Transport in climate/weather models

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Some opportunities at NCAR

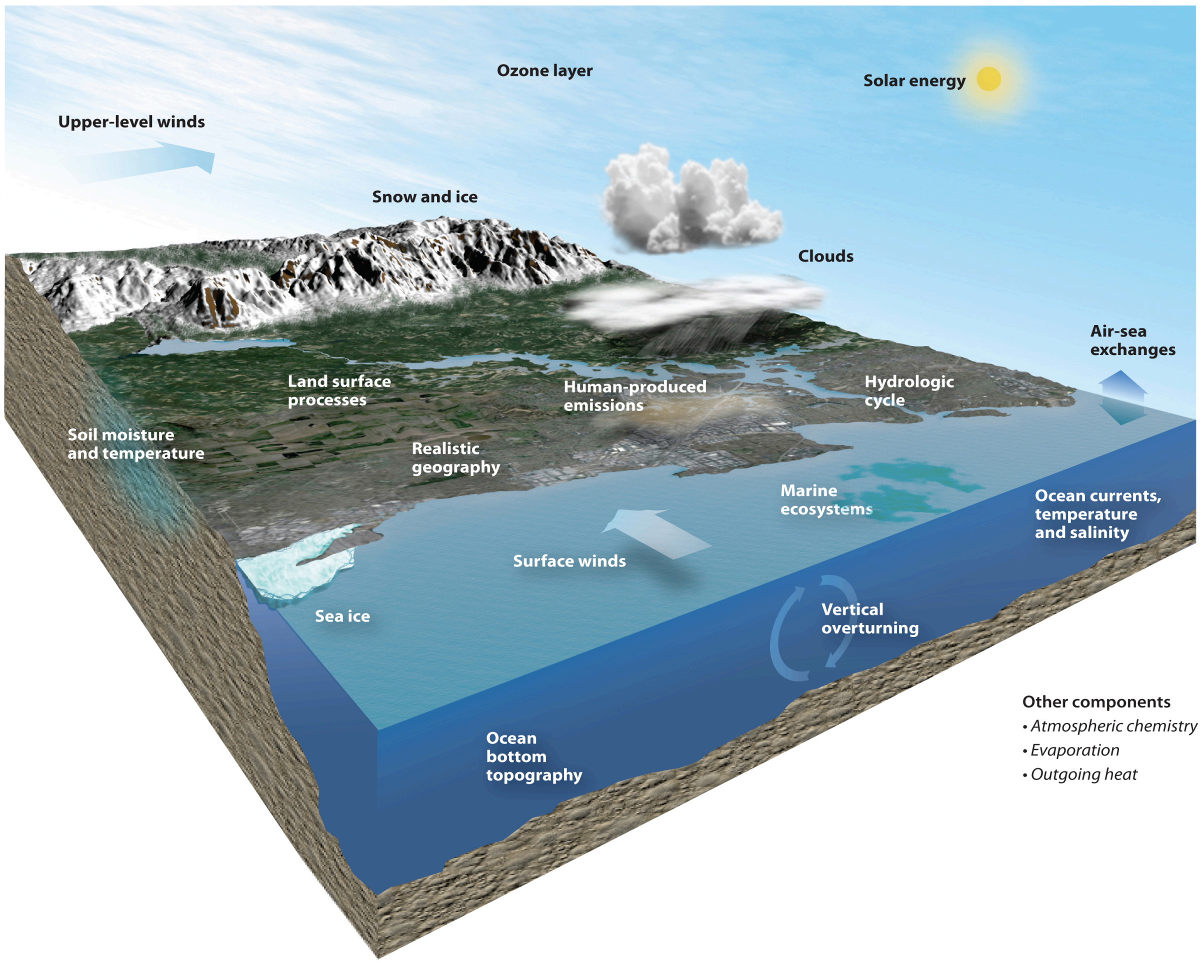
SIParCS
Summer Internships in Parallel Computational Science
BOULDER • CO

Summer Internships in Parallel Computational Science

Advanced Study Program

- **ASP Postdoctoral fellowships**
- **Graduate student visitor program**

NCAR's CESM
(Community Earth System Model)



Community Atmosphere Model (CAM)

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Three talks on transport:

1. **Transport in climate-weather models**

   What do we transport in climate/climate-chemistry models? Why?

2. **Desirable properties of transport schemes**

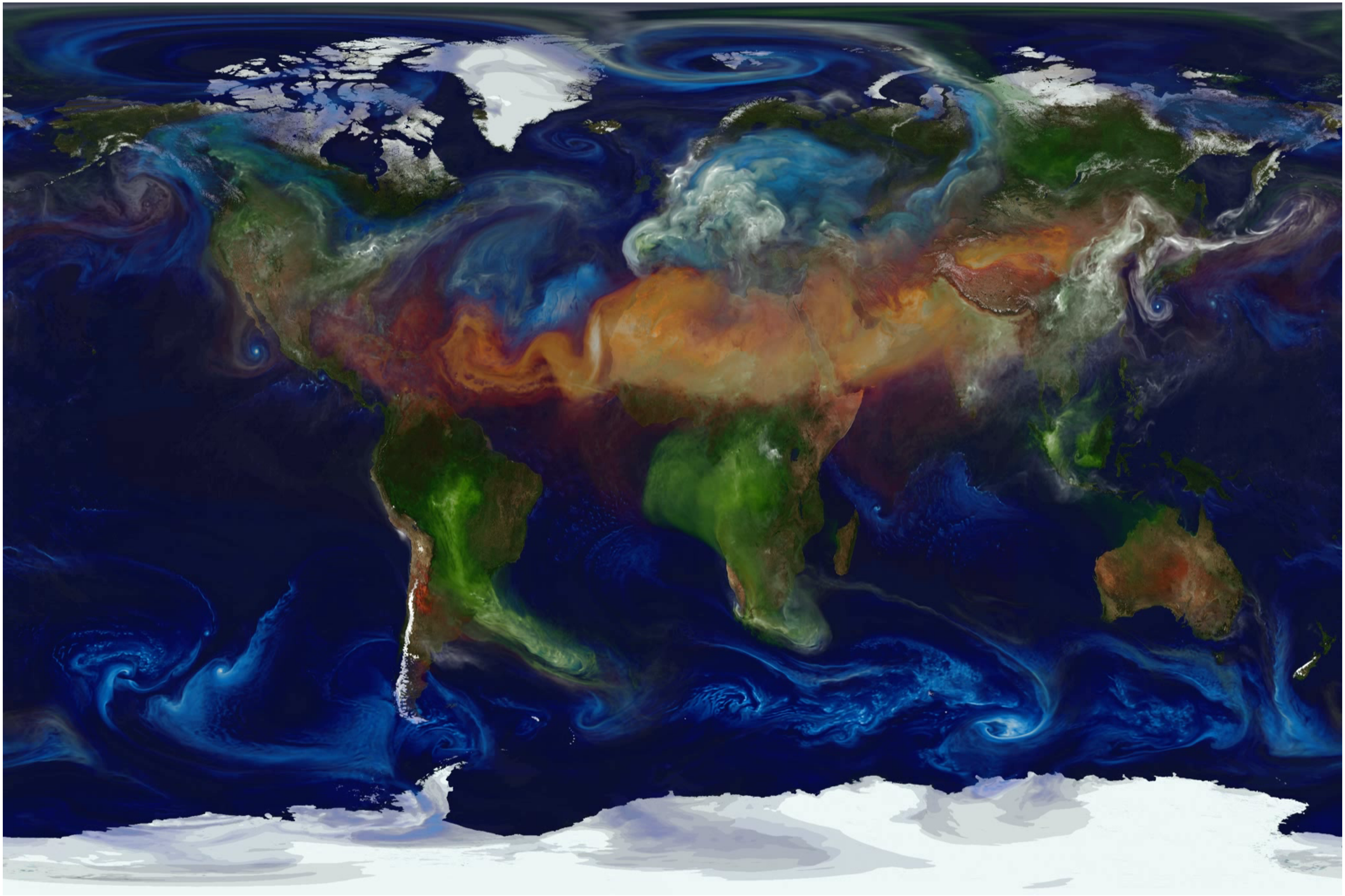
   What physical properties of the continuous equation of motion are important to respect in discretization schemes?

3. **Numerical methods for tracer advection**

   James Kent's lecture

GEOS-5 simulation: winds transporting aerosols (5/2005-5/2007)

In general, dust appears in shades of orange, sea salt blue, sulfates white, and carbon green



The most important continuity equation in modeling

Consider the continuity equation for dry air

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (1)$$

where ρ_d is the density of dry air (mass per unit volume of Earth's atmosphere) and $\mathbf{v}$ is a 3D velocity vector.

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where ρ_d is dry air (mass per unit volume of Earth's atmosphere velocity vector.

Dry air makes up 99.75% of the mass of the atmosphere:

mean mass of dry air = 5.1352 ± 0.0003 x 10^{18} kg

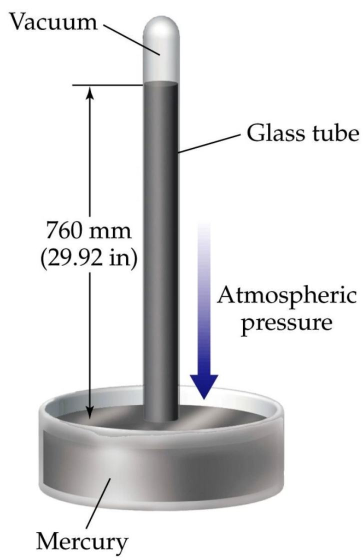
mean mass of atmosphere = 5.1480 x 10^{18} kg

Trenberth and Smith (2005)

The dry hydrostatic surface pressure, $p_{s,d}$, is the force exerted by the dry air above per unit area

$$p_{s,d} = \int_{z=z_s}^{z=z_{top}} g \rho_d \, dz.$$

where g is the acceleration of gravity and p_d is dry pressure.



Simple Mercury Barometer

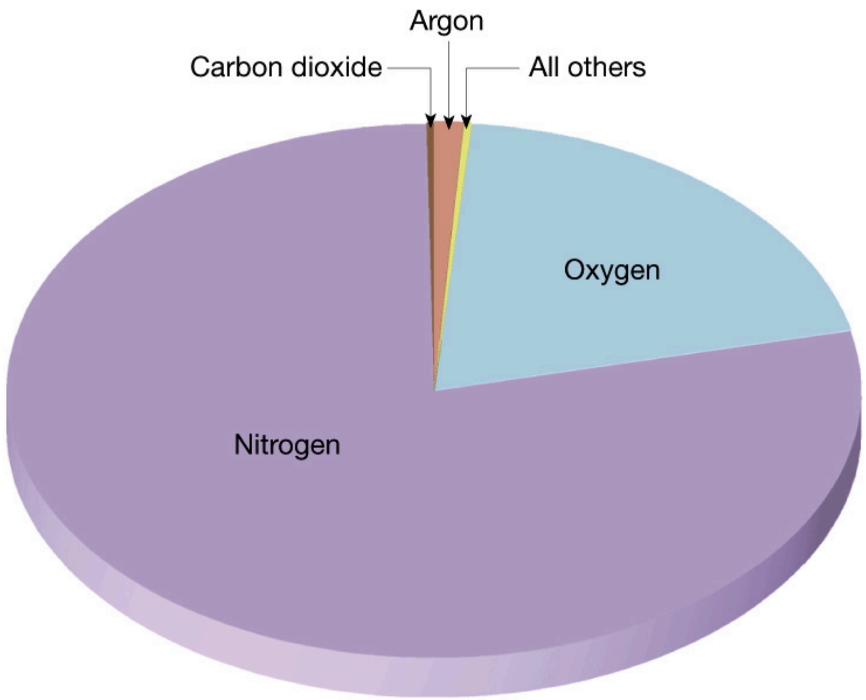
Mean $p_{s,d}$ = 982hPa

Mean p_s = 984.8hPa
(total surface pressure)

Table 1–2 Principal gases of dry air

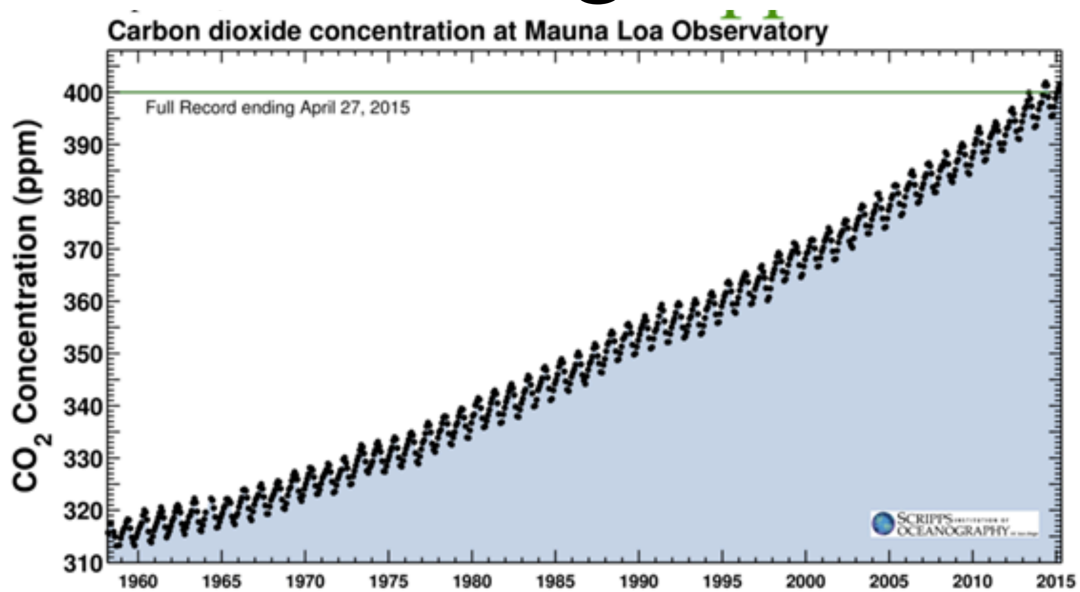
Constituent	Percent by Volume	Concentration in Parts Per Million (PPM)
Nitrogen (N_2)	78.084	780,840.0
Oxygen (O_2)	20.946	209,460.0
Argon (Ar)	0.934	9,340.0
Carbon dioxide (CO_2)	0.036	360.0
Neon (Ne)	0.00182	18.2
Helium (He)	0.000524	5.24
Methane (CH_4)	0.00015	1.5
Krypton (Kr)	0.000114	1.14
Hydrogen (H_2)	0.00005	0.5

Atmospheric composition is changing …



Source: http://www.ux1.eiu.edu/~cfjps/1400/atmos_origin.html

The Keeling curve



Burning fossil fuels add CO_2 to the atmosphere, however, it also removes oxygen, and so the added mass is 37.5% of the oxygen used. The added mass from this process alone would amount to about 0.03 hPa. This is offset by the fact that roughly half of the carbon dioxide generated by fossil fuel burning does not remain in the atmosphere but is taken up by the oceans and biosphere. The latter gives back the oxygen in photosynthesis, while the carbon dioxide entering the ocean may be taken out of the system as carbonate. **The net change in mass is likely to be less than 0.01 hPa in surface pressure** and is more likely a net loss than a gain in mass.

Source:http://serc.carleton.edu/eslabs/carbon/7a.html

The most important continuity equation in modeling

Consider the continuity equation for dry air

Accurate to approximately 0.01hPa globally

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \qquad (1)$$

where ρ_d is the density of dry air (mass per unit volume of Earth's atmosphere) and $\mathbf{v}$ is a 3D velocity vector.

The most important continuity equation in modeling

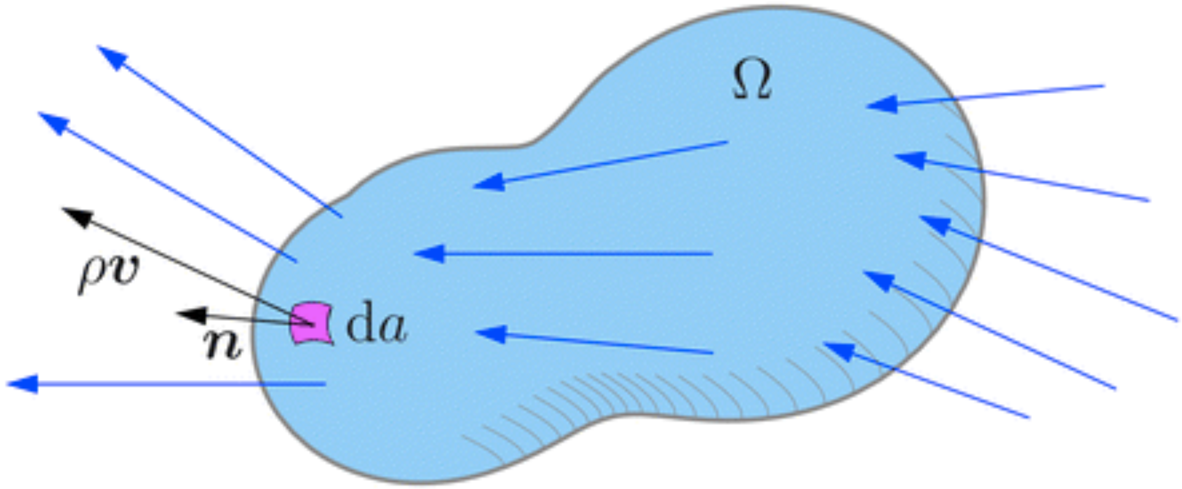
Consider the continuity equation for dry air

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (1)$$

where ρ_d is the density of dry air (mass per unit volume of Earth's atmosphere) and $\mathbf{v}$ is a 3D velocity vector.

Note that the continuity equation for air is "tightly" coupled with momentum and thermodynamic equations

To solve (1) we need to know the velocity field!



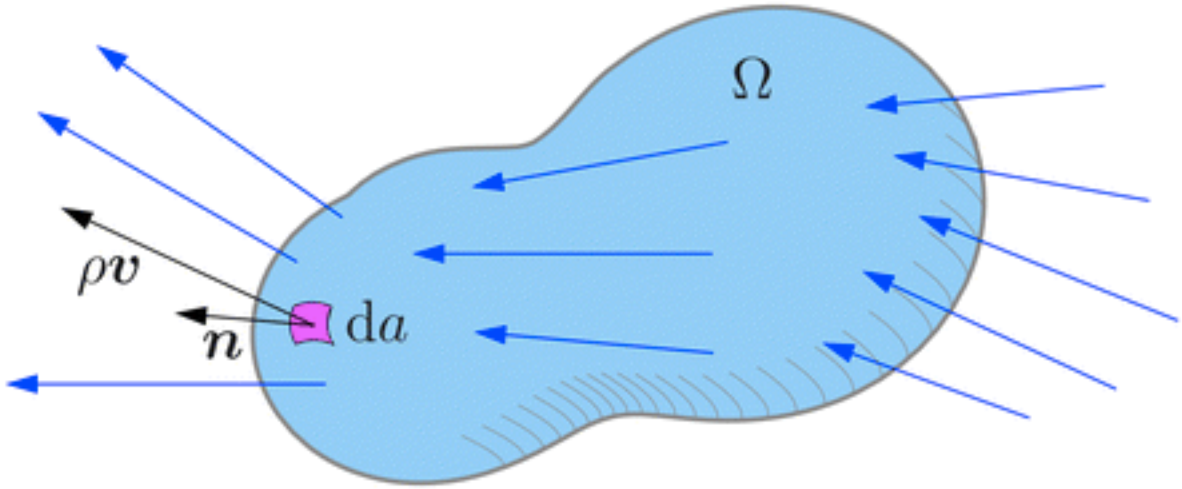
Eulerian version:

Ω stays fixed
in local coordinate system

- The continuity equation is a conservation law for mass:

$$\begin{aligned}\frac{\partial}{\partial t}\iiint_\Omega \rho_d \, dV &= -\iiint_\Omega \nabla\cdot(\rho_d \mathbf{v})\, dV,\\ &= -\oiint_{\partial\Omega} (\rho_d \mathbf{v})\cdot\mathbf{n}\, dS,\end{aligned}$$

where Ω is a fixed volume, ∂Ω the surface of Ω and **n** is outward pointing unit vector normal to the local surface.
⇒ The flux of mass through the area *da* is *da* times $\rho_d \mathbf{v}\cdot\mathbf{n}$.



Lagrangian version:

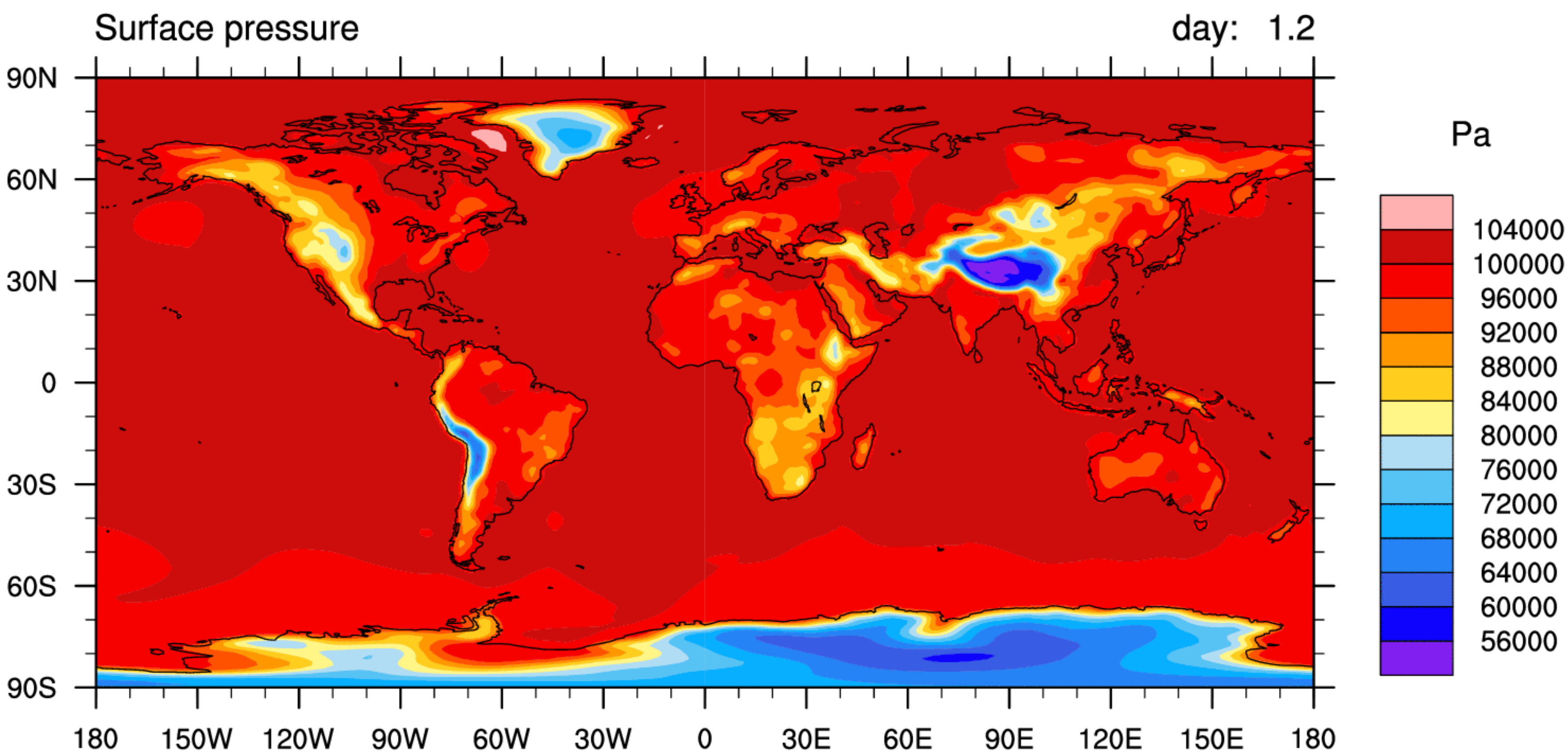
Ω moves with the flow

- The continuity equation is a conservation law for mass:

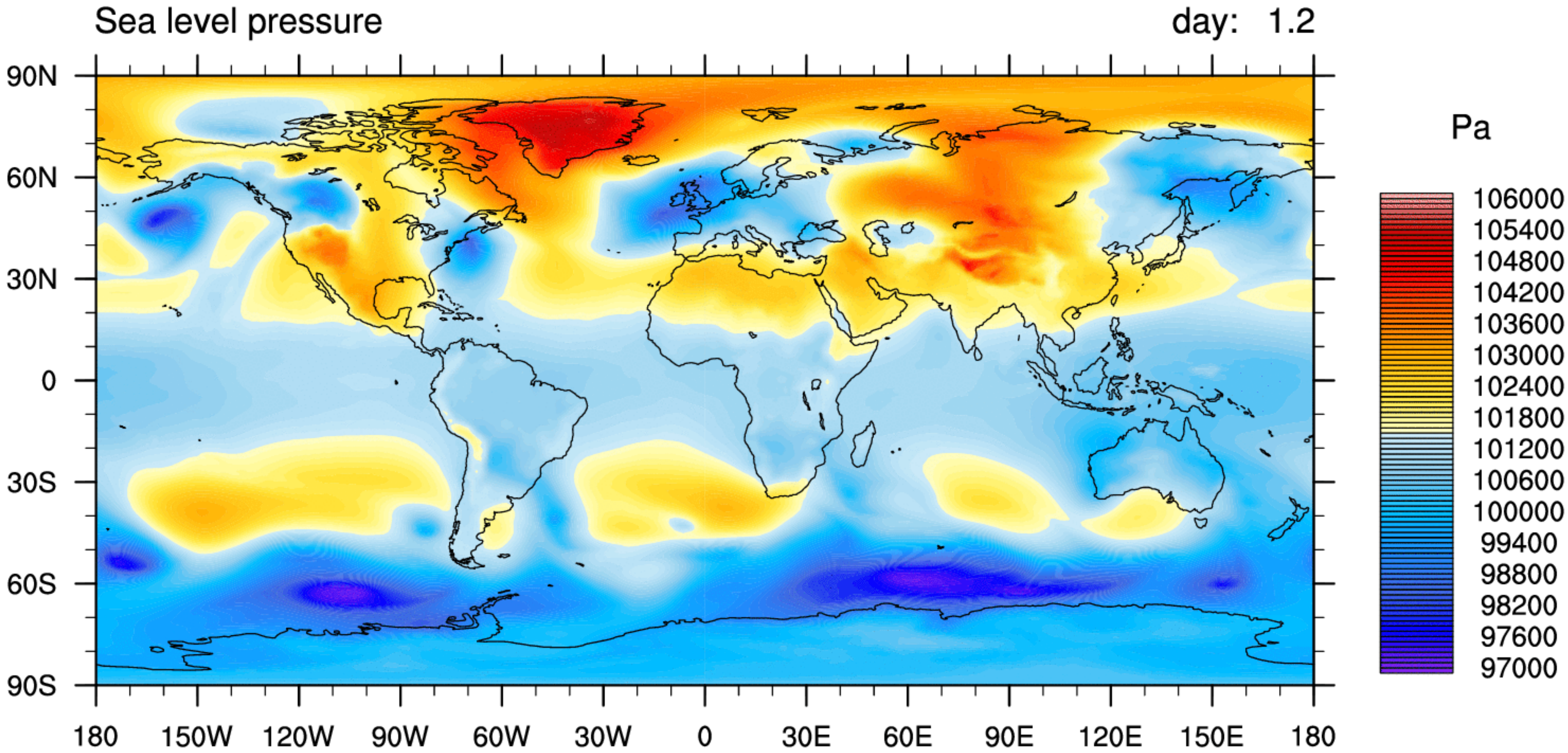
$$\frac{\partial}{\partial t}\iiint_{\Omega} \rho_d dV = -\iiint_{\Omega} \nabla\cdot(\rho_d \mathbf{v})\, dV,$$

$$= -\oiint_{\partial\Omega} (\rho_d \mathbf{v})\cdot\mathbf{n}\, dS,$$

FV dycore, CAM5 physics



FV dycore, CAM5 physics



Water in the atmosphere

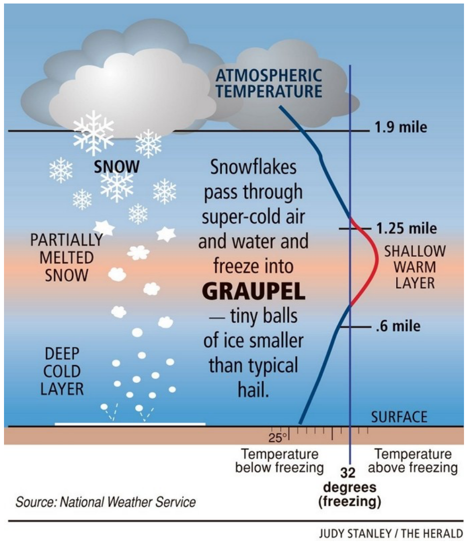
1. Water vapor (gaseous phase of water): weight of water vapor in the atmosphere corresponds to approximately ~2.4hPa

2. Liquid water (clouds): condensation of water vapor form droplets

3. Frozen water / ice (clouds): ice crystals

Cirrus clouds (high clouds)

High resolution models also transport graubel, hail, snow, …



Water substance X, where $X = v, cl, ci$ (water vapor, cloud liquid and cloud ice), is represented with mixing ratio variable:

$$m_X \equiv \frac{\rho_X}{\rho_d},$$

where ρ_d is the mass of dry air per volume of moist air.

- m_X is mixing ratio of water substance of type X with respect to dry air (not moist air!)
- The mass of moist air in a unit volume, including all water substances, is simply the sum of the individual components

$$\rho = \rho_d + \rho_v + \rho_{cl} + \rho_{ci} = \rho_d \left(1 + m_v + m_{cl} + m_{ci}\right).$$

- Some models (and/or parameterizations) use specific humidities

$$q_X = \frac{\rho_X}{\rho}.$$

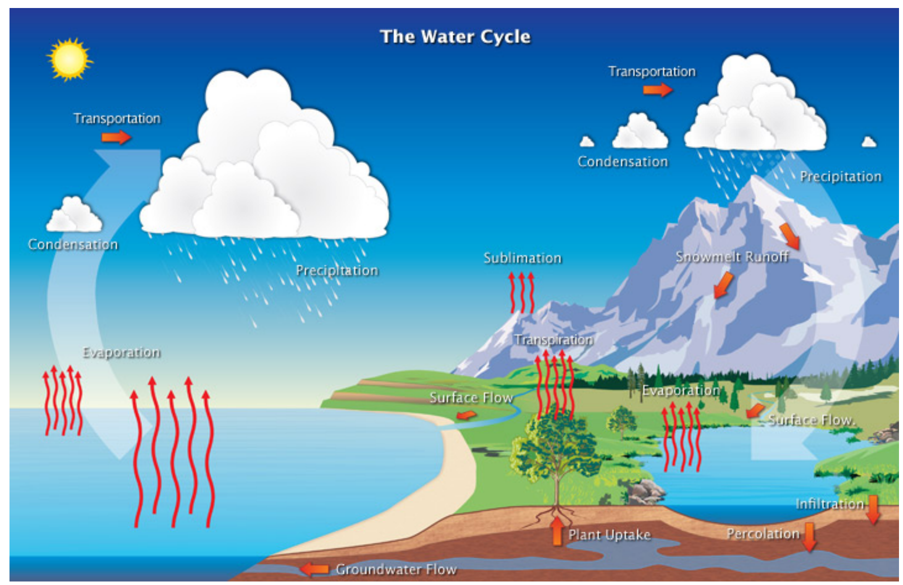
The budget equation for water substance X is

$$\frac{\partial}{\partial t}(m_x \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = \rho_d \, S^{m_X}, \tag{2}$$

where S^{m_X} is source of water substance X.

Water variable sources/sinks:

- **Changes of state**
- **Precipitation formation (and**
- **evaporation)**
- **Unresolved transports by turbulence and convection**
- **Surface fluxes**



Some models solve the continuity equation for 'total air density' ($\rho = \rho_d + \sum_{X=(v,cl,ci)} \rho_X$) rather than ρ_d, in which case there are source terms:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = \sum_{X=(v,cl,ci)} S^{\rho_X}. \quad (3)$$

Similarly, if specific humidities $q_X \equiv \frac{\rho_X}{\rho}$ are used in the prognostic variables instead of 'dry' mixing ratios $m_X \equiv \frac{\rho_X}{\rho_d}$, then the continuity equation for water substance X is

$$\frac{\partial}{\partial t}(q_X \rho) + \nabla \cdot (q_X \rho \mathbf{v}) = \rho S^{q_X} + q_X \sum_{X=(v,cl,ci)} S^{\rho_X}, \quad (4)$$

which is considerably more complicated than

$$\frac{\partial}{\partial t}(m_x \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = \rho_d \, S^{m_X}. \quad (5)$$

Some models solve the continuity equation for 'total air density' ($\rho = \rho_d + \sum_{X=(v,cl,ci)} \rho_X$) rather than ρ_d, in which case there are source terms:

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Similarly, if specific humidities $q_X \equiv \frac{\rho_X}{\rho}$ are variables instead of 'dry' mixing ratios $m_X \equiv$ continuity equation for water substance X is

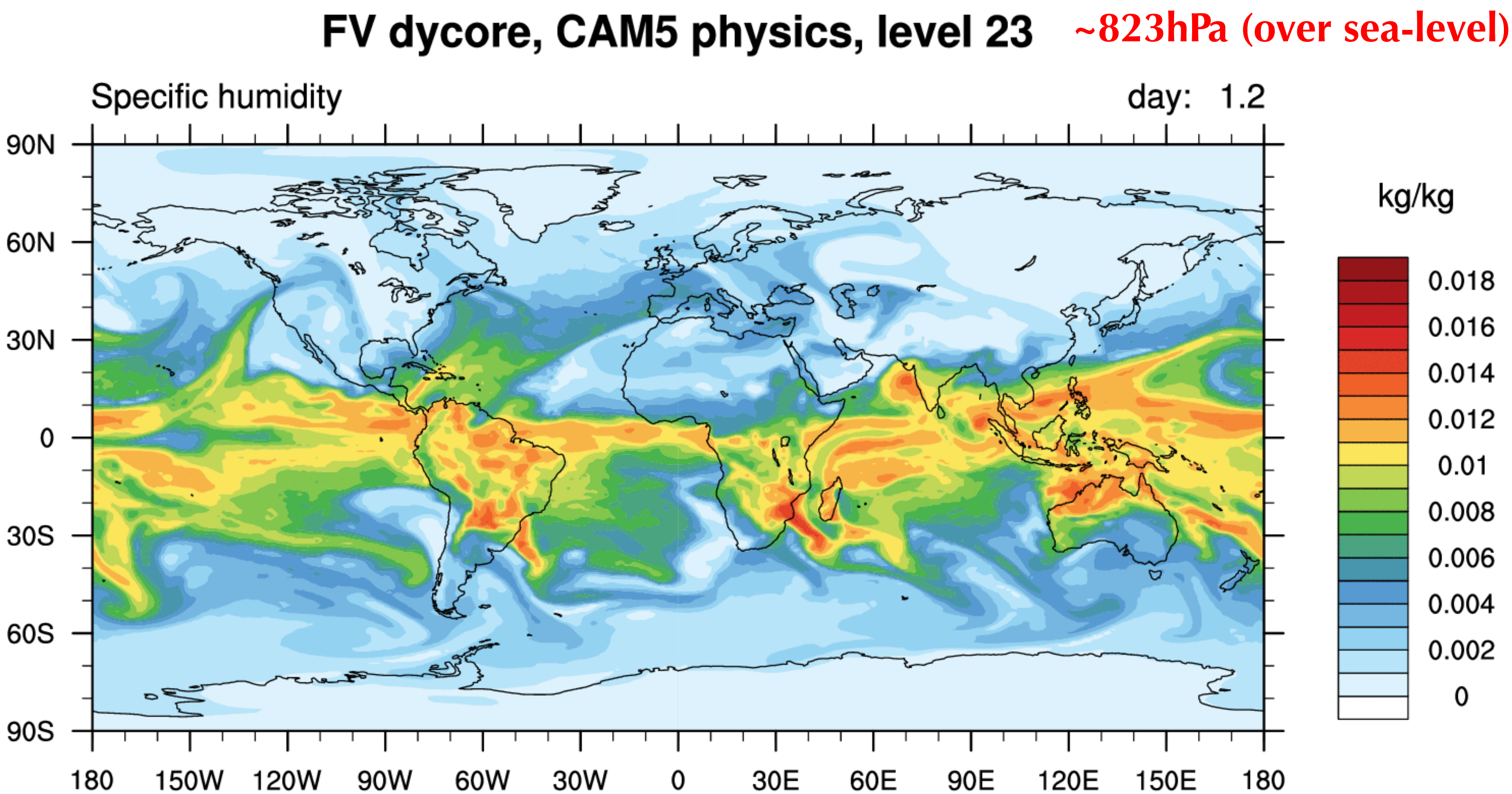
Complicates physics-dynamics coupling!

$$\frac{\partial}{\partial t}(q_X \rho) + \nabla \cdot (q_X \rho \mathbf{v}) = \rho S^{q_X} + q_X \sum_{X=(v,cl,ci)} S^{\rho_X}, \qquad (4)$$

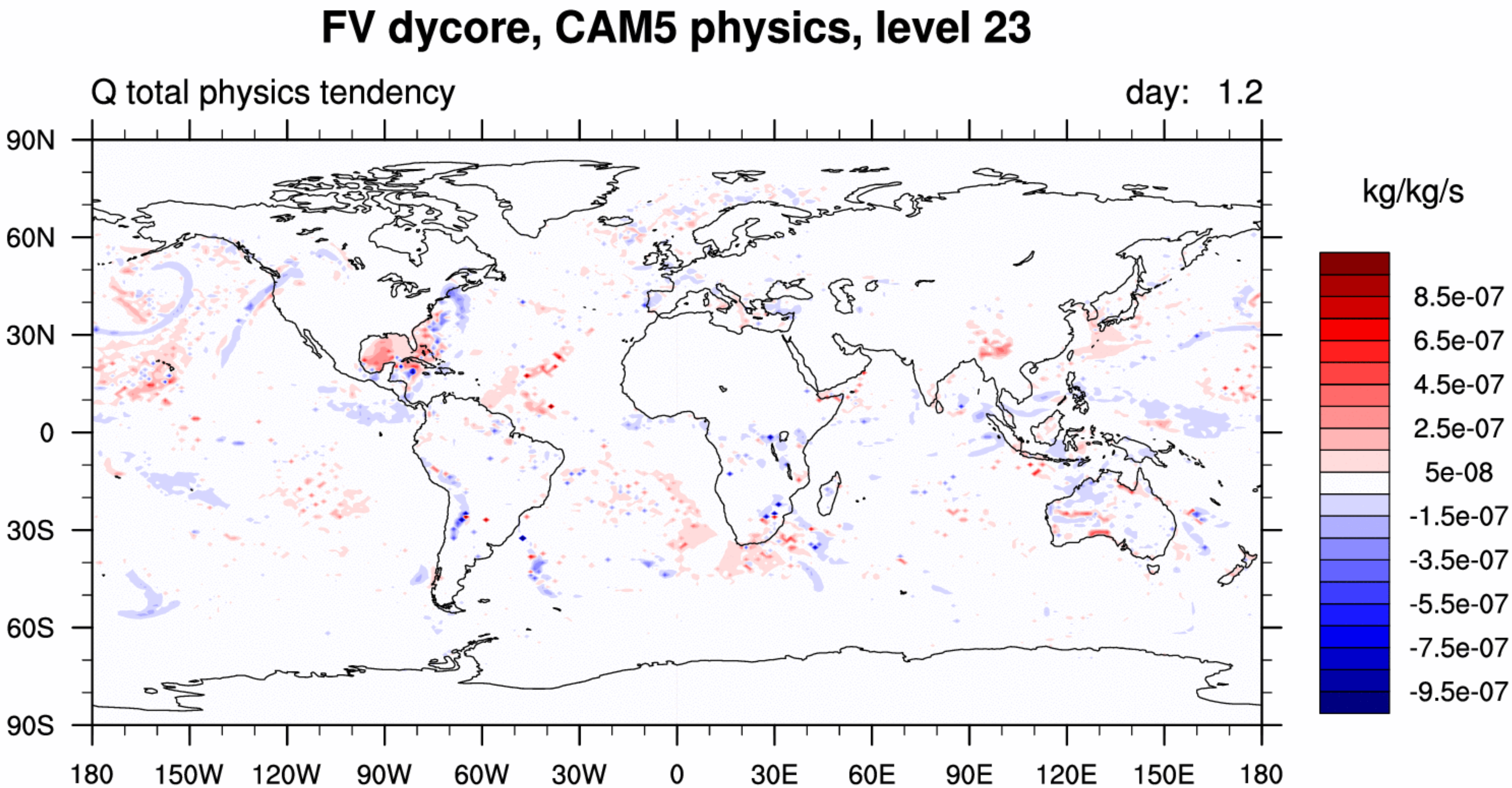
which is considerably more complicated than

$$\frac{\partial}{\partial t}(m_x \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = \rho_d S^{m_X}. \qquad (5)$$

q_v


FV dycore, CAM5 physics, level 23
~823hPa (over sea-level)
Specific humidity
day: 1.2
90N
60N
30N
0
30S
60S
90S
180
150W
120W
90W
60W
30W
0
30E
60E
90E
120E
150E
180
kg/kg
0.018
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0

$$S^{q_v}$$



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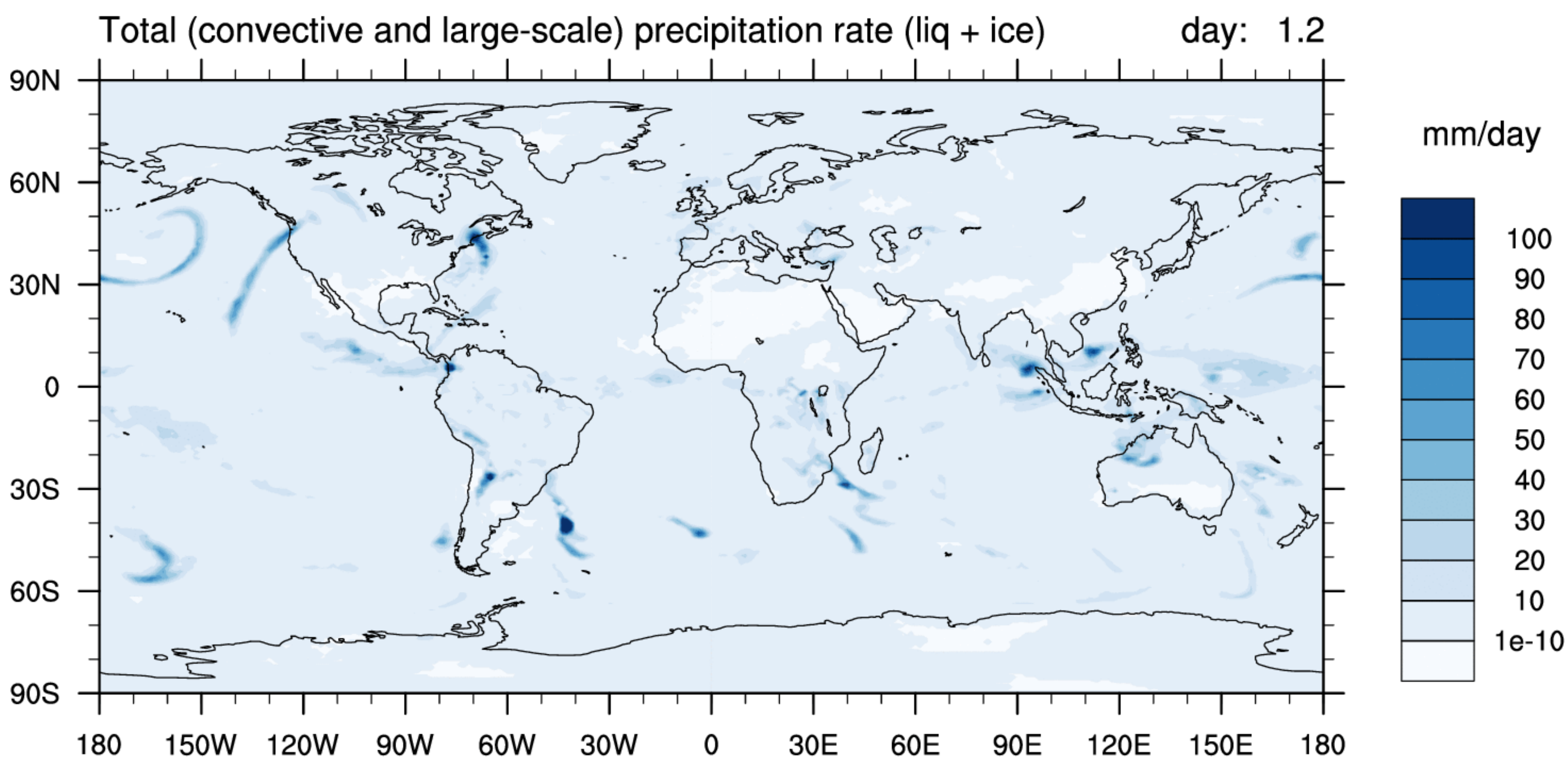
FV dycore, CAM5 physics



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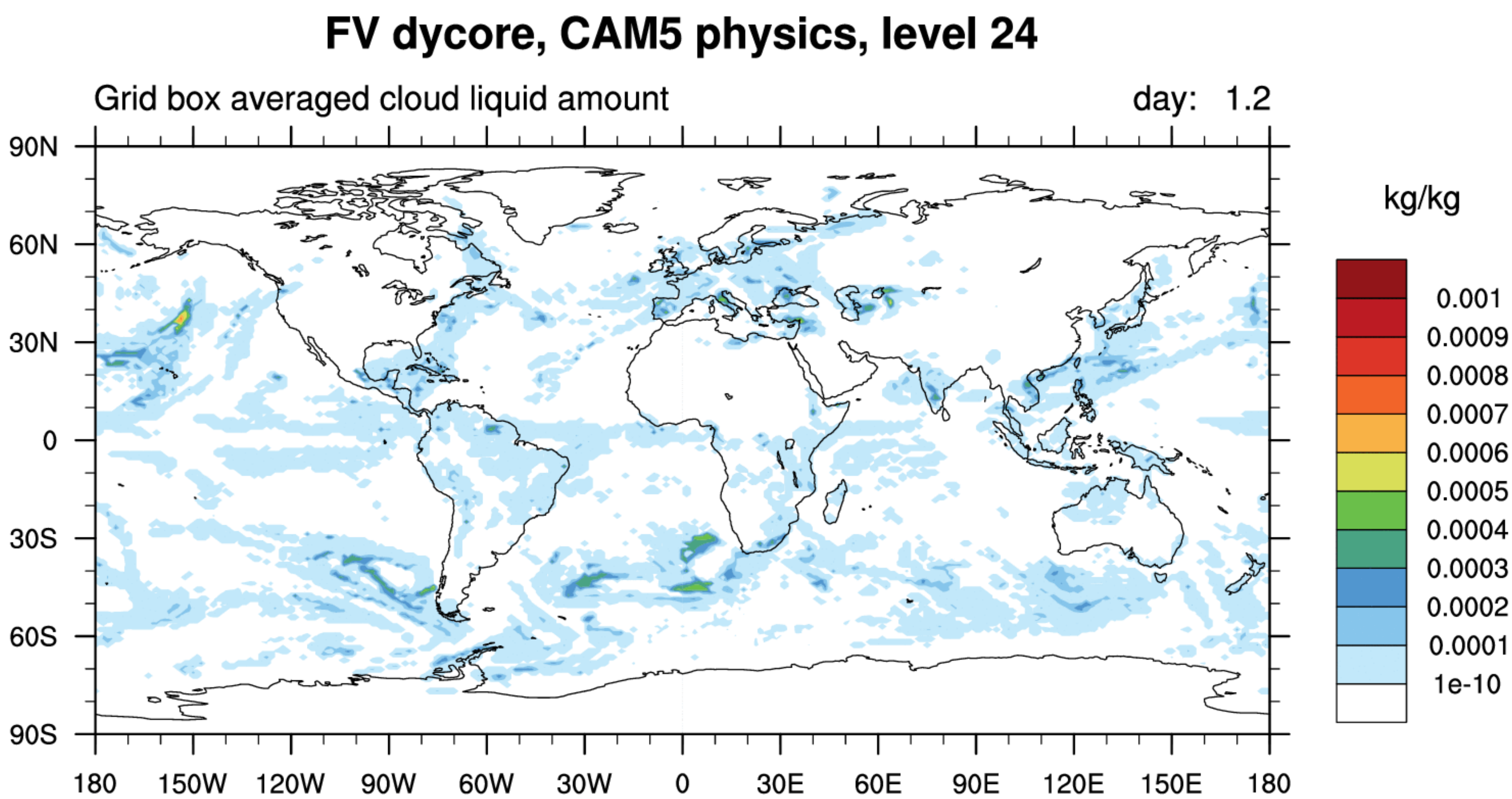
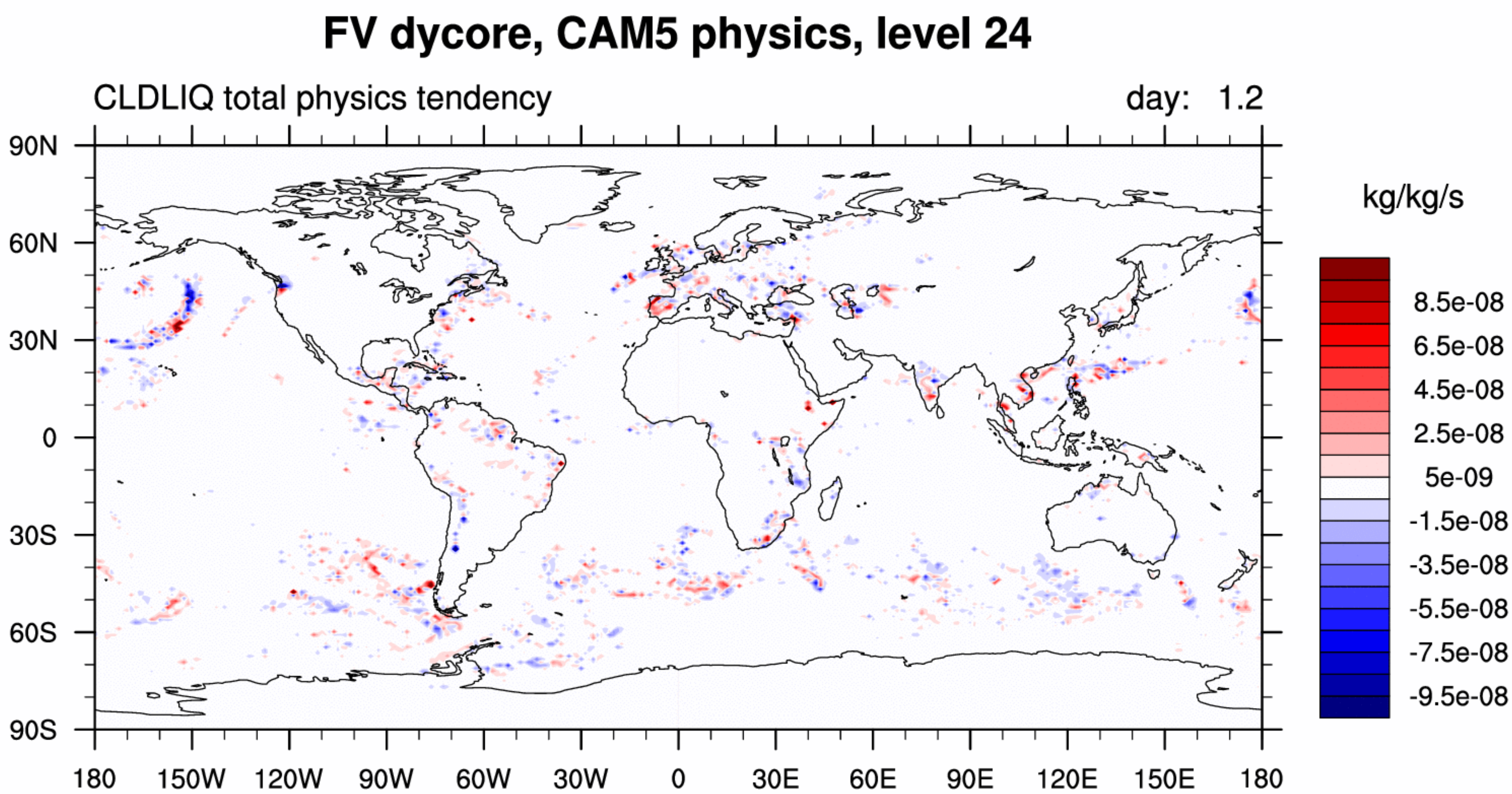
q_{cl}

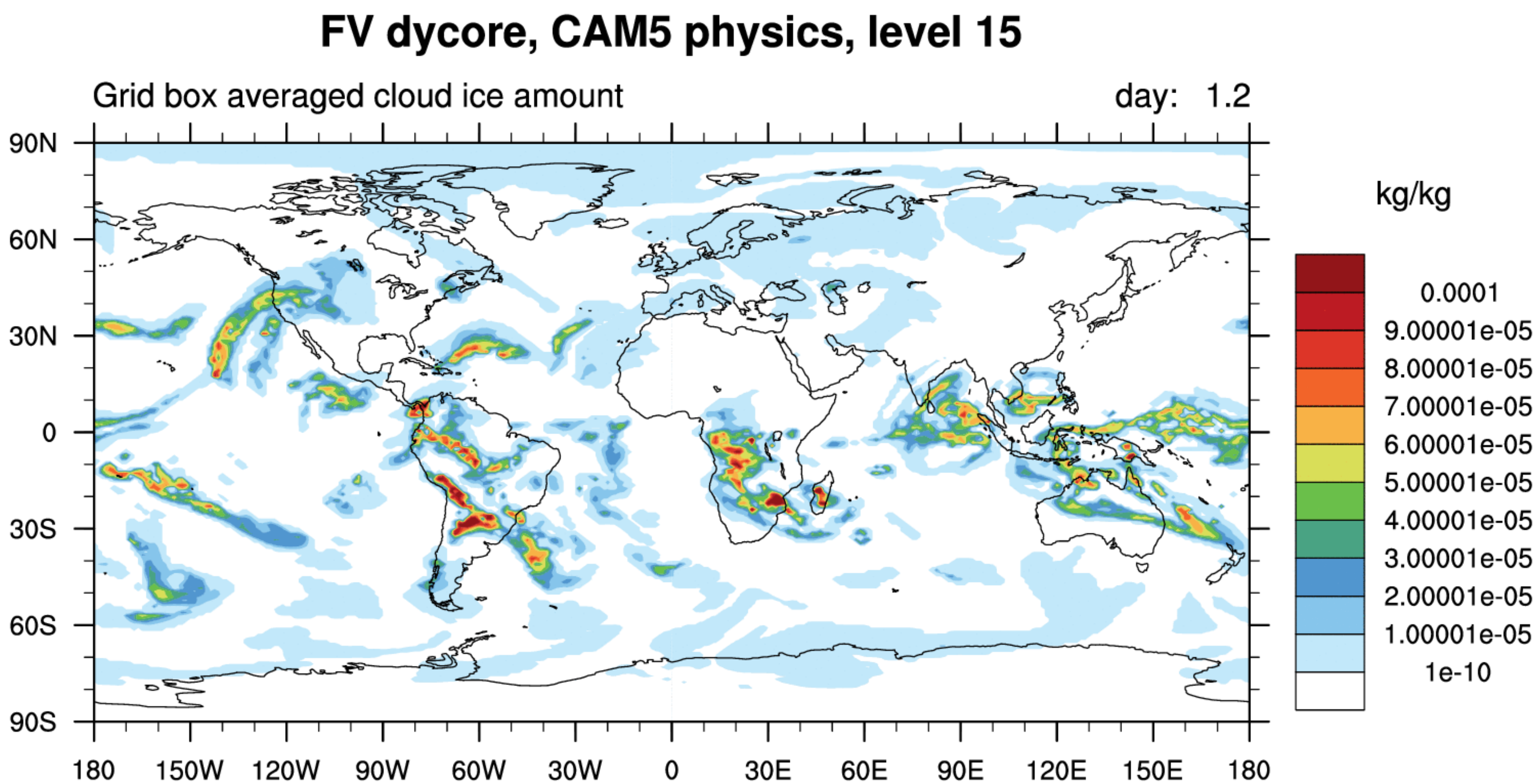

FV dycore, CAM5 physics, level 24
Grid box averaged cloud liquid amount
day: 1.2
90N
60N
30N
0
30S
60S
90S
180
150W
120W
90W
60W
30W
0
30E
60E
90E
120E
150E
180
kg/kg
0.001
0.0009
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
1e-10

$S^{q_{cl}}$

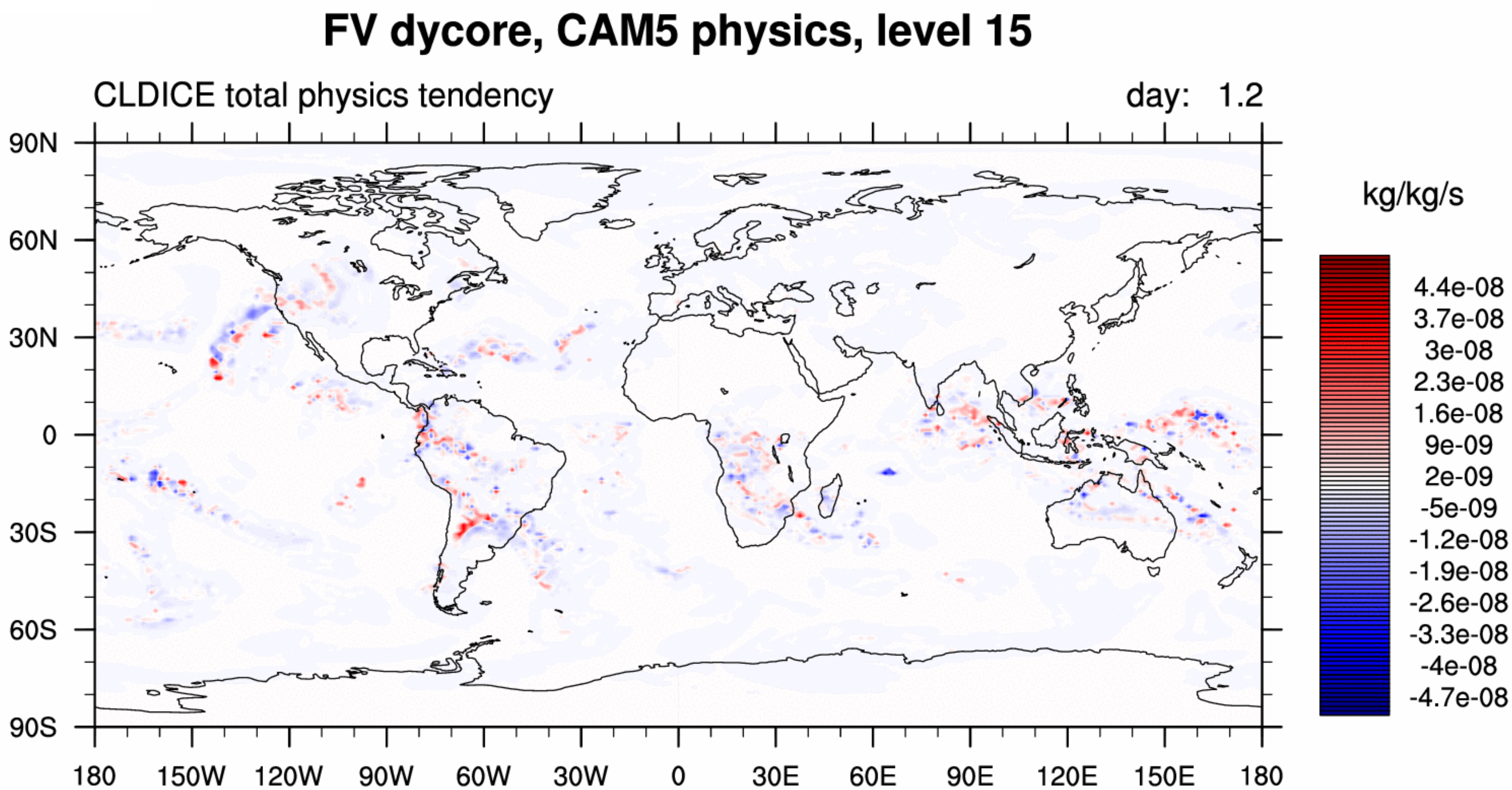


FV dycore, CAM5 physics, level 24
CLDLIQ total physics tendency
day: 1.2
kg/kg/s
8.5e-08
6.5e-08
4.5e-08
2.5e-08
5e-09
-1.5e-08
-3.5e-08
-5.5e-08
-7.5e-08
-9.5e-08
90N
60N
30N
0
30S
60S
90S
180
150W
120W
90W
60W
30W
0
30E
60E
90E
120E
150E
180

q_{ci}


FV dycore, CAM5 physics, level 15
Grid box averaged cloud ice amount
day: 1.2
90N
60N
30N
0
30S
60S
90S
180
150W
120W
90W
60W
30W
0
30E
60E
90E
120E
150E
180
kg/kg
0.0001
9.00001e-05
8.00001e-05
7.00001e-05
6.00001e-05
5.00001e-05
4.00001e-05
3.00001e-05
2.00001e-05
1.00001e-05
1e-10

$S^{q_{ci}}$

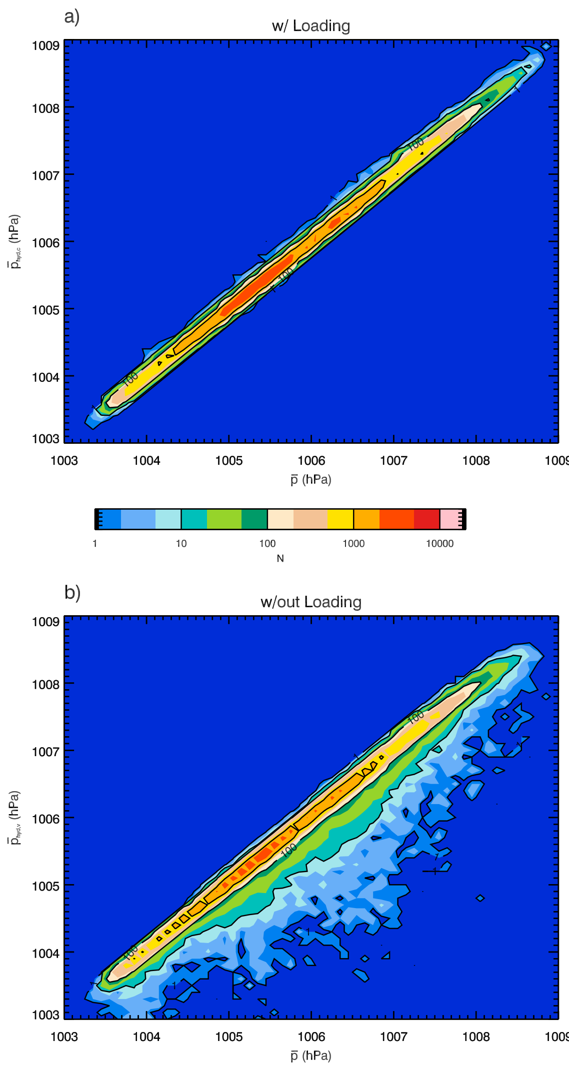

FV dycore, CAM5 physics, level 15
CLDICE total physics tendency
day: 1.2
kg/kg/s
4.4e-08
3.7e-08
3e-08
2.3e-08
1.6e-08
9e-09
2e-09
-5e-09
-1.2e-08
-1.9e-08
-2.6e-08
-3.3e-08
-4e-08
-4.7e-08
90N
60N
30N
0
30S
60S
90S
180
150W
120W
90W
60W
30W
0
30E
60E
90E
120E
150E
180

$$\rho = \rho_d + \rho_v$$

versus

$$\rho = \rho_d + \rho_v + \rho_{cl} + \rho_{ci}$$

Condensate loading (CL) and surface pressure (P_s) (Bacmeister et al., 2012)



Experiment setup

Model = WRF (NCAR weather research forecast model) with 'all' water variables prognostic as well as non-hydrostatic dynamics; $\Delta x = \Delta y = 500$m horizontal resolution, 5 day simulation.

Non-hydrostatic effects at $\Delta x = 25$km

Figure (upper): Joint frequency distributions of WRF pressure (x-axis) and hydrostatic pressure (y-axis) coarse-grained to 25 km.

Non-hydrostatic effects not significant!

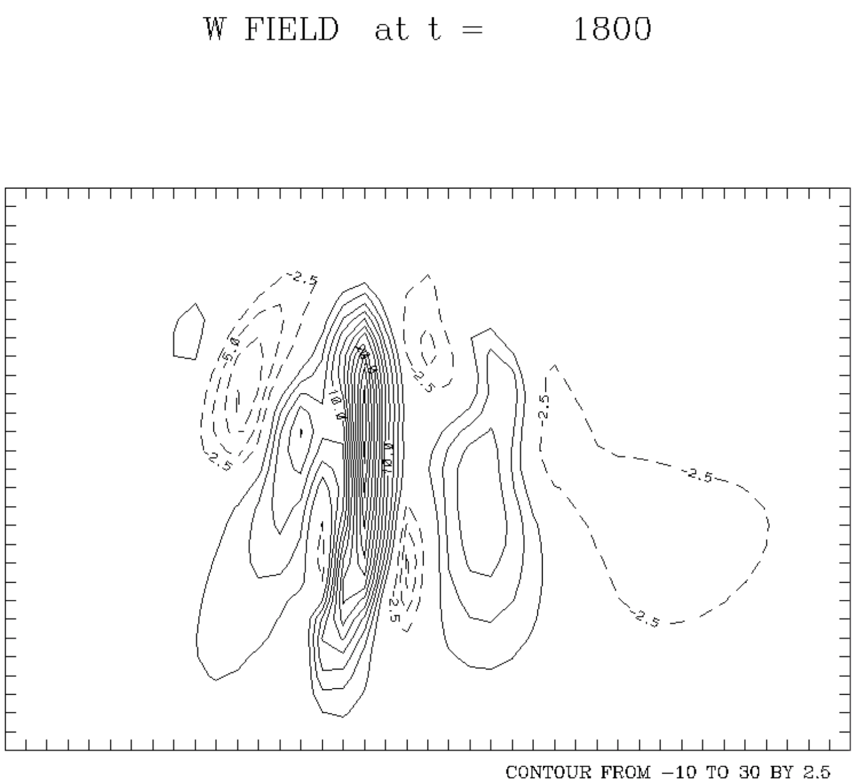
What is the effect of CL on P_s?

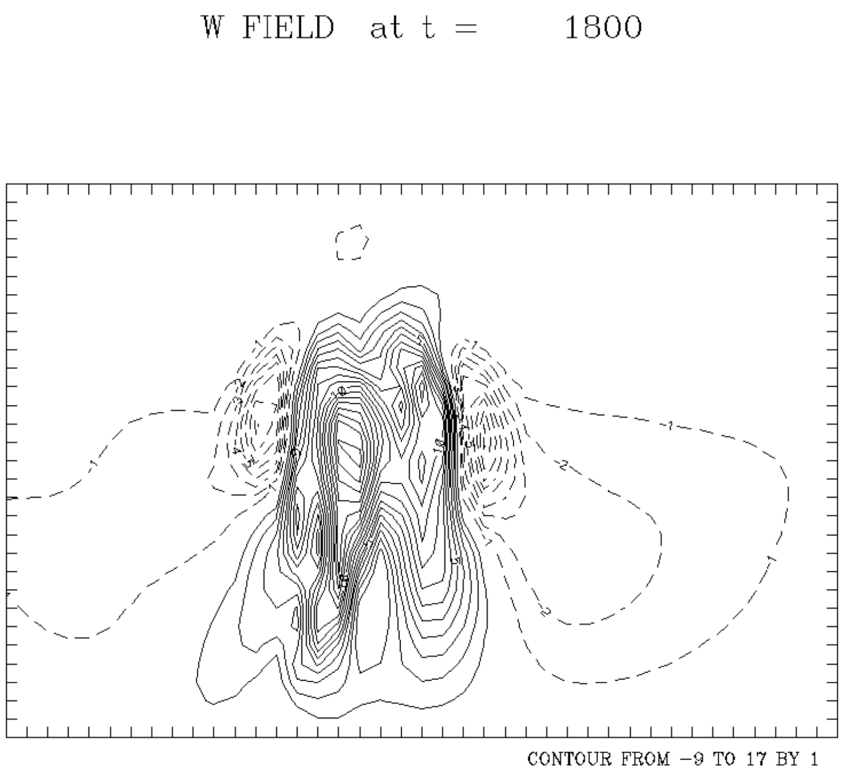
Figure (lower): Same as upper but hydrostatic pressure ignores CL (y-axis).

$\Rightarrow$ frequent, large ($\mathcal{O}$(hPa)) underestimates of P_s compared to WRF P_s.

A clear implication of this result is that high-resolution climate model surface pressures in regions of strong precipitation may be systematically underestimated by several hPa.

Idealized squall-line simulation (2D)



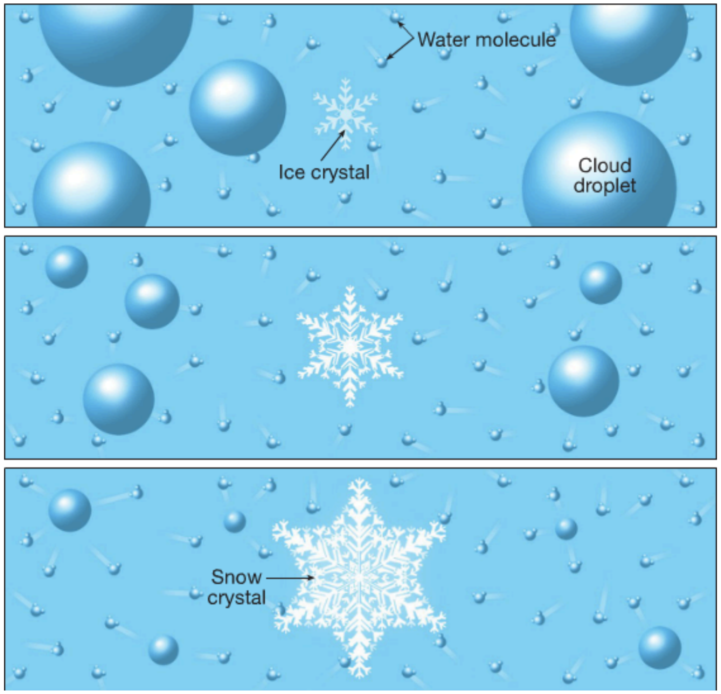


Δx=1km

Figure courtesy of J. Klemp (NCAR)

Cloud microphysics

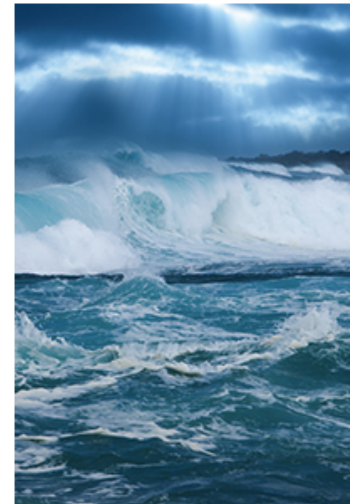
Modern cloud microphysics parameterizations also require tracers for number concentrations of cloud liquid and cloud ice in addition to the mixing ratios for cloud liquid and ice.



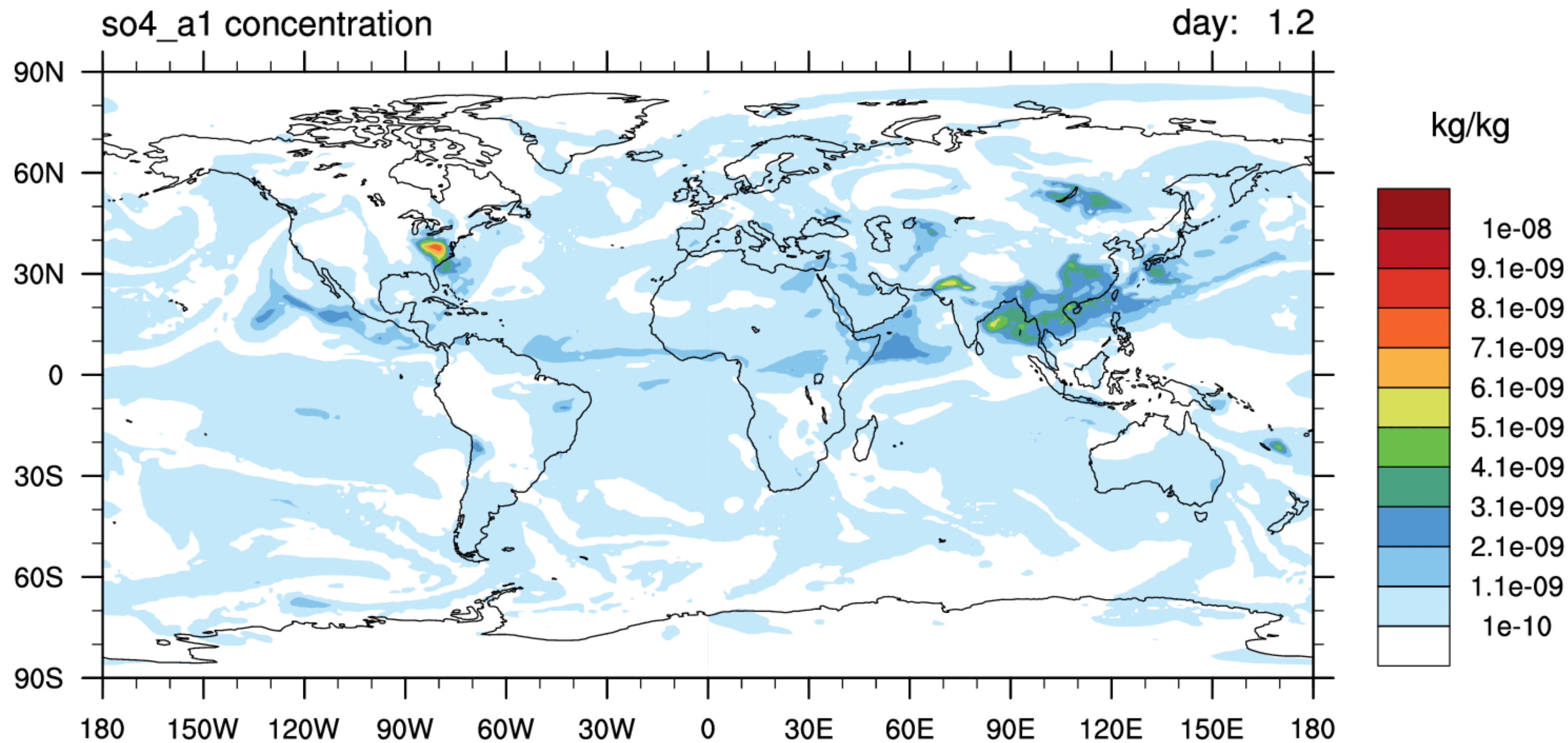
Source: https://www.studyblue.com/notes/note/n/section-18-3/deck/1357832

Examples of non-water tracers

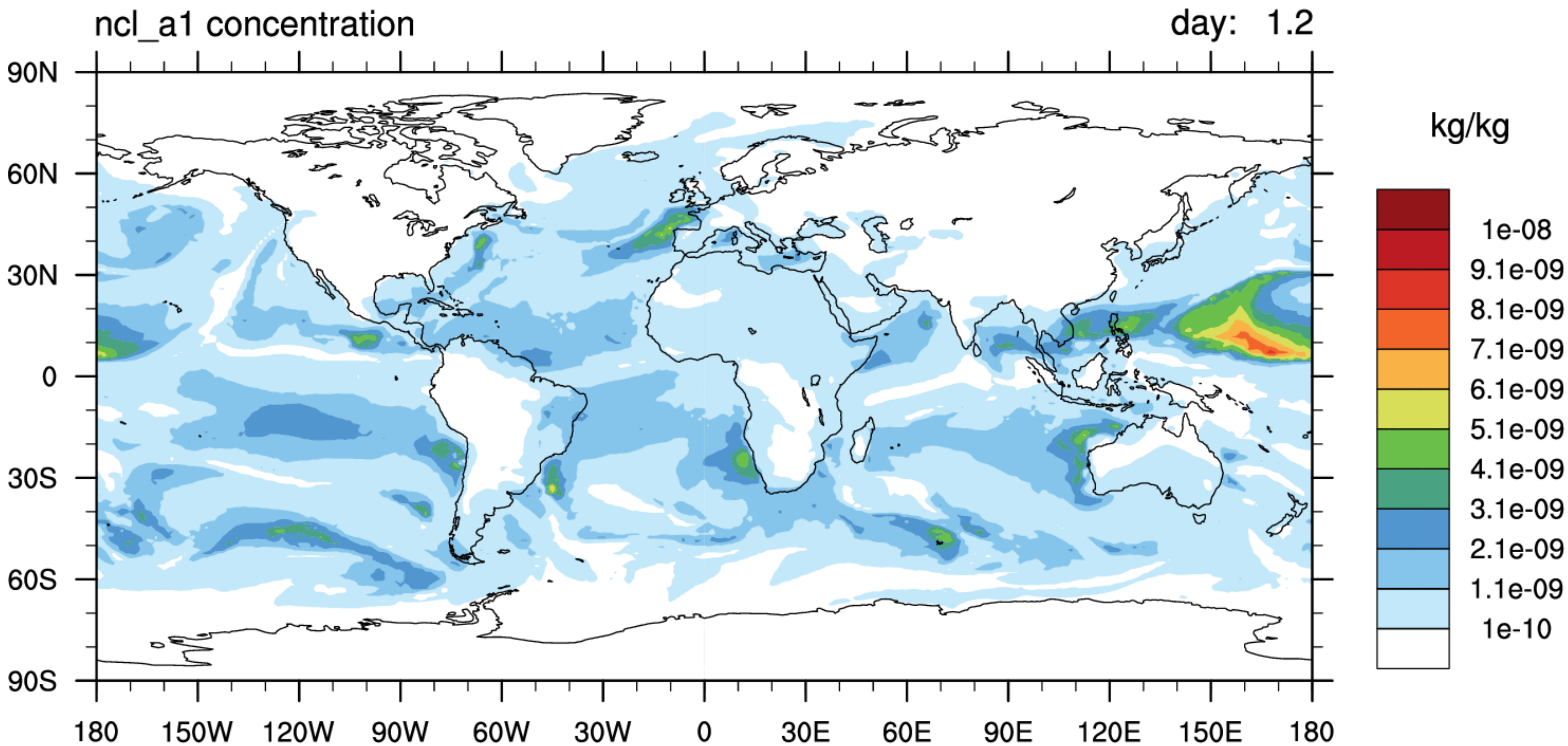
- Sea-salt
- SO_2, SO_4
- Carbon dioxide
- DMS: Dimethylsulfite – biogenic sulfur compound
- SOAG: Secondary Organic Aerosol
- O_3
- ....



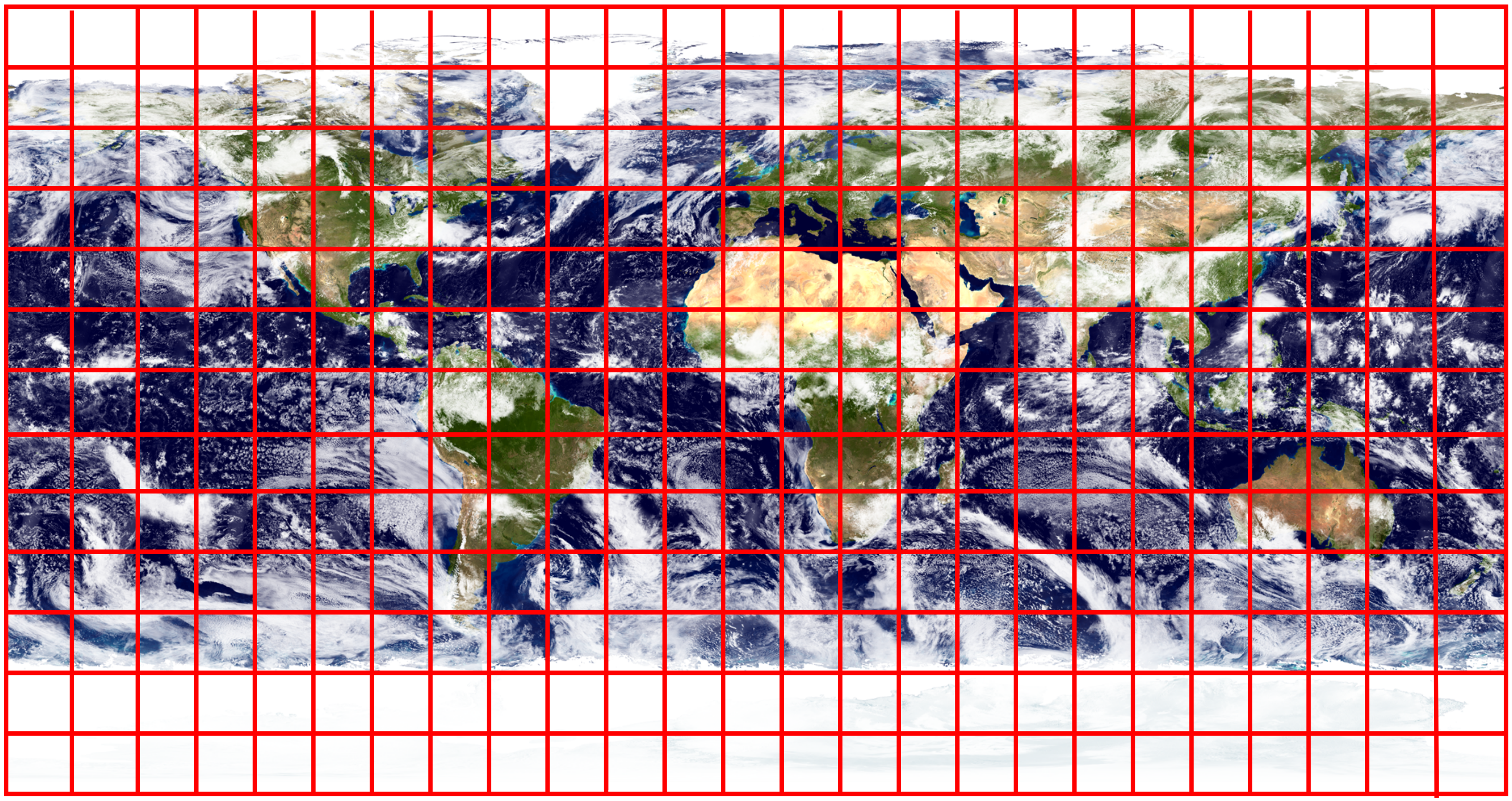
FV dycore, CAM5 physics, level 24



FV dycore, CAM5 physics, level 30



Sub-grid-scale redistribution of tracer mass



$$\frac{\partial}{\partial t}(m_x \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = \rho_d \, S^{m_X}$$

Vertical transport by deep convection

Convection is an effective way of mixing tracers in the vertical (e.g. Mahowald et al., 1995; Collins et al., 1999), e.g., convective updrafts can transport a tracer from the surface to the upper troposphere on time scales of $\mathcal{O}(1h)$.

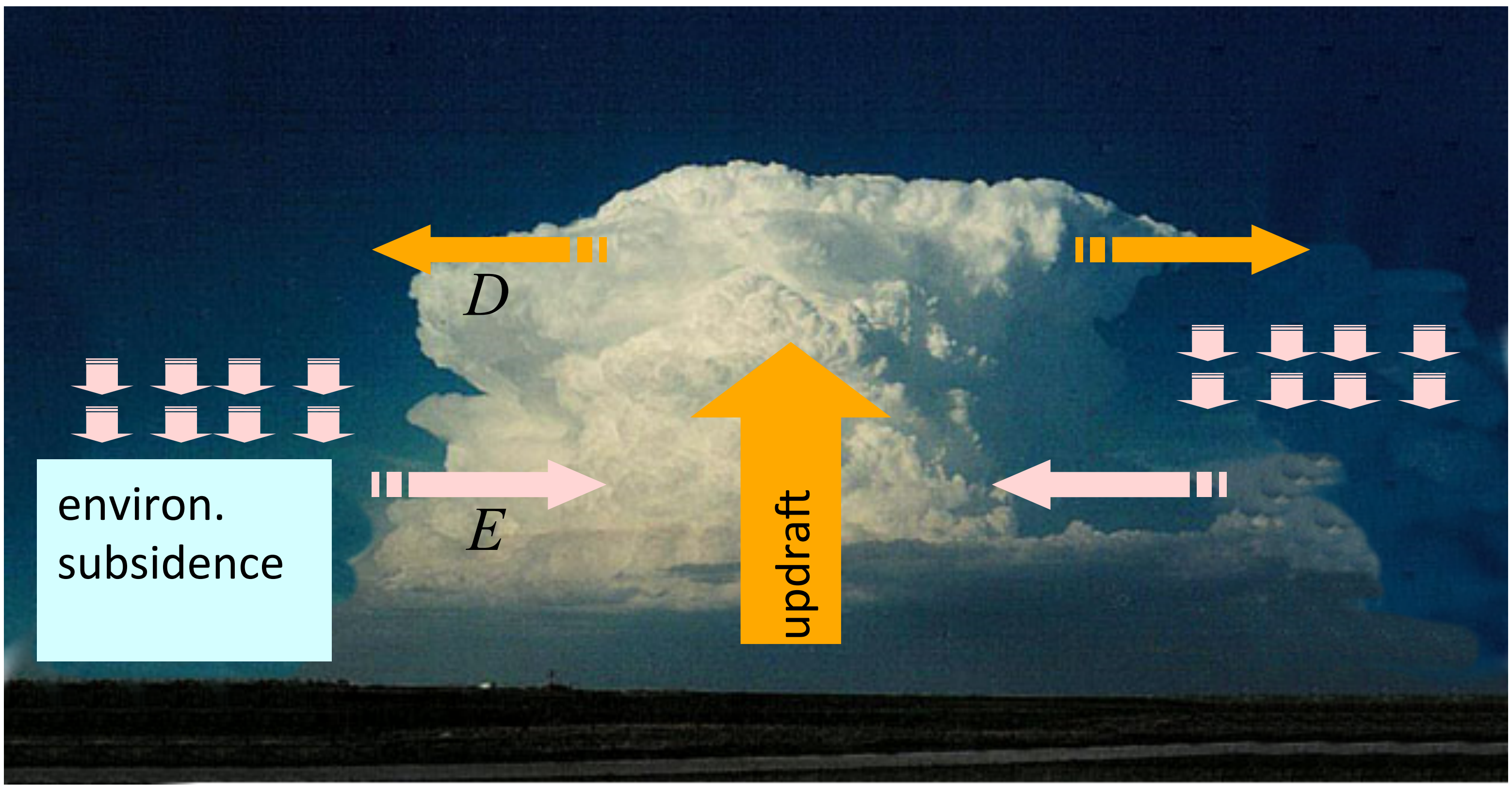
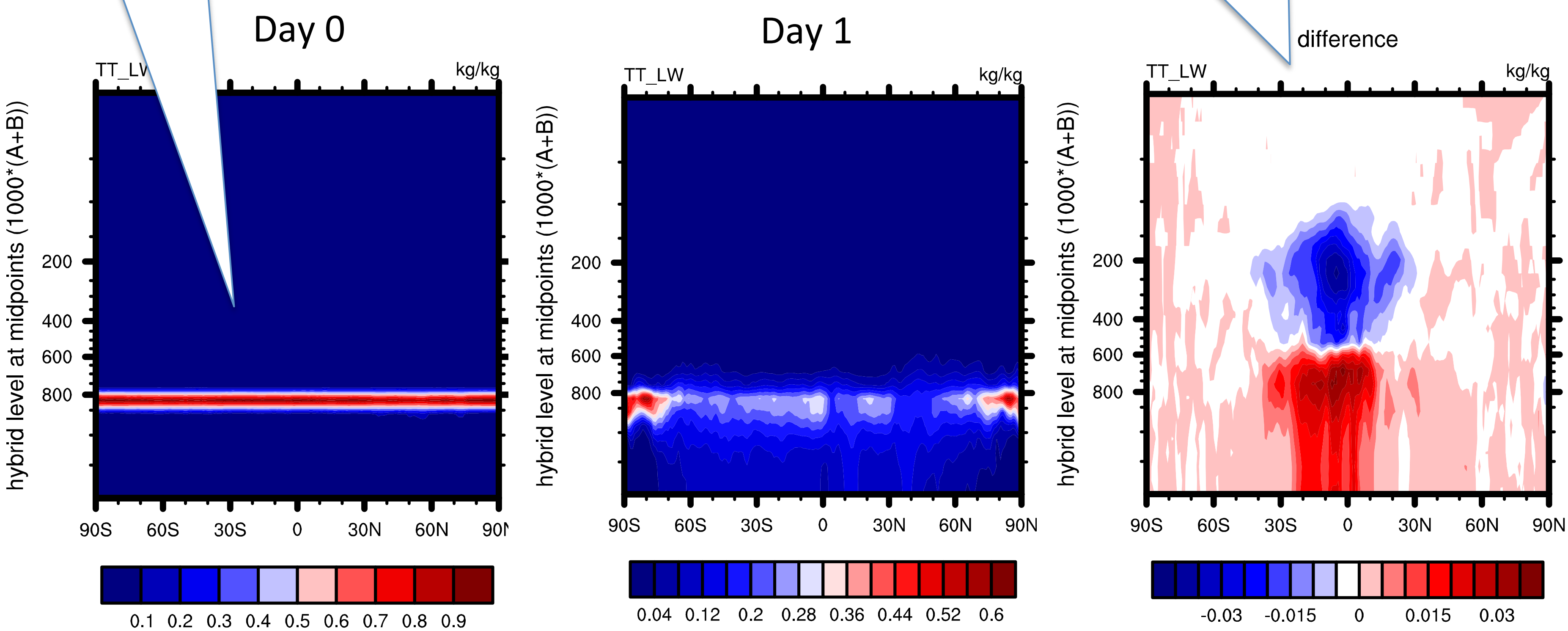


Figure courtesy of J. Bacmeister (NCAR)

Rasch et al. (2006) setup

Mixing ratio 1 in one layer and 0 elsewhere

Difference between simulation without deep convective transport and with



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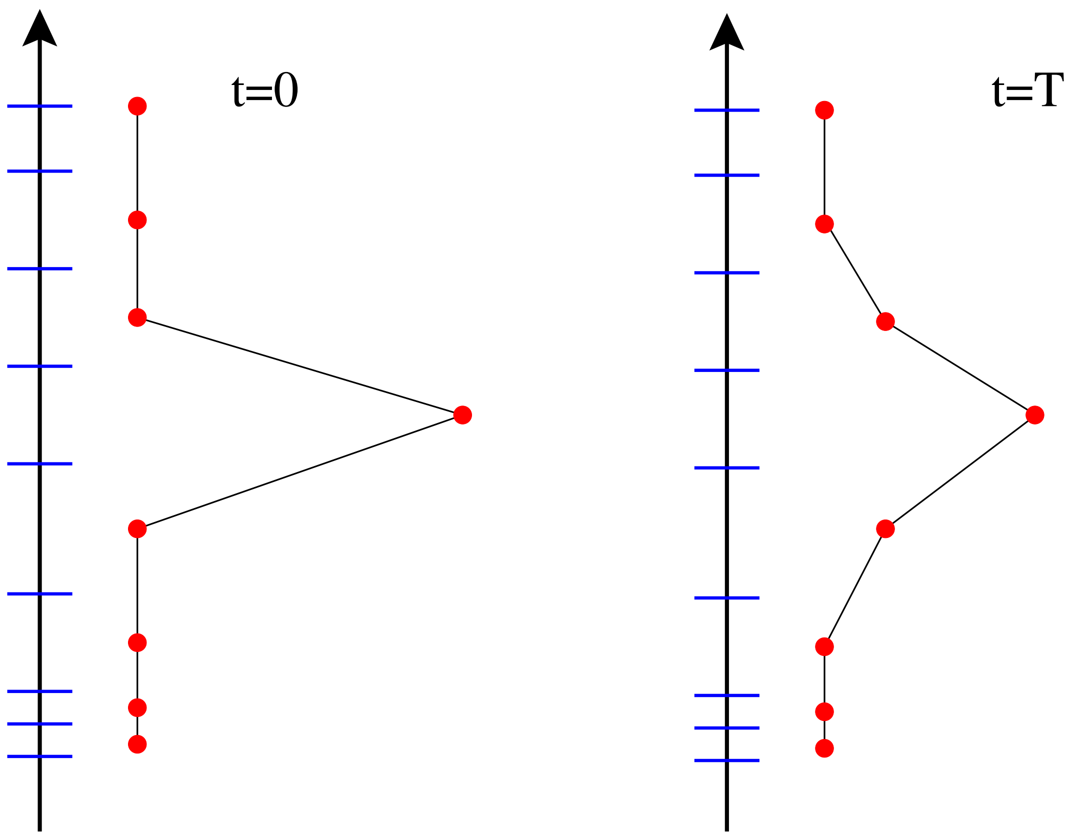
Turbulent diffusion

Given vertical profile of eddy diffusion coefficient $K(p)$:

$$\frac{\partial \overline{\varphi}}{\partial t} = \frac{\partial}{\partial p}\left[K(p)\frac{\partial \overline{\varphi}}{\partial p}\right]$$

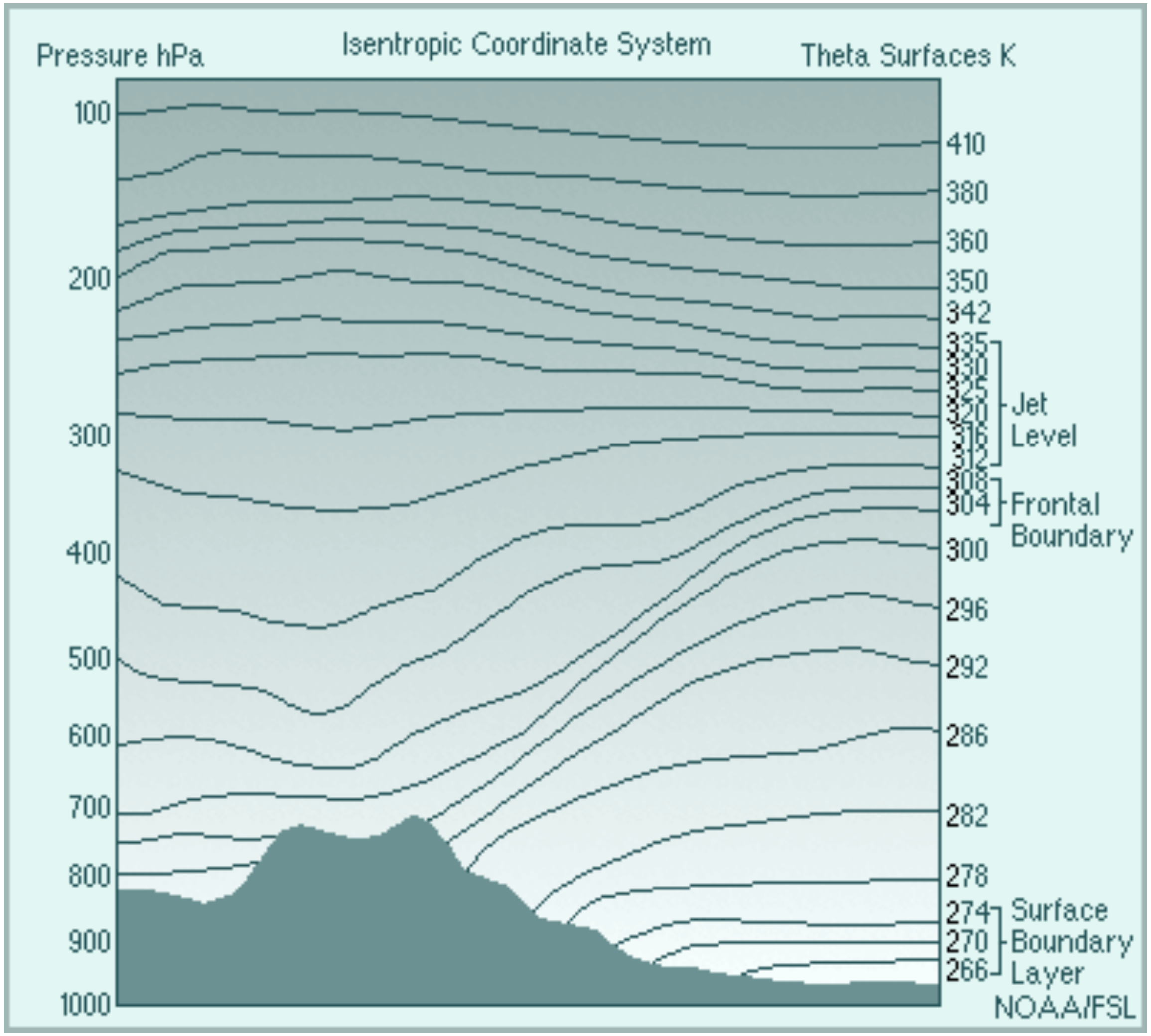
Contrary to convective tracer transport turbulent diffusion is a local process!



Vertical coordinates and tracer transport

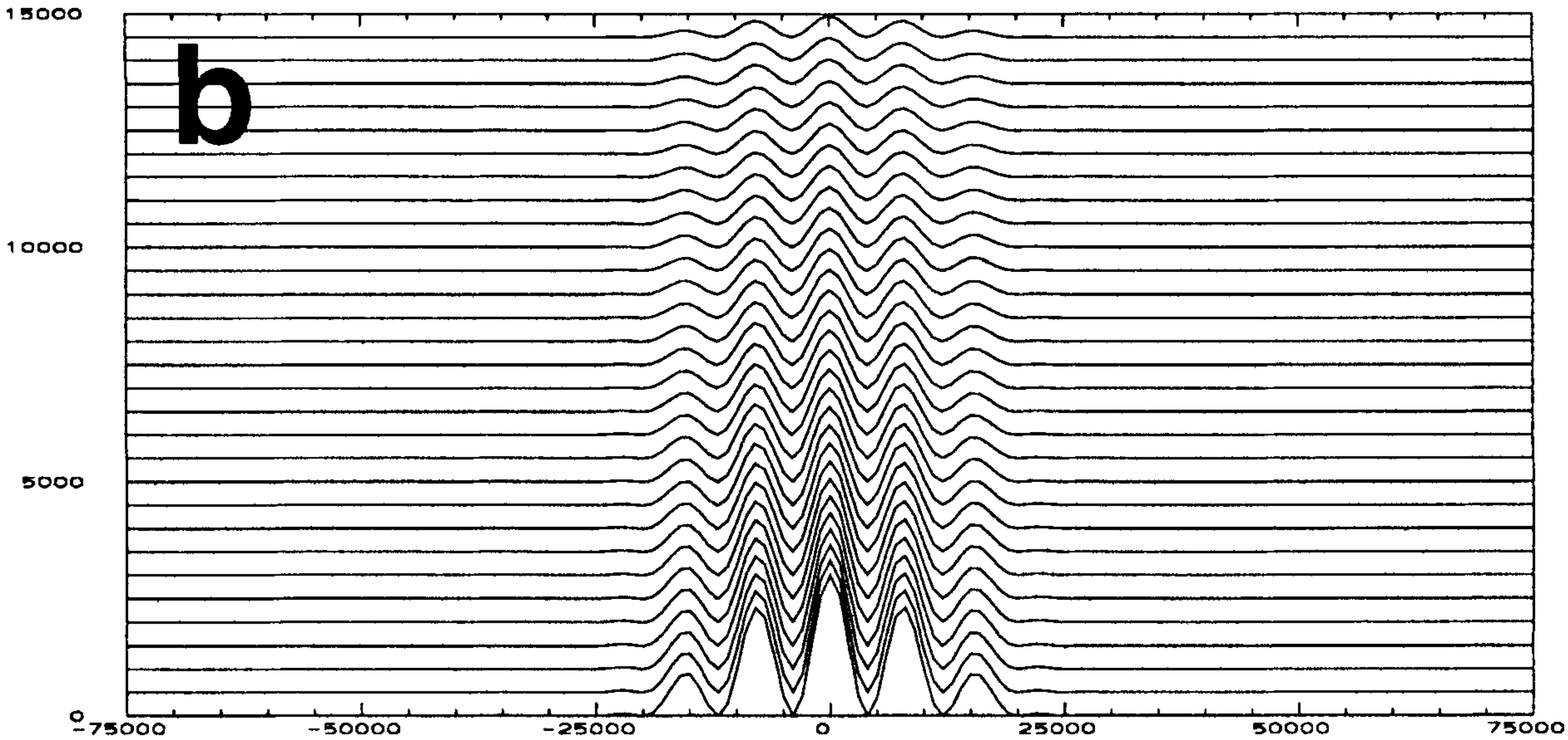
$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \qquad (1)$$

Vertical coordinates: isentropes



http://www.met.tamu.edu/class/metr452/models/2001/vertres.html

Vertical coordinates and topography



Schaer et al. (2002)

Vertical coordinates

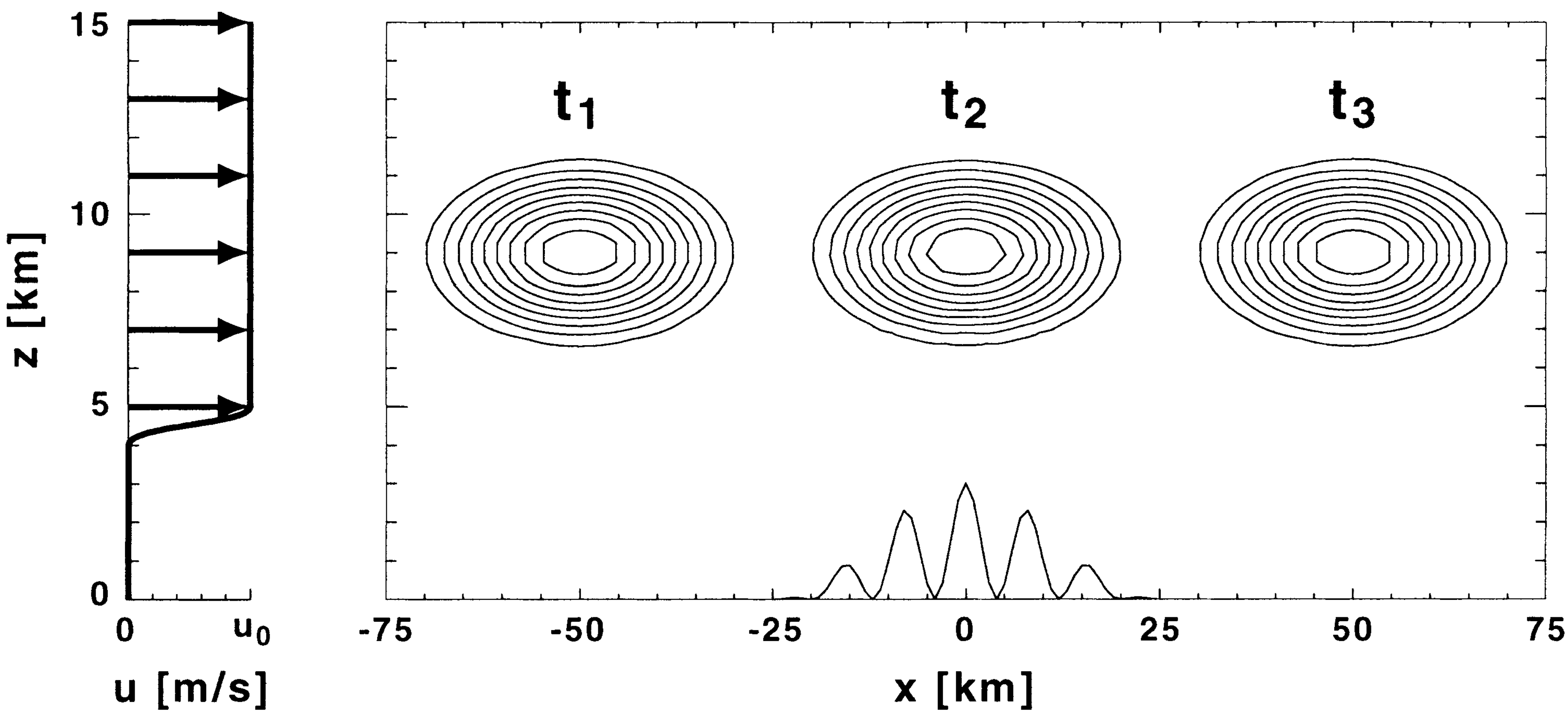
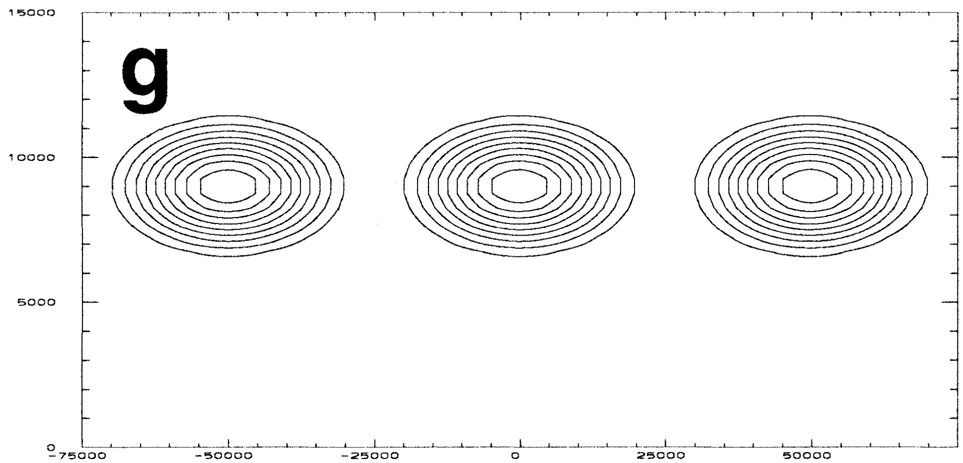
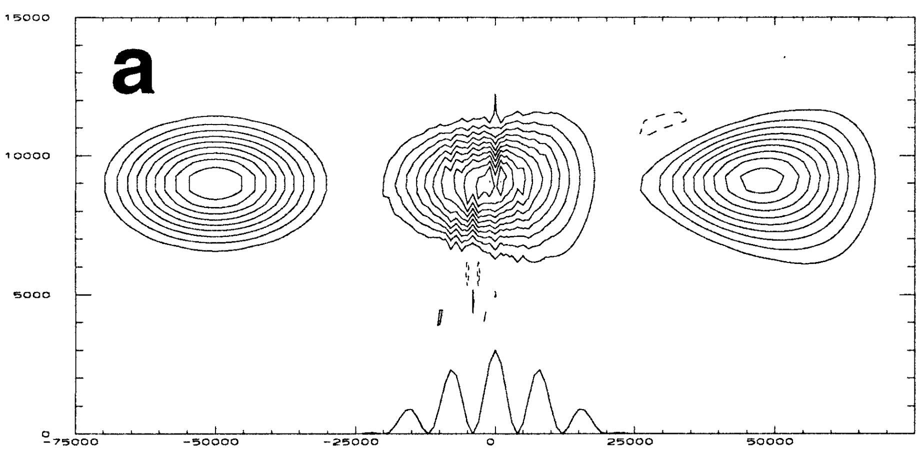


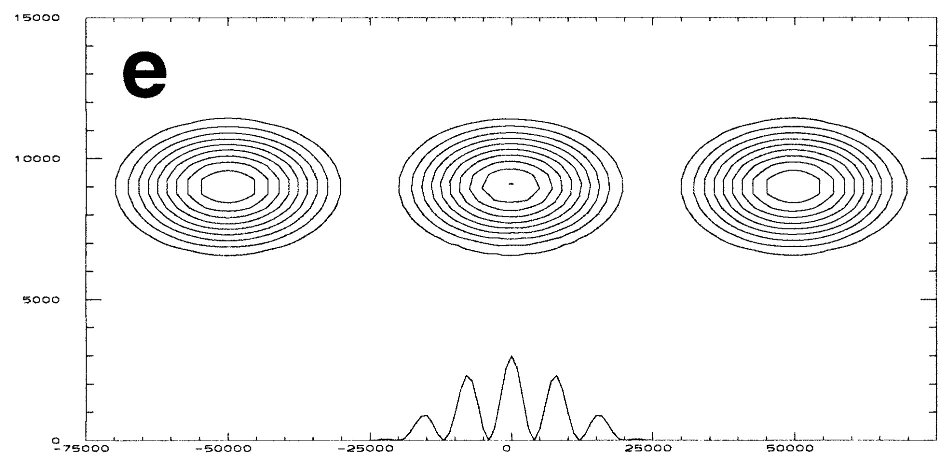
FIG. 4. Vertical cross section of the idealized two-dimensional advection test. The topography is located entirely within a stagnant pool of air, while there is a uniform horizontal velocity aloft. The analytical solution of the advected anomaly is shown at three instances.

Schaer et al. (2002)

Vertical coordinates

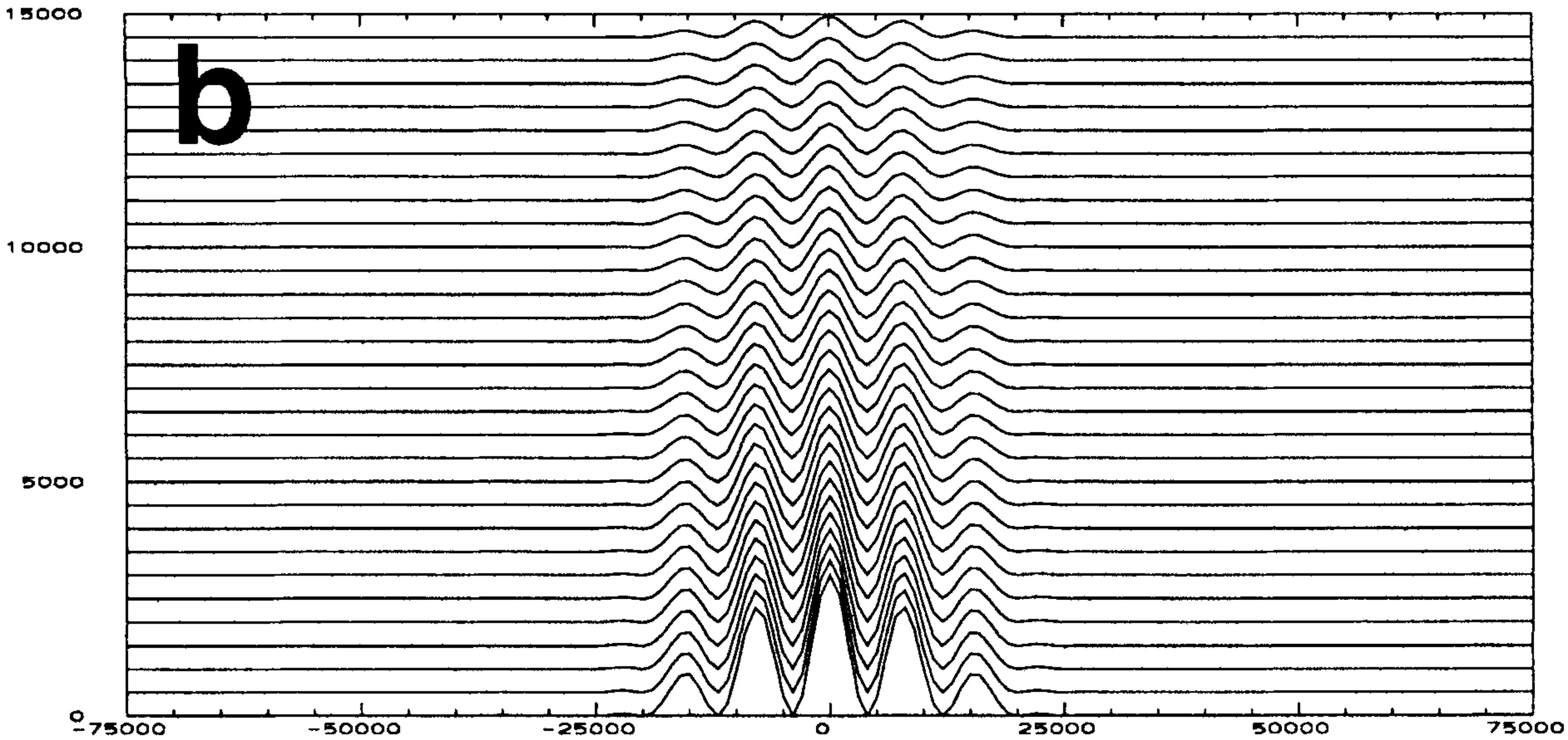






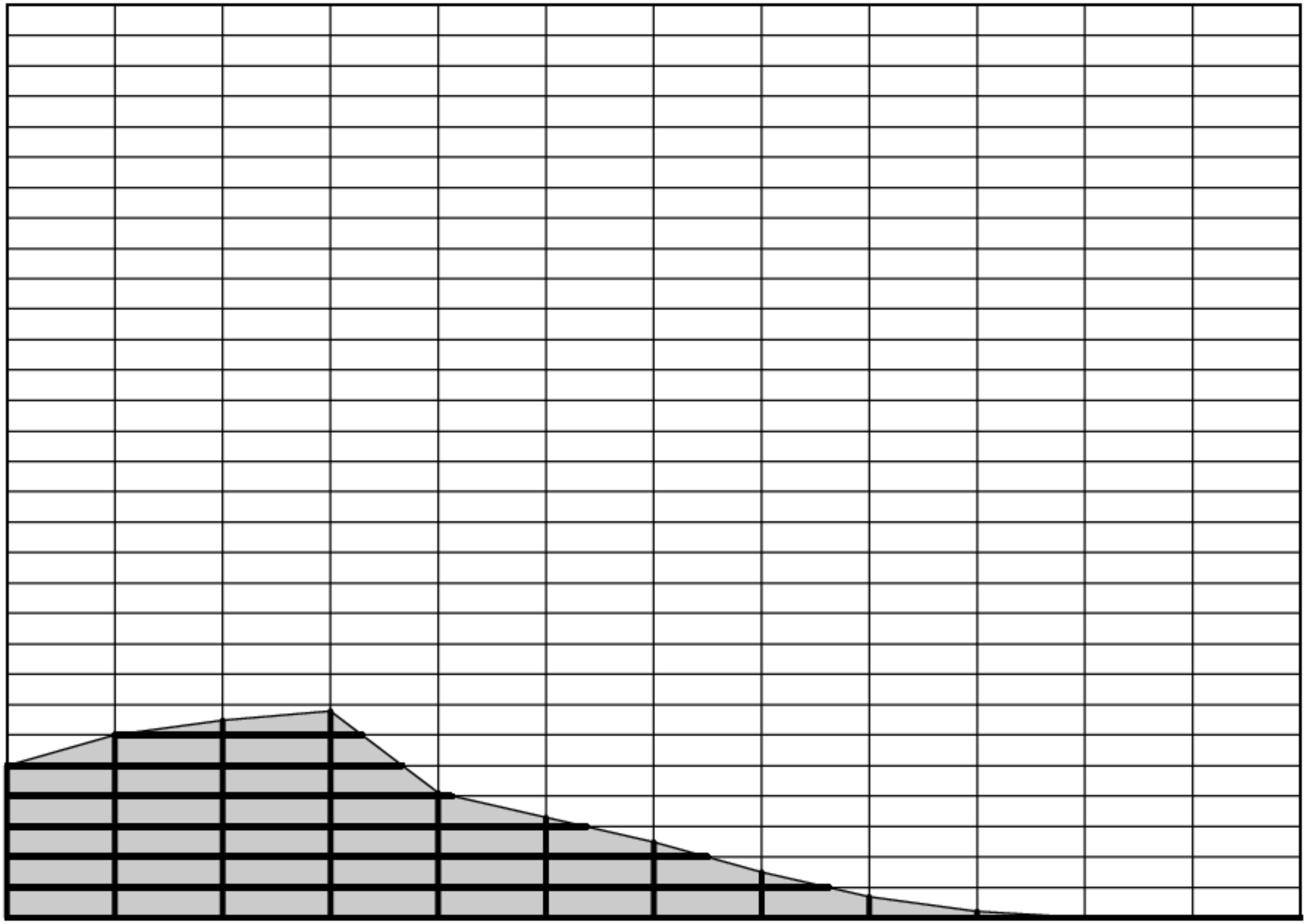
Schaer et al. (2002)

Vertical coordinates and topography



Schaer et al. (2002)

Vertical coordinates and topography



From R. Walko

What tracers need to be prognosed

Minimal set: The water species - crucial for predicting the dynamics and moist thermodynamics of the atmosphere (e.g., CAM4 has 3 tracers: humidity, cloud liquid and cloud ice)

What else? Depends on the problem you wish to study with you model ...

- **Aerosol indirect effects: e.g. CAM5 - approximately 27 more tracers**

CAM5 configuration

Fixed: (N_2, O_2 H_2O,) O_3, OH, NO_3, HO_2
(prescribed with monthly mean values)

Chemically active: H_2O_2, H_2SO_4, SO_2, DMS, SOAG

Chemistry: photolysis of H_2O_2, DMS,
[usr_HO2_HO2] $HO_2 + HO_2 \rightarrow H_2O_2$
$H_2O_2 + OH \rightarrow H_2O + HO_2$
[usr_SO2_OH] $SO_2 + OH \rightarrow H_2SO_4$
$DMS + OH \rightarrow SO_2$

Aerosol formation of SO_4:
Chemically: from SO_2 -> H_2SO4
aq-phase (H_2O_2, O_3), nucleation, from H_2SO_4
H_2SO_4 deposition

Slide courtesy of S.Tilmes (NCAR)

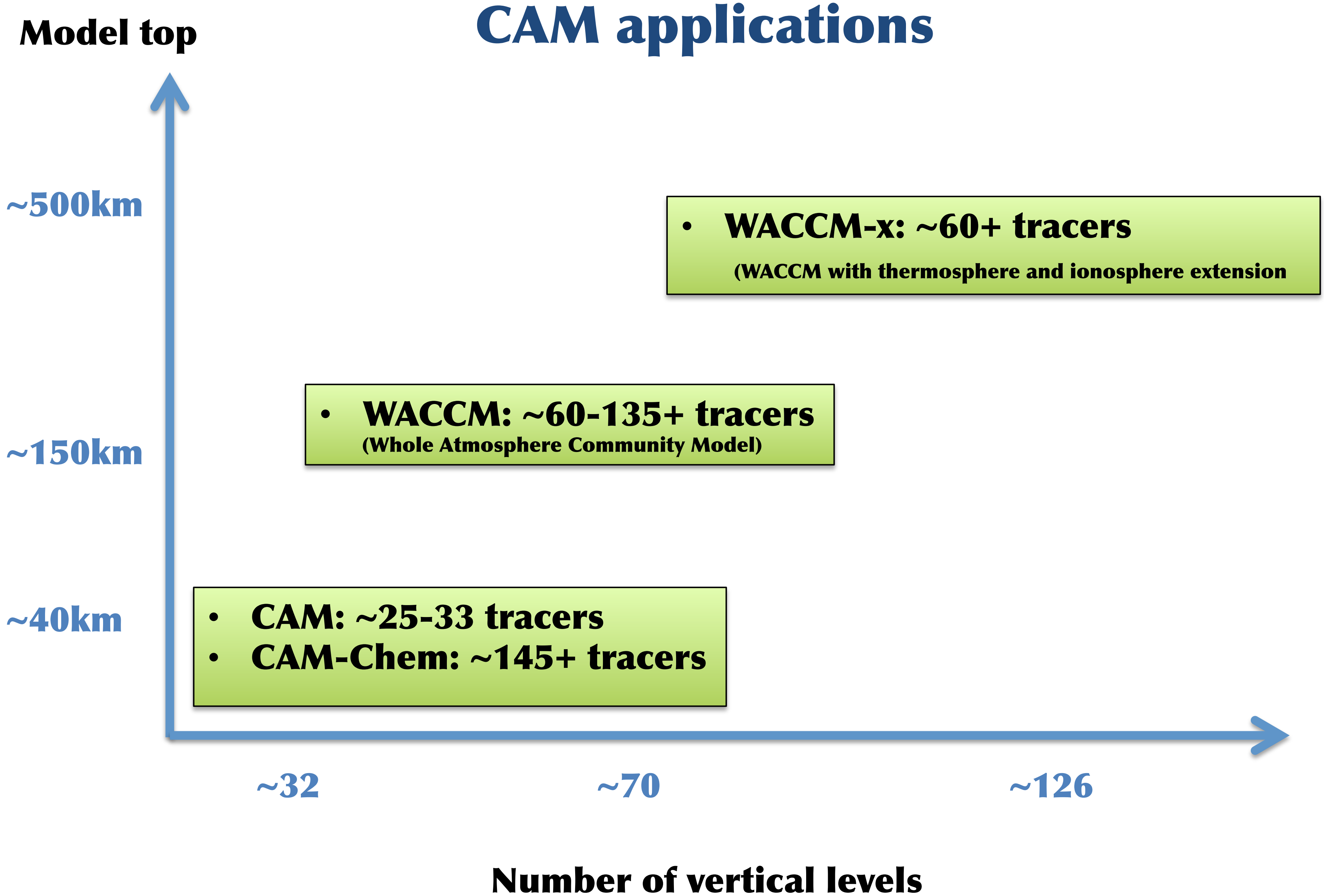
What tracers need to be prognosed

Minimal set: The water species - crucial for predicting the dynamics and moist thermodynamics of the atmosphere (e.g., CAM4 has 3 tracers: humidity, cloud liquid and cloud ice)

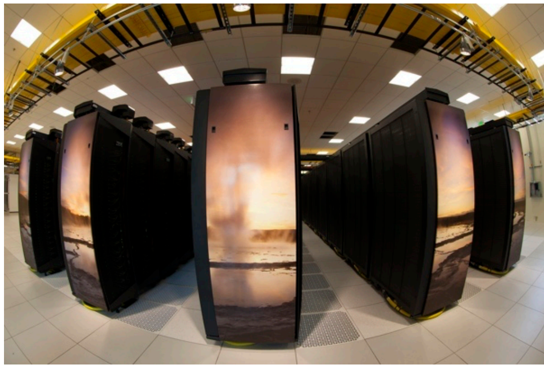
What else? Depends on the problem you wish to study with you model …

- **Aerosol indirect effects: e.g. CAM5 - approximately 27 more tracers**
- **Comprehensive tropospheric and stratospheric chemistry (including H2O2 and Ozone), and improved aerosol formation representation: e.g., CAM5-Chem – approximately 145 aerosol/chemical species**

CAM applications



Computational cost of tracer transport is a significant fraction of overall runtime cost

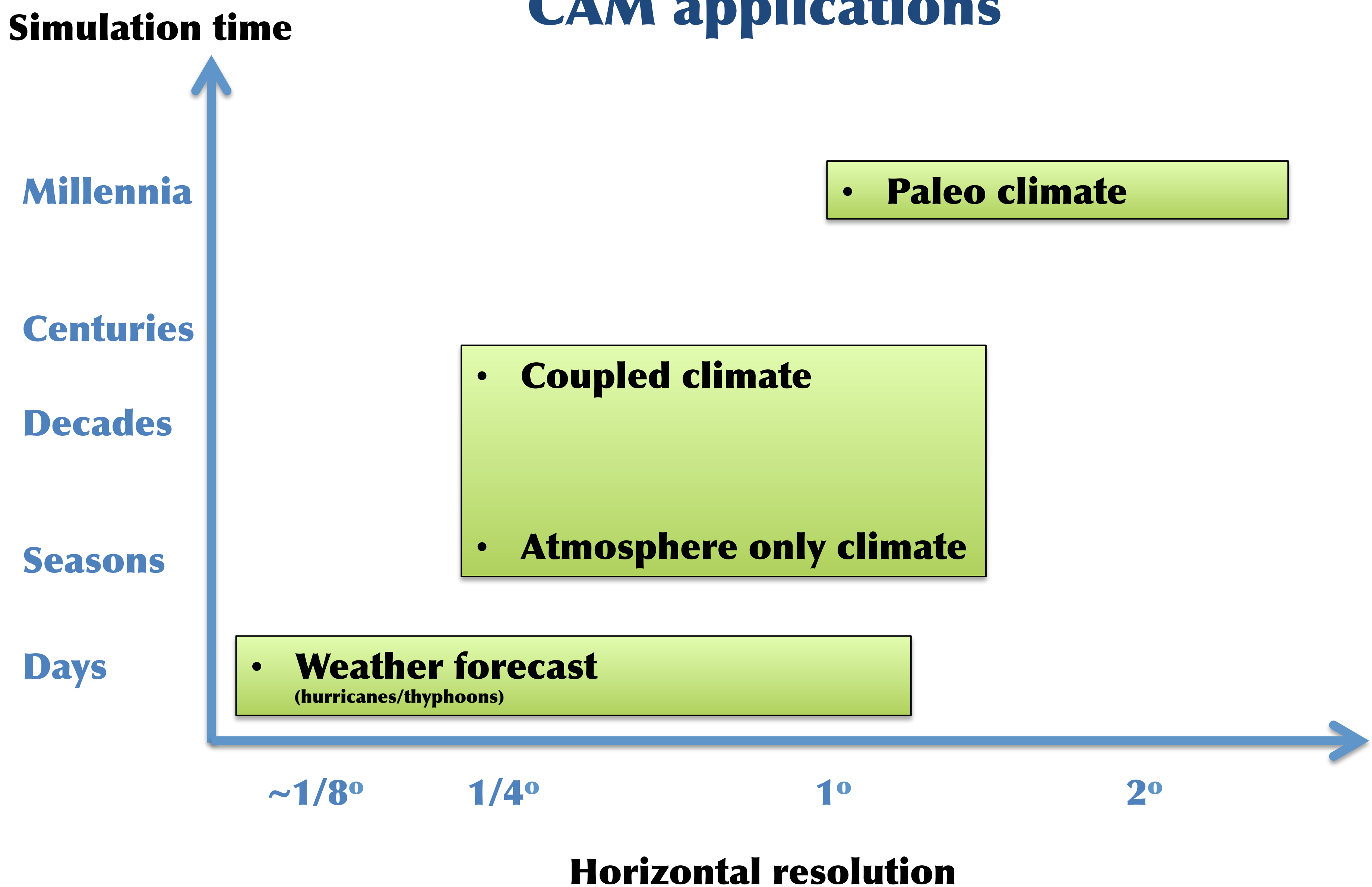


- **Scalability:**

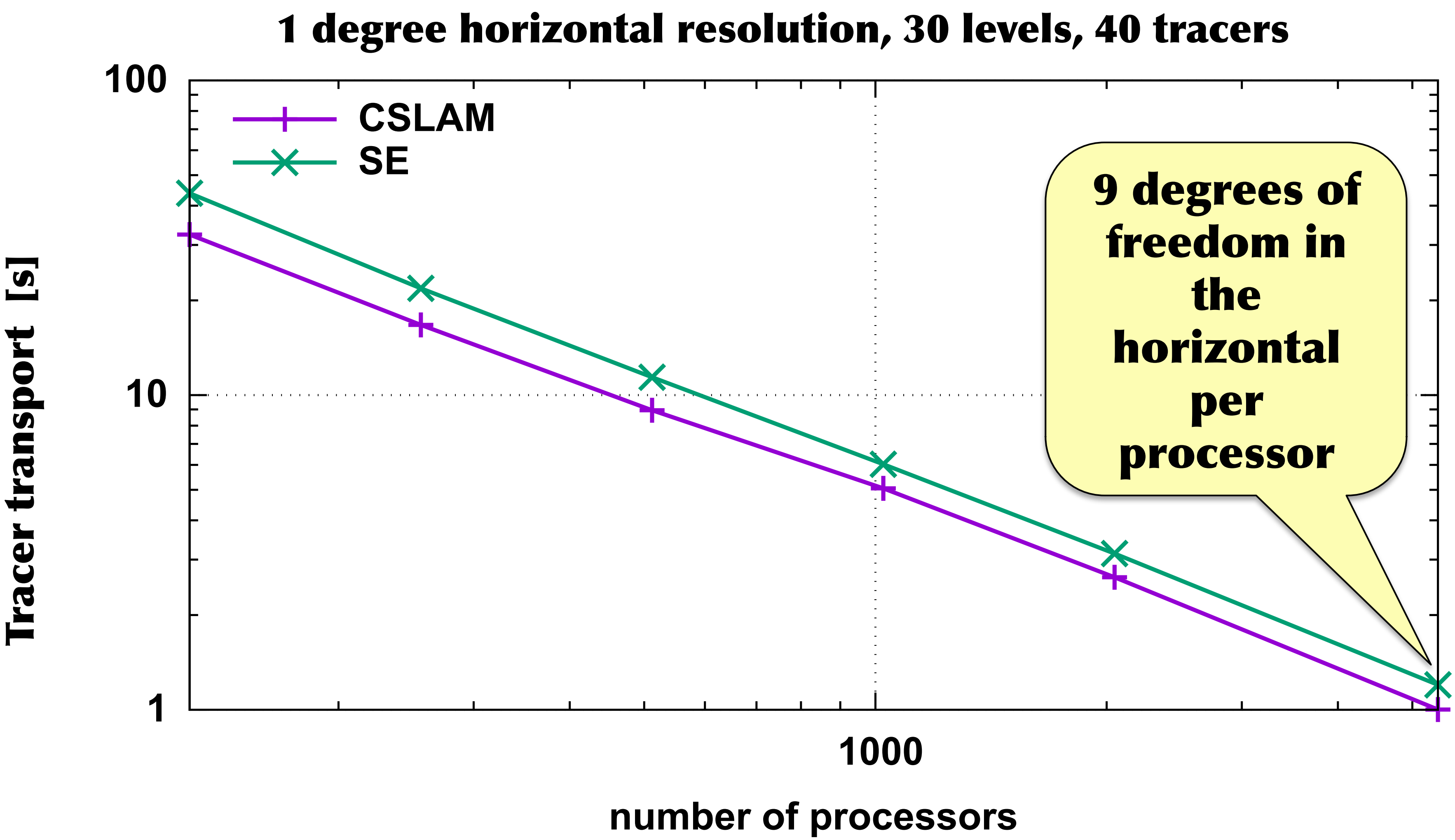
  - weak scaling (as the number of cores is increased the problem size is also increased)
  - strong scaling (as the number of cores is increased the problem size remains the same)

- **Cost per tracer matters for large tracer counts**

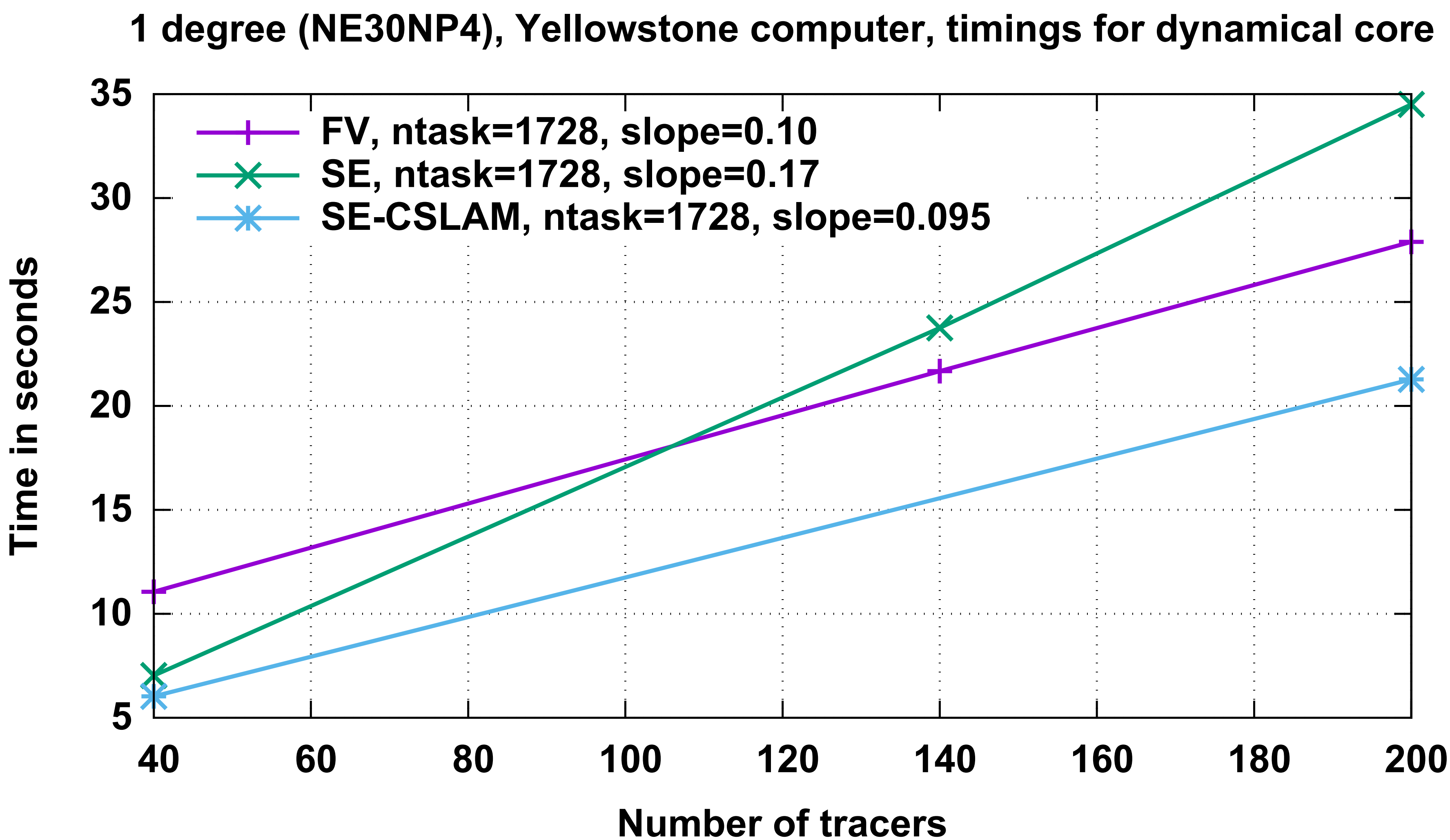
CAM applications



Performance: strong scaling



Cost per tracer: slope



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