Separating dynamics, physics and tracer transport grids in a global climate model

Peter Hjort Lauritzen

Atmospheric Modeling and Predictability Section
Climate and Global Dynamics Laboratory
National Center for Atmospheric Research

Workshop on Multiscale Modeling and its Applications:
From Weather and Climate Models to Models of Materials Defects
April 24, 2016
The Fields Institute, Toronto

NCAR UCAR | National Center for Atmospheric Research Climate & Global Dynamics climate • models • society

Thanks to my collaborators

Internal collaborators

Computational & Information Systems Laboratory

R. Kelly (Consulting Services Group)
R.D. Nair (Institute for Mathematics Applied to Geosciences)
J. Dennis (Application Scalability and Performance Group)

NCAR UCAR | National Center for Atmospheric Research
Climate & Global Dynamics — climate • models • society

S. Goldhaber (Atmospheric Modeling & Predictability Section)

National Center for Atmospheric Research
Atmospheric Chemistry Observations & Modeling

J.-F. Lamarque & A. Conley
(Atmospheric Chemistry Observations & Modeling Laboratory)

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

External collaborators

M.A. Taylor (Sandia National Laboratories)
P.A. Ullrich (University of California, Davis)
T. Dubos (École Polytechnique , France)
C. Erath (Technische Universität Darmstadt, Germany)
J. Overfelt (Sandia National Laboratories)

NCAR UCAR | National Center for Atmospheric Research
Climate & Global Dynamics — climate • models • society

Overview

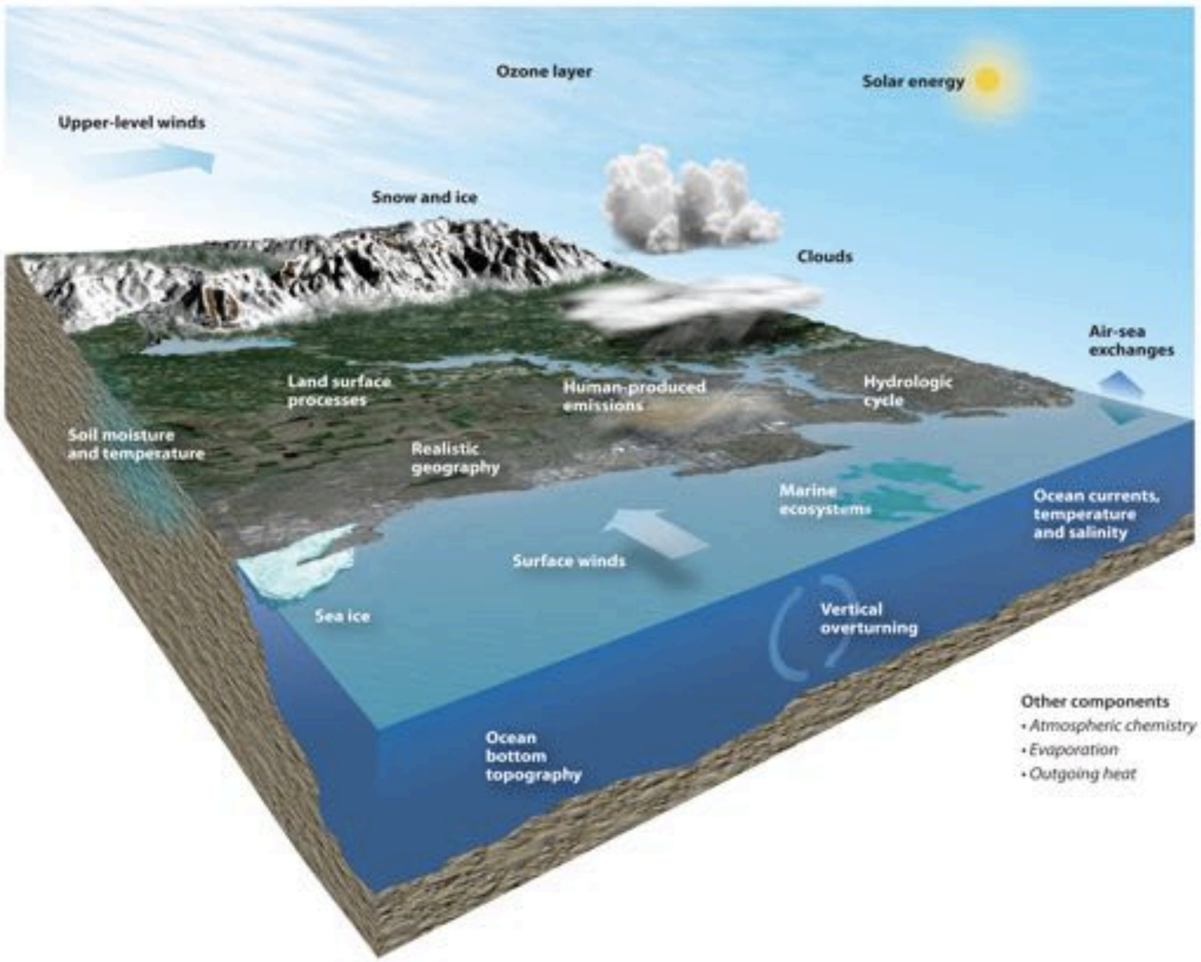
1. Long introduction

- **NCAR global climate model applications**
- **Define dynamical core and physics**
- **Physics-dynamics coupling**
- **Conservation from a climate modelers perspective!**

2. Separating dynamics and tracer grids (motivated by efficiency and accuracy concerns)

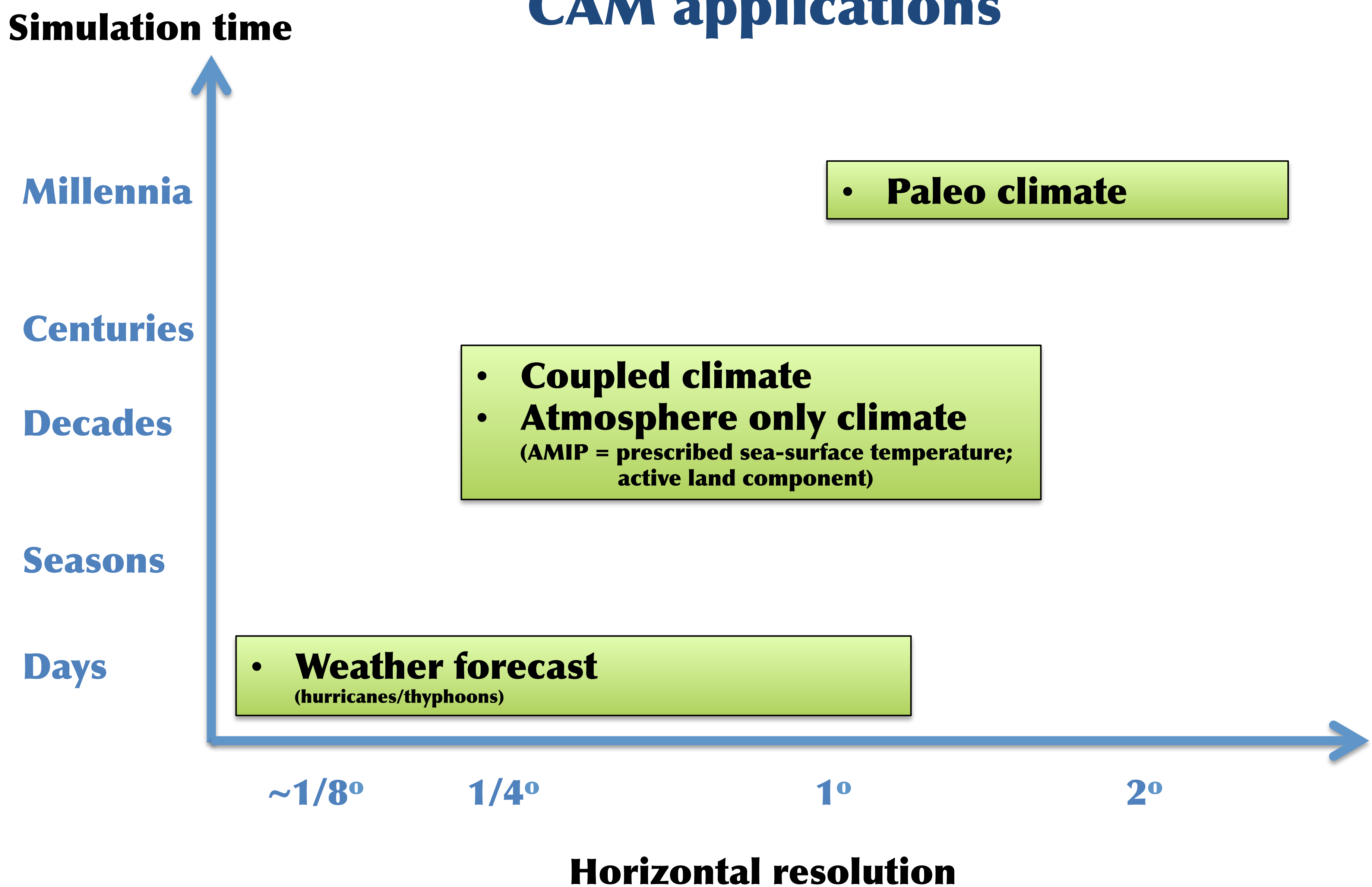
3. Separating physics and dynamics grids

Setting the stage: NCAR's CESM
(Community Earth System Model)

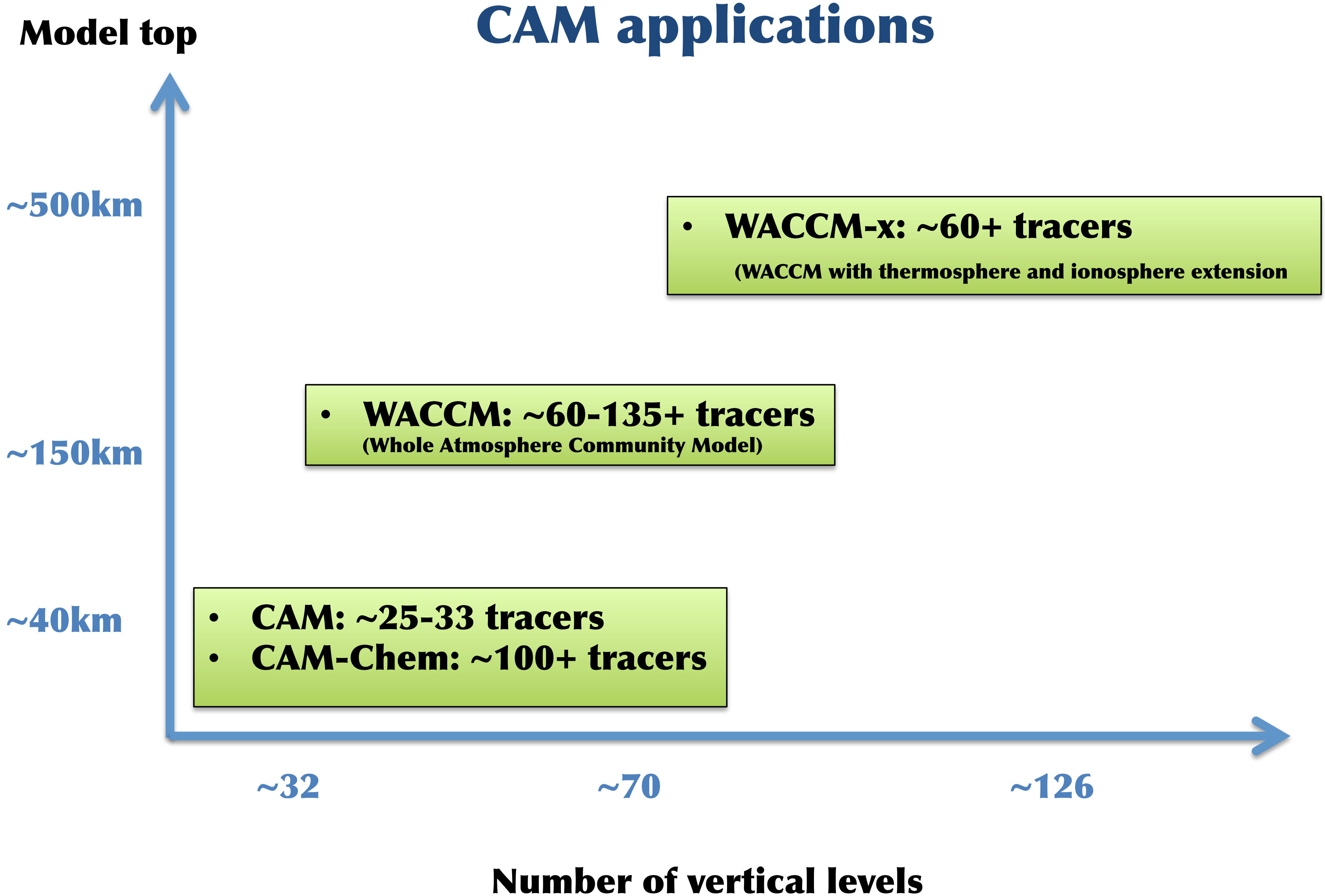


Community Atmosphere Model (CAM)

CAM applications



CAM applications



Separation of scales in CAM

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t} + (\zeta + f)\,\hat{k}\times\vec{u} + \nabla\left(\frac{1}{2}\vec{u}^2 + \Phi\right) + \frac{1}{\rho}\nabla p = \nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T - \frac{1}{c_p\rho}\omega = \nu\nabla^4 T,,$$

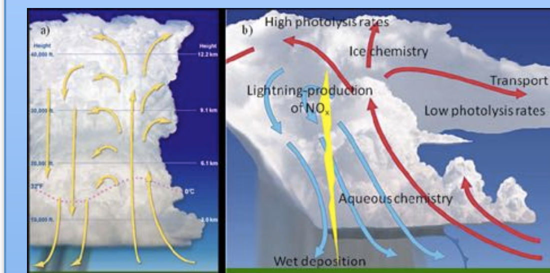
$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right) = \nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right) = \nu\nabla^4\left(m_i\right), \quad i = v, cl, ci, \ldots$$

Approximates the solution to the adiabatic equations of motion:

- **Momentum (u,v)**
- **Thermodynamic equation (T)**
- **Continuity equation for air (p)**
- **Continuity equation for**
  - **forms of water (water vapor, cloud liquid, cloud ice, rain, …)**
  - **quantities needed to represent aerosols**
  - **chemical species**

Physics module



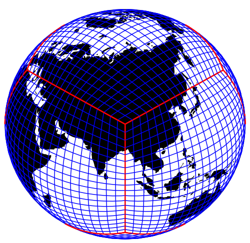
Radiation
Boundary layer turbulence
Orographic drag
Shallow and deep convection
Aerosol processes
Vertical mixing
…

Physics-dynamics coupling layer

Separation of scales in CAM

"Workhorse" dynamical core in CAM is **CAM-FV** (Lin, 2004).

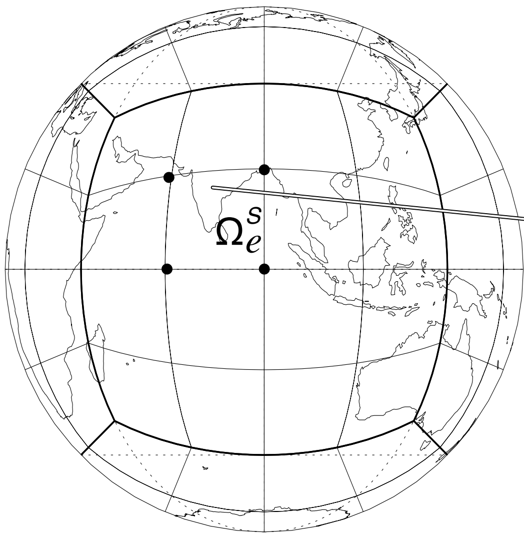
To improve CAM scalability the spectral-element (SE) dynamical core was implemented/imported into CAM (NCAR/DOE) - referred to as **CAM-SE**.



- quantities needed to represent aerosols
- chemical species

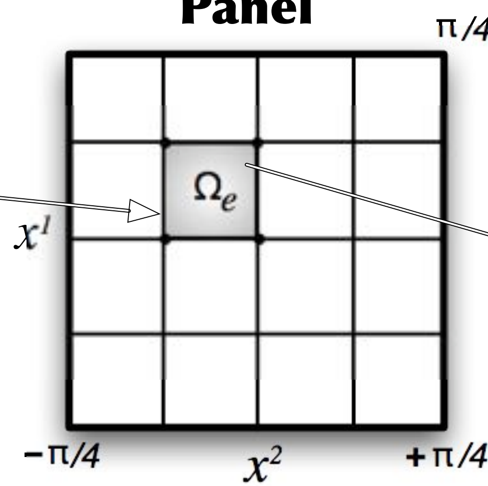
Physics-dynamics coupling layer

The spectral-element method: discretization grid



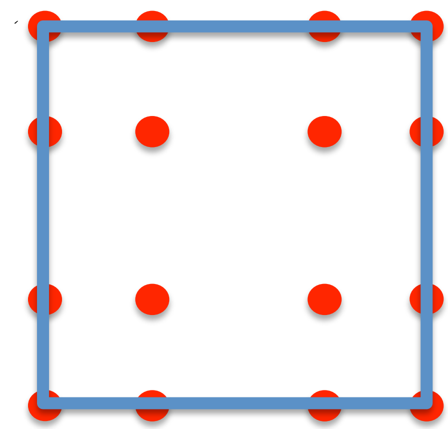
Physical Domain

Panel



Computational Domain

Element



GLL Quadrature Grid

Nodal 1D polynomial basis functions

GLL=Gauss-Lobatto-Legendre

The spectral-element method: discretization grid

Panel π/4 **Element**

For any arbitrary variable f (e.g., T, u, v, p, ...) one can approximate f as a function of a tensor product of 1D basis functions on the 2D GLL grid:

$$f(x,y) = \sum_{i,j} f_{i,j} h_i(x_i) h_j(y_j),$$

where $f_{i,j}$ is grid point values of f.

Physical Domain Computational Domain GLL Quadrature Grid

Nodal 1D polynomial basis functions

GLL=Gauss-Lobatto-Legendre

Separation of scales in CAM

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t} + (\zeta + f)\,\hat{k}\times\vec{u} + \nabla\left(\frac{1}{2}\vec{u}^2 + \Phi\right) + \frac{1}{\rho}\nabla p = \nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T - \frac{1}{c_p\rho}\omega = \nu\nabla^4 T, ,$$

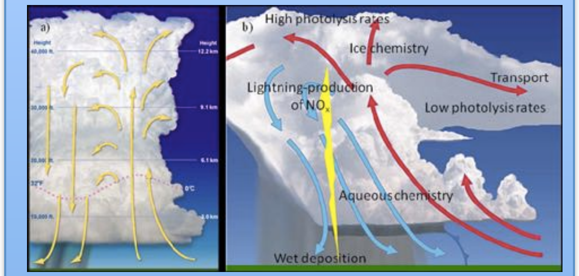
$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right) = \nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right) = \nu\nabla^4\left(m_i\right), \quad i = v, cl, ci, ...$$

Approximates the solution to the adiabatic equations of motion:

- **Momentum (u,v)**
- **Thermodynamic equation (T)**
- **Continuity equation for air (p)**
- **Continuity equation for**
  - **forms of water (water vapor, cloud liquid, cloud ice, rain, …)**
  - **quantities needed to represent aerosols**
  - **chemical species**

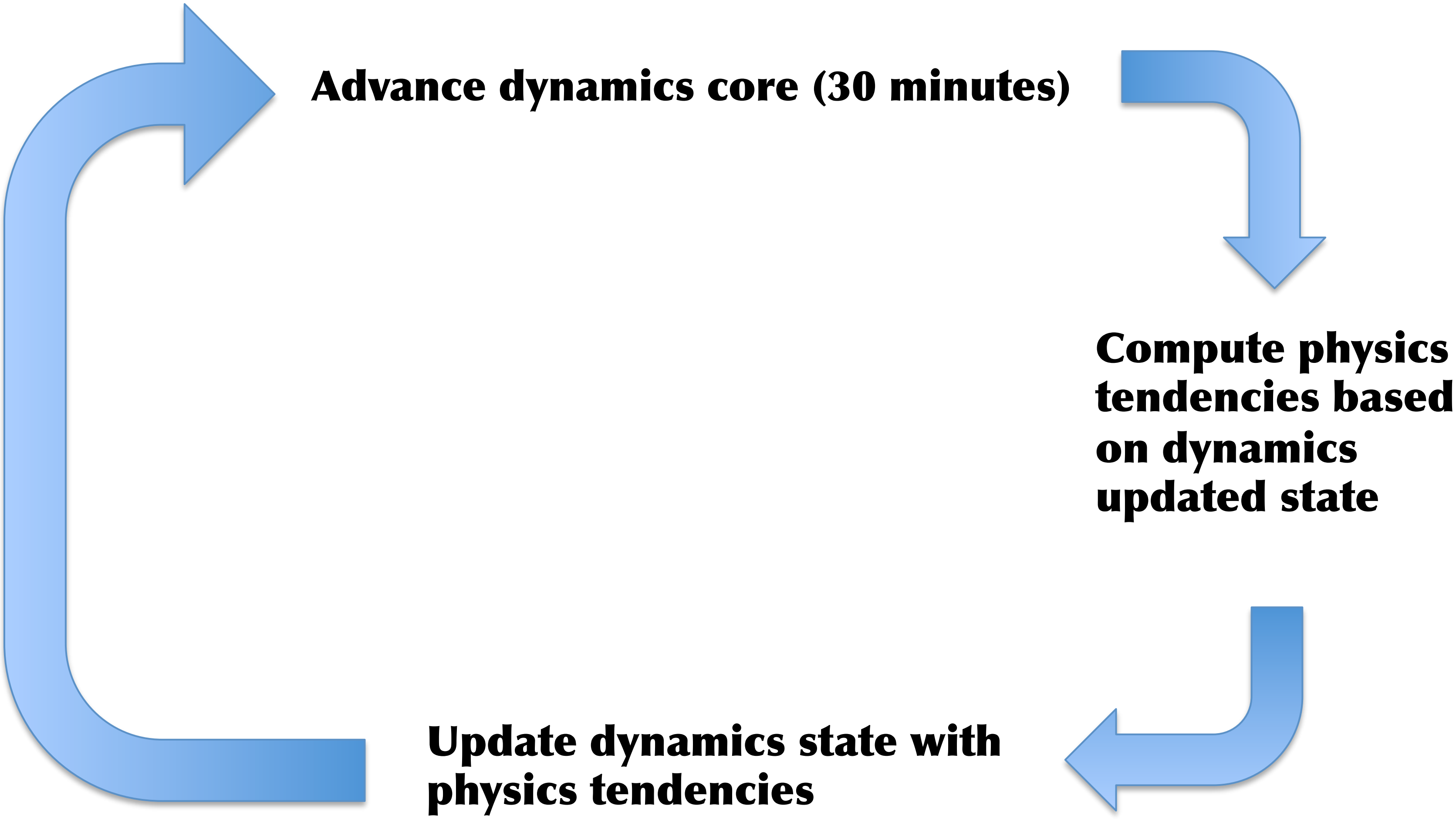
Physics module



Radiation
Boundary layer turbulence
Orographic drag
Shallow and deep convection
Aerosol processes
Vertical mixing
….

Physics-dynamics coupling layer

Physics dynamics coupling methods



Physics dynamics coupling methods

Advance dynamics core (30 minutes)

Compute physics tendencies based on dynamics updated state

Update dynamics state with physics tendencies

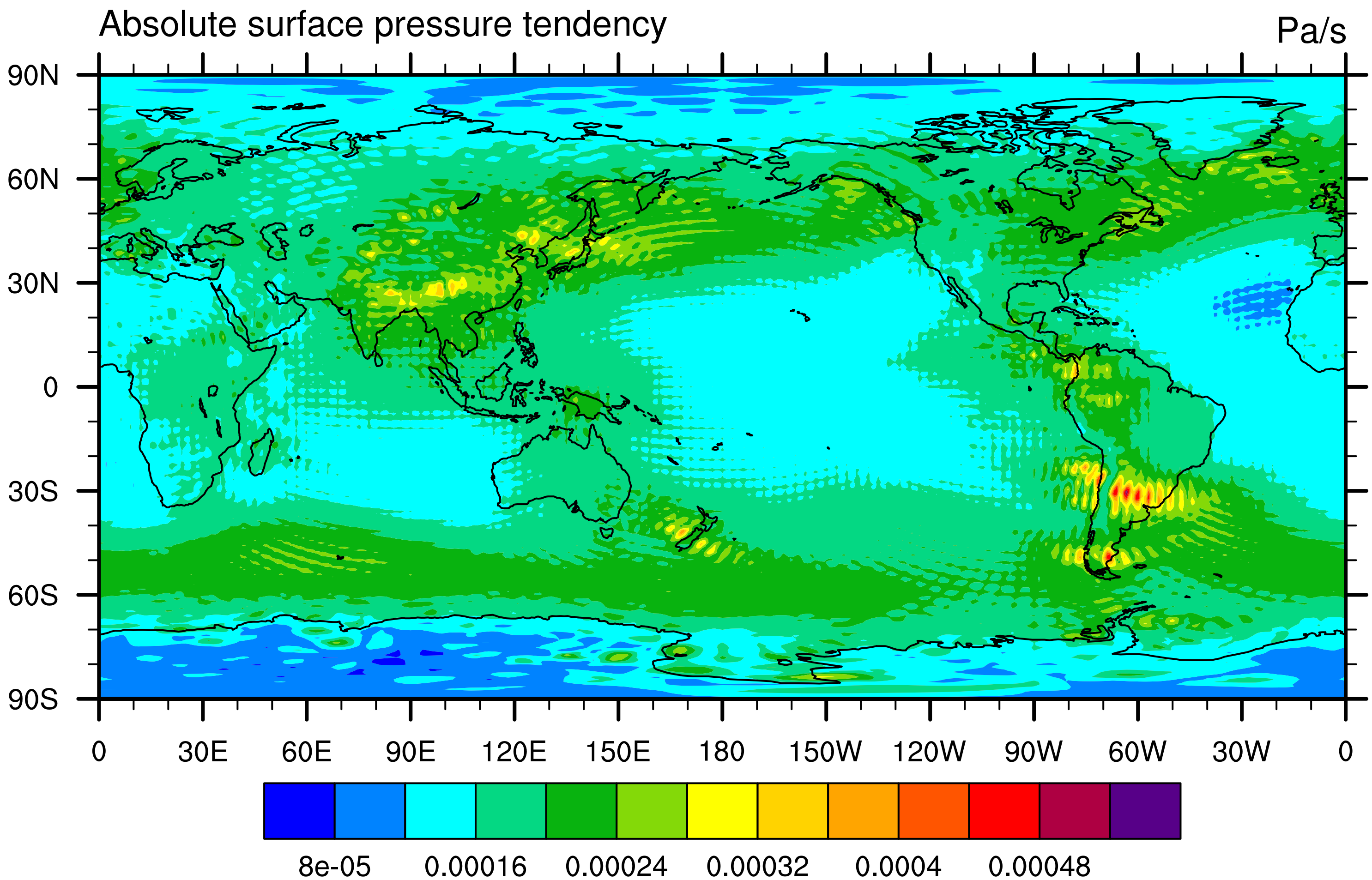
For long physics time-steps and less diffusive dynamical cores this can create spurious noise!

Noise can be detected by computing

$$\frac{d}{dt}|p_s|$$

Physics dynamics coupling methods

10 year average of $\frac{d}{dt}|p_s|$ from AMIP run



Physics dynamics coupling methods

Advance dynamics core (30 minutes): add physics tendency "chunks" during the dynamics time-stepping - every 15 minutes in this example (I refer to it as "dribbling")

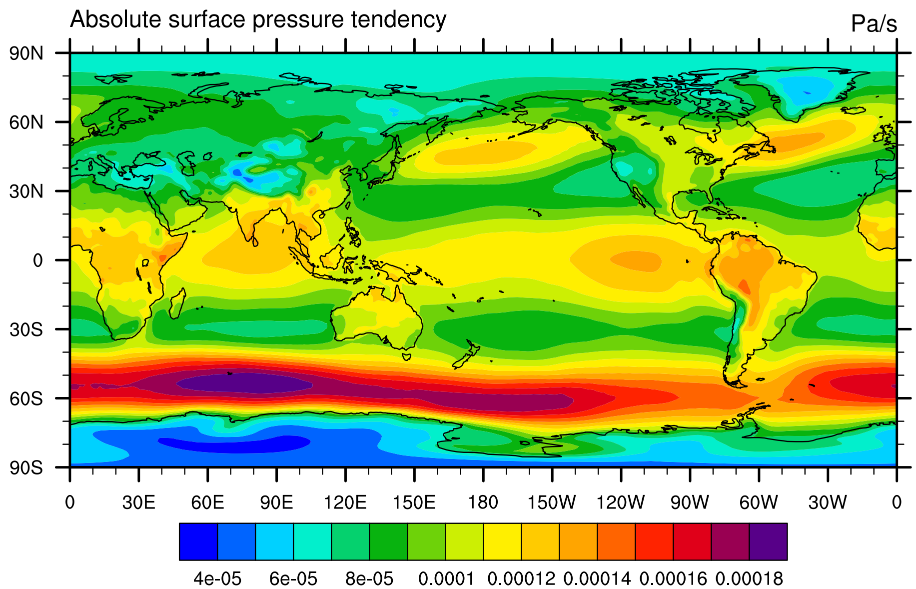
Compute physics tendencies based on dynamics updated state

Split physics tendencies into a number of "chunks"

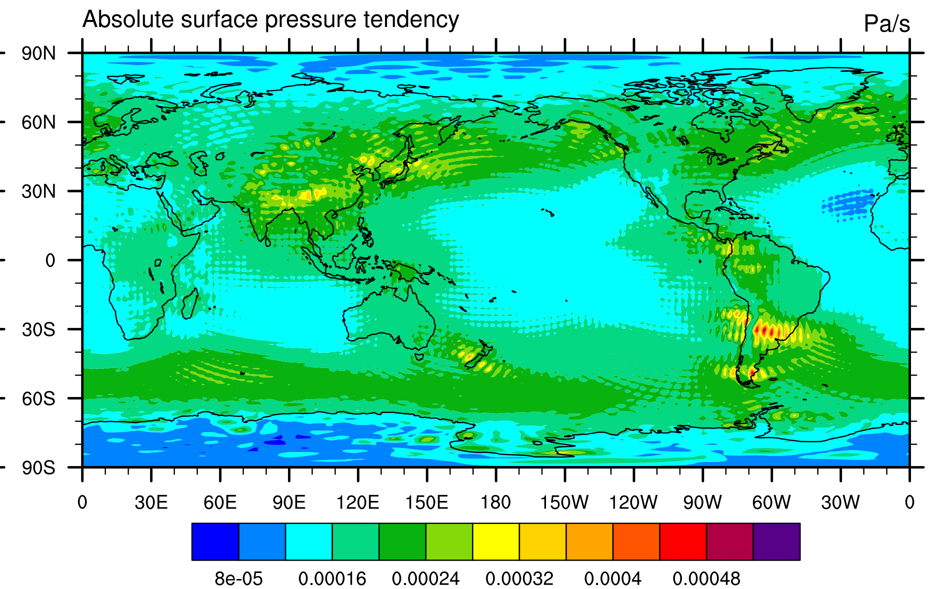
Physics dynamics coupling methods

10 year average of $\frac{d}{dt}|p_s|$ **from AMIP run**

"Dribbling" physics tendencies



State updated every 30 minutes



Separation of scales in CAM

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t} + (\zeta + f)\,\hat{k}\times\vec{u} + \nabla\left(\frac{1}{2}\vec{u}^2 + \Phi\right) + \frac{1}{\rho}\nabla p = \nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T - \frac{1}{c_p\rho}\omega = \nu\nabla^4 T,,$$

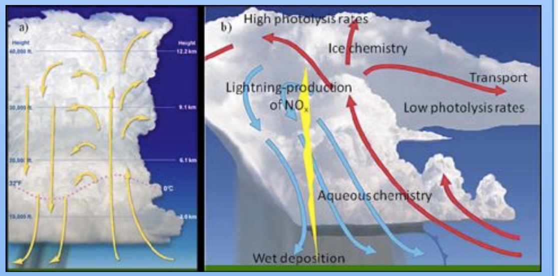
$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right) = \nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right) = \nu\nabla^4\left(m_i\right), \quad i = v, cl, ci, \ldots$$

Approximates the solution to the adiabatic equations of motion:

- **Momentum (u,v)**
- **Thermodynamic equation (T)**
- **Continuity equation for air (p)**
- **Continuity equation for**
  - **forms of water (water vapor, cloud liquid, cloud ice, rain, …)**
  - **quantities needed to represent aerosols**
  - **chemical species**

Physics module



Radiation
Boundary layer turbulence
Orographic drag
Shallow and deep convection
Aerosol processes
Vertical mixing

Physics-dynamics coupling layer

Separation of scales in CAM

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t} + (\zeta + f)\,\hat{k}\times\vec{u} + \nabla\left(\frac{1}{2}\vec{u}^2 + \Phi\right) + \frac{1}{\rho}\nabla p = \nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T - \frac{1}{c_p\rho}\omega = \nu\nabla^4 T,,$$

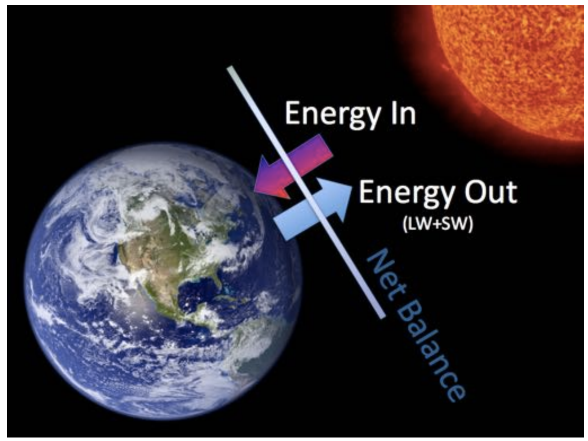
$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right) = \nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right) = \nu\nabla^4\left(m_i\right), \quad i = v, cl, ci, \ldots$$

Approximates the solution to the adiabatic equations of motion:

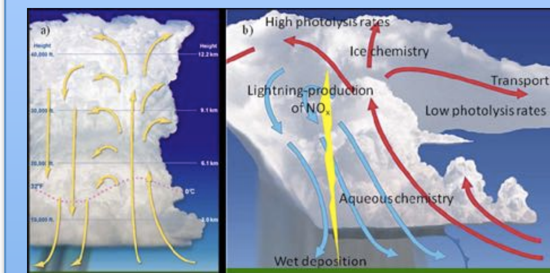
- **Momentum (u,v)**
- **Thermodynamic equation (T)**
- **Continuity equation for air (p)**
- **Continuity equation for**
  - **- forms of water (water vapor, cloud liquid, cloud ice, rain, …)**
  - **- quantities needed to represent aerosols**
  - **- chemical species**

Balancing energy and mass budgets is very very important



Physics-dynamics coupling layer

Physics module



Radiation
Boundary layer turbulence
Orographic drag
Shallow and deep convection
Aerosol processes
Vertical mixing

Aside: Energy conservation

For a coupled climate model total energy conservation is important (otherwise climate will drift)

=> Need to satisfy

$$\frac{d}{dt}\left(K + c_p T + \Phi\right) = \frac{1}{\rho}\frac{\partial p}{\partial t} + F_{net}$$

where K kinetic energy, \rho is density, p pressure, T temperature, \Phi geopotential height and F_{net} are net fluxes computed by parameterization (e.g., heating and momentum forcing).

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t} + (\zeta + f)\,\hat{k}\times\vec{u} + \nabla\left(\frac{1}{2}\vec{u}^2 + \Phi\right) + \frac{1}{\rho}\nabla p = \nu\nabla^4\vec{u},$$

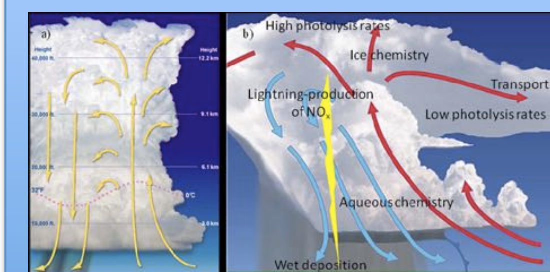
$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T - \frac{1}{c_p\rho}\omega = \nu\nabla^4 T,,$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right) = \nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right) = \nu\nabla^4\left(m_i\right), \quad i = v, cl, ci, \ldots$$

Physics-dynamics coupling layer

Physics module



...ide: Energy conservation

Frictional heating rate is calculated from K energy tendency produced from momentum diffusion and added to T

For a coupled climate model total energy conservation is important (otherwise climate will drift)

=> Need to satisfy

$$\frac{d}{dt}\left(K+c_pT+\Phi\right)=\frac{1}{\rho}\frac{\partial p}{\partial t}+F_{net}$$

where K kinetic energy, \rho is density, p pressure, T temperature, \Phi geopotential height and F_{net} are net fluxes computed by parameterization (e.g., heating and momentum forcing).

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t}+(\zeta+f)\,\hat{k}\times\vec{u}+\nabla\left(\frac{1}{2}\vec{u}^2+\Phi\right)+\frac{1}{\rho}\nabla p=\nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t}+\vec{u}\cdot\nabla T-\frac{1}{c_p\rho}\omega=\nu\nabla^4 T,,$$

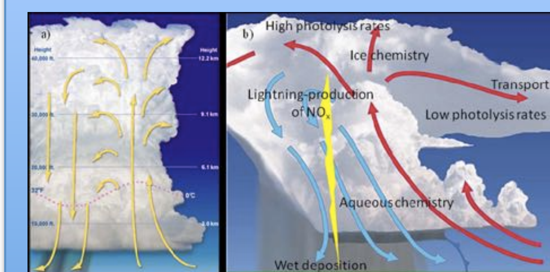
$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right)+\nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right)=\nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right)+\nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right)=\nu\nabla^4\left(m_i\right),\quad i=v,cl,ci,...$$

The dynamical core may not conserve energy due to inherent numerical dissipation, non-conservation due to time truncation errors, etc.

Physics-dynamics coupling layer

Physics module



Aside: Energy conservation

For a coupled climate model total energy conservation is important (otherwise climate will drift)

=> Need to satisfy

$$\frac{d}{dt}\left(K+c_pT+\Phi\right)=\frac{1}{\rho}\frac{\partial p}{\partial t}+F_{net}$$

where K kinetic energy, \rho is density, p pressure, T temperature, \Phi geopotential height and F_{net} are net fluxes computed by parameterization (e.g., heating and momentum forcing).

Note that weather model parameterizations do not conserve total energy

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t} + (\zeta + f)\,\hat{k}\times\vec{u} + \nabla\left(\frac{1}{2}\vec{u}^2 + \Phi\right) + \frac{1}{\rho}\nabla p = \nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T - \frac{1}{c_p\rho}\omega = \nu\nabla^4 T,,$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right) = \nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right) + \nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right) = \nu\nabla^4\left(m_i\right), \quad i = v, cl, ci, \ldots$$

The dynamical core may not conserve energy due to inherent numerical dissipation, non-conservation due to time truncation errors, etc.

Physics-dynamics coupling layer

Physics module

CAM physics does not change surface pressure – under that assumption each paramerization conserves energy (i.e. energy change due to state variables changing is exactly balanced by net fluxes).

However, changes in water variables does change pressure => When pressure is updated energy conservation is violated

Aside: Energy conservation

For a coupled climate model total energy conservation is important (otherwise climate will drift)

=> Need to satisfy

$$\frac{d}{dt}\left(K+c_pT+\Phi\right)=\frac{1}{\rho}\frac{\partial p}{\partial t}+F_{net}$$

where K kinetic energy, \rho is density, p pressure, T temperature, \Phi geopotential height and F_{net} are net fluxes computed by parameterization (e.g., heating and momentum forcing).

Energy conservation can be violated in physics-dynamics coupling if the physics tendencies are added during the time-stepping (underlying pressure changes!)

Note that weather model parameterizations do not conserve total energy

Dynamical core module

$$\frac{\partial \vec{u}}{\partial t}+(\zeta+f)\,\hat{k}\times\vec{u}+\nabla\left(\frac{1}{2}\vec{u}^2+\Phi\right)+\frac{1}{\rho}\nabla p=\nu\nabla^4\vec{u},$$

$$\frac{\partial T}{\partial t}+\vec{u}\cdot\nabla T-\frac{1}{c_p\rho}\omega=\nu\nabla^4 T,,$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}\right)+\nabla\cdot\left(\frac{\partial p_d}{\partial \eta}\vec{u}\right)=\nu\nabla^4\left(\frac{\partial p_d}{\partial \eta}\right),$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p_d}{\partial \eta}m_i\right)+\nabla\cdot\left(\frac{\partial p_d}{\partial \eta}m_i\vec{u}\right)=\nu\nabla^4\left(m_i\right),\quad i=v,cl,ci,...$$

The dynamical core may not conserve energy due to inherent numerical dissipation, non-conservation due to time truncation errors, etc.

Physics-dynamics coupling layer

Physics module

CAM physics does not change surface pressure – under that assumption each paramerization conserves energy (i.e. energy change due to state variables changing is exactly balanced by net fluxes).

However, changes in water variables does change pressure => When pressure is updated energy conservation is violated

Aside: Energy budgets in CAM-SE

10 year averages from AMIP simulation (specified SSTs cycling over same year)

Dynamical core module

- **Rate of energy change due to explicit dissipation (hyperviscosity)**

  dE/dt = 0.0729 W/m^2

- **Frictional heating rate is calculated from K tendency produced from momentum diffusion and added to T:**

  dE/dt = 0.6997 W/m^2

- **Vertical remapping**

  dE/dt = -0.1547 W/m^2

Total loss of energy in dynamics

dE/dt = -0.0723 W/m^2

Rate of energy change due to "dribbling" physics tendencies in the dynamics

dE/dt = 0.056 W/m^2

Physics-dynamics coupling layer

Physics module

- **"physical" changes in energy due to water change**

  dE/dt = -0.0016 W/m^2

- **Change in energy due to change in pressure due to water vapor change ("dme_adjust")**

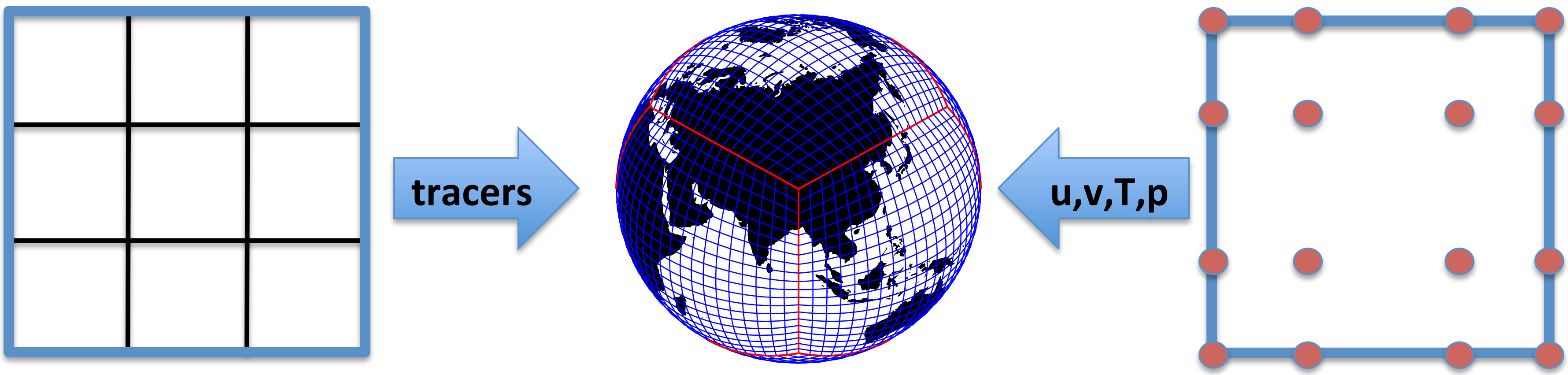
  dE/dt = 0.2667 W/m^2

- **Energy fixer**

  dE/dt = -0.1843

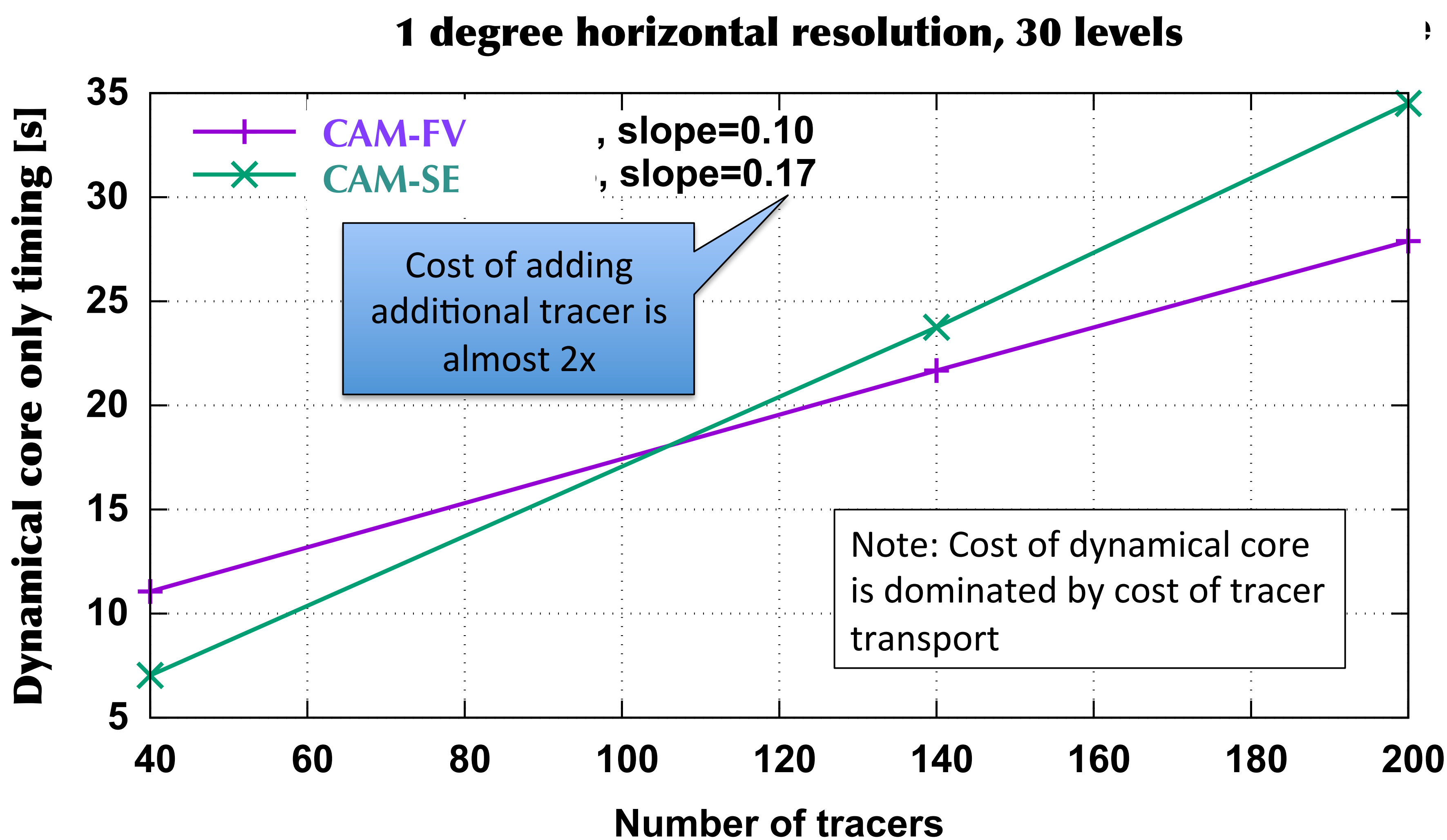
  (= loss in dynamics + dme_adjust)

Part I: separating transport and dynamics grids/methods in CAM-SE



Why?

Cost per additional tracer
(dynamical core timings using 1728 tasks)



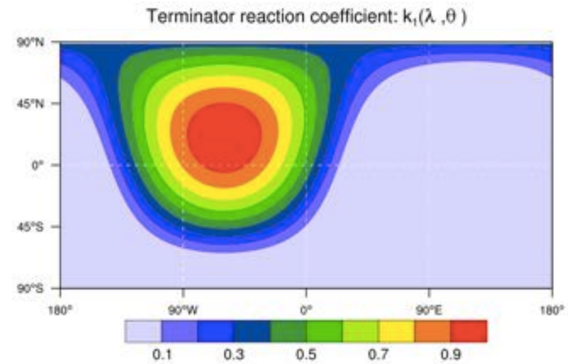
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

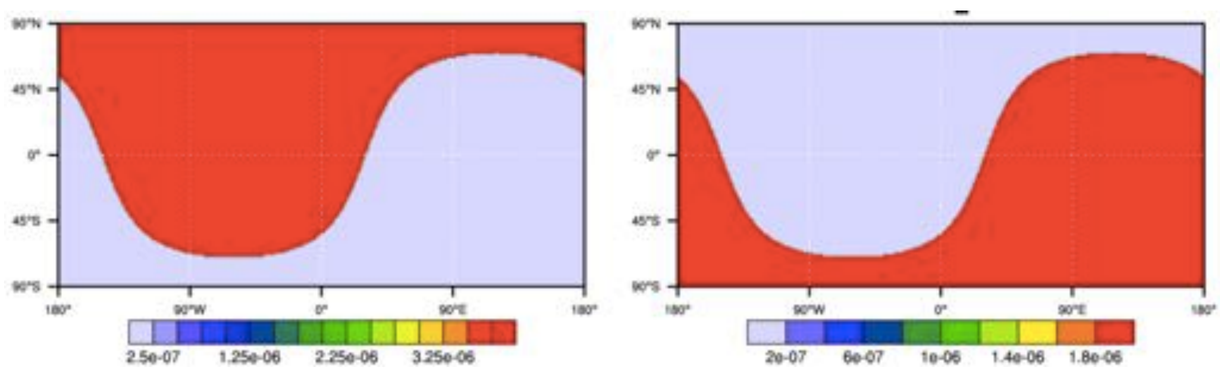
See: http://www.cgd.ucar.edu/cms/pel/terminator.html

- Consider 2 reactive chemical species, Cl and Cl_2 :

$$Cl_2 \rightarrow Cl + Cl : k_1$$
$$Cl + Cl \rightarrow Cl_2 : k_2$$



- Steady-state solution (no flow):

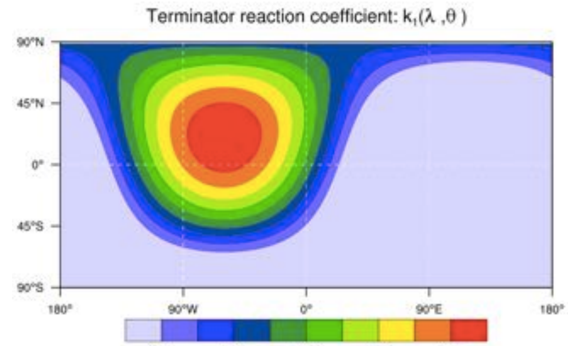


- In any flow-field Cl_y=Cl+2*Cl_2 should be constant at all times (correlation preservation)

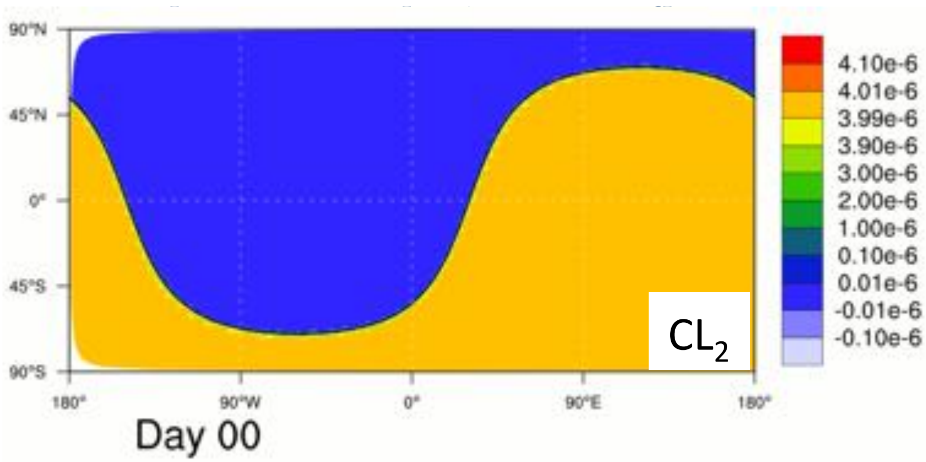
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

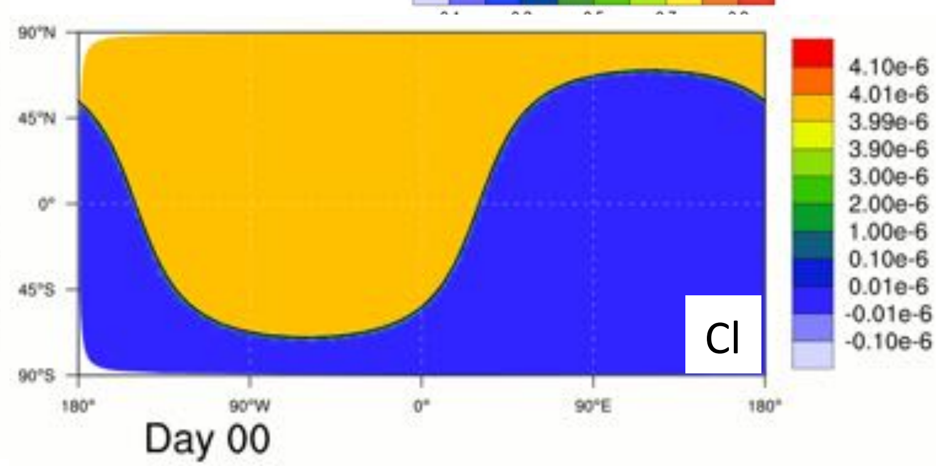
(Lauritzen et al., 2015)
See: http://www.cgd.ucar.edu/cms/pel/terminator.html

- Consider 2 reactive chemical species, Cl and Cl_2 :



$$Cl_2 \rightarrow Cl + Cl : k_1$$
$$Cl + Cl \rightarrow Cl_2 : k_2$$





- In any flow-field $Cl_y=Cl+2*Cl_2$ should be constant at all times (correlation preservation).

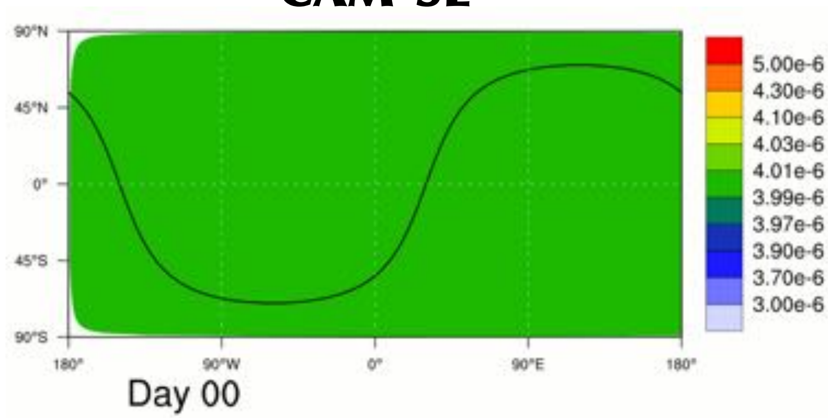
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

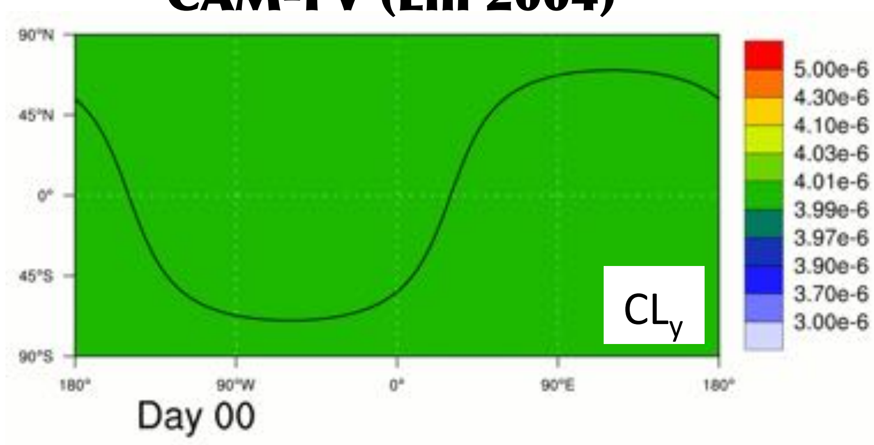
See: http://www.cgd.ucar.edu/cms/pel/terminator.html

Errors are due to non-conservation of linear correlations in tracer transport scheme and/or physics-dynamics coupling

CAM-SE



CAM-FV (Lin 2004)



- **In any flow-field $Cl_y = Cl + 2*Cl_2$ should be constant at all times (correlation preservation).**

Problem formulation

Improve the efficiency and accuracy of tracer transport in CAM-SE

Solution?

Note: It is easy to make an efficient model that is inaccurate or an accurate model that is inefficient (at least for smooth problems) …

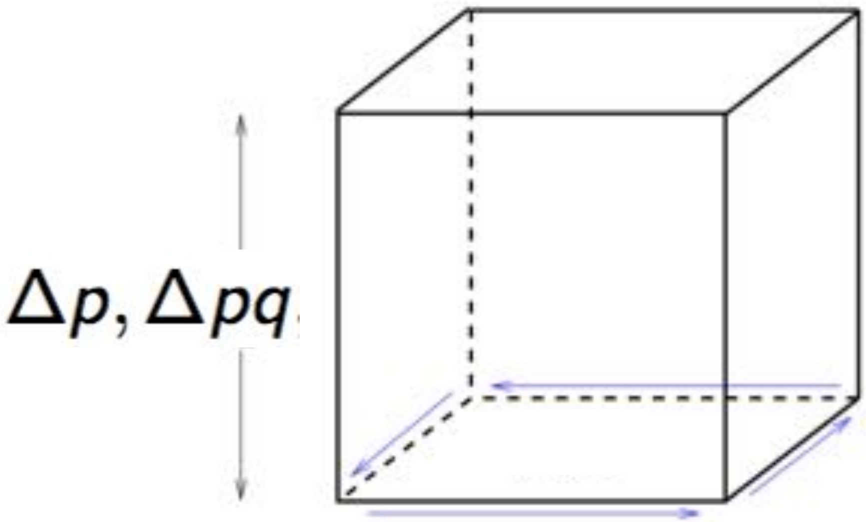
Tracer transport: Continuity equation

Consider the continuity equation of air mass (pressure level thickness Δp), and tracer mass (Δpq, where q mixing ratio)

$$\frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \vec{v}) = 0, \qquad \psi = \Delta p, \Delta pq,$$

respectively, where $\vec{v}$ wind vector.

No sources/ sinks



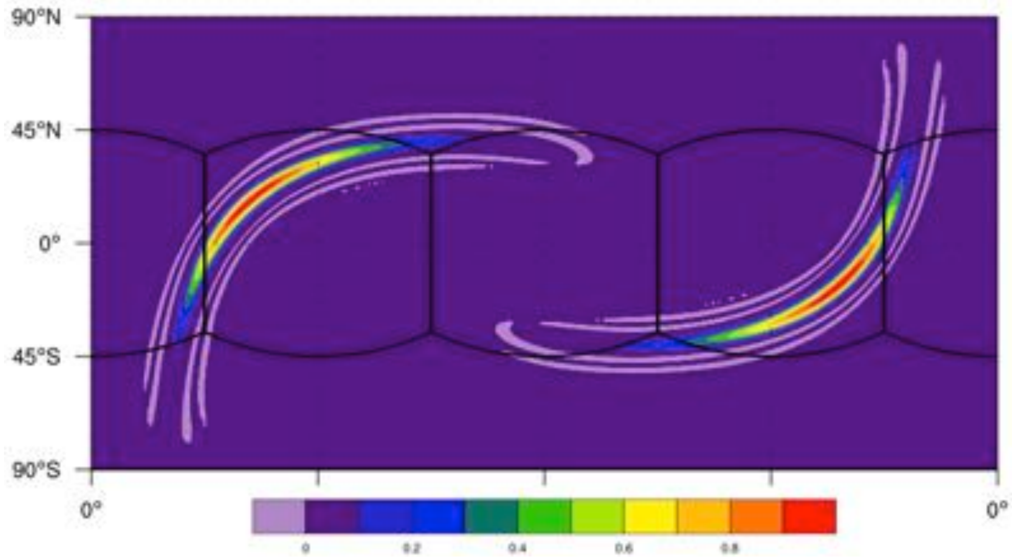
Requirements for transport schemes intended for global climate/climate-chemistry applications:

1. Global (and local) Mass-conservation

The solution to the continuity equation without sources/sinks must conserve mass. Very important!

2. Physical realizable solutions (shape-preservation)

Scheme must not produce new extrema (in particular negatives) in q



Example of unphysical solution

Requirements for transport schemes intended for global climate/climate-chemistry applications:

3. Preservation of functional relations between tracers

Transport scheme preserves $q_2 = f(q_1)$

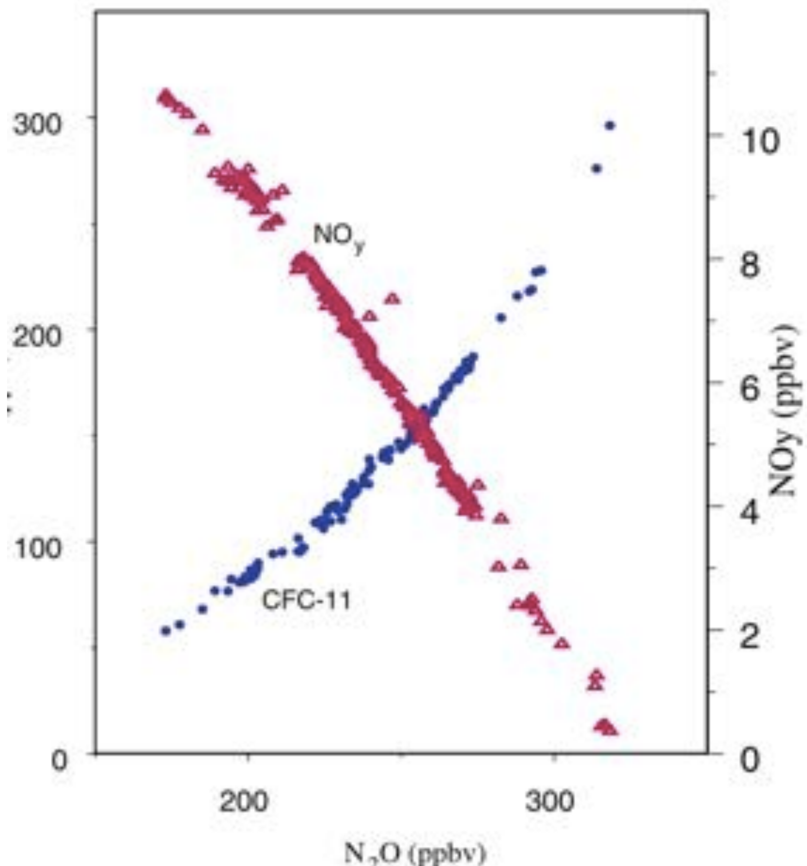


Figure: Aircraft observations of long-lived species in the stratosphere

Tracer transport scheme should not unphysically perturb these relations between tracers

Plumb (2007)

Requirements for transport schemes intended for global climate/climate-chemistry applications:

4. Consistency (tracer and air mass are coupled!)

Continuity equations for air mass and tracer mass:

$$\frac{\partial(\Delta p)}{\partial t} + \nabla \cdot (\Delta p \vec{v}) = 0, \quad (1)$$

$$\frac{\partial(\Delta p q)}{\partial t} + \nabla \cdot (\Delta p q \vec{v}) = 0, \quad (2)$$

If $q = 1$ then the transport scheme should reduce to the continuity equation for air.

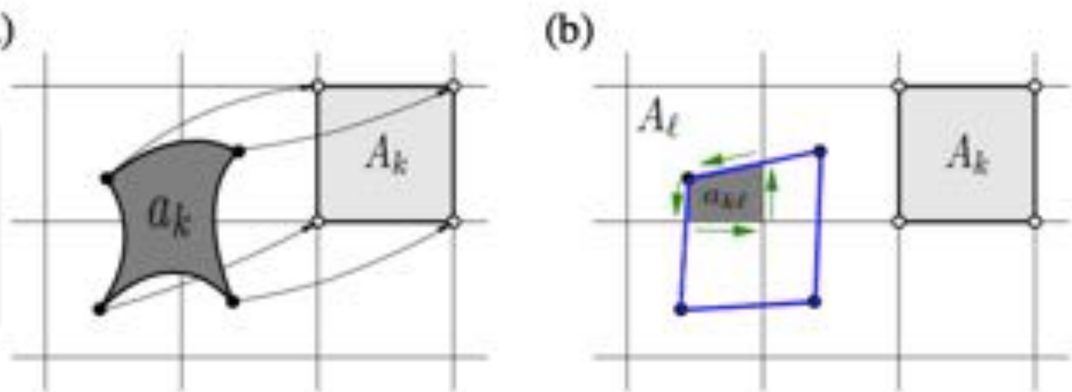
In model consistency is non-trivial if:

- **Using prescribed wind and mass fields from , e.g., re-analysis.**
- **(2) is solved with a different numerical method than (1)**

A way to accelerate tracer transport:

Conservative Semi-LAgrangian Multi-tracer (CSLAM)

$$\frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \vec{v}) = 0,$$



Finite-volume Lagrangian form of continuity equation for air (pressure level thickness, Δp), and tracer (mixing ratio, q):

$$\int_{A_k} \psi_k^{n+1}\, dA = \int_{a_k} \psi_k^n\, dA \quad = \quad \sum_{\ell=1}^{L_k} \left[\int_{a_{k\ell}} \psi_{k\ell}^n(x,y)\, dA \right], \quad \psi = \Delta p, \Delta p\, q,$$

where n time-level, $a_{k\ell}$ overlap areas, L_k #overlap areas, and $\psi_{k\ell}^n(x,y)$ reconstruction function in cell $k\ell$.

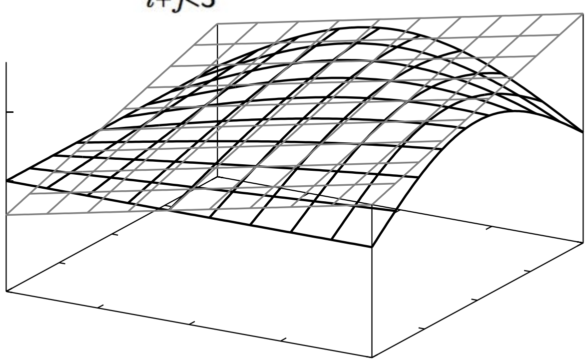
A way to accelerate tracer transport:

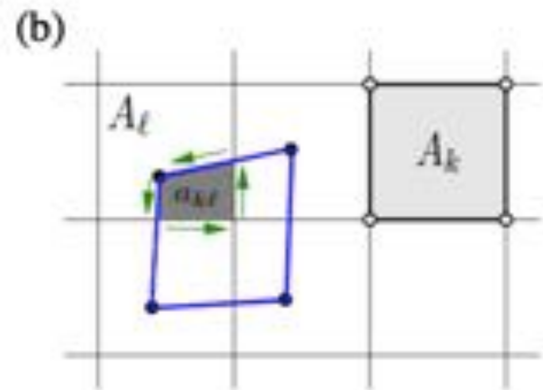
Basic formulation | Lauritzen et al. (2010)

Conservative Semi-LAgrangian Multi-tracer (CSLAM)

$$\psi^n_{k\ell}(x,y) = \sum_{i+j<3} c^{(i,j)} x^i y^j$$

3rd order





Finite-volume Lagrangian form of continuity equation for air (pressure level thickness, Δp), and tracer (mixing ratio, q):

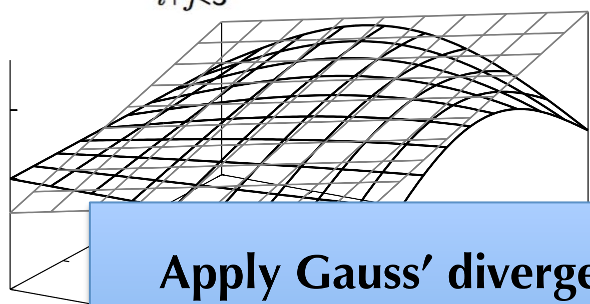
$$\int_{A_k} \psi_k^{n+1}\, dA = \int_{a_k} \psi_k^n\, dA \;=\; \sum_{\ell=1}^{L_k} \left[\int_{a_{k\ell}} \psi^n_{k\ell}(x,y)\, dA \right], \quad \psi = \Delta p, \Delta p\, q,$$

where n time-level, $a_{k\ell}$ overlap areas, L_k #overlap areas, and $\psi^n_{k\ell}(x,y)$ reconstruction function in cell $k\ell$.

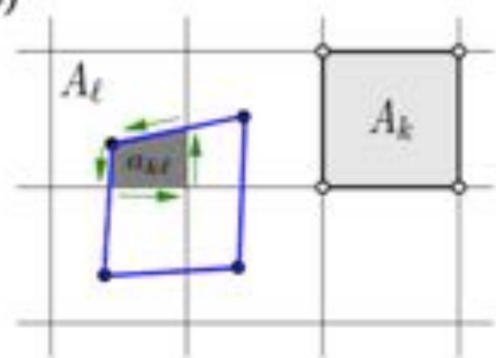
A way to accelerate tracer transport:

Conservative Semi-LAgrangian Multi-tracer (CSLAM)

$$\psi^n_{k\ell}(x,y) = \sum_{i+j<3} c^{(i,j)} x^i y^j,$$



(b)



Apply Gauss' divergence theorem to convert area integrals into line-integrals

Finite-volume Lagrangian … of continuity equation for air (pressure level thickness, Δp), and tracer (mix… ratio, q):

$$\int_{A_k} \psi_k^{n+1}\, dA = \int_{a_k} \psi_k^n\, dA \;=\; \sum_{\ell=1}^{L_k} \left[\int_{a_{k\ell}} \psi^n_{k\ell}(x,y)\, dA \right], \quad \psi = \Delta p, \Delta p\, q,$$

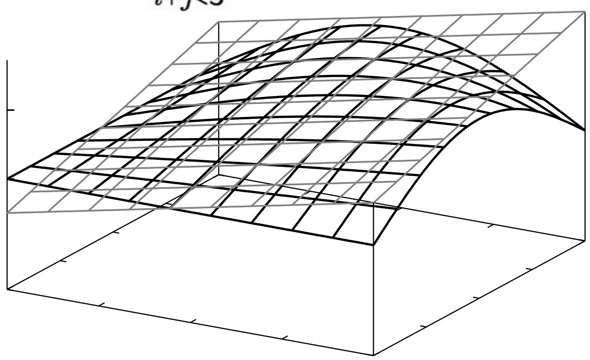
where n time-level, $a_{k\ell}$ overlap areas, L_k #overlap areas, and $\psi^n_{k\ell}(x,y)$ reconstruction function in cell $k\ell$.

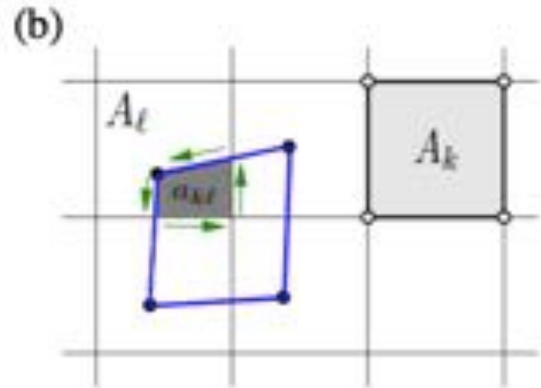
A way to accelerate tracer transport:

Basic formulation | Lauritzen et al. (2010)

Conservative Semi-LAgrangian Multi-tracer (CSLAM)

$$\psi_{k\ell}^{n}(x,y) = \sum_{i+j<3} c^{(i,j)} x^i y^j,$$





$$\int_{A_k} \psi_k^{n+1}\, dA = \int_{a_k} \psi_k^{n}\, dA = \sum_{\ell=1}^{L_k} \left[\sum_{i+j\leq 2} c_\ell^{(i,j)} w_{k\ell}^{(i,j)} \right], \quad \psi = \Delta p, \Delta p\, q,$$

- Multi-tracer efficient: $w_{k\ell}^{(i,j)}$ re-used for each additional tracer (Dukowicz and Baumgardner, 2000).
- Scheme allows for large time-steps (flow deformation limited).
- Conserves mass, shape, linear correlations (Lauritzen et al., 2014).

A way to accelerate tracer transport:

Basic formulation | Lauritzen et al. (2010)

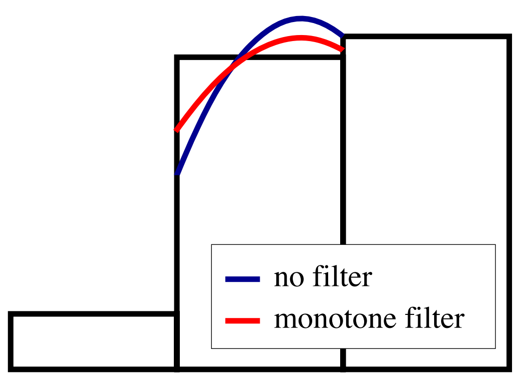
Conservative Semi-LAgrangian Multi-tracer (CSLAM)

Shape-preservation

- Apply limiter to mixing ratio sub-grid cell distribution:

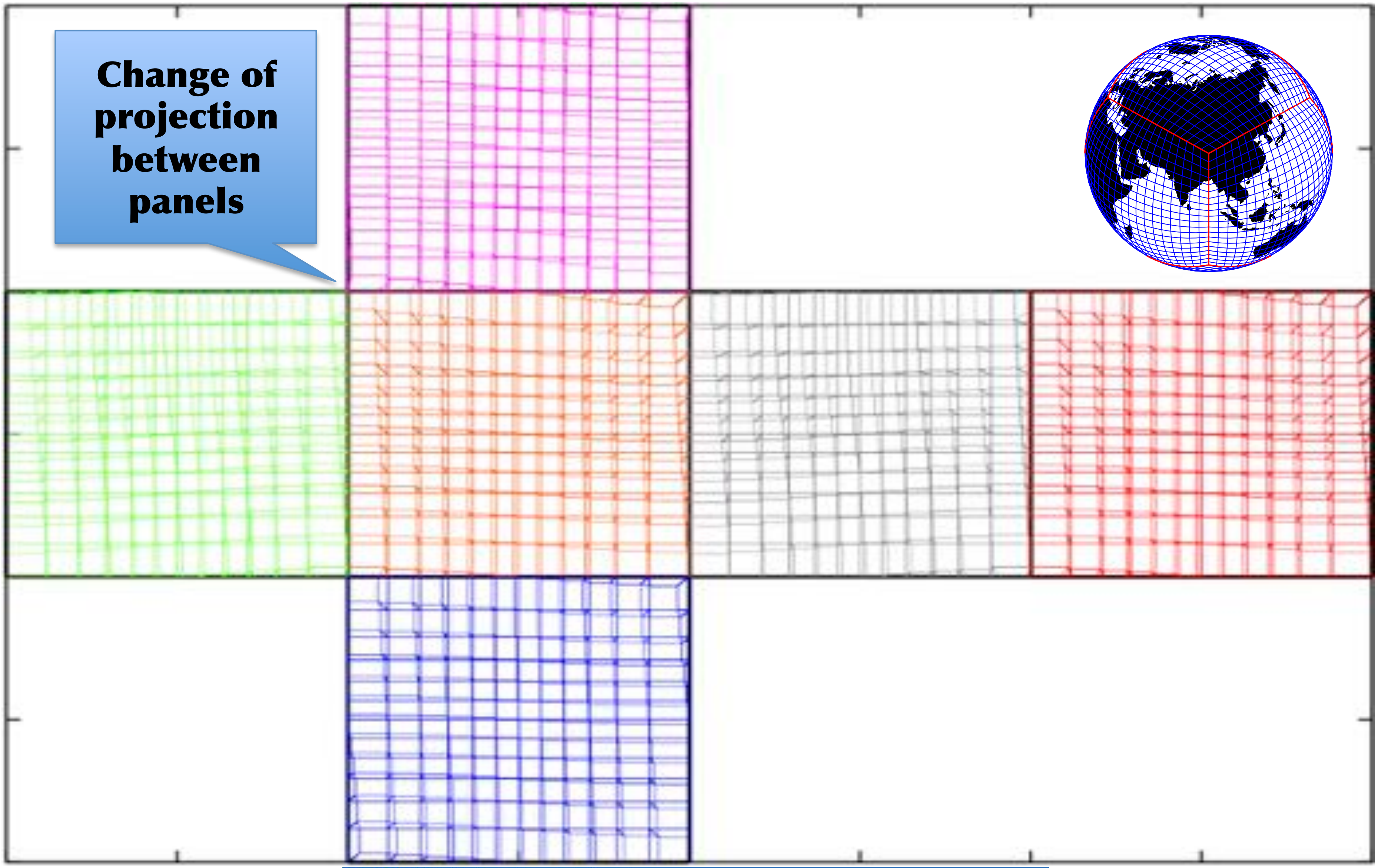
$$q(x,y) = \sum_{\imath+\jmath<3} c^{(\imath,\jmath)} x^{\imath} y^{\jmath},$$

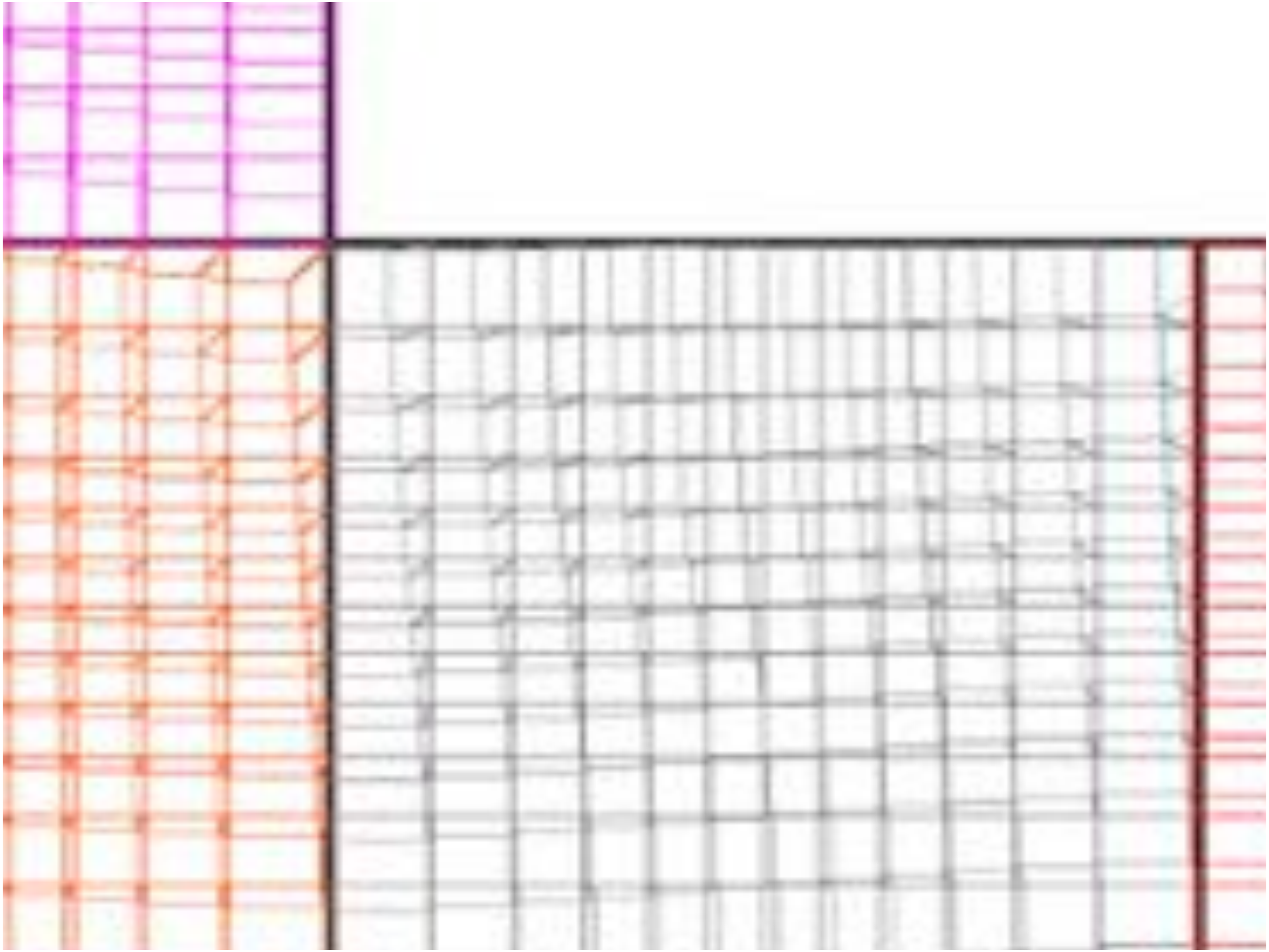
(Barth and Jespersen, 1989) so that extrema of $q(x,y)$ are within range of neighboring $\overline{q}$.



Extension to cubed-sphere:

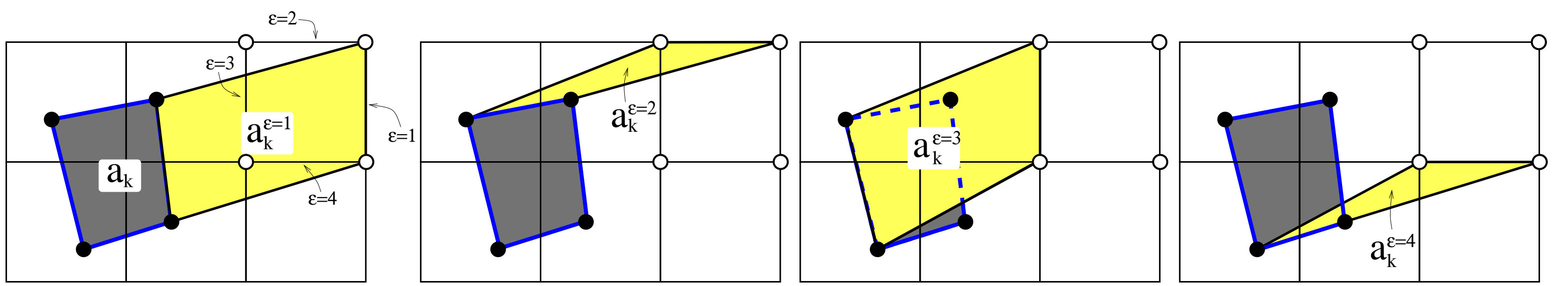
Figure shows upstream Lagrangian grid





A way to accelerate tracer transport:

Flux-form CSLAM ≡ Lagrangian CSLAM



$$\int_{A_k} \psi_k^{n+1}\, dA = \int_{A_k} \psi_k^n\, dA - \sum_{\epsilon=1}^{4} s_{k\ell}^{\epsilon} \int_{a_k^{\epsilon}} \psi\, dA, \quad \psi = \Delta p, \Delta p\, q.$$

where

- a_k^{ϵ} = 'flux-area' (yellow area) = area swept through face ϵ
- $s_{k\ell}^{\epsilon}$ = 1 for outflow and -1 for inflow.

Flux-form and Lagrangian forms of CSLAM are equivalent (Lauritzen et al., 2011).

Coupling finite-volume semi-Lagrangian transport with spectral element dynamics

4. Consistency (tracer and air mass are coupled!)

Continuity equations for air mass and tracer mass:

Spectral elements

$$\frac{\partial(\Delta p)}{\partial t} + \nabla \cdot (\Delta p \vec{v}) = 0,$$

CSLAM

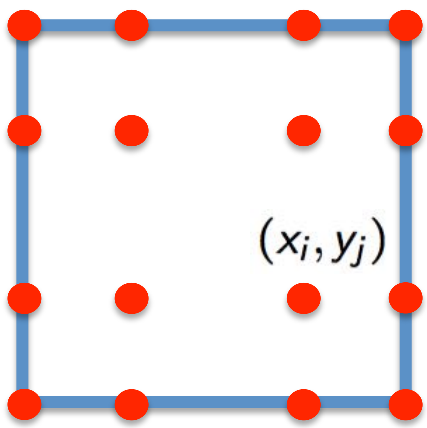
$$\int_{A_k} (\Delta p q)_k^{n+1}\, dA = \int_{a_k} (\Delta p q)^n\, dA.$$

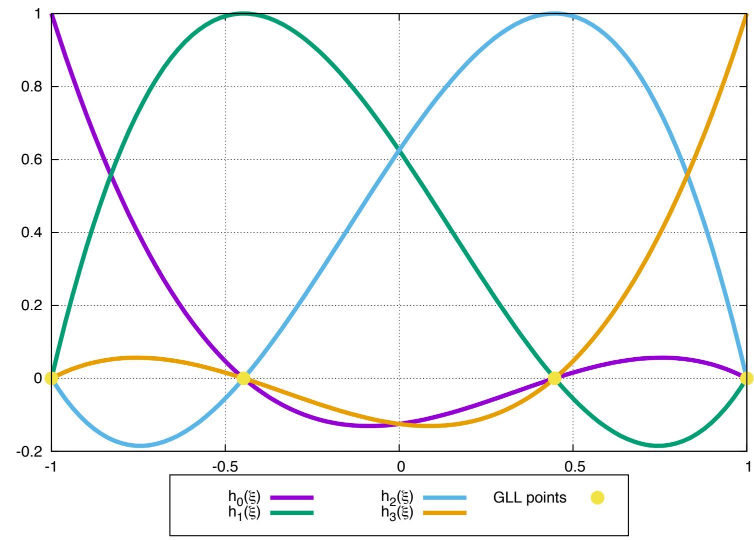
If $q = 1$ then the transport scheme should reduce to the continuity equation for air.

We need to couple without violating mass-conservation, shape-preservation, and consistency

The spectral-element method

Spectral-Element Method (SEM)



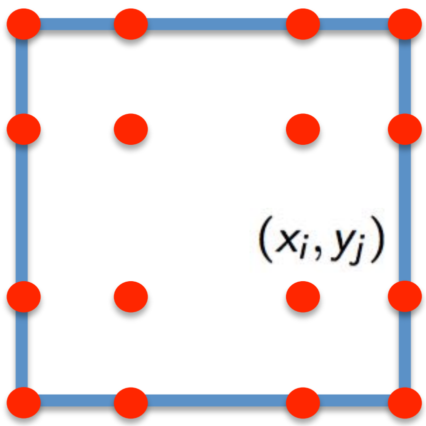


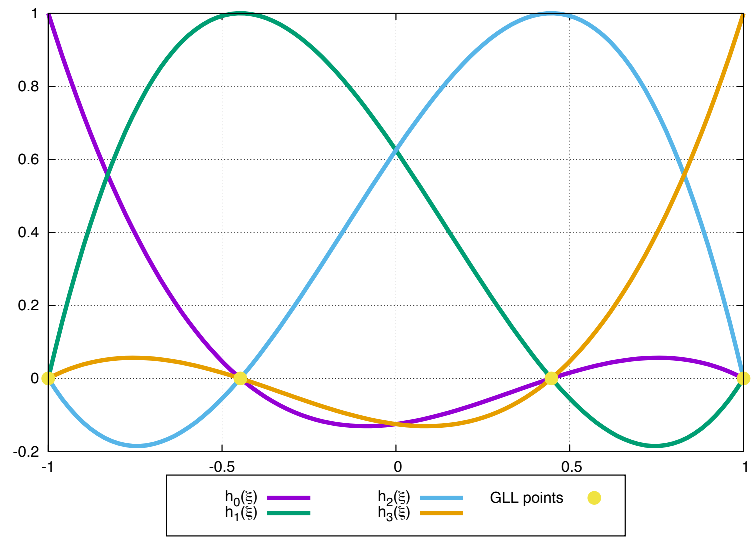
Continuity equation for Δp:

$$\frac{\partial \Delta p}{\partial t} = -\nabla \cdot \Delta p \vec{v} + \tau \nabla^4 \Delta p.$$

The spectral-element method

Spectral-Element Method (SEM)





Continuity equation for Δp:

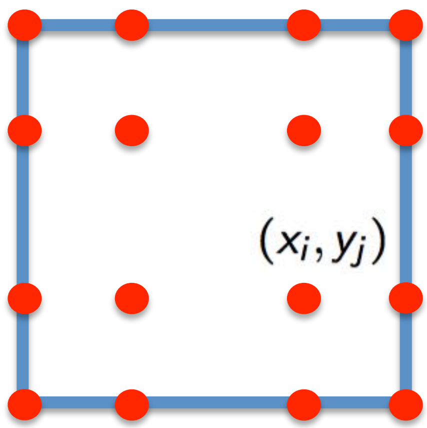
$$\left\langle h_k, \frac{\partial \Delta p}{\partial t} \right\rangle = \langle h_k, -\nabla \cdot \Delta p \vec{v} \rangle + \left\langle h_k, \tau \nabla^4 \Delta p \right\rangle,$$

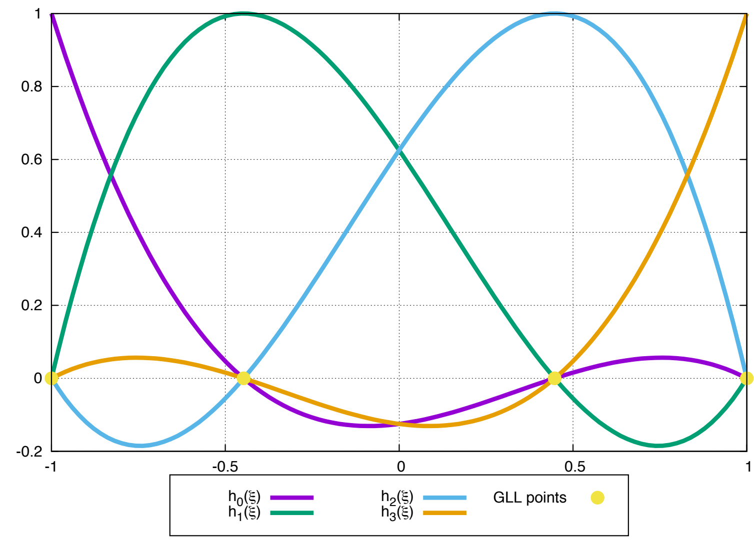
where $\langle h_k, \cdot \rangle$ is inner product

$$\langle h_k, f \rangle = \sum_{i,j} w_{i,j} h_k(x_i, y_j) f(x_i, y_j) \sim \iint h_k f \, dA.$$

The spectral-element method

Spectral-Element Method (SEM)



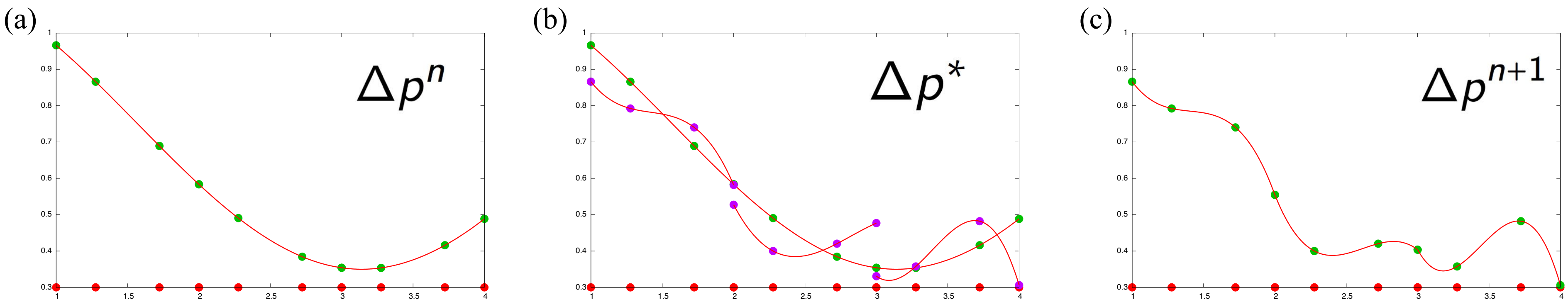


Continuity equation for Δp:

$$\left\langle h_k, \frac{\Delta p^* - \Delta p^n}{\Delta t} \right\rangle = \langle h_k, -\nabla \cdot \Delta p \vec{v} \rangle + \langle h_k, \tau \nabla^4 \Delta p \rangle .$$

Temporal discretization: multi-stage Runge-Kutta time-stepping

The spectral-element method

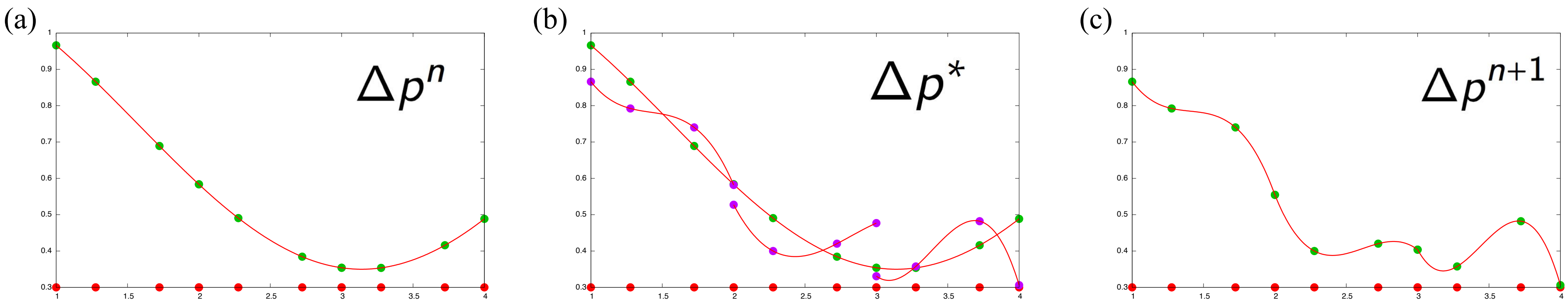


Continuity equation for Δp:

$$\left\langle h_k, \frac{\Delta p^* - \Delta p^n}{\Delta t} \right\rangle = \langle h_k, -\nabla \cdot \Delta p \vec{v} \rangle + \langle h_k, \tau \nabla^4 \Delta p \rangle .$$

Temporal discretization: multi-stage Runge-Kutta time-stepping

The spectral-element method



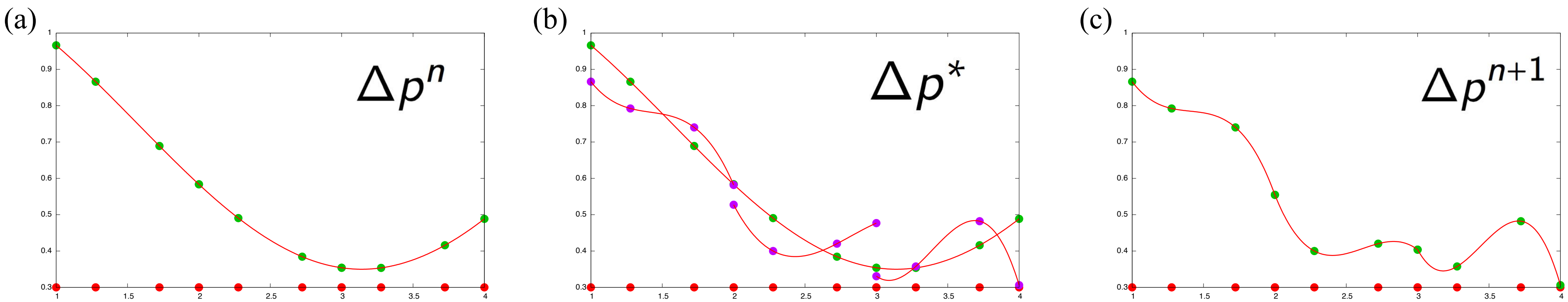
- Projection step

$$\Delta p^{n+1} = DSS\,(\Delta p^*)$$

  where *DSS* refers to *Direct Stiffness Summation* (also referred to as assembly or inverse mass matrix step).

- Choice of GLL quadrature based inner product and nodal basis functions gives a diagonal mass matrix (Maday and Patera, 1987).

The spectral-element method

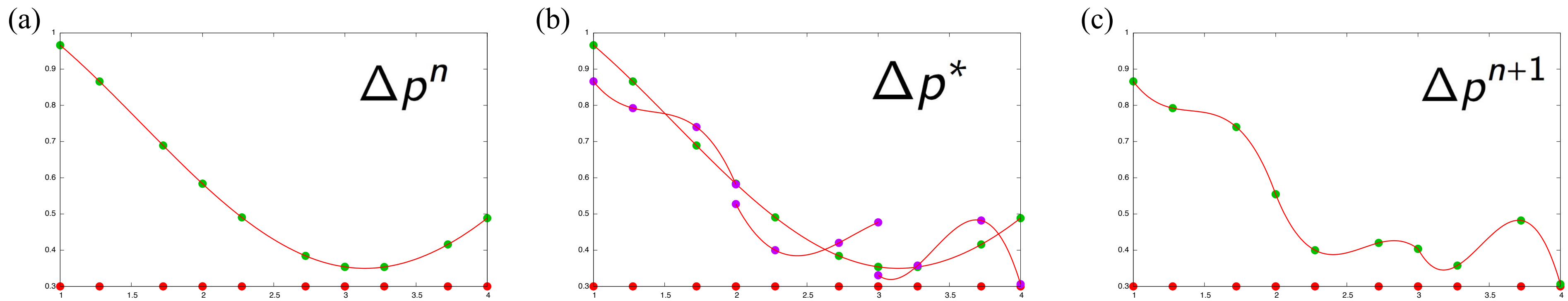


Continuity equation for Δp:

$$\left\langle h_k, \frac{\Delta p^{n+1} - \Delta p^n}{\Delta t} \right\rangle = \langle h_k, -\nabla \cdot \Delta p \vec{v} \rangle + \langle h_k, \tau \nabla^4 \Delta p \rangle + \langle h_k, D \rangle .$$

Temporal discretization: multi-stage Runge-Kutta time-stepping

The spectral-element method

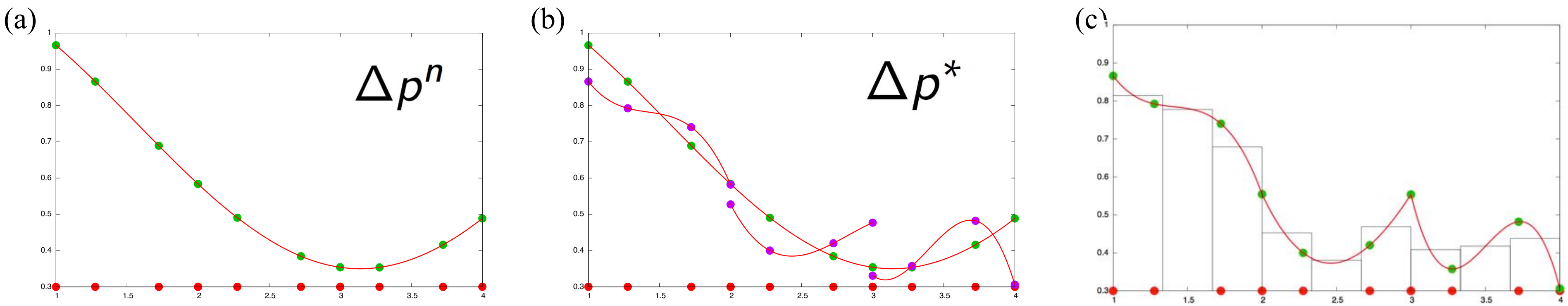


Continuity equation for Δp:

$$\left\langle h_k, \frac{\Delta p^{n+1} - \Delta p^n}{\Delta t} \right\rangle = \langle h_k, F \rangle + \langle h_k, G \rangle + \langle h_k, D \rangle .$$

Temporal discretization: multi-stage Runge-Kutta time-stepping

The spectral-element method



Setting basis function to 1 yields the mass change in each element

Continuity equation for Δp:

$$\left\langle h_k, \frac{\Delta p^{n+1} - \Delta p^n}{\Delta t} \right\rangle = \langle h_k, F \rangle + \langle h_k, G \rangle + \langle h_k, D \rangle .$$

Temporal discretization: multi-stage Runge-Kutta time-stepping

Diagnosing fluxes from spectral-element method

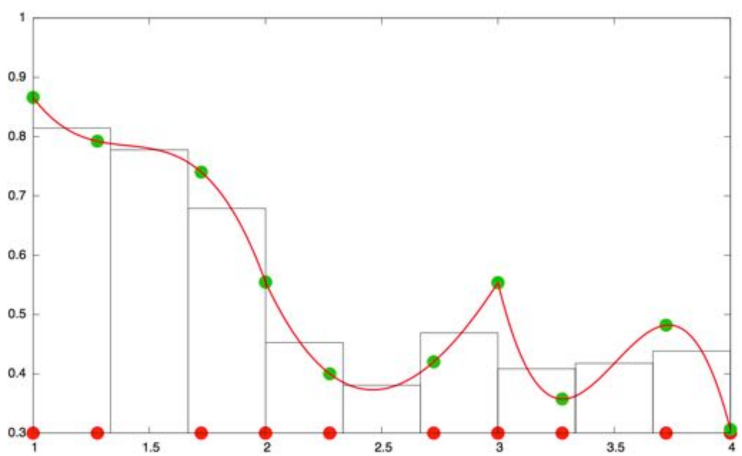
- There exist a basis ϕ_k so that

$$\left\langle \phi_k, \frac{\Delta p^{n+1} - \Delta p^n}{\Delta t} \right\rangle = \langle \phi_k, F \rangle + \langle \phi_k, G \rangle + \langle \phi_k, D \rangle,$$

gives the change of mass in each CSLAM control volume.

- Moreover, each term on right-hand side can be expressed in terms of edge fluxes:

$$\left(\Delta p^{n+1} - \Delta p^n\right) \Delta A_k = \sum_{\epsilon=1}^{4} \left[\mathcal{F}_F^{(\epsilon)} + \mathcal{F}_G^{(\epsilon)} + \mathcal{F}_D^{(\epsilon)}\right].$$



The story so far

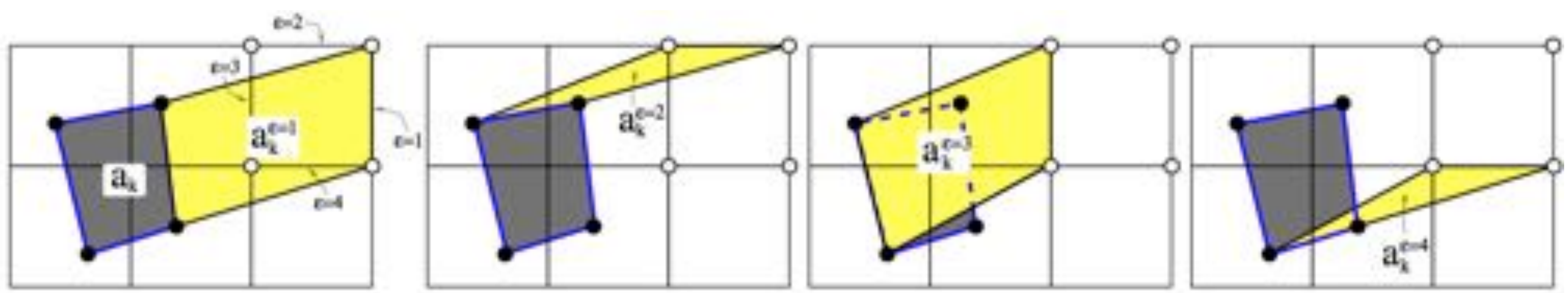
Spectral-Element Method: CAM-SE

Mass change over CSLAM control volume A_k implied by SE

$$\left(\Delta p^{n+1} - \Delta p^{n}\right)\Delta A_k = \sum_{\epsilon=1}^{4}\left[\mathcal{F}_F^{(\epsilon)} + \mathcal{F}_G^{(\epsilon)} + \mathcal{F}_D^{(\epsilon)}\right],$$

(Lauritzen et al., 2016; in prep).

Finite-Volume Method: CSLAM



CSLAM discretization is given by

$$\left(\widetilde{\Delta p}^{n+1} - \widetilde{\Delta p}^{n}\right)\Delta A_k = \sum_{\epsilon=1}^{4}\left[\mathcal{F}_{CSLAM}^{(\epsilon)}\right] = -\sum_{\epsilon=1}^{4} s_{k\ell}^{\epsilon}\int_{a_k^{\epsilon}} \Delta p^{n}\, dA.$$

Lauritzen et al., (2011)

The story so far

Spectral-Element Method: CAM-SE

Mass change over CSLAM control volume A_k implied by SE

$$\left(\Delta p^{n+1} - \Delta p^{n}\right)\Delta A_k = \sum_{\epsilon=1}^{4}\left[\mathcal{F}_F^{(\epsilon)} + \mathcal{F}_G^{(\epsilon)} + \mathcal{F}_D^{(\epsilon)}\right],$$

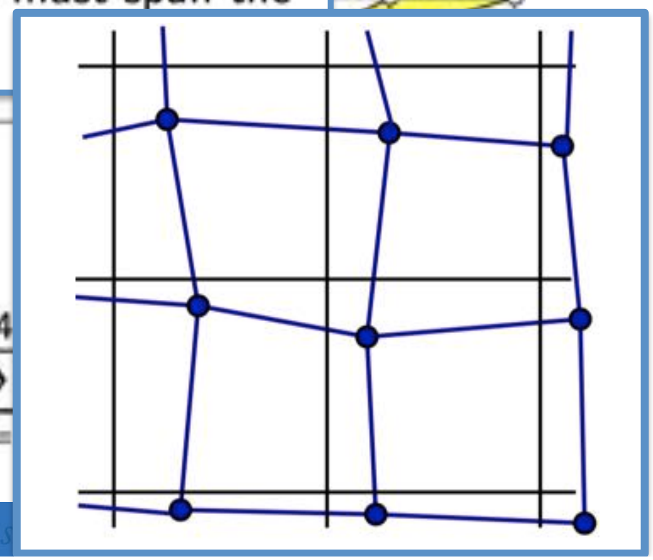
(Lauritzen et al., 2016; in prep).

Fir

For each face ϵ in cell a_k, find a swept area $a_k^{(\epsilon)}$ so that

$$\mathcal{F}_{CSLAM}^{(\epsilon)} = \mathcal{F}_F^{(\epsilon)} + \mathcal{F}_G^{(\epsilon)} + \mathcal{F}_D^{(\epsilon)}.$$

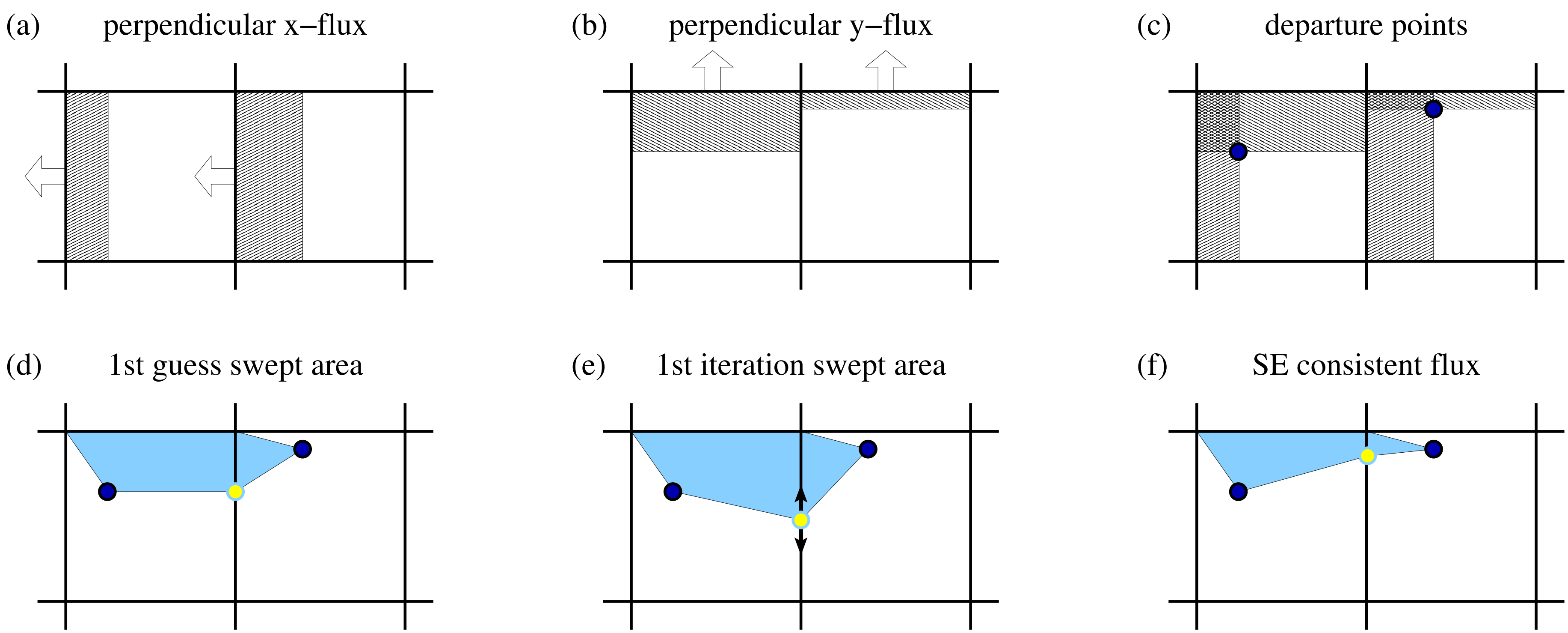
Lagrangian consistency constraint: The upstream areas must span the sphere without cracks or overlaps



CSLAM discretization is given by

$$\left(\widetilde{\Delta p}^{n+1} - \widetilde{\Delta p}^{n}\right)\Delta A_k = \sum_{\epsilon=1}^{4}\left[\mathcal{F}_{CSLAM}^{(\epsilon)}\right] = -\sum_{\epsilon=}^{4}$$

Consistent SE-CSLAM algorithm: step-by-step example



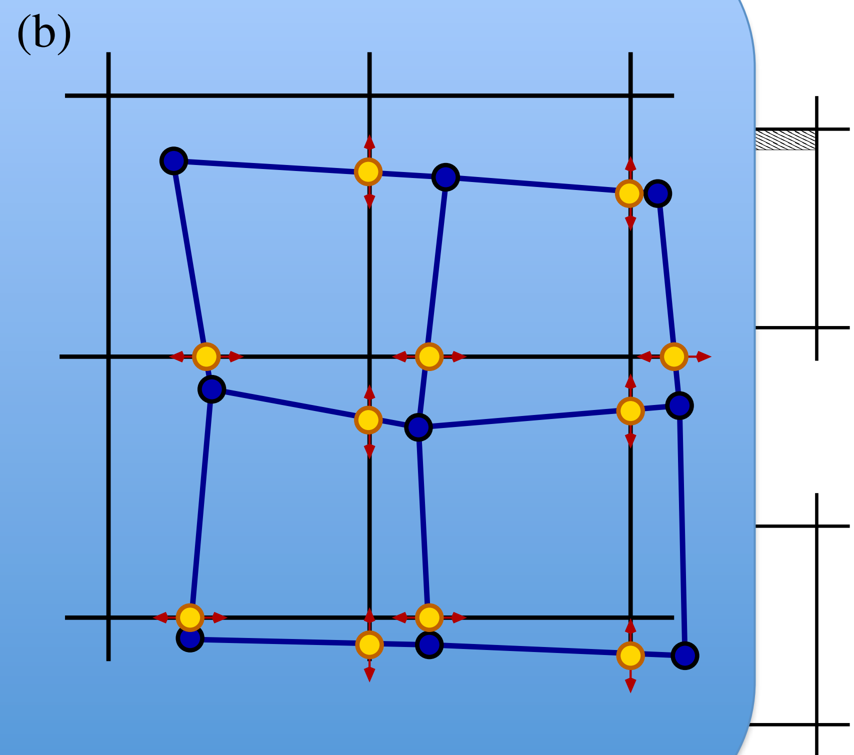
Well-posed? As long as flow deformation $\left|\frac{\partial u}{\partial x}\right| \Delta t \lesssim 1$ (Lipschitz criterion)

Lauritzen et al., 2016 (in prep.)

Consistent SE-CSLAM algorithm: step-by-step example

Local iteration problem generating an upstream grid that spans the sphere without cracks and overlaps

=> all CSLAM technology from Lauritzen et al. (2010) can be used



Well-posed? As long as flow deformation $\left|\frac{\partial u}{\partial x}\right| \Delta t \lesssim 1$ (Lipschitz criterion)

Consistent CSLAM algorithm is general

In principle, the consistent CSLAM algorithm can be made consistent with any fluxes that obey the Lipschitz criterion …

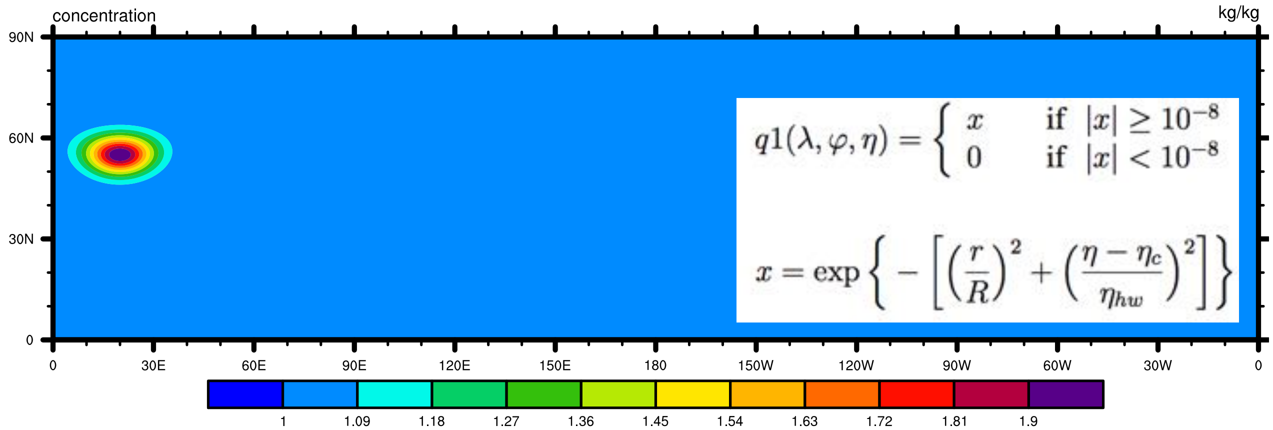
NCAR

Idealized baroclinic wave test

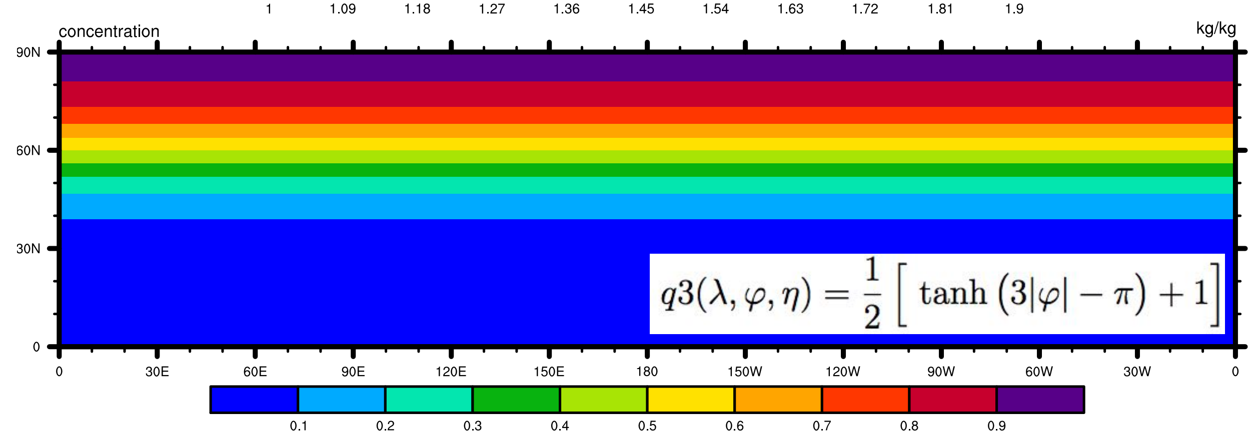
No sub-grid-scale forcing, dry, balanced initial condition with perturbation
Jablonowski and Williamson (2006)

Surface pressure computed with CSLAM is identical to SE (to round-off)

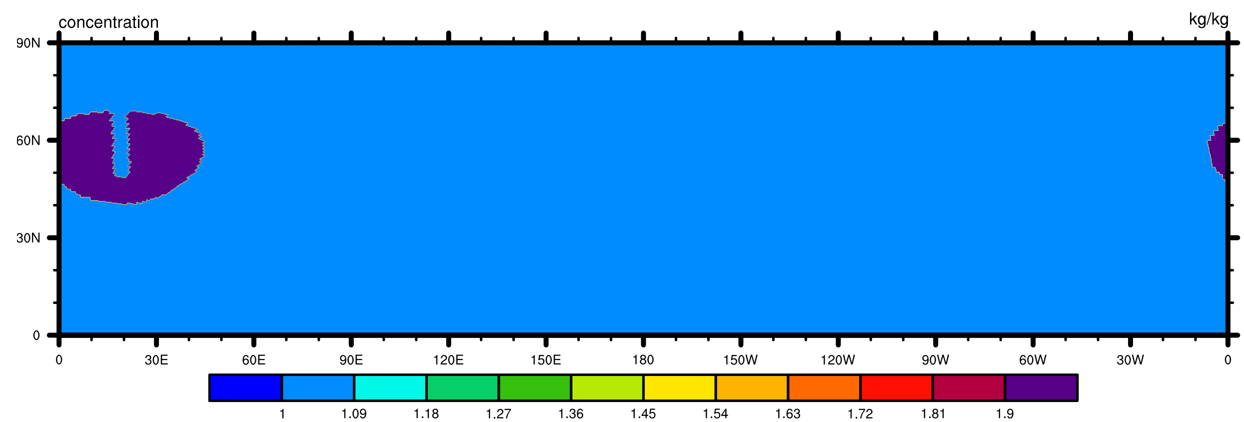
3 tracers: initial conditions



Gaussian "ball"

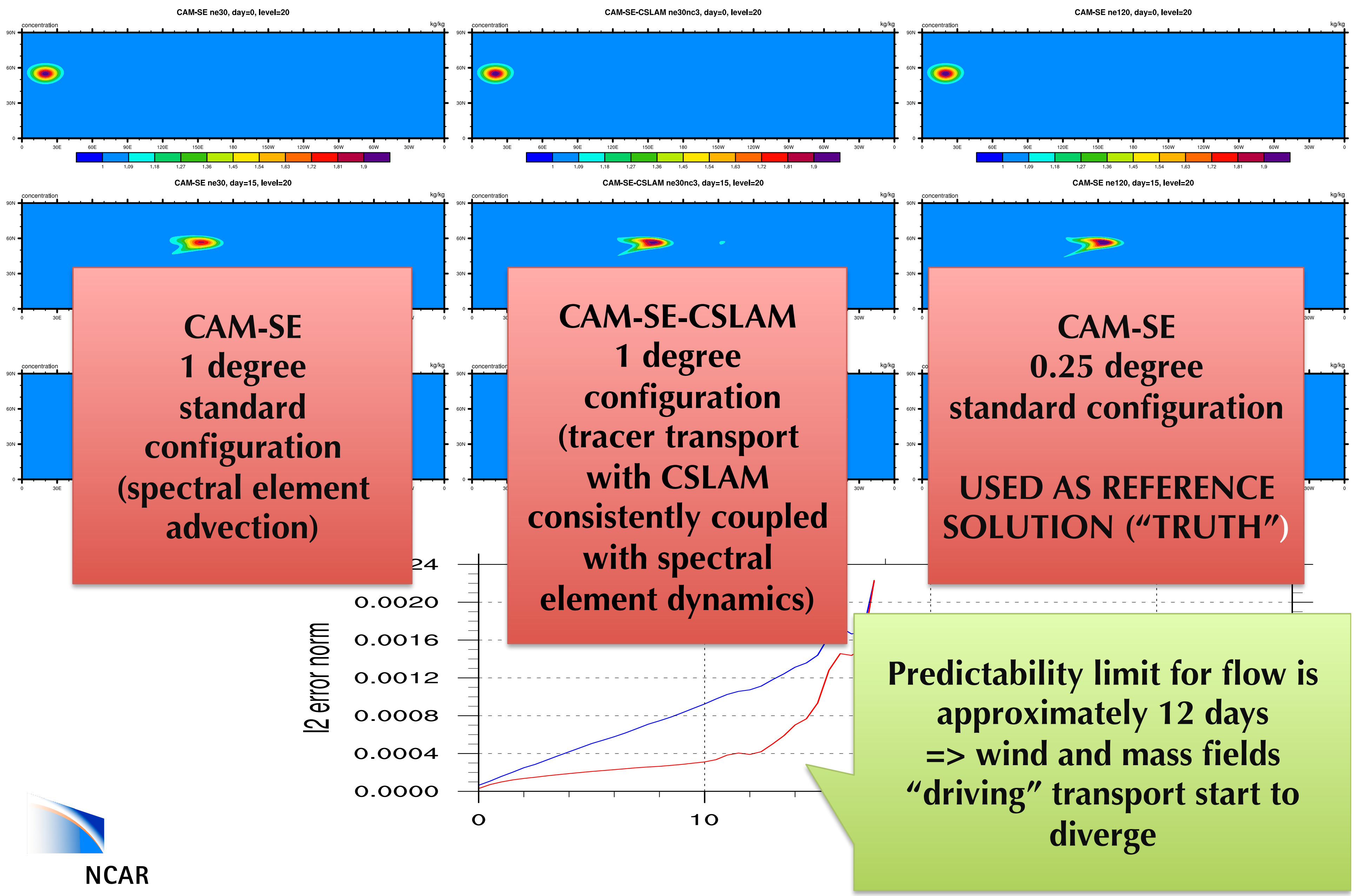


Zonally symmetric (smooth)



Slotted cylinder (non-smooth)

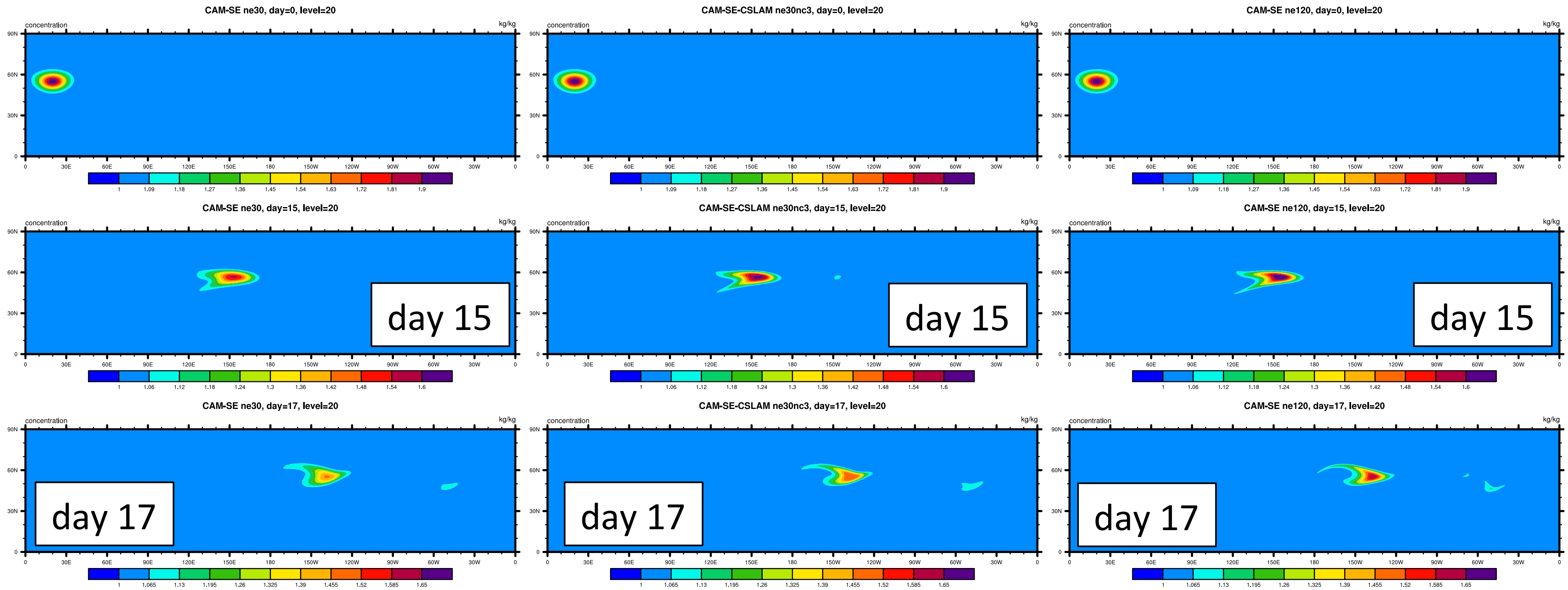
NCAR

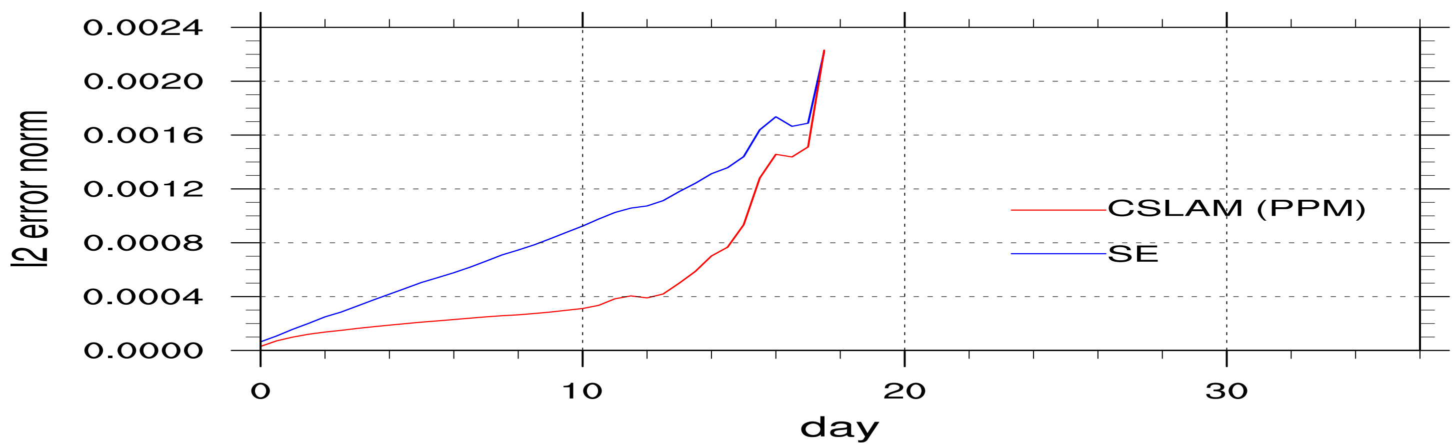


CAM-SE ne30, day=0, level=20
CAM-SE-CSLAM ne30nc3, day=0, level=20
CAM-SE ne120, day=0, level=20
CAM-SE ne30, day=15, level=20
CAM-SE-CSLAM ne30nc3, day=15, level=20
CAM-SE ne120, day=15, level=20
concentration
kg/kg
CAM-SE
1 degree
standard
configuration
(spectral element
advection)
CAM-SE-CSLAM
1 degree
configuration
(tracer transport
with CSLAM
consistently coupled
with spectral
element dynamics)
CAM-SE
0.25 degree
standard configuration
USED AS REFERENCE
SOLUTION ("TRUTH")
l2 error norm
0.0020
0.0016
0.0012
0.0008
0.0004
0.0000
0
10
Predictability limit for flow is
approximately 12 days
=> wind and mass fields
"driving" transport start to
diverge

NCAR

CAM-SE | CAM-SE-CSLAM | CAM-SE reference

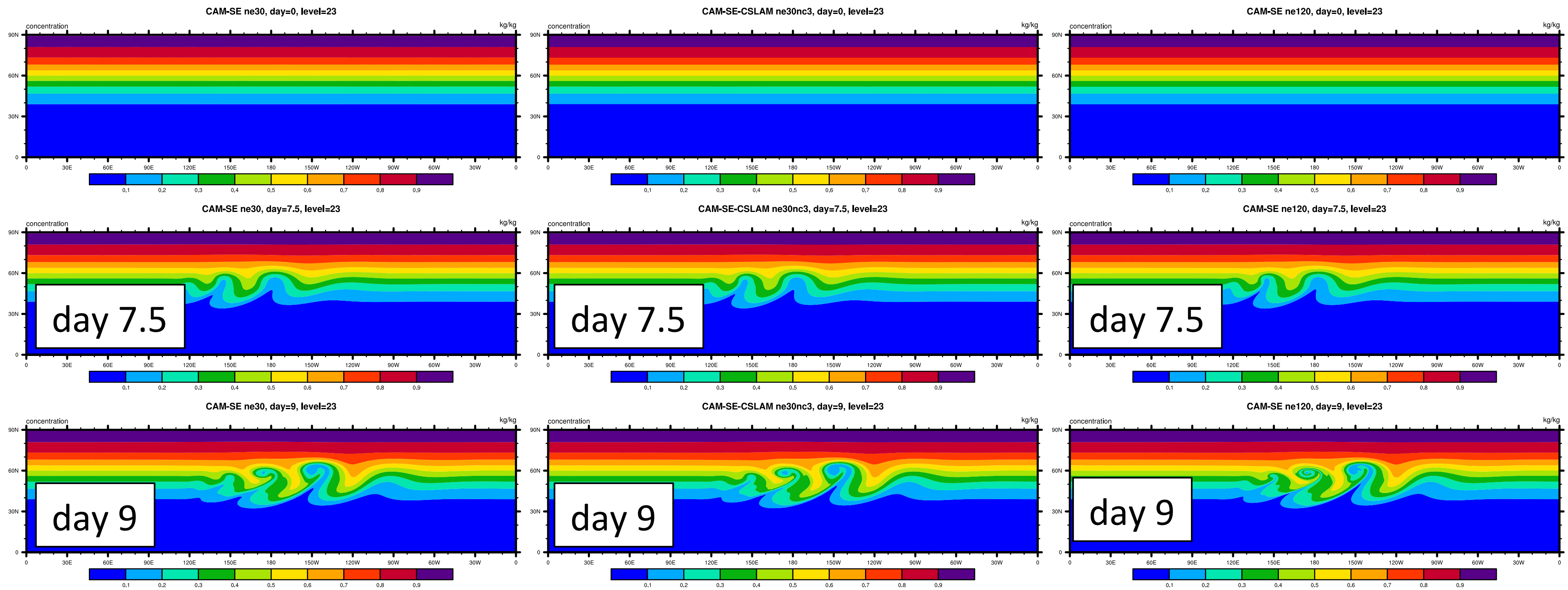


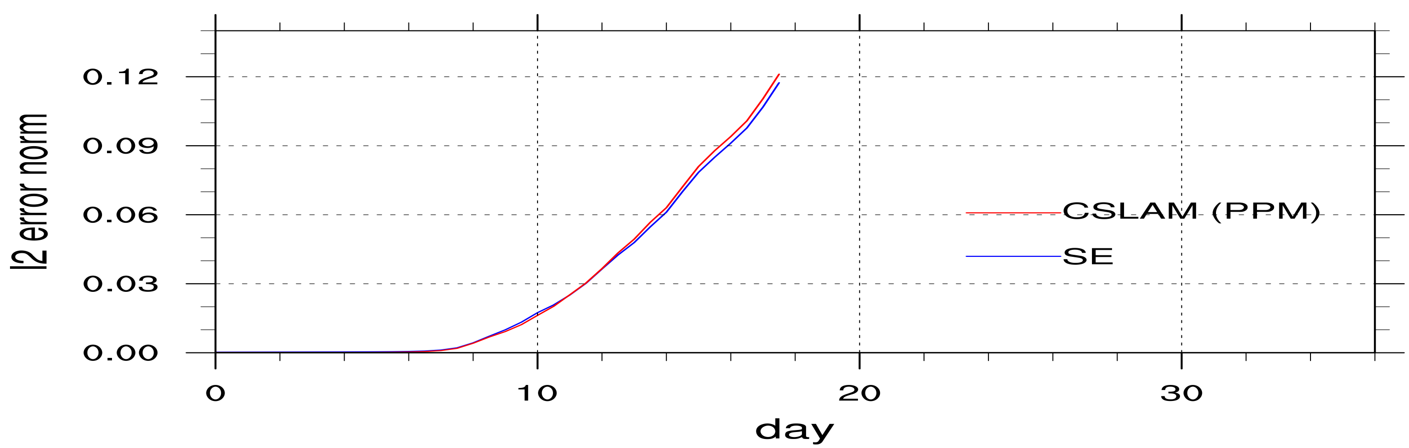


NCAR

Lauritzen et al., 2016 (in prep.)

CAM-SE	CAM-SE-CSLAM	CAM-SE reference

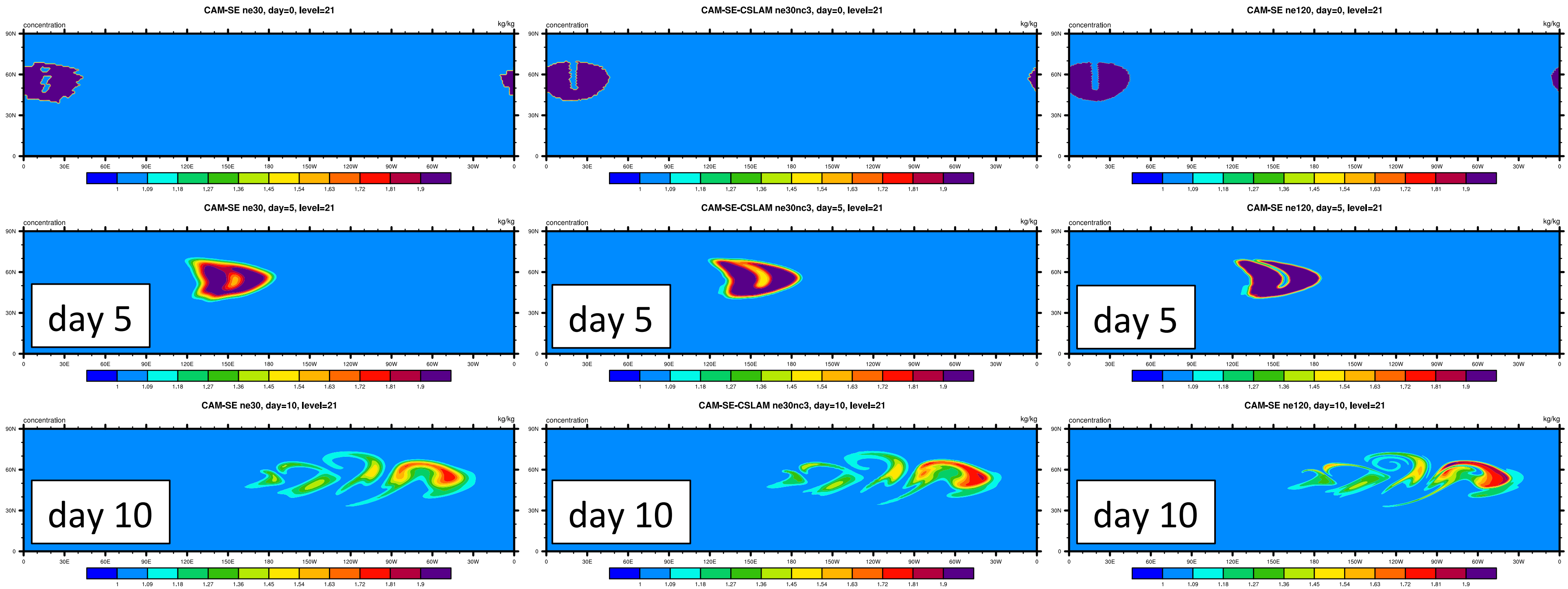


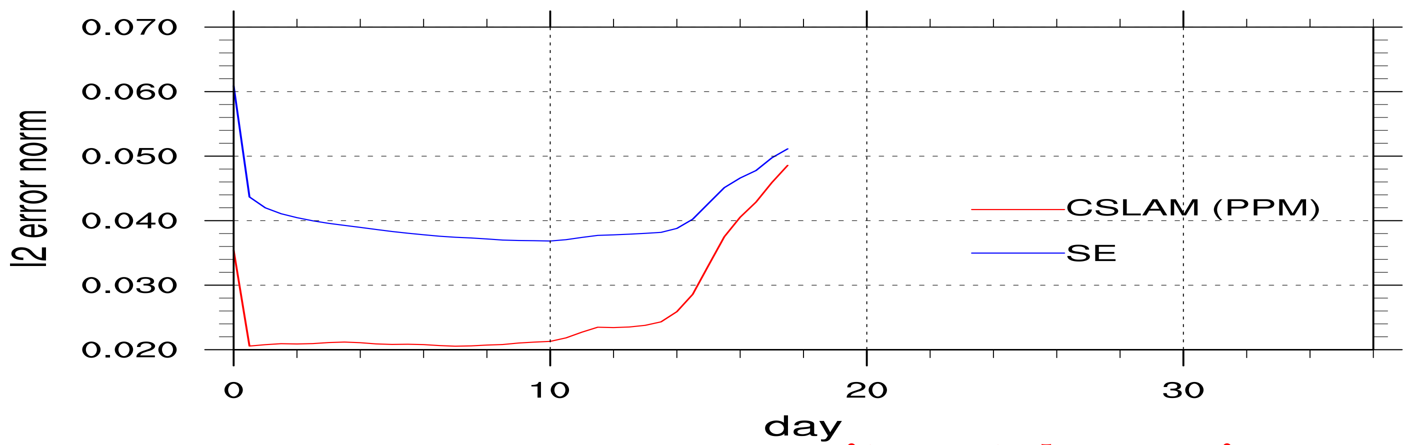


Lauritzen et al., 2016 (in prep.)

NCAR

CAM-SE | CAM-SE-CSLAM | CAM-SE reference





NCAR

Lauritzen et al., 2016 (in prep.)

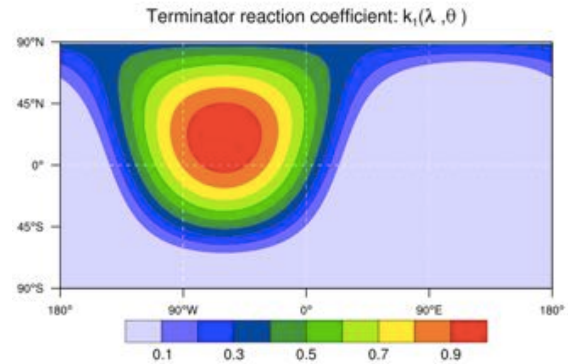
The terminator ‘toy’-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

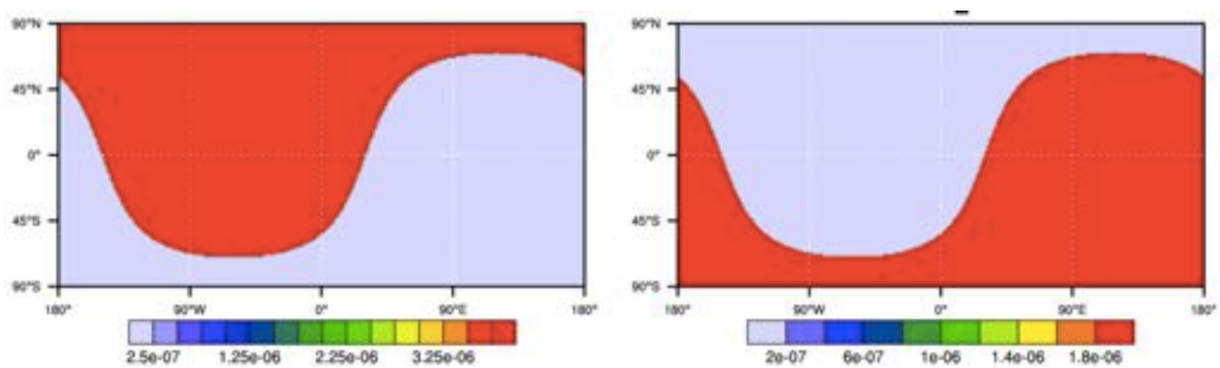
See: http://www.cgd.ucar.edu/cms/pel/terminator.html

- Consider 2 reactive chemical species, Cl and Cl_2 :

$$Cl_2 \rightarrow Cl + Cl : k_1$$
$$Cl + Cl \rightarrow Cl_2 : k_2$$

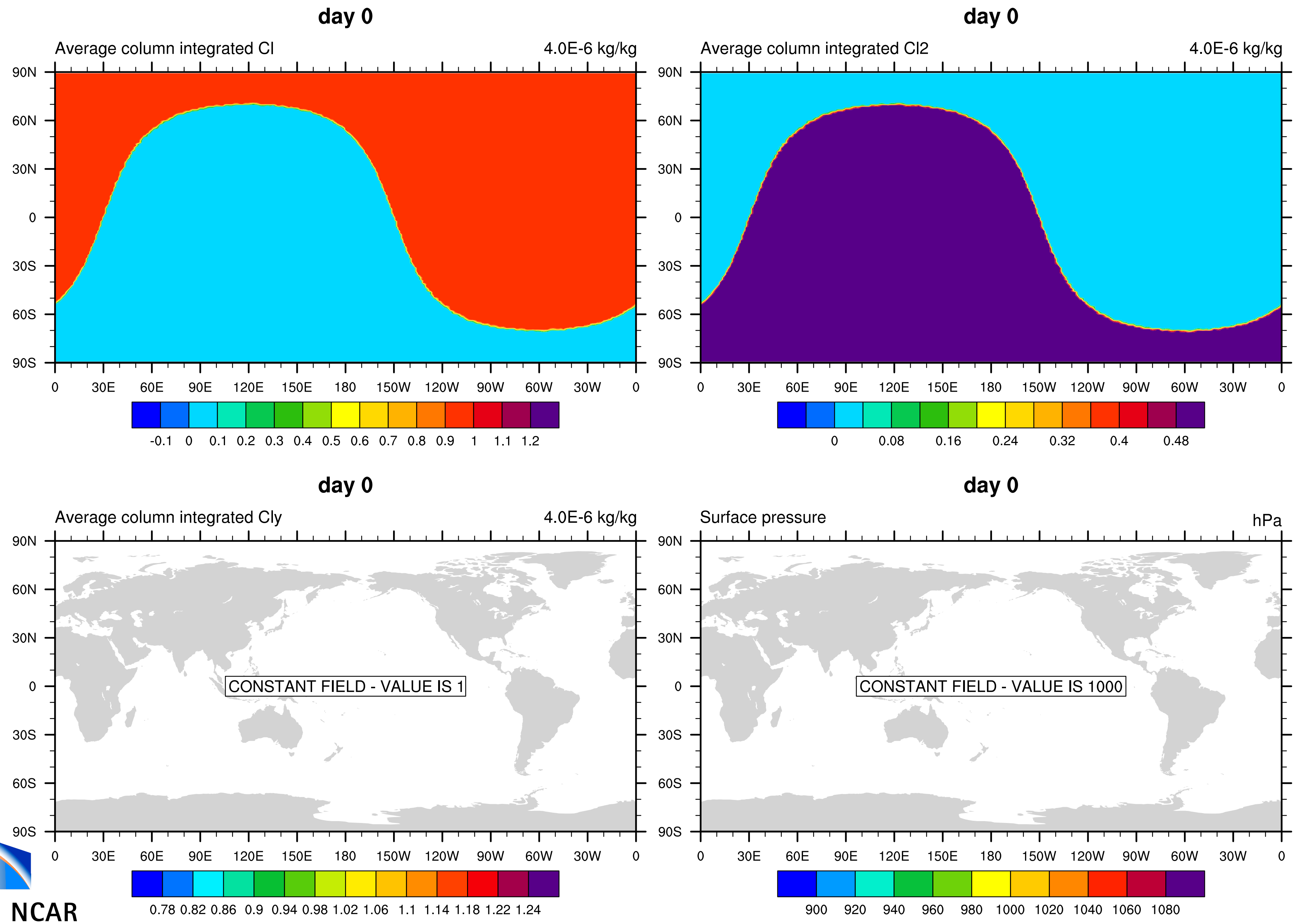


- Steady-state solution (no flow):



- In any flow-field $Cl_y = Cl + 2*Cl_2$ should be constant at all times (correlation preservation)

Initial condition

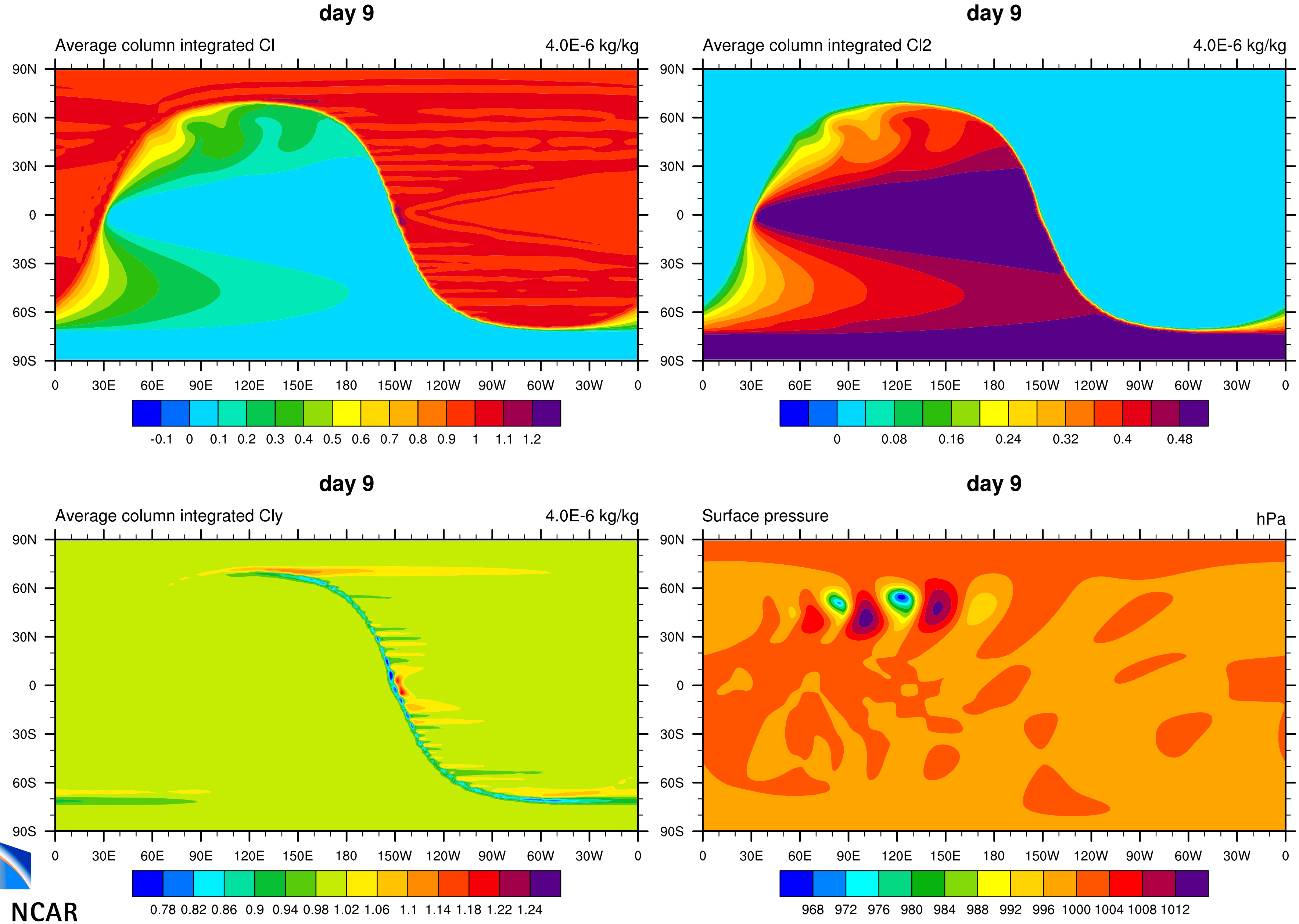


Lauritzen et al., 2016 (in prep.)

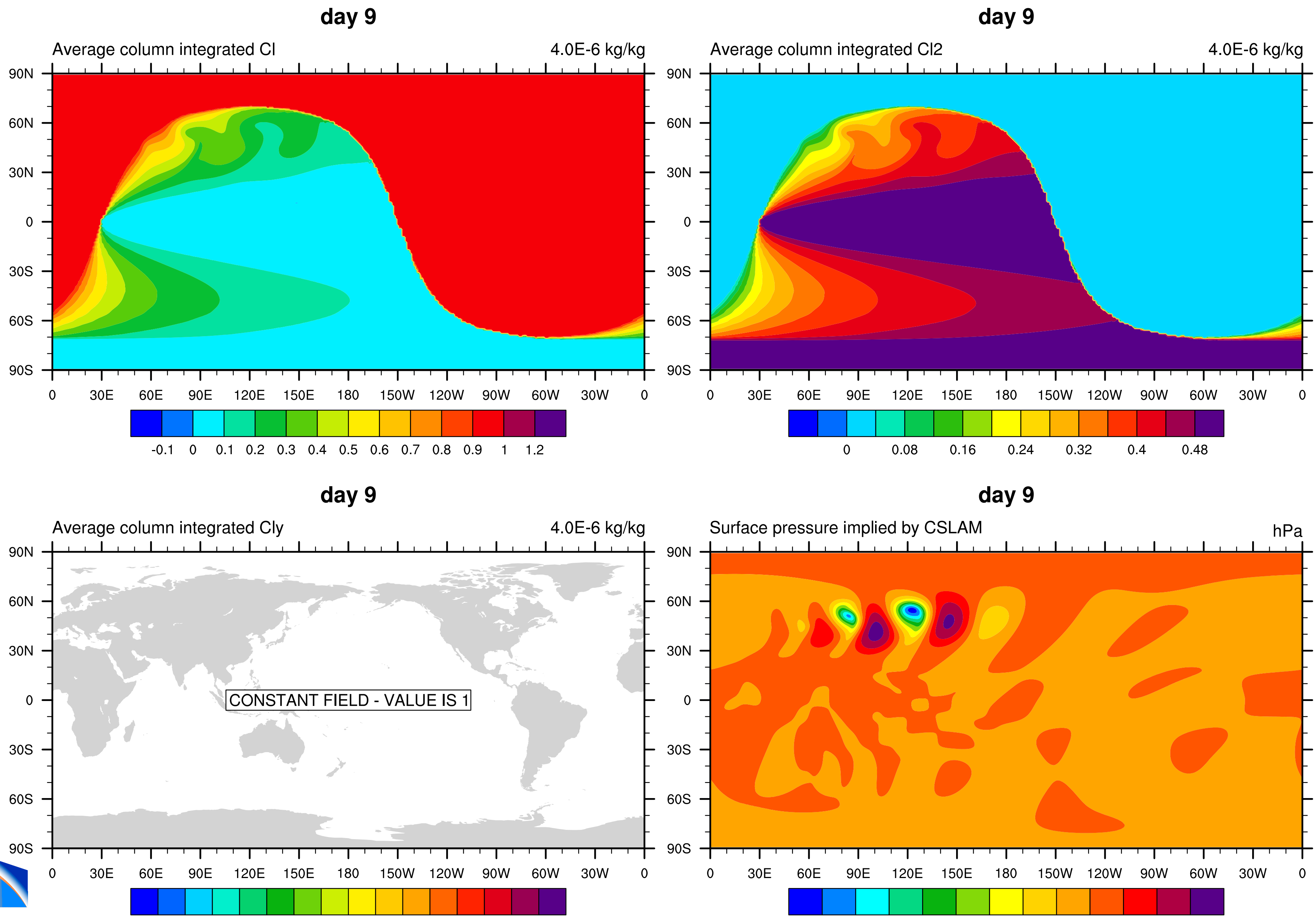
NCAR

CAM-SE

Lauritzen et al., 2016 (in prep.)



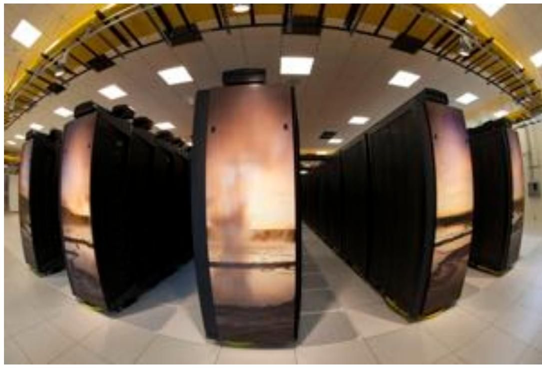
CAM-SE-CSLAM



Lauritzen et al., 2016 (in prep.)

NCAR

Performance



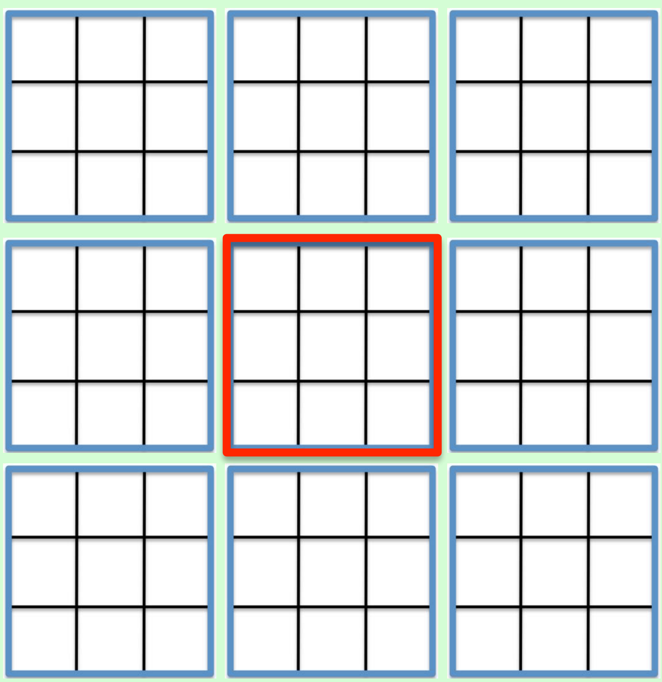
- **All simulations run on NCAR's Yellowstone computer**
- **No exploration of threading**

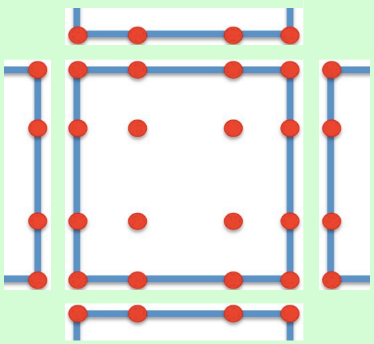
MPI communication

For every 30 minute physics time-step:

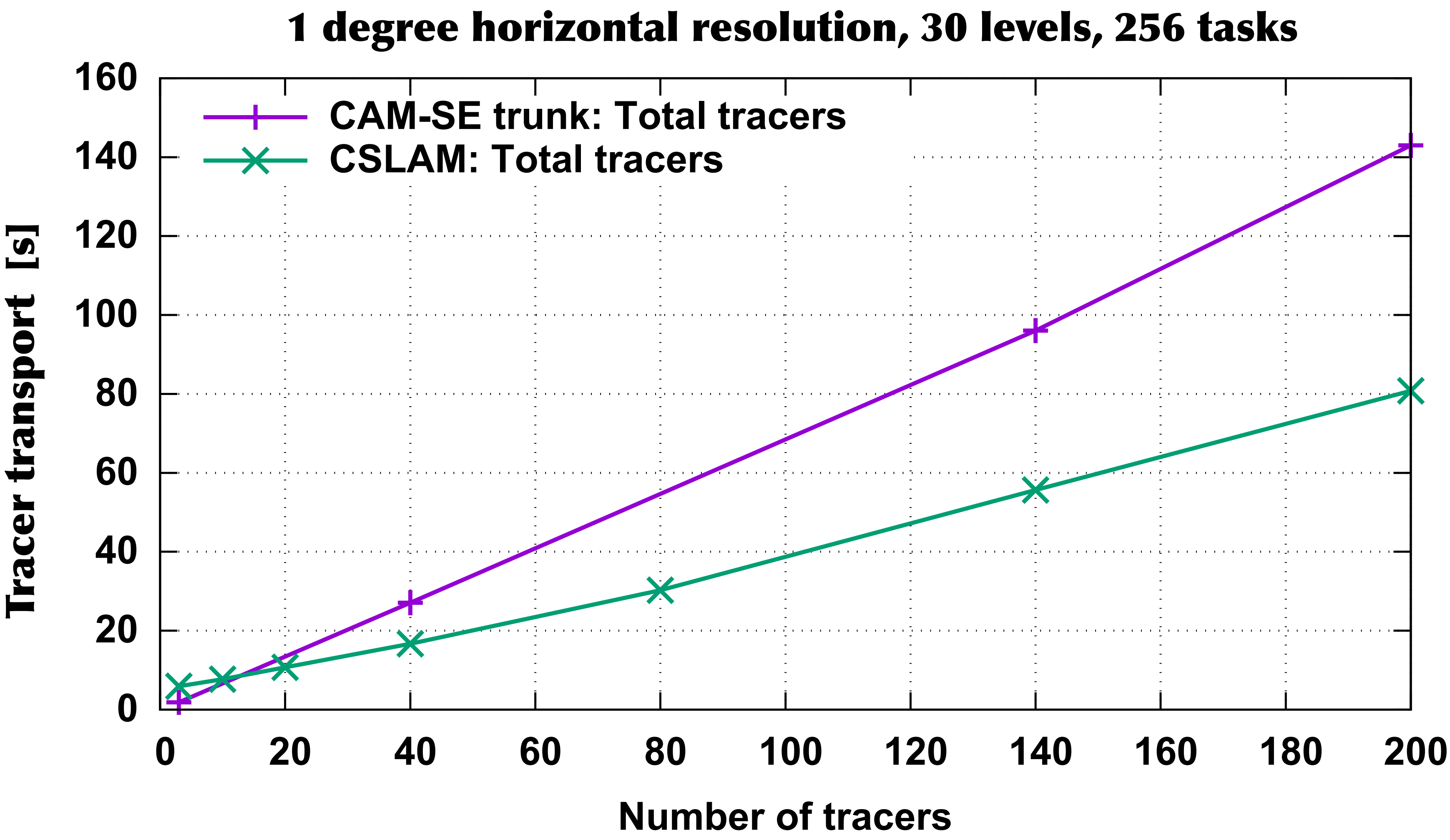
- SE performs 6 tracer time-steps (dt=300s) => 42 MPI calls (7 per tracer dt)
- CSLAM performs 2 tracer time-steps (dt=900s) => 2 MPI calls (1 per tracer dt)

That said, CSLAM needs a much larger halo than SE:

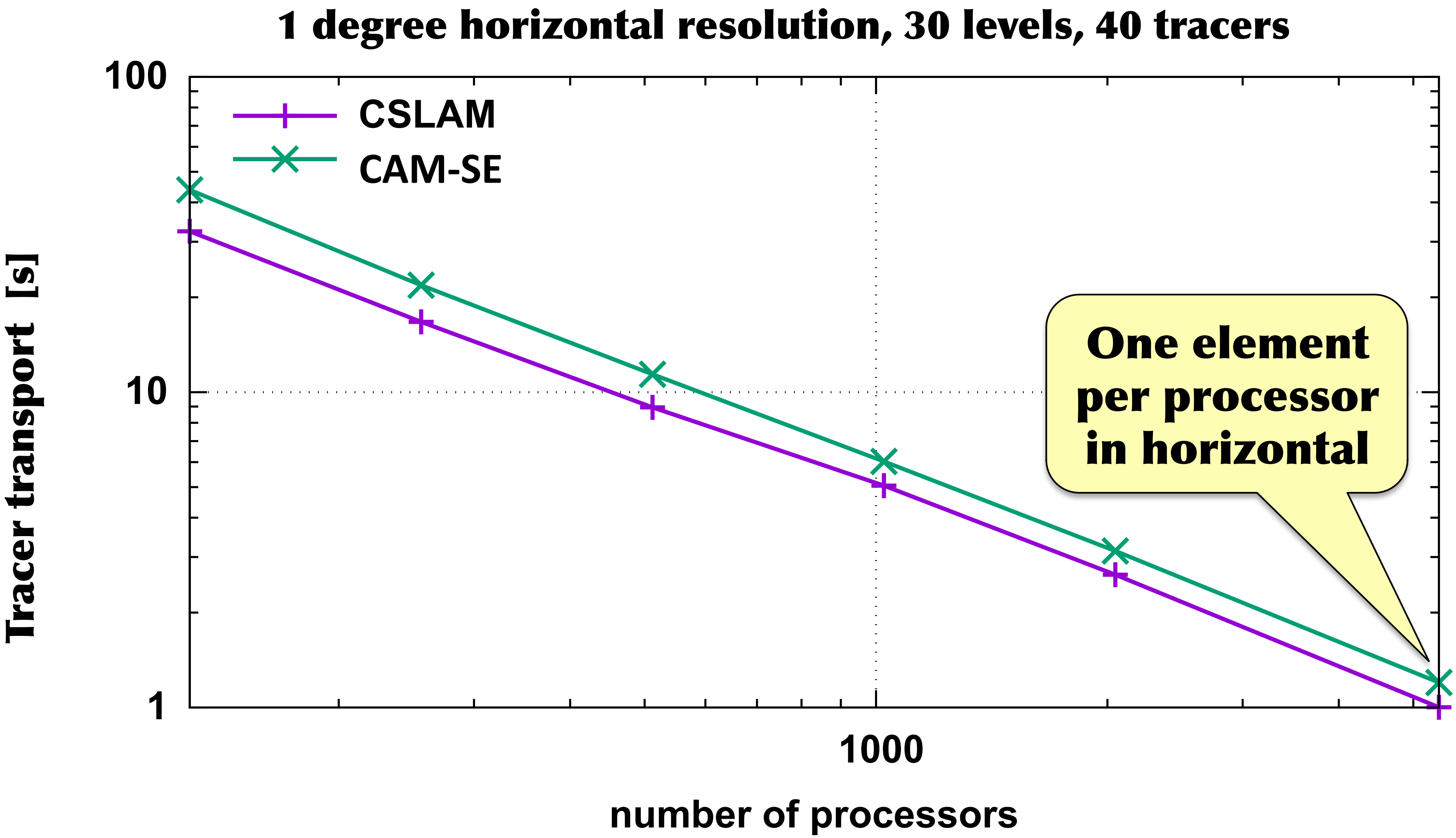




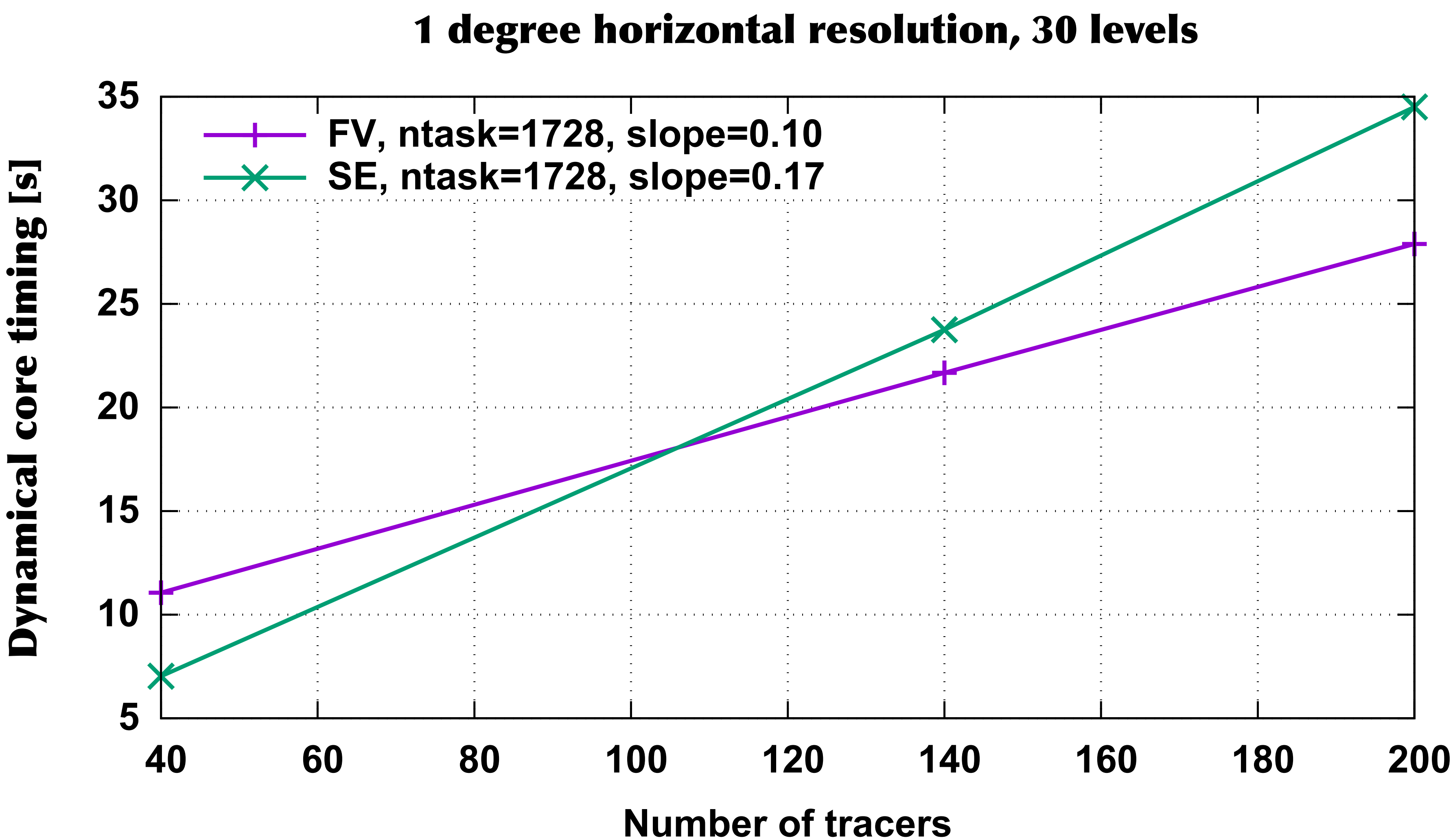
Performance



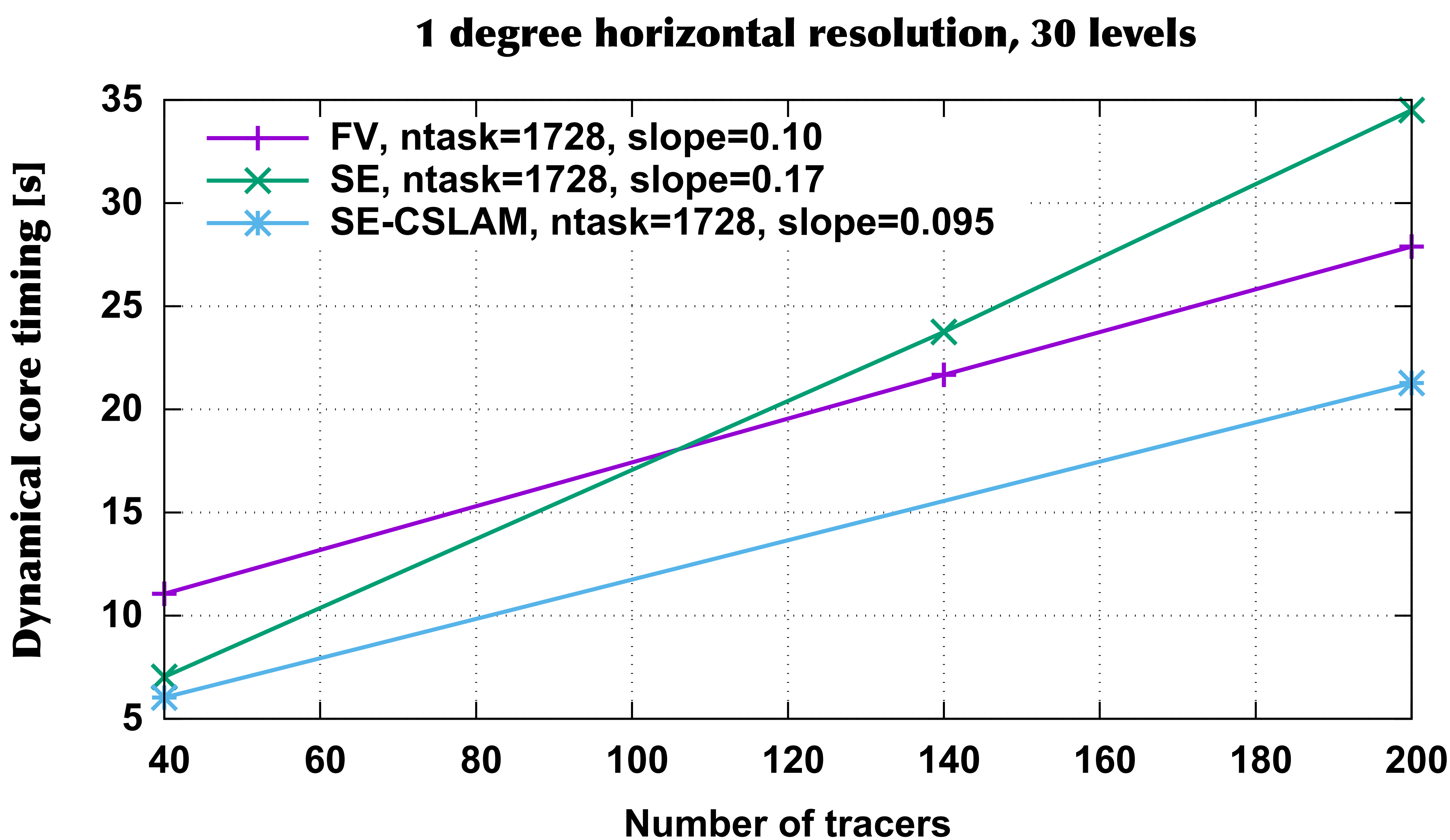
Performance: strong scaling



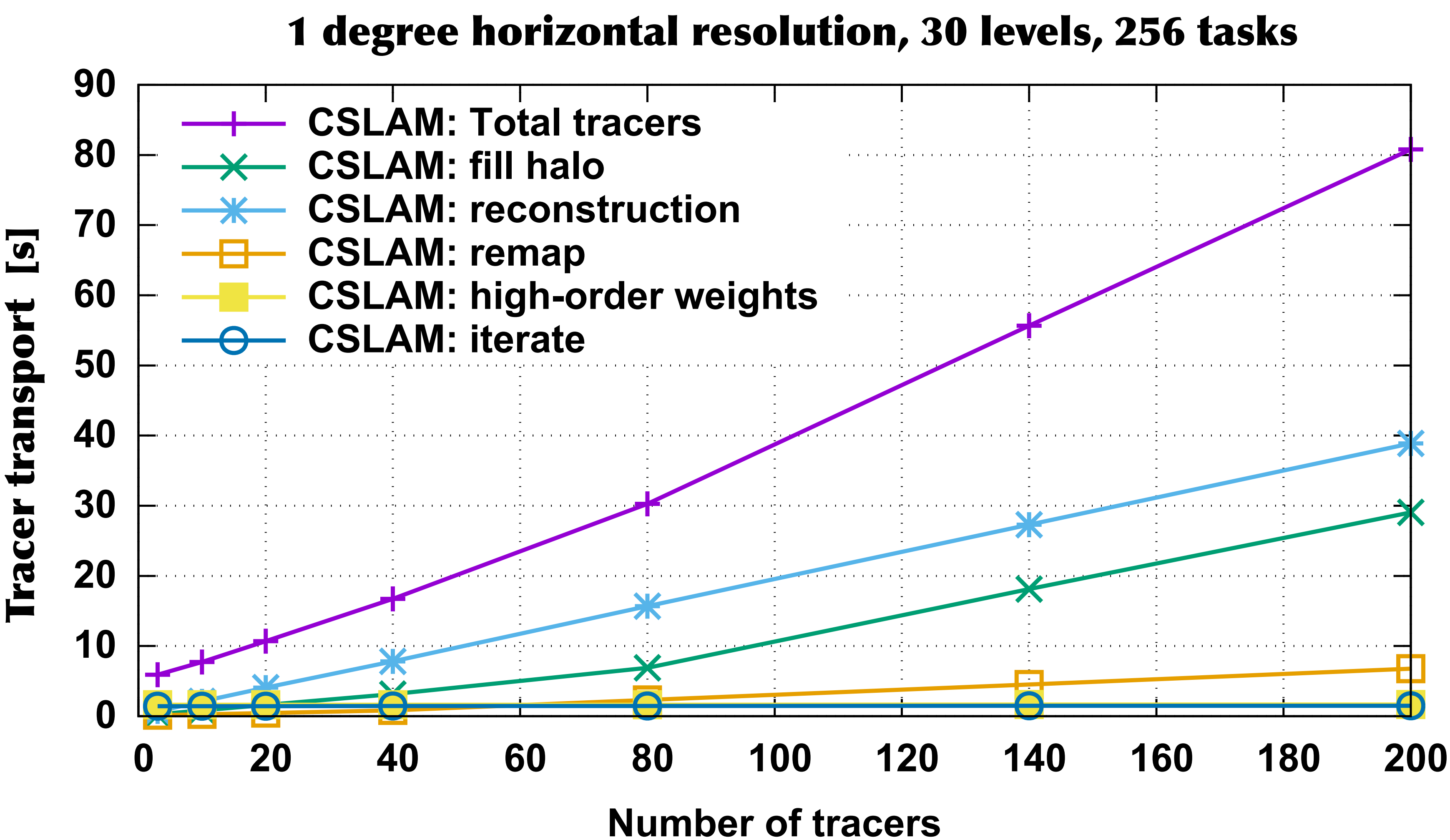
How do we compare with CAM-FV (dynamical core timings using 1728 tasks)



How do we compare with CAM-FV (dynamical core timings using 1728 tasks)

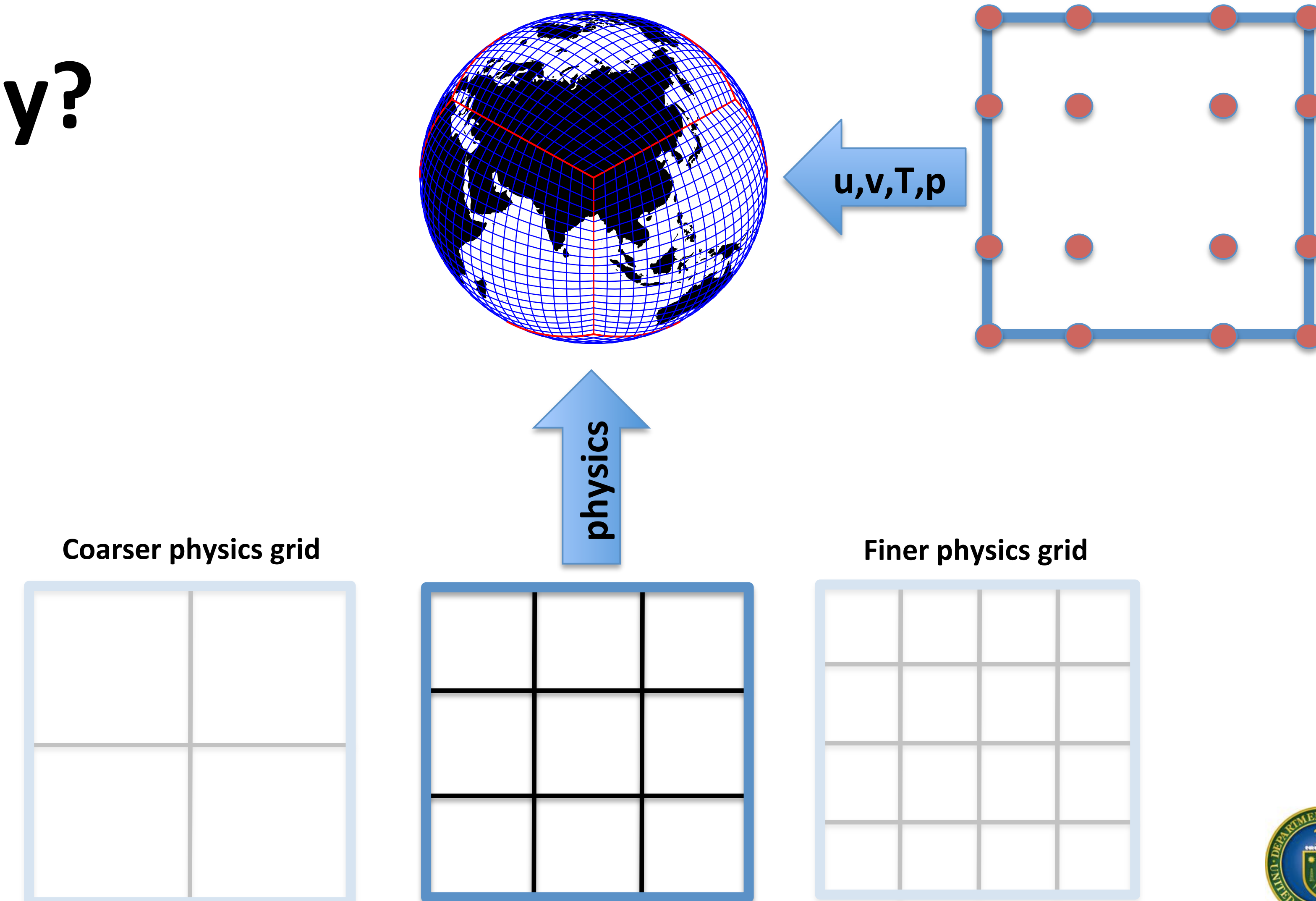


Performance: break-down of CSLAM algorithm



Part II: Coupling to physics

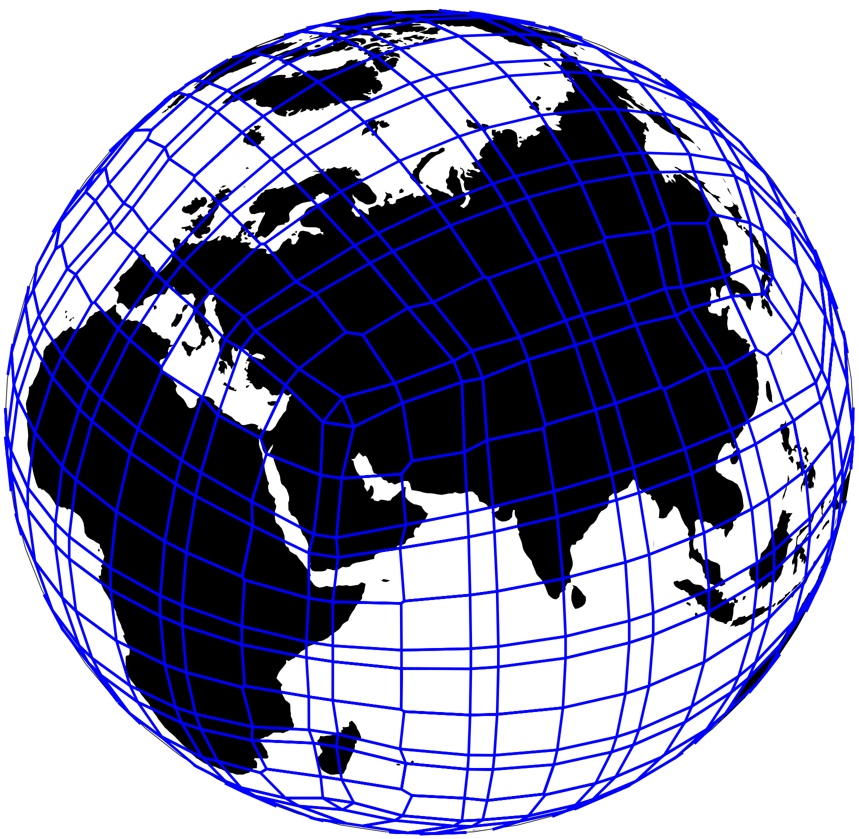
Why?

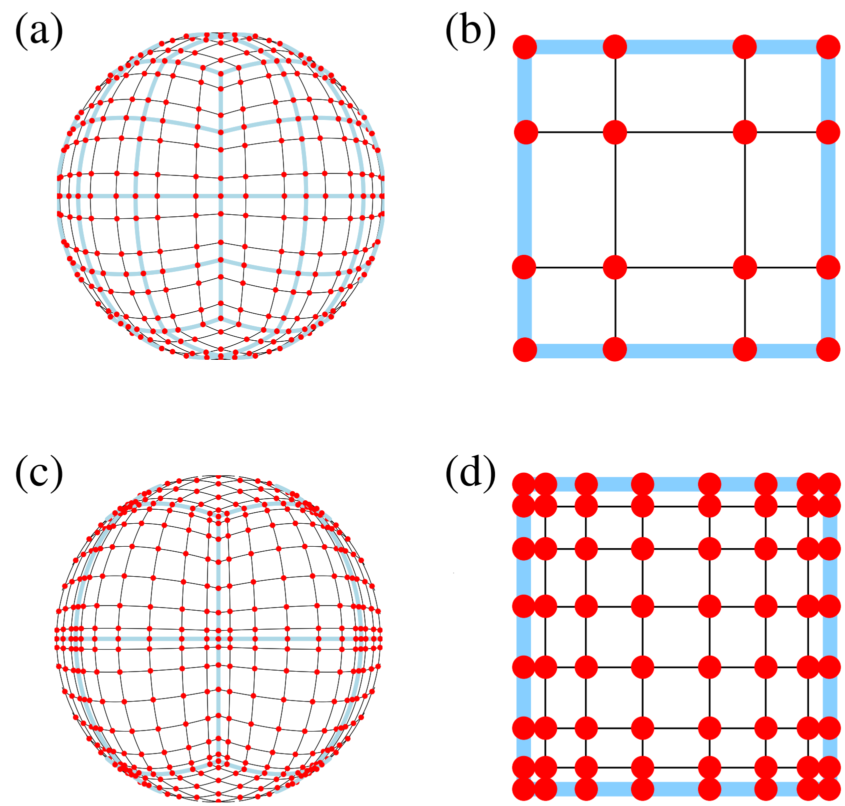


Non-uniform sampling of atmospheric state

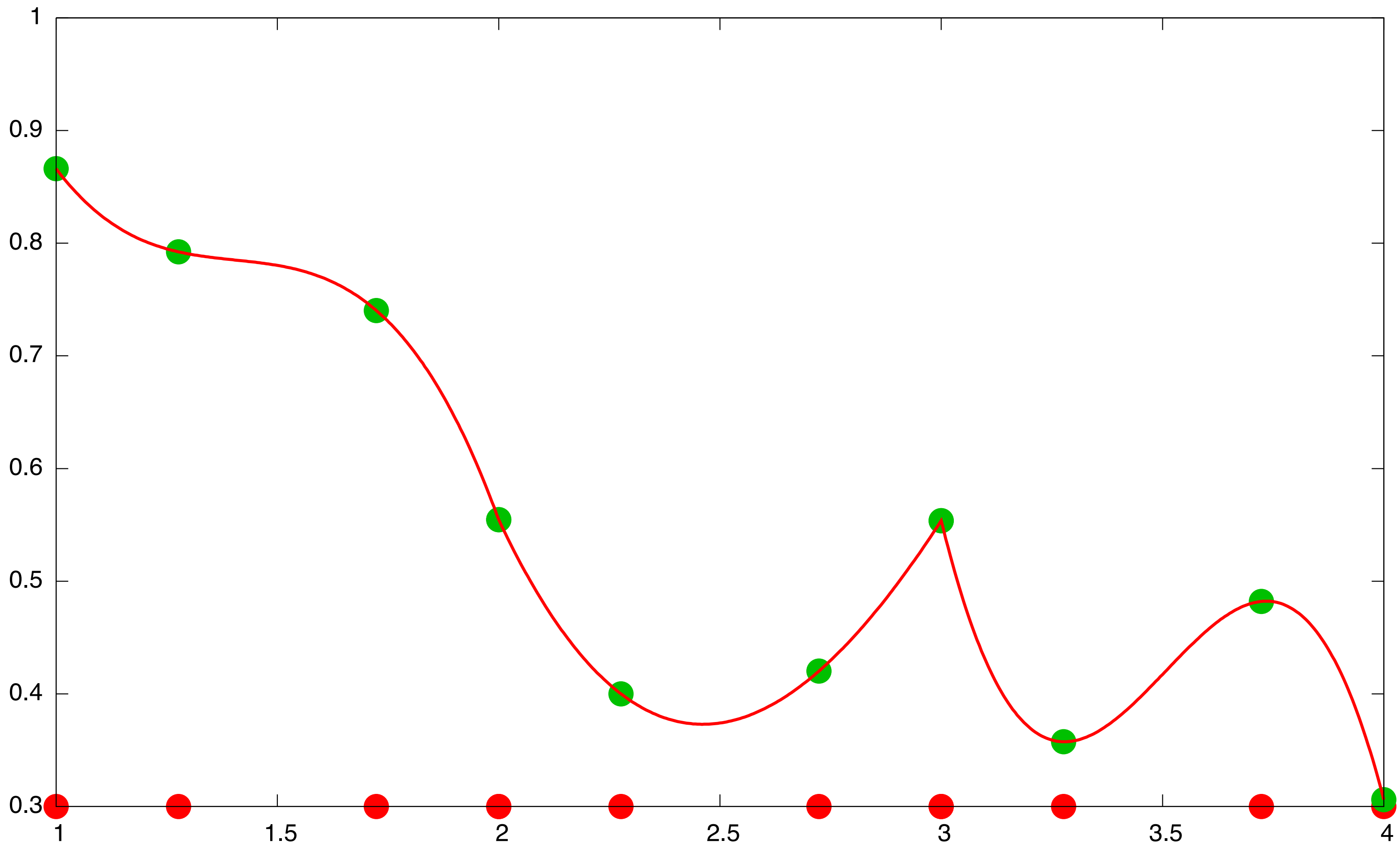
Gets worse with increasing order!

Current physics/“coupler” grid

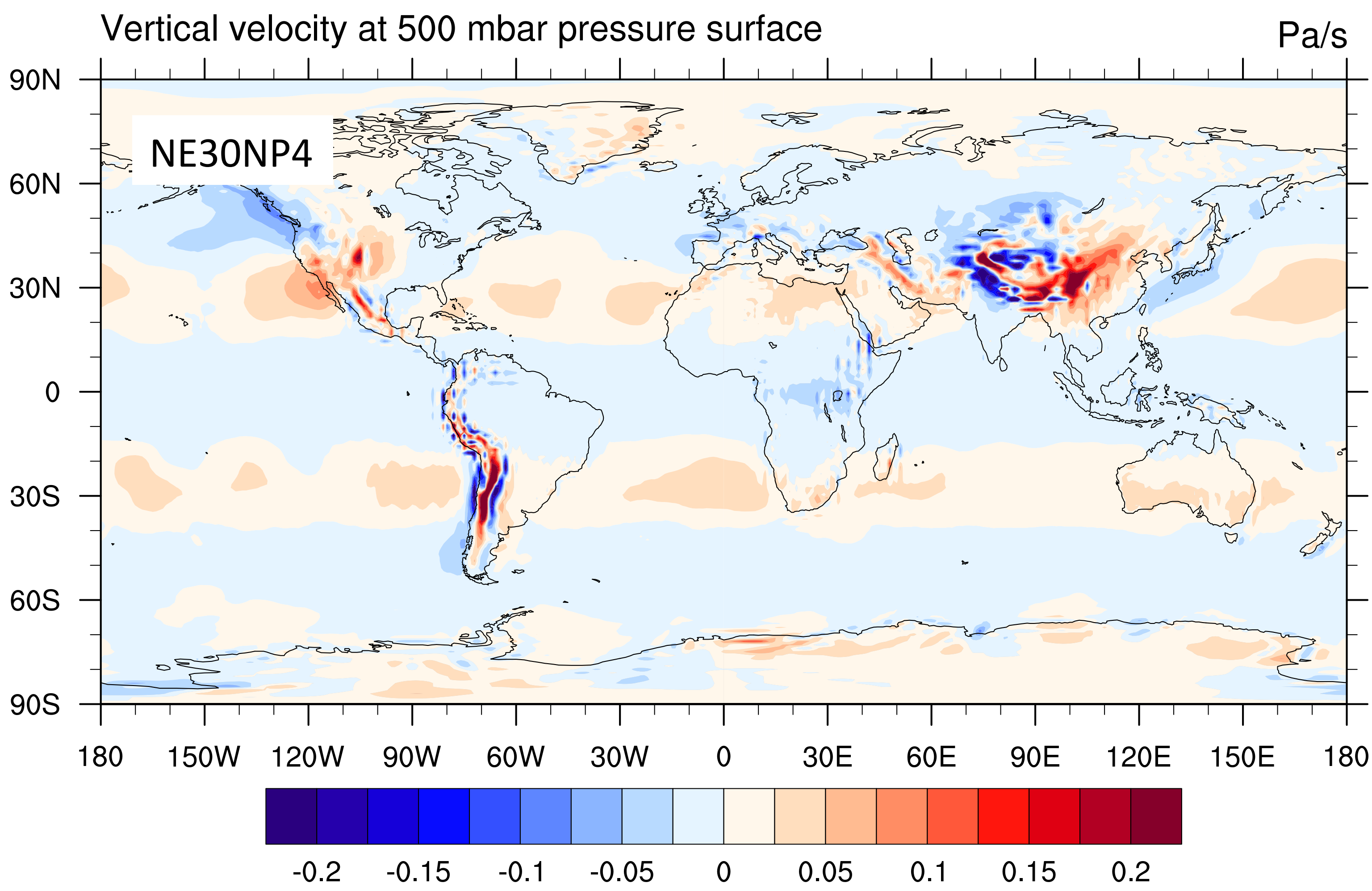




Grid-scale forcing



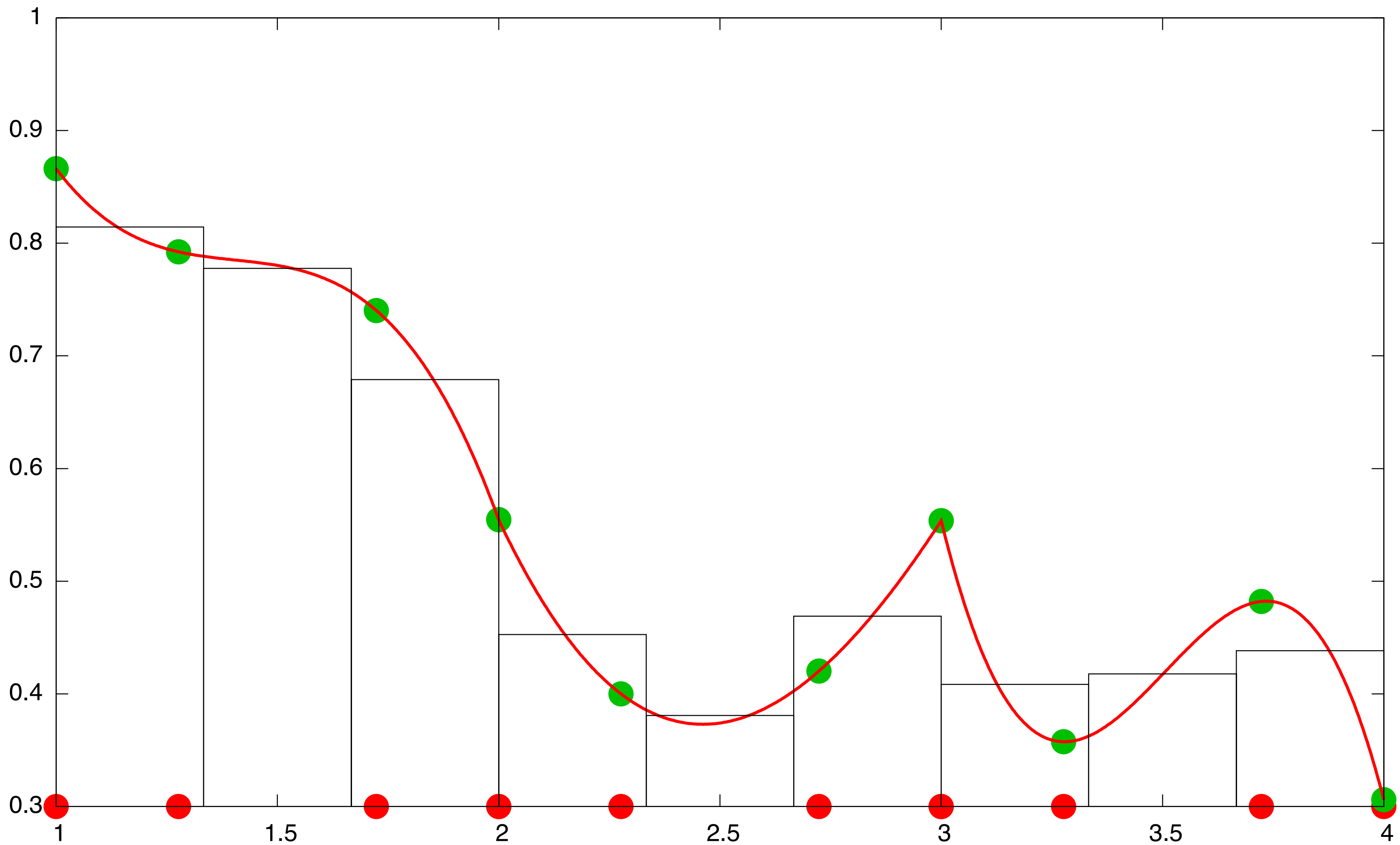
Held-Suarez with topography

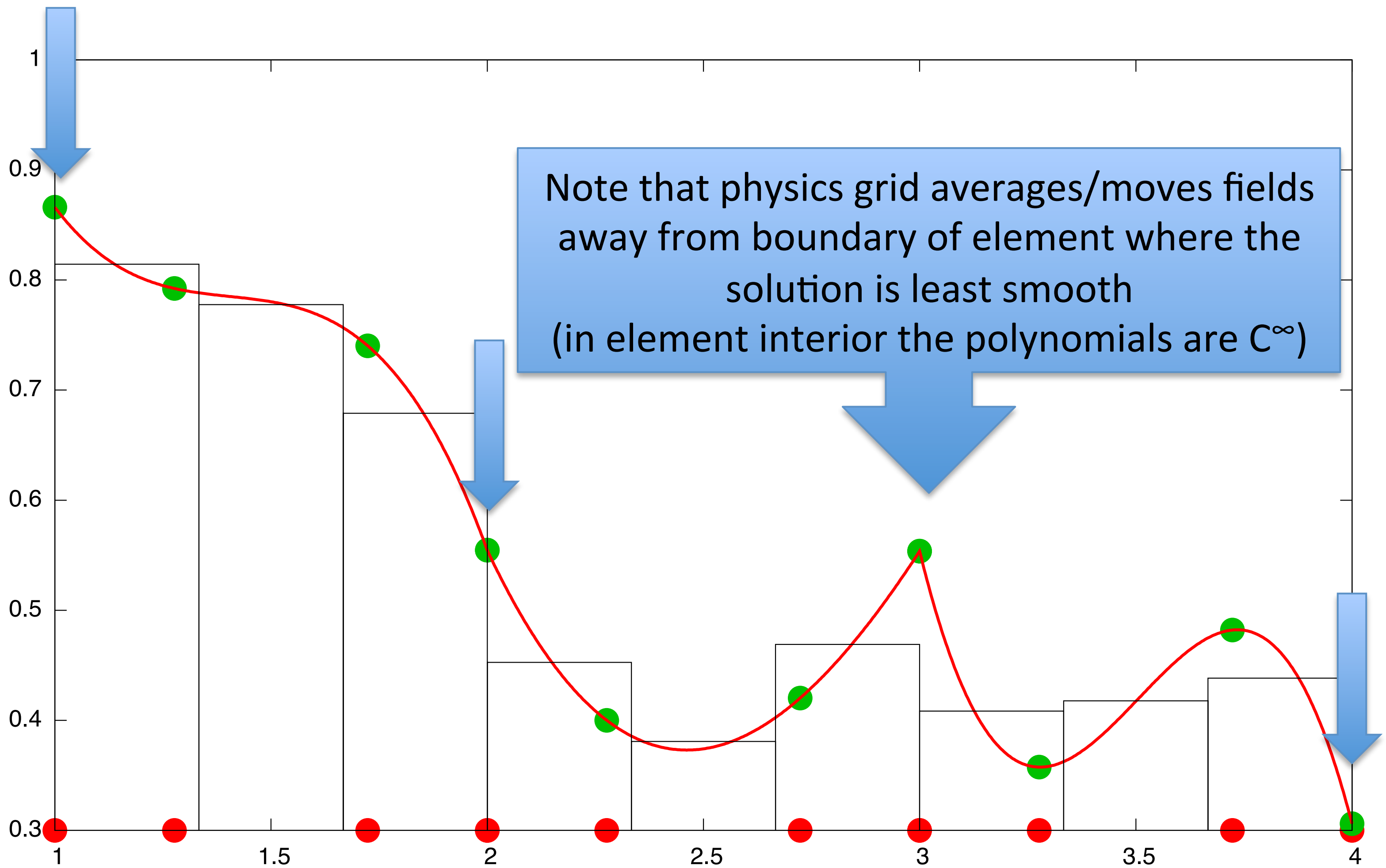


NCAR UCAR | National Center for Atmospheric Research Climate & Global Dynamics climate • models • society

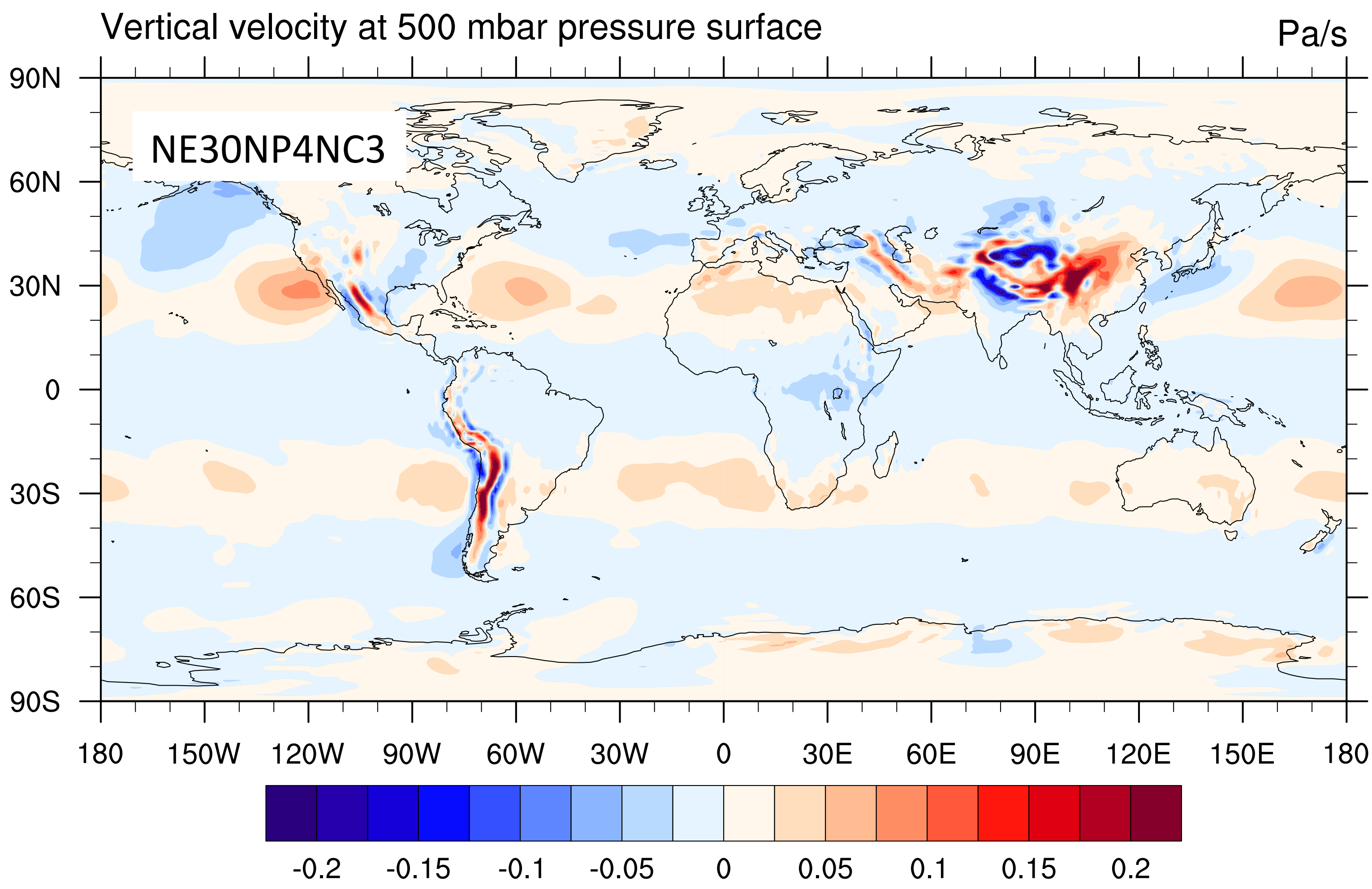
SciDAC
Scientific Discovery through
Advanced Computing

NSF




1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
1
1.5
2
2.5
3
3.5
4
Note that physics grid averages/moves fields away from boundary of element where the solution is least smooth
(in element interior the polynomials are C∞)

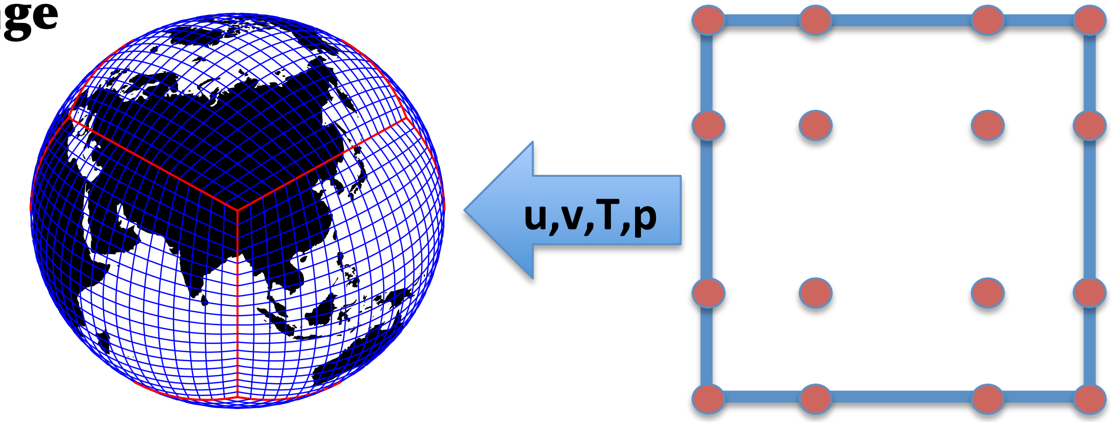
Held-Suarez with topography



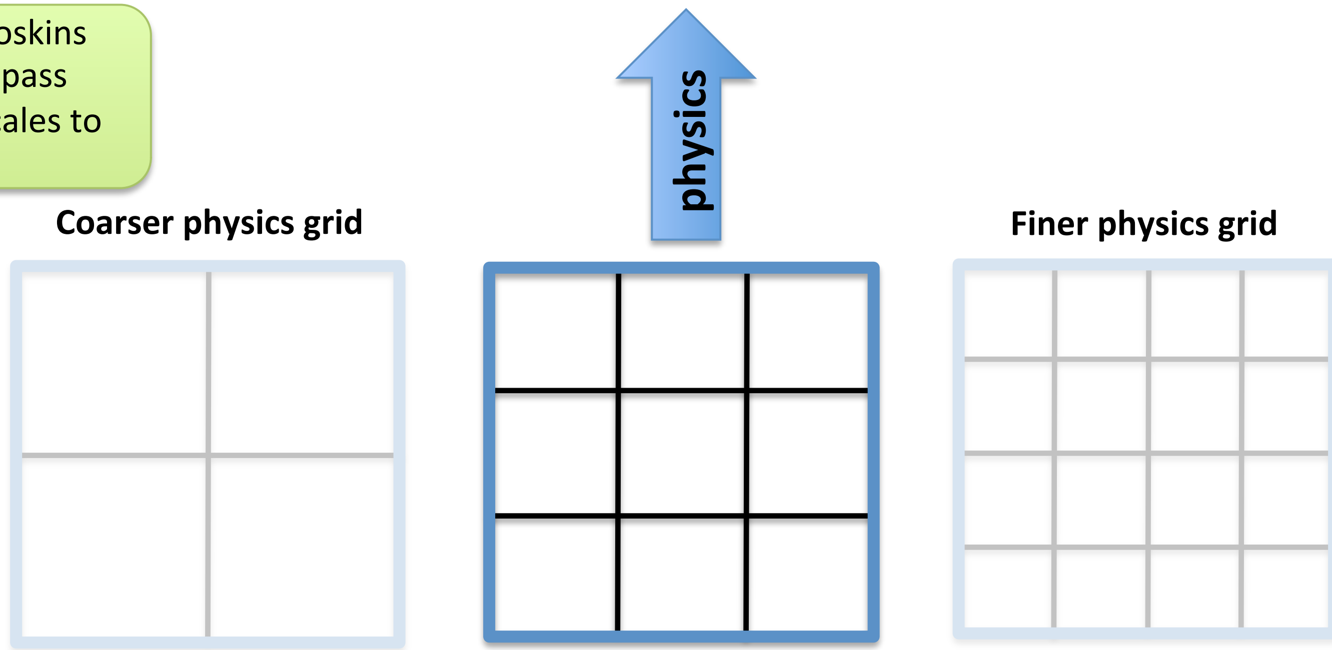
NCAR UCAR | National Center for Atmospheric Research | Climate & Global Dynamics | climate • models • society

CAM-SE-physgrid

- Implemented dry-mass vertical coordinates in CAM-SE (vertical levels do not change during physics-dynamics coupling)
- Inherently conservative mapping between grids (Ullrich and Taylor, 2015)
- Capability to run physics on 2x2,3x3,4x4,… grids



Lander and Hoskins (1997): only pass "believable" scales to physics!



Wet mass vertical coordinates

2.1. **Definition of vertical coordinate.** Consider a (wet mass) terrain following hybrid vertical coordinate where the pressure p is given by

$$p(\eta) = A(\eta)p_0 + B(\eta)ps, \tag{24}$$

where $A(\eta)$ and $B(\eta)$ define the vertical level spacing, p_0 the pressure at the top of the model atsmophere, and ps is the moist (full) surface pressure. We choose a floating vertical coordinate so that

$$\dot{\eta} = 0. \tag{25}$$

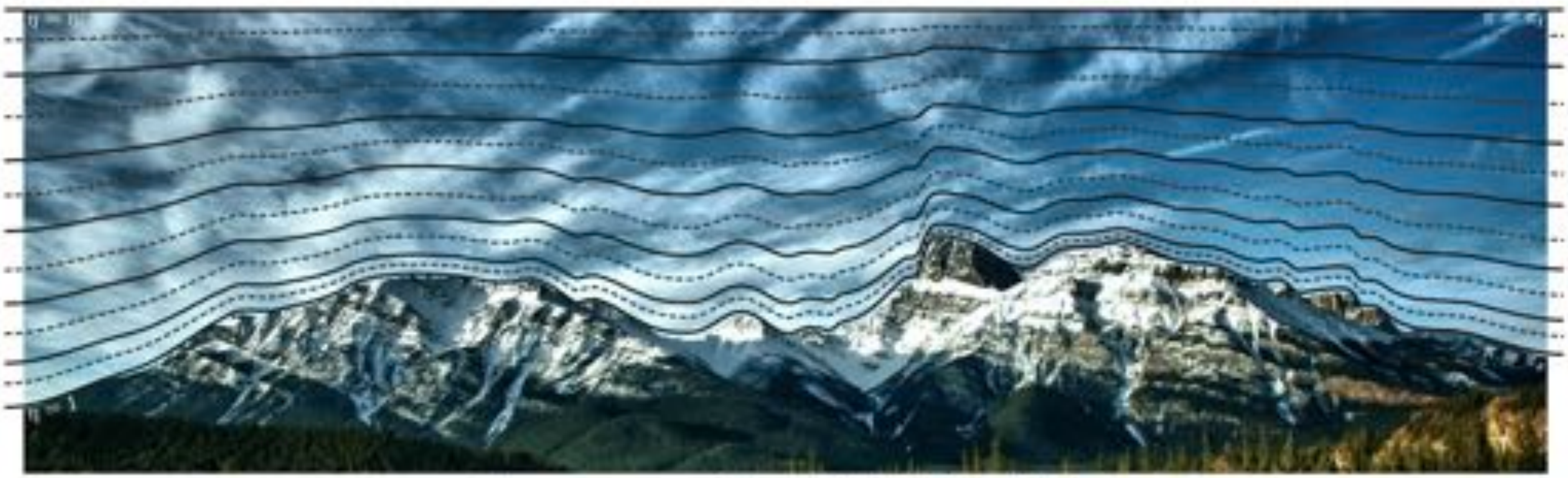
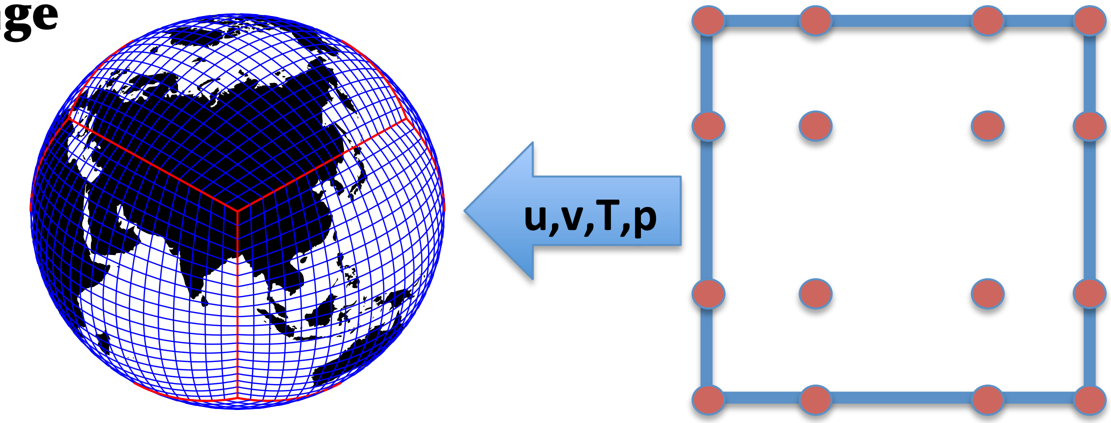


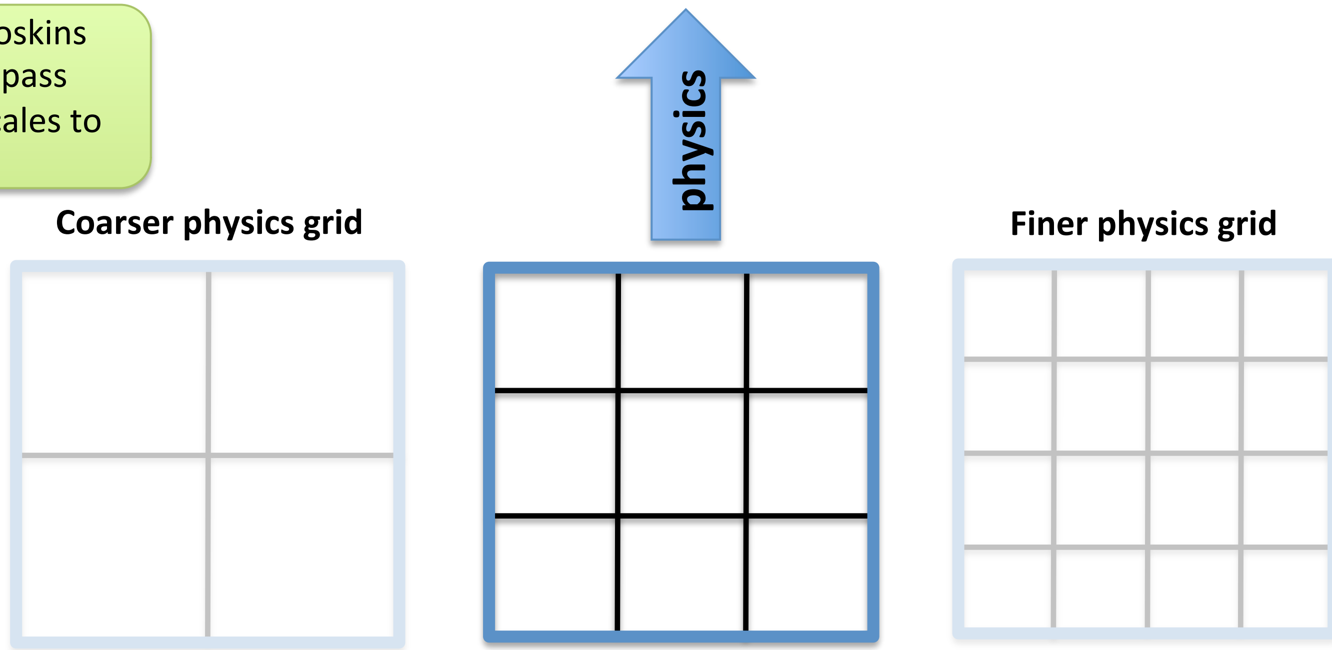
Figure courtesy of David Hall (CU Boulder).

CAM-SE-physgrid

- **Implemented dry-mass vertical coordinates in CAM-SE (vertical levels do not change during physics-dynamics coupling)**
- **Inherently conservative mapping between grids** **(Ullrich and Taylor, 2015)**
- **Capability to run physics on 2x2,3x3,4x4,... grids**



Lander and Hoskins (1997): only pass "believable" scales to physics!



Summary

- Presented algorithm to consistently couple spectral-element dynamics with remap finite-volume transport
- Accuracy is improved for "non-smooth" tracer distributions when using CAM-SE-CSLAM compared to CAM-SE.
- Note that our modeling framework is quite unique in the sense that we support finite-volume and high-order Galerkin methods in the same framework
- Capability to run physics on different grid than dynamics
- CAM-SE physgrid and CAM-SE-CSLAM (uses physgrid) are scheduled to be released with CESM2 later this year

More information: http://www.cgd.ucar.edu/cms/pel

Email: pel@ucar.edu