EXA-SCALE CHALLENGES AND OPPORTUNITIES FROM THE ATMOSPHERIC CHEMISTRY AND CHEMISTRY CLIMATE MODELLING PERSPECTIVE

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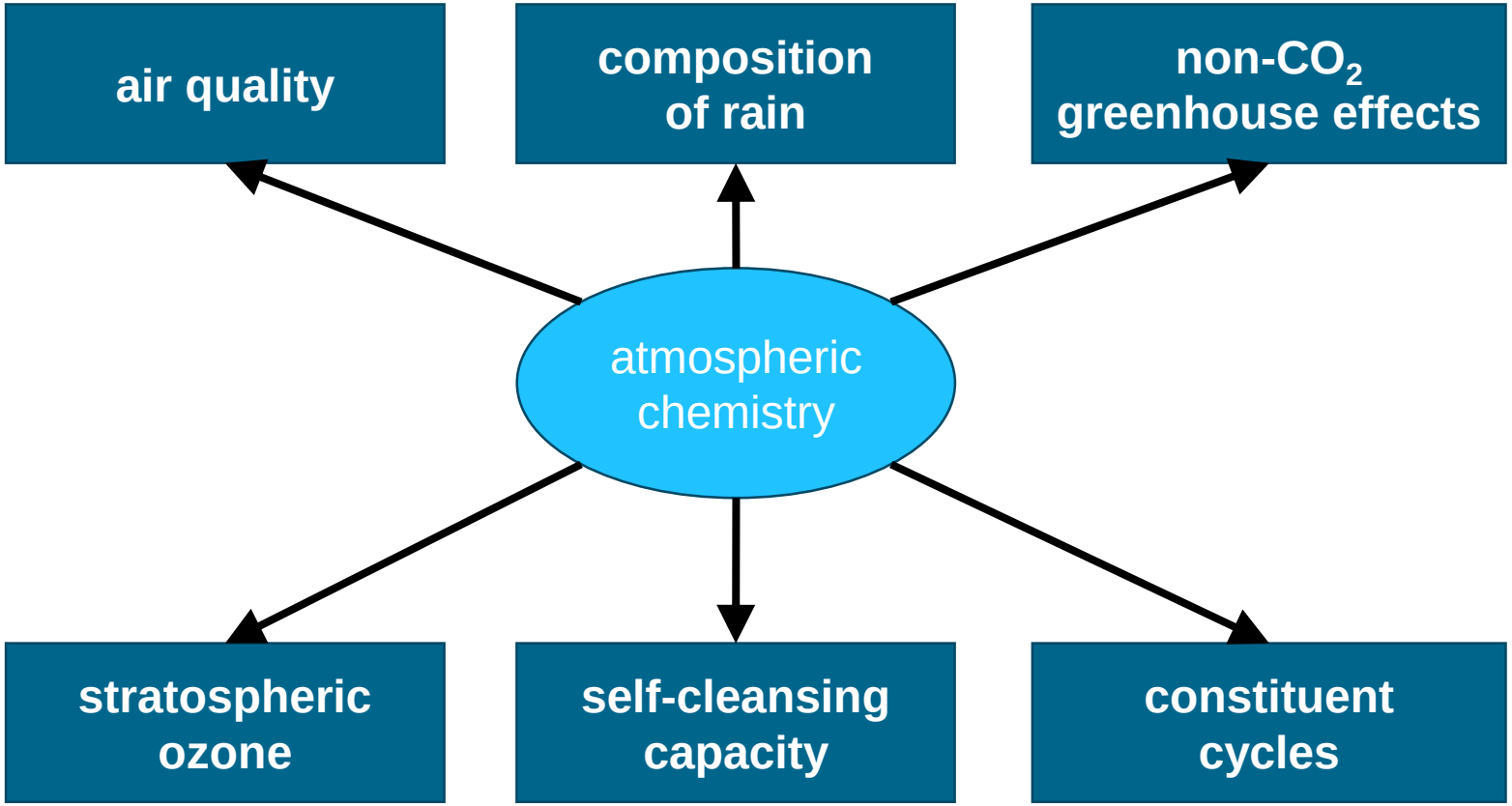
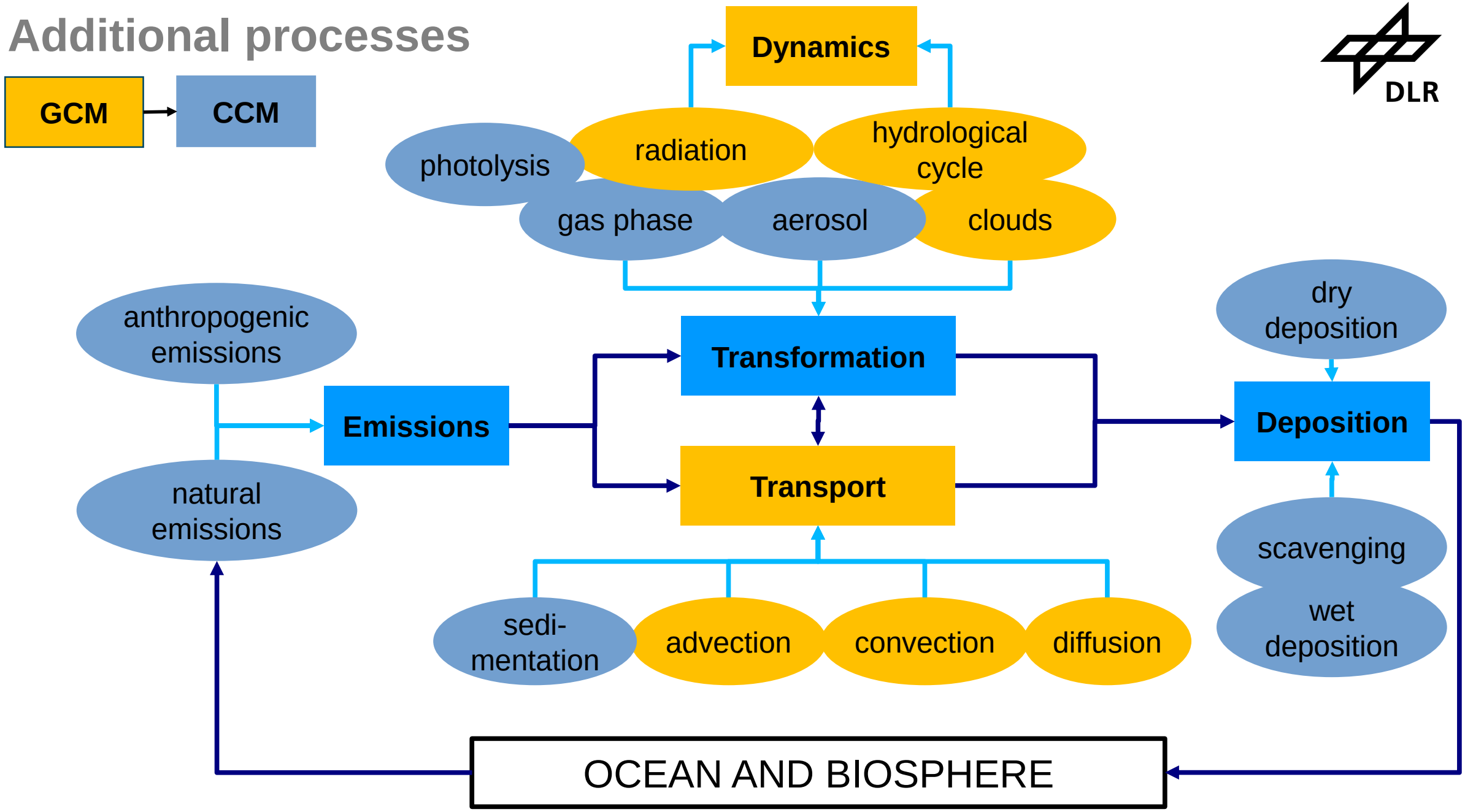
DKRZ User Workshop, Oct 12, 2022, Hamburg

Atmospheric Chemistry



Additional processes



Additional processes

- Tracers (=prognostic variables) describing the chemical compounds (large scale advection, convective transport, diffusion, …)
- Kinetic system(s) describing the chemical reactions in gas-, liquid-, and aerosol phase
- calculation of photolysis rates and heterogeneous reaction rates (incl. PSCs)
- aerosol micro-physics and interaction with clouds
- Sources of chemical compounds
  - Prescribed gridded data of emission fluxes (mostly reactive species), and/or
  - Prescribed gridded lower boundary condition of mixing ratio (mostly long lived)
  - on-line calculation (lightning NOx, dust, sea-salt aerosol, biogenic organics, soil-NOx, air-sea exchange, …)
- Sinks of chemical compounds
  - dry deposition
  - wet deposition
  - sedimentation (aerosol)
- Feedback on radiation, hydrological cycle, clouds, …

- + additional on-line diagnostics

Number of prognostic variables

	GCM	CCM	CCM+	CCM+AQ
Stratospheric chemistry	--	Ozone + CH_4/H_2O PSCs	Ozone + CH_4/H_2O PSCs + VSLS	Ozone + CH_4/H_2O PSCs + VSLS + sulphur cycle
Tropospheric chemistry - **gas phase** - **aqueous phase** - **aerosol phase**	 -- -- --	 -- -- --	 HOx/NOx , C_4 + Isoprene ++ --	 … + >C_5 + S … + ~C_4 + S + … … + ~C_4 + S + …
# of prognostic variables	~ 10	~ 50	~100 – 500	2500
# chemical reactions	--	< 100 + 0 + 0	~ 300 + ~100 + 0	~ 2000 + ~300 + ~300
			CCMI + CMIP6	

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12.10.2022

MESSy Consortium

ESM Advanced Earth System Modelling Capacity

ExaESM Pilot Lab Exascale Earth System Modelling

ccmi chemistry-climate model initiative

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	GCM	CCM	CCM+	CCM+AQ
Stratospheric chemistry	--	Ozone + CH_4/H_2O PSCs	Ozone + CH_4/H_2O PSCs + VSLS	Ozone + CH_4/H_2O PSCs + VSLS + sulphur cycle
Tropospheric chemistry	-- -- --	-- -- --	HOx/NOx , C_4 + Isoprene ++ --	… + >C_5 + S … + ~C_4 + S + … … + ~C_4 + S + …
# of prognostic variables	~ 10	~ 50	~100 – 500	2500
# chemical reactions		~ 0 + 0 + 0	~ 300 + ~100 + 0	~ 2000 + ~300 + ~300
			CCMI + CMIP6	

x 10

memory/core & I/O

FLOPS

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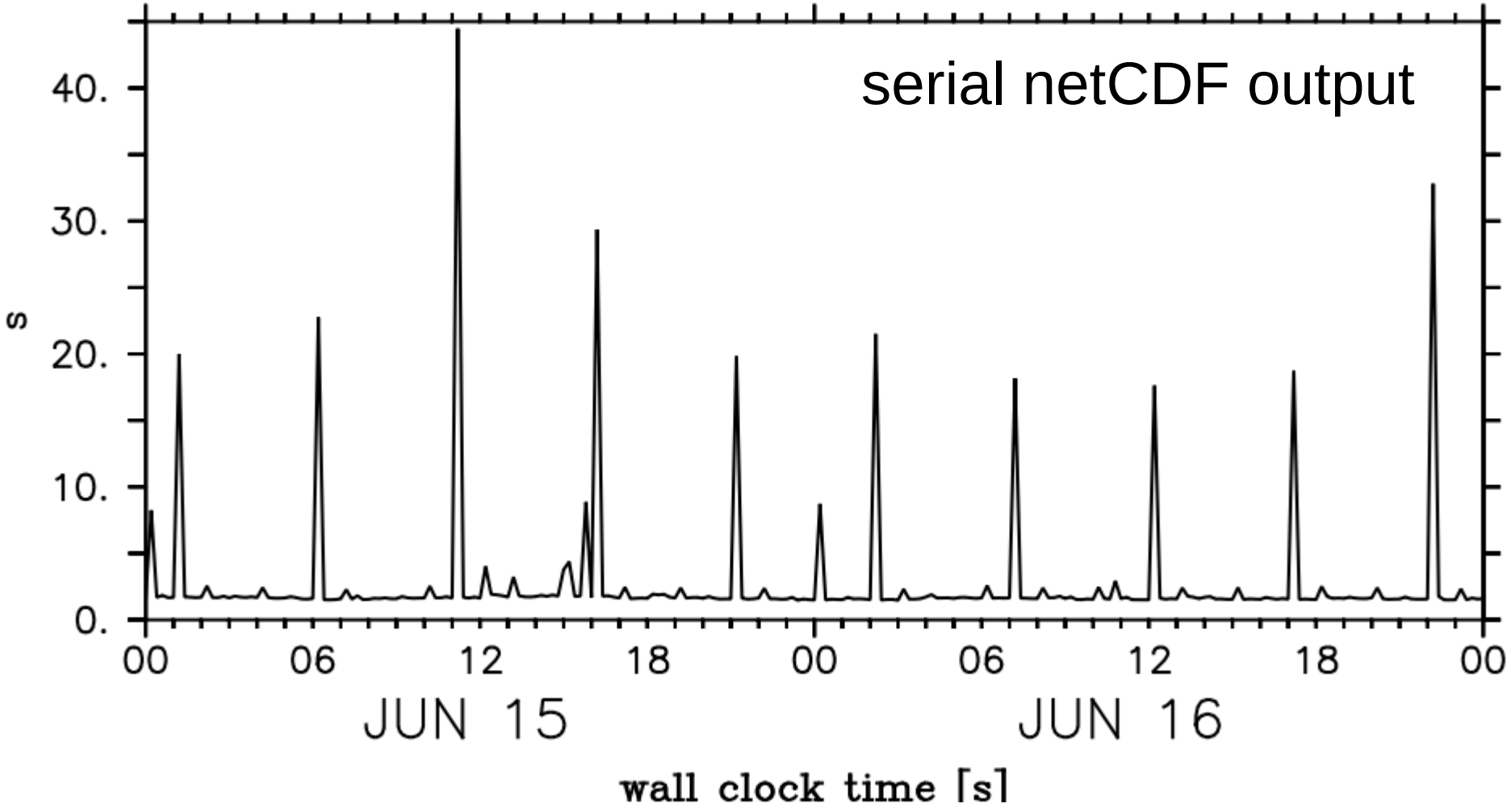
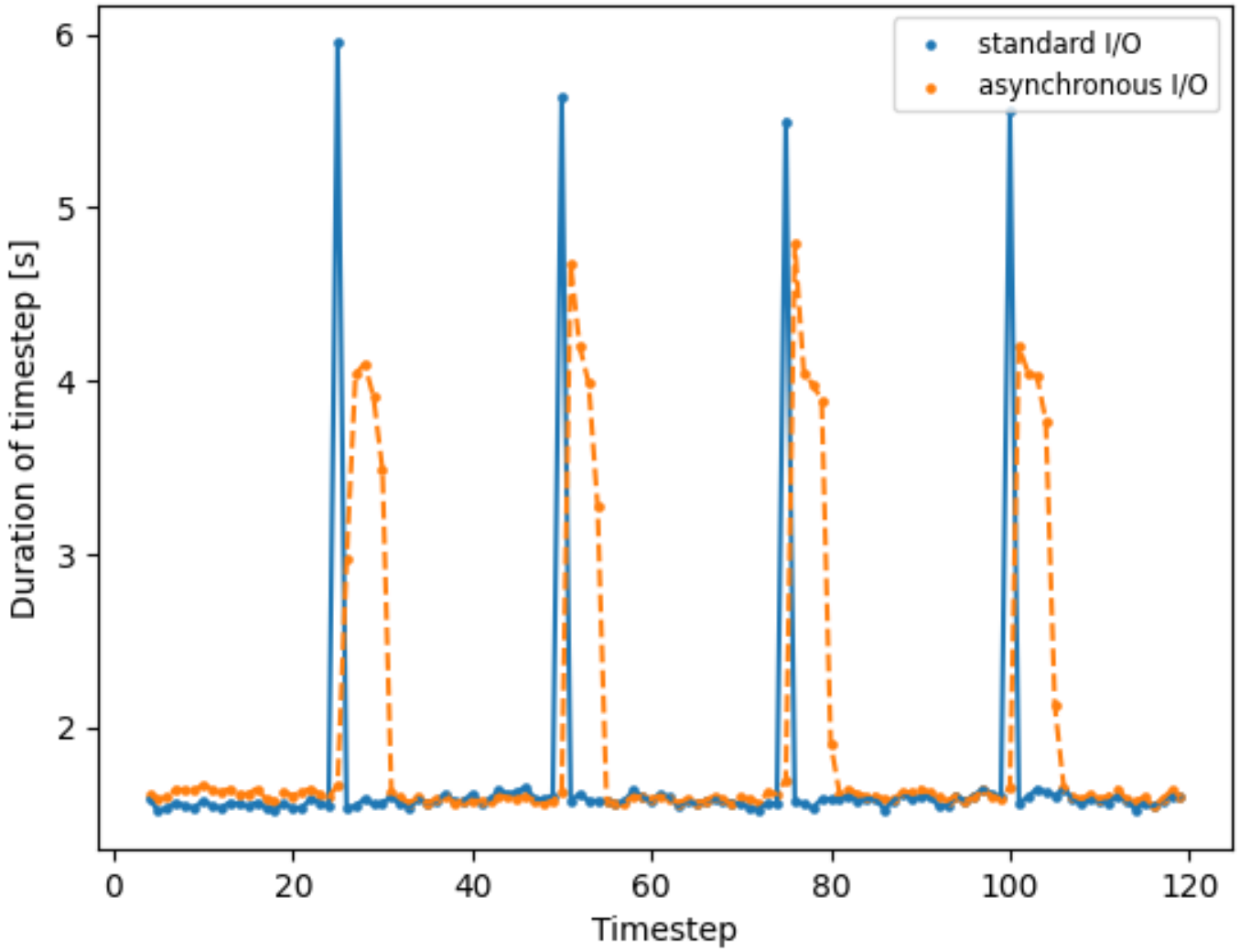
Wall clock time per simulated time step
Example: EMAC T42L90MA, Δt = 12 min, RD1SD-made3-01
512 MPI tasks on 4 levante nodes



6 TByte/year

→

- parallel or distributed &
- asynchronous



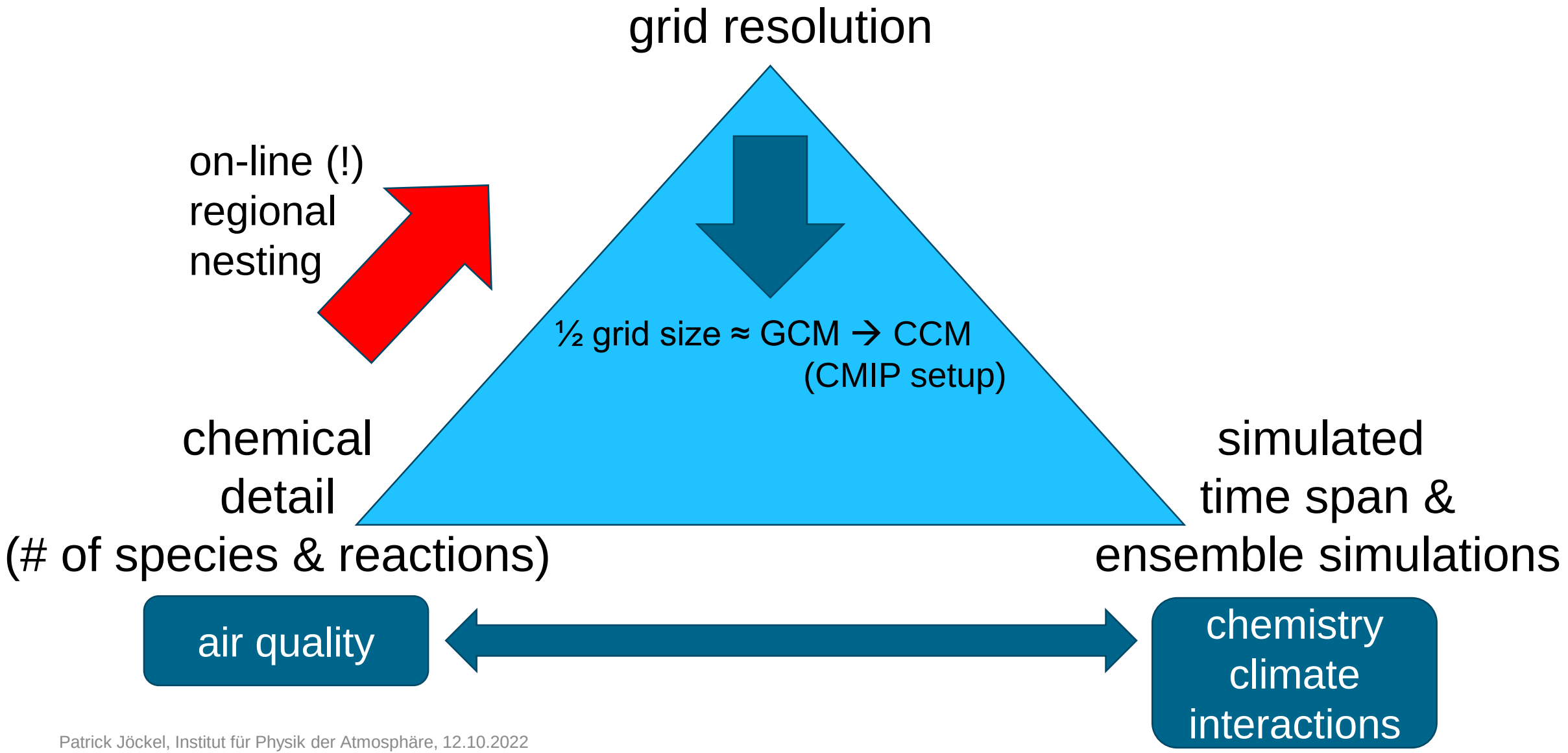
- CPU time
- wall-clock time reduced by 5%
- not yet distributed

Profile

(*courtesy of T. Kirfel (FZJ-IEK8), K. Hartung (DLR-PA)*)

Submodel	Process	Using KPP	% of subgrid_loop CCMI-2	% of subgrid_loop MOM
MECCA	Gas phase chemistry	**Yes**	**67.9**	**83.6**
SCAV	Wet deposition & liquid phase chemistry	**Yes**	**16.0**	**8.3**
CONVECT	Convection		4.8	2.3
CVTRANS	Convection tracer transport		4.8	4.5
RAD	Radiation		1.4	0.2
E5VDIFF	Vertical turbulent exchange		1.2	0.5
MSBM	Multiphase stratospheric box model		1.0	0.1
JVAL	Photolysis rate		0.6	0.1

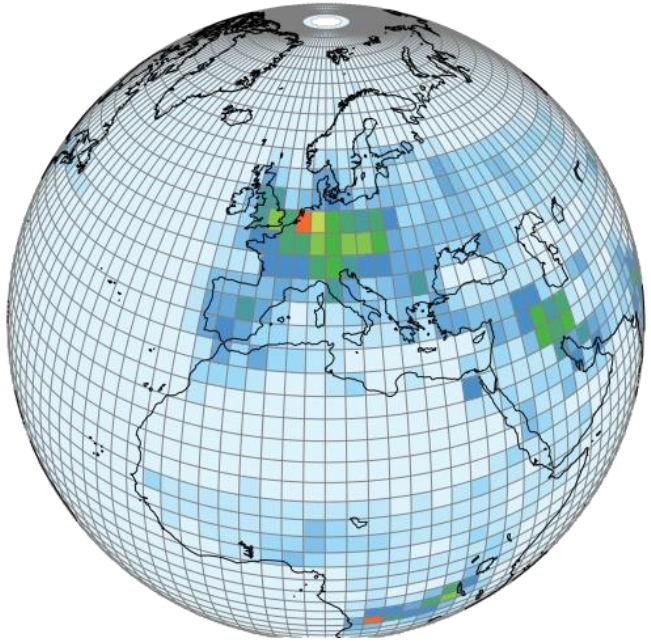
Compromises



On-line nesting (MPMD setup, high coupling frequency)

CLIMATE

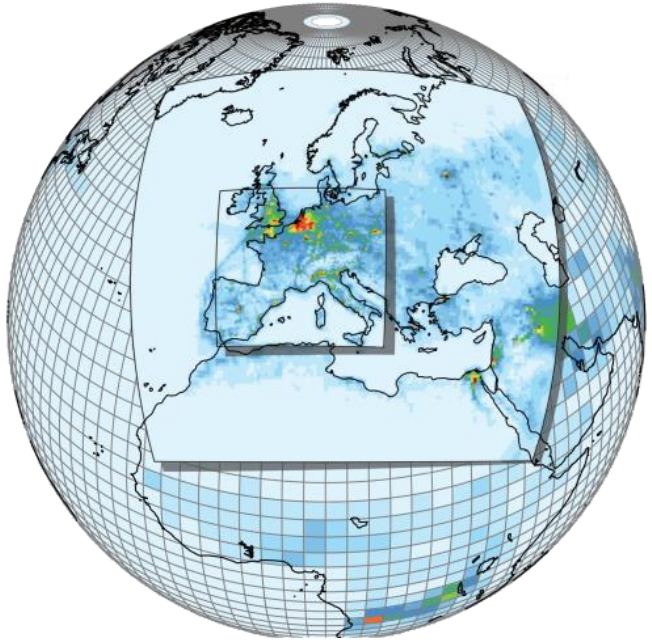
EMAC



ECHAM/**M**ESSy
Atmospheric **C**hemistry CCM

on-line nesting

MECO(n)



MESSy-fied **E**CHAM and
COSMO models nested ***n*** times

AIR-QUALITY

- consistency (through common submodels)
- dynamical & chemical boundary conditions consistent on short time scales
- multiple nests possible
- external coupling: name space & (almost) arbitrary grid sizes possible

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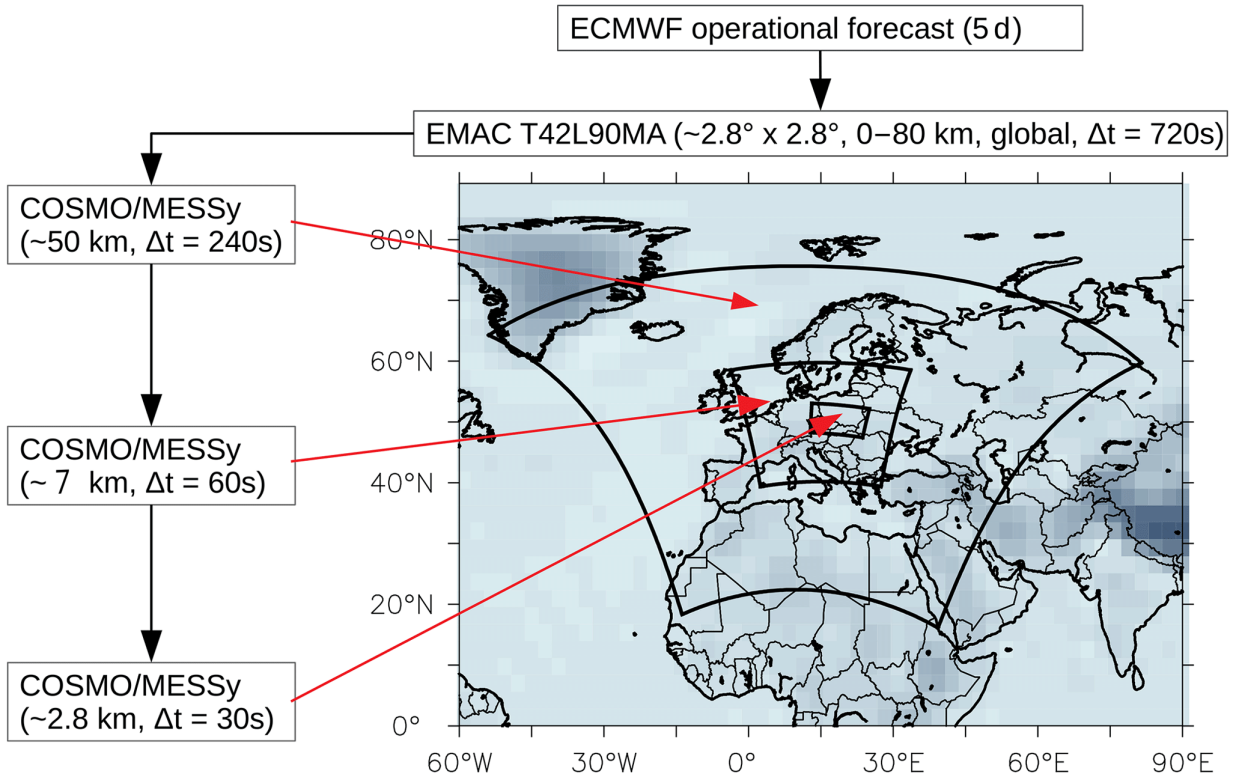
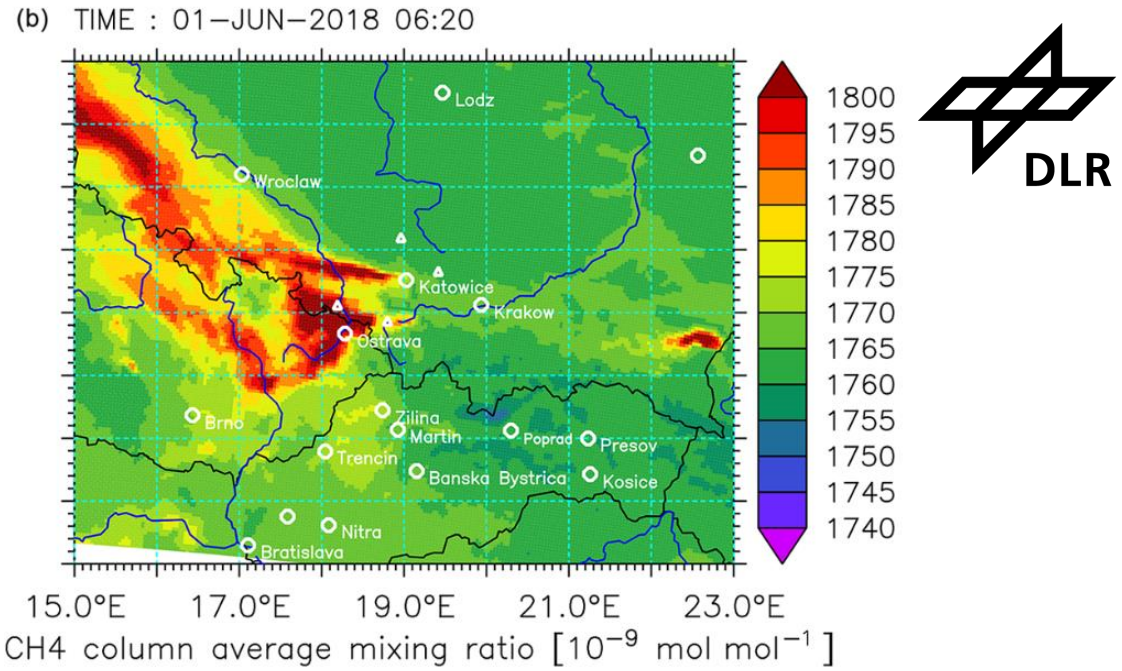
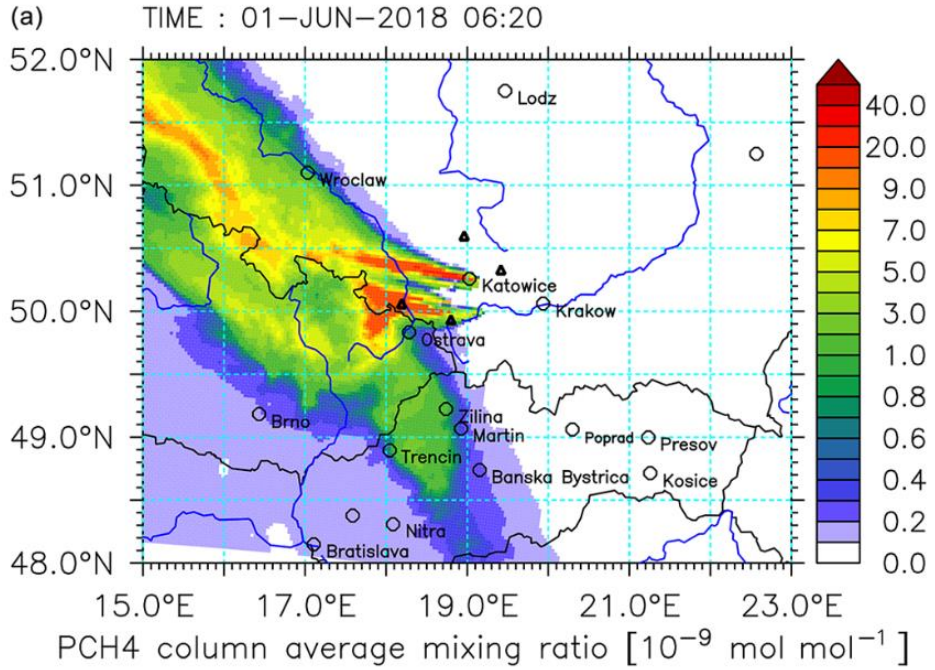
On-line nesting: Example







CH_4 forecast for CoMet 1.0 flight campaign

(Nickl et al., GMD, 2020)

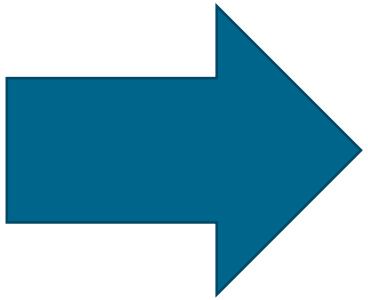
Opportunities on Exa-Scale HPC Systems

- increased resolution (globally) and/or more/finer nested regions
  (Note: “lag” behind standard GCMs w.r.t. global resolution will probably remain!)
- longer simulated time spans with nested regions (decades)
- more detailed chemistry
  - beyond C_4, SOA, …
  - isotopologues
- more detailed diagnostics (e.g. “tagging” of emissions by sector and region)
- ensemble simulations of CCMI / CMIP type with comprehensive atmospheric chemistry

Technical challenges

Tackling the scientific questions of chemistry climate & air quality feedback require:

- higher resolution (**globally !**): ½ grid size → factor 8 operations
- more detailed chemical kinetics (# of species & reactions)
- ensemble (~10 members) simulations (to address the uncertainty!)
  - aim: integration of decades to centuries (pre-industrial to 2100) [CCMI, CMIP]



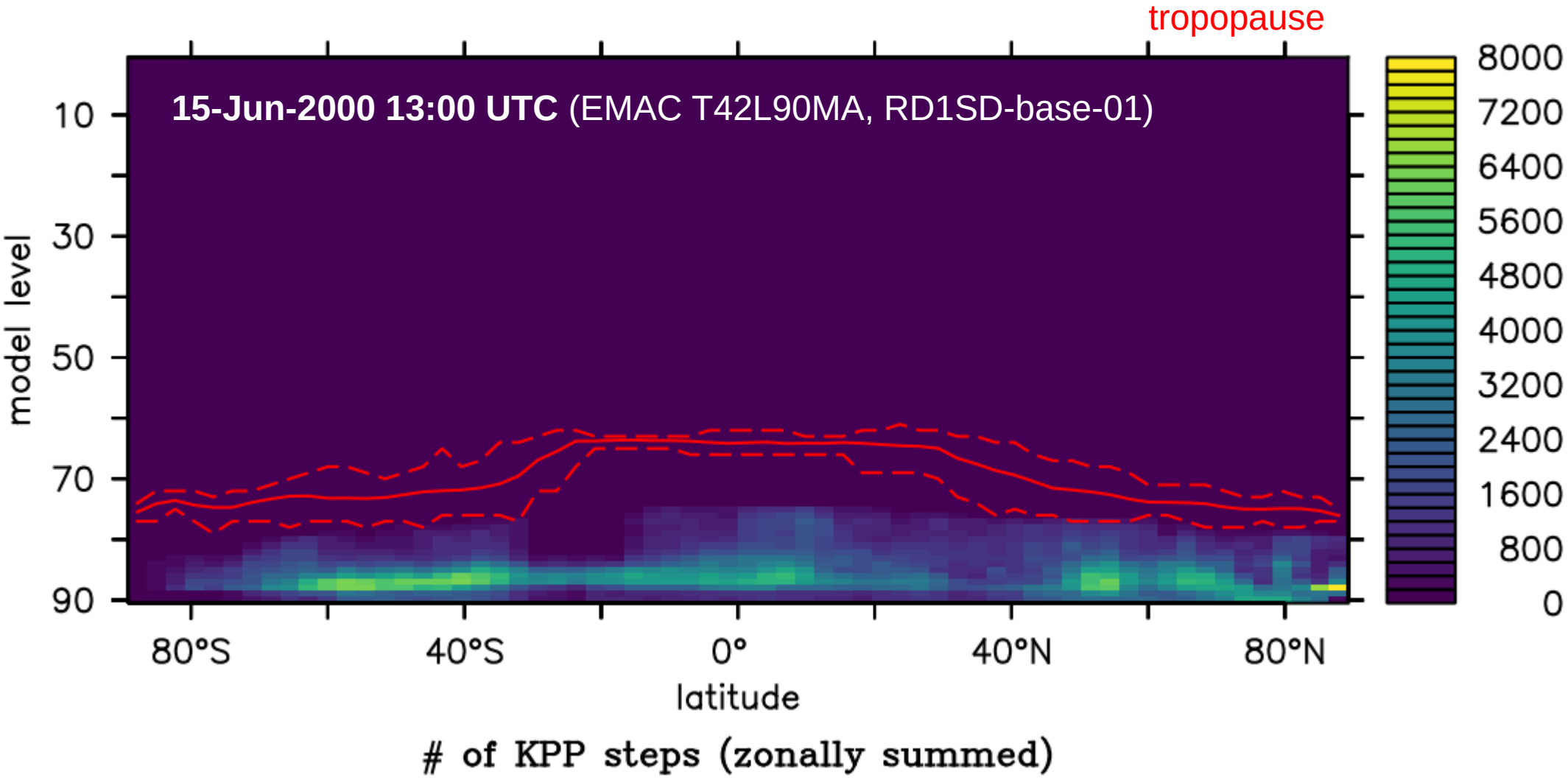
- memory per core
- FLOPs — massively parallel / accelerated
- I/O — asynchronous & parallel

ODE Solver (kinetic Systems)

- A + B → C + D ; k(p,T,…) ➔ $\frac{d[A]}{dt} = -k(p,T,\ldots)[A][B]$ ➔ stiff[1] ODE system
- Solver: 3rd order Rosenbrock solver with automatic time-stepping
  - Fortran code automatically generated from equation system (KPP)
  - automatic time stepping within model time step length Δt
  - the further away from the chemical equilibrium, the stiffer the system
  - the stiffer the system, the more (sub)time-steps are required
- In MESSy: different ODE solvers in operator splitting approach:
  - gas phase chemistry (MECCA)
  - aqueous phase chemistry (in clouds and rain, SCAV)
  - ice phase chemistry (SCAV)
  - aerosol phase chemistry (GMXE)

[1]https://en.wikipedia.org/wiki/Stiff_equation

Dynamic Load Imbalance of ODE Solver (kinetic systems)
Example: liquid phase (clouds & rain, LS & CV) [SCAV]



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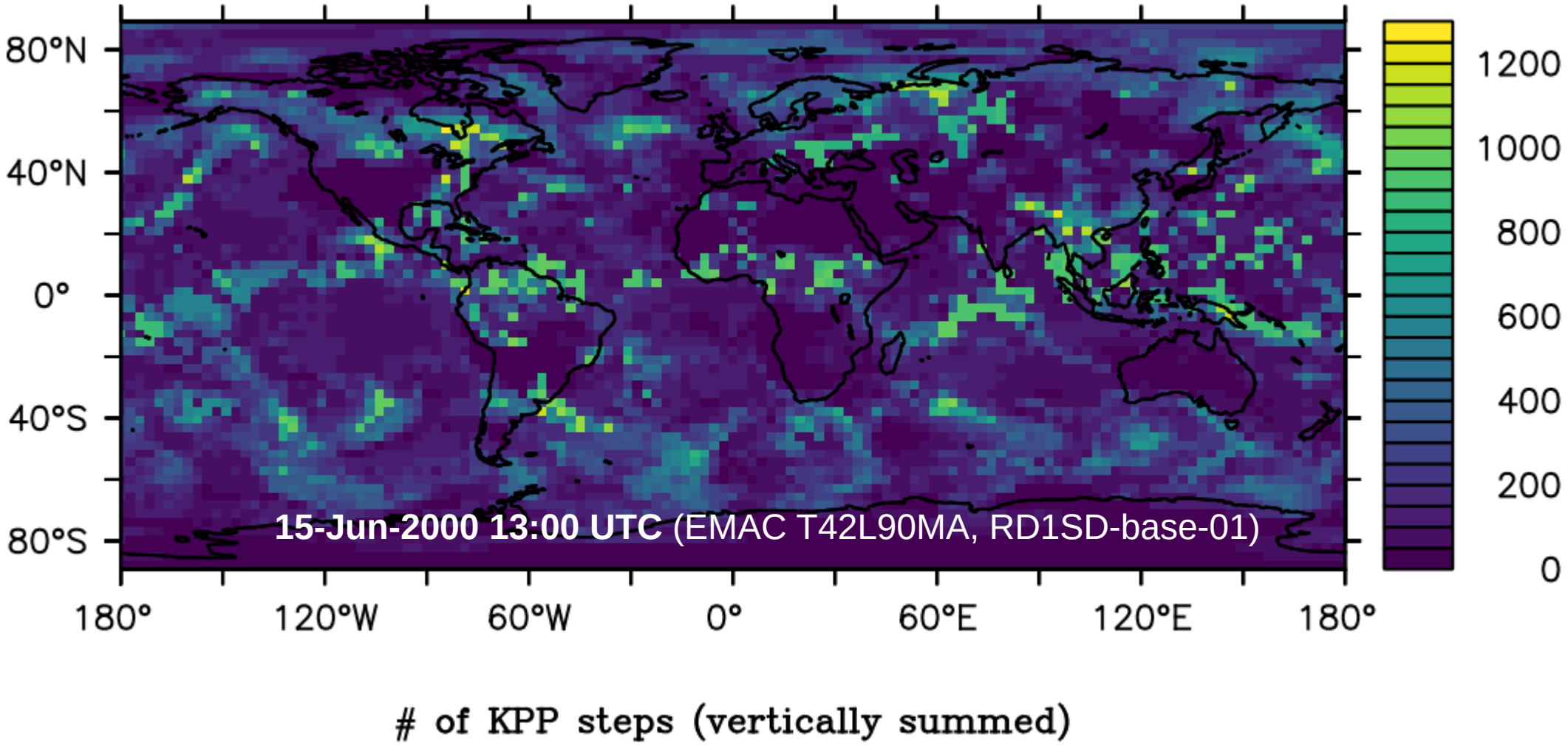
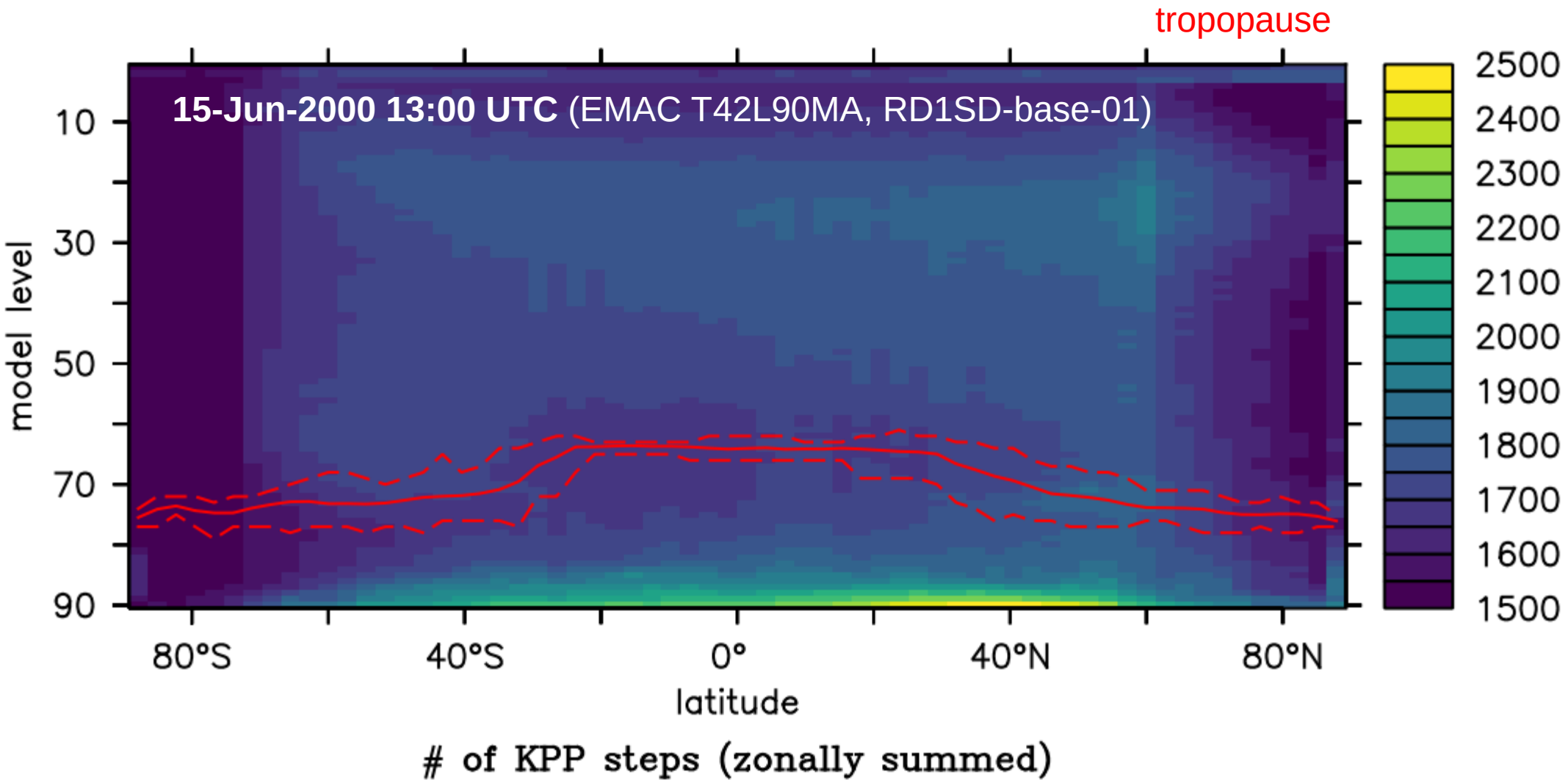


Dynamic Load Imbalance of ODE Solver (kinetic systems)
Example: gas phase [MECCA]



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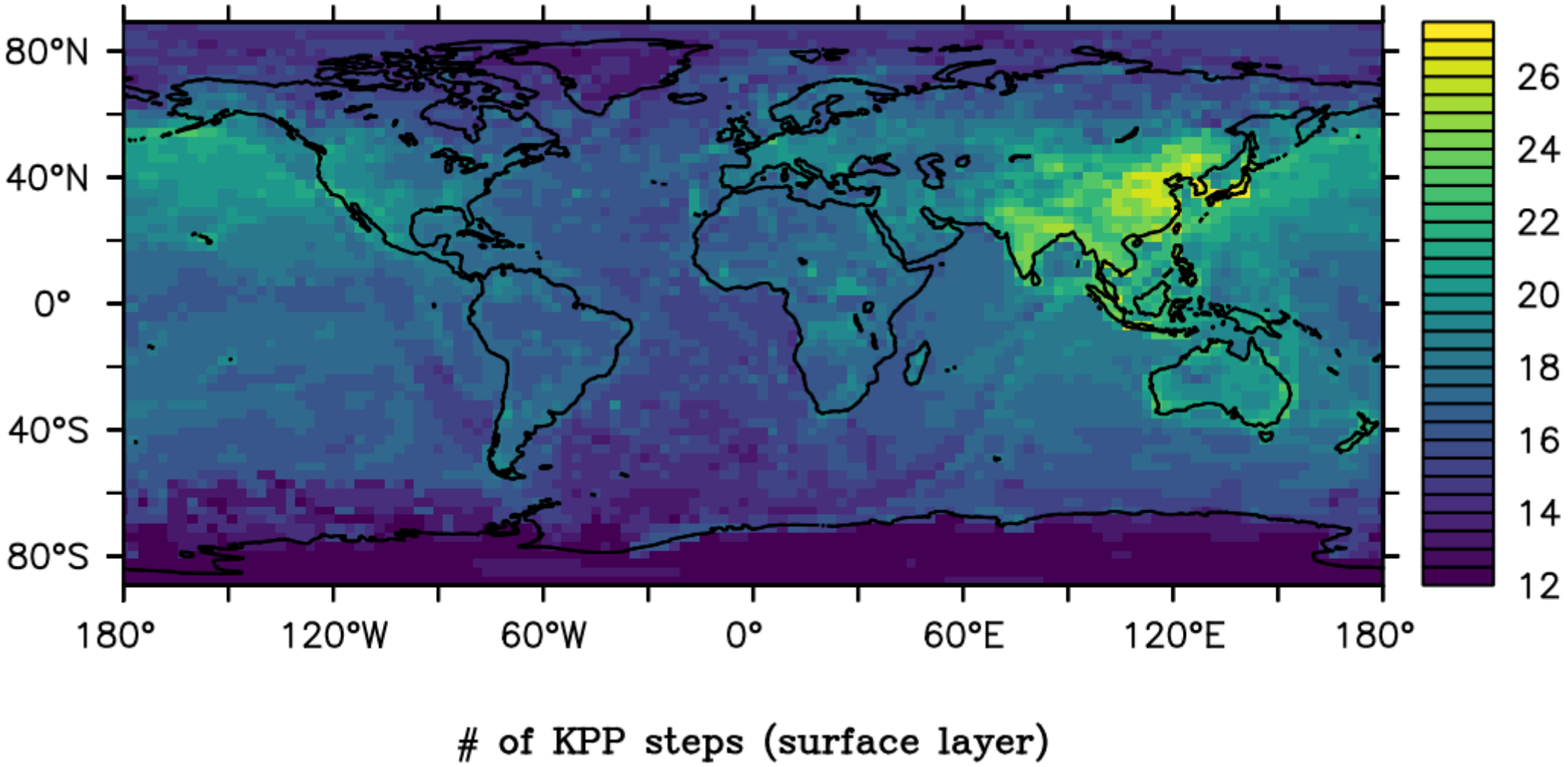

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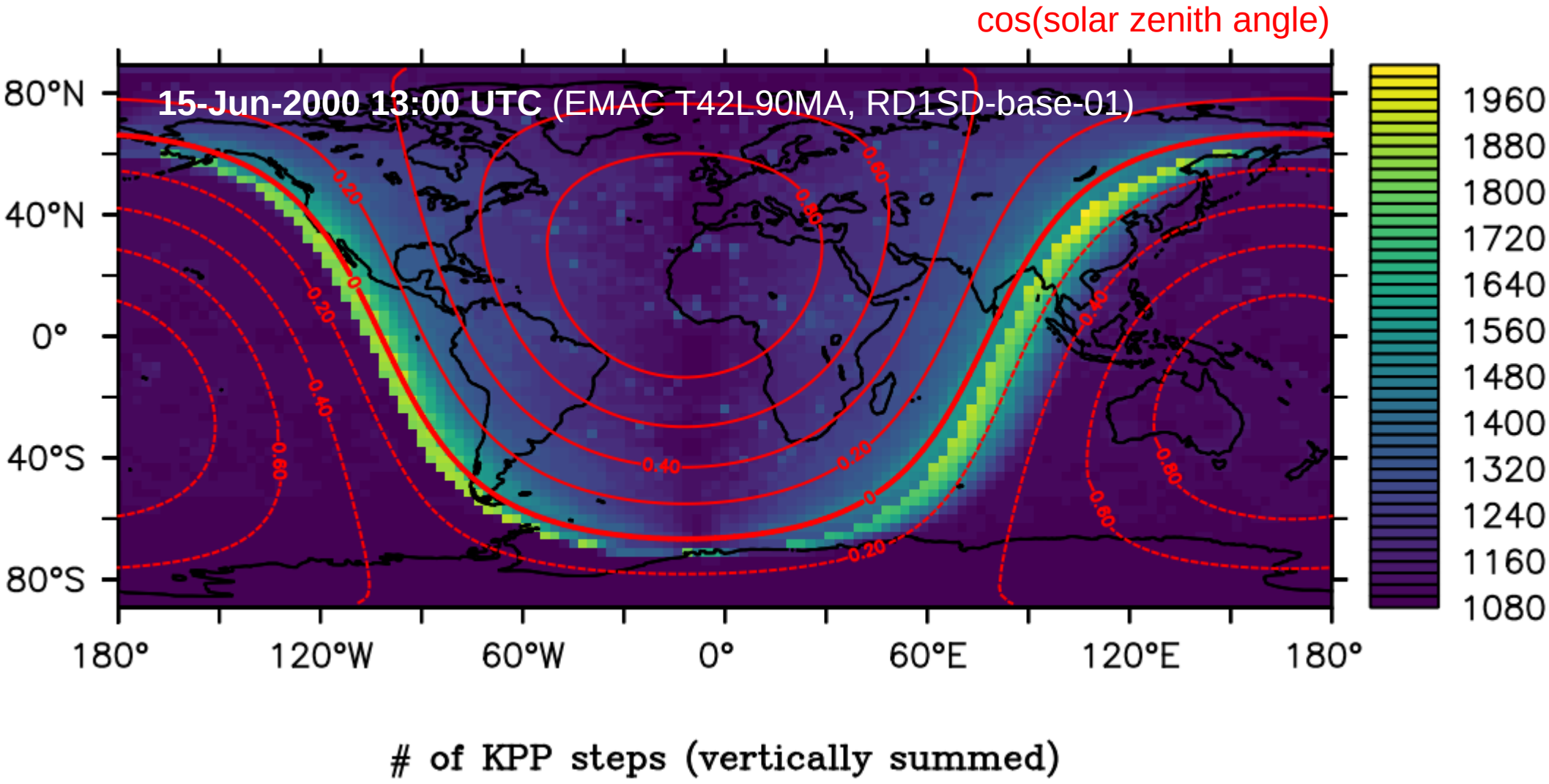
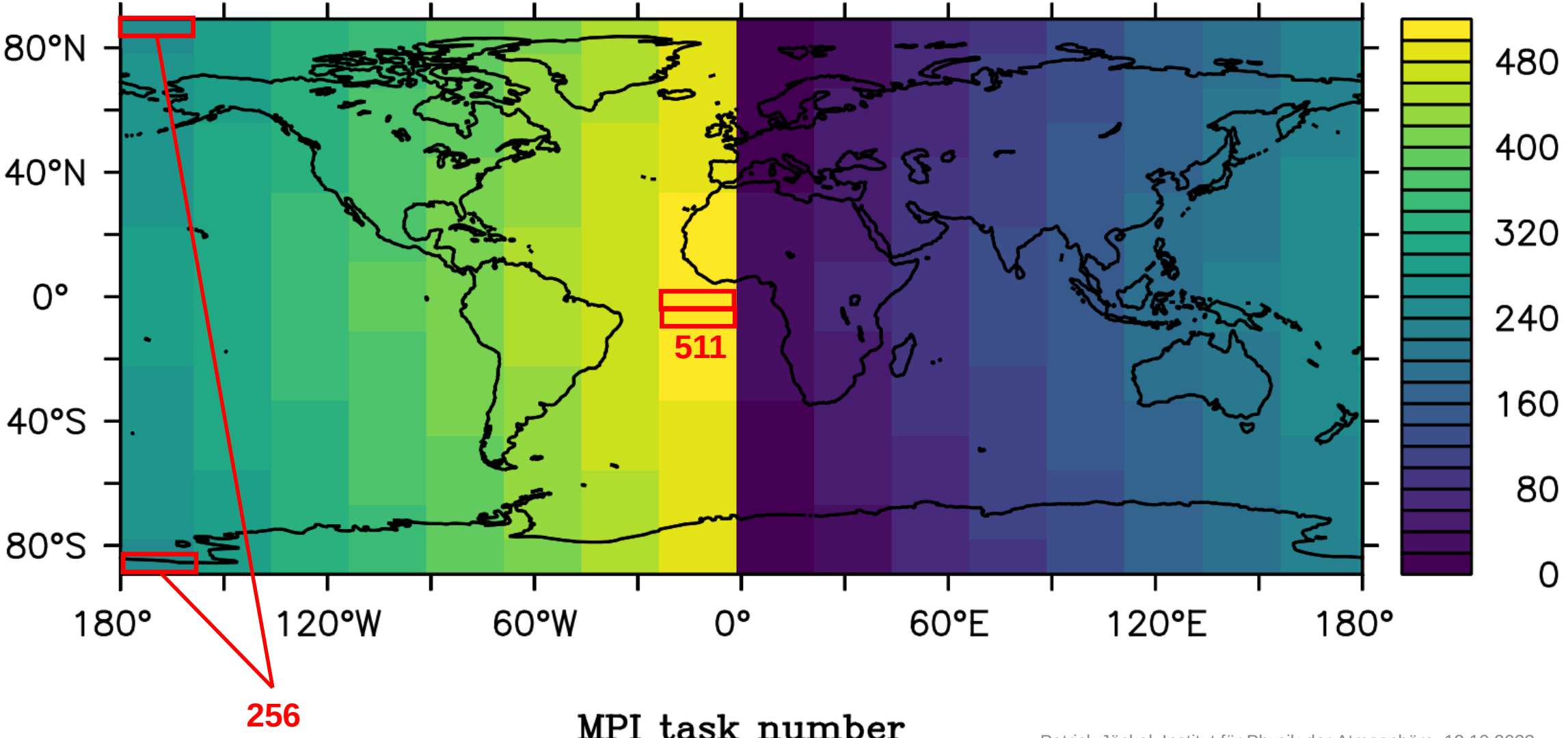
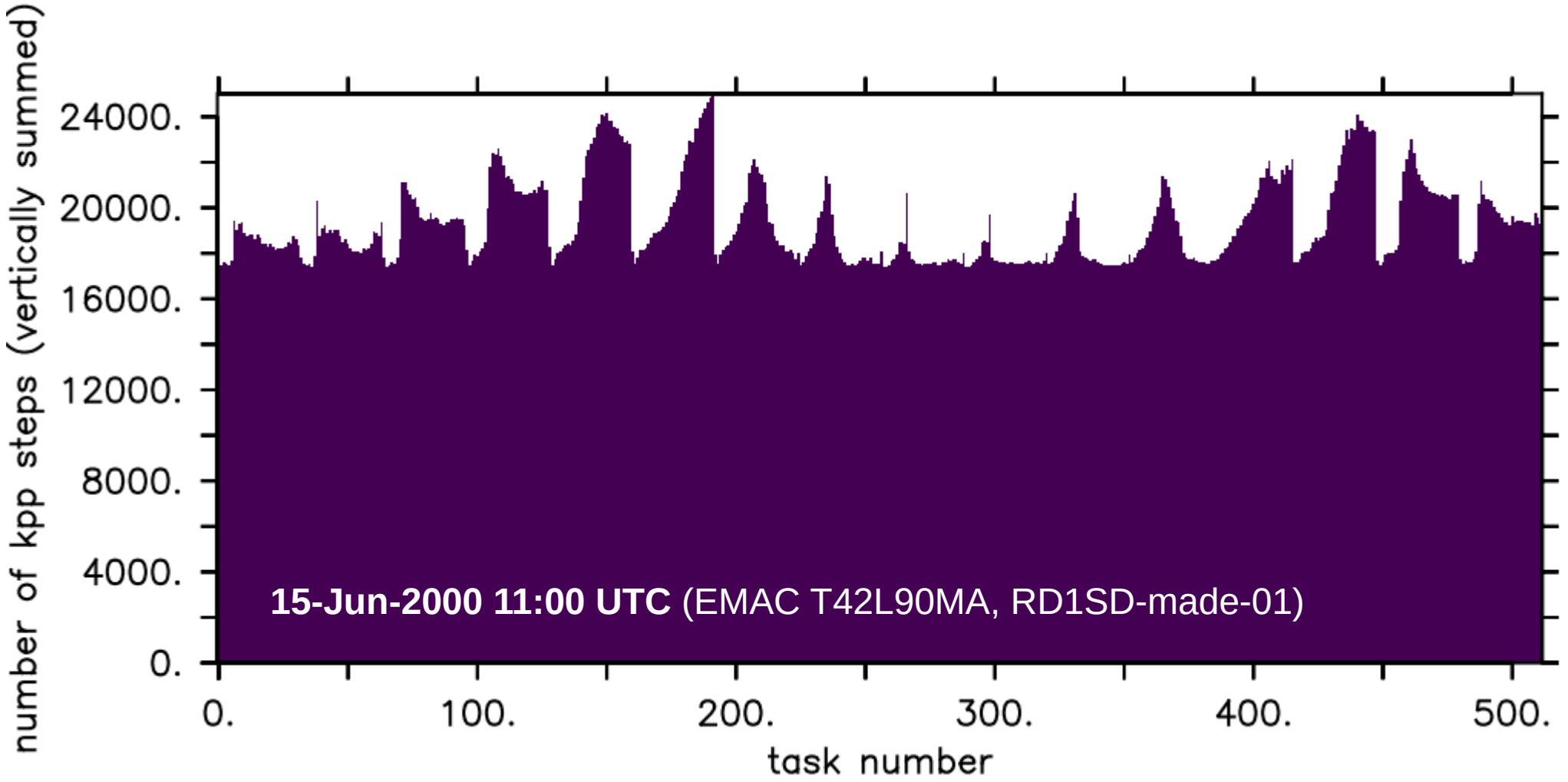


Horizonal domain decomposition
Example: EMAC T42L90MA on 4 nodes of levante
512 tasks ➔ 16 x 32 → 16 columns per task



Number of KPP steps per task



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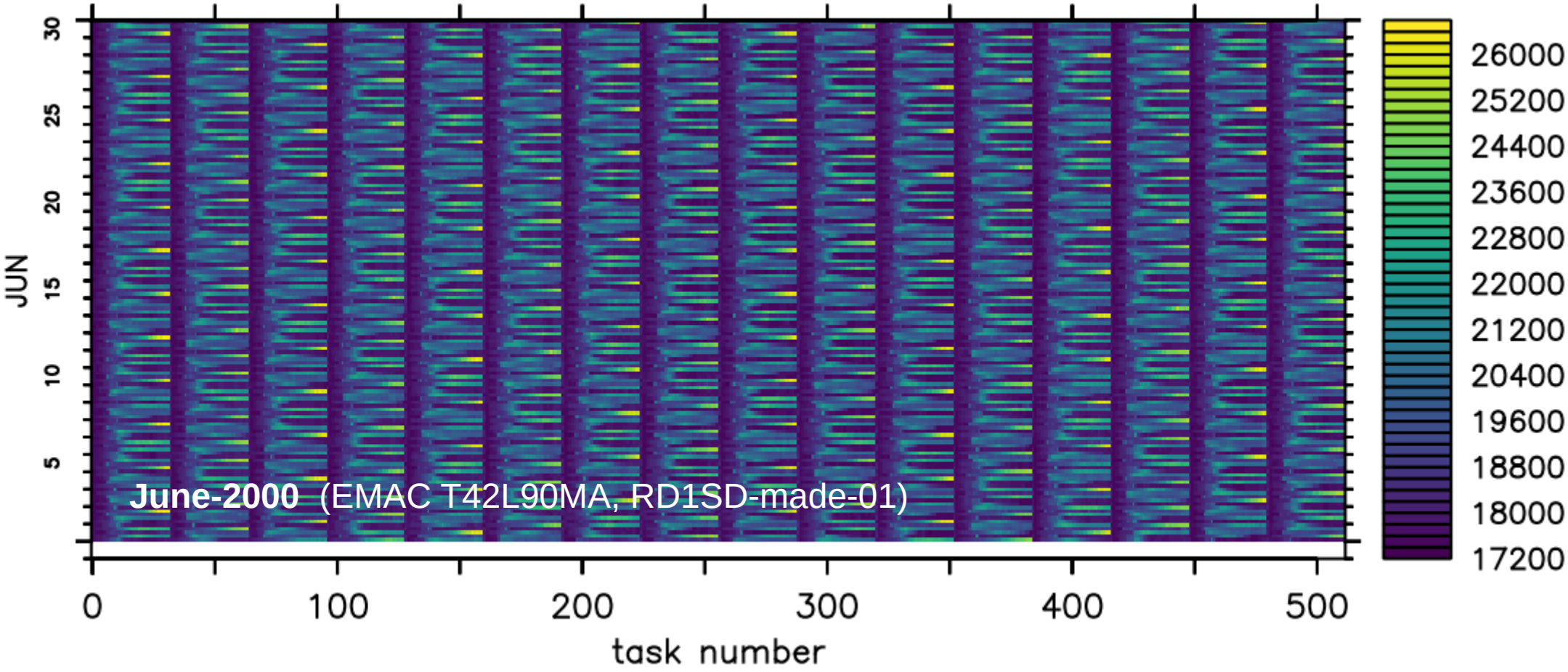

Dynamic Load Imbalance of ODE Solver (kinetic systems)
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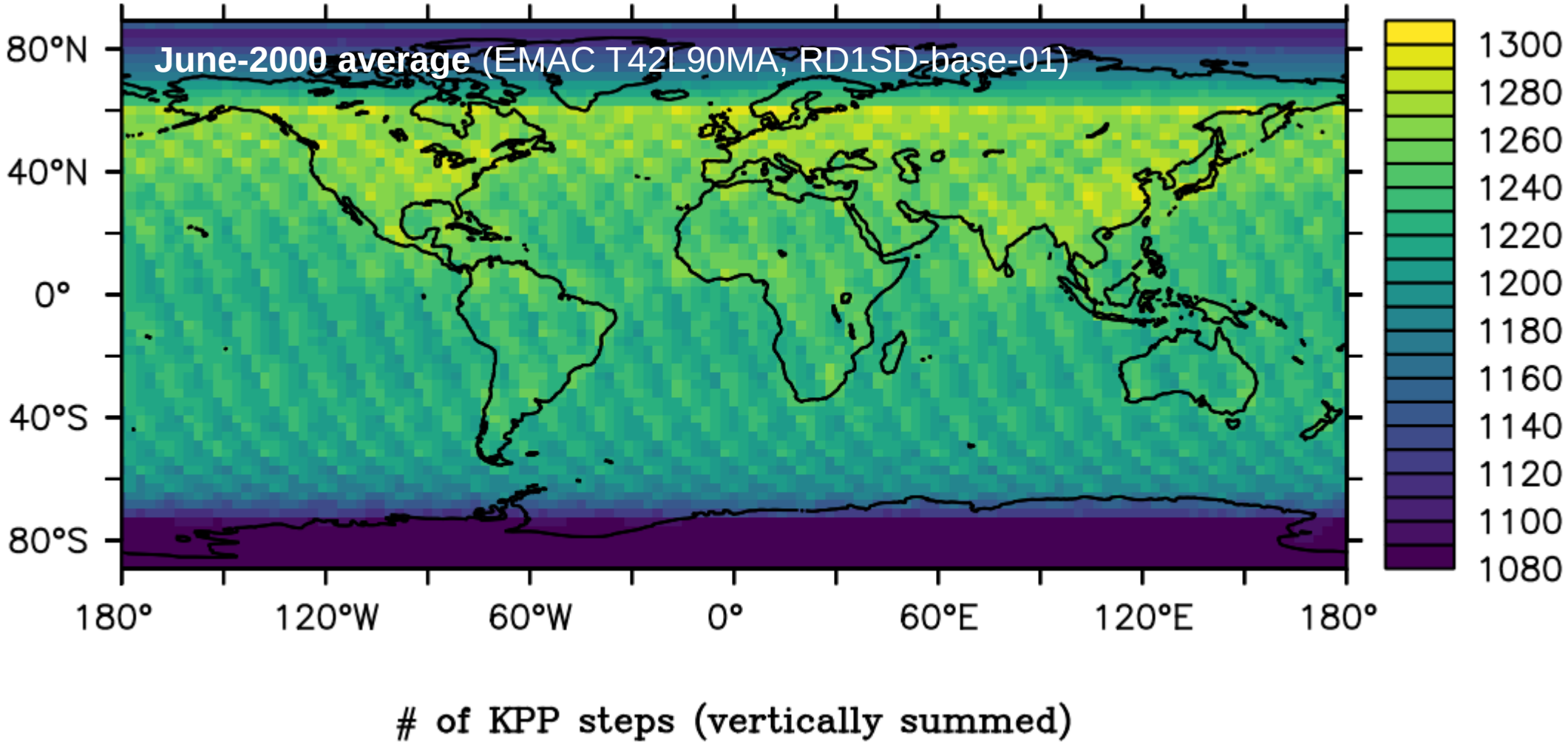

Dynamic Load Imbalance

- „adaptive“ parallel horizontal domain decomposition
  - → alternative decomposition for „chemistry“
    - 1st step: static → YAXT
    - 2nd step: dynamic ?, scheduling for accelerators ?
  - challenge: transport of tracers (large scale advection) with its own „basemodel“-decomposition
    - frequent data transpositions create communication overhead!
- **or:**
  “use” idling cores for other “tasks”, such as asynchronously scheduled I/O

Take home messages

CCMs are fundamentally different from GCMs w.r.t. HPC demands:

- x 10 .. x 100 more prognostic (and diagnostic) variables
  - larger memory/core and I/O requirements → parallel & asynchronous I/O, data reduction
- more processes, in particular “expensive” kinetic solvers
  - CCMs require (at a given resolution) per simulated time span ~ 10x (or more) CPU-time
  - equivalent to doubling the resolution (at least!) → resolution sacrificed for detailed, explicit chemistry
  - external on-line nesting for increased regional resolution; arbitrary nesting steps
  - kinetics is “embarrassingly” parallel, but other processes (e.g. advection of tracers) are not
  - large dynamic load imbalance → requires dynamic parallel decomposition or asynchronous/specific scheduling

Impressum

Thema:	Exa-scale challenges and opportunities from the atmospheric chemistry and chemistry climate modelling perspective
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