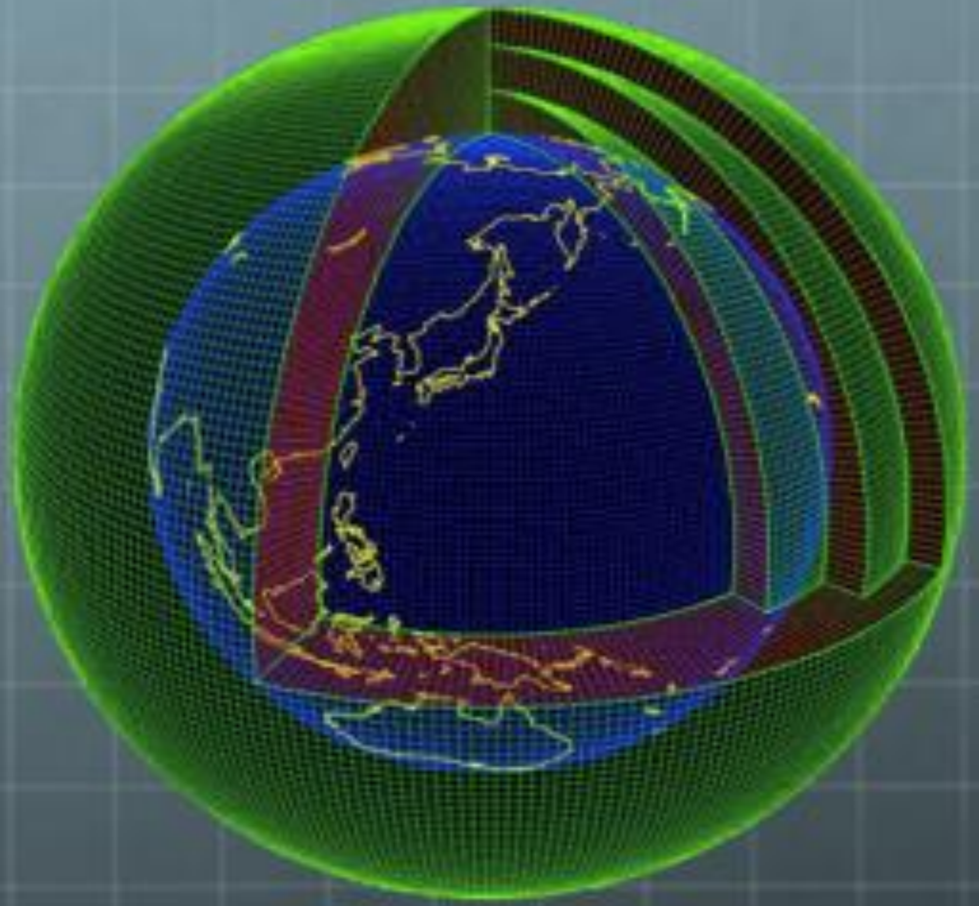
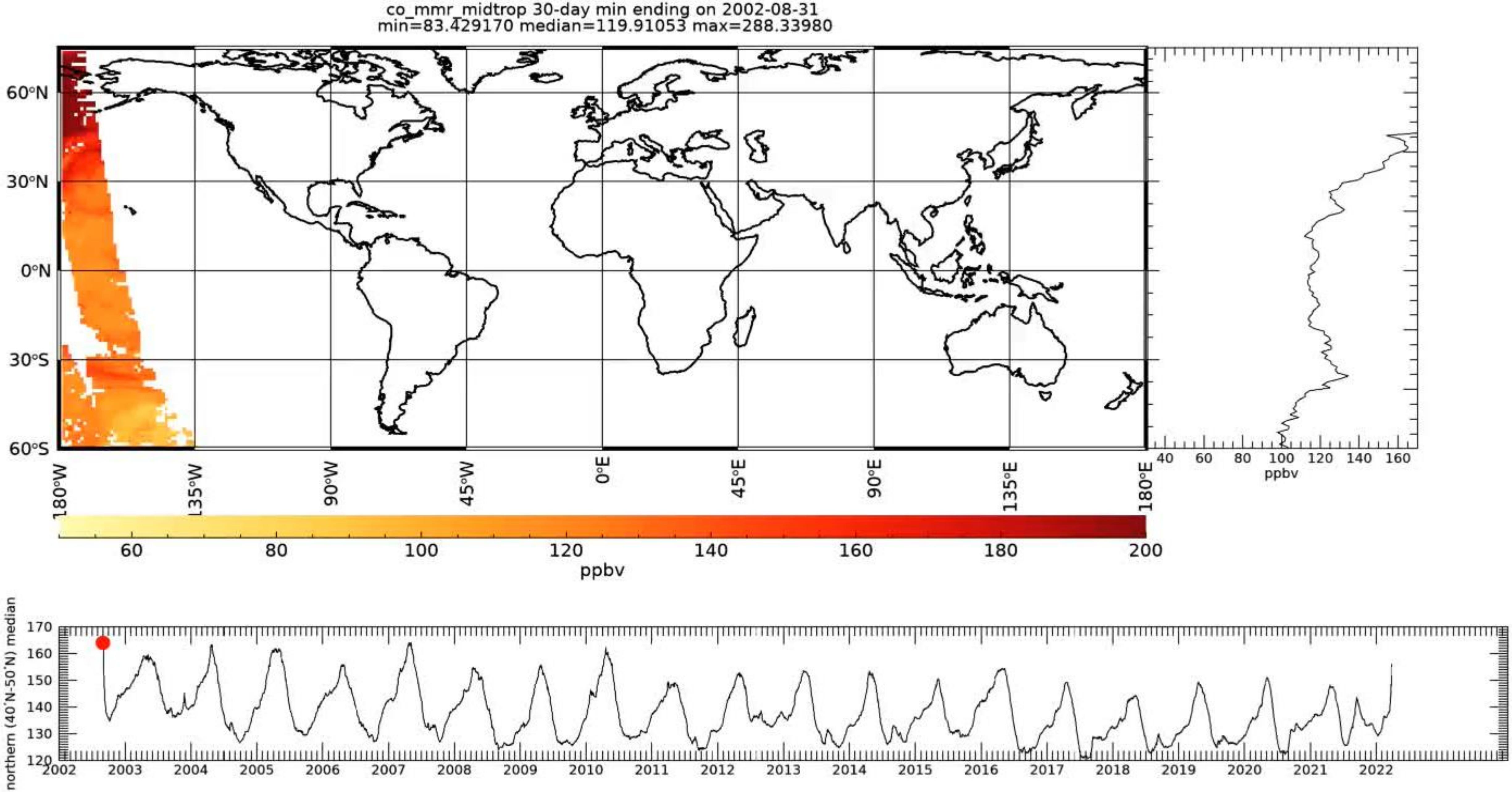
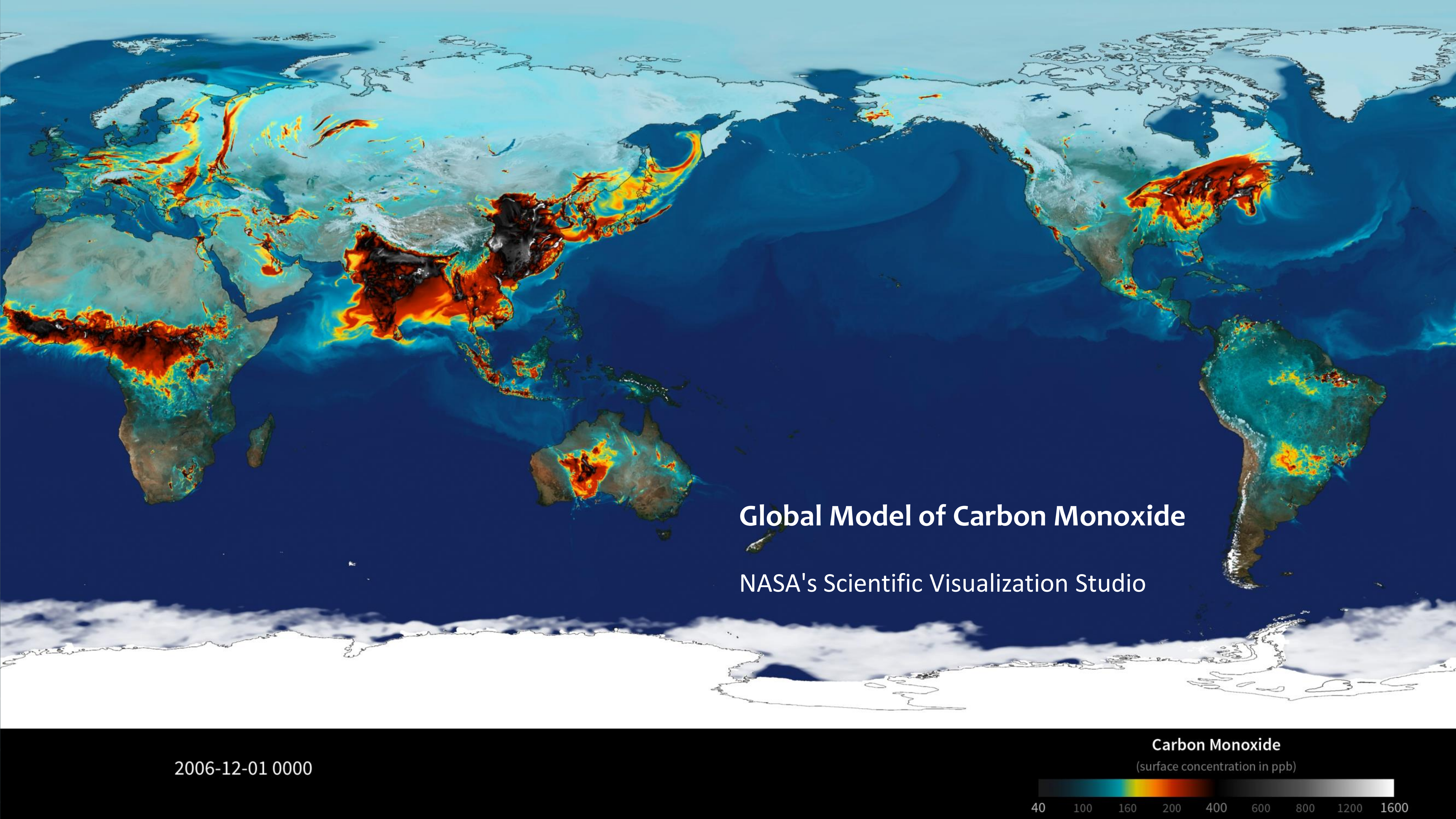


Atmospheric Chemistry: Mathematical Modeling

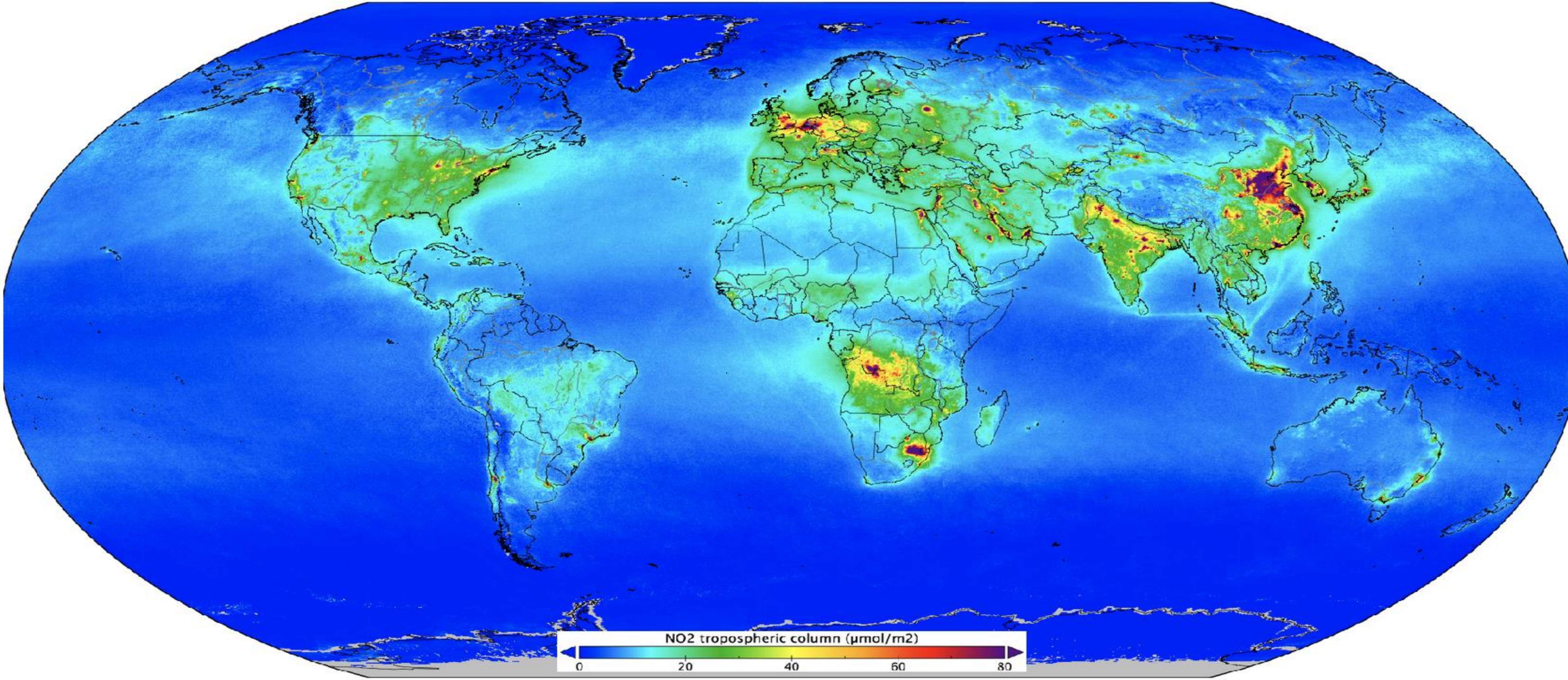
Guy P. Brasseur

Carbon Monoxide measured by AIRS



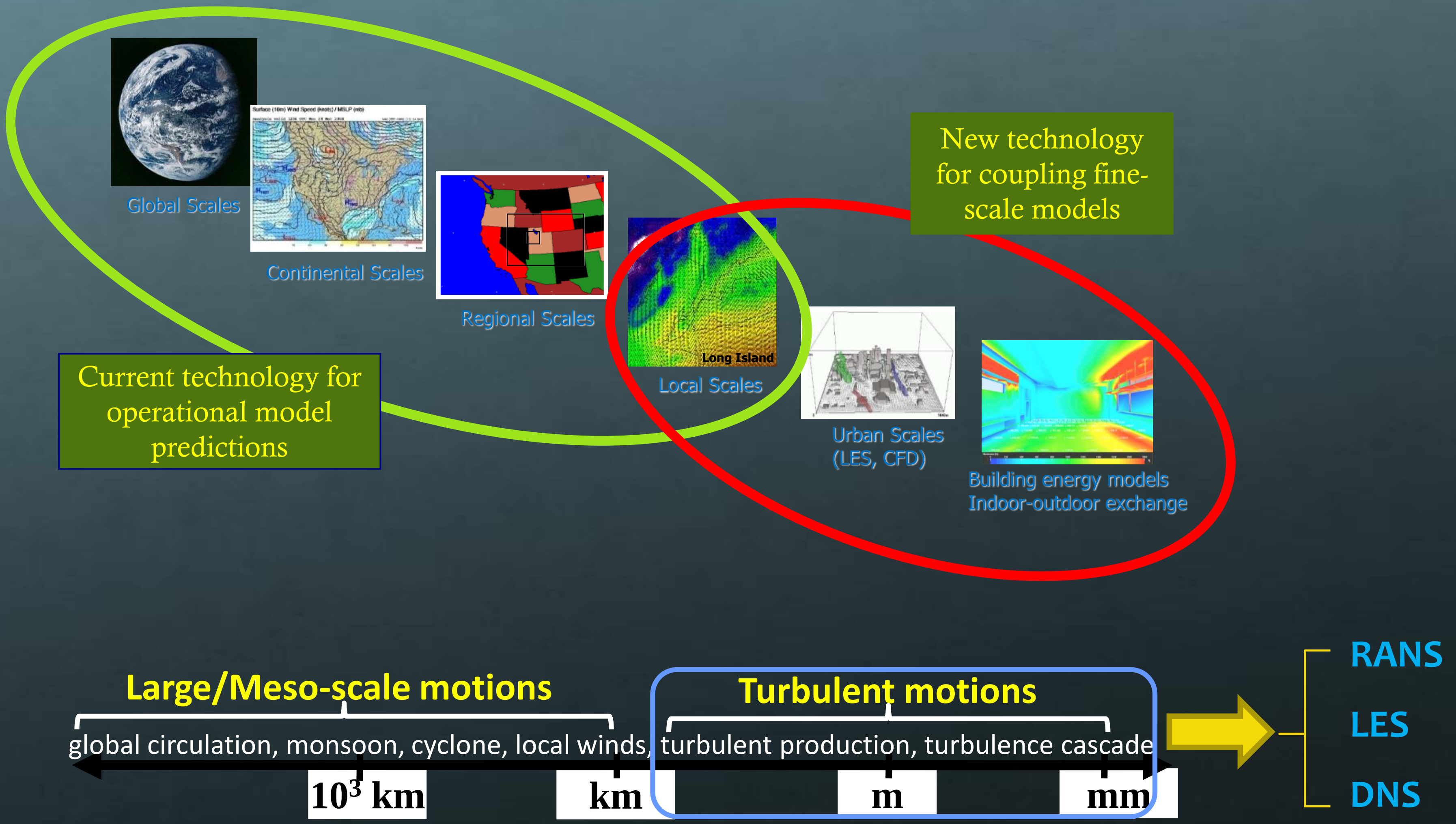

Global Model of Carbon Monoxide
NASA's Scientific Visualization Studio
2006-12-01 0000
Carbon Monoxide
(surface concentration in ppb)
40 100 160 200 400 600 800 1200 1600

Nitrogen Oxides Tropospheric Column TROPOMI



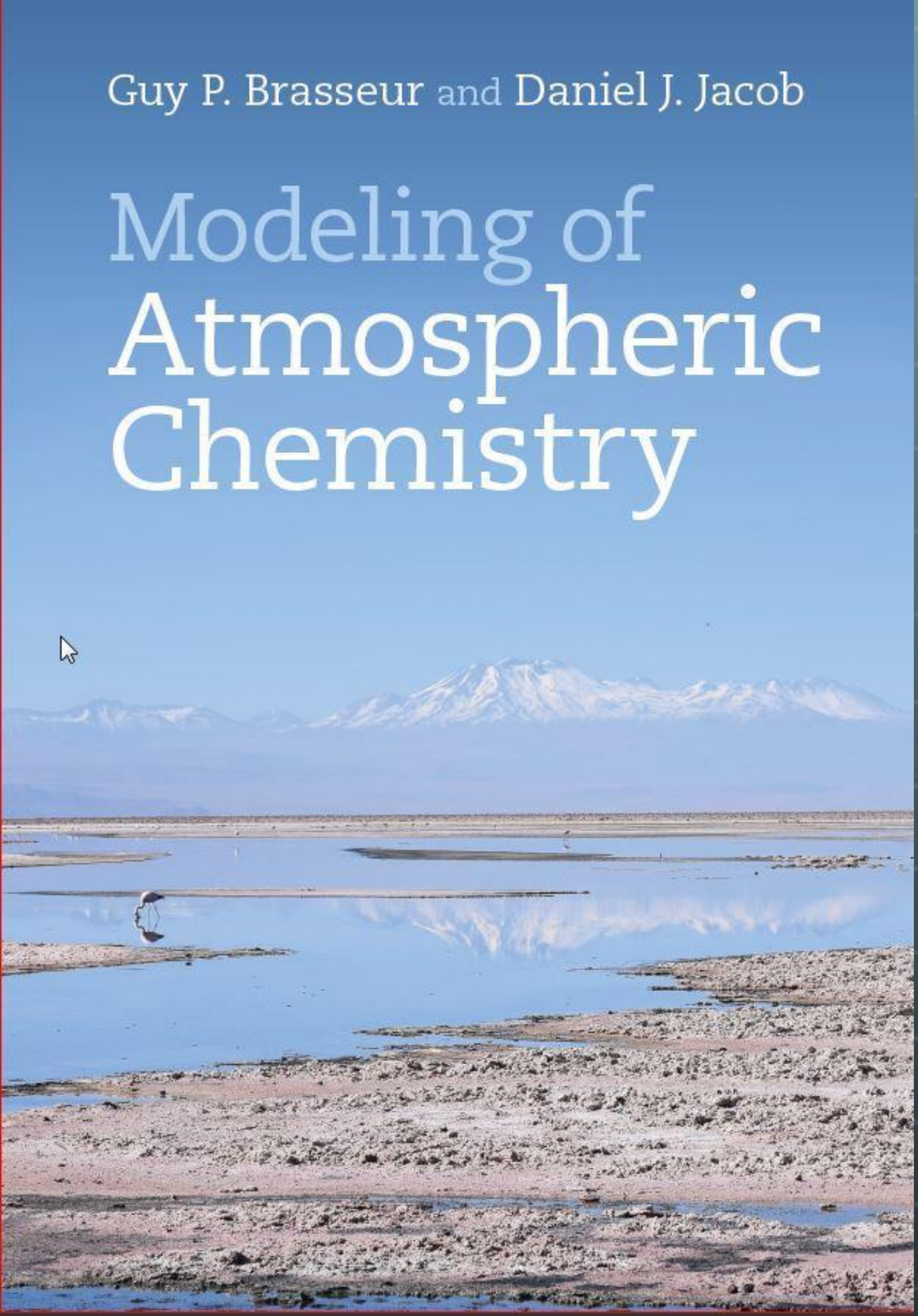
The physical/chemical modeling system: ----A spectrum of coupled scales

From: Xuemei Wang, Jinan University



Outline

- What is a Model?
- Types of Chemical Transport Models
- Fundamental Equations
- Modeling of Chemical Processes
- Modeling of Resolved Transport
- Modeling of Subscale- Processes

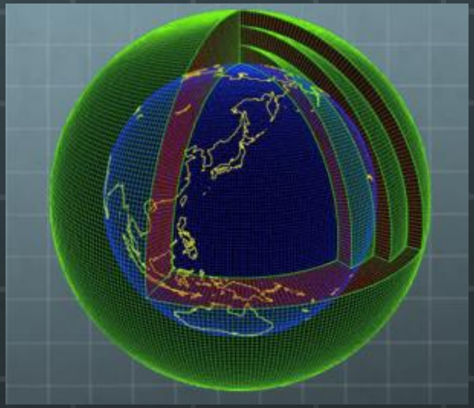


Reading Material

- 1. The concept of model
- 2. Atmospheric structure and dynamics
- 3. Chemical processes in the atmosphere
- 4. Model equations and numerical approaches
- 5. Formulations of radiative, chemical, and aerosol rates
- 6. Numerical methods for chemical systems
- 7. Numerical methods for advection
- 8. Parameterization of subgrid-scale processes
- 9. Surface fluxes
- 10. Atmospheric observations and model evaluation
- 11. Inverse modeling for atmospheric chemistry
- Appendix: brief mathematical review

Cambridge University Press, 2017, 606 pp.

1. What is a Model ?



What is a Model?

Magritte
Belgian painter:

This is not a pipe

What is a Model?

- A model is a **representation** of part of the Universe in which we live and evolve.
- Physical models can be viewed as **mathematical representations of the fundamental laws** that govern a system under study.
- These laws express some **fundamental concepts** (such as conservation of energy)

What is a Model?

- Models do not produce new concepts or laws that are not already included in the model formulation or input.
- By combining a large amount of information, they produce a system behavior that cannot be anticipated from simple considerations.
- Models can be used to *generate knowledge*
- Models are used as *diagnostic* tools to analyze a system and understand observational data, or as *prognostic* tools to predict the behavior of a system under yet unknown situations.

What is a Model?

- Models often capture limited aspects of the functioning of a system; they simplify reality and focus on a particular issue; they may not be fully "objective" and may "embellish" reality.
- The solutions of the model equations are not easily obtained. Since in most cases, no solution exists, numerical approximations must be found.
- A system can be deterministic (predictable once initial conditions are specified) or chaotic (when the solution is strongly influence by initial conditions).

Different Types of Models

- **Conceptual Models** that help to assess the consequences of some hypotheses. These models are usually very simple and focused on some issue, but trigger interest and sometimes new research. There is no attempt to reproduce perfectly the real world.
- **Detailed Models** that try to reproduce as closely as possible the real world. Their success depends on the level of fidelity in representing real situations. Examples: Numerical Weather Forecast Models.

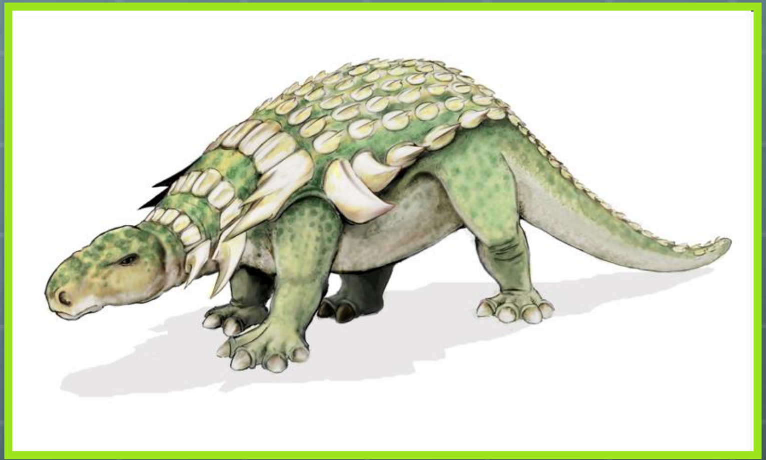
What is a Model?

- Simulation modeling represents a way to create virtual copies of the Earth in cyberspace. These virtual copies (often supported by computing devices) can be submitted to all kinds of forcings and experiments without jeopardizing the true specimen.
- For example, it is possible to explore the domains in the Earth system "phase space" that are reachable without creating catastrophic and irreversible damage to mankind.

Forward and Inverse Problem

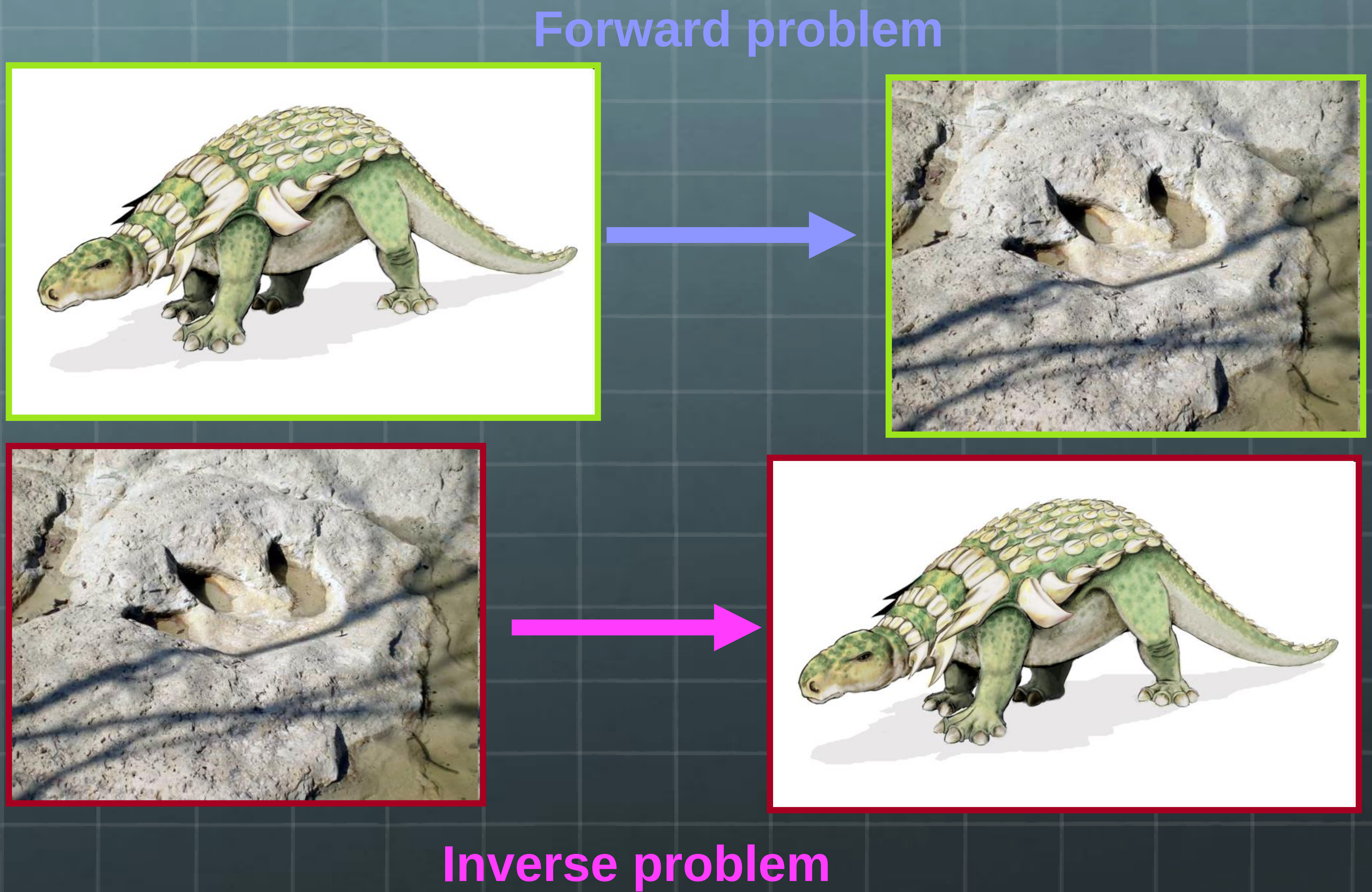
Forward and Inverse Problem

Forward problem



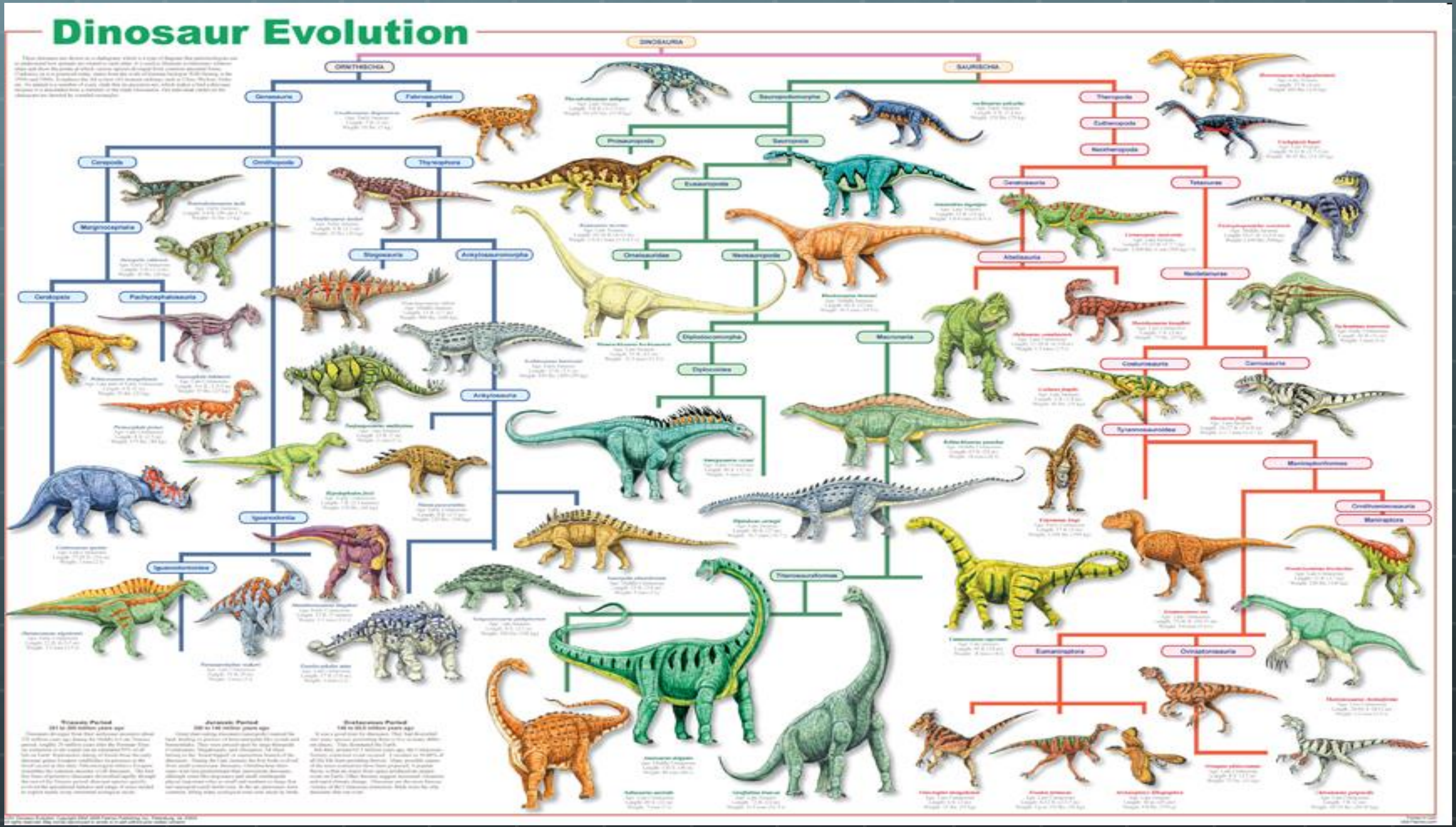
From Cathy Clerbaux.

Forward and Inverse Problem

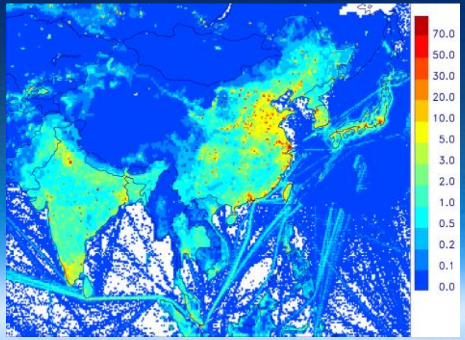


From Cathy Clerbaux.

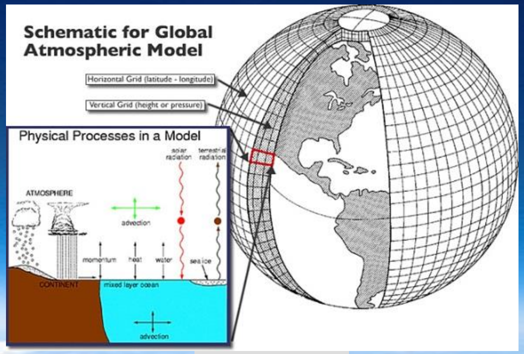
A Priori Knowledge



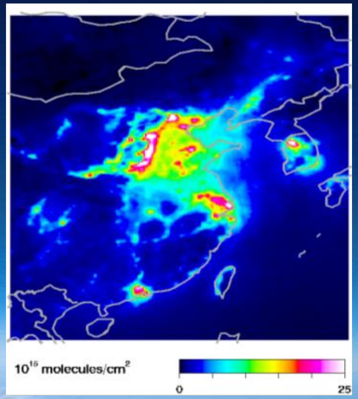
Forward and Inverse Problem



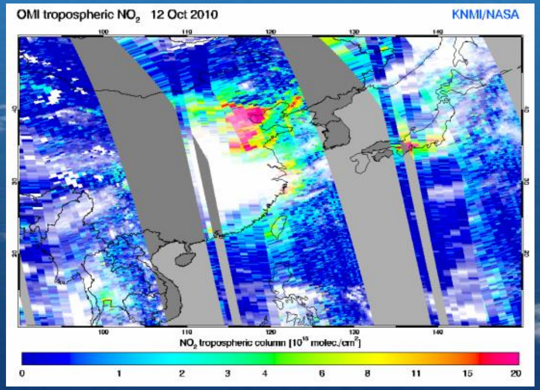
A priori emissions



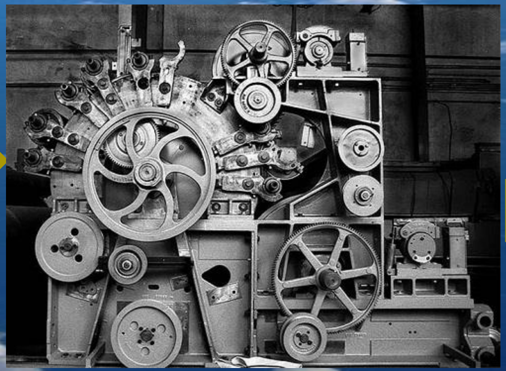
CTM



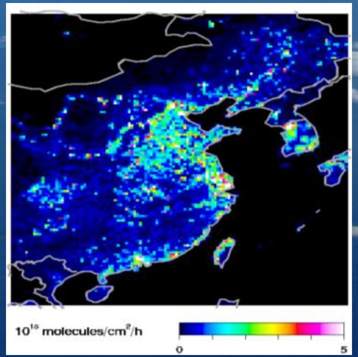
Concentrations



Satellite observations

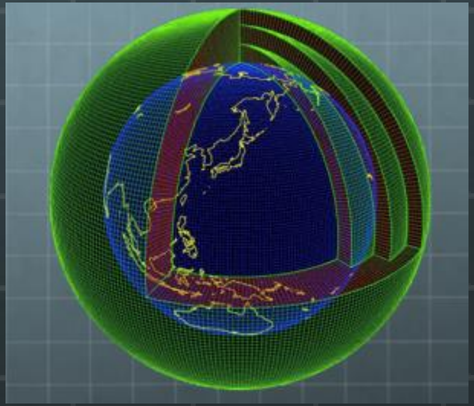


Inversion algorithm



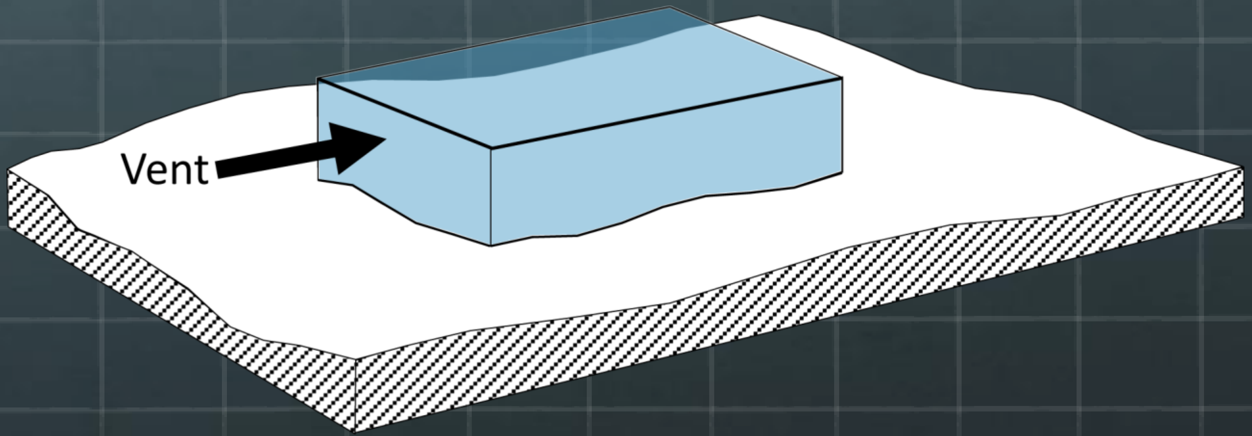
Updated Emissions

2. Types of Chemical Transport Models

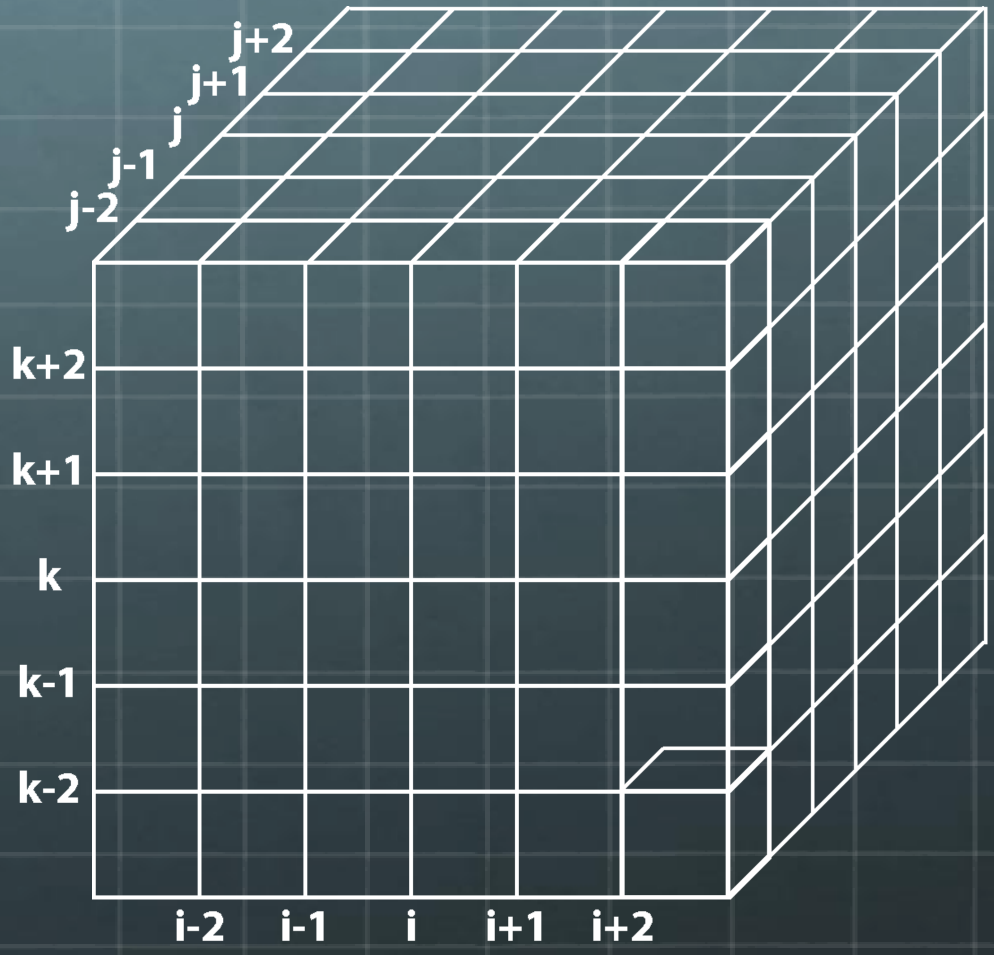


Eulerian Models

- We are following the evolution of the concentration of chemical species in a fixed volume (fixed framework).
- → 0D, 1D, 2D, 3 fixed grids



Type of Models

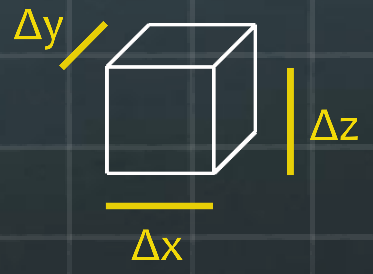


$f_i(t)$ = 0D = 'box'

$f_i(z,t)$ = 1D

$f_i(x,z,t)$ = 2D

$f_i(x,y,z,t)$ = 3D

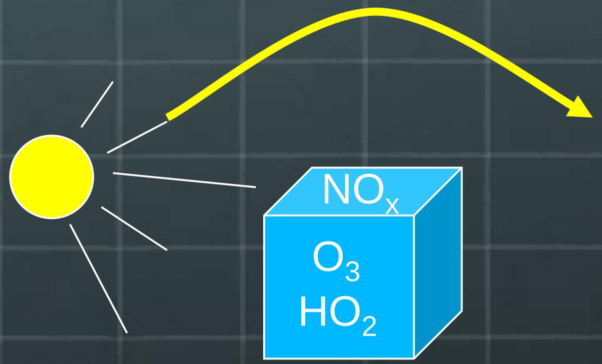


Zero-D (point) Models

Idea: investigate the chemistry in an „air parcel“ without regarding advection or diffusion processes

Advantage: computationally very fast, allows for comprehensive chemical mechanism, Monte Carlo simulations, etc.

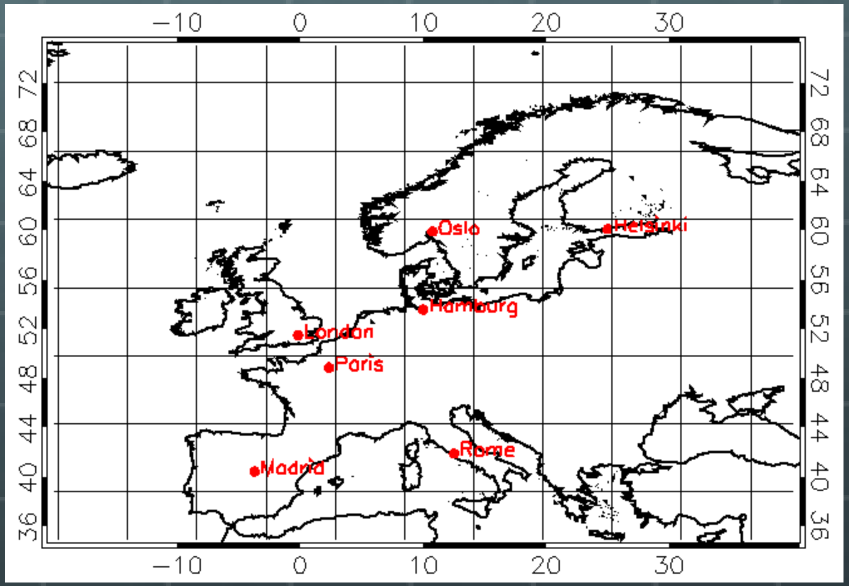
Disadvantage: does not take transport into account

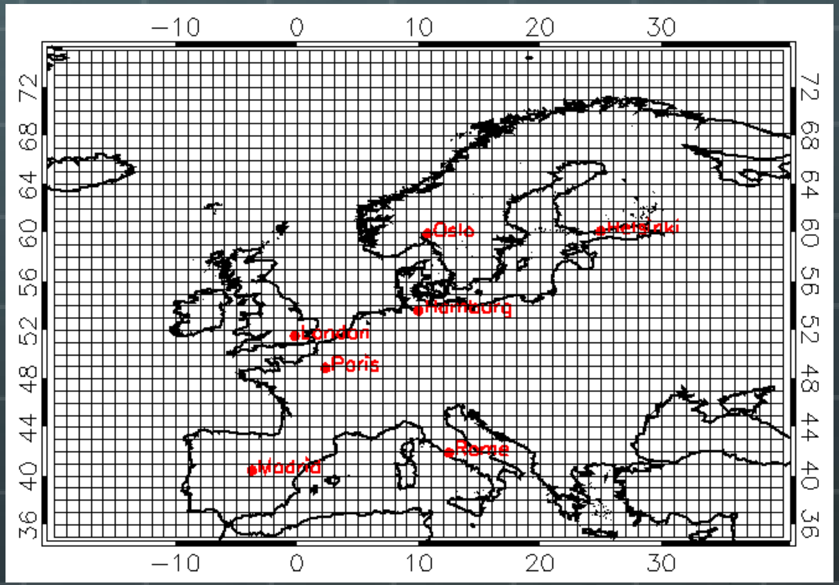


Three-dimensional Eulerian Models

This model type represents the most comprehensive, but also computationally most expensive type of models. The earth' atmosphere is divided into thousands of „grid boxes" of more or less regular shape.

Examples:

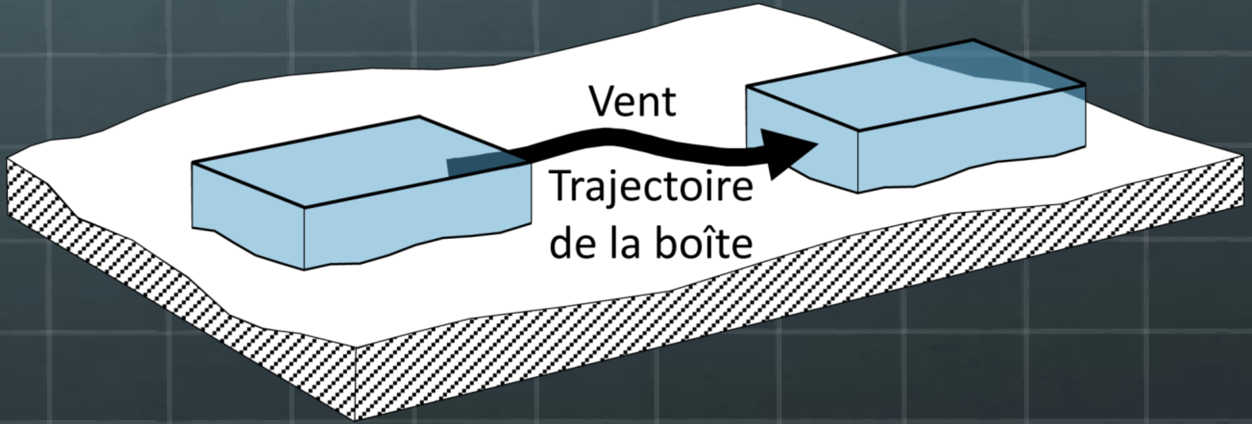




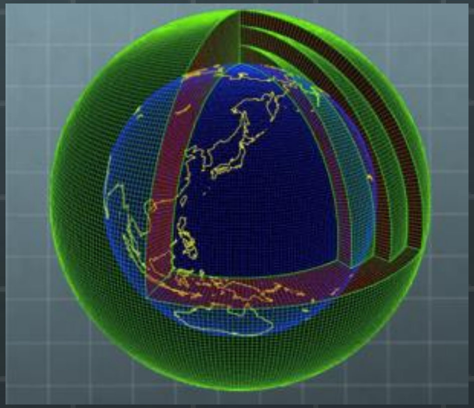
Grid box boundaries over Europe with 64x32 boxes (left), and a 1°x1° grid (right)

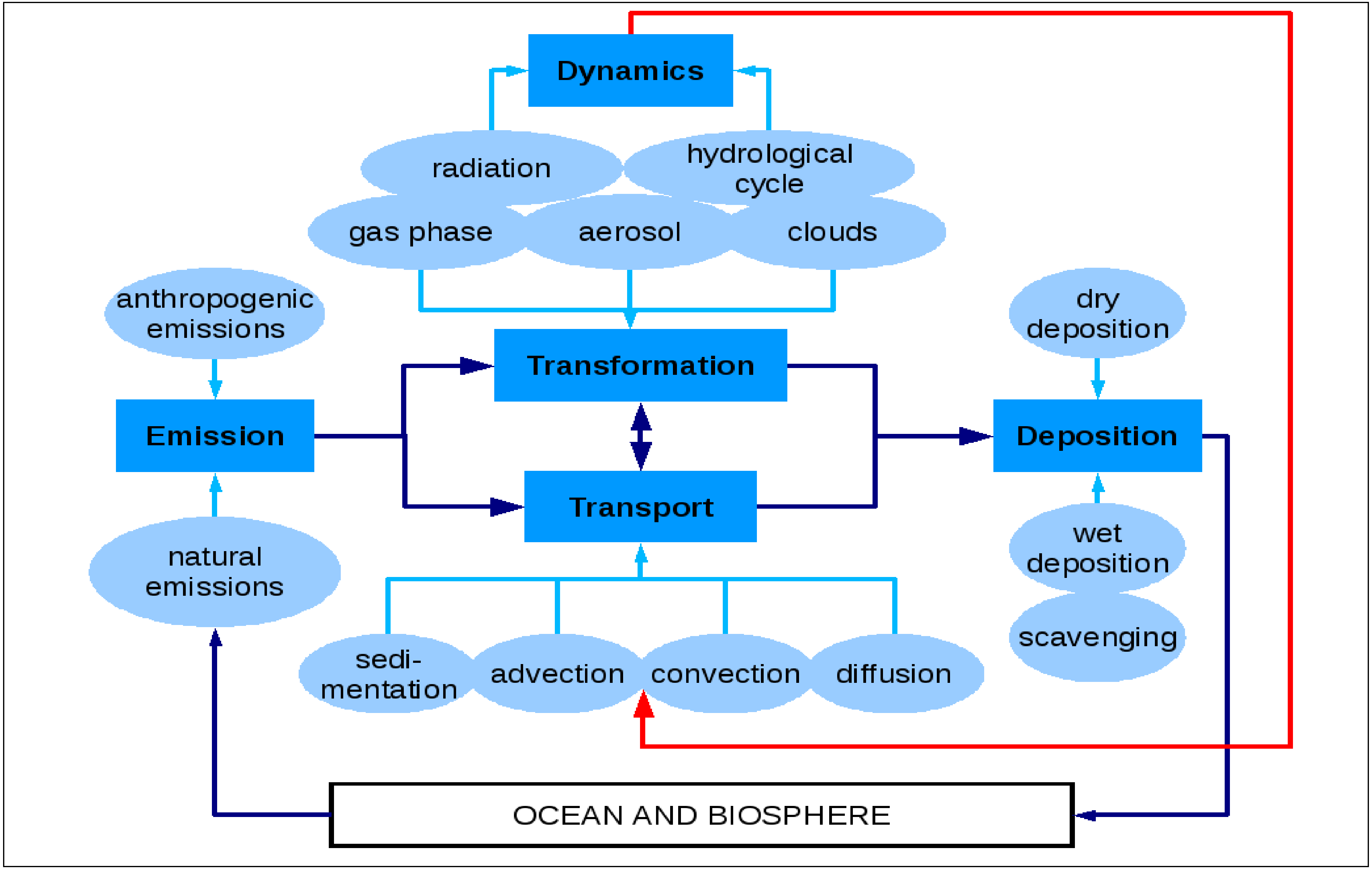
Lagrangian Model

- We follow the displacement of a large number of air parcels, and derive the evolution of the concentration of chemical species in each air parcel. The frame follows the air parcels

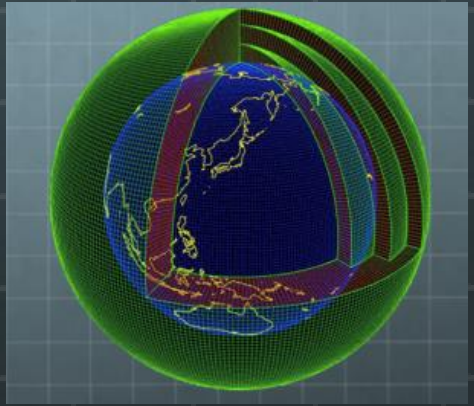


4. The Fundamental Equations




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

4.1 The Momentum Equations
Conservation of Momentum
(Newton's second law)



neric

$\vec{\nabla} p + \vec{g}$

avitati

force

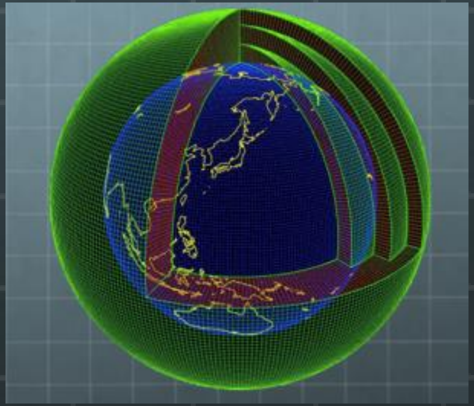
deriv

$\vec{V}$ $+ \vec{v}.$

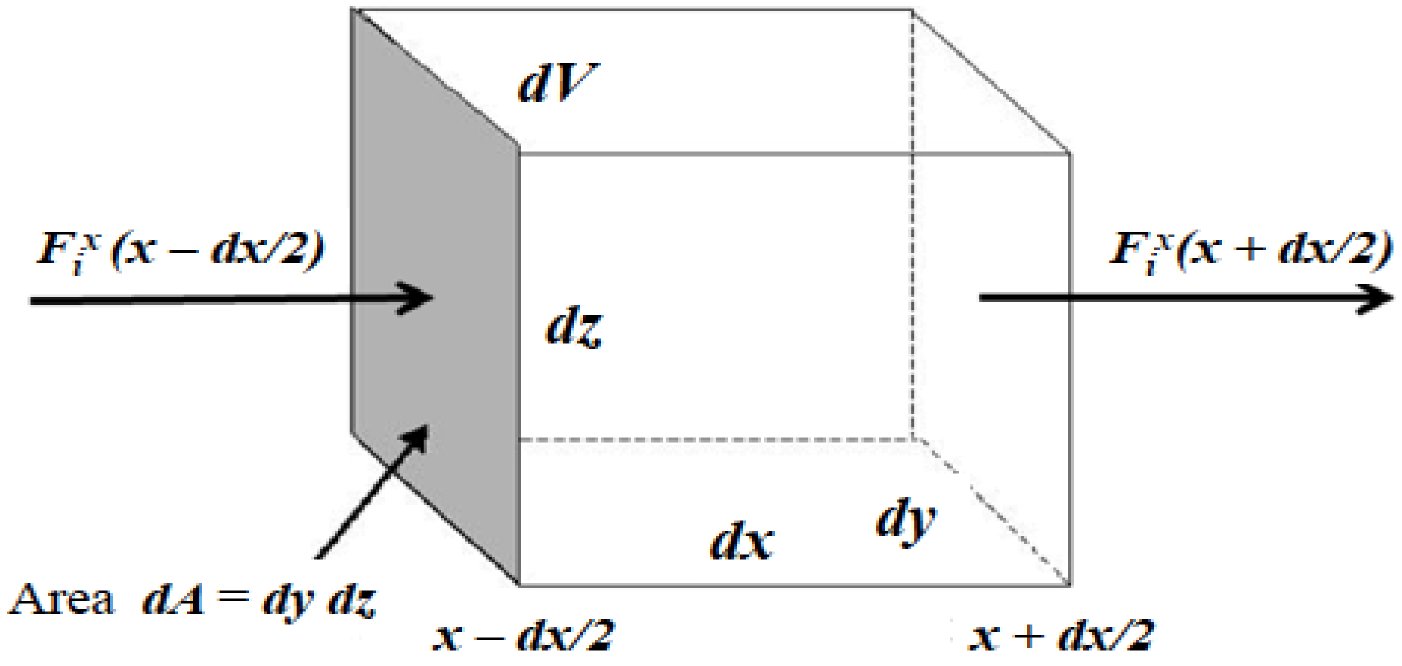
Newton. Euler

Navier Stokes

4.2 The Continuity Equation
Conservation of Mass



The Continuity Equation (Mass Conservation)



$$\left[\frac{\partial \rho_i}{\partial t}\right]_{adv} = \frac{[F_i^x(x - dx/2) - F_i^x(x + dx/2)]\ dx\ dy}{dx\ dy\ dz} = -\frac{\partial(\rho_i u)}{\partial x}$$

Atmospheric Model

(4) The continuity equation or the conservation of mass

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla}.\left(\rho \vec{v}\right)$$

Local changes

Term related to transport

(5) The conservation of water vapour mass

$$\frac{\partial \rho q}{\partial t} = -\vec{\nabla}.(\rho \vec{v} q) + \rho(E - C)$$

Local changes

Term related to transport

Moisture source/sink

Atmospheric Model

(6) The continuity equation or the conservation of mass for chemical species

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla}.\left(\rho\vec{v}\right) + P - L$$

Local changes

Term related to transport

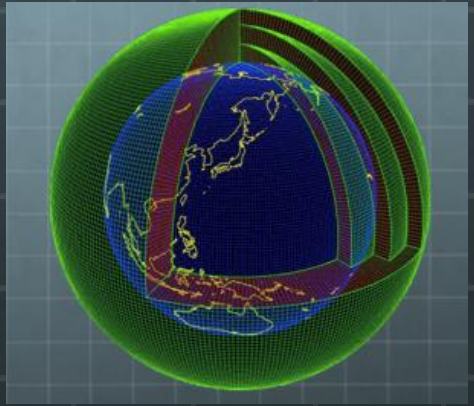
Local production and loss terms

Here ρ represents now the concentration of N chemical species that are related through chemical reactions.

ρ is therefore a vector of N elements.

L is generally expressed as the product of a matrix by a concentration vector

4.3 The Energy Equations
Conservation of Energy



Atmospheric Model

(6) The first law of thermodynamics (the conservation of energy)

$$C_p \frac{dT}{dt} = Q + \frac{1}{\rho}\frac{dp}{dt}$$

Changes in internal energy

Heat input

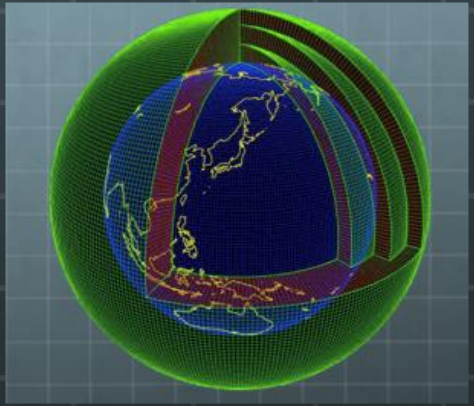
Work

(7) The equation of state

$$p = \rho R_g T$$

+ model "physics": parameterisation of subgrid-scale processes, radiative fluxes, turbulent fluxes, etc.

5. Resolution of Model Equations

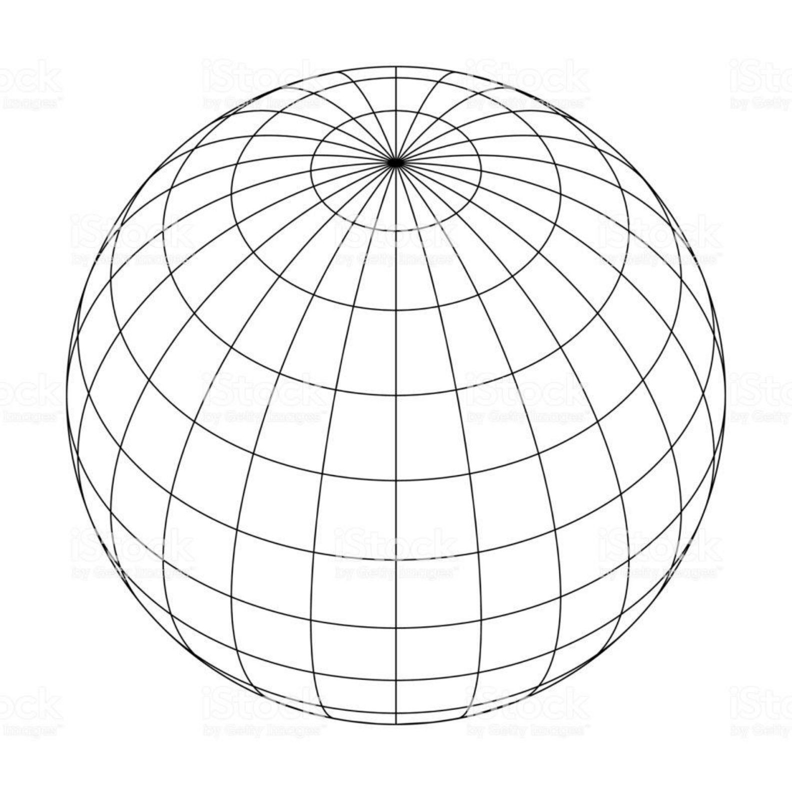


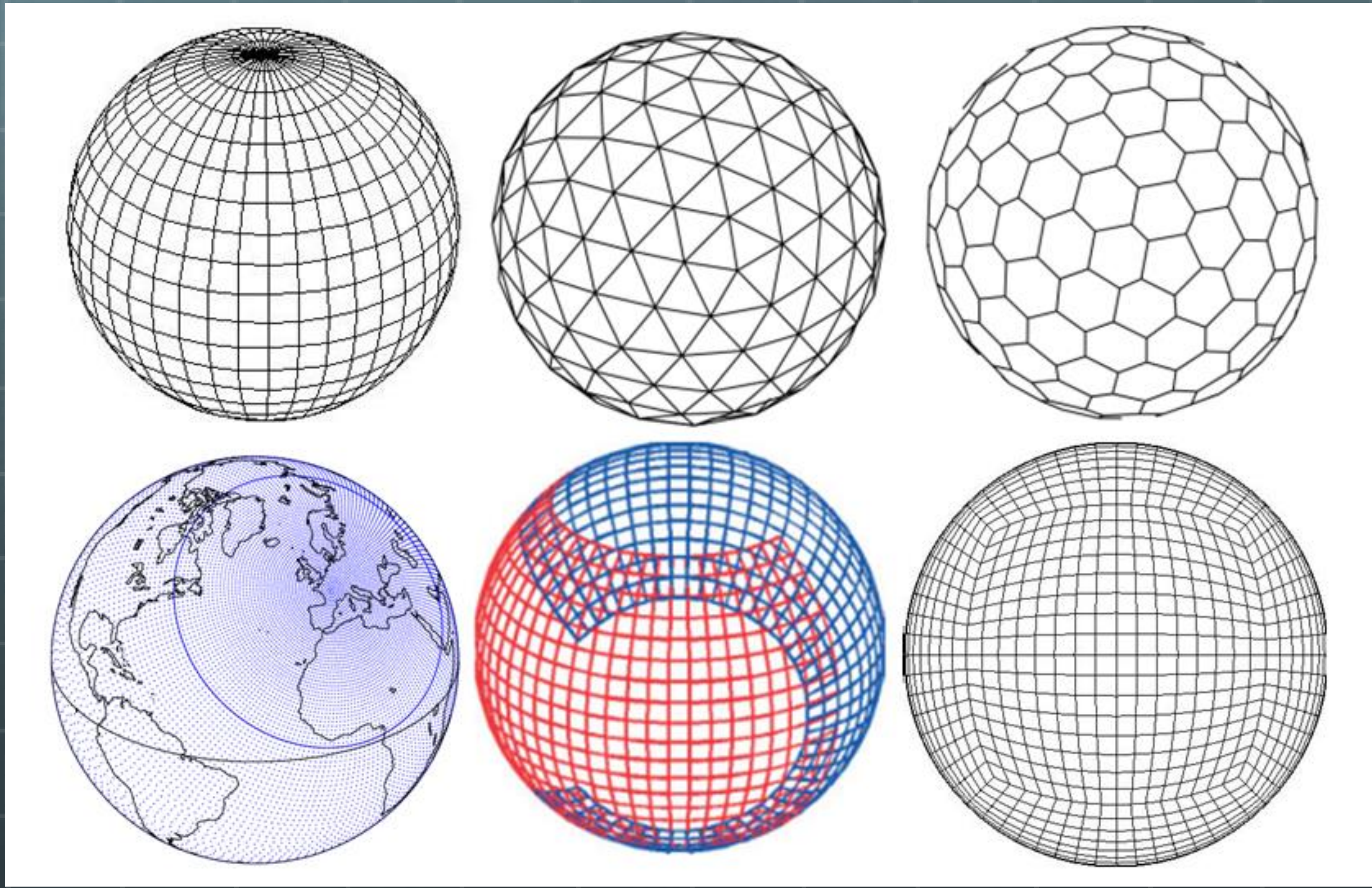
Representation in a Model of the Atmospheric Quantities

- The analytic solution of the atmospheric equations is not available, and these equations have to be solved by numerical methods.
- Equations can be discretized and solved at finite locations and finite time intervals. The locations can be points on a numerical grid or finite volumes (average values in a small volume of the domain).
- Another approach in global models is to expand on the sphere the quantities as a finite series of waves. These are the spectral models.

Representation of Atmospheric Variables on a Numerical Grid

Grid-point models





Problem at the poles !

Spectral Methods

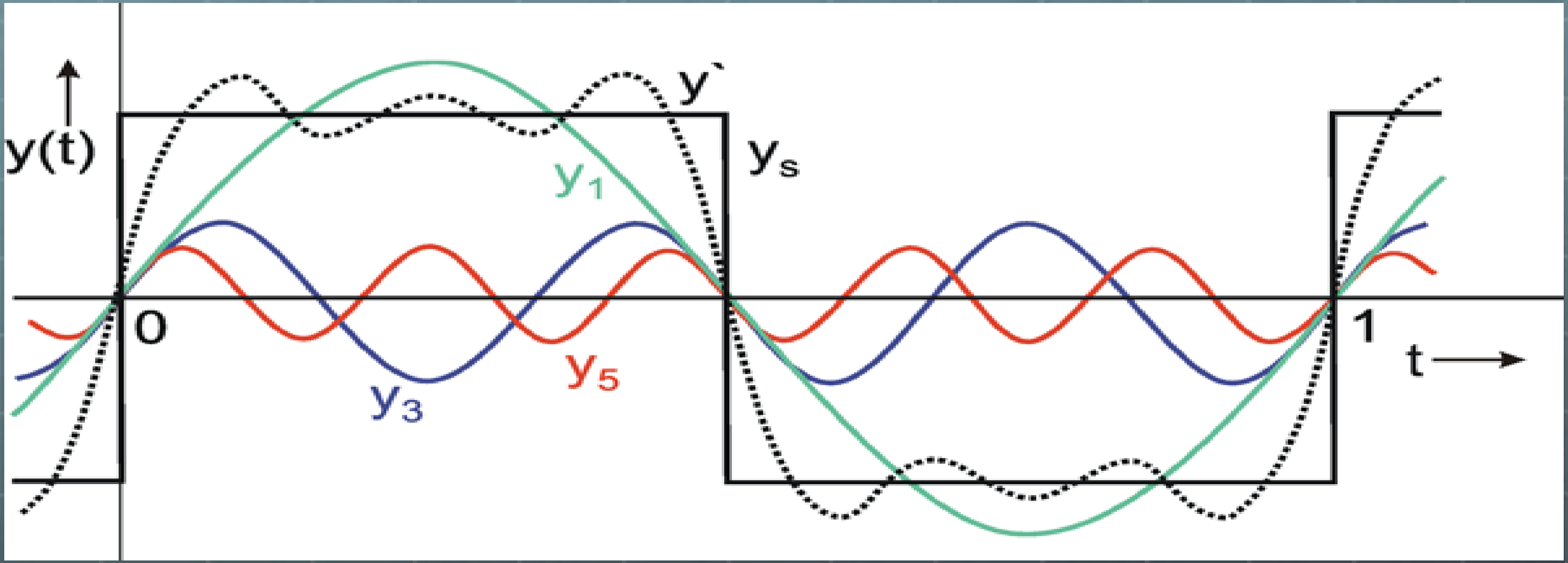
Over a periodic 1-D domain, we can express any function $\Psi(x)$ (such as the temperature) as the sum over all wavenumbers k of sine functions with different amplitudes d_k and phases φ_k :

$$\Psi(x,t) = \sum_0^\infty a_k(t) \sin[kx + \varphi_k]$$

The component with the lowest frequency is called the fundamental. With higher frequencies, the components are the harmonics.

When all variables are replaced by expressions of that type, the resulting system of equation is reduced to a system of ordinary differential equation for the unknown $a_k(t)$ which depends only on time.

Fourier decomposition of a square function



Fourier decomposition of a square function y_s with the fundamental

$$y_1 = 3/\pi \sin 2\pi t,$$

and the two harmonics

$$y_3 = 4/(3\pi) \sin 6\pi t$$
$$y_5 = 4/(5\pi) \sin 10\pi t$$

the sum

$$y' = y_1 + y_2 + y_3 \text{ (dotted line).}$$

Spectral Method on a Sphere

Application of the spectral method to the sphere can be done by expanding the functional forms $\Psi(\lambda, \mu, t)$ of the different variables as a function of longitude λ [0, 2π] and sine of latitude μ [–1, 1]) using normalized *spherical harmonics* $Y_n^m(\lambda, \mu)$ (see Figure 4.21):

$$\Psi(\lambda, \mu, t) = \sum_{m=-M}^{M} \sum_{n=|m|}^{N(m)} a_n^m(t)\, Y_n^m(\lambda, \mu) \tag{4.252}$$

where $a_n^m(t)$ are the spectral coefficients, which are the unknowns to be determined as a function of time t. The choice of parameters M and $N(m)$ define the truncation of the expansion.

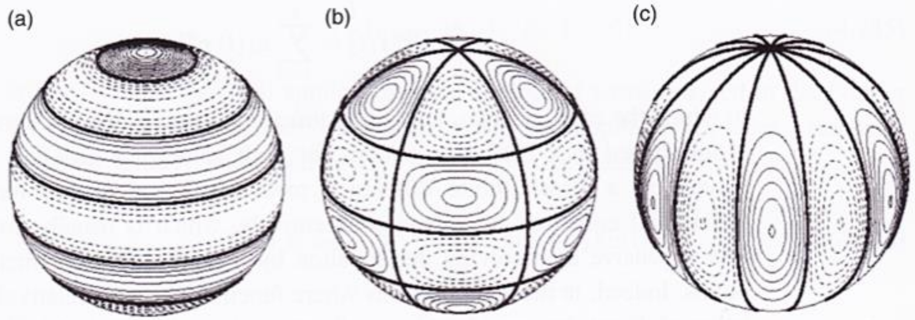
Spectral Method on a Sphere: Y_n^m (λ,μ)

They are expressed as a combination of sines and cosines (or equivalently by complex exponentials) to represent the periodic variations in the zonal direction, and by real associated Legendre functions of the first kind $P_n^m(\mu)$ (see Box 4.11) to account for the variations in the meridional direction. Thus,

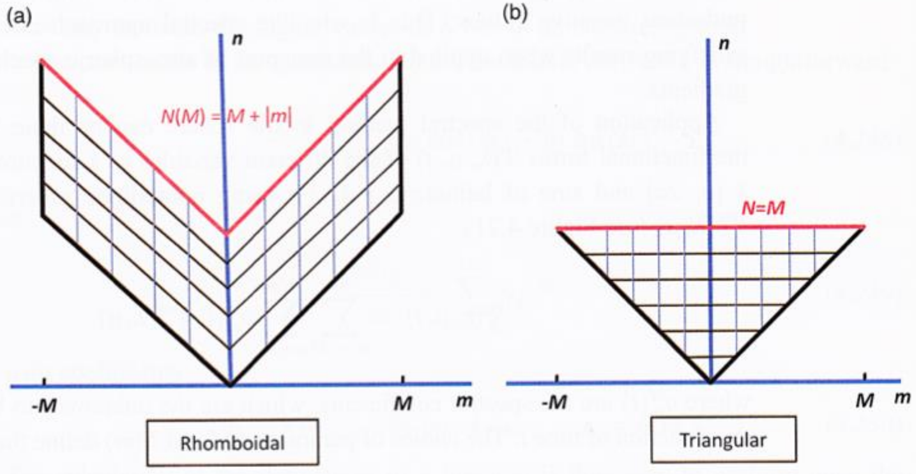
$$Y_n^m(\lambda, \mu) = P_n^m(\mu)e^{im\lambda} \qquad (4.254)$$

Here, index m represents the zonal wavenumber; its highest value M specifies the number of waves retained in the zonal direction. Index $n - |m|$ is called the meridional nodal number.

The type of truncation to be adopted for expression (4.252) is determined by the relation between the number of waves allowed in the zonal and the meridional directions. If N is chosen to be equal to M, the truncation is said to be *triangular*. If it is such that $N = M + |m|$, it is called *rhomboidal* (Figure 4.22).



Representation of the characteristics of three spherical harmonics with total wavenumber $n = 6$. (a): zonal wavenumber $m = 0$, (b): $m = 3$ and (c): $m = 6$. From Williamson and Laprise (1998).



Spectral Methods versus Grid Models

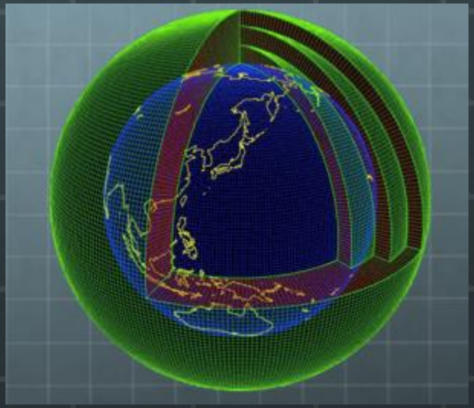
The advantage of the spectral methods is that the space derivatives can be calculated exactly. Numerical integration is only over time.

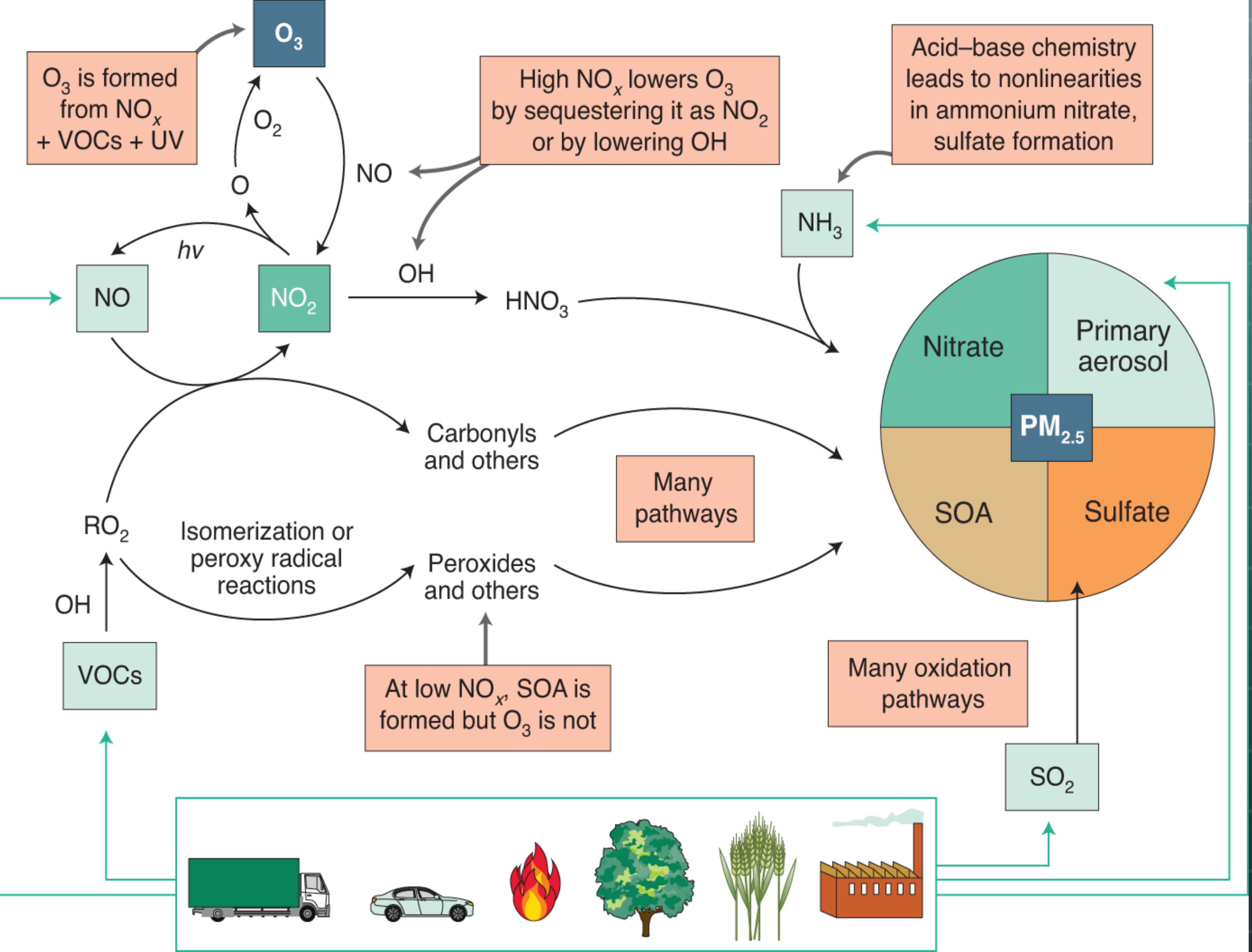
With the proper choice of parameters, the **spectral method** provides accurate and stable results; it can be conservative. It is therefore widely used in general circulation models of the atmosphere.

The method is not well suited for new computer architecture with massively parallel processors.

In addition, it is not shape preserving (monotonic, positive definite). Overshoots and undershoots (negative values) can be produced. There, it not used in chemical transport models. **Grid models** are preferred to treat local chemical processes.

6. Modeling of Chemical Processes





Tropospheric Chemistry

Chemistry

Chemical systems are assumed to be represented by a system of *N* nonlinear equations, where *N* is the number of species included in the model. In global chemical transport models, *N* is typically 100-200, but in complex box models, it can reach several thousands.

Because of the very different chemical lifetimes involved, the system is said to be stiff. Appropriate numerical methods must be adopted to solve stiff systems

Explicit and Implicit Algorithms

Consider a generic function **Ψ**(t) that represents the concentration (vector of N elements) for *N* chemical compounds. The equation for the system is:

$$\frac{d\boldsymbol{\psi}(t)}{dt} = \mathbf{s}(\boldsymbol{\psi}, t)$$

with the specified initial condition $\boldsymbol{\psi}(t_o)$

Explicit Method

$$\boldsymbol{\psi}^{\mathbf{n+1}} = \boldsymbol{\psi}^{\mathbf{n}} + \Delta t\ \mathbf{s}(t_n, \boldsymbol{\psi}^n)$$

Implicit Method

$$\boldsymbol{\psi}^{n+1} = \boldsymbol{\psi}^n + \Delta t\ \mathbf{s}(t_{n+1}, \boldsymbol{\psi}^{n+1})$$

Explict versus Implicit Methods

Fully explicit Methods:

- Simple to solve, but stability considerations constrain the integration time steps to prohibitively small values.
- The positivity of the solution is not guaranteed.

Fully Implicit Methods:

- Unconditionally stable, so that the time step can be large, limited by accuracy considerations.
- Require the resolution of a system of algebraic equations at each time step and each grid point

“Stiff systems”

Here: the stiffness is = 1000

$$\frac{du}{dt} = 998\,u + 1998\,v$$

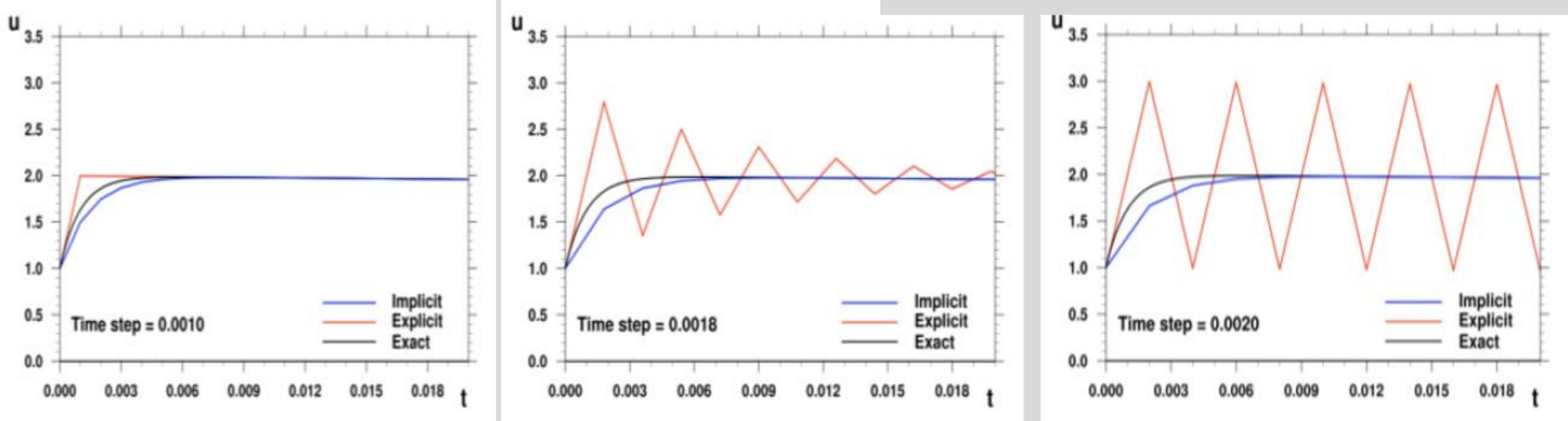
$$\frac{dv}{dt} = -999\,u - 1999\,v$$

with the initial conditions $u(0) = 1$ and $v(0) = 0.$

The analytic solution is

$$u(t) = 2e^{-t} - e^{-1000t}$$

$$v(t) = -e^{-t} + e^{-1000t}$$



The Gear Method

Accuracy and stability can be increased through multi-level methods (here K time levels):

$$\psi^{n+1} = \sum_{k=0}^{\mathcal{K}} \alpha_k \psi^{n-k} + \Delta t \sum_{k=-1}^{\mathcal{K}} \gamma_k \mathbf{s}(t_{n-k}, \psi^{n-k})$$

A specific application is the Gear algorithm:

$$\psi^{n+1} = \sum_{k=0}^{\mathcal{K}} \alpha_k \psi^{n-k} + \Delta t\, \gamma\, \mathbf{s}(t_{n+1}, \psi^{n+1})$$

This implicit equation is solved by an iterative method:

$$(\mathbf{I} - \Delta t\, \gamma\, \mathbf{J}) \bullet \left(\psi_{(r+1)}^{n+1} - \psi_{(r)}^{n+1} \right) = -\psi_{(r)}^{n+1} + \Delta t\, \gamma\, \mathbf{s}(t_{n+1}, \psi_{(r)}^{n+1}) + \sum_{k=0}^{\mathcal{K}} \alpha_k \psi^{n-k}$$

Automatic adjustment of the order of the method and of the time step to maximize stability and accuracy

Tropospheric Chemical Mechanisms

- Typical 3D model used for air quality:

  100 - 200 reactions

- Typical 0D (box) models used for sensitivity studies:

  5,000 - 10,000 reactions

- Fully explicit (computer-generated) mechanisms:

  10^6 - 10^7 reactions

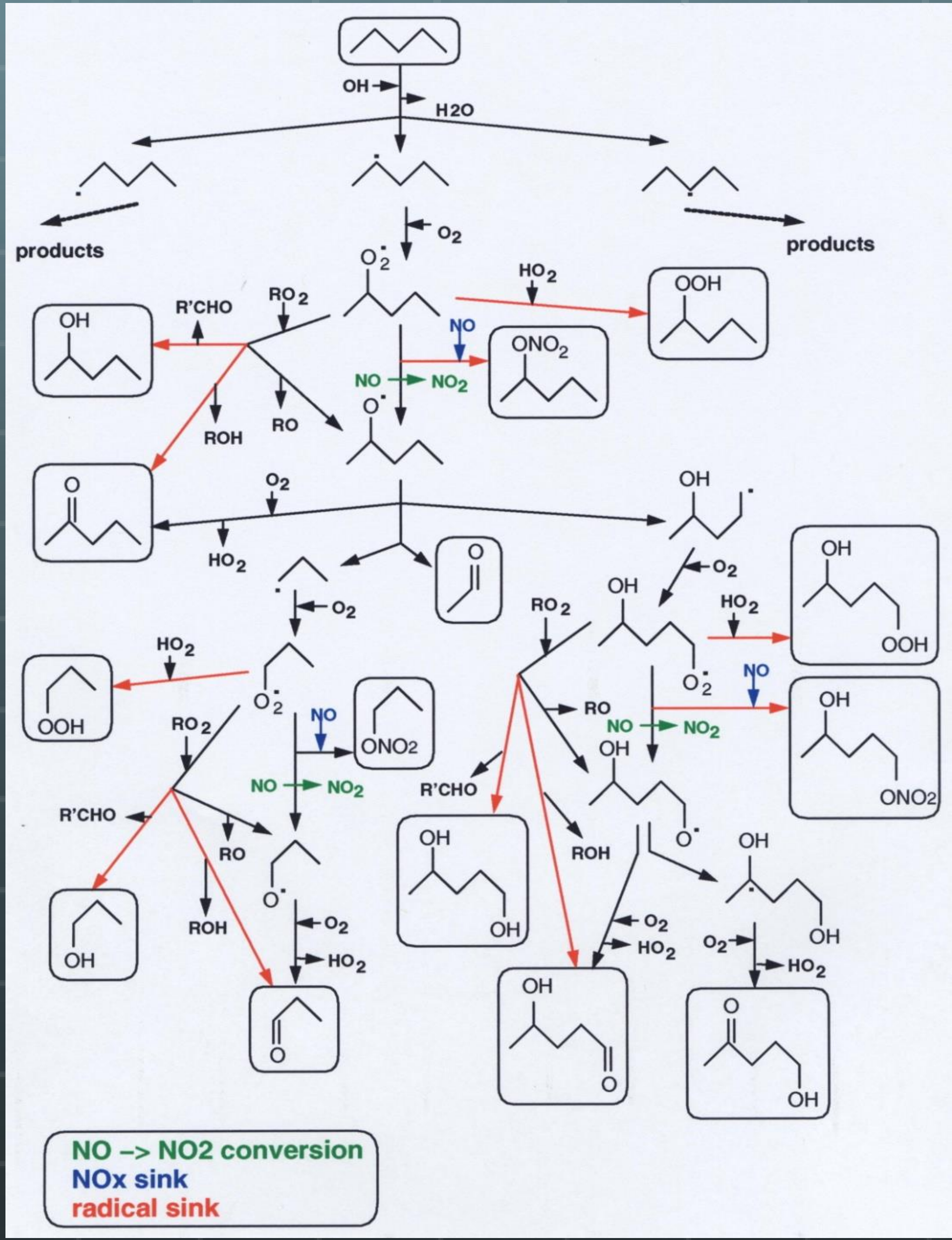
Simplified Mechanism for Pentane (C_5H_{12})

Multiple NO→NO_2 conversions produce O_3

Organic nitrates allow long-range transport of NOx

Radical sinks:
Some are temporary, producing HOx later

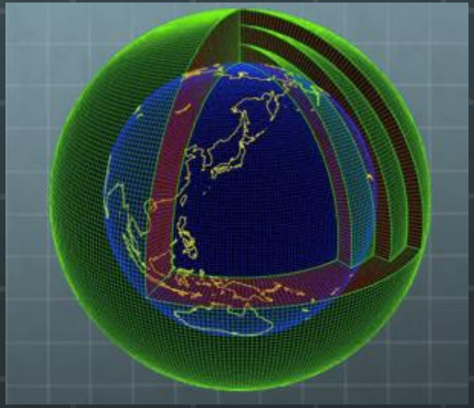
Some have low vapor pressures, can make organic aerosols



Some Chemical Mechanisms

- **Heuristic**
  - Most textbooks [e.g. *Seinfeld and Pandis*, 1997]
- **Lumped**
  - CB-IV [*Gery*, 1989]
  - RADM, RACM [*Stockwell*, 1990; 1997]
  - SAPRC99 [*Carter*, 2000]
- **Explicit**
  - NCAR Master Mechanism [*Madronich and Calvert*, 1989]
  - Leeds Master Mechanism [*Jenkin et al.*, 1997]
  - Self-Generating Mechanism [*Aumont et al.*, 2005]

7. Modeling of Transport

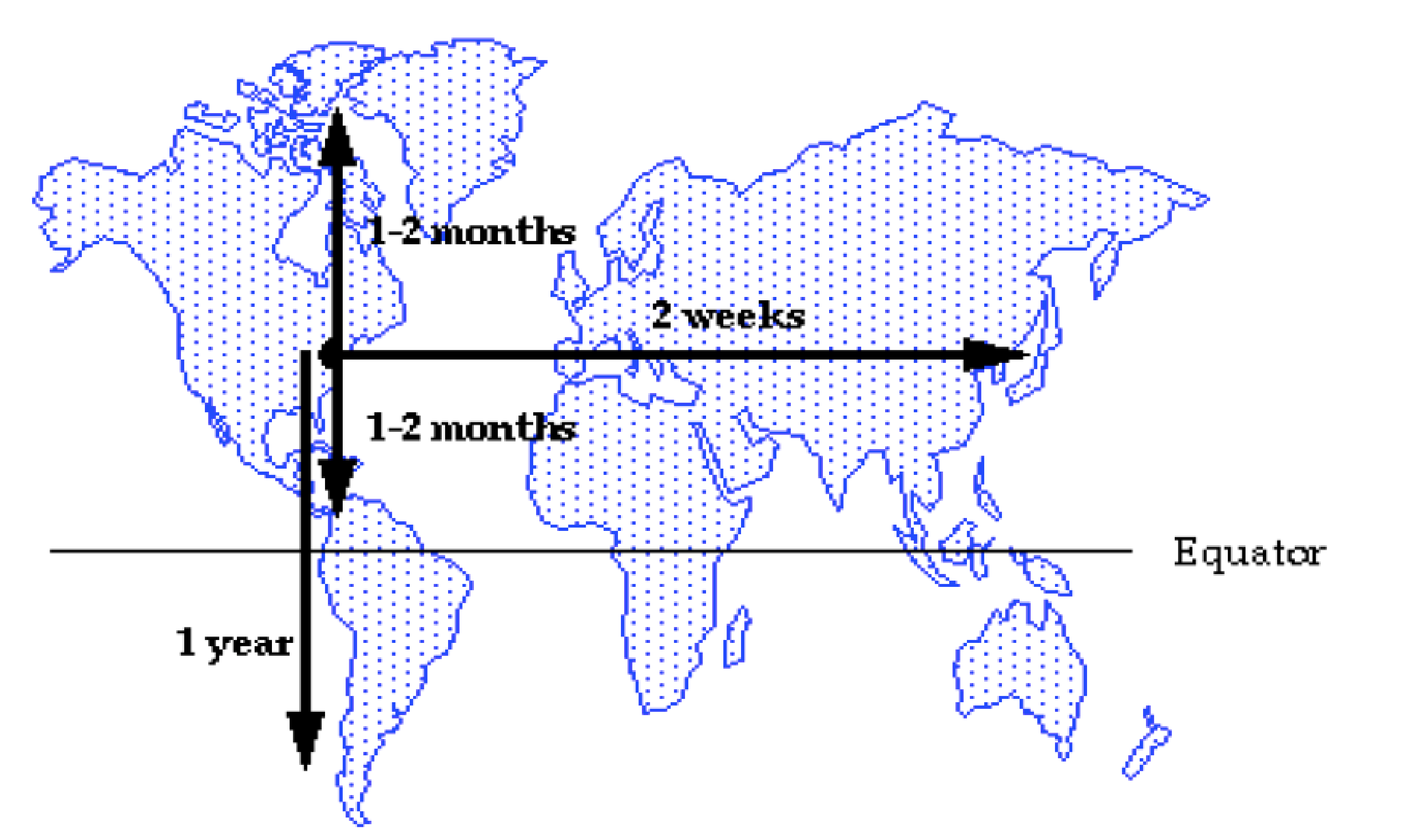


Transport

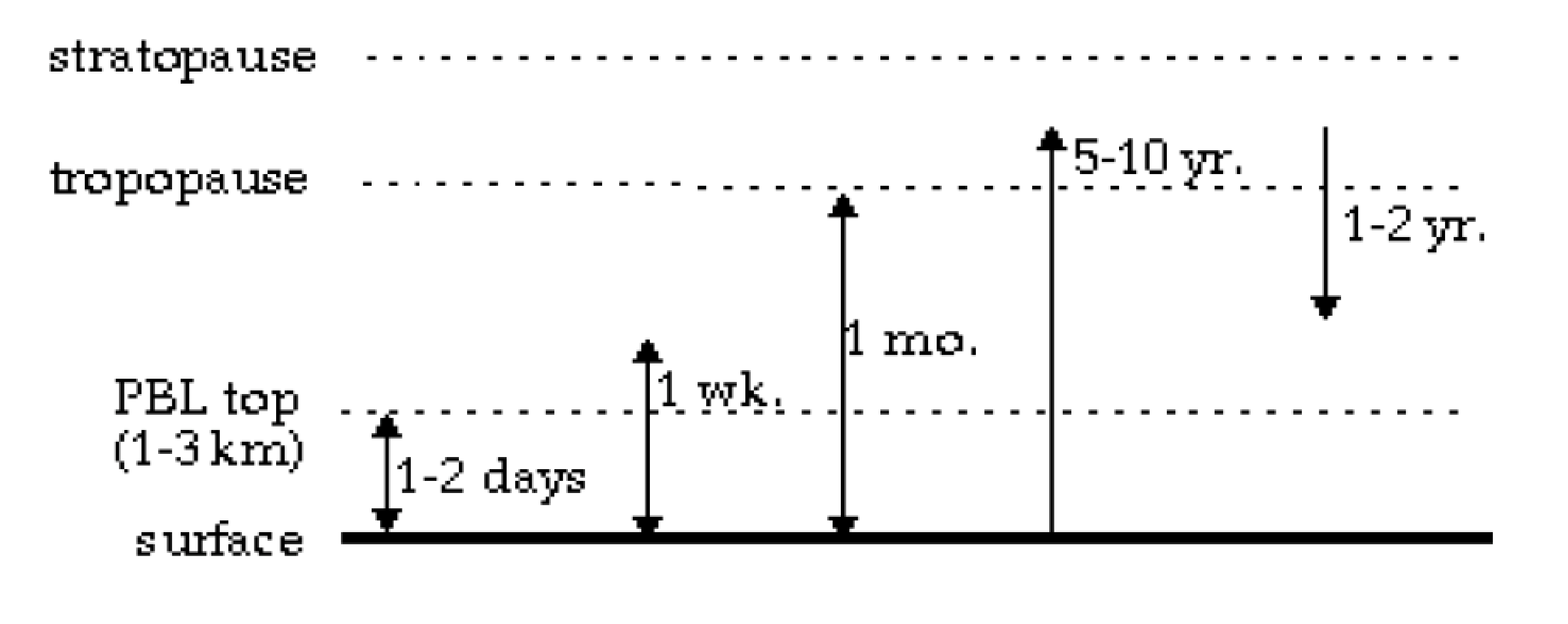
Advection: resolved transport

Mixing: Sub-grid (unresolved) transport

Horizontal Transport Timescales



Timescales for vertical exchanges



7.1. Advection

Requirements for a scheme of Numerical Advection

- **Accuracy:** Solution close to the true solution
- **Stability:** Solution should not diverge from its true state
- **Monotonicity:** No spurious extremum
- **Conservation:** Mass must be conserved if no source/sink
- **Transportivity:** transport must be downwind
- **Locality:** Solutions not affected by perturbations far away
- **Correlativity:** Relations between species preserved
- **Flexibility:** Implemented for different grids and resolutions
- **Efficiency:** Computationally fast

The (1-D) Advection Equation

Consider the advection of function Ψ(*x*) along direction *x* with a constant velocity *c*

$$\frac{\partial \Psi}{\partial t} + c\frac{\partial \Psi}{\partial x} = 0$$

The *initial distribution* de the function is given by G(*x*)

$$\Psi(x,0) = G(x)$$

The problem is well-posed if the value of function Ψ is provided as time evolves (upstream *boundary condition*)

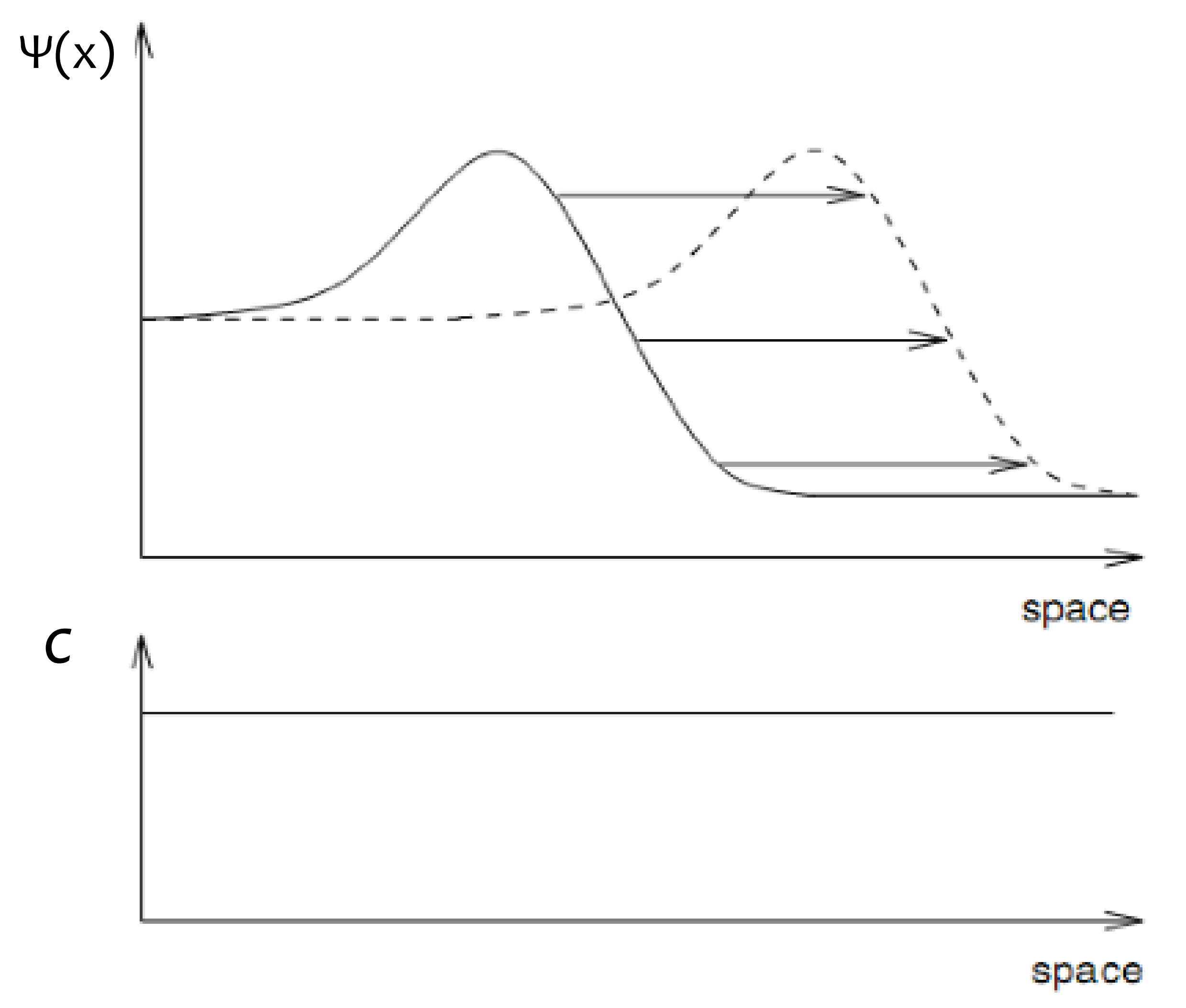
$$\Psi(0,t) = H_0(t)$$

The analytic solution of the 1-D advection equation is

$$\Psi(x,t) = G(x - ct)$$

(Translation of the signal)

1-D Advection of a signal with a constant velocity



Methods with Space-Centered Differences

We approximate the space derivative by a centered difference

$$\frac{\partial \Psi}{\partial x} = \frac{\Psi_{j+1} - \Psi_{j-1}}{2\Delta x} + O(\Delta x^2)$$

The discretized form of the advection equation is

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t} = -c\frac{\Psi_{j+1}^n - \Psi_{j-1}^n}{2\,\Delta x}$$

or $$\Psi_j^{n+1} = \Psi_j^n - \frac{\alpha}{2}\left(\Psi_{j+1}^n - \Psi_{j-1}^n\right)$$ with $$\alpha = c\frac{\Delta t}{\Delta x}$$

This algorithm is **unconditionally unstable** (for all values of α)

Methods with Space-Uncentered Differences

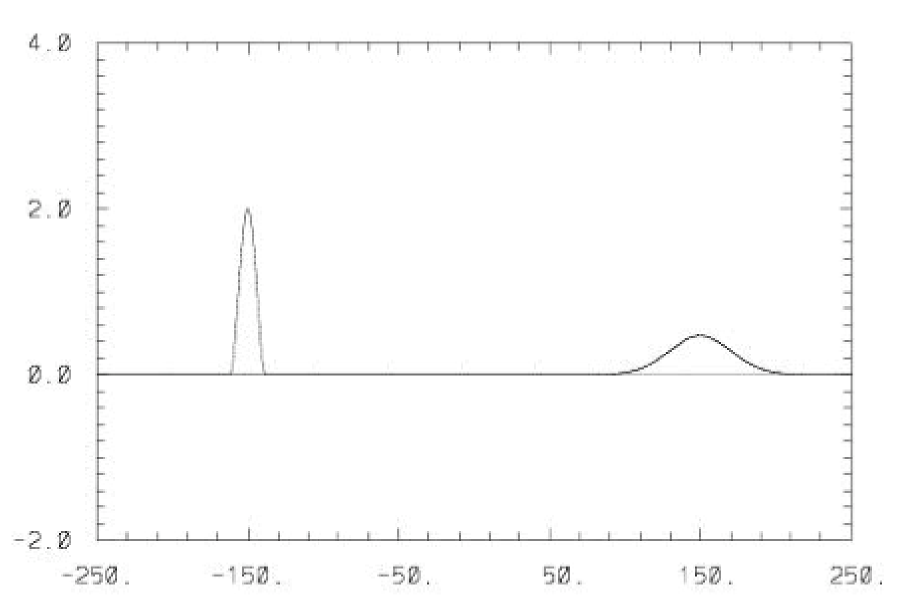
$$\frac{\partial \Psi}{\partial x} = \frac{\Psi_j - \Psi_{j-1}}{\Delta x} + O(\Delta x)$$

This method assumes that the value of the function at point *j* is affected only by the value at the upwind point *j*-1

Stable if $\alpha = \boxed{c\frac{Dt}{Dx} \le 1}$ **CFL criteria**

$$\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t} = -c\frac{\Psi_j^n - \Psi_{j-1}^n}{\Delta x} \quad \textit{for } c > 0$$

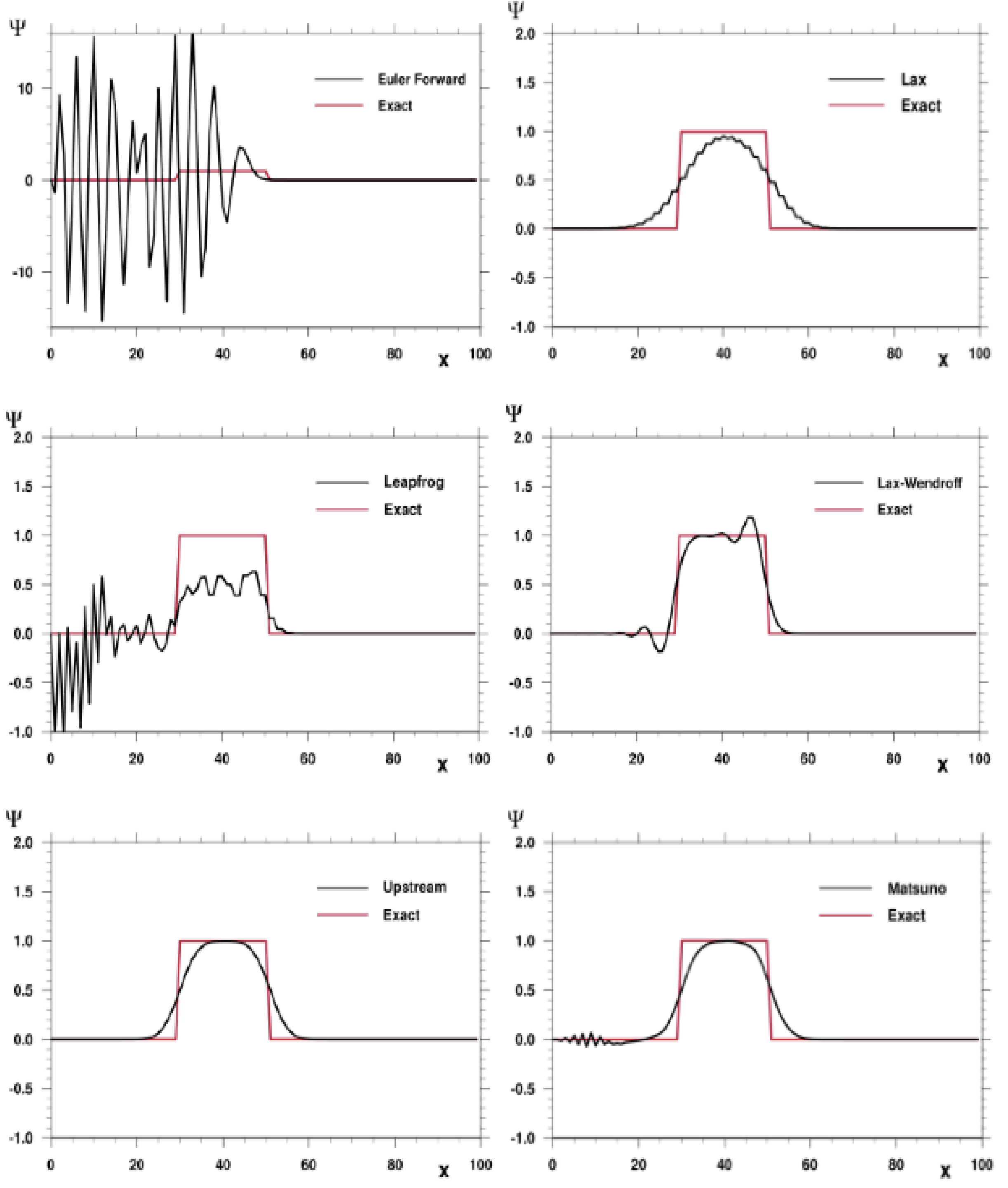
$$\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t} = -c\frac{\Psi_{j+1}^n - \Psi_j^n}{\Delta x} \quad \textit{for } c < 0$$



The method is positive definite, but very **diffusive**

Method	Algorithm	Stability	Accuracy	Remarks
Euler Forward (FTCS)	$\Psi_j^{n+1} = \Psi_j^n - \alpha/2\,(\Psi_{j+1}^n - \Psi_{j-1}^n)$	Unconditionally unstable	Δt, Δx^2	
Lax	$\Psi_j^{n+1} = ½\,(\Psi_{j+1}^n + \Psi_{j-1}^n) - \alpha/2\,(\Psi_{j+1}^n - \Psi_{j-1}^n)$	Stable for $\alpha < 1$	Δt, Δx^2	Dissipative
Leapfrog	$\Psi_j^{n+1} = \Psi_j^{n-1} - \alpha(\Psi_{j+1}^n - \Psi_{j-1}^n)$	Stable for $\alpha < 1$	Δt^2 ,Δx^2	Dispersive
Lax-Wendroff	$\Psi_j^{n+1} = \Psi_j^n - \alpha/2\,(\Psi_{j+1}^n - \Psi_{j-1}^n)$ $+ ½\,\alpha^2\,(\Psi_{j+1}^n - 2\,\Psi_j^n + \Psi_{j-1}^n)$	Stable for $\alpha < 1$	Δt^2, Δx^2	
Implicit	$\Psi_j^{n+1} = \Psi_j^n - \alpha/2\,(\Psi_{j+1}^{n+1} - \Psi_{j-1}^{n+1})$	Unconditionally stable	Δt, Δx^2	
Crank-Nicholson	$\Psi_j^{n+1} = \Psi_j^n - \alpha/4\,[(\Psi_{j+1}^{n+1} - \Psi_{j-1}^{n+1})$ $+ (\Psi_{j+1}^n - \Psi_{j-1}^n)]$	Unconditionally stable	Δt^2, Δx^2	
Matsuno	$\Psi_j^{n+1} = \Psi_j^n - \alpha/2\,(\Psi_{j+1}^n - \Psi_{j-1}^n)$ $+ \alpha^2/4\,(\Psi_{j+2}^n - 2\,\Psi_j^n + \Psi_{j-2}^n)$	Stable for $\alpha < 1$	Δt, Δx^2	Dissipative
Heun	$\Psi_j^{n+1} = \Psi_j^n - \alpha/2\,(\Psi_{j+1}^n - \Psi_{j-1}^n)$ $+ \alpha^2/8\,(\Psi_{j+2}^n - 2\,\Psi_j^n + \Psi_{j-2}^n)$	Unconditionally unstable	Δt^2, Δx^2	
Kurihara	$\Psi_j^{n+1} = \Psi_j^n - \alpha/4[(\Psi_{j+1}^{n-1} - \Psi_{j-1}^{n-1})$ $+ (\Psi_{j+1}^n - \Psi_{j-1}^n)]$ $+ \alpha^2/4\,(\Psi_{j+2}^n - 2\,\Psi_j^n + \Psi_{j-2}^n)$	Stable for $\alpha < 1$	Δt^2, Δx^2	Not dissipative
Fourth-order (implicit)	$\Psi_j^{n+1} = \Psi_j^n - \alpha/12\,[\Psi_{j-2}^{n+1} - 8\,\Psi_{j-1}^{n+1}$ $+ 8\Psi_{j+1}^{n+1} - \Psi_{j+2}^{n+1}]$	Unconditionally stable	Δt, Δx^4	
Upstream (α>0)	$\Psi_j^{n+1} = \Psi_j^n - \alpha\,(\Psi_j^n - \Psi_{j-1}^n)$	Stable for $\alpha < 1$	Δt, Δx	Monotonic Dissipative
Upstream (α<0)	$\Psi_j^{n+1} = \Psi_j^n - \alpha\,(\Psi_{j+1}^n - \Psi_j^n)$	Stable for $\alpha < 1$	Δt, Δx	Monotonic Dissipative

Comparison of the performance of different elementary methods to treat the linear advection algorithm



Which method should we use?

Centered methods are not positive definite, and characterized by noise.
Some algorithms (Euler-forward method) is unconditionally unstable.
Other algorithms can be stable under the CFL condition, but are not free of oscillations.

Uncentered methods (upwind or upstream) are free of oscillation (no phase lag), thus positive definite, but are diffusive. Usually stable for the CFL condition.

More advanced methods have been developed to address some of these problems. The best strategy is to improve the upwind method.

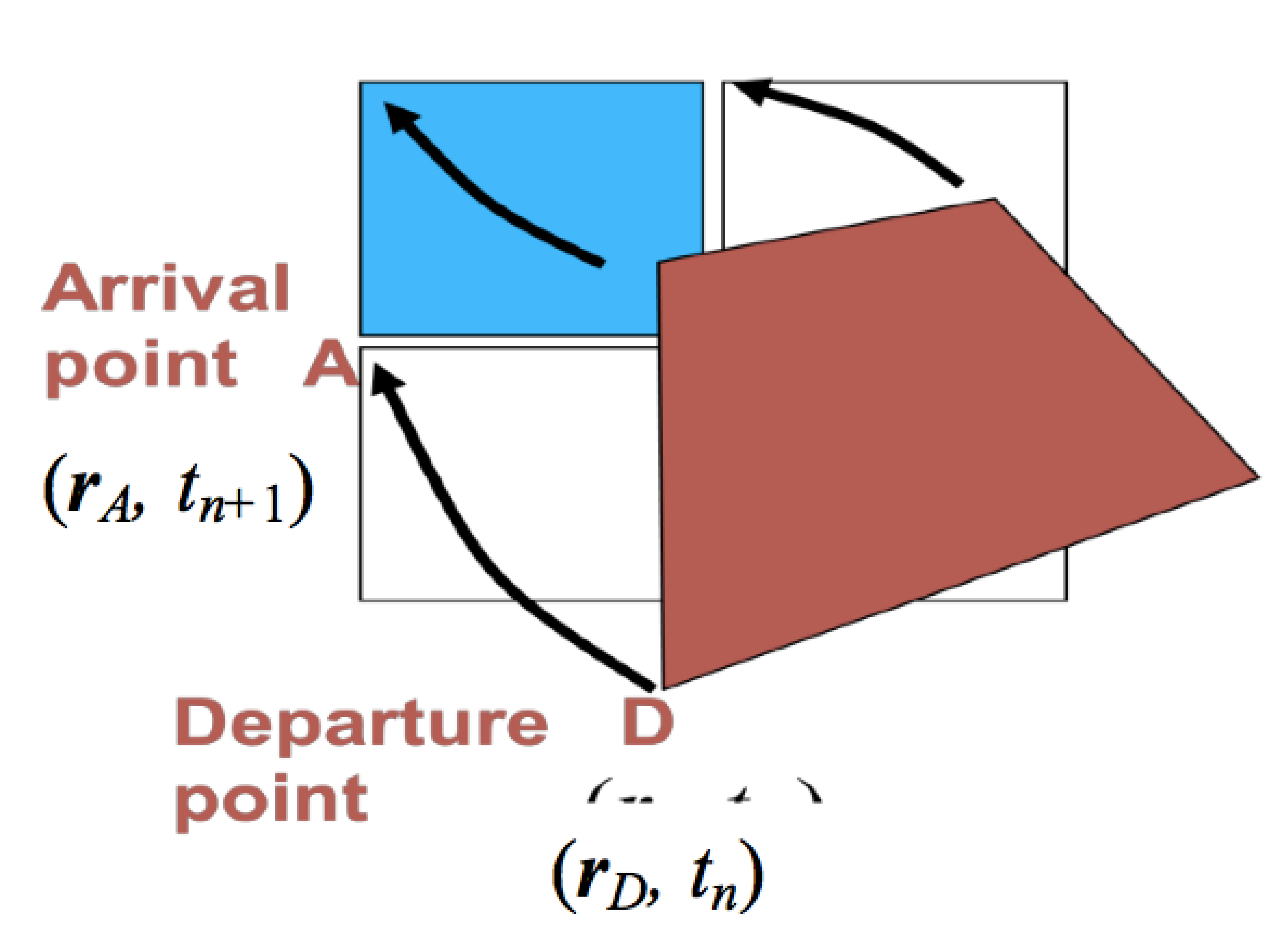
Higher Order Approaches: The Prather Method

The distribution of the function $\psi(x,y)$ inside a grid box $\Delta x\ \ \Delta y$ is represented by a second-order polynomial:

$$\Psi(x,y) = a_0 + a_1\,x + a_2\,x^2 + b_1\,y + b_2\,y^2 + c\,xy$$

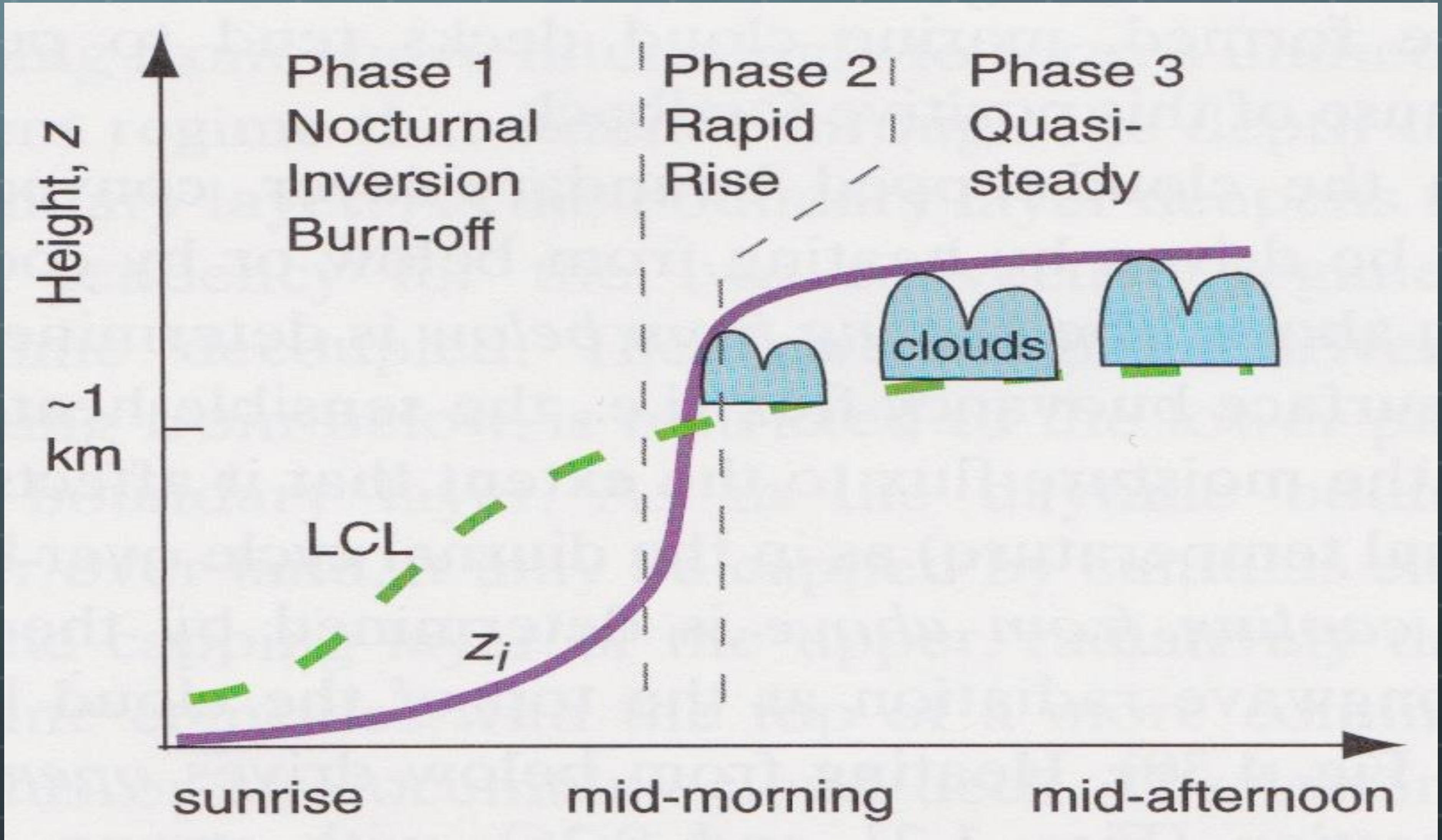
During a time step Δt, we use the upstream method and advect successively in each direction x and y the mean value as well as the first derivative (slope) and second derivative (curvature). The method has the advantages of the upwind method but is much less diffusive.

The semi-Lagrangian Method

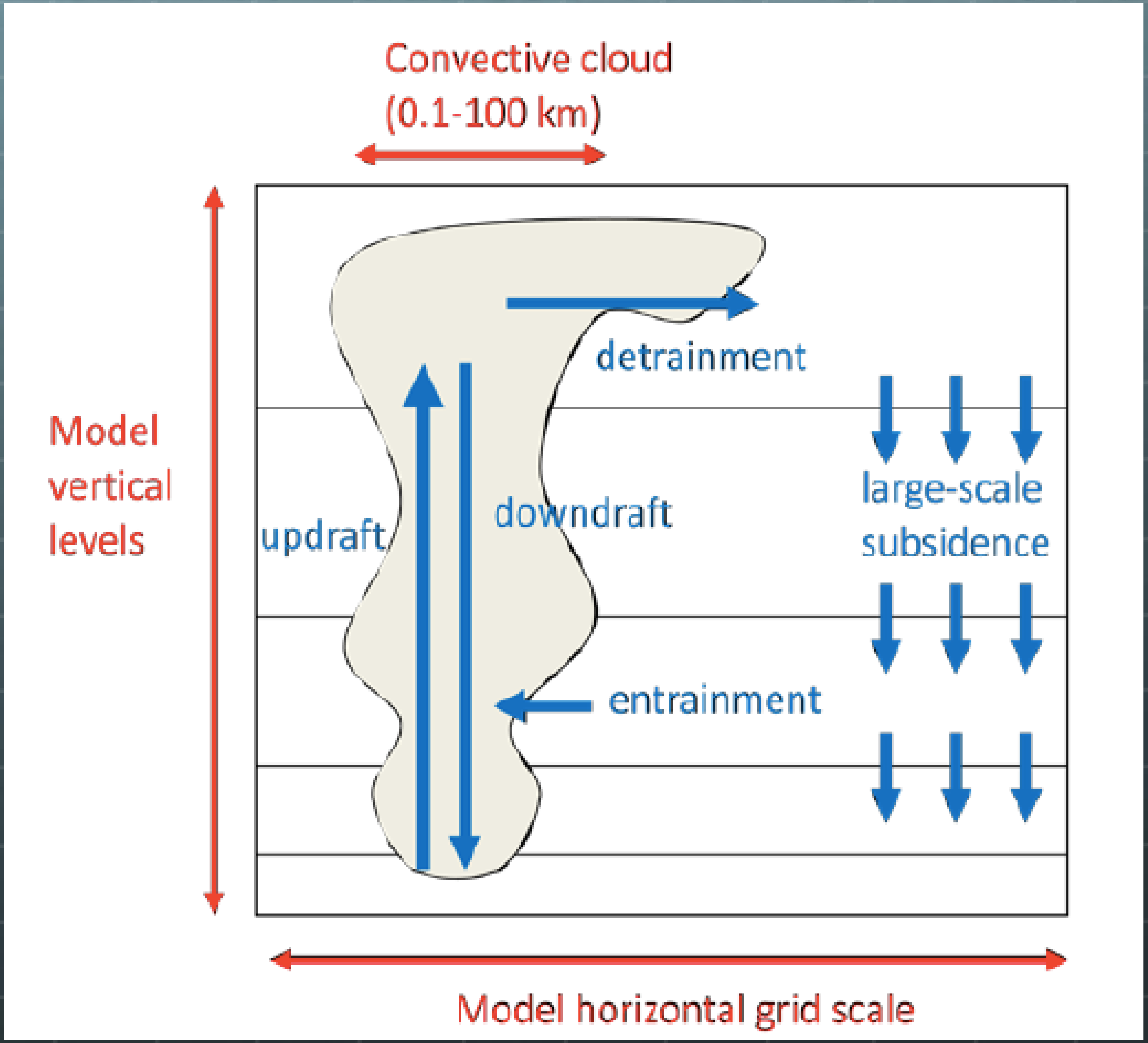


7.2. Sub-grid Exchanges

Exchanges between the Boundary layer and the Free troposphere



Convective Vertical Exchanges



Reynolds Decomposition

Reynolds Decomposition: Turbulence

Any variable is decomposed as a mean (resolved) component and a subscale (unresolved) component (whose mean is zero):

$$A = \bar{A} + A'$$

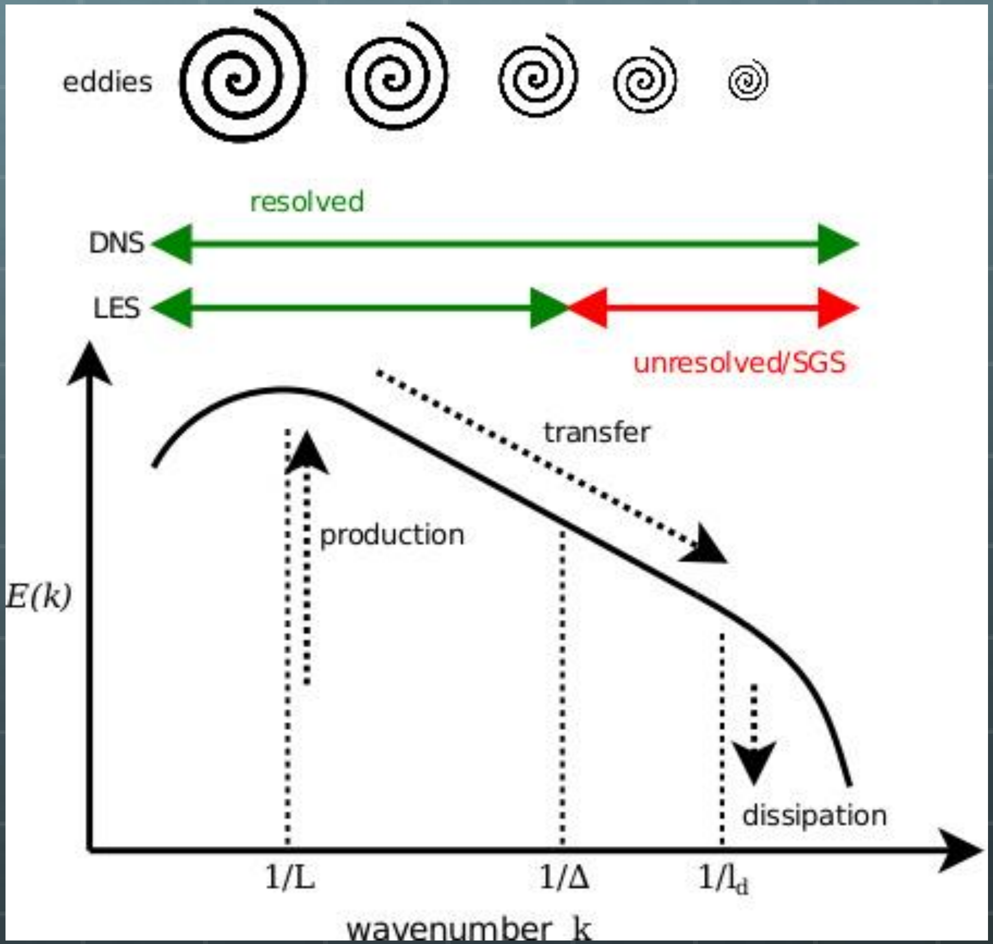
Flux of chemical species: Flux = $\overline{\rho V} = (\bar{\rho}\,\bar{V} + \overline{\rho' V'})$

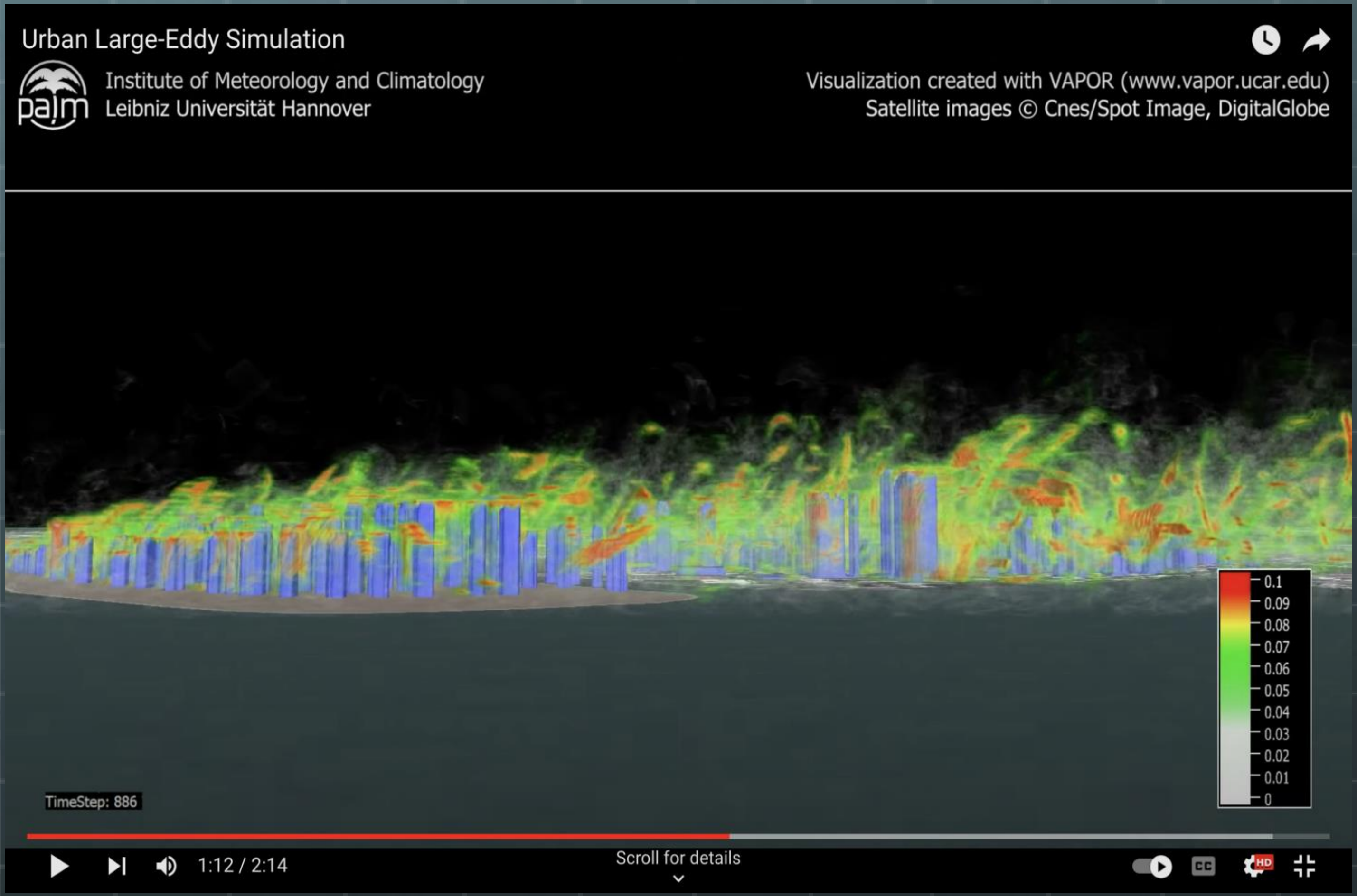
Parameterization $\overline{\rho' V'} \div -\boldsymbol{K}\,\nabla\rho$

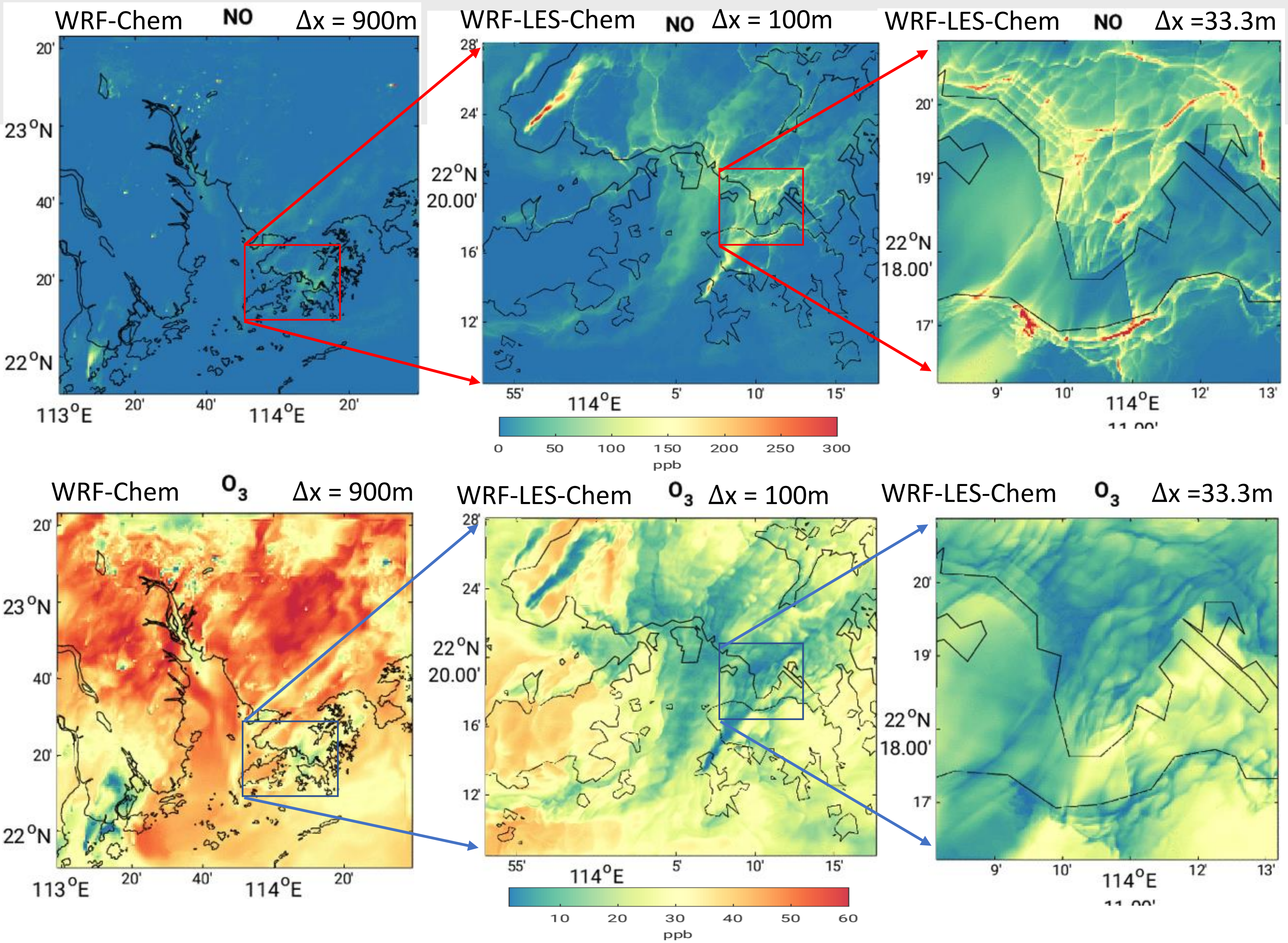
Reaction between A and B: $A + B \rightarrow C$

Mean chemical rate: $k\overline{AB} = k\bar{A}\,\bar{B} + k\overline{A'B'}$

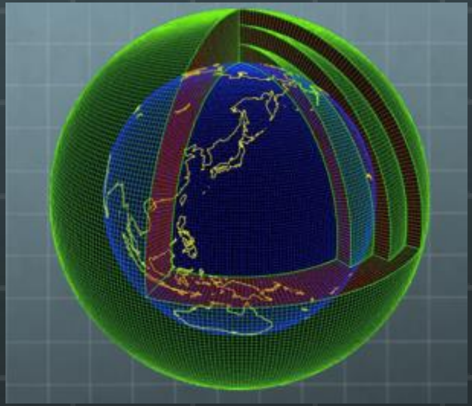
Treating Turbulence: Large Eddy Simulations for high-resolution boundary layer simulations



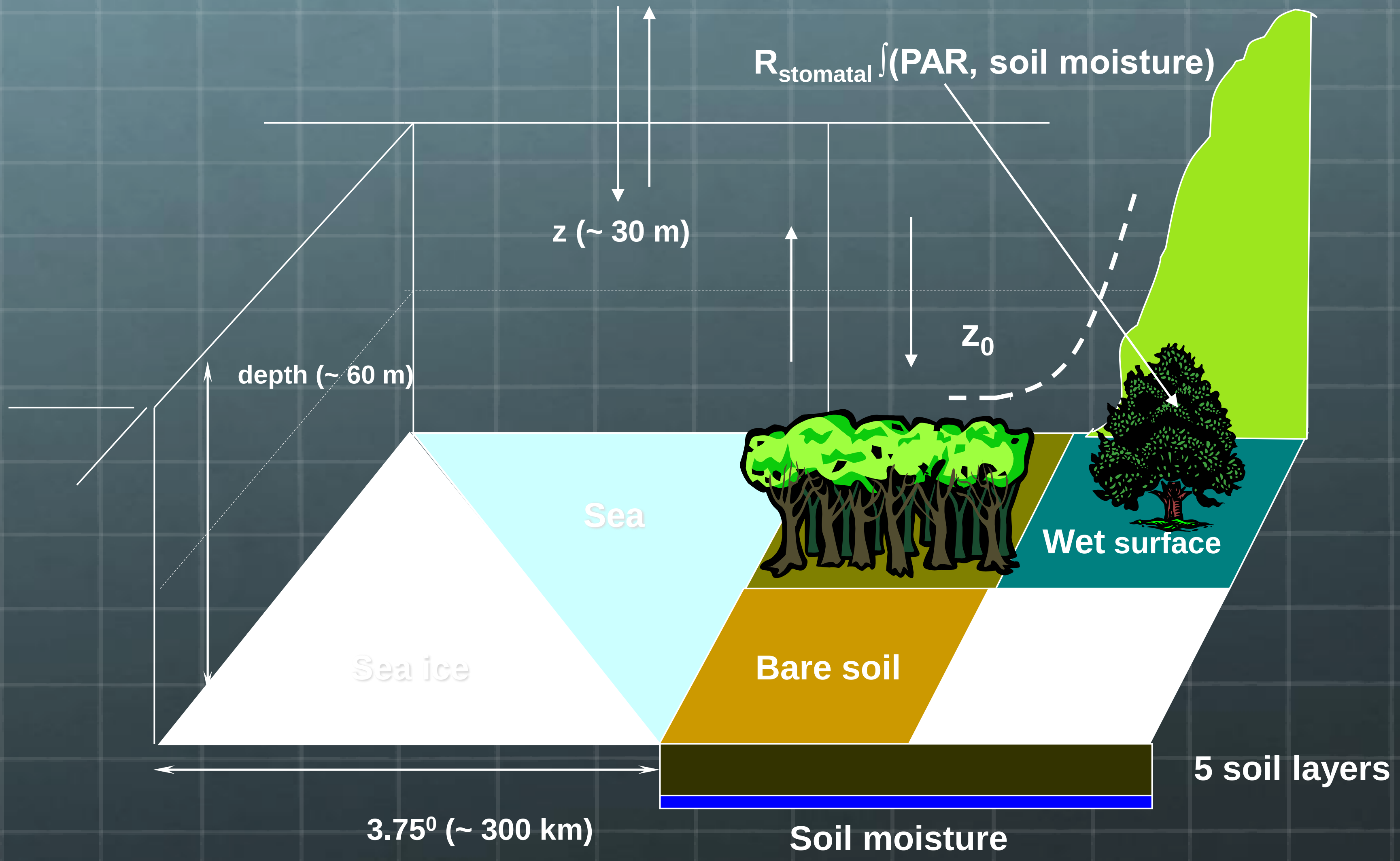



WRF-Chem NO Δx = 900m
WRF-LES-Chem NO Δx = 100m
WRF-LES-Chem NO Δx =33.3m
ppb
WRF-Chem O3 Δx = 900m
WRF-LES-Chem O3 Δx = 100m
WRF-LES-Chem O3 Δx =33.3m
ppb

8. Modeling of Surface Exchanges



Surface Exchanges: Representation of the Surface



8.1. Emissions

Emissions (1)

- In current models, emissions are typically specified as monthly mean mass fluxes with a spatial resolution of several kilometers.
- In contemporary models, natural emissions are often calculated from emission models (ex. wildfires)
- The compilation of emissions inventories is a labor-intensive task; these inventories constitute one of the major uncertainties in modeling.
- Attempts have been made to estimate “top-down” emissions based on satellite and in-situ observations and using „inverse“ models.

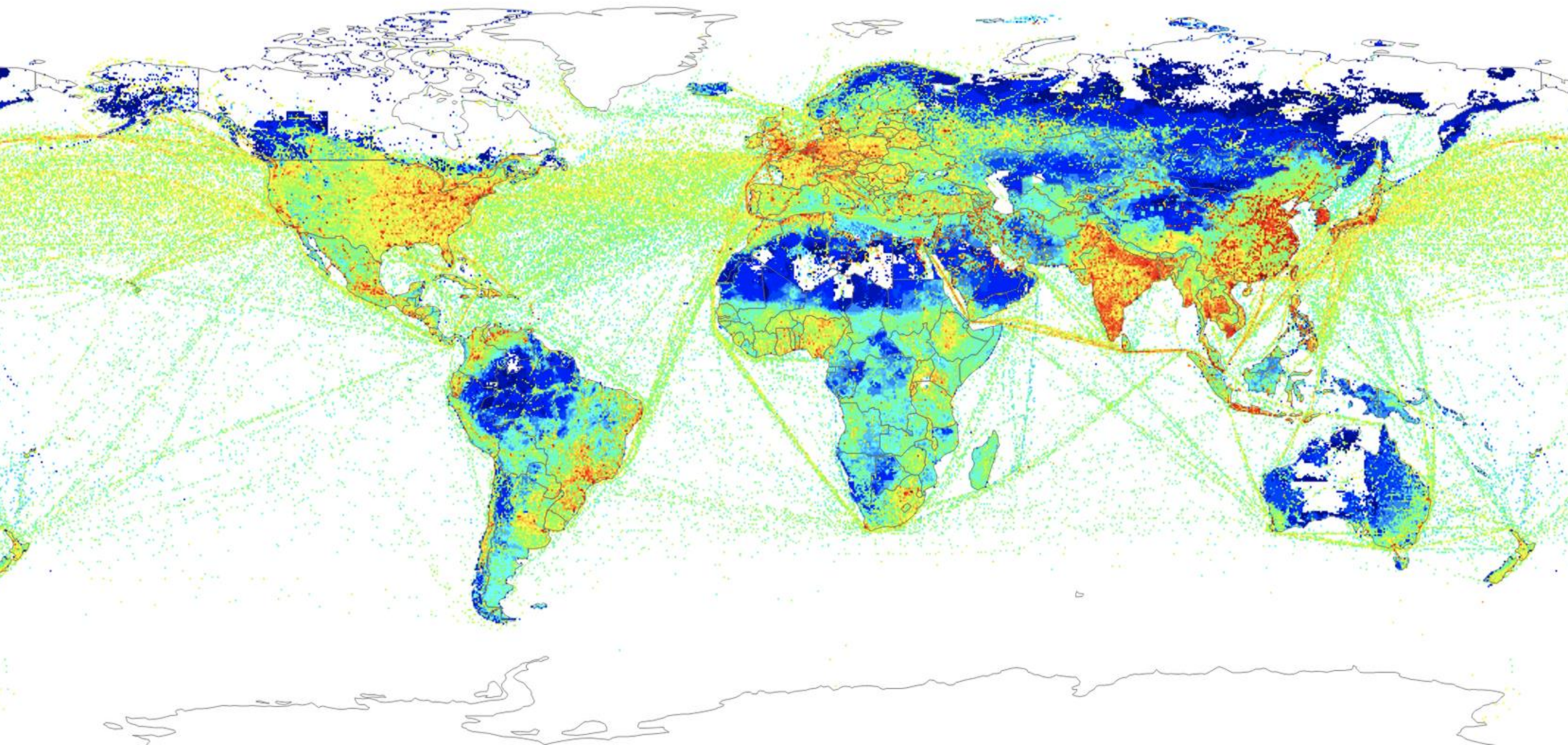
Emissions (2)

Typical categories of emissions inventories include:

- fossil fuel combustion
- biofuel combustion
- vegetation fires
- biogenic emissions (plants and soils)
- volcanic emissions
- oceanic emissions
- agricultural emissions (incl. fertilisation)

etc.

NOx Emissions



8.2. Dry Deposition

Dry Deposition

Transport of gaseous and particulate species from the atmosphere onto surfaces in the absence of precipitation

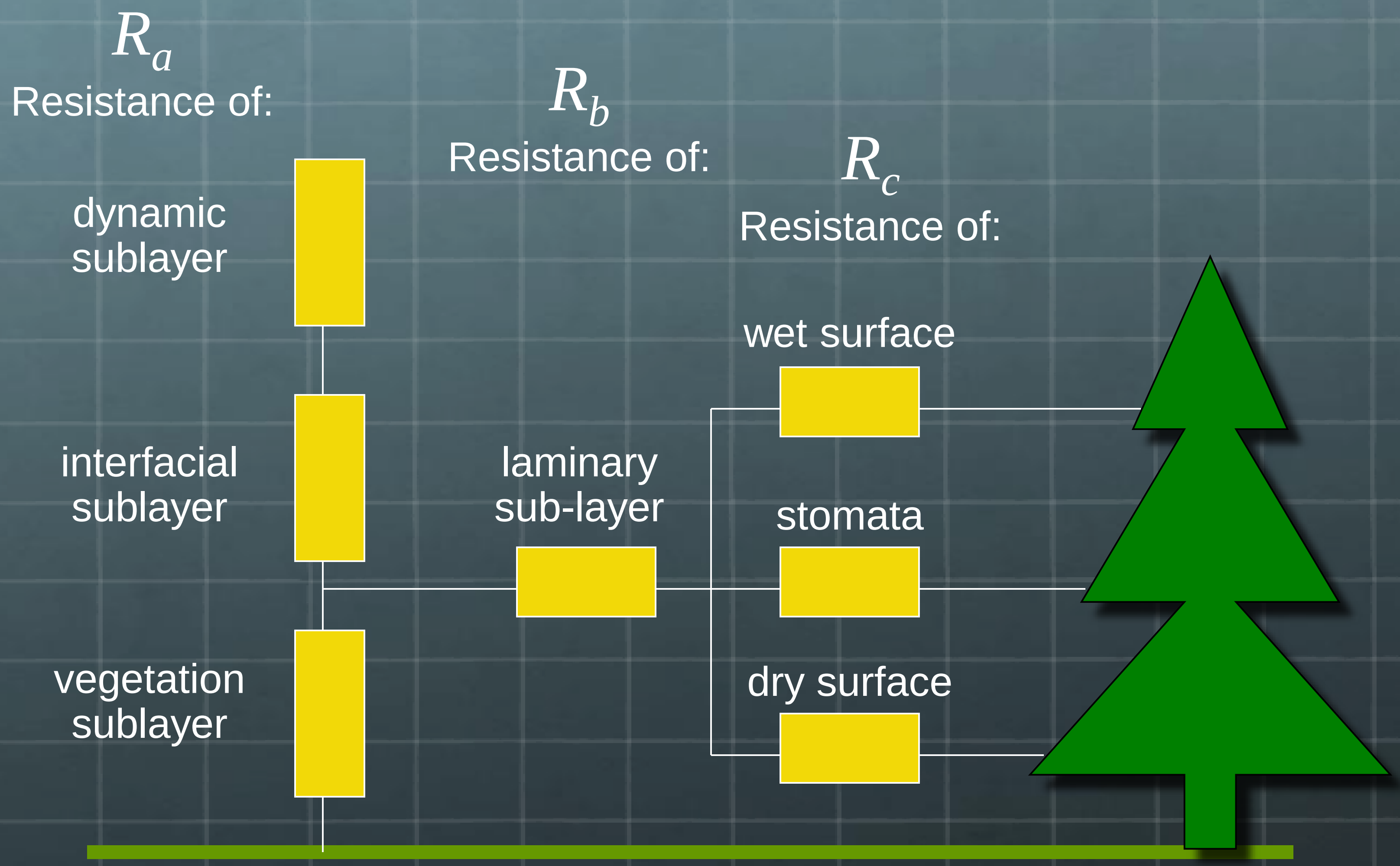
Controlling factors: atmospheric turbulence, chemical properties of species, and nature of the surface

Deposition flux: $$F = -v_d C$$

v_d: deposition velocity
C: concentration of species at reference height (~10 m)

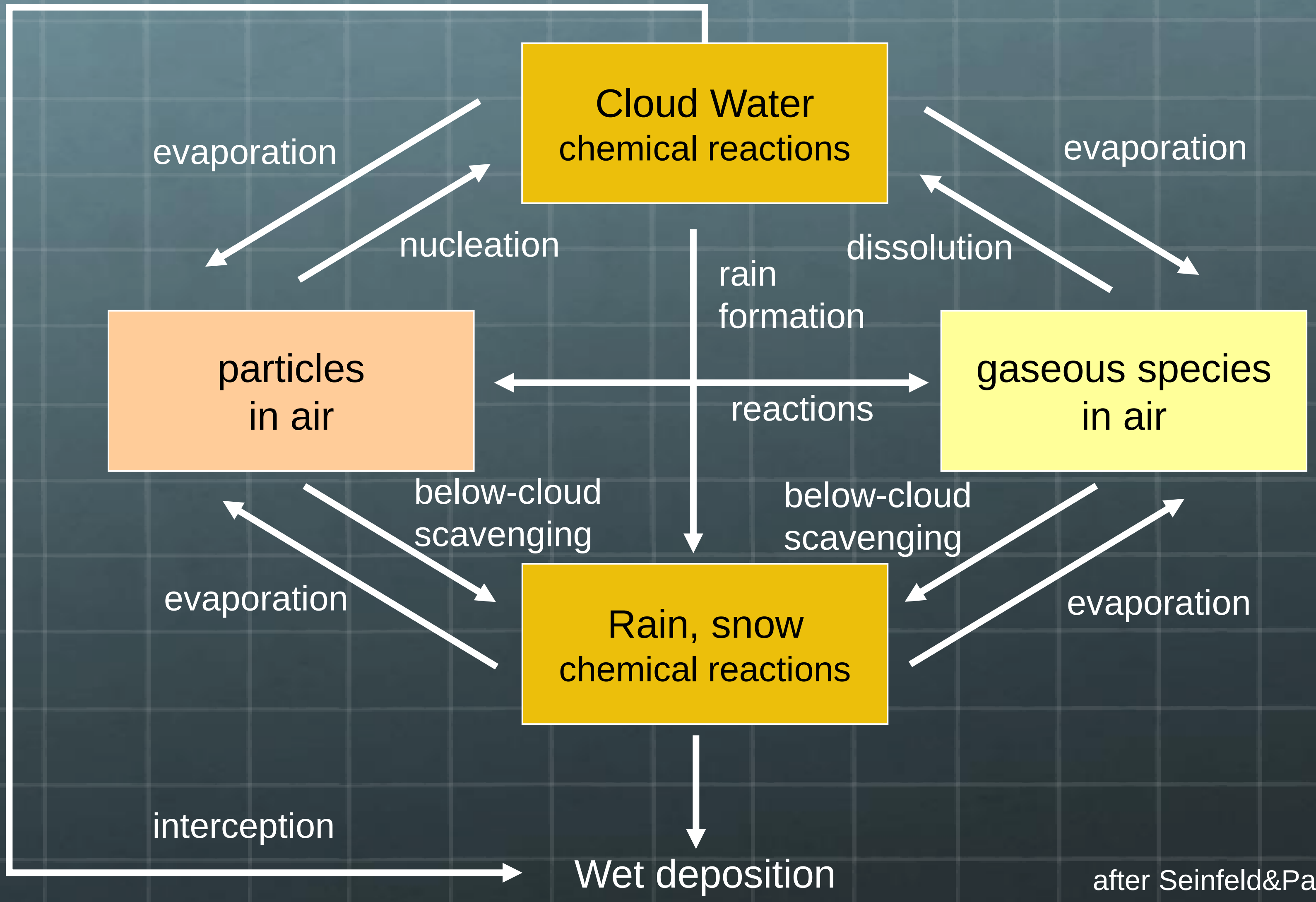
Dry deposition velocity

$$V_d = \frac{1}{R_a + R_b + R_c}$$



8.3. Wet Deposition

Wet deposition



after Seinfeld&Pandis, 1998

Thank You