Earth System Models: Challenges in a changing HPC environment

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Outline

- Introduction

- “Coupling”: An attempt to classify different methods

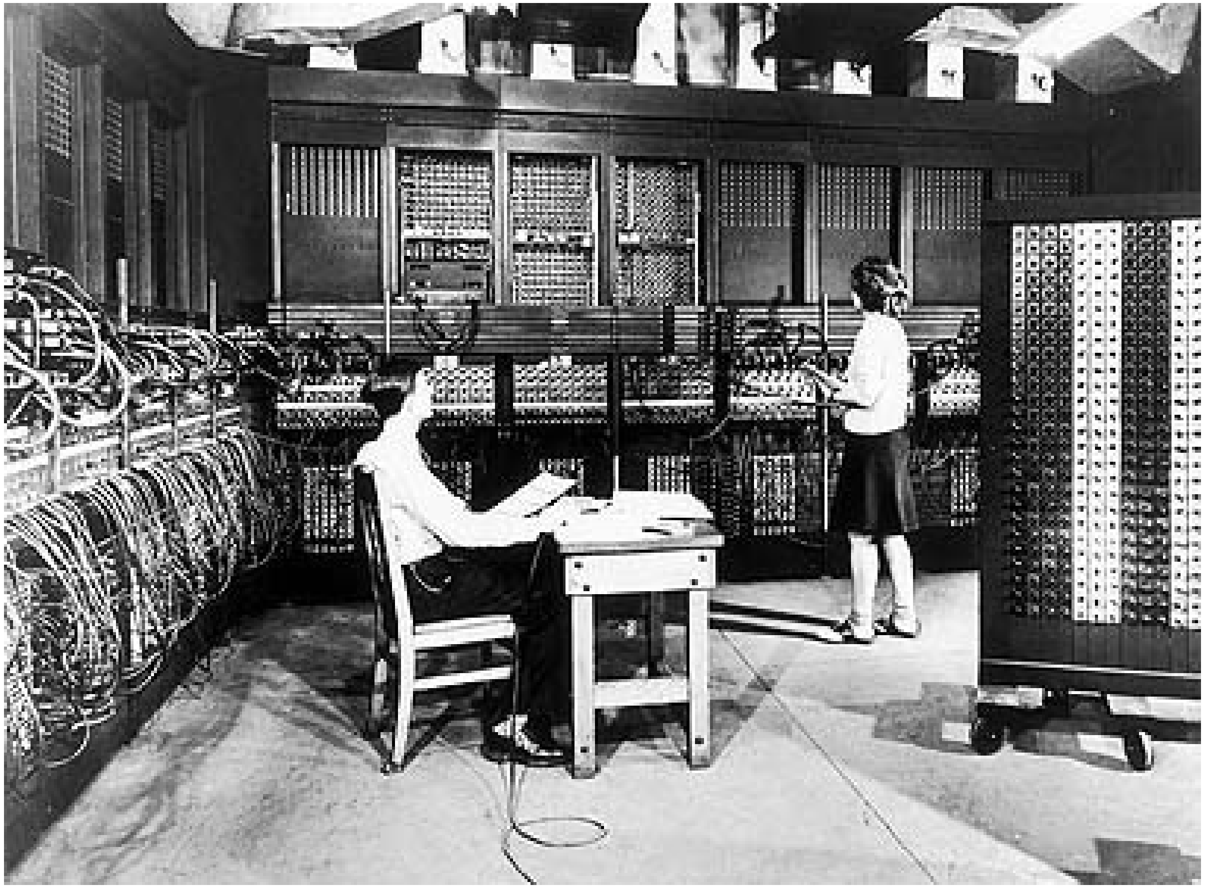
- Examples, challenges (and solutions)
    1. Atmospheric Chemistry in the Earth System
    2. Atmosphere – Ocean System
    3. On-line nesting: an alternative way to higher resolution

- Summary and Outlook

Computational Earth System Science
(numerical weather prediction and climate simulations)
was from the beginning on exploiting HPC up to the limits …

1950 (Charney, Fjørtoft, von Neumann):
first numerical weather forecast on ENIAC (Electronic Numerical Integrator and Computer)

forecast time: 24 hours
computation: 24 hours



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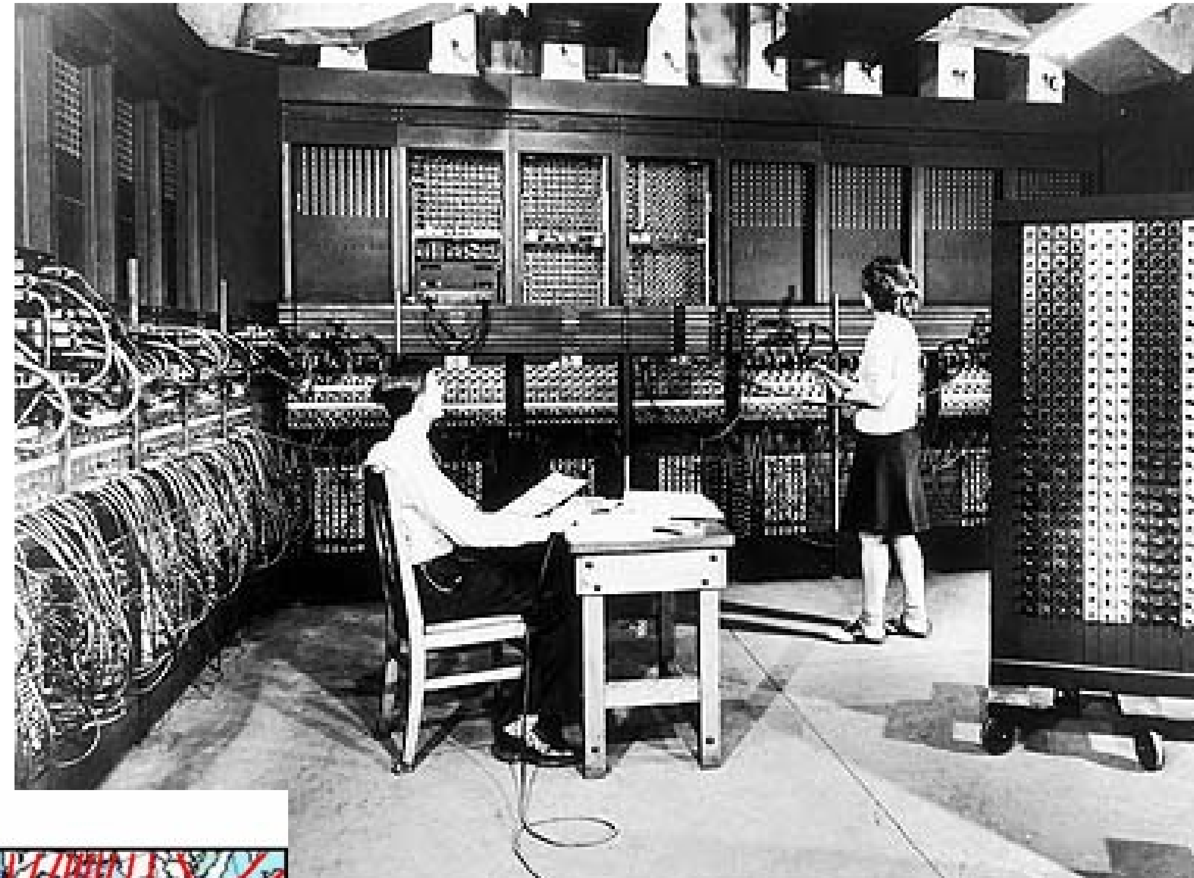

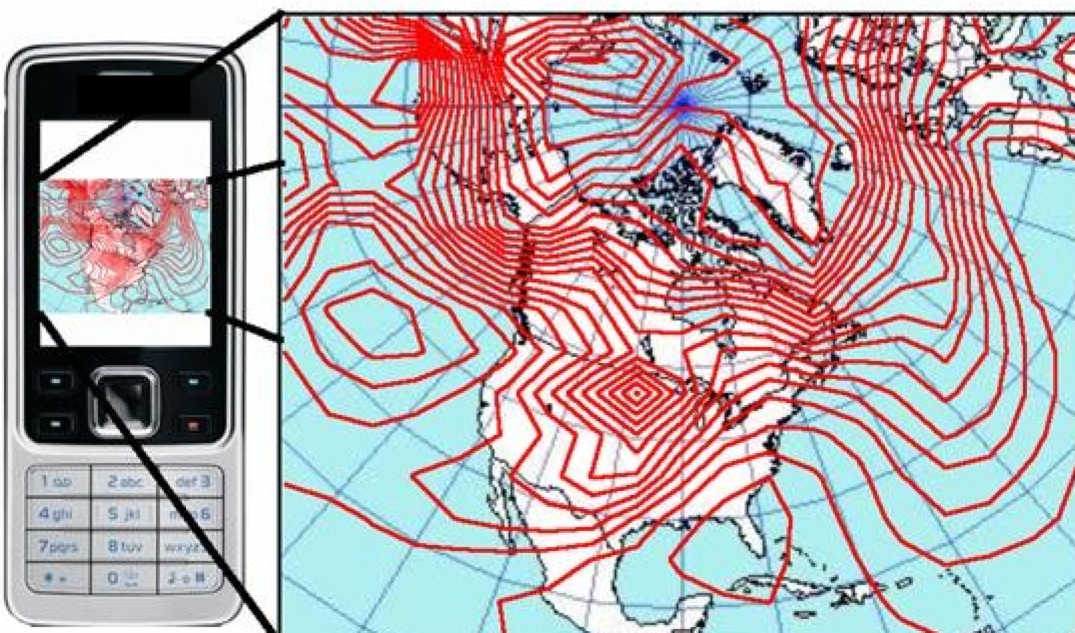

2008 (Lynch & Lynch):
reconstruction on mobile-phone (JAVA-application):

forecast time: 24 hours
computation: < 1 second (!!!)

Lynch & Lynch, Weather 63, 324-326, 2008.
http://mathsci.ucd.ie/~plynch/eniac/phoniac.html

Deutsches Klimarechenzentrum (DKRZ)

8448 Cores
158 TFlops/s

Top 500
June 2009: no. 27
Nov 2011: no. 98

http://www.dkrz.de

Computational Earth System Science
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… mainly for two reasons:

increasing resolution of numerical discretisation(s)
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increasing complexity by incorporating more and more
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→ *"coupling"*

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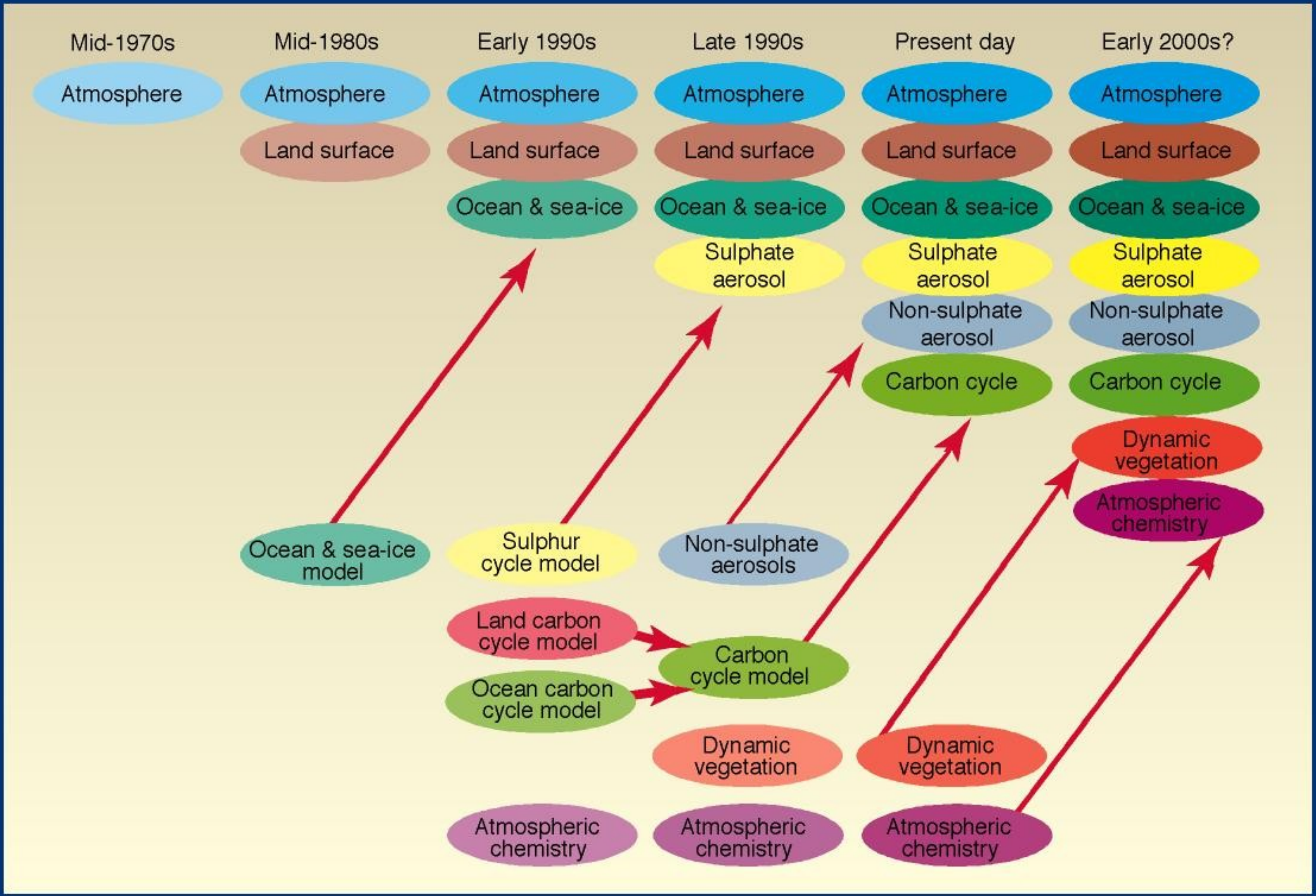
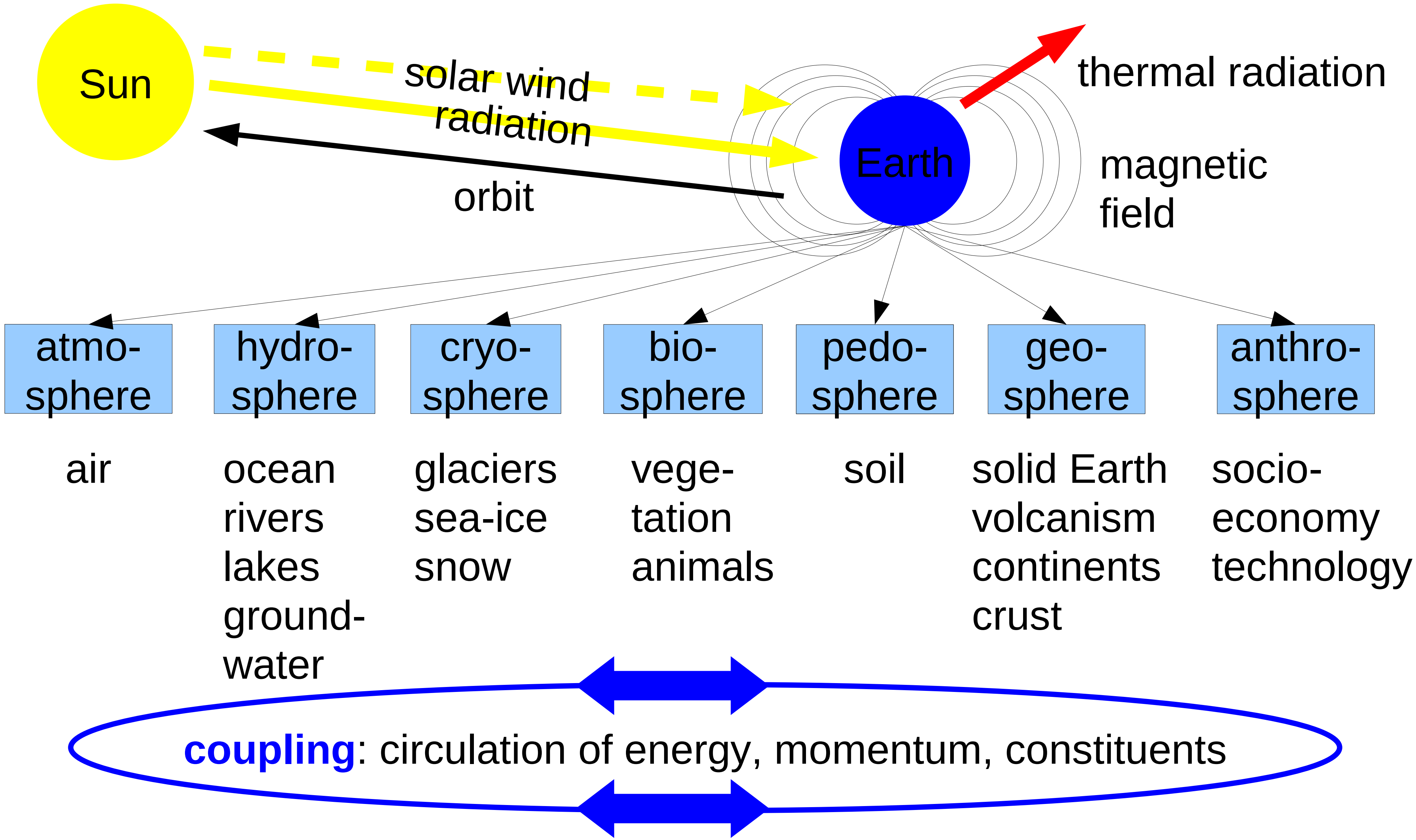
The development of climate models, past, present and future



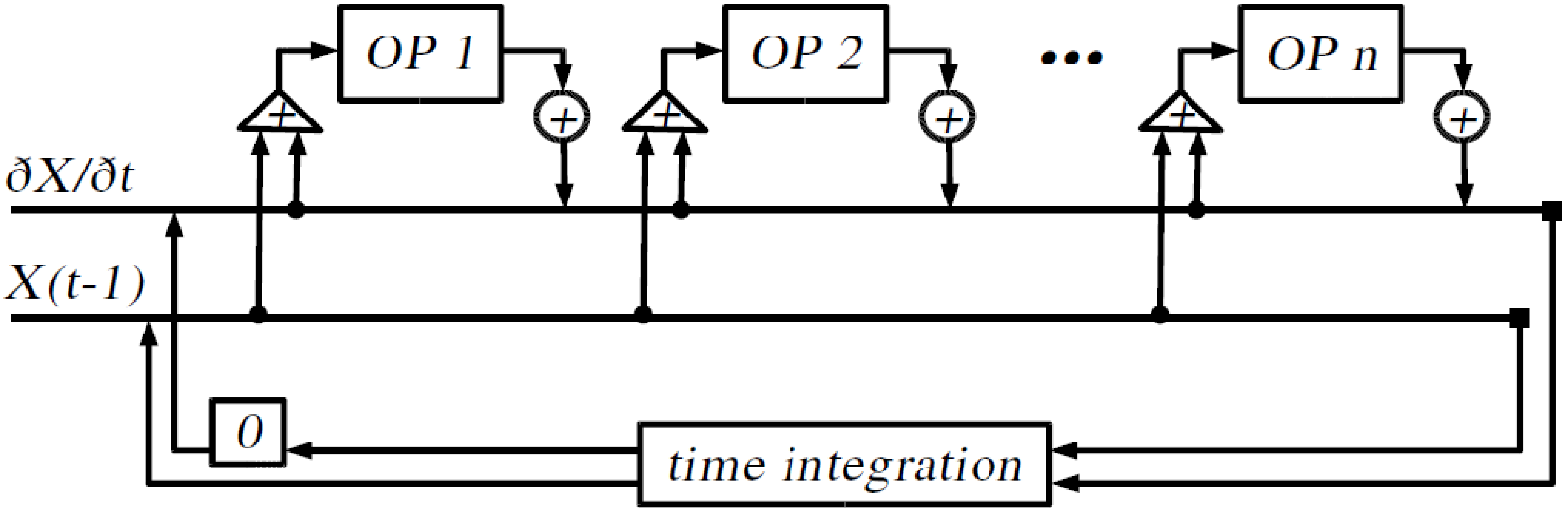
WG1 - TS BOX 3
FIGURE 1



change of state variables by physical, chemical, biological, socio-economic processes

Coupling ...

… the prerequisite is the *operator splitting* concept



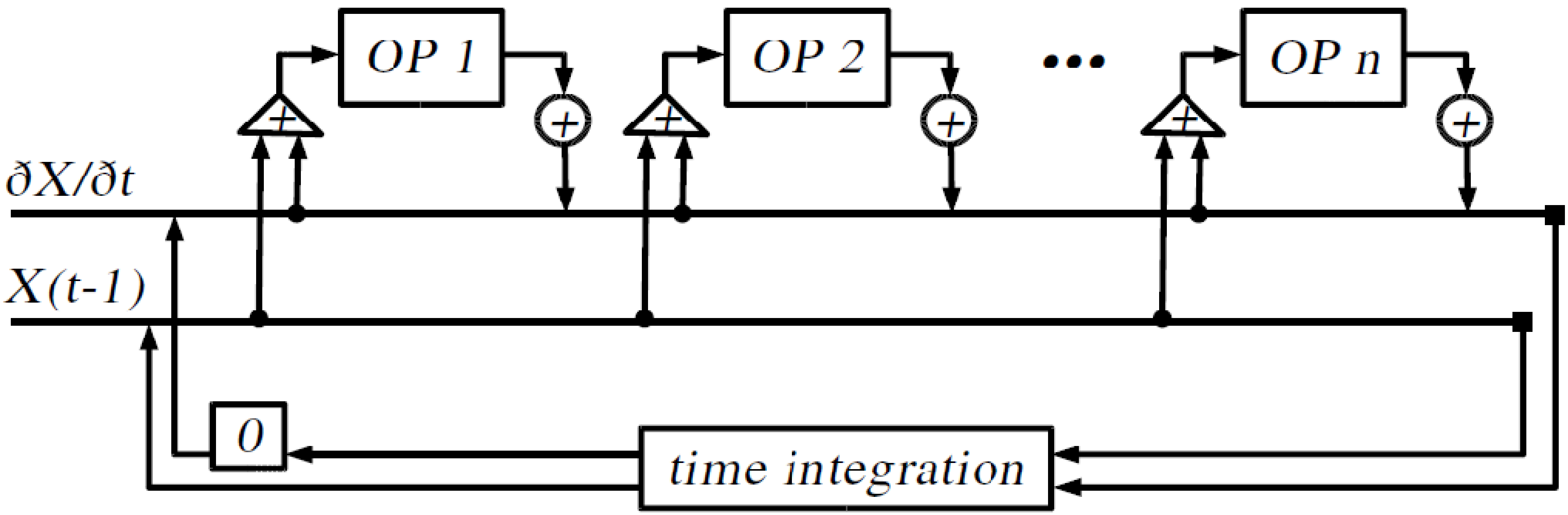
(Jöckel et al., ACP, 2005)

Coupling ...

… the prerequisite is the *operator splitting* concept

Example:
X = air
temperature

radiation convection ... diffusion

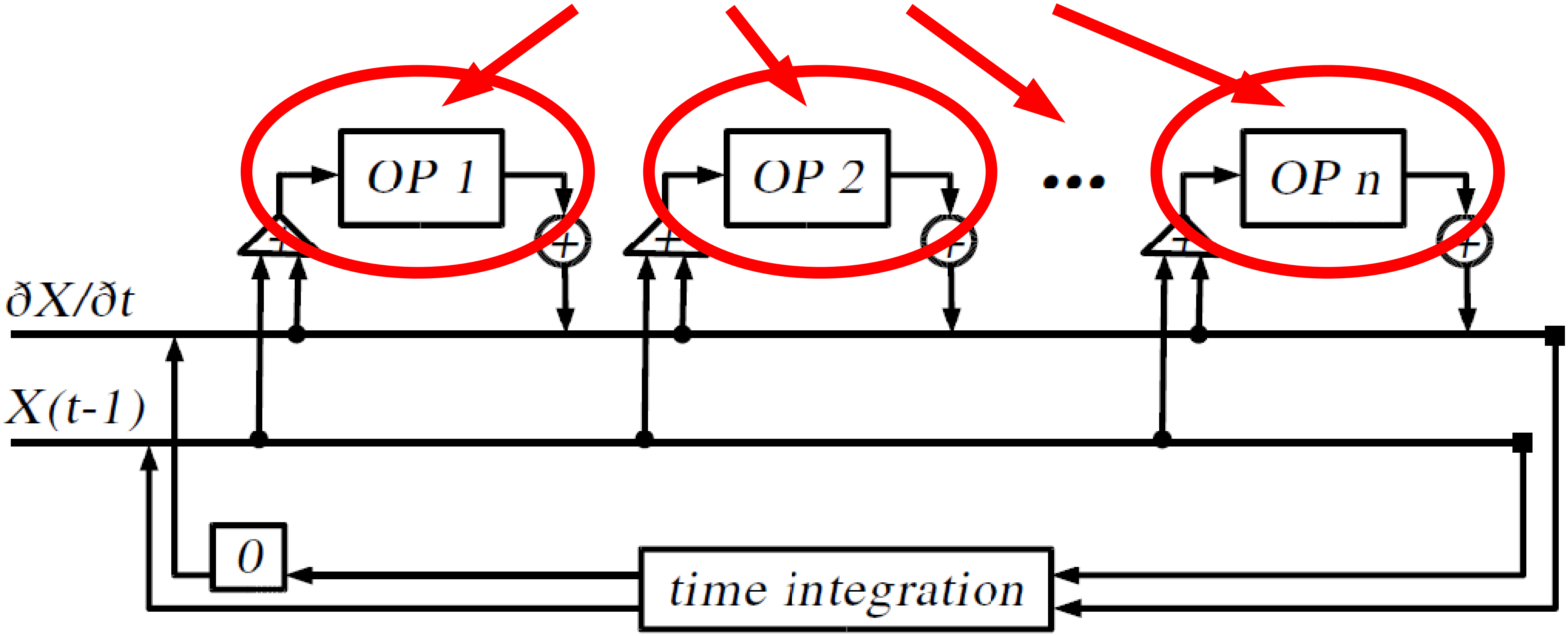


(Jöckel et al., ACP, 2005)

Coupling ...

… the prerequisite is the *operator splitting* concept

different numerical algorithms (discretisation, parallel decomposition, cache/vector blocking, ...)



(Jöckel et al., ACP, 2005)

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Coupling ...

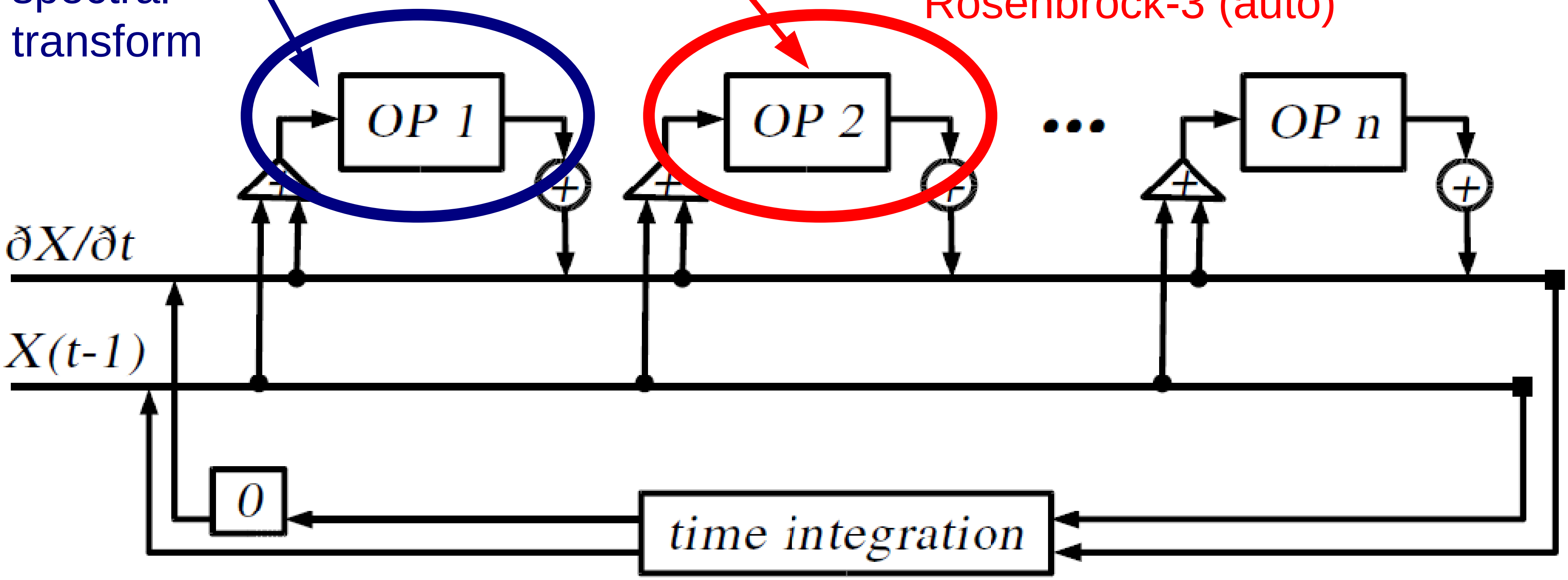
Example:

basic (dynamical) equations → coupled PDE system

reaction kinetics (chemistry) → coupled ODE system

spectral transform

Rosenbrock-3 (auto)



(Jöckel et al., ACP, 2005)

Coupling … a classification (of the “way” how operators “communicate”)

internal coupling ⟷ **external coupling**

internal coupling

- Os are part of the *same program unit* (“task”)
- data exchange via *working memory*

{ on-line, direct }

external coupling

- Os are split into *different program units* (“tasks”)

off-line

- data exchange via *external storage* (files)

on-line

- data exchange via *working memory*

indirect

- involves an *add. external* program (“*coupler*”)

direct

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  - **off-line**
    - data exchange via *external storage* (files)
  - **on-line**
    - data exchange via *working memory*
      - **indirect**
        - involves an *add. external* program ("*coupler*")
      - **direct**

choice depends on:
- application
- implementation effort (legacy code!)
- desired sustainability, flexibility, re-usability

→ compromise in minimizing computational and communication overheads

Example 1: internal coupling

Language level: CALL subroutine_1(..., A, …) [INTENT(OUT)]

↓

CALL subroutine_2(..., A, …) [INTENT(IN)]

more formal: standard model infrastructure + coding standard

- Earth System Modeling Framework (ESMF) (*http://www.earthsystemmodeling.org*)
- Modular Earth Submodel System (MESSy) (*http://www.messy-interface.org*, *Jöckel et al., ACP, 2005*)
- … (many others)

key: strict separation of *model infrastructure (4 layer!)* (memory management, I/O, parallel decomp., time control, etc.) from *“process” (and “diagnostic”) formulations*

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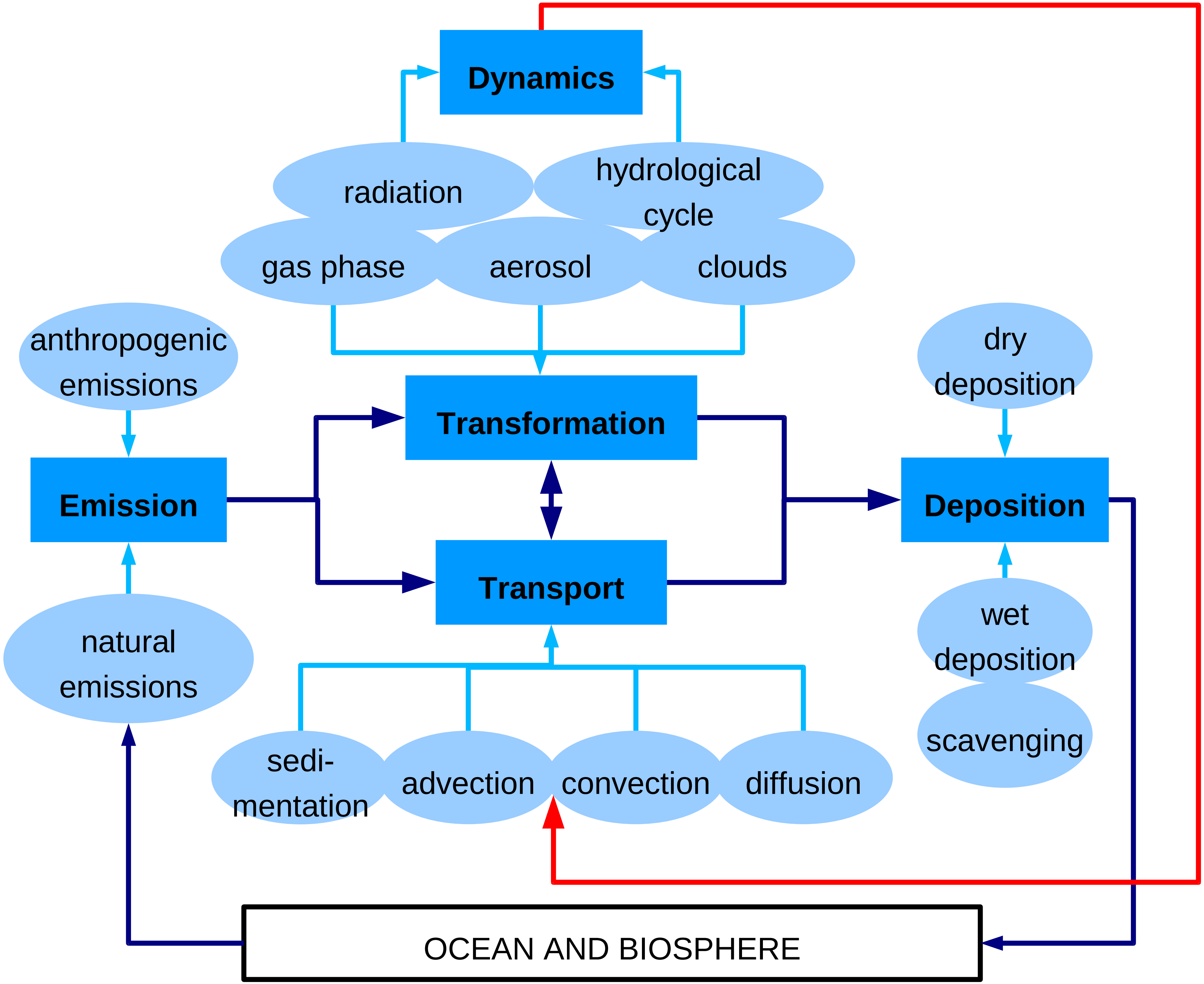
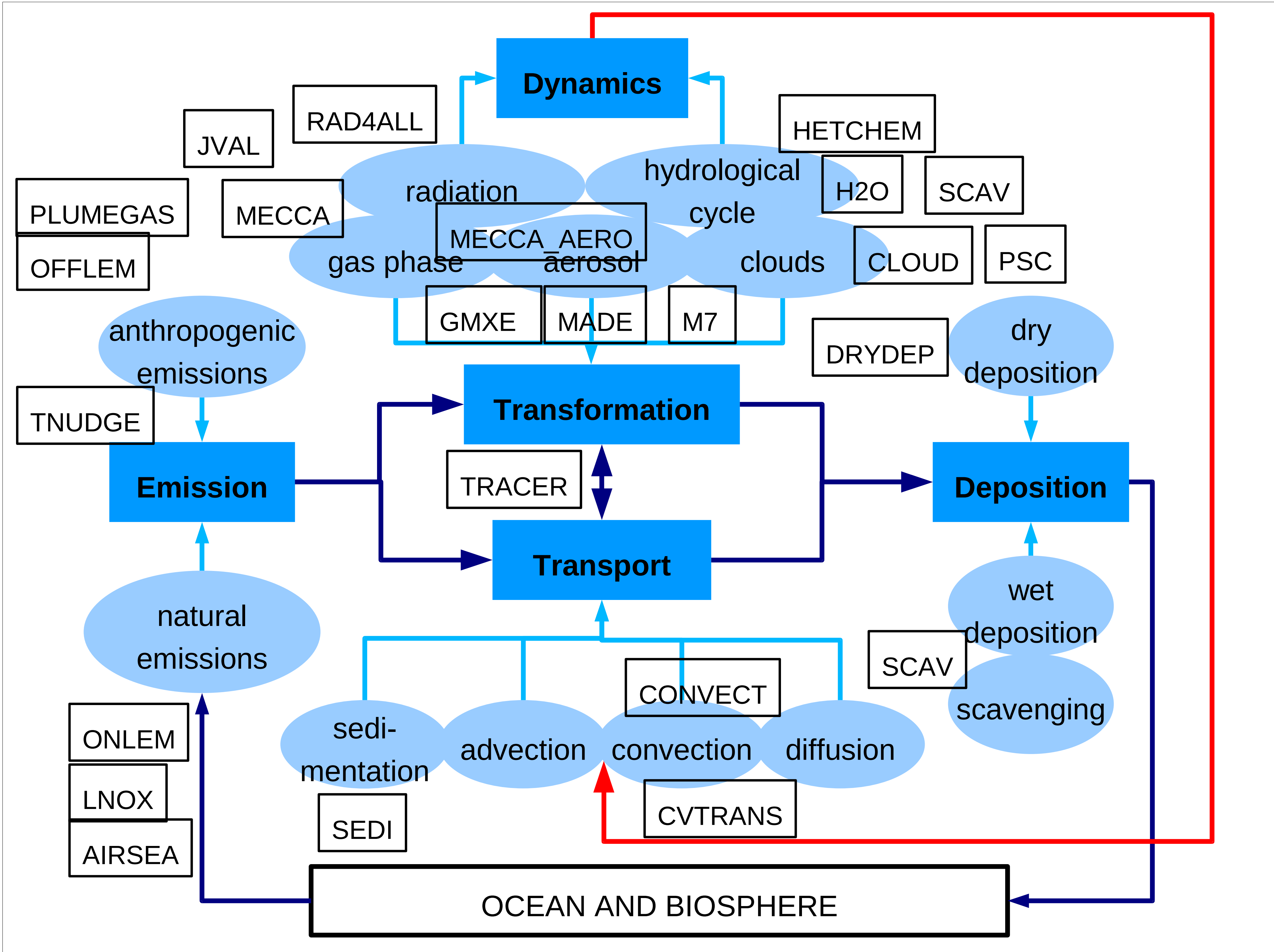
Example 1a: internal coupling of Atmospheric Chemistry in MESSy

coupling via model infrastructure (nearly object oriented)

- TIMER
- CHANNEL (pointer based memory management and I/O)
- TRACER (special for chemical constituents)
- …

“operators” = “processes” = “submodels”


Dynamics
radiation
hydrological cycle
gas phase
aerosol
clouds
anthropogenic emissions
dry deposition
Transformation
Emission
Deposition
Transport
natural emissions
wet deposition
scavenging
sedi-mentation
advection
convection
diffusion
OCEAN AND BIOSPHERE


Dynamics
RAD4ALL
JVAL
HETCHEM
PLUMEGAS
MECCA
radiation
hydrological cycle
H2O
SCAV
OFFLEM
MECCA_AERO
gas phase
aerosol
clouds
CLOUD
PSC
GMXE
MADE
M7
DRYDEP
anthropogenic emissions
dry deposition
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Emission
TRACER
Deposition
Transport
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SCAV
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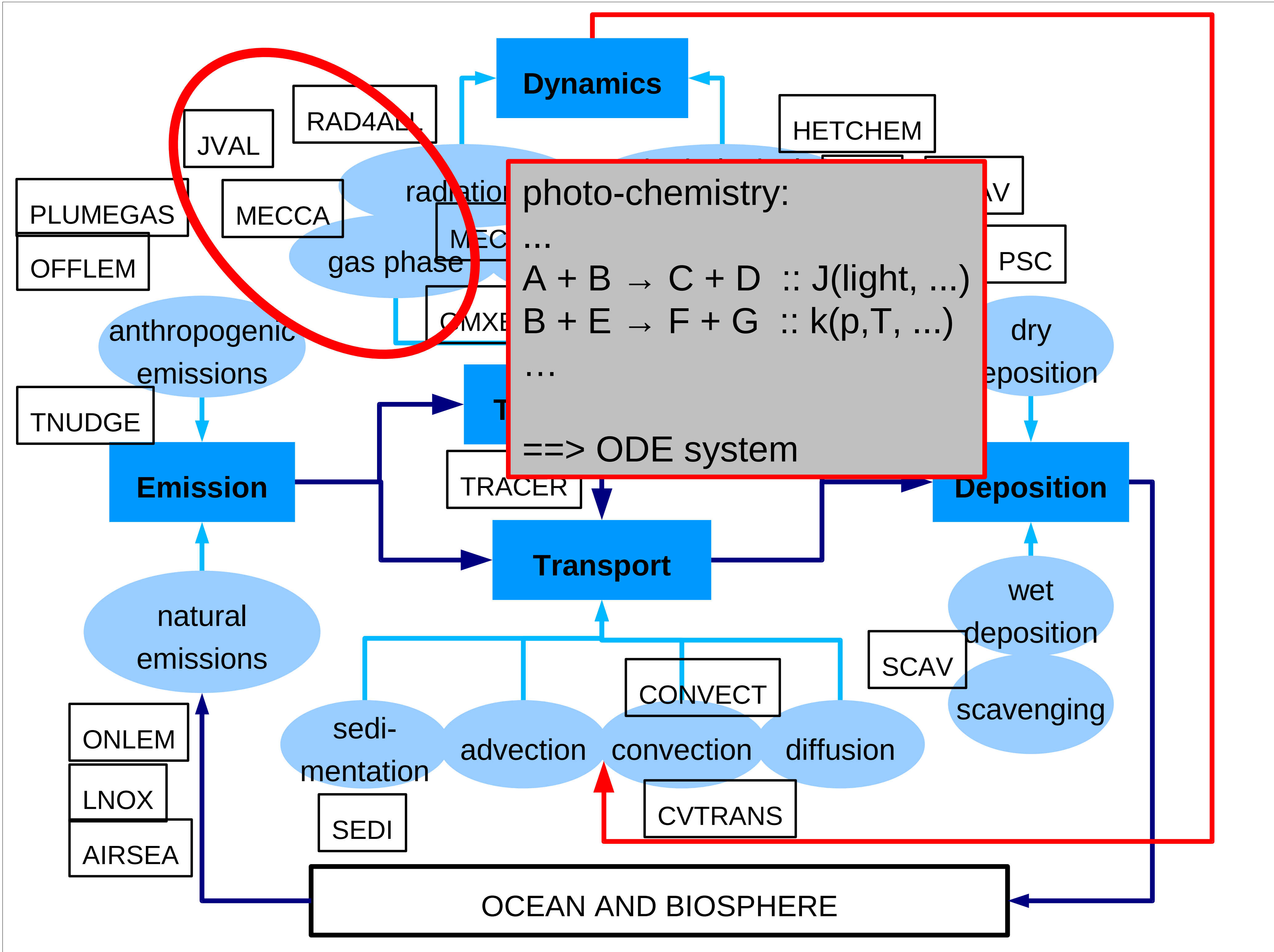
CONVECT
ONLEM
sedi-mentation
advection
convection
diffusion
LNOX
SEDI
CVTRANS
AIRSEA
OCEAN AND BIOSPHERE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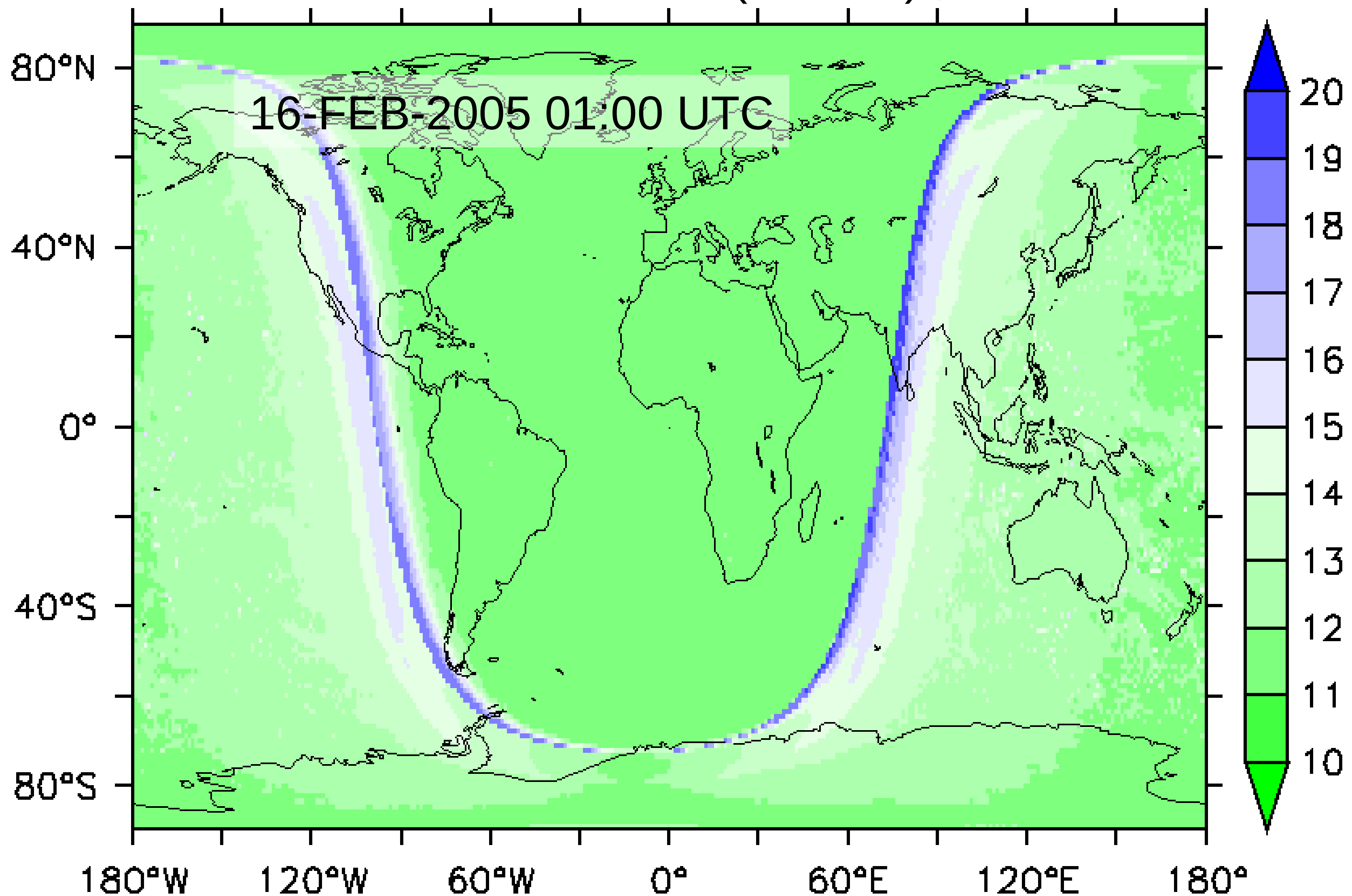
SCAV
scavenging
CONVECT
sedi-mentation
advection
convection
diffusion
ONLEM
LNOX
AIRSEA
SEDI
CVTRANS
OCEAN AND BIOSPHERE
photo-chemistry:
...
A + B → C + D :: J(light, ...)
B + E → F + G :: k(p,T, ...)
...
==> ODE system

Number* of sub-time steps of the ODE solver for the kinetic system

T106L90MA → ~ 1.125° x 1.125° x 90 (~80 km) ; Δt = 6 min

*vertical average



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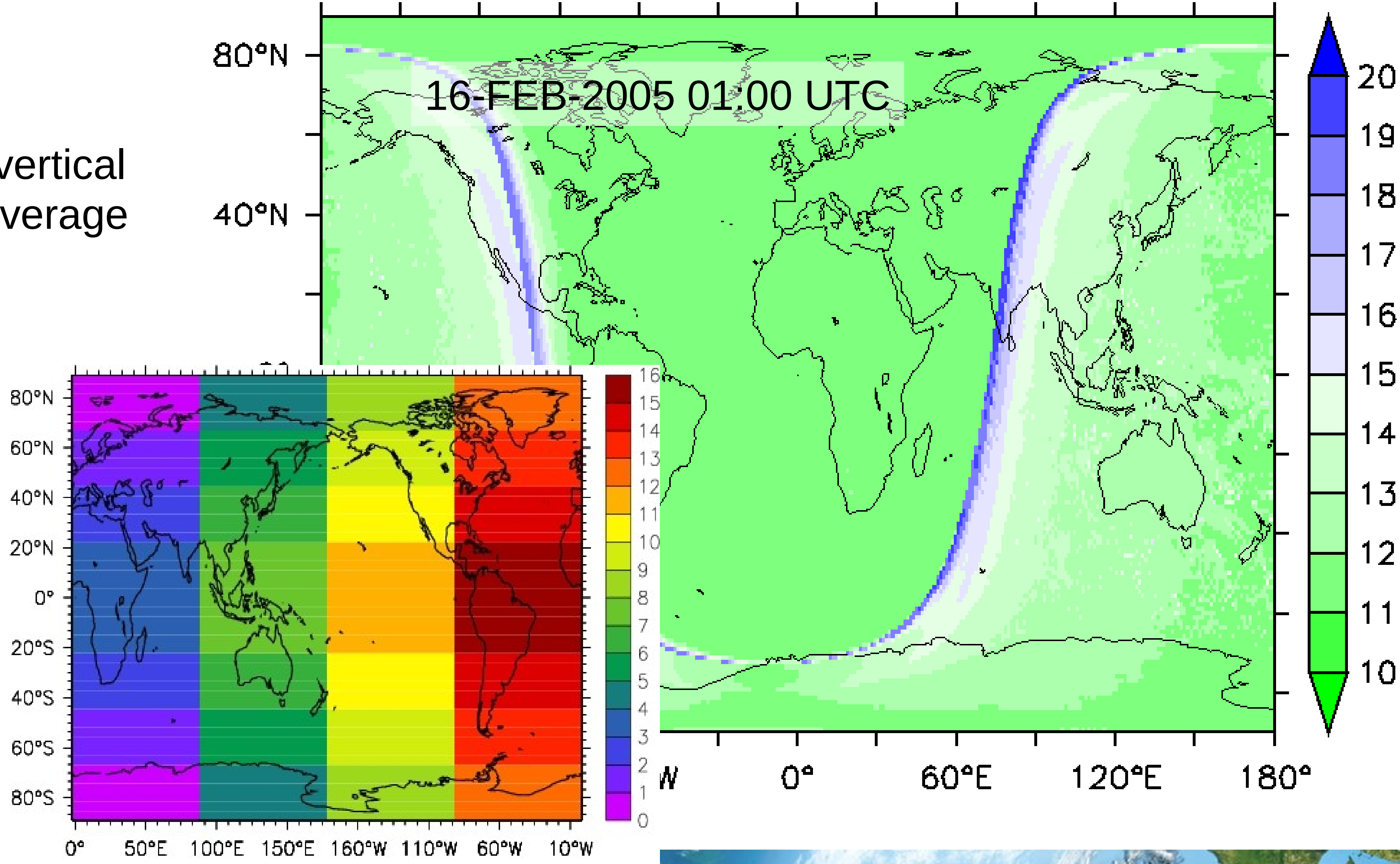

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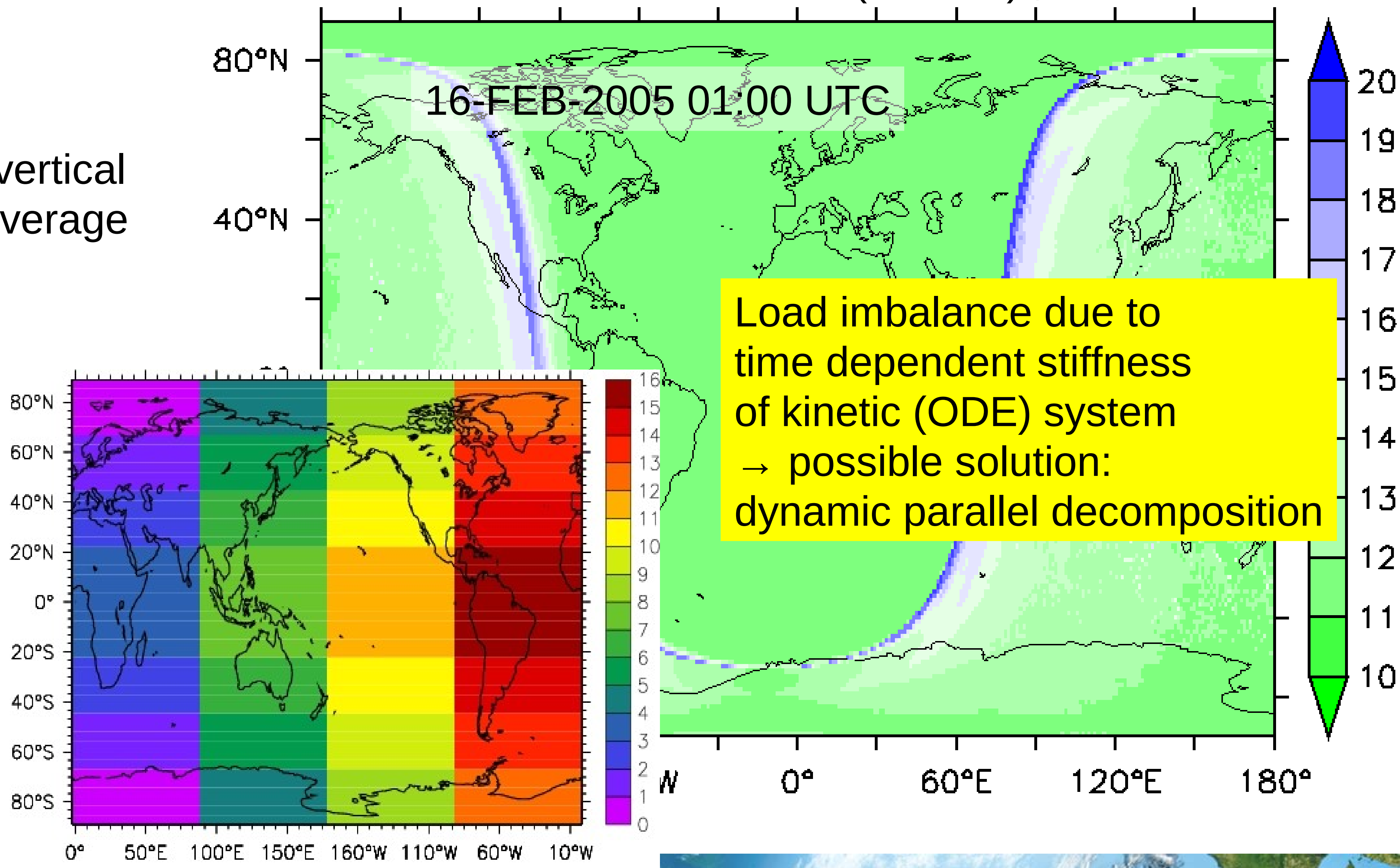


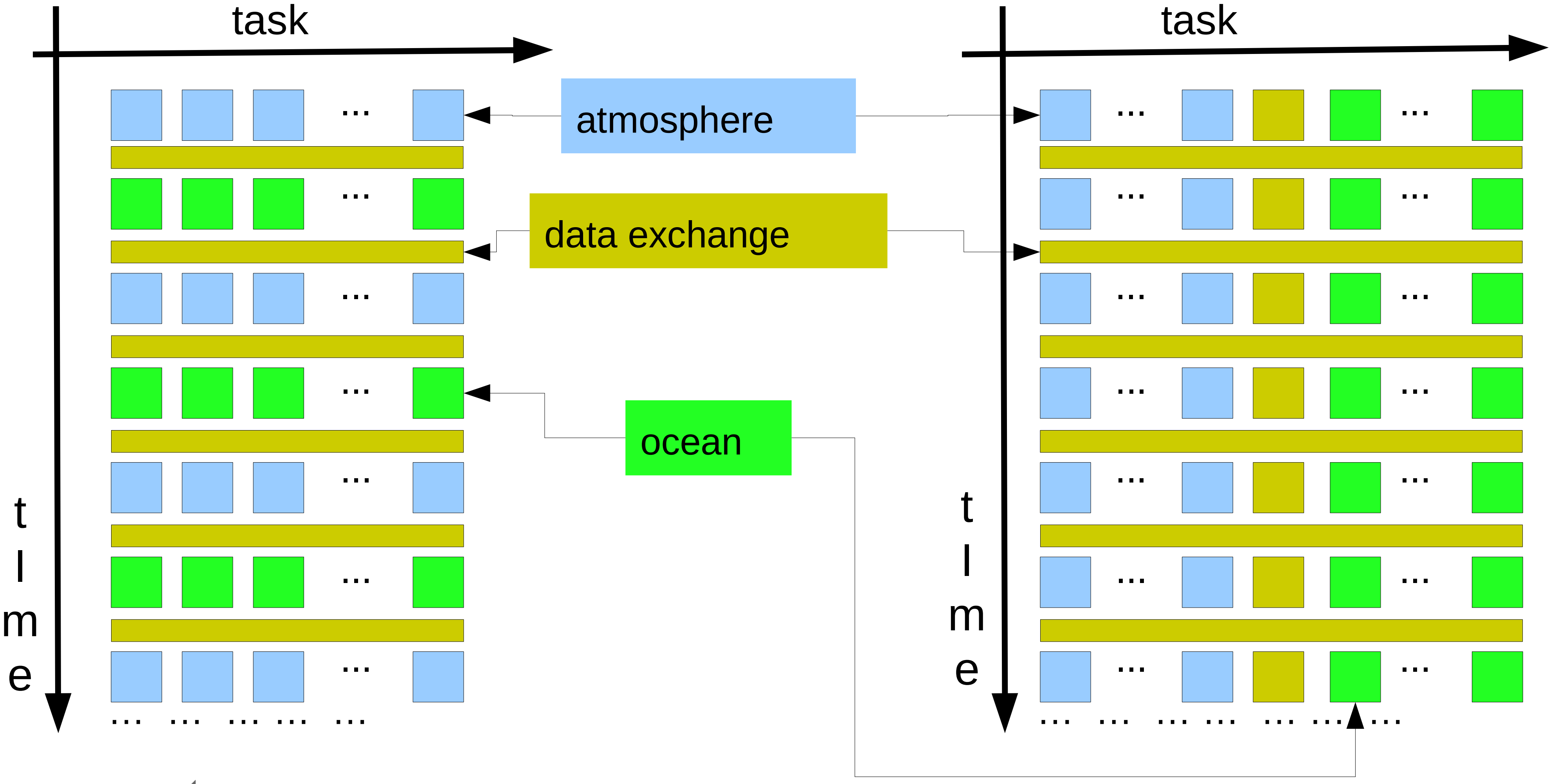
Load imbalance due to
time dependent stiffness
of kinetic (ODE) system
→ possible solution:
dynamic parallel decomposition

Example 2: internal coupling **versus** indirect external coupling

of an Atmosphere – Ocean System (domain coupling)

MPIOM as MESSy submodel
“coupled to” ECHAM5

MPIOM – OASIS3 – ECHAM5



Example 2: internal coupling **versus** indirect external coupling

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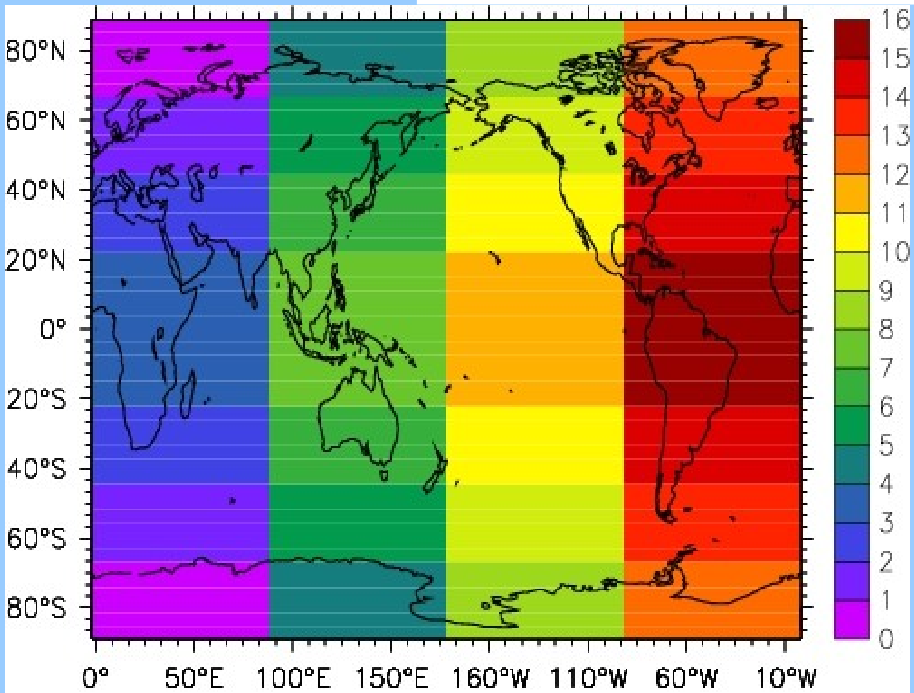
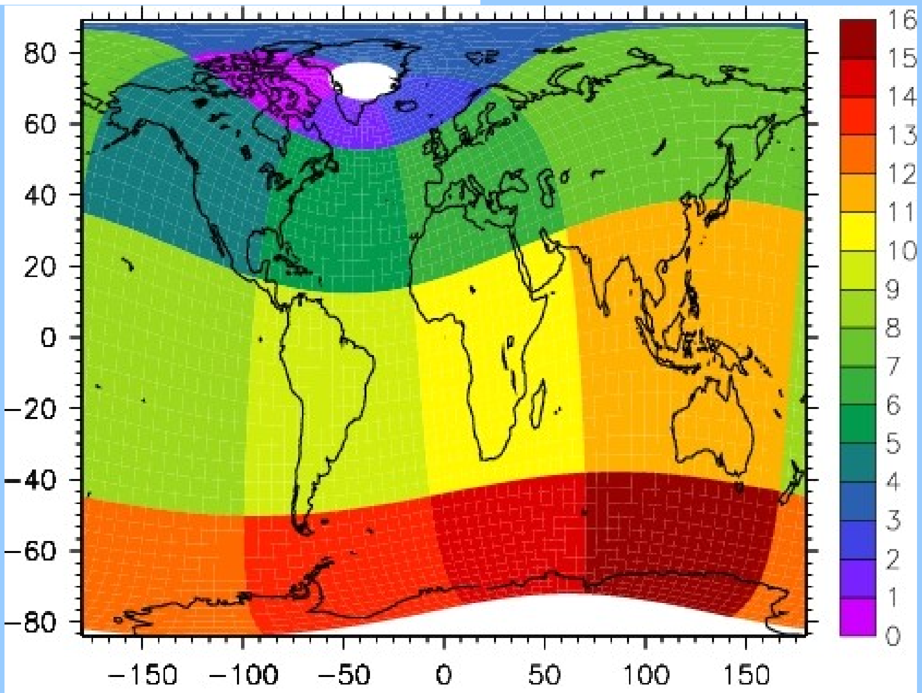
Processor ID # for 4 x 4 decomposition



Atmosphere



Ocean (rotated grid)

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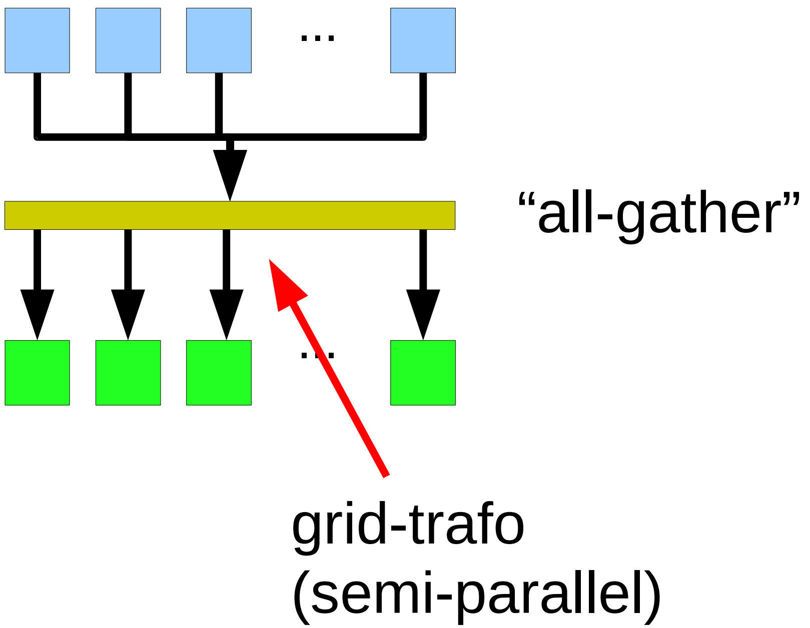
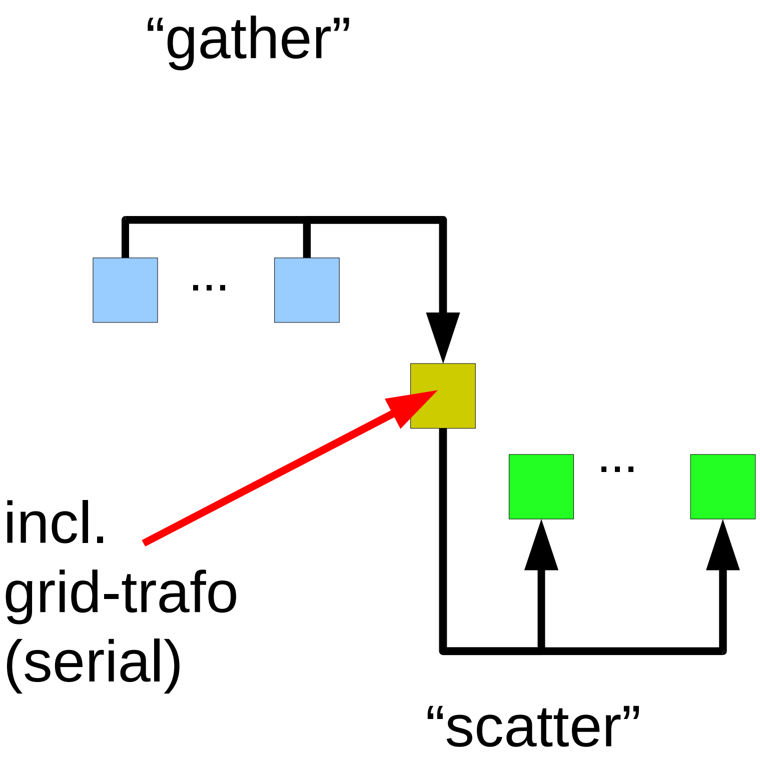
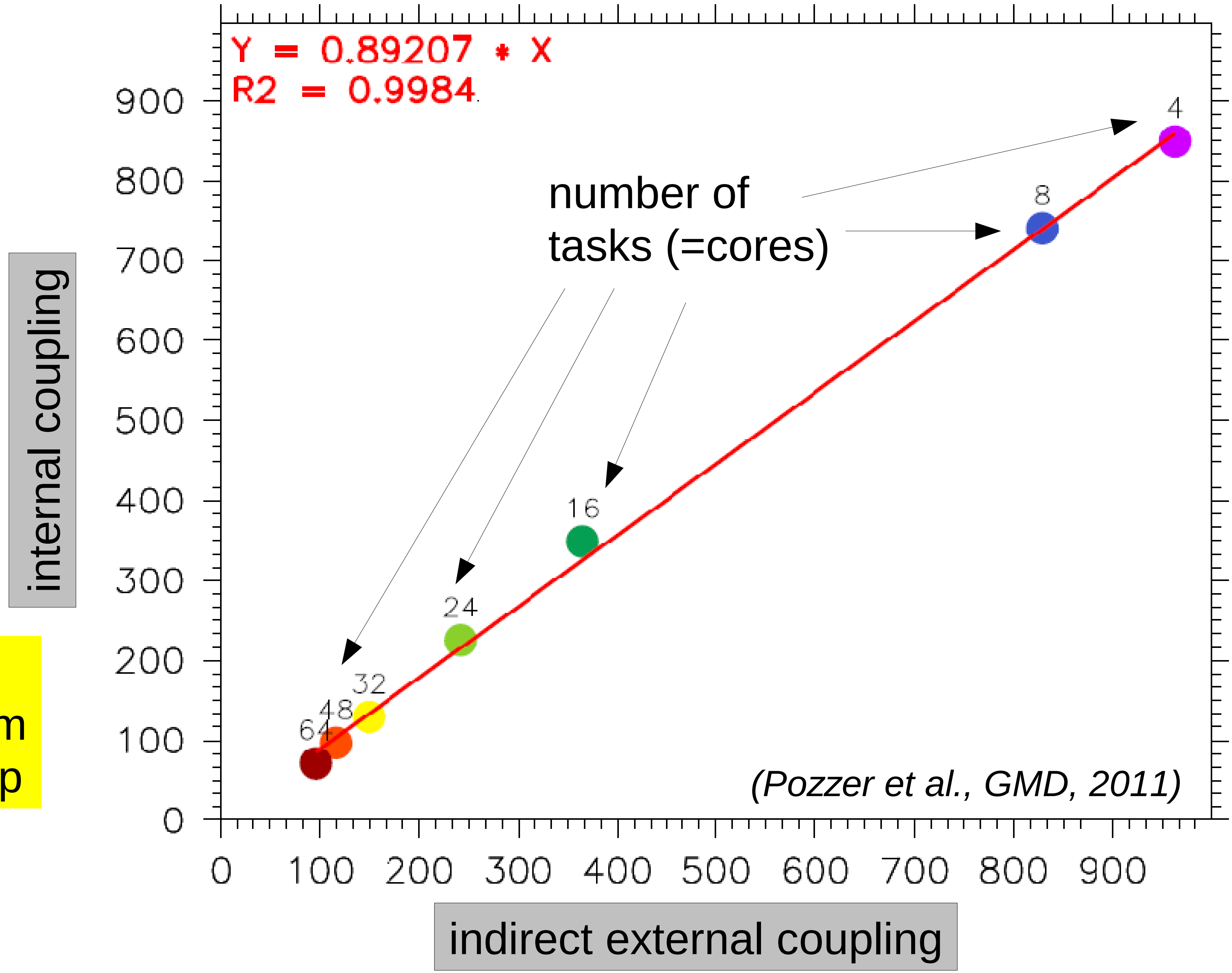




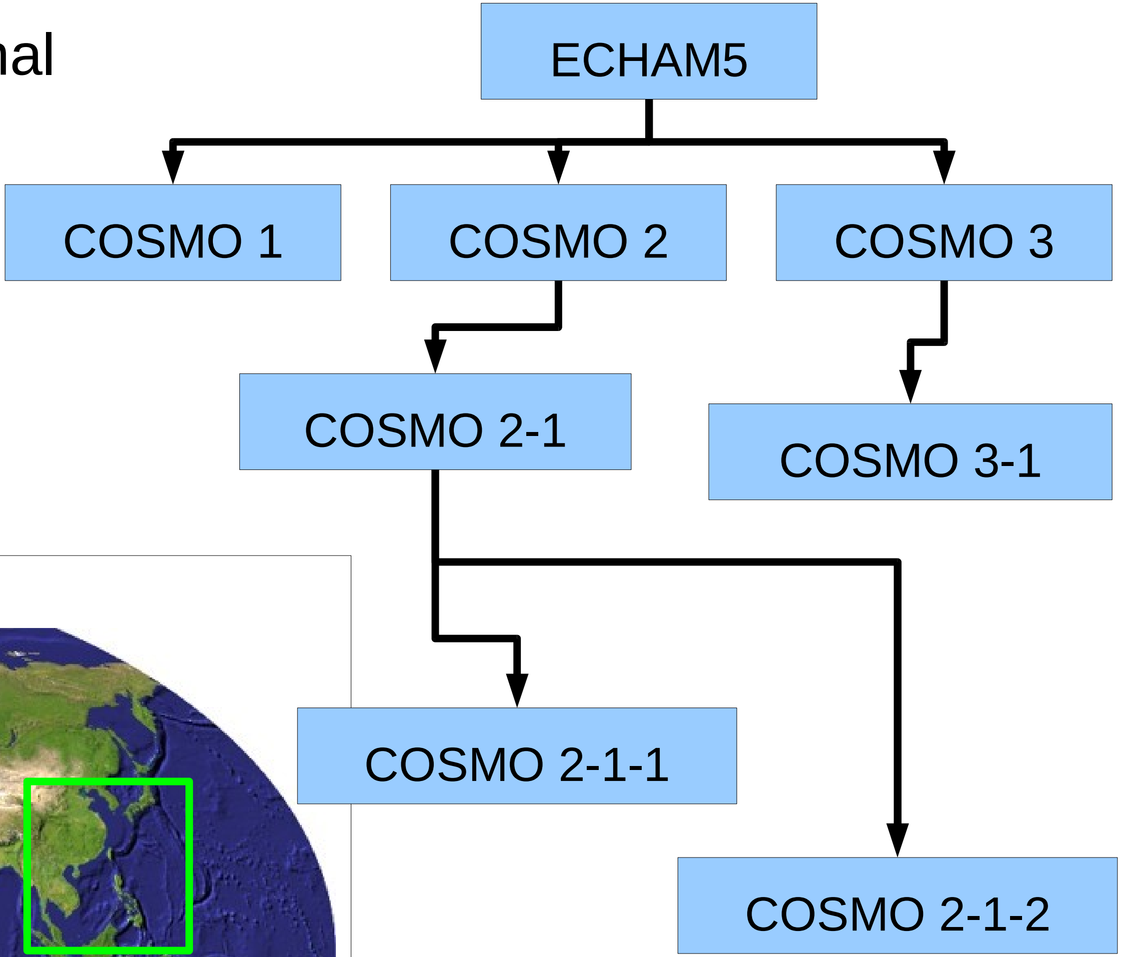
Example 2: Performance (seconds per simulated month)

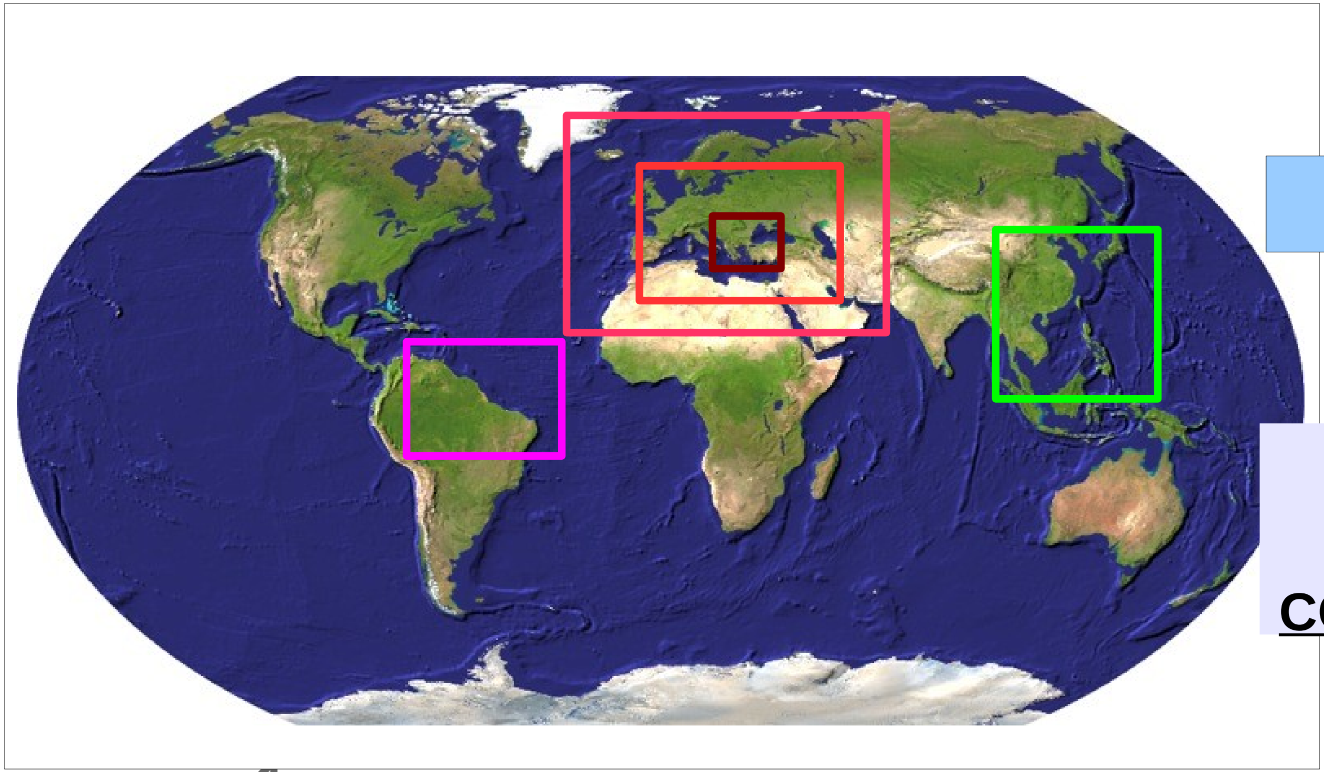


depends on:
- HPC system
- model setup

Example 3: On-line nesting: an alternative way to higher resolution

- 1-way on-line nested global-regional atmospheric model system (zoom)
- multiple instances possible due to client – server architecture of MMD ...





MECO(n):
<u>M</u>ESSy-fied <u>E</u>CHAM and
<u>CO</u>SMO models <u>n</u>-times nested

(Kerkweg & Jöckel, GMD, 2012a,b; Hofmann et al., GMD, 2012)

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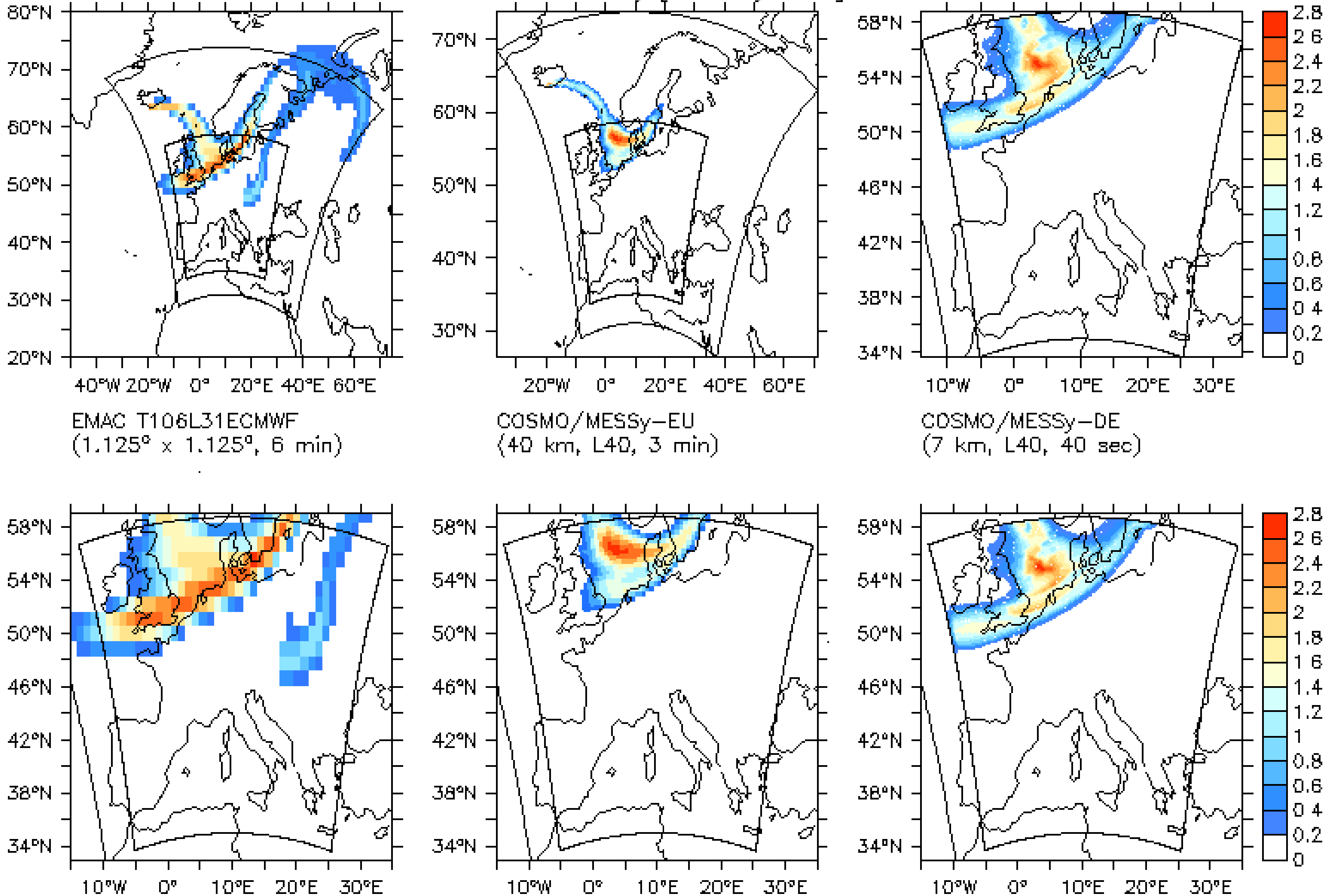
MECO(2) simulation of **Eyjafjallajokull eruption plume 2010**

TIME : 17-APR-2010 00:00 column density [arbitrary units]



(c) Patrick Joeckel, DLR, Aug 2011

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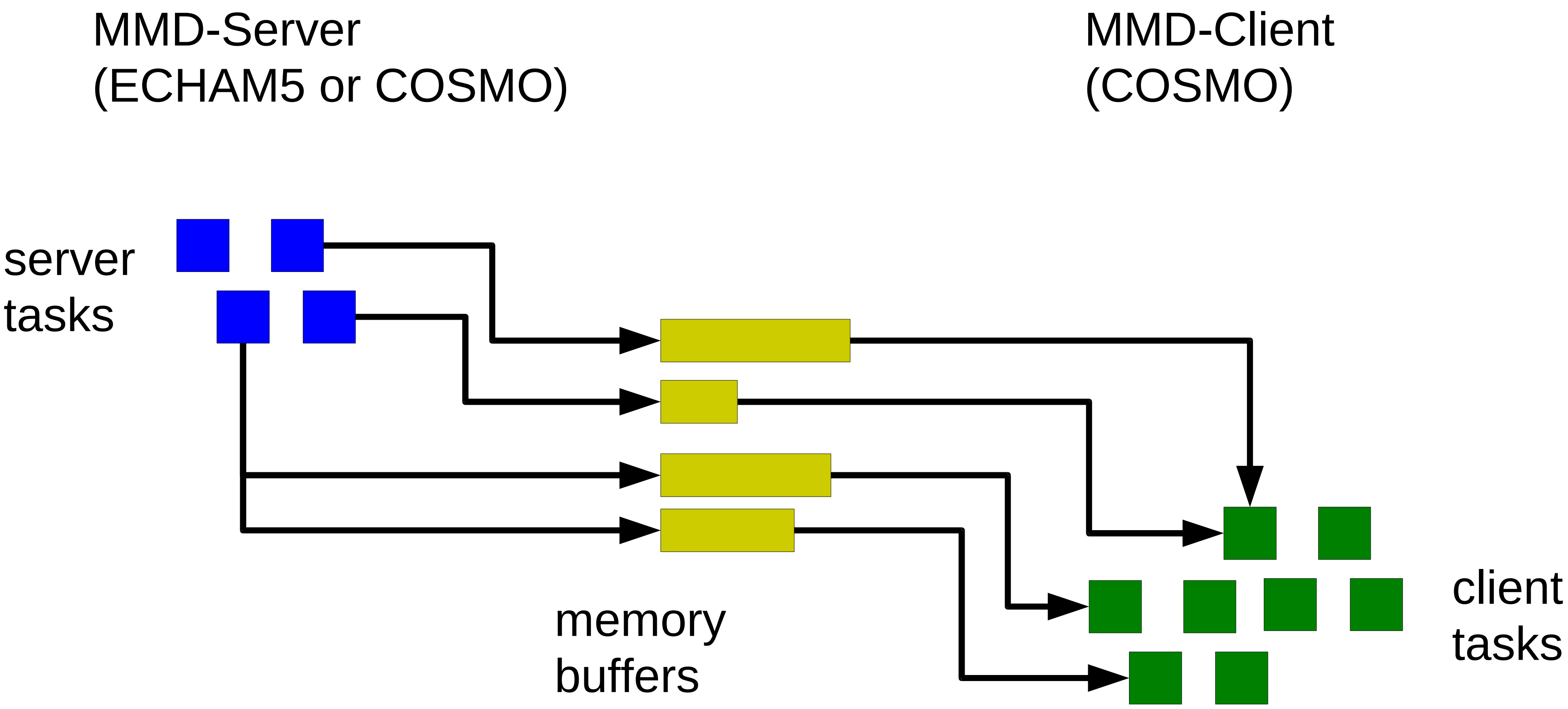
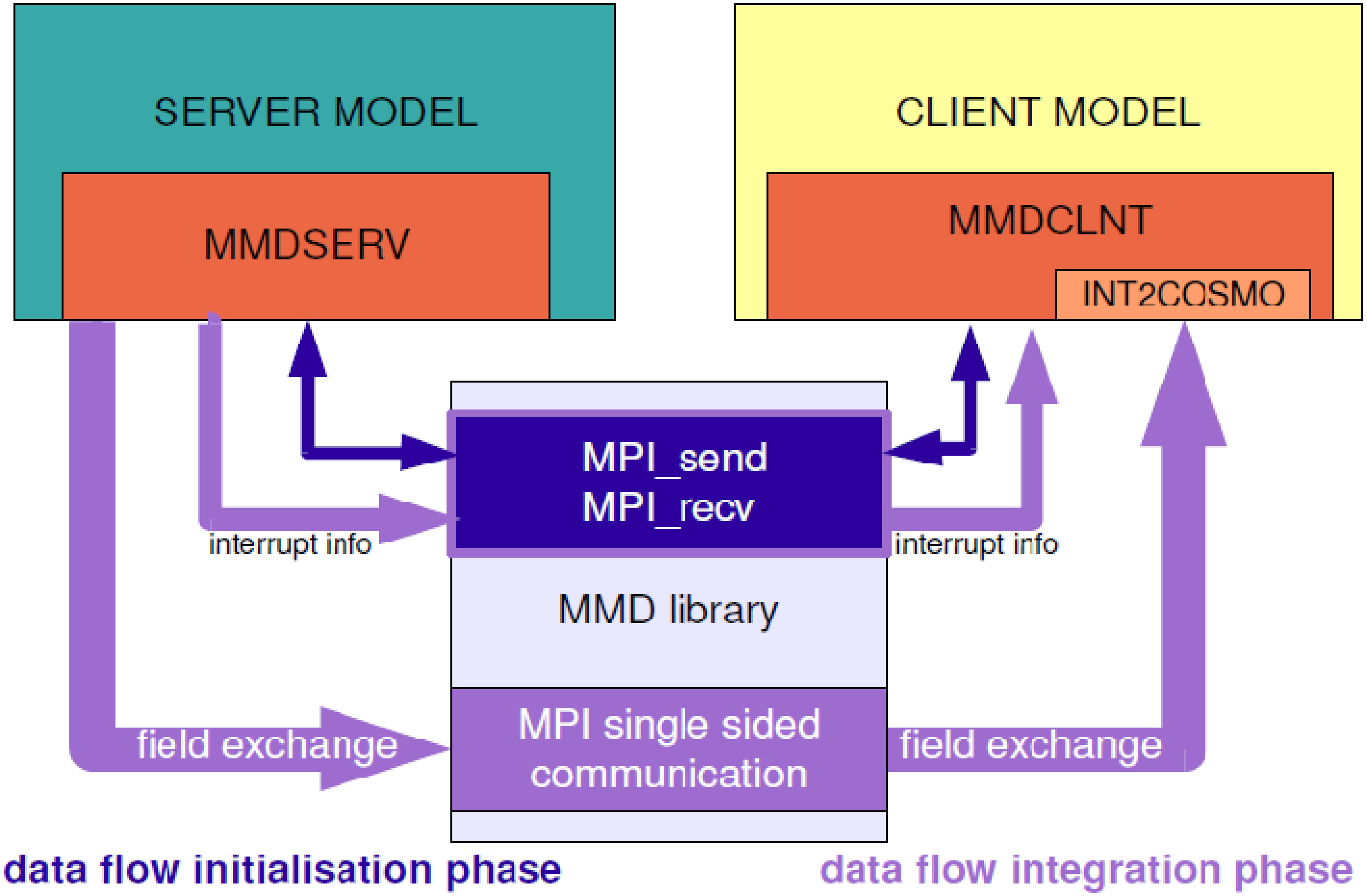


MPI based, single sided “point-to-point” communication between c&s tasks with overlapping grids

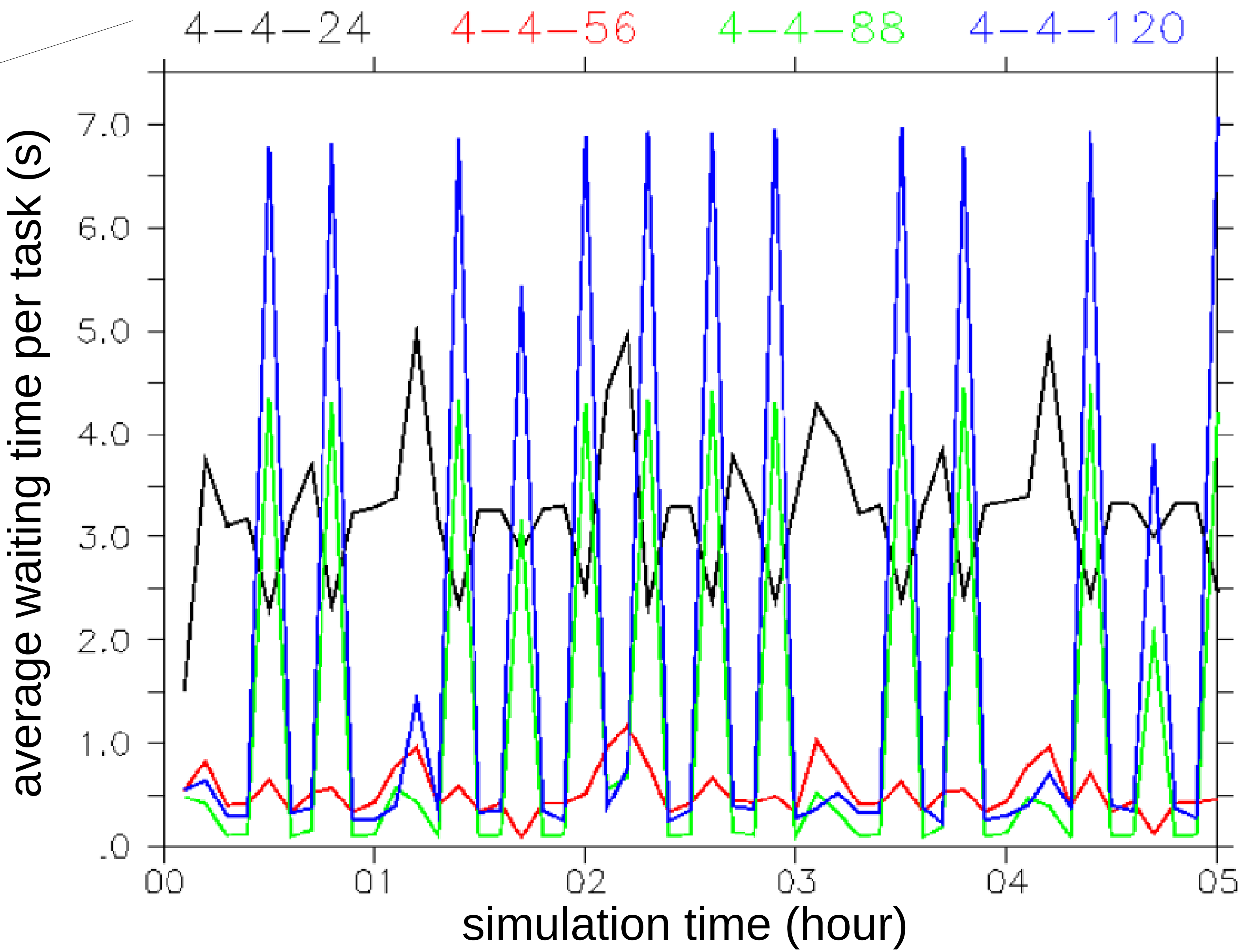
Example 3: On-line nesting: an alternative way to higher resolution



(Kerkweg & Jöckel, GMD, 2012b)

Example 3: On-line nesting: an alternative way to higher resolution

no. of tasks
ECHAM-
COSMO-40 km
COSMO-7 km



4-4-56
is most
efficient !

additional
effort to
optimize
efficiency !

Summary

- ESMs are computationally demanding due to *continuously increasing complexity*
- *Operator splitting* is basis for coupling of model components
- Different coupling methods exist;
  challenge: efficiency – computation versus communication
- Exemplary challenges:
  - Atmospheric Chemistry: *internal coupling*
    → Load Imbalance (parallel decomp.)
  - Atmosphere – Ocean System: *internal* vs. *indirect external* coupling
    → both feasible, best choice depends on model (legacy code!), model setup, HPC-system
  - Global – Regional Nesting: *direct on-line coupling* (client – server approach)
    → complex timing, add. effort to achieve efficiency
- (exascale parallelisation, parallel I/O, memory/core reduction)