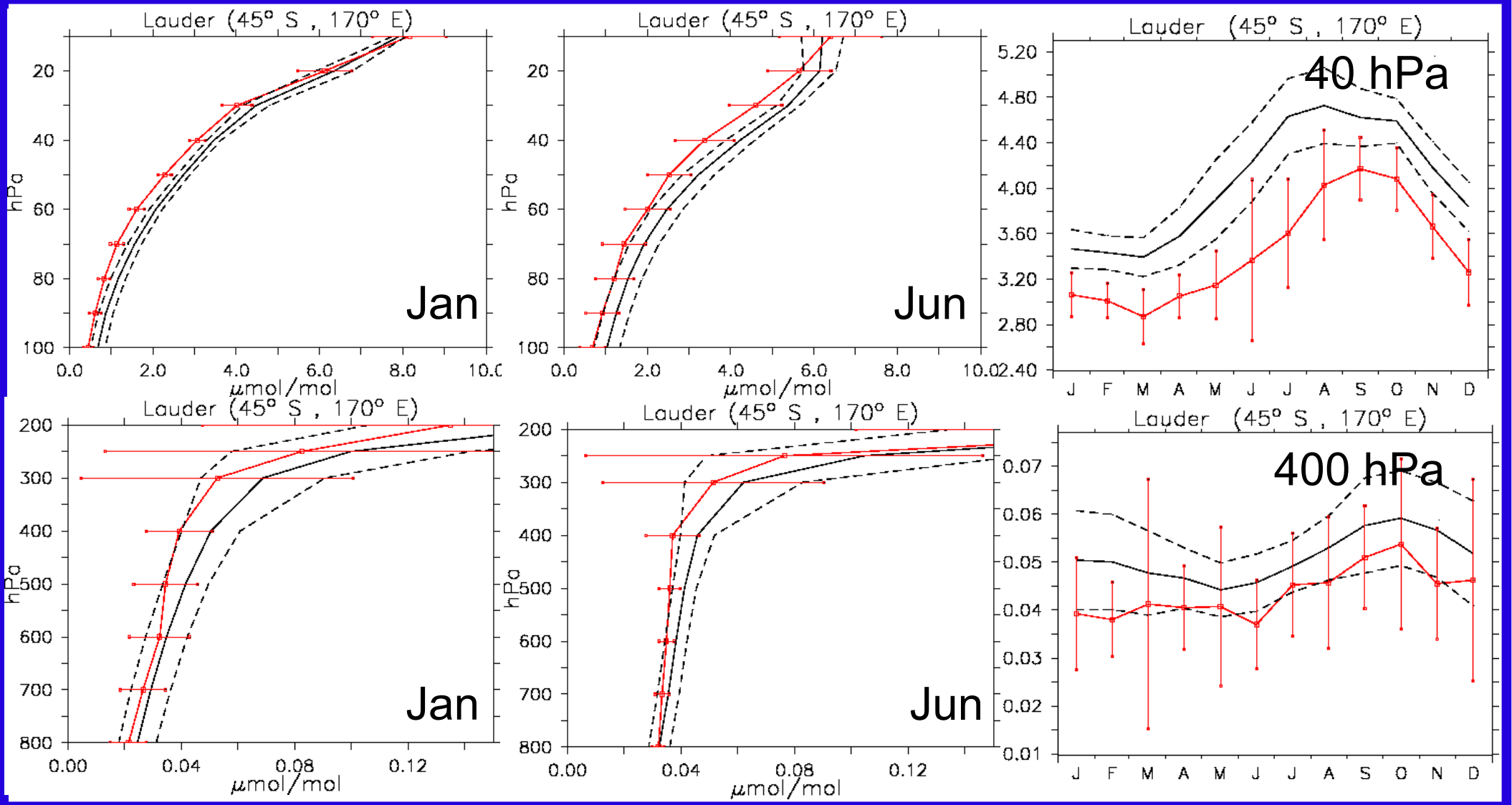
Ozone

Comparison with O_3 database (monthly averages)



Logan et al., JGR, 1999; Jöckel et al., ACP, 2006

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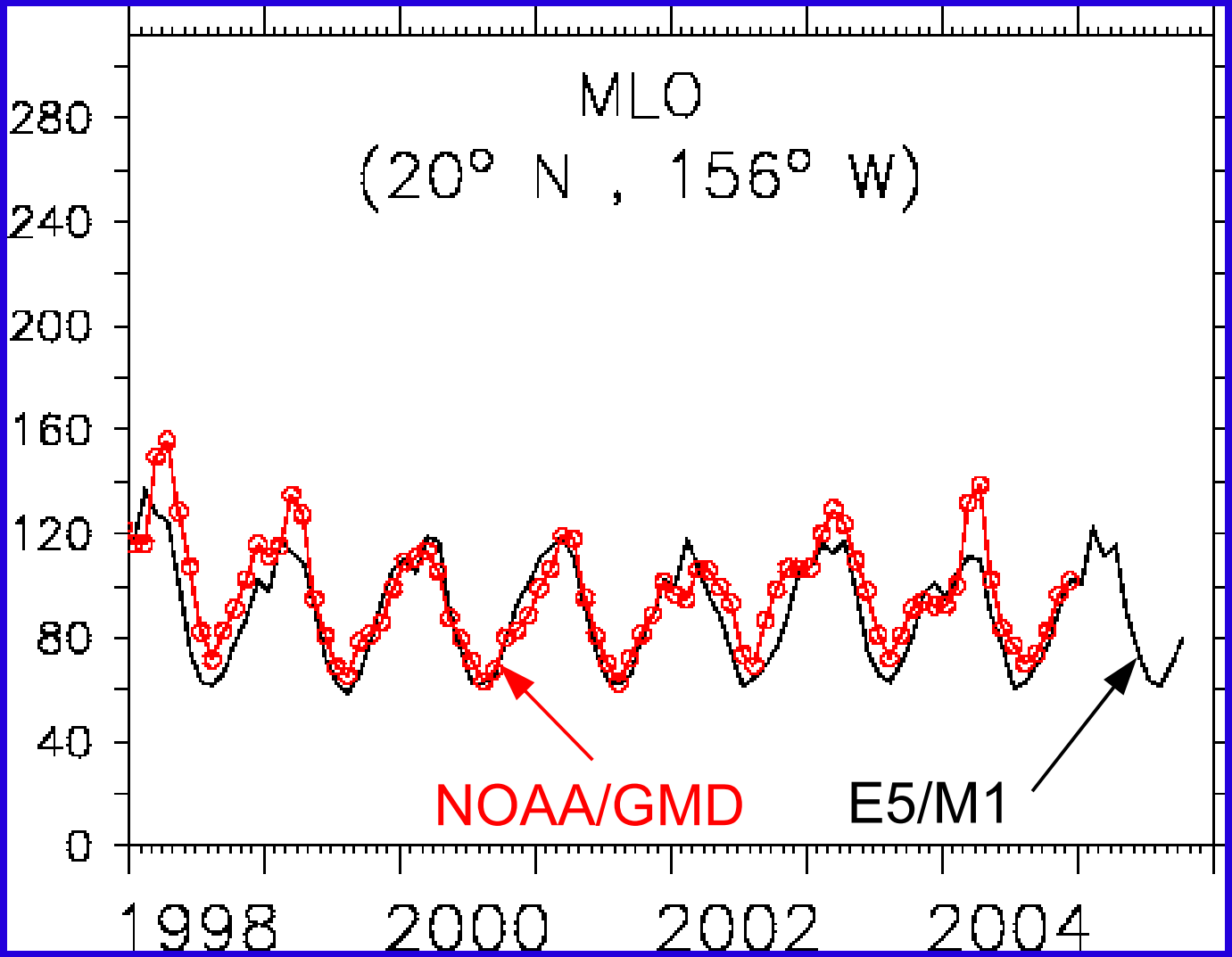
Carbon monoxide

Example:
tropospheric CO



Novelli et al., JGR, 1998
Jöckel et al., ACP, 2006
Pozzer et al., ACP, 2007

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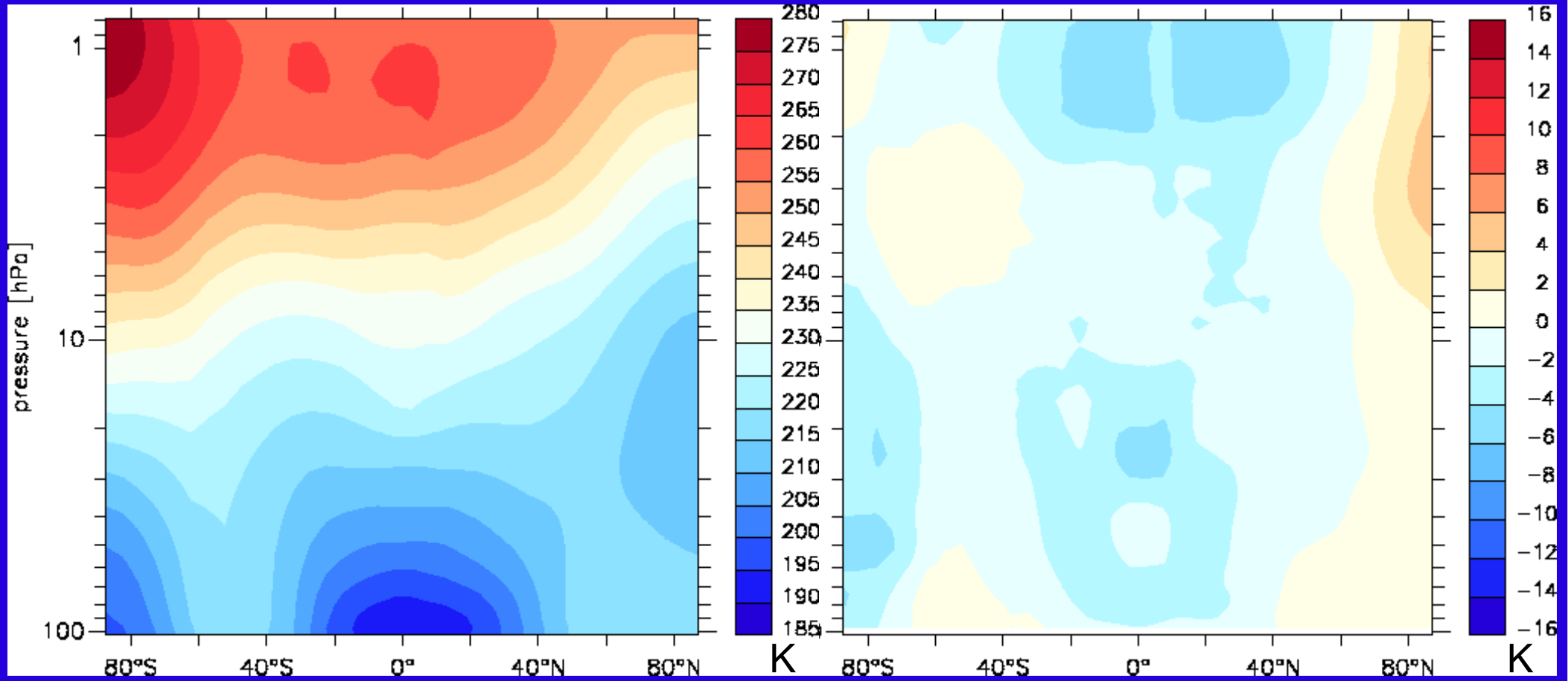
Temperature

Example: stratospheric temperature (SON 2003)

E5/M1 (S2)

E5/M1 - MIPAS



Jöckel et al., ACP, 2006

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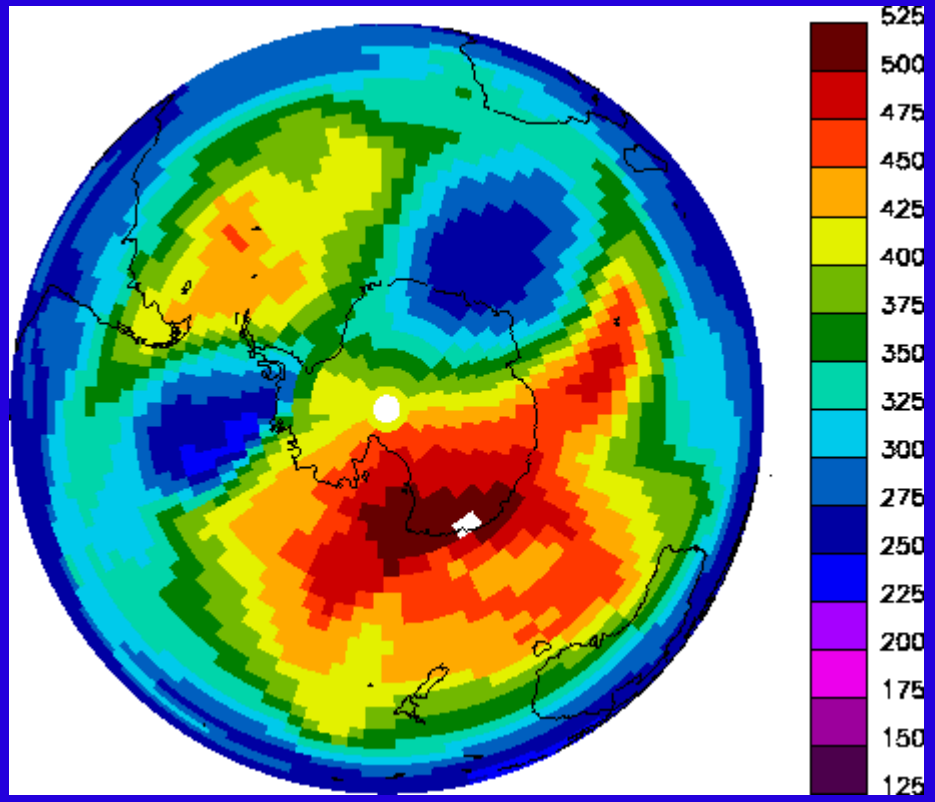
SH vortex split 2002

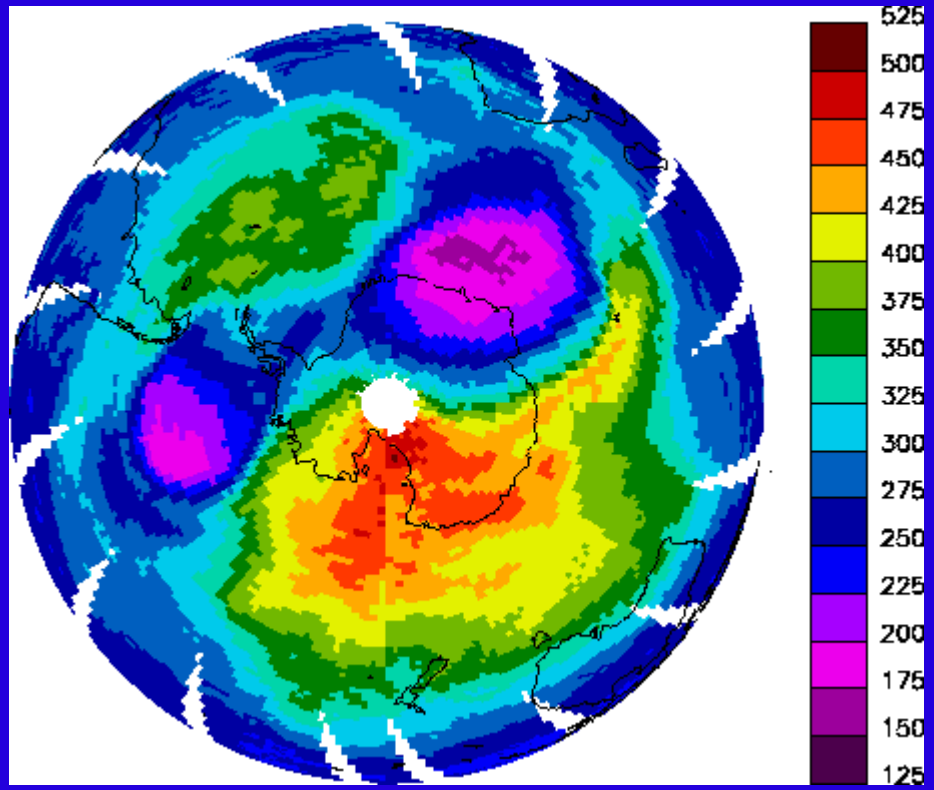
SH vortex split 2002 reproduced

Total Ozone [DU] 26 Sep 2002

E5/M1 (S2)



TOMS



Jöckel et al., ACP, 2006

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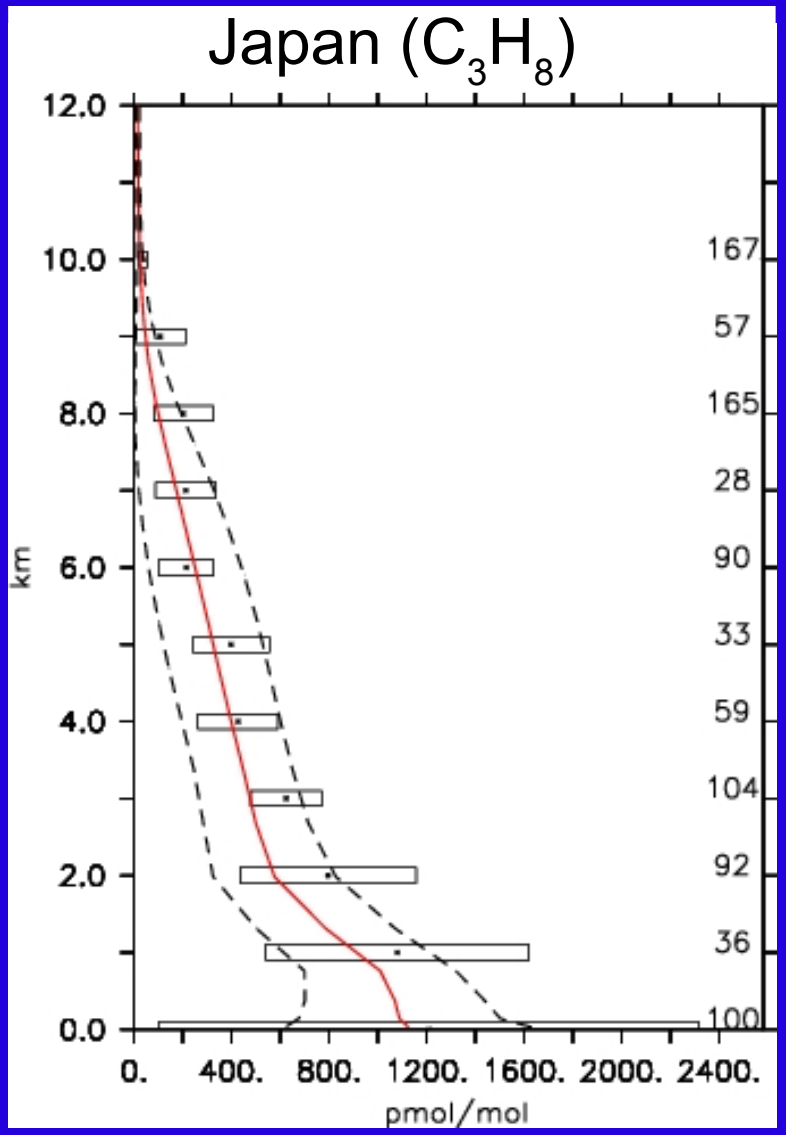
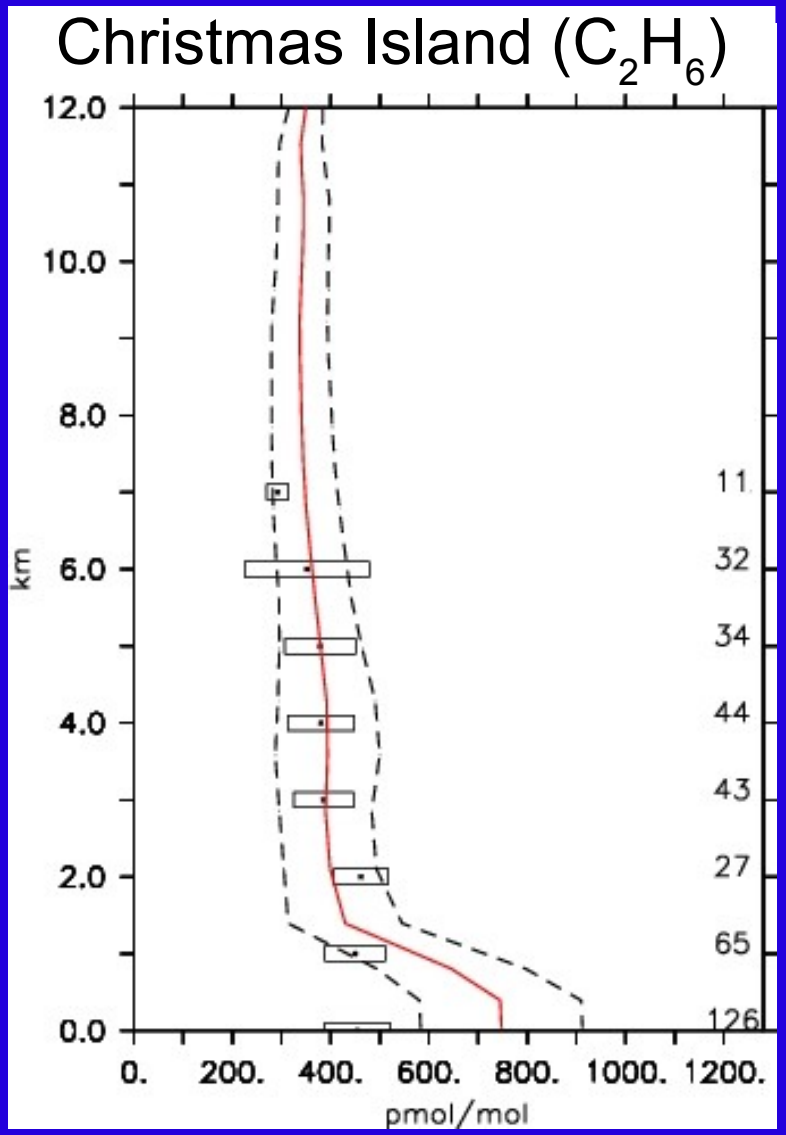
Organic species

Organic species

Example: Propane



Example: Ethane



Emmons et al.,JGR, 2000; Pozzer et al., ACP, 2007

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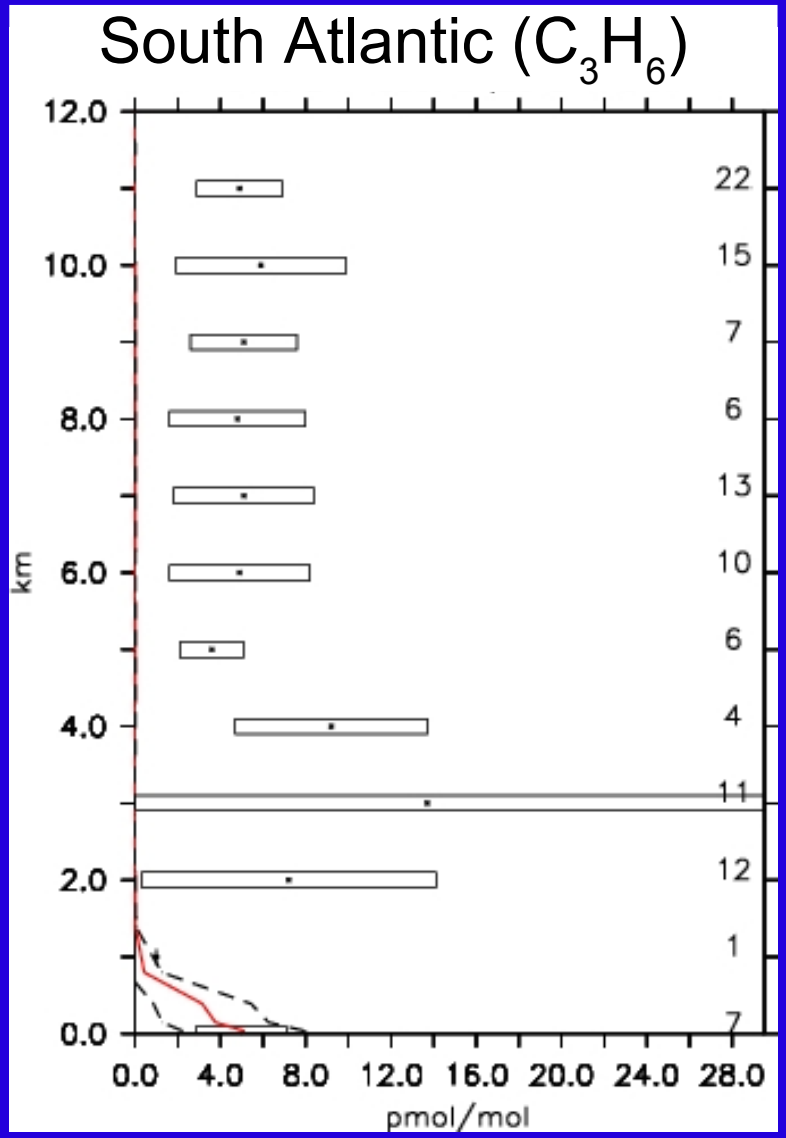
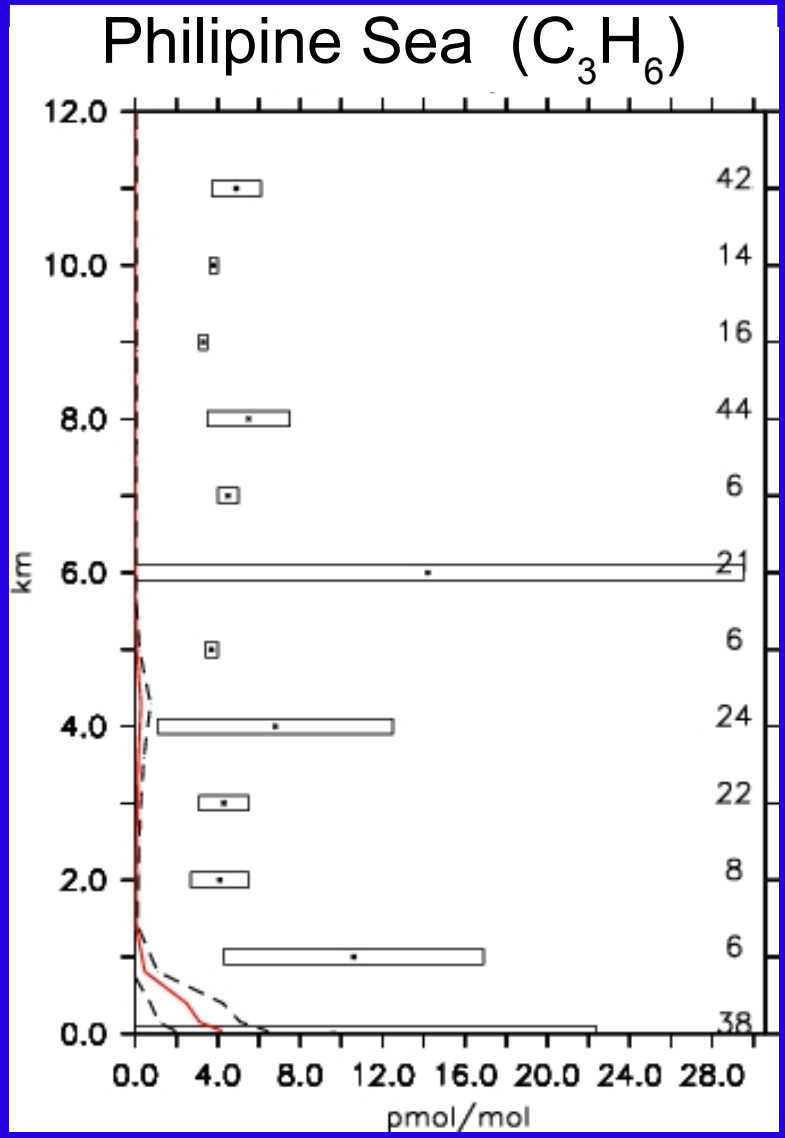
Organic species

...
some
fail
...

Example: Propene





Emmons et al.,JGR, 2000; Pozzer et al., ACP, 2007

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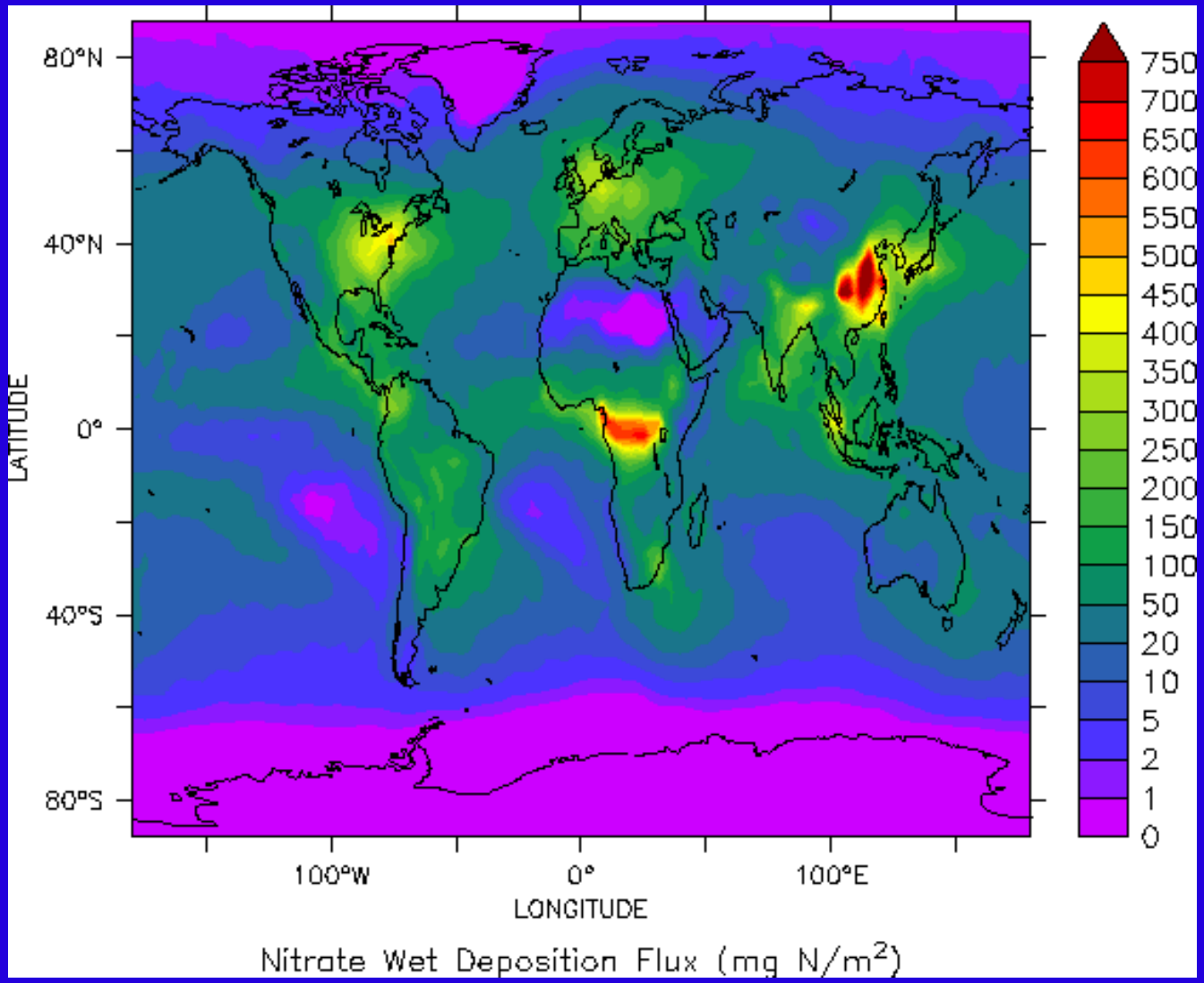
Wet deposition

Example: Nitrate [mg(N)/m^2/year]



Tost et al., ACP, 2007

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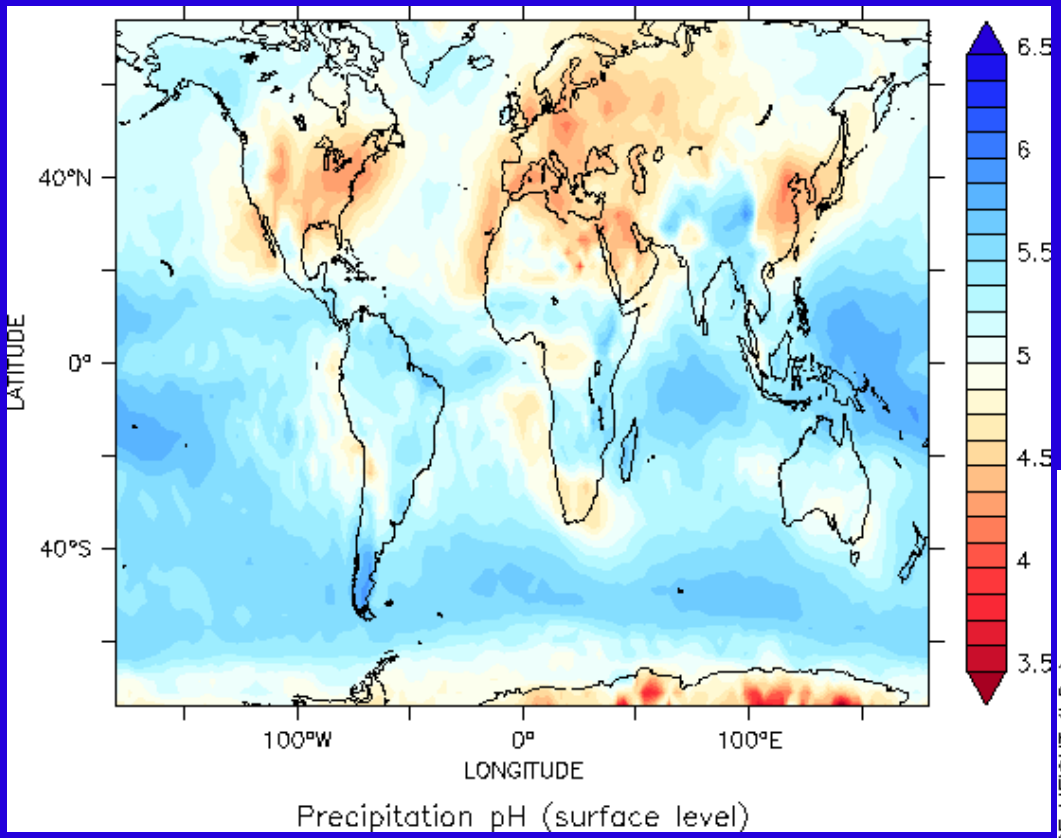
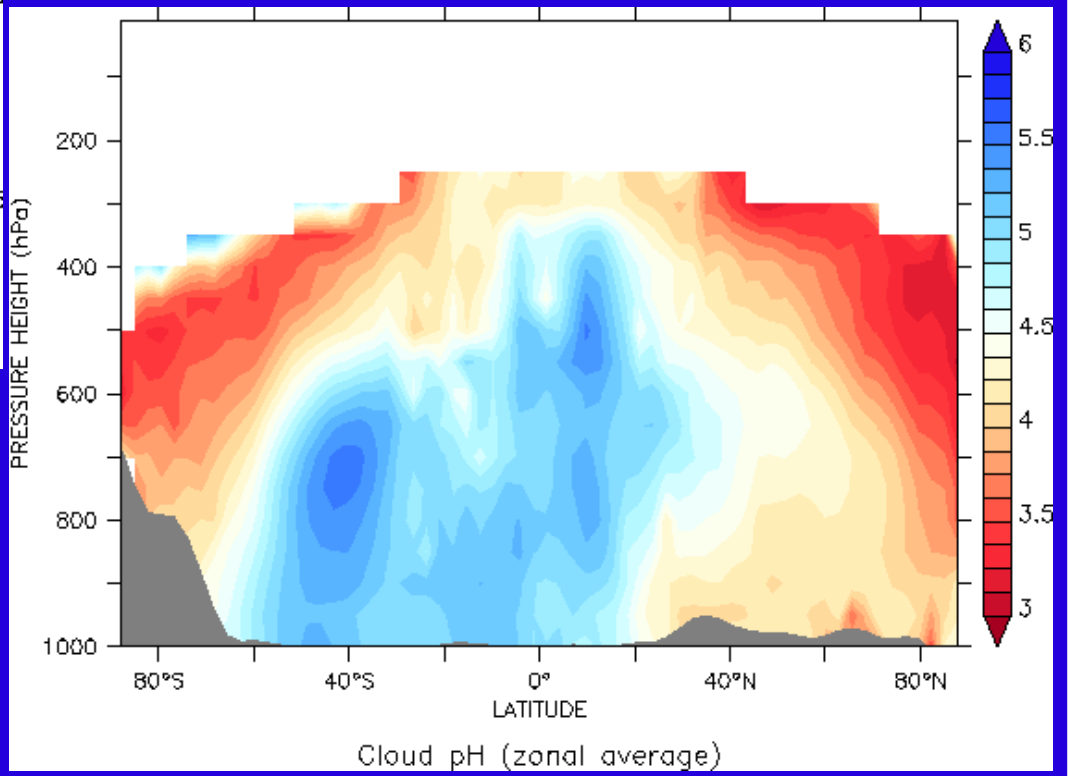
pH



precipitation pH

cloud pH



Tost et al., ACP, 2007

V. Some notes on the implementation and performance

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Performance

... is highly dependent on the chosen setup ...

Evaluation simulation (S1):

- ECHAM5/MESSy T42L90MA, 1998-2005
- IBM P4 “regatta”; 256 CPUs; (psi @ RZG):
  - ~ 8 hours (wall clock) / simulation month
  - ~ 1 Tb output / simulation year

>>> 70-80% of CPU time consumed by chem. kinetics

>>> high I/O load (MPI, dedicated I/O CPU, gather)
-> parallel-netCDF (MPI-2); work in progress

>>> parallelisation of ECHAM5:

- regional decomposition in grid-point space
  NCPUS = NPROCA x NPROCB
- “vector”-packing on every CPU:
  (NGPBLKS-1)xNPROMA + NPROMZ

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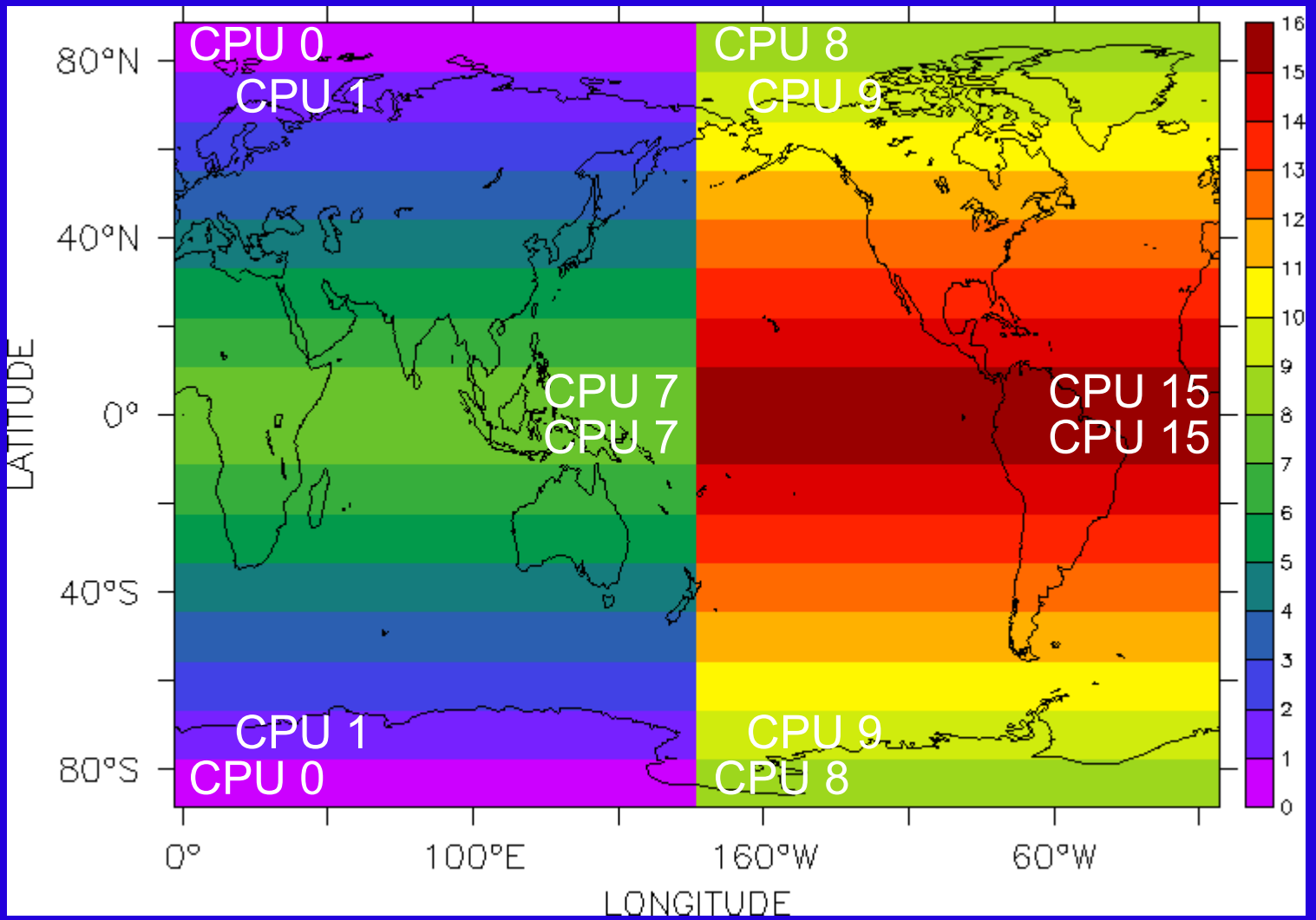
Parallelisation

EXAMPLE: T21L19 >>> 64 longitudes x 32 latitudes x 19 levels

NCPUS=16

NPROCB = 2

NPROCA = 8



choice of NPROCA NPROCB (NCPUS) limited by advection

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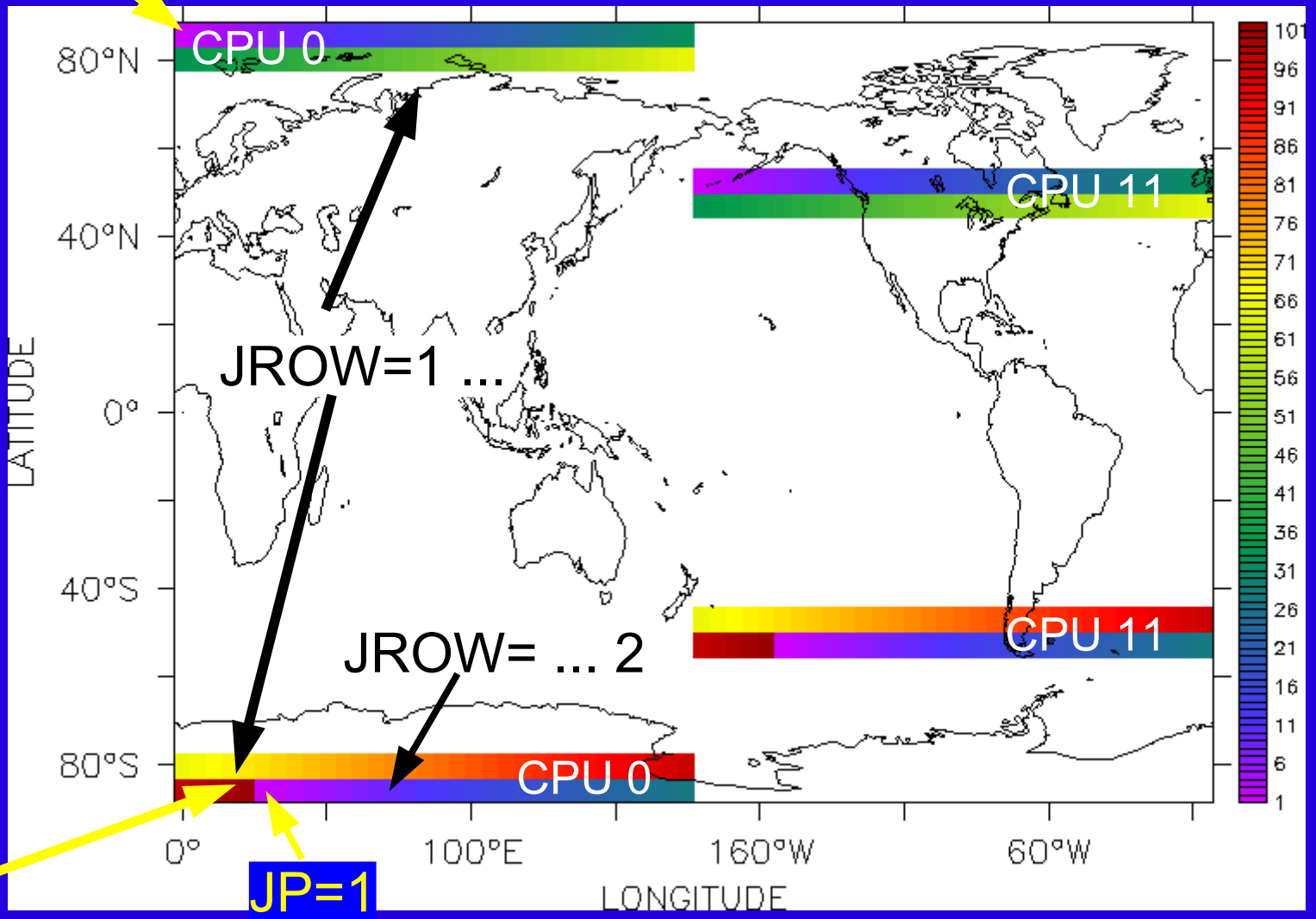
Vectorisation

on each CPU ...

optimal choice of NPROMA ?

vector-architectures: as large as possible

scalar-architecture: cache ???



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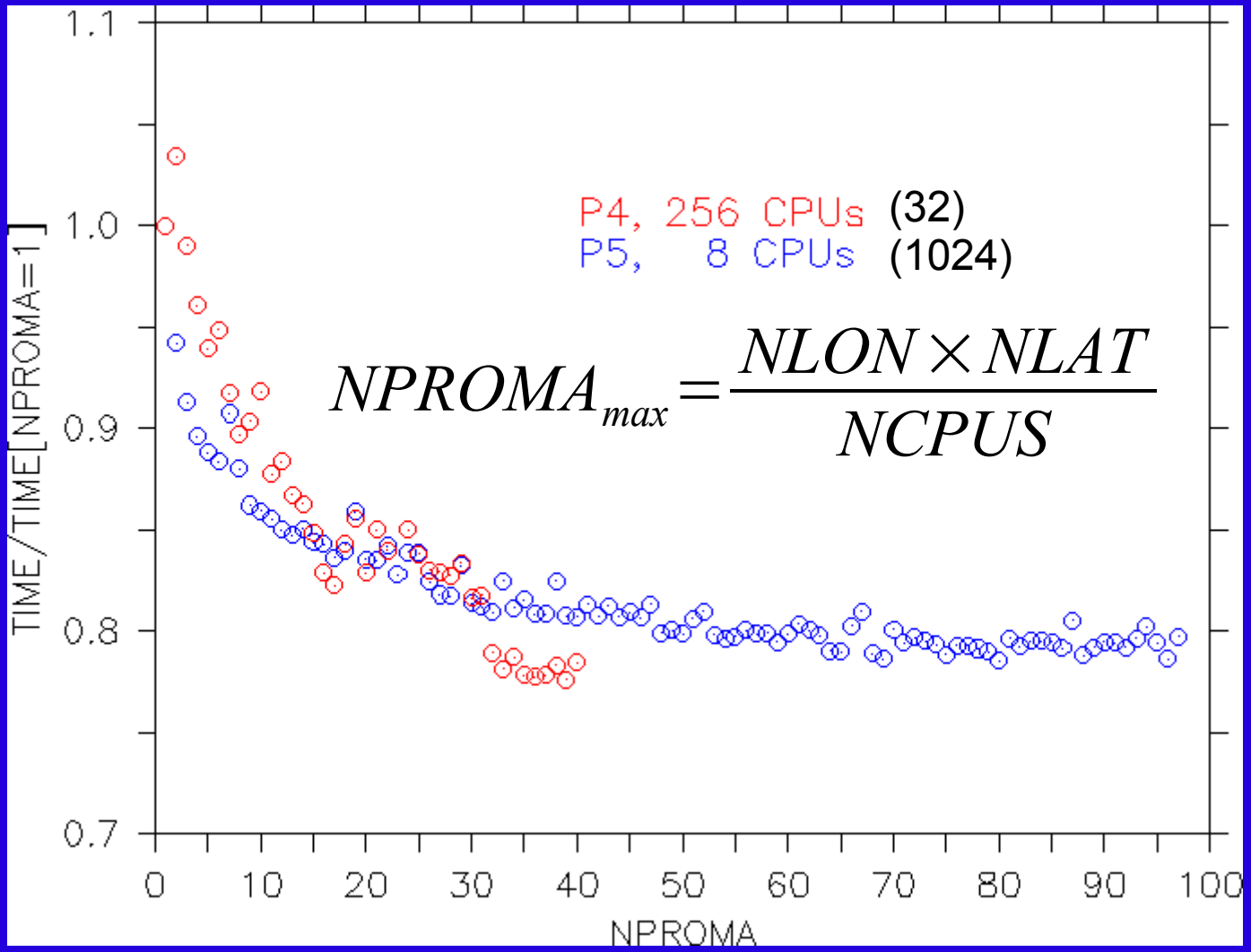
Vectorisation

Example: T42L90MA (128 longitudes x 64 latitudes x 90 levels)
WITH complex chemistry setup



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Performance issues

Problem (with parallelisation):

role of involved processes (with different computational demands) varies with space and time

Examples:

- convection / convective transport / scavenging
  - >>> tropics vs. polar region
- chemical transformations
  - >>> annual and diurnal cycle (photo-chemistry !)
  - >>> involved species
  - ~ ~ ~ stiffness of the ODE system describing the chemical kinetics ...
    (reaction rates vary over several orders of magnitude)
    SOLVER: - 'fast'
    - 'reliable', accurate
    - stable (!)

>>> 3rd order Rosenbrock with automatic time stepping

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Automatic time-stepping

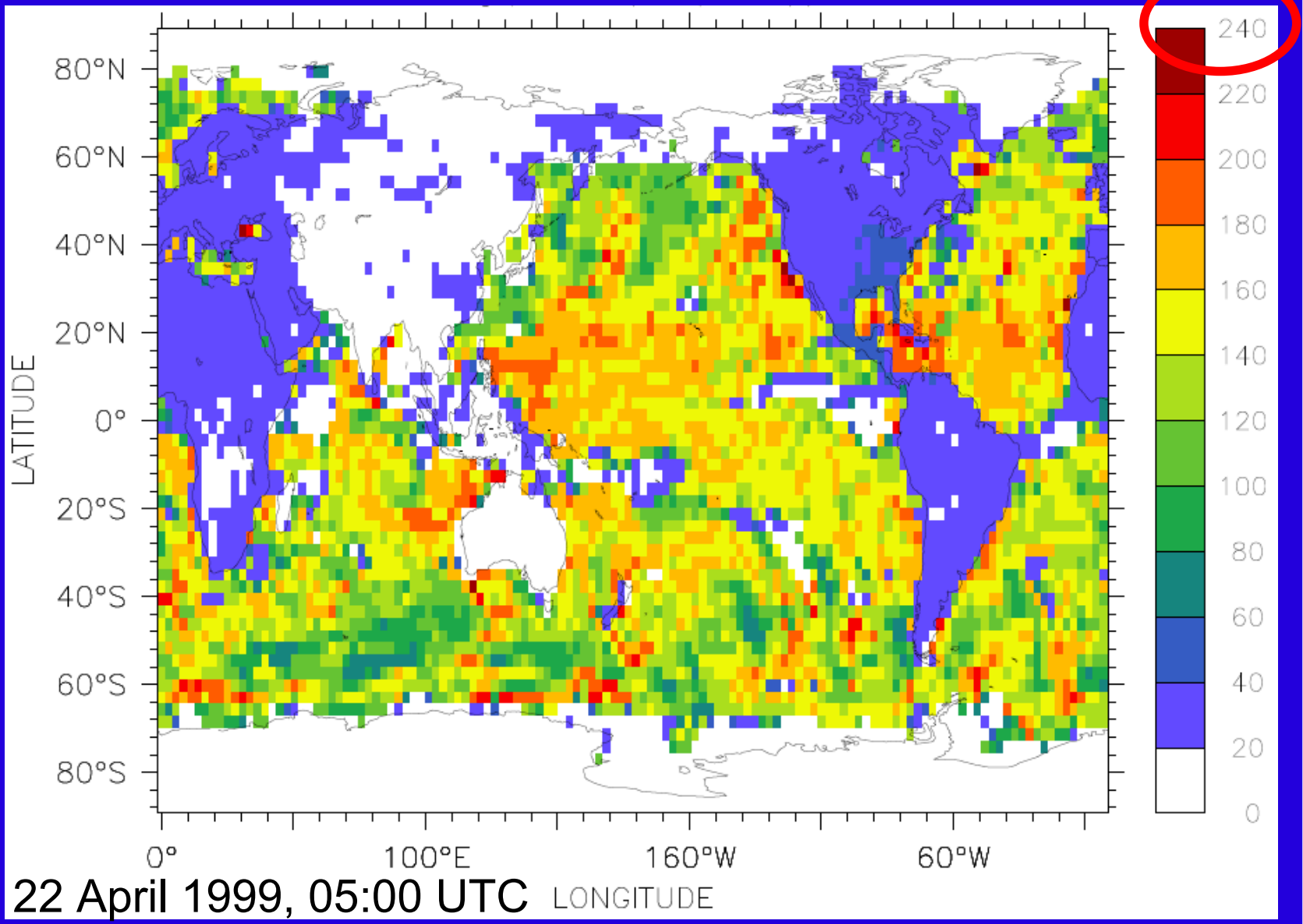
number of kpp (ros3-auto) substeps

Kerkweg et al., ACP, 2007

lowest model layer (~ 70m) with (sea-salt-) aerosol chemistry

>>>

very stiff ODE system



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Automatic time-stepping

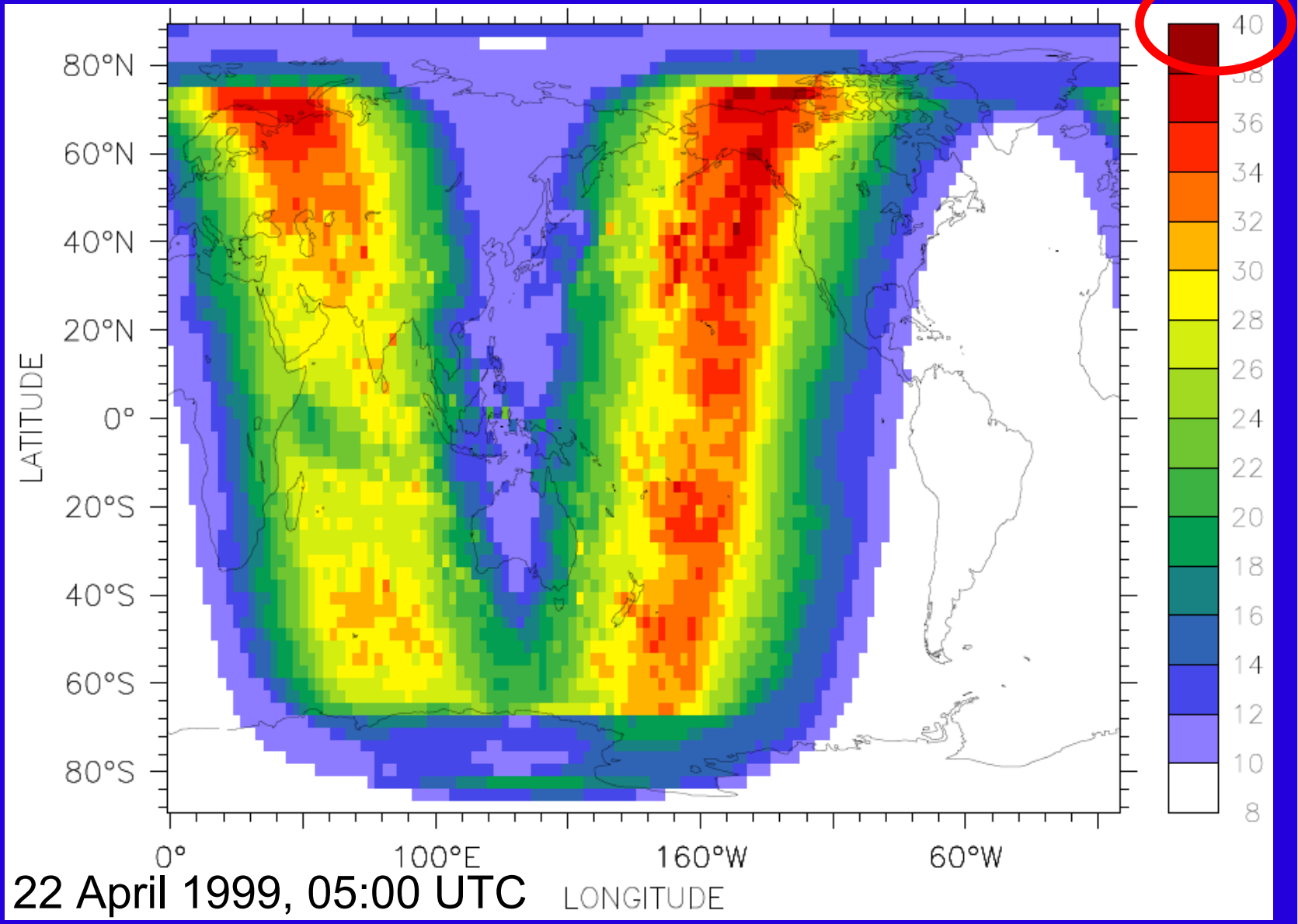
Kerkweg et al., ACP, 2007

number of kpp (ros3-auto) substeps

70 hPa
(~ 50 km)
only gas
phase
chemistry

>>>

lower stiffnes
of the ODE
system



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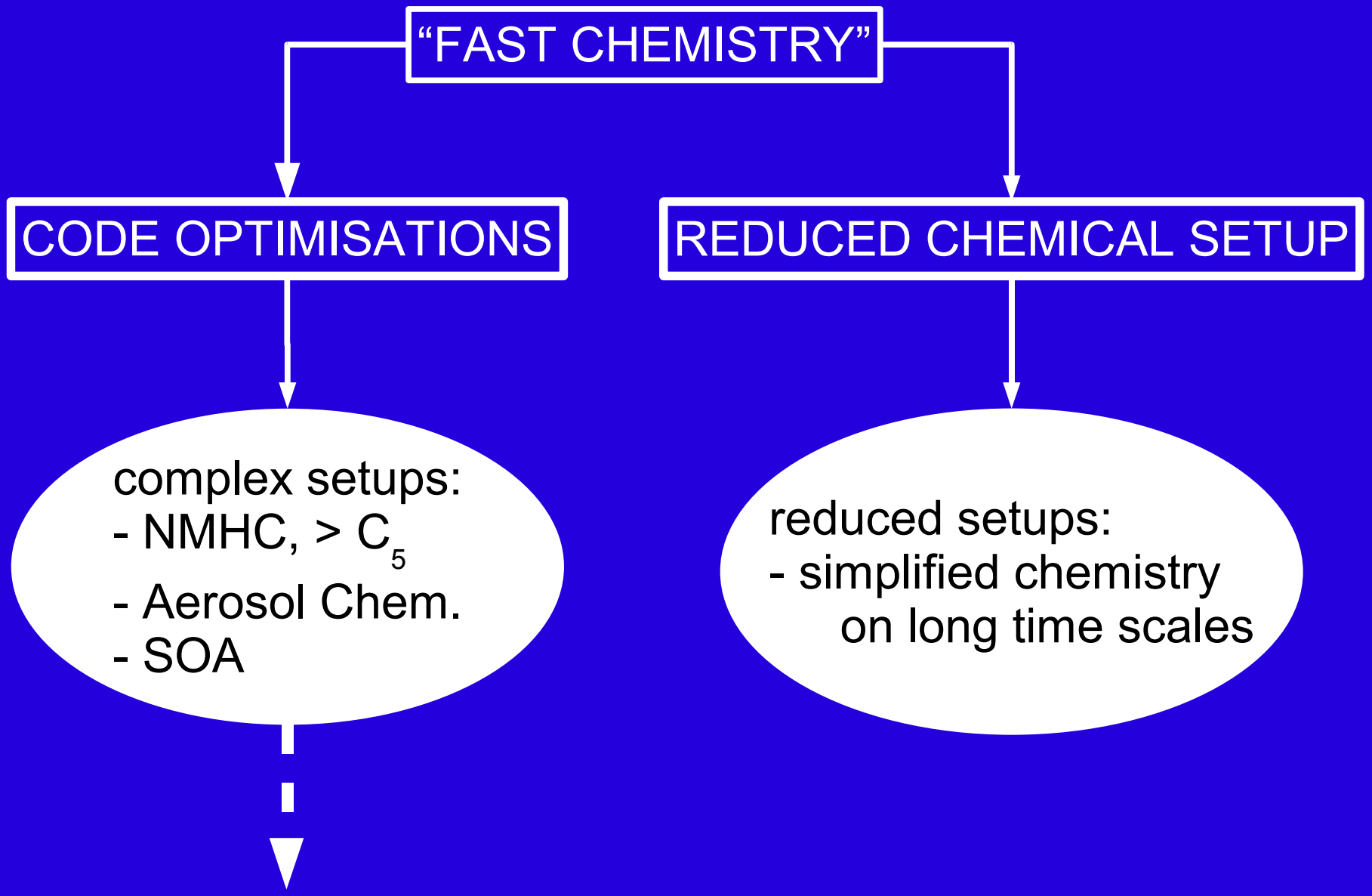
Performance ???



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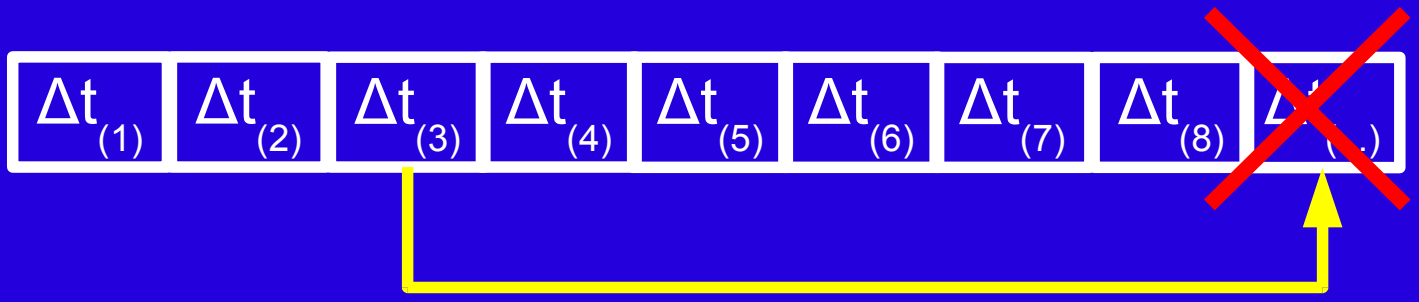
Vectorisation of KPP code

OUTER LOOP: grid-box
INNER LOOP: solver (automatic time stepping)

"**scalar**" implementation

OUTER LOOP: solver (automatic time stepping)
(applied to vector of grid-boxes)
+ (de-)compression algorithm



"**vector**" implementation

"sort-out" every box for which solver finished time-stepping

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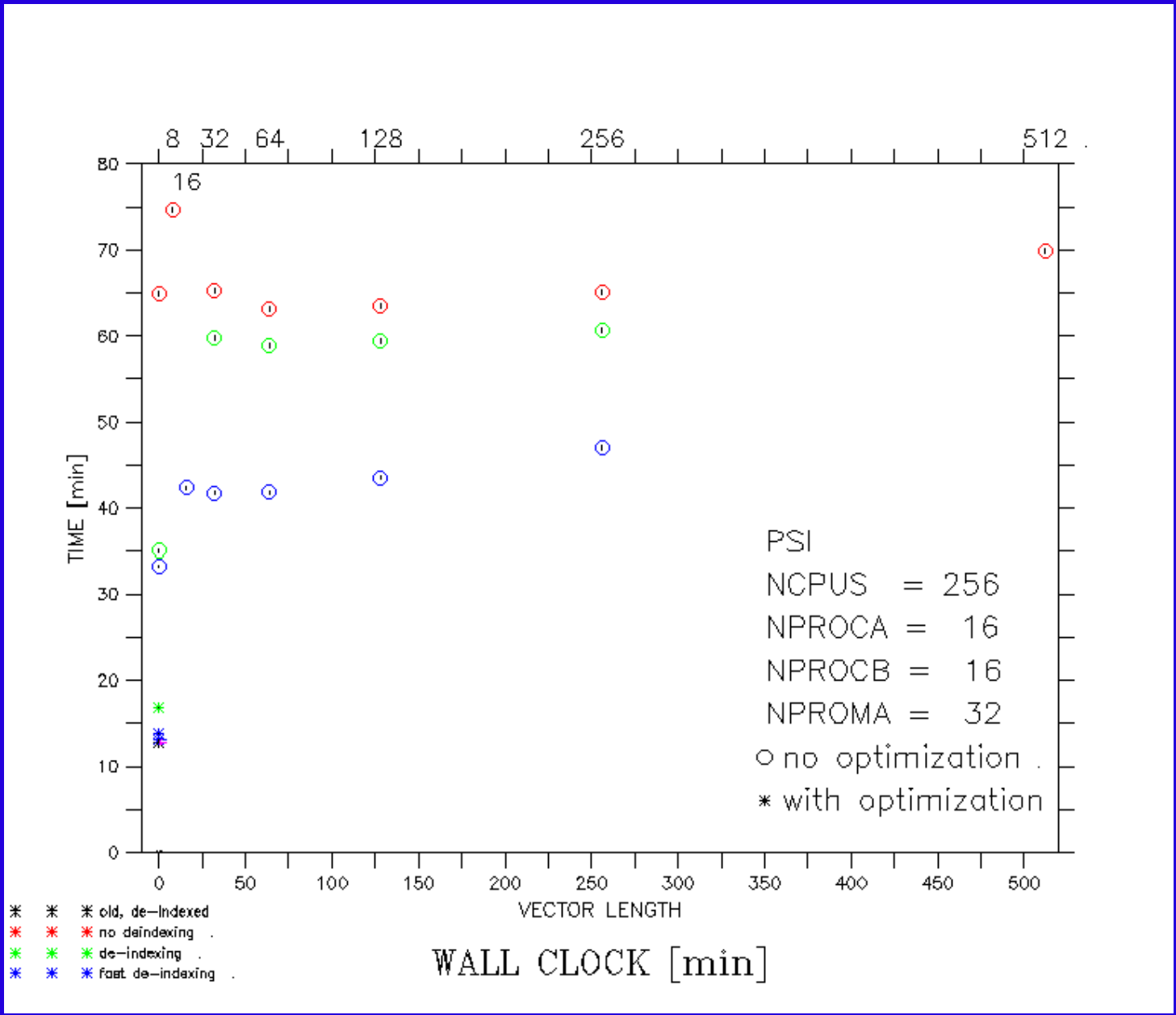
Vectorisation of KPP code

on p4/p5:

scalar implementation is much faster than vector implementation

>>>

overhead of (de-compression) exceeds gain of cache usage optimisation



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scalar sparse LU-decomposition

... loop with indirect indexing ... replaced by sequence of operations

average wall-clock time
per simulation time step

p4
256 CPUs
T42L90MA
complex chemistry

no de-indexing	64.97s	-qnoopt
de-indexing (1)	35.08 s	-qnoopt
de-indexing (2)	13.84 s	
de-indexing (2)	13.04 s	JVS(:) -> JVS(LU_NONZERO)
de-indexing (2)	13.11 s	JVS(:) -> JVS(LU_NONZERO) -Q-kppdecomp
de-indexing (1)	12.85 s	JVS(:) -> JVS(LU_NONZERO) -Q-kppdecomp

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Scaling

Example: T42L90MA (128 longitudes x 64 latitudes x 90 levels)
WITH complex chemistry setup (1 day integration) ;
measured with “-pg” - Option on p4/p5

256 / (2*8) = 16

	P5 (8 CPUs) (CPU 2)	P4 (256 CPUs) (CPU 40)	
TOTAL	6938 s	645 s	10.76
CHEM. SOLVER	5382 s	262 s	20.54
ADVECTION	381 s	23 s	16.57

!!! preliminary results: choice of arbitrary CPU for comparison is NOT appropriate

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www.messy-interface.org

special issue in Journal of Atmospheric Chemistry and Physics

http://www.atmos-chem-phys.net/special_issue22.html

Thank you very much for your attention !