Mass-conserving and positive-definite semi-Lagrangian advection in NCEP GFS: *Decomposition for massively parallel computing without halo*

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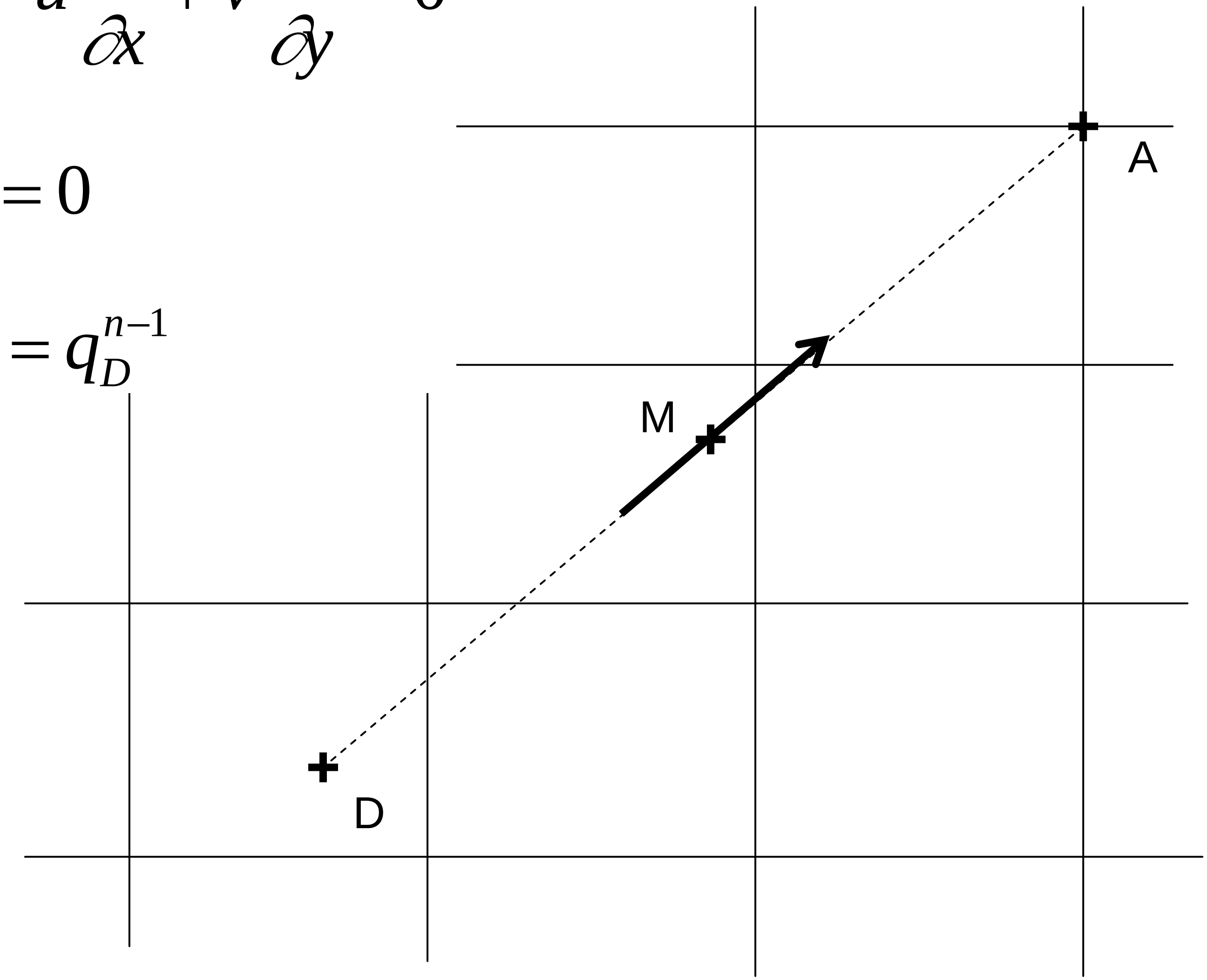
Introduction

- The common elements for traditional semi-Lagrangian method are
  - Iteration to find departure and/or mid-point values
  - Interpolation from regular grid points to departure and/or mid-points
  - Require halo grids in MPP
- Advantage of semi-Lagrangian Method
  - Allowable larger time step, saving time
  - Use linear grid in spectral model; same grid-point with higher resolution of spectral truncation

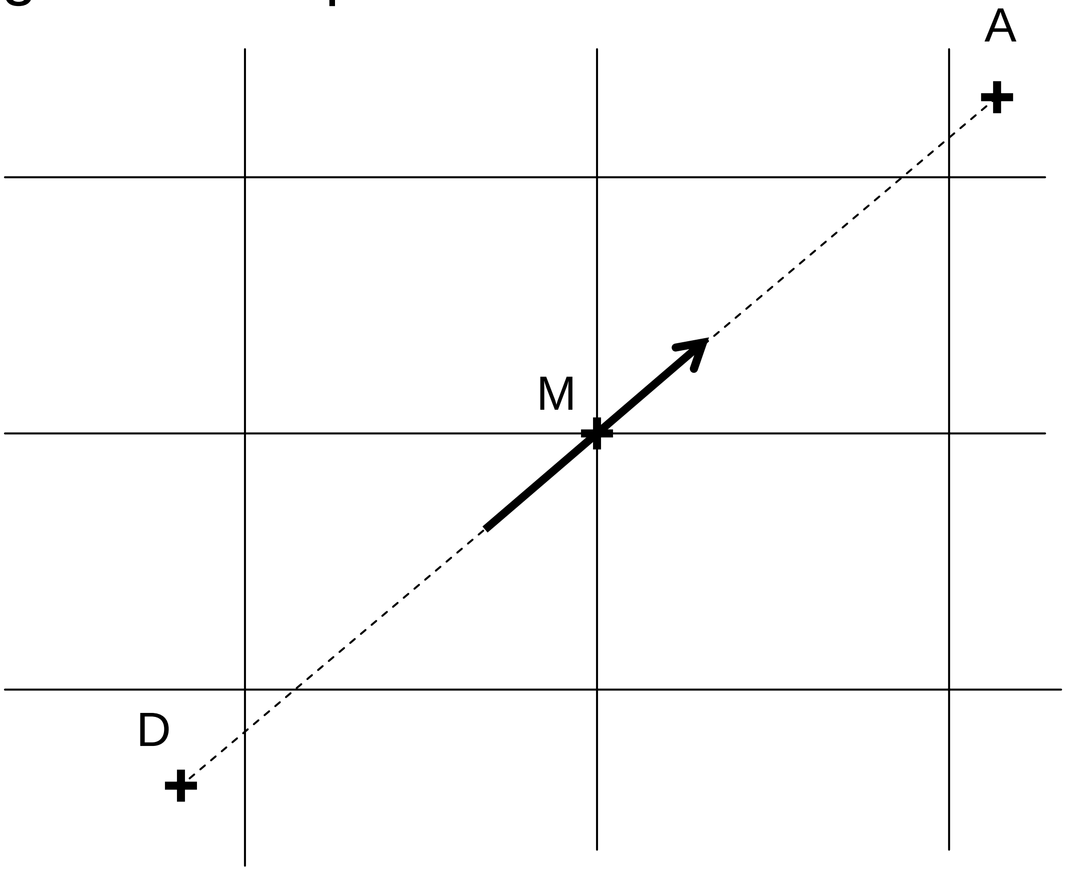
$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} = 0$$

$$\frac{Dq}{Dt} = 0$$

$$q_A^{n+1} = q_D^{n-1}$$



Starting from mid-point



No guessing and no iteration

but one 2-D interpolation and one 2-D remapping

Proposed Method

- Splitting semi-Lagrangian advection
  - advection in one direction first
  - then advection in another direction
  - temporal and spatial splitting
- Advantage
  - no guessing and no iteration
  - 1-D interpolation and remapping
  - possible no halo (with transpose)
  - incremental implementation
- Possible to add mass conservation and positive definite advection

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} = 0$$

$$\left(\frac{\partial q}{\partial t}\right)_{X-direction} + \left(\frac{\partial q}{\partial t}\right)_{Y-direction} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} = 0$$

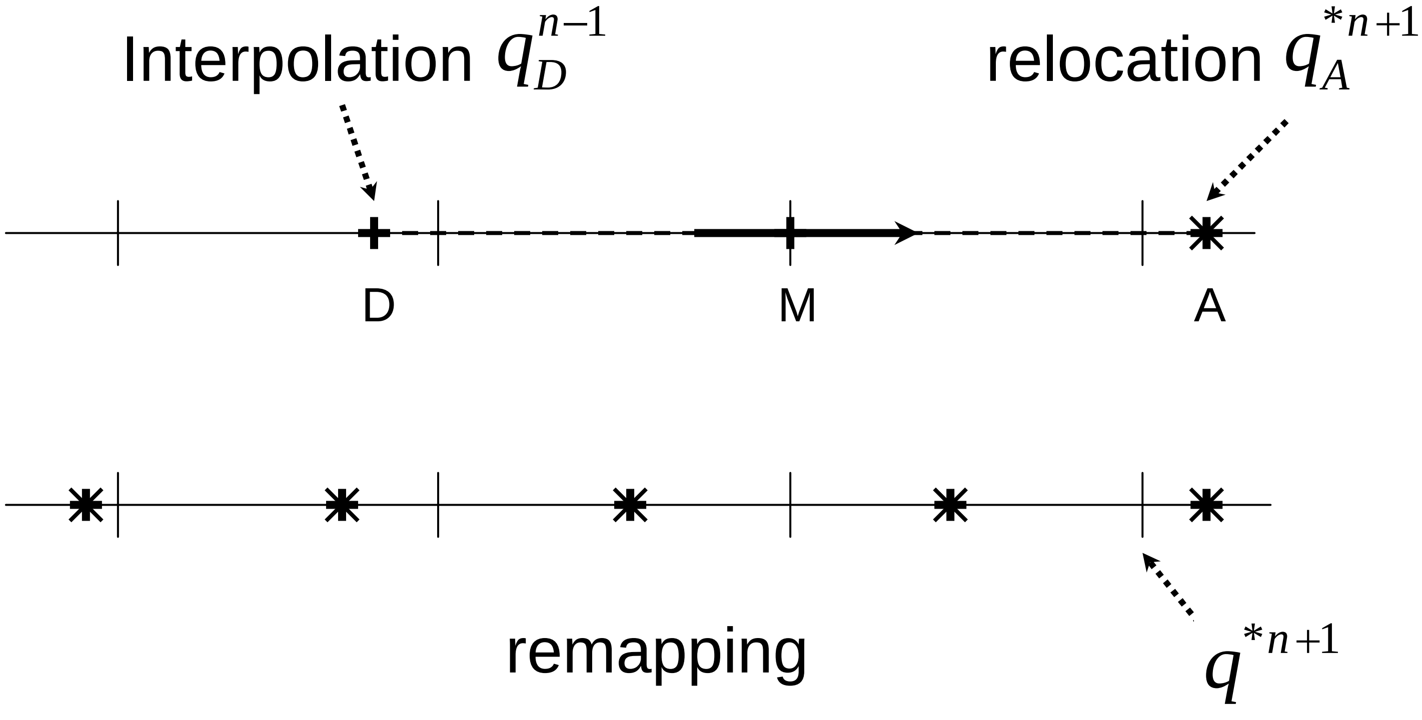
$$\left\langle\left(\frac{\partial q}{\partial t}\right)_{X-direction} + u\frac{\partial q}{\partial x}\right\rangle + \left\langle\left(\frac{\partial q}{\partial t}\right)_{Y-direction} + v\frac{\partial q}{\partial y}\right\rangle = 0$$

$$\left(\frac{Dq}{Dt}\right)_{X-direction} + \left(\frac{Dq}{Dt}\right)_{Y-direction} = 0$$

$$X_D = X_M - U_M \Delta t$$

$$X_A = X_M + U_M \Delta t$$

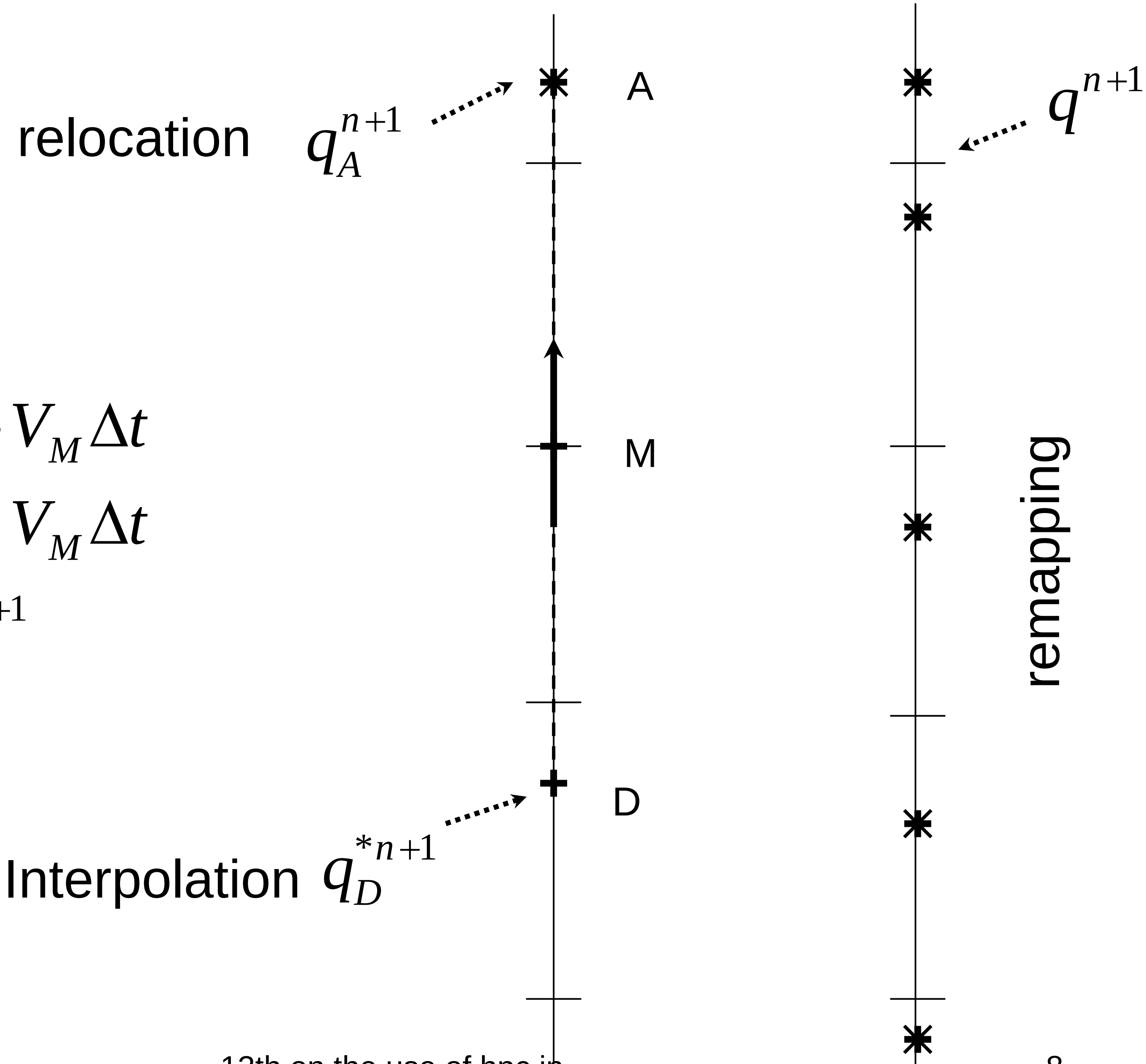
$$q_A^{*n+1} = q_D^{n-1}$$

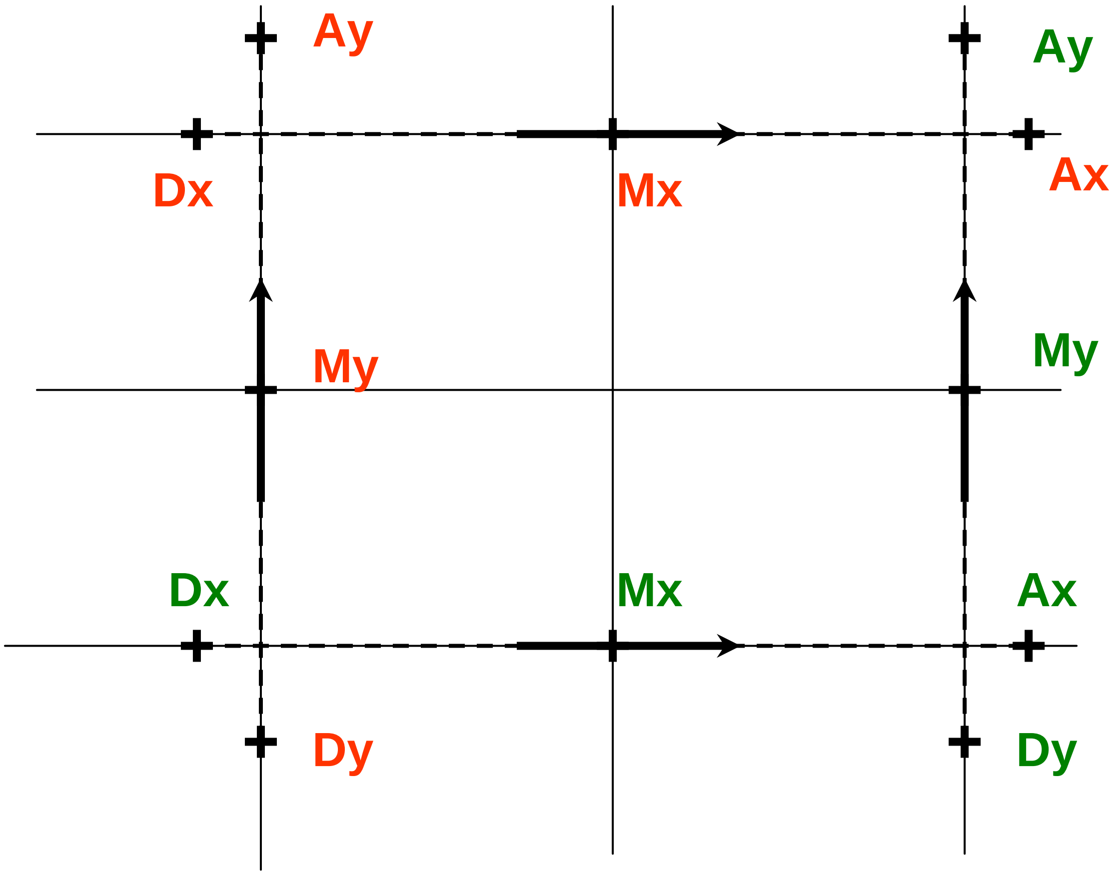


$$Y_D = Y_M - V_M \Delta t$$

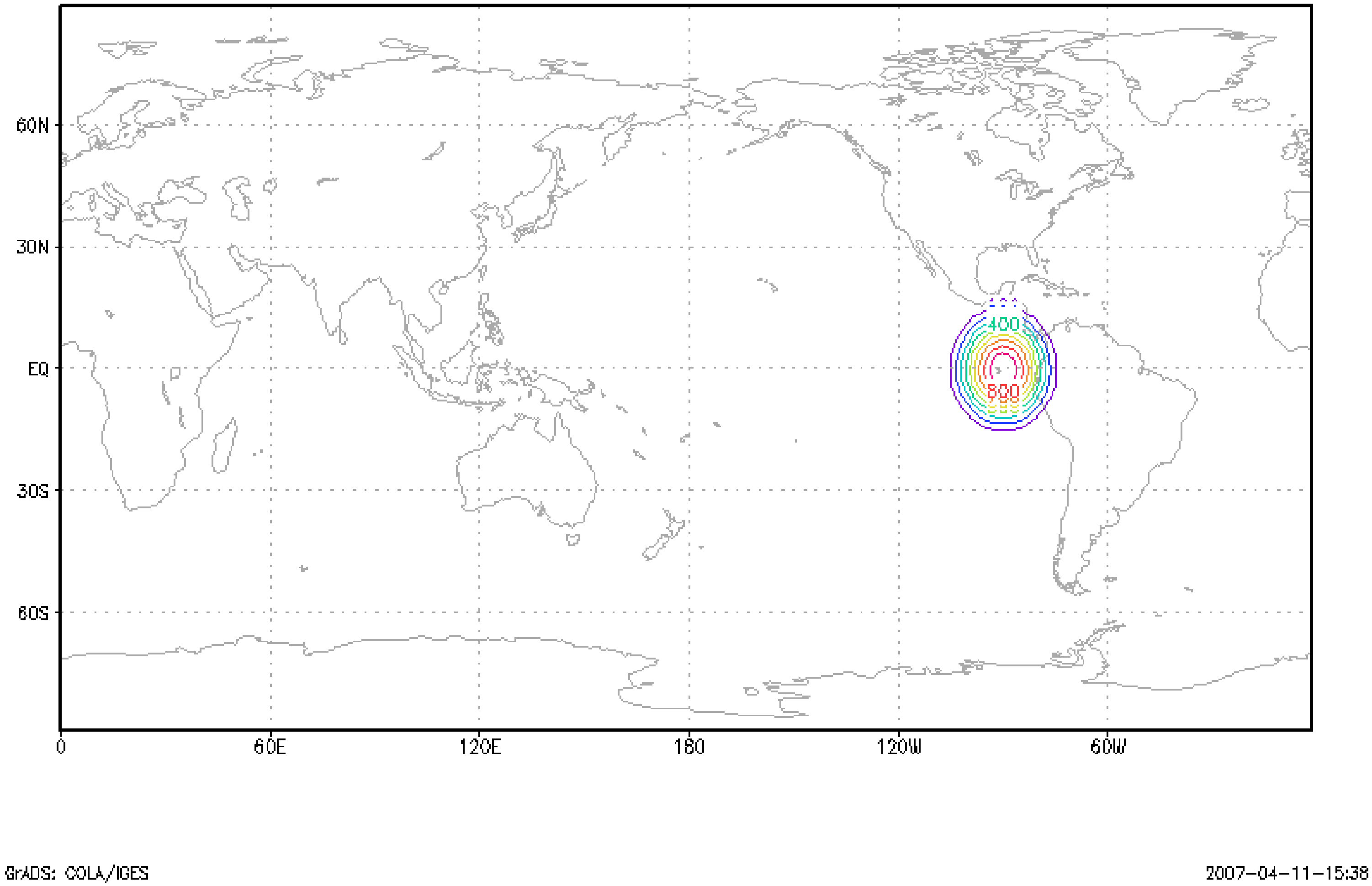
$$Y_A = Y_M + V_M \Delta t$$

$$q_A^{n+1} = q_D^{*n+1}$$

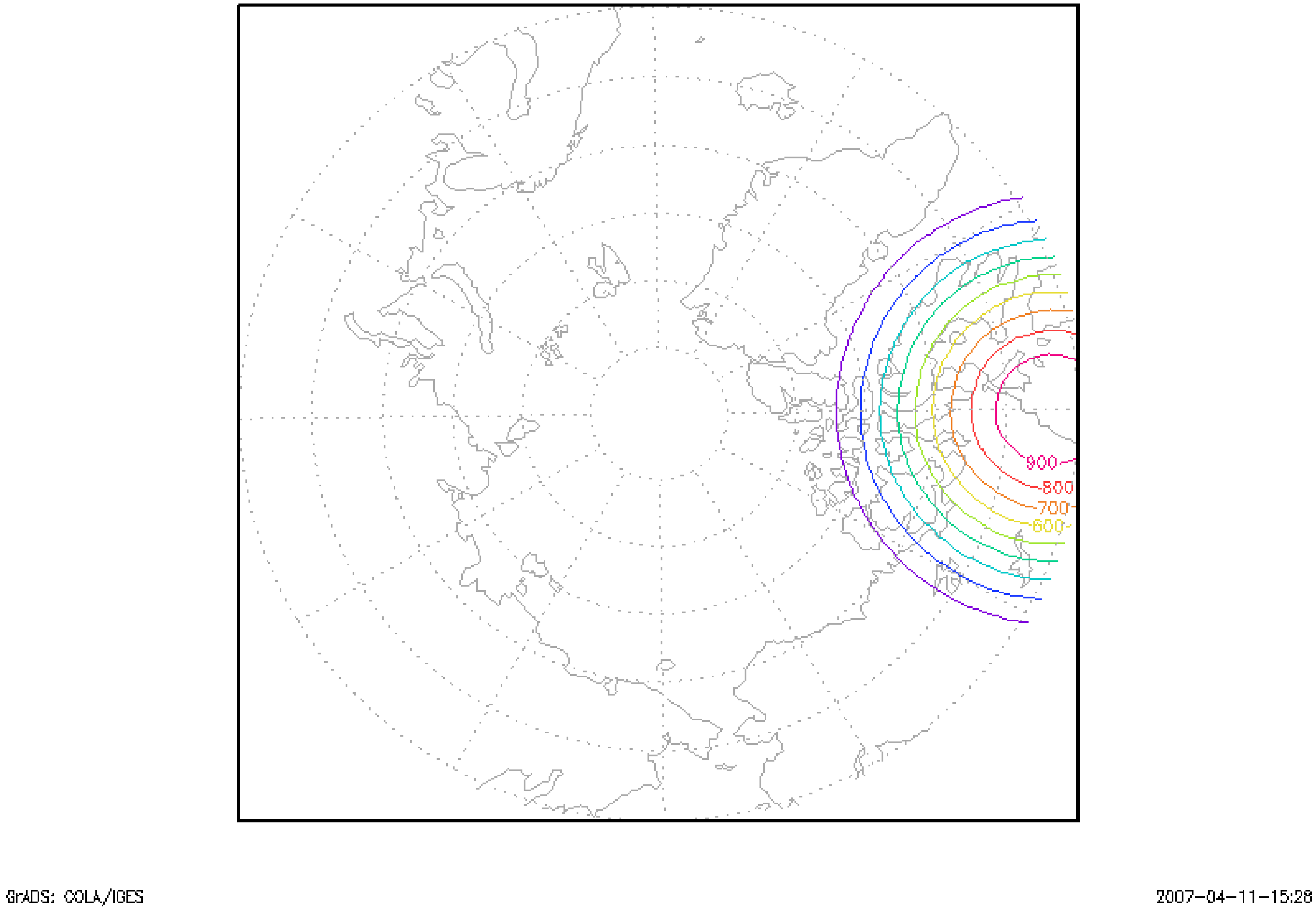



Ay
Ay
Dx
Mx
Ax
My
My
Dx
Mx
Ax
Dy
Dy

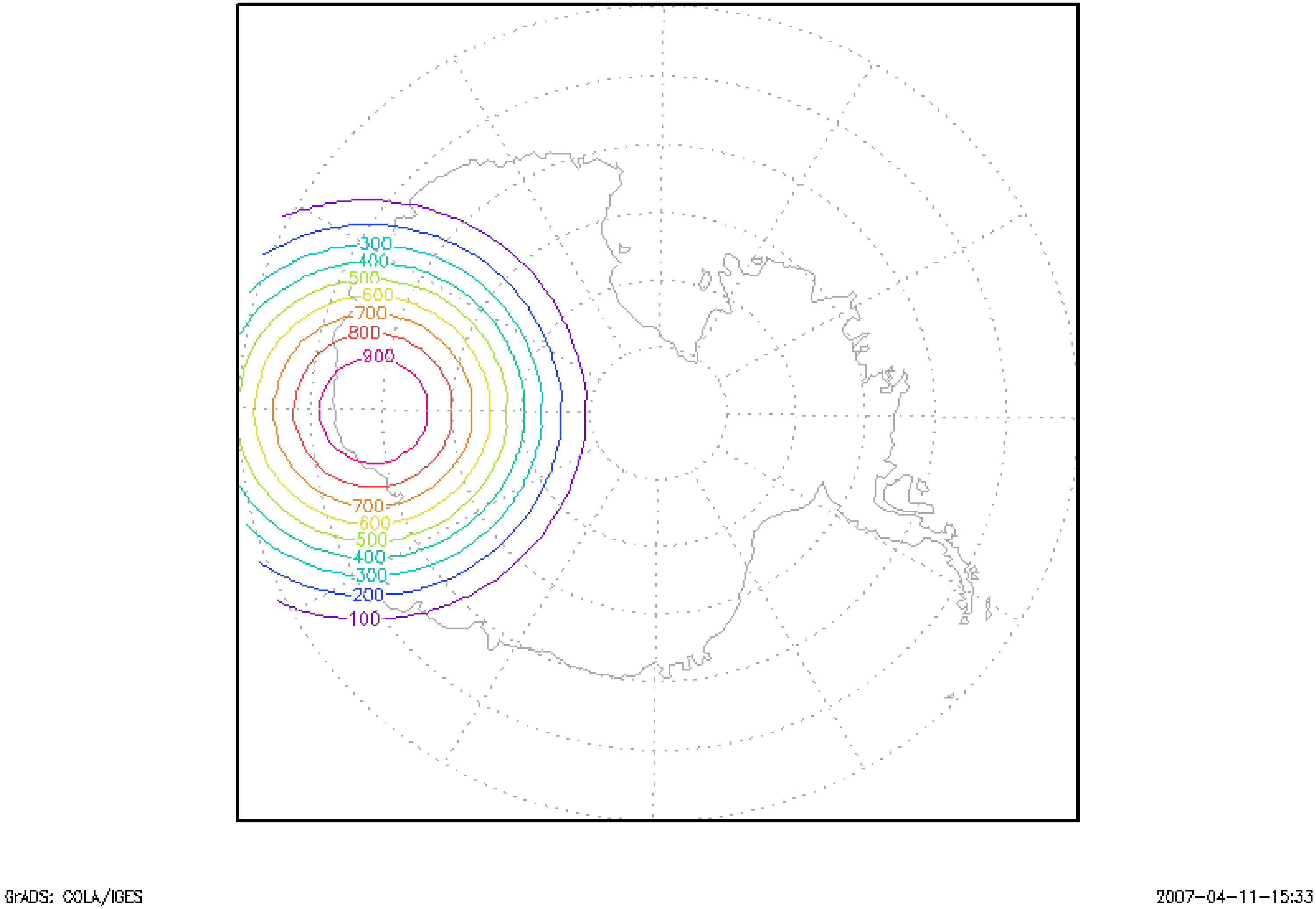
Gaussian 256 x 128 with time step of 1800 sec



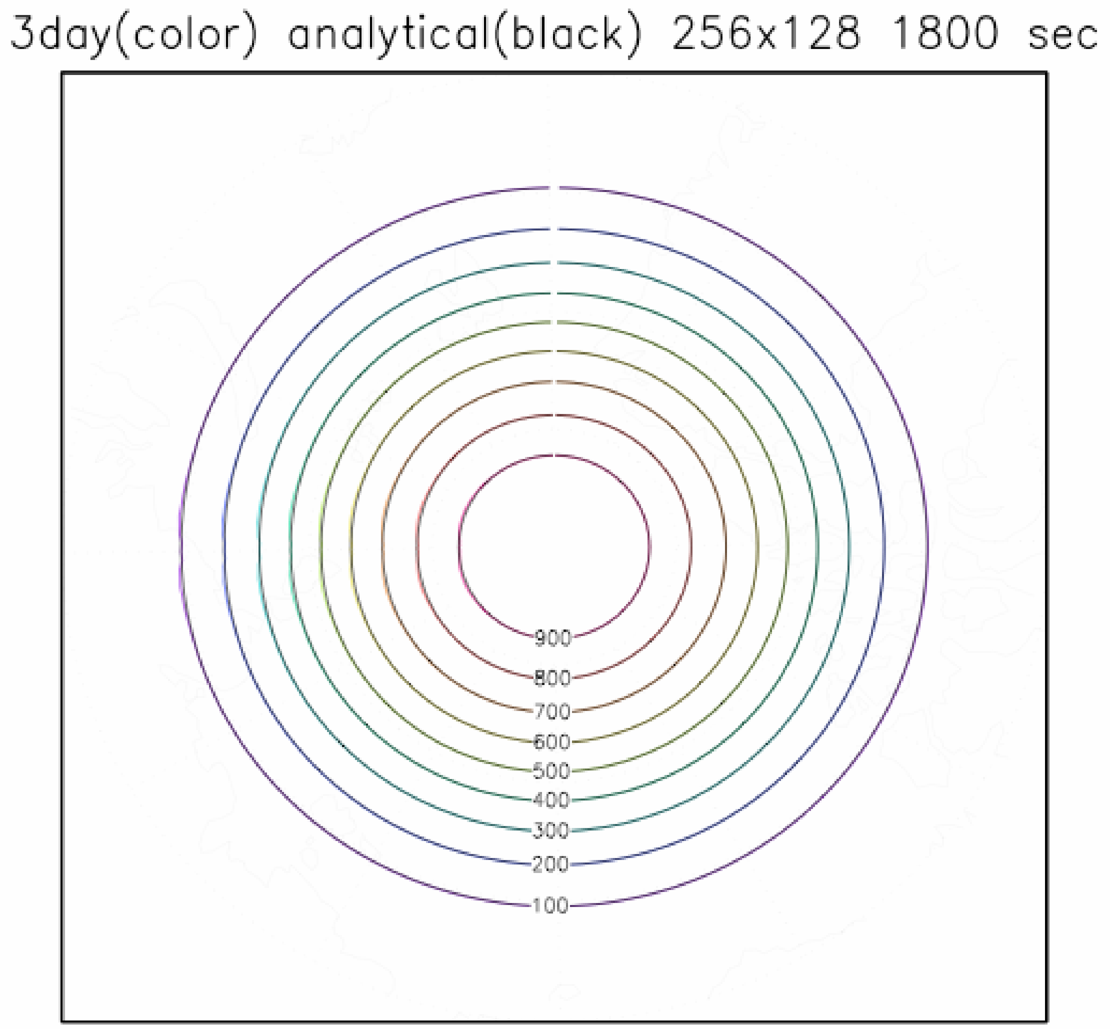
Gaussian 256 x 128 with time step of 1800 sec
Across north pole



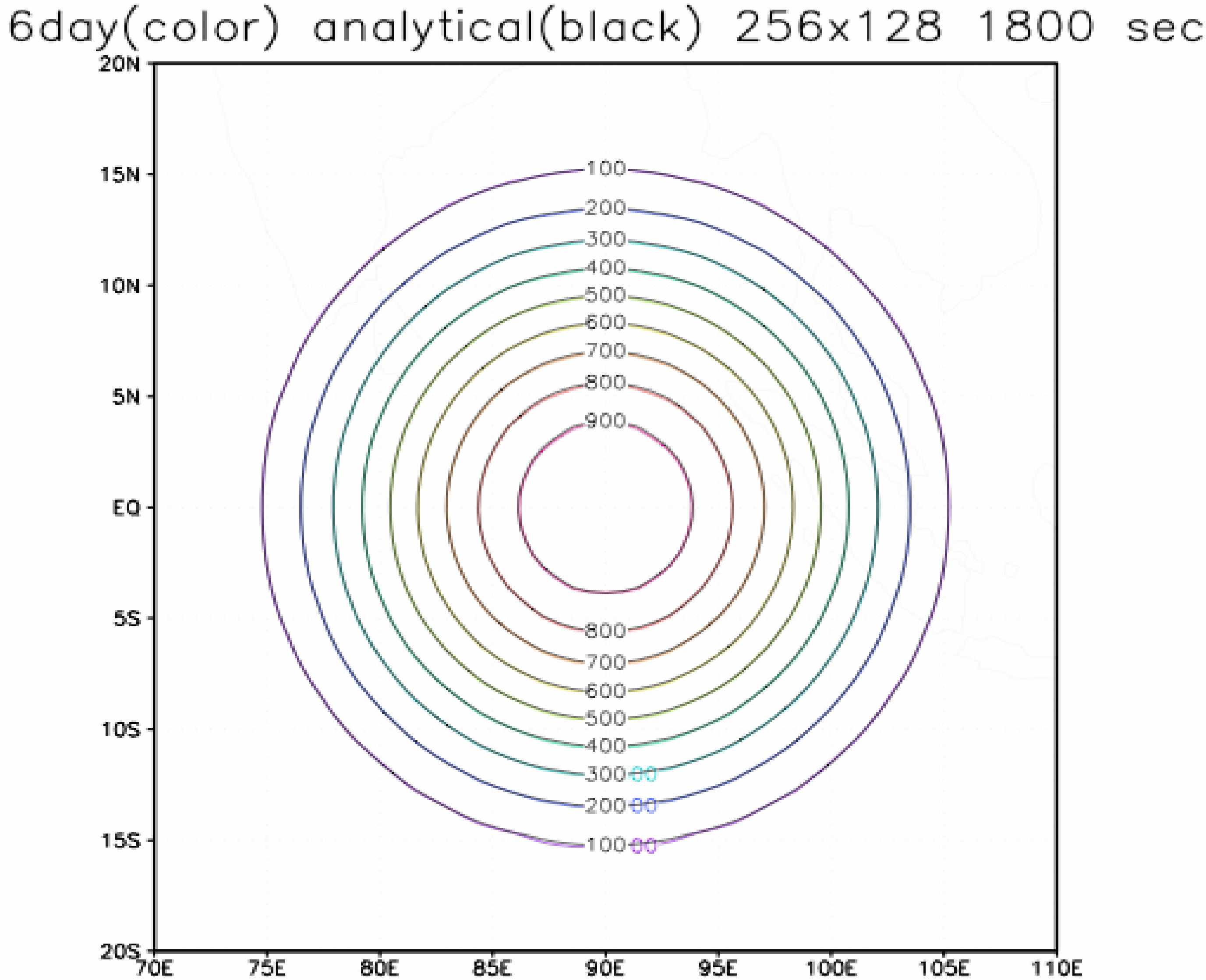
Gaussian 256 x 128 with time step of 1800 sec
Across south pole



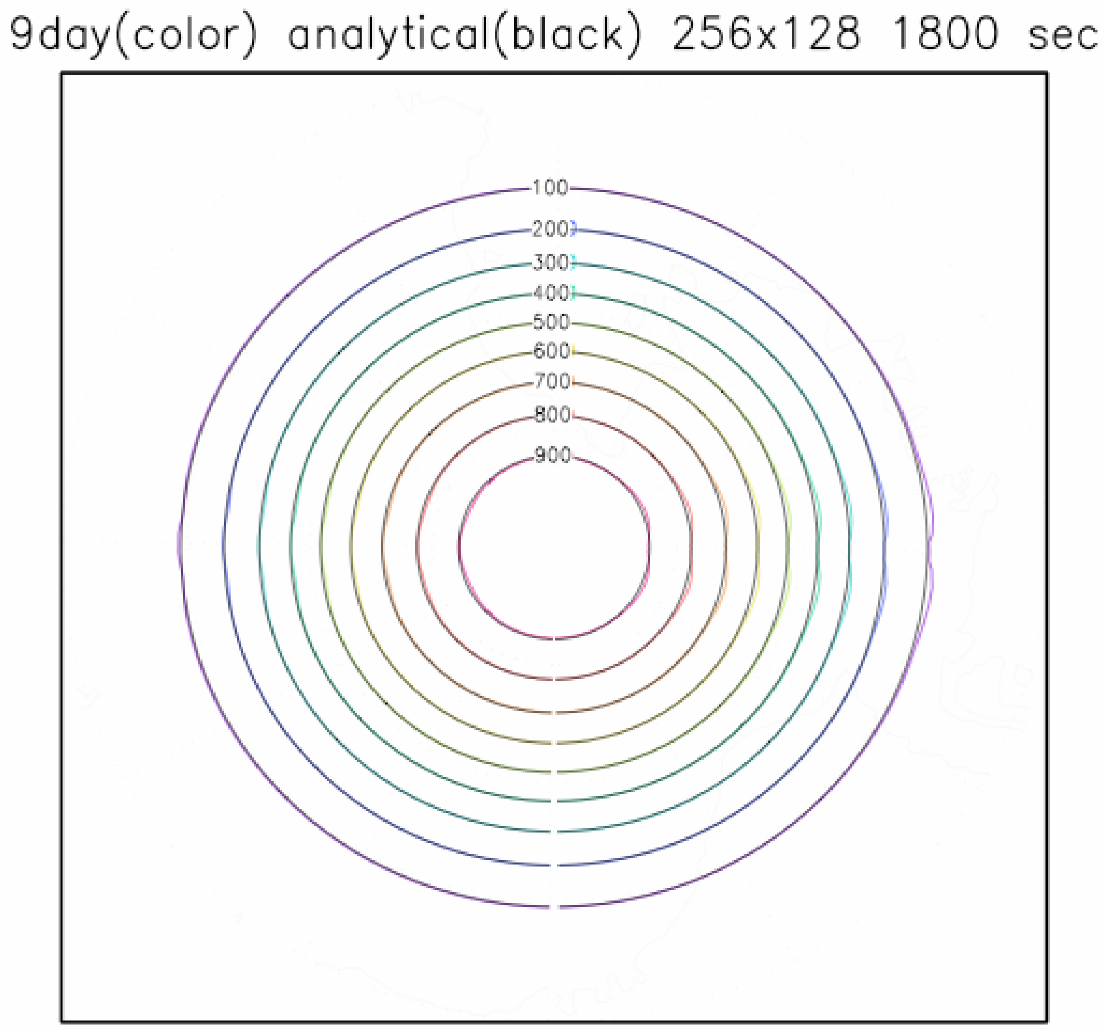
at north pole



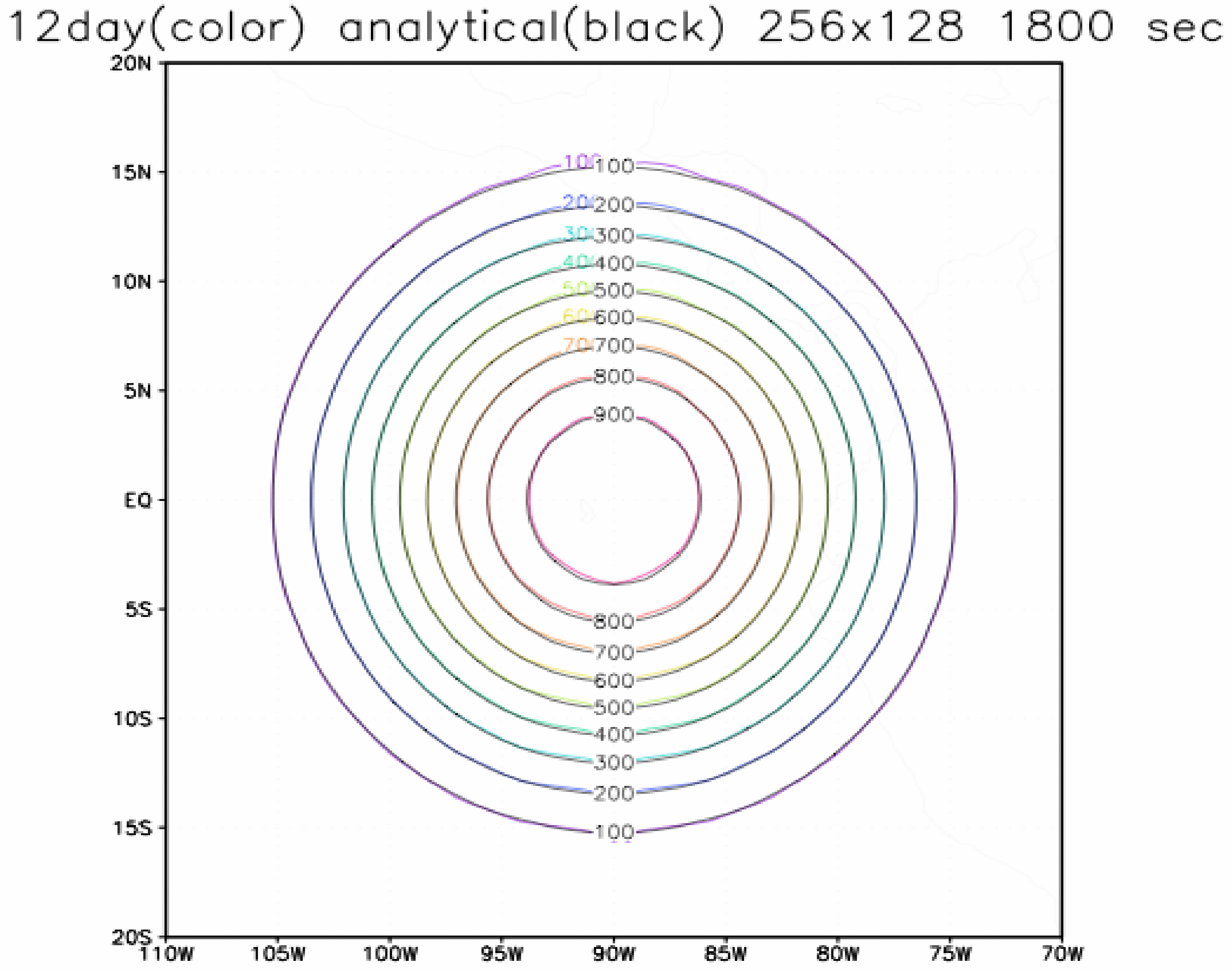
at equator


6day(color) analytical(black) 256x128 1800 sec
20N
15N
10N
5N
EQ
5S
10S
15S
20S
70E
75E
80E
85E
90E
95E
100E
105E
110E
100
200
300
400
500
600
700
800
900

at south pole



one complete revolution



$$L_1 = \frac{I\left[|q - q_T|\right]}{I\left[|q_T|\right]}$$

$$L_2 = \frac{\left\langle I\left[(q - q_T)^2\right]\right\rangle^{\frac{1}{2}}}{\left\langle I\left[(q_T)^2\right]\right\rangle^{\frac{1}{2}}}$$

$$L_\infty = \frac{Max\left[|q - q_T|\right]}{Max\left[|q_T|\right]}$$

$$\max = \frac{Max[q] - Max[q_T]}{Max[q_T] - Min[q_T]}$$

$$\min = \frac{Min[q] - Min[q_T]}{Max[q_T] - Min[q_T]}$$

where

$$I[A] = \frac{1}{4\pi a^2} \iint_{\phi\lambda} A \cos\phi \, d\phi \, d\lambda$$

$$Max[A] = global\_\mathrm{max}\_of\_A$$

$$Min[A] = global\_\mathrm{min}\_of\_A$$

Compare Errors

	min	max	L_1	L_2	L_∞
FFSL-5 128x64	-1.3E-3	-0.053	0.047	0.041	0.053
FFSL-3 256x128	-5.82E-4	0.040	0.020	0.020	0.040
NISL 128x64	-2.26E-4	-0.017	0.037	0.050	0.052
NISL 256x128	-7.67E-5	-0.0021	0.018	0.013	0.014
NISL 512x256	-2.72E-5	-0.00026	0.0053	0.0046	0.0070

For mass conservation, let's start from continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho \dot{\zeta}}{\partial \zeta} = 0$$

$$\left\langle \left(\frac{\partial \rho}{\partial t} \right)_{(X)} + \frac{\partial \rho u}{\partial x} \right\rangle + \left\langle \left(\frac{\partial \rho}{\partial t} \right)_{(Y)} + \frac{\partial \rho v}{\partial y} \right\rangle + \left\langle \left(\frac{\partial \rho}{\partial t} \right)_{(Z)} + \frac{\partial \rho \dot{\zeta}}{\partial \zeta} \right\rangle = 0$$

Consider 1-D and rewrite it in advection form, we have

$$\left(\frac{\partial \rho}{\partial t} \right)_{(X-direction)} + u \frac{\partial \rho}{\partial x} = -\rho \frac{\partial u}{\partial x}$$

Advection form is for semi-Lagrangian,
but it is not conserved if divergence is treated as force at mid-point,
So divergence term should be treated with advection

Divergence term in Lagrangian sense is the change of the volume if mass is conserved, so we can write divergence form as

$$\left(\frac{\partial u}{\partial x}\right)_{Lagrangian\_sense} = \frac{1}{\Delta_x}\frac{d\Delta_x}{dt}$$

Put it into the previous continuity equation, we have

$$\left(\frac{d\rho\Delta_x}{dt}\right)_{X-direction} = 0$$

$$\left(\frac{\partial\rho\Delta_x}{\partial t}\right)_{X-direction} + u\frac{\partial\rho\Delta_x}{\partial x} = 0$$

which can be seen as $\left(\rho\Delta_x\right)_{departure} = \left(\rho\Delta_x\right)_{arrival}$

How about mass conservation for tracer ?

If we use tracer and continuity equation as following together

$$\frac{\partial q}{\partial t}+u\frac{\partial q}{\partial x}+v\frac{\partial q}{\partial y}+\dot{\zeta}\frac{\partial q}{\partial \zeta}=0$$

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x}+\frac{\partial \rho v}{\partial y}+\frac{\partial \rho \dot{\zeta}}{\partial \zeta}=0$$

Then density weighted tracer can be treated as conservation as

$$\frac{\partial \rho q}{\partial t}+\frac{\partial \rho q u}{\partial x}+\frac{\partial \rho q v}{\partial y}+\frac{\partial \rho q \dot{\zeta}}{\partial \zeta}=0$$

Combine it with continuity equation, we can have conserved tracer advection

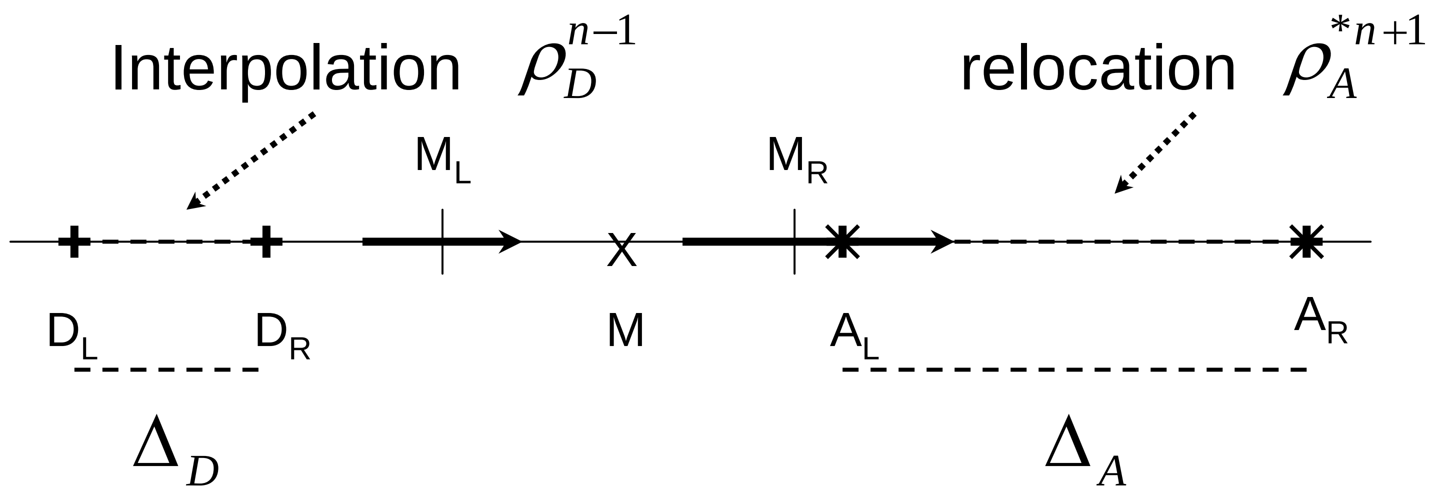
$$\frac{d\rho q\Delta}{dt}=0 \qquad \frac{d\rho\Delta}{dt}=0$$

We do

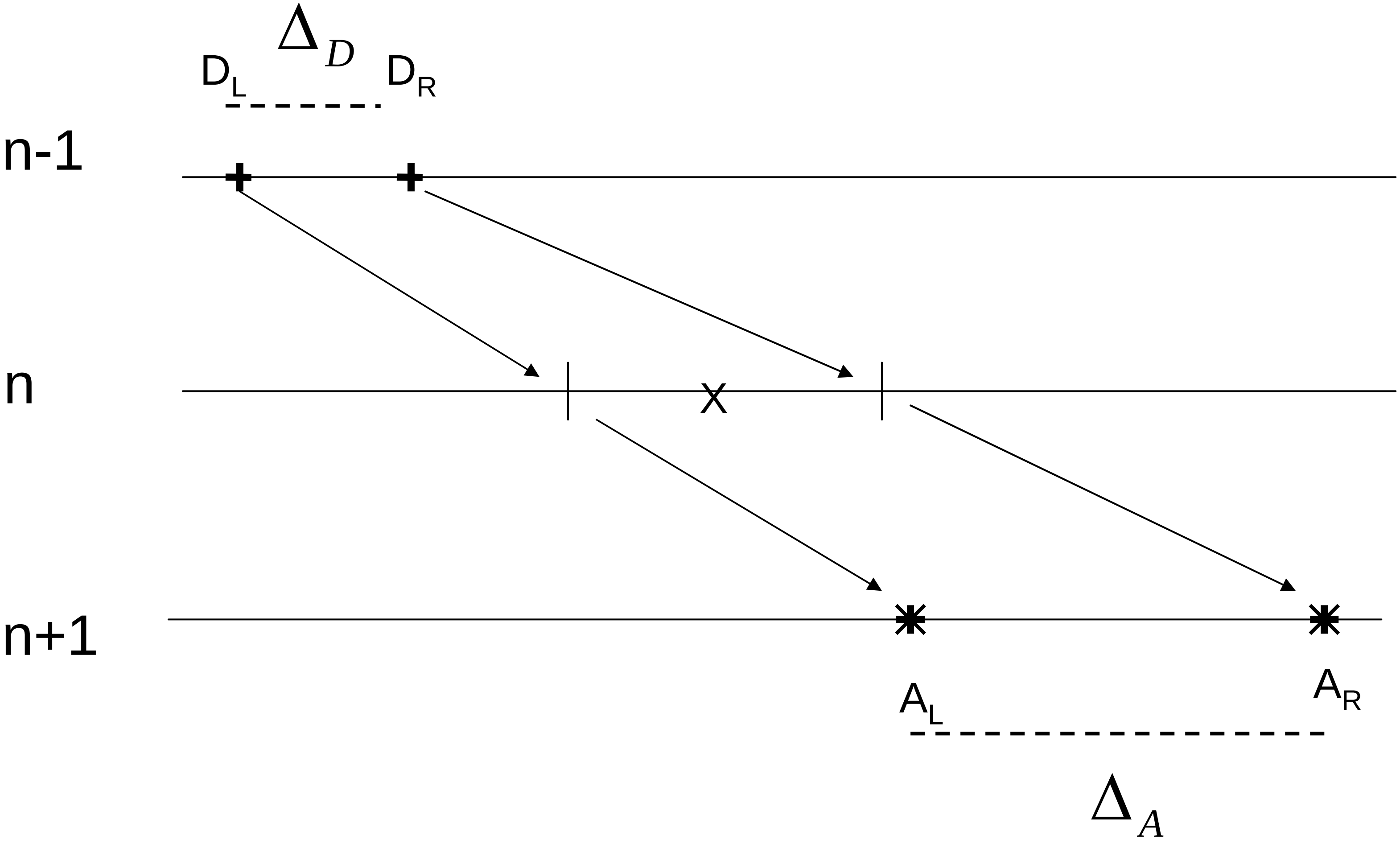
$$X_L^D = X_L^M - U_L^M \Delta t \qquad X_L^A = X_L^M + U_L^M \Delta t$$

$$X_R^D = X_R^M - U_R^M \Delta t \qquad X_R^A = X_R^M + U_R^M \Delta t$$

$$\Delta_D = X_R^D - X_L^D \qquad \Delta_A = X_R^A - X_L^A$$



$$\rho_D^{n-1} \Delta_D = \rho_A^{n+1} \Delta_A$$



$$\rho_D^{n-1}\Delta_D = \rho_A^{n+1}\Delta_A$$

The given value can be presented piece-wisely by

$$\rho = S(x)$$

so the previous mass equality can be replaced as following

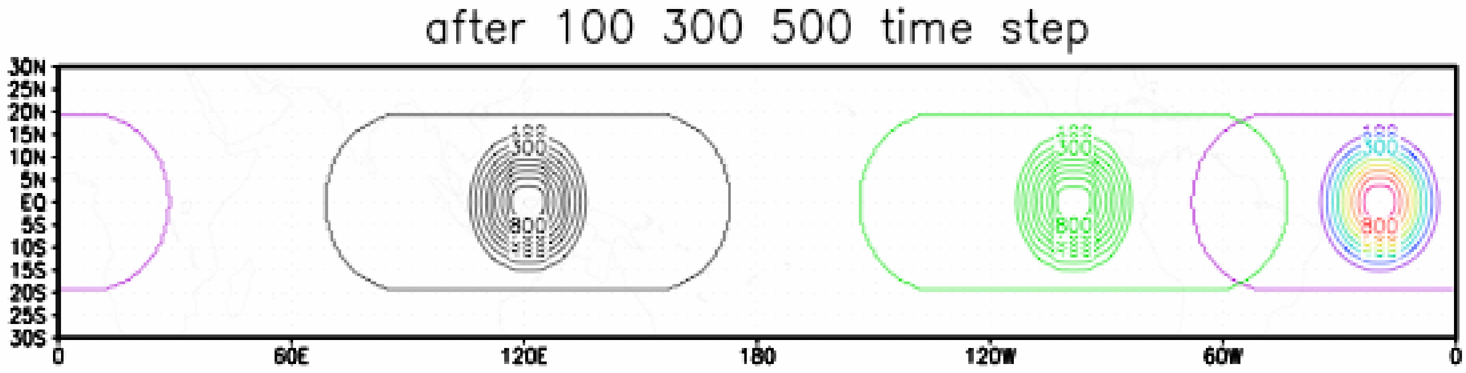
$$\int_{D_L}^{D_R} S_D^{n-1}(x)dx = \int_{A_L}^{A_R} S_A^{n+1}(x)dx$$

Also we want to make sure that total mass is conserved as

$$\oint S_R^{n-1}(x)dx = \oint S_D^{n-1}(x)dx = \oint S_A^{n+1}(x)dx = \oint S_R^{n+1}(x)dx$$

where subscript R is regular grid
D is departure grid
A is arrival grid for

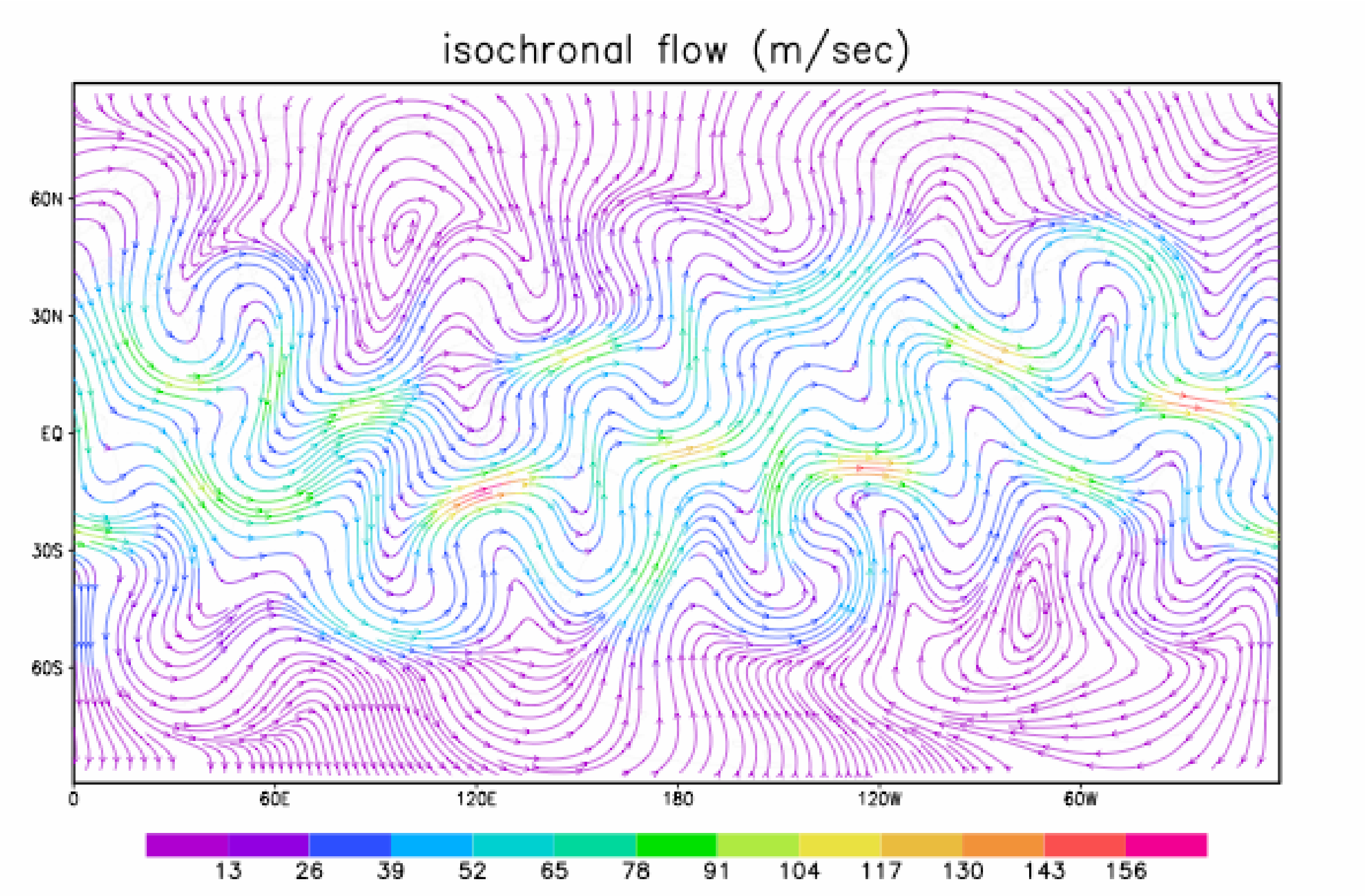
This implies that mass conservation should be used during interpolation from regular cell to departure cell and from arrival cell to regular cell. thus, we apply **monotonic PPM** for S(x).

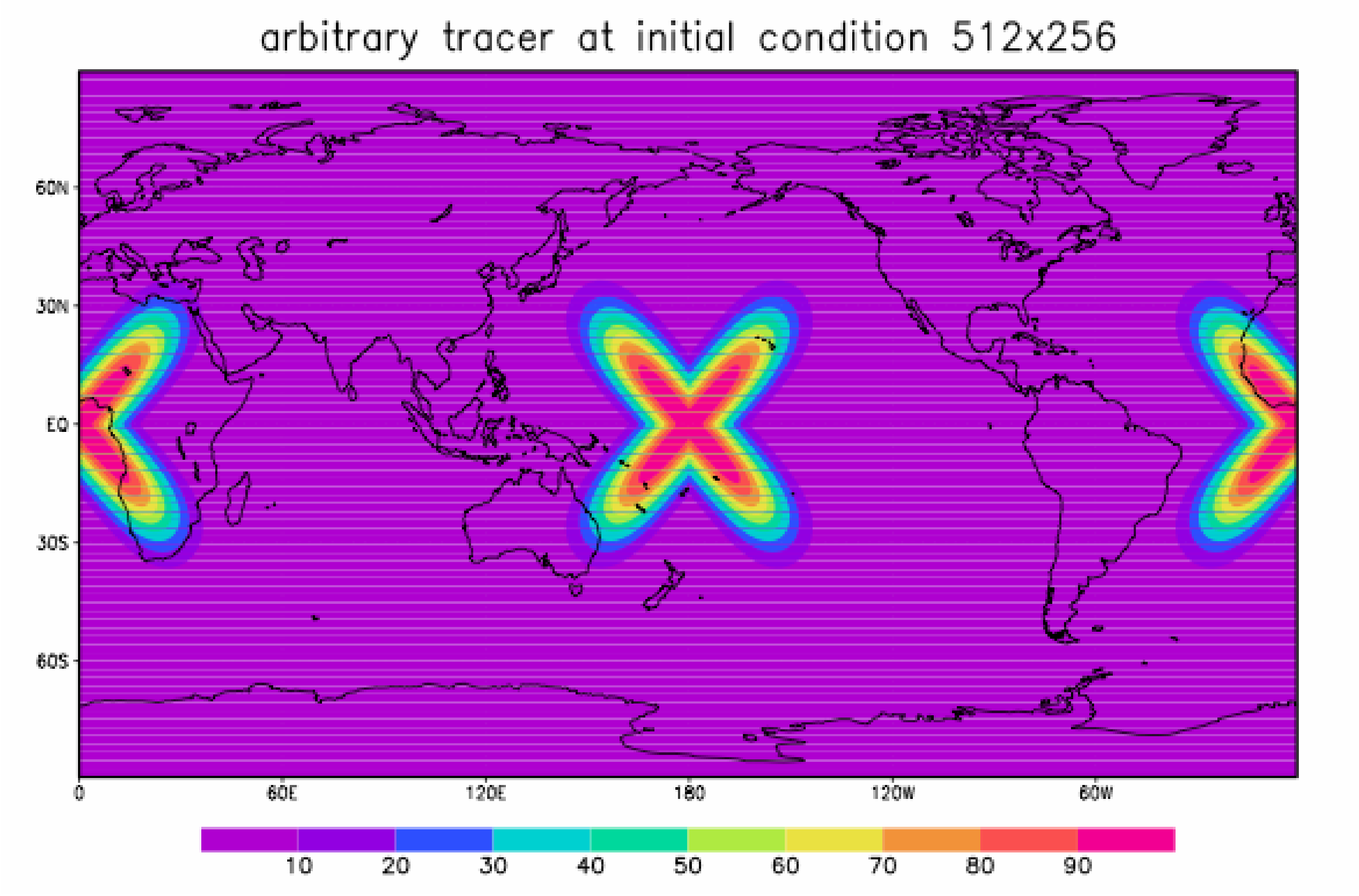


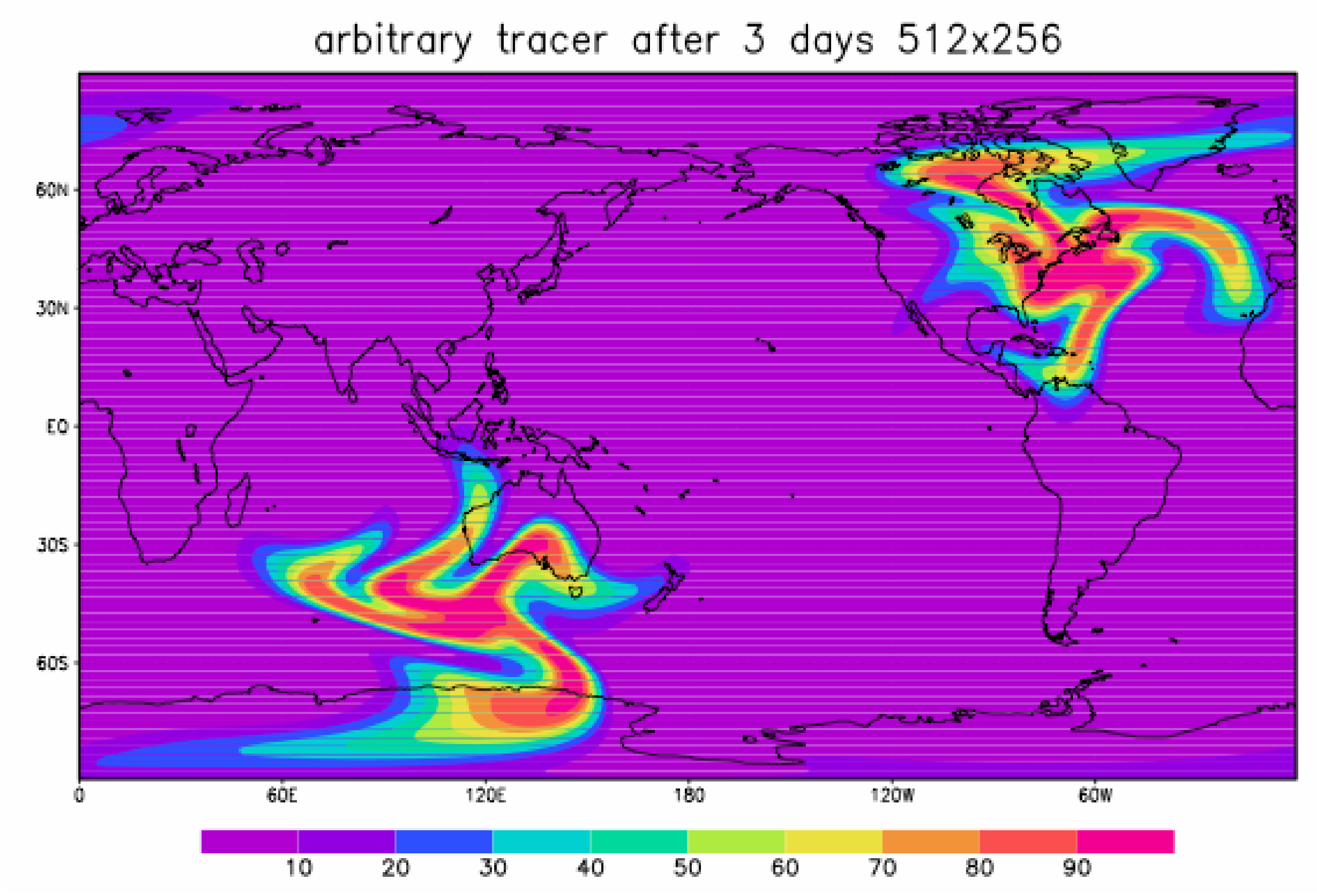
$$\frac{(total\ \ mass)-(initial\ \ total\ \ mass)}{(initial\ \ total\ \ mass)} \approx 10^{-15}$$

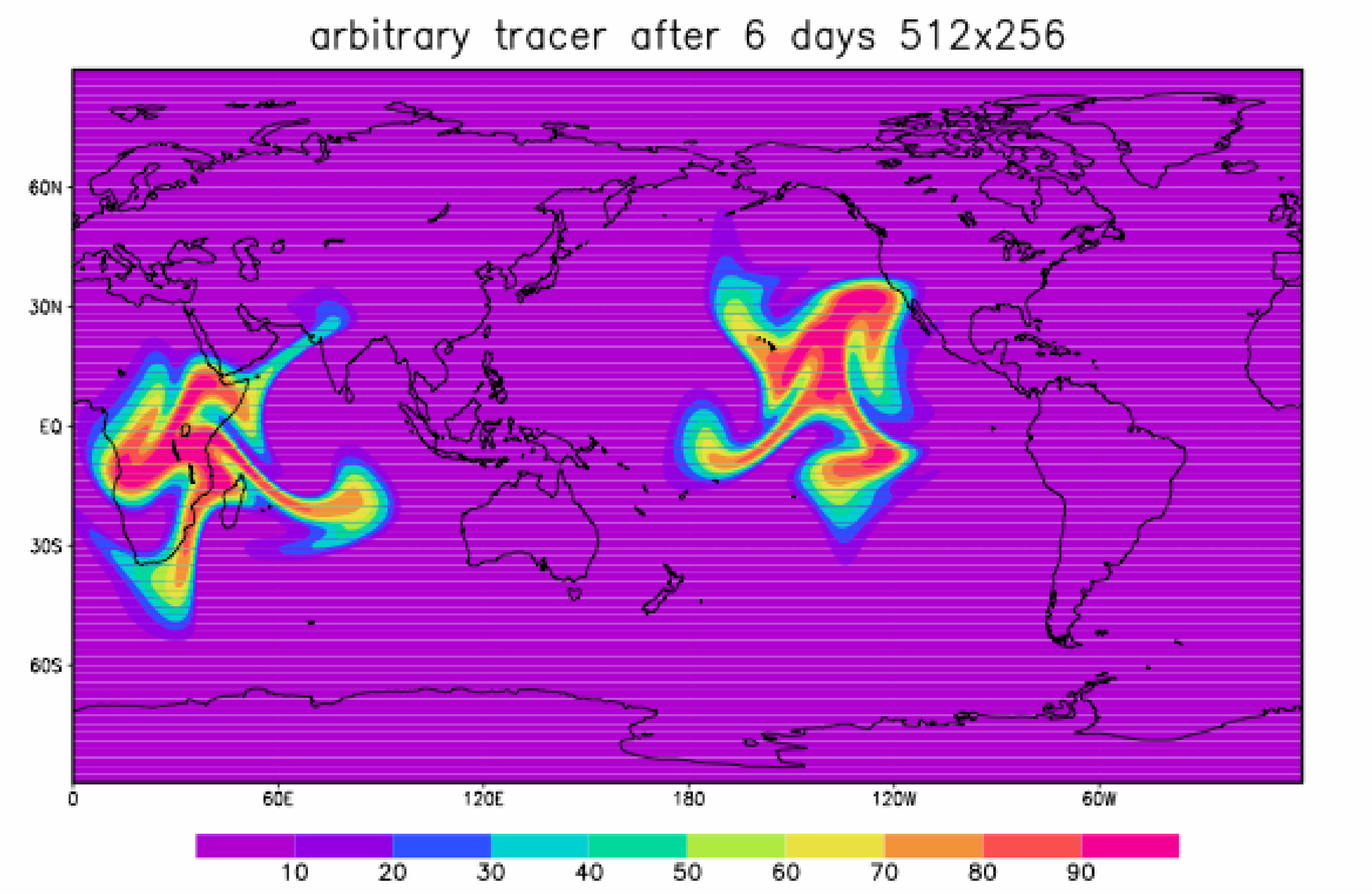
Isochronal flow

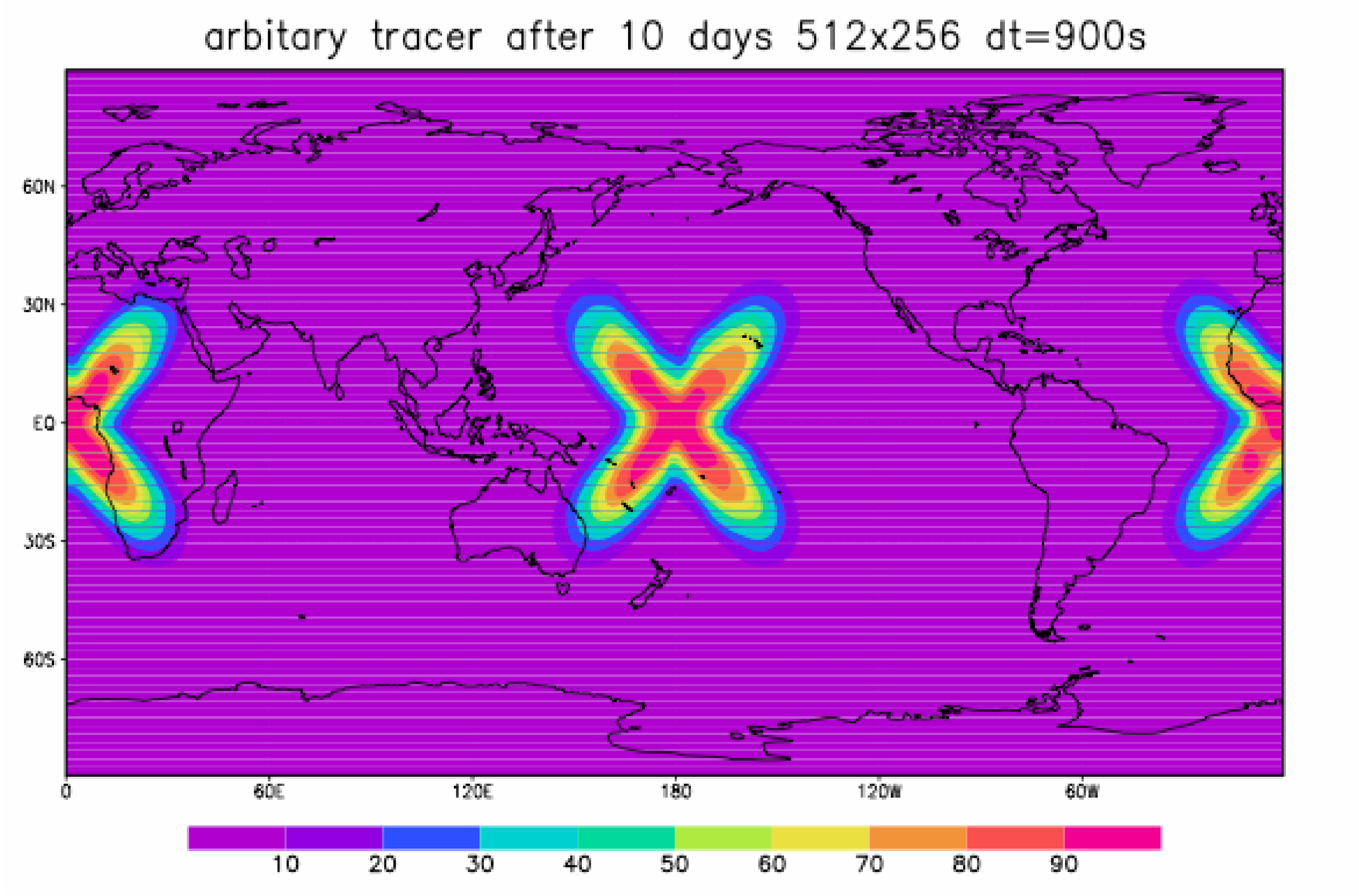
- Any given point will return to its original location after a given period of time.
- Gaussian grid dimensioned 512 x 256.
- Rotate coordinates so “equator” goes through (39N,77W), thus giving flow over real poles.
- Apply non-divergent global wave number 4-20 perturbation displacement (of standard deviation size 0.1-0.2 non-dimensional vorticity) using a random number generator.
- Set return period to 10 days.


isochronal flow (m/sec)
60N
30N
EQ
30S
60S
0
60E
120E
180
120W
60W
13
26
39
52
65
78
91
104
117
130
143
156


arbitrary tracer at initial condition 512x256
60N
30N
EQ
30S
60S
0
60E
120E
180
120W
60W
10
20
30
40
50
60
70
80
90


arbitrary tracer after 3 days 512x256
60N
30N
EQ
30S
60S
0
60E
120E
180
120W
60W
10
20
30
40
50
60
70
80
90


arbitrary tracer after 6 days 512x256
60N
30N
EQ
30S
60S
0
60E
120E
180
120W
60W
10
20
30
40
50
60
70
80
90

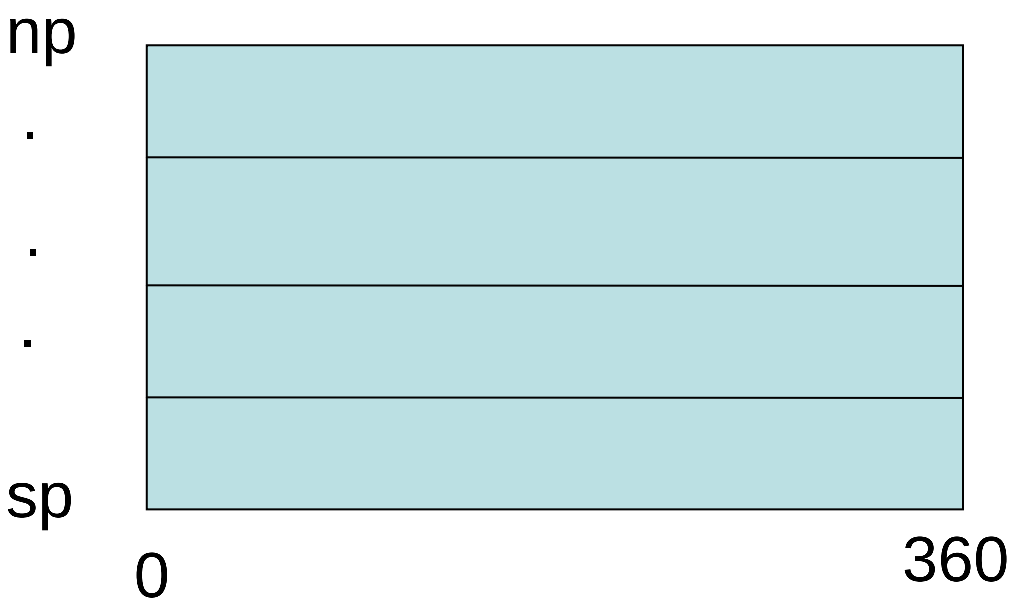

arbitary tracer after 10 days 512x256 dt=900s
60N
30N
EQ
30S
60S
0
60E
120E
180
120W
60W
10
20
30
40
50
60
70
80
90

Decomposition in NCEP GFS

- Current NCEP GFS uses 1D decomposition with MPI and thread with OpenMP.
- Transpose with MPI_AllToAllv is used to move between two sub-domains for spectral transform.
- First sub-domain has some given latitudes with all longitudes grids, which is for FFT in longitudinal direction.
- Second sub-domain has some given zonal wave numbers with all meridian wave numbers, which is for Legendre transform in meridian direction.
- Transpose between two sub-domains, thus there is no halo required.

Implement into NCEP GFS

- The same first sub-domain is used to compute semi-Lagrangian advection in any given latitudinal global circle. All departure and arrival points are in the same circle, so no halo is needed.
- Then transpose first sub-domain to another grid-point sub-domain, which has all Gaussian latitude points but some longitude points. Therefore semi-Lagrangian advection can be computed in any given longitude with all latitude points, so, again, no halo is required.
- The PPM mass conserving between reduced grid and full grid in any given latitude is also applied.



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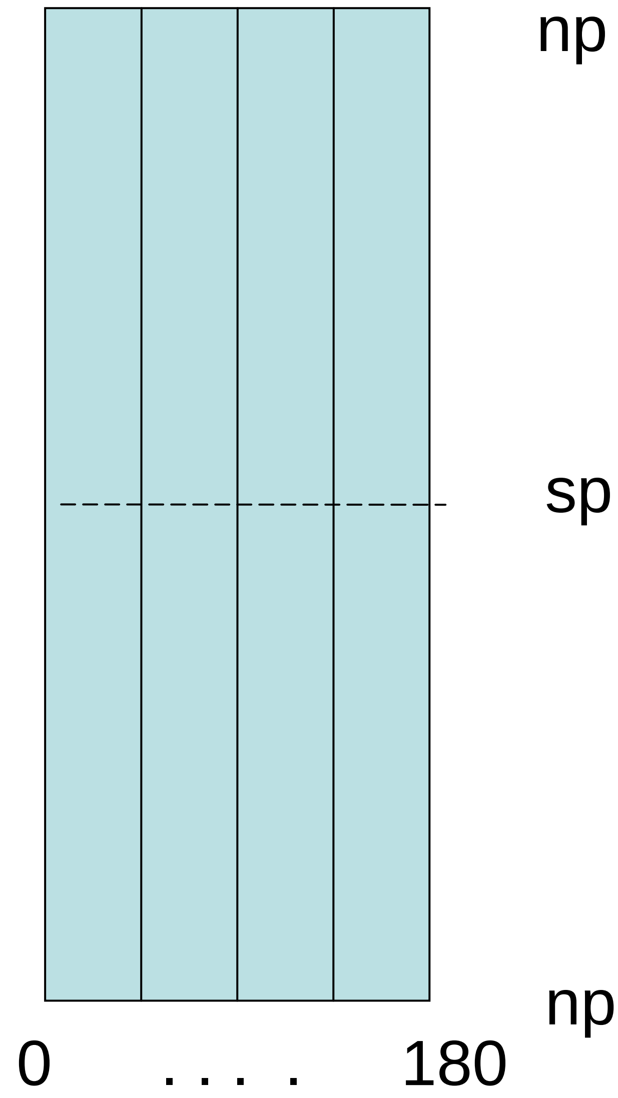
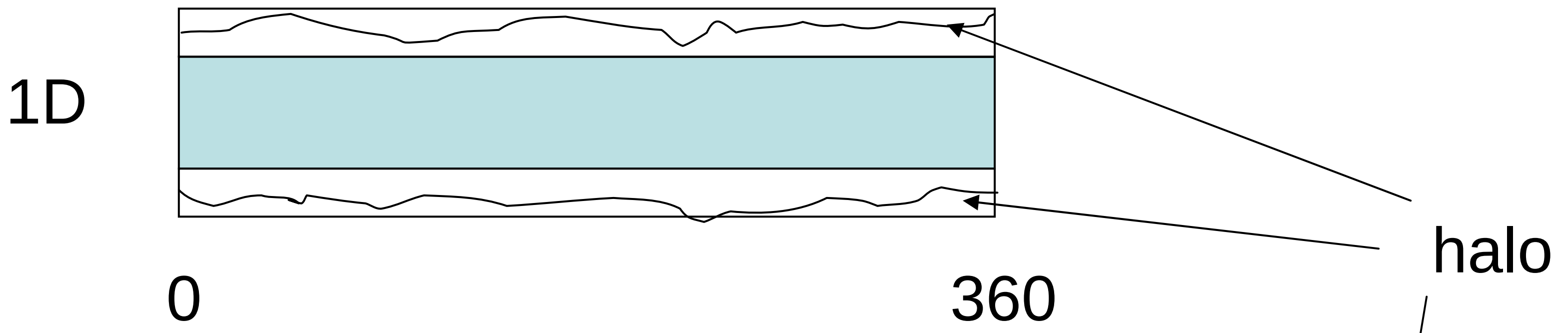


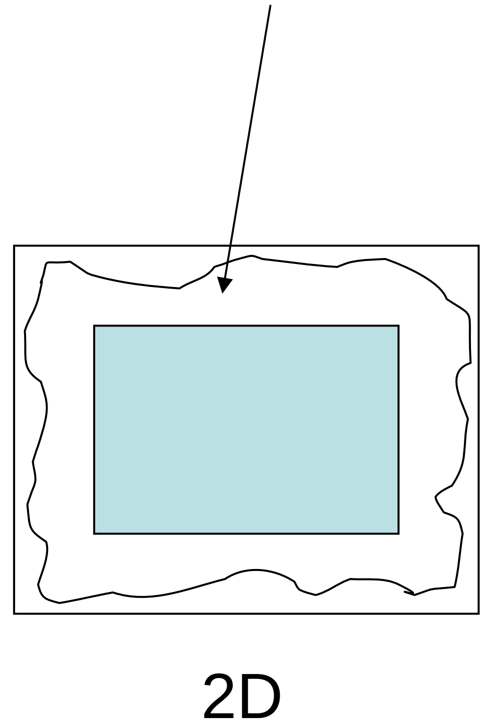
Transpose

No halo is required
No increasing memory with
Increasing number of PE(cpu)



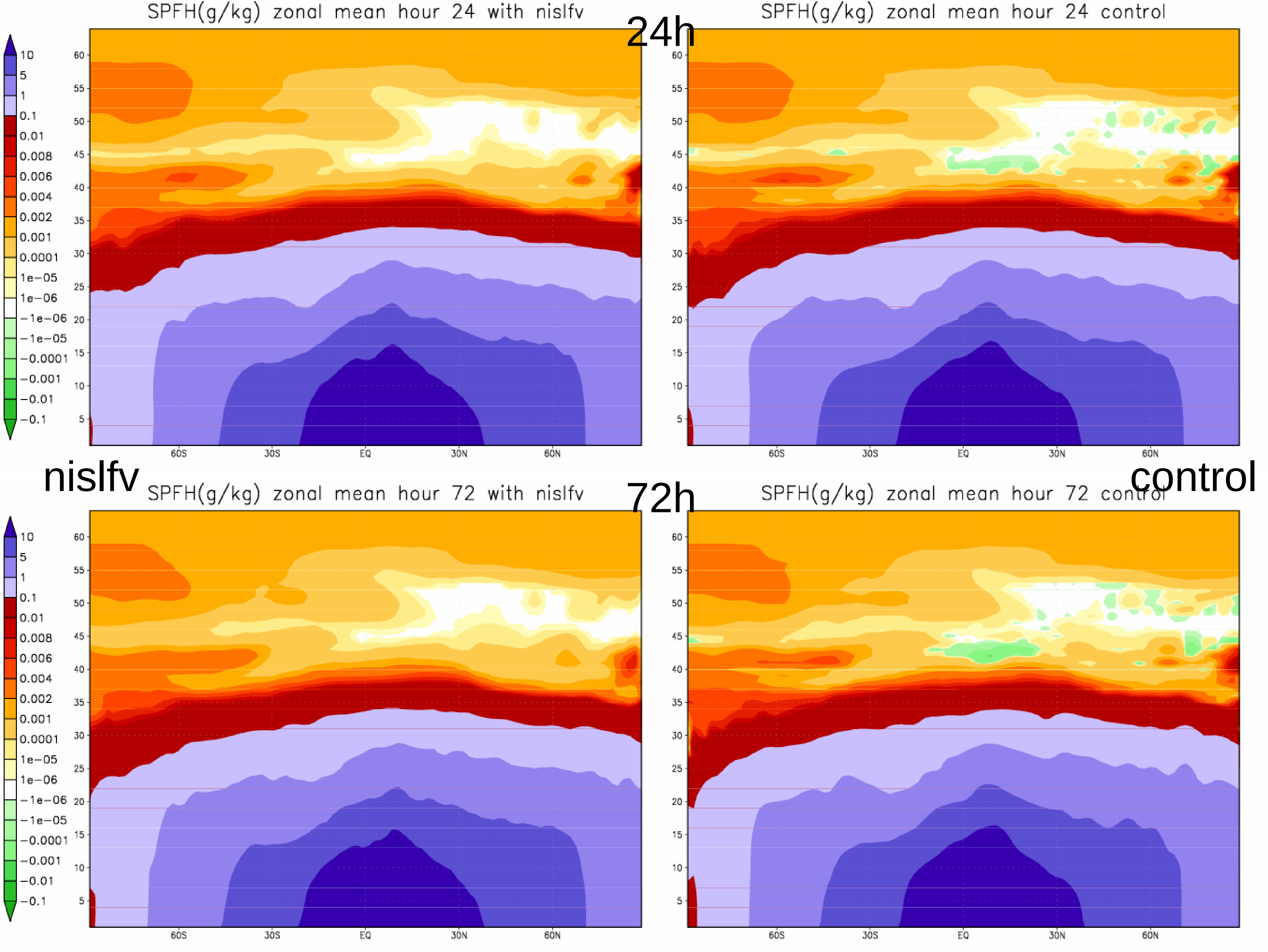
Halo Exchange

Extra memory is required,
which may be as huge
as computing grid while number of
MPP cpu increases.

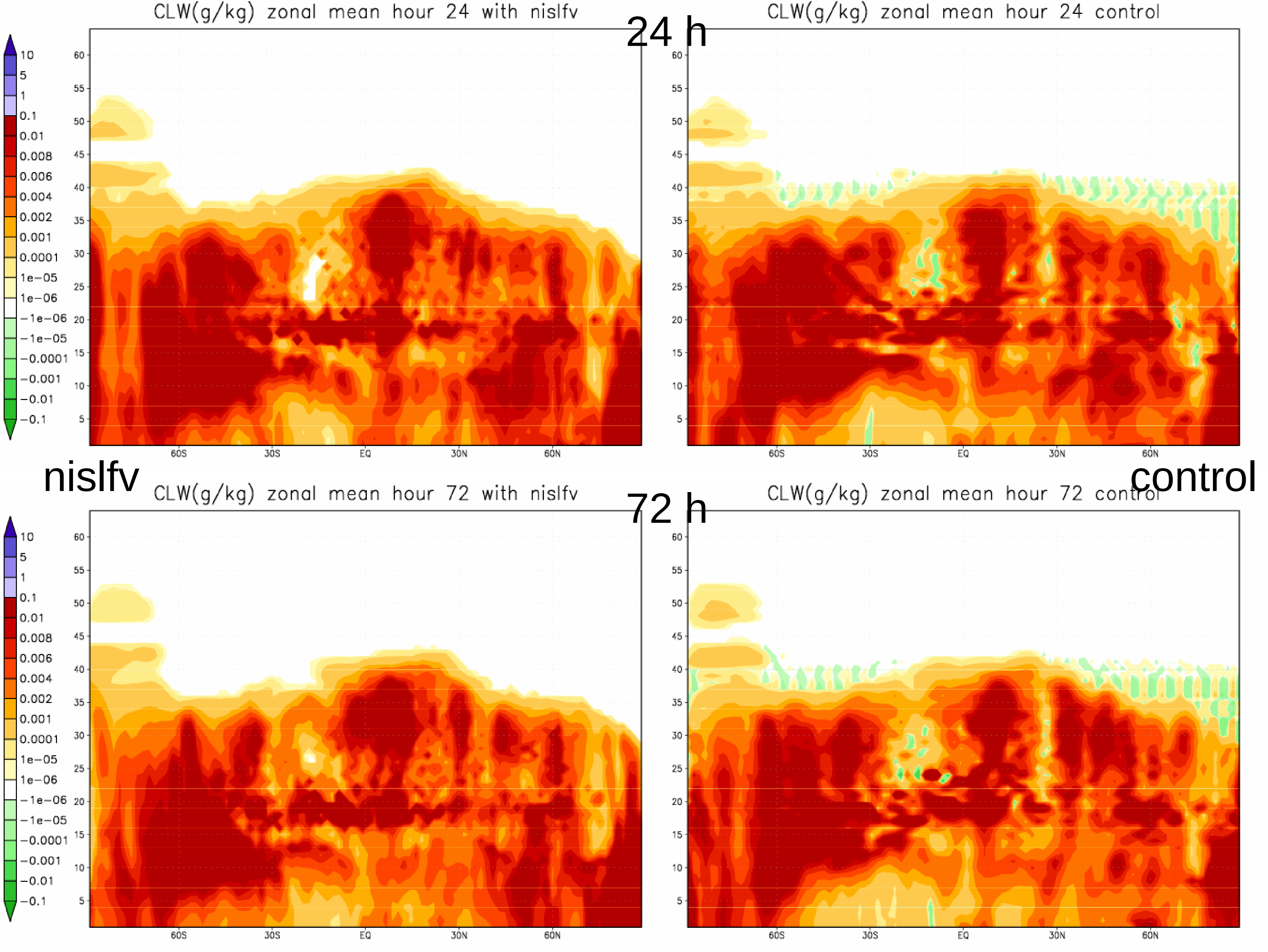


Case test in NCEP GFS

- Arbitrary date is selected.
- Modify NCEP GFS IO into grid-point data.
- Negative tracers are replaced with zero value at the initial time.
- T126 L64 resolution is tested.
- Model physics is included.
- Two runs are compared;
  - **control**: Spectral advection in horizontal, finite difference in vertical asoperational GFS.
  - **nislfv**: Non-iteration mass conserving positive definite semi-Lagrangian on tracers.

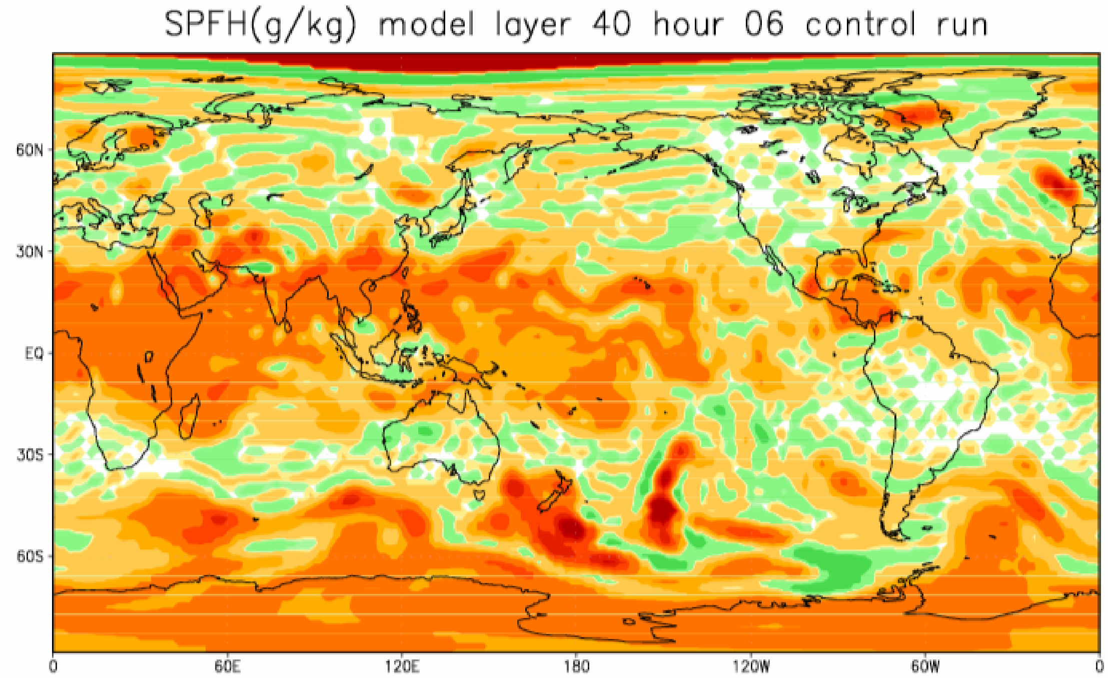


24h
72h
nislfv
control
SPFH(g/kg) zonal mean hour 24 with nislfv
SPFH(g/kg) zonal mean hour 24 control
SPFH(g/kg) zonal mean hour 72 with nislfv
SPFH(g/kg) zonal mean hour 72 control
10
5
1
0.1
0.01
0.008
0.006
0.004
0.002
0.001
0.0001
1e−05
1e−06
−1e−06
−1e−05
−0.0001
−0.001
−0.01
−0.1
60
55
50
45
40
35
30
25
20
15
10
5
60S
30S
EQ
30N
60N



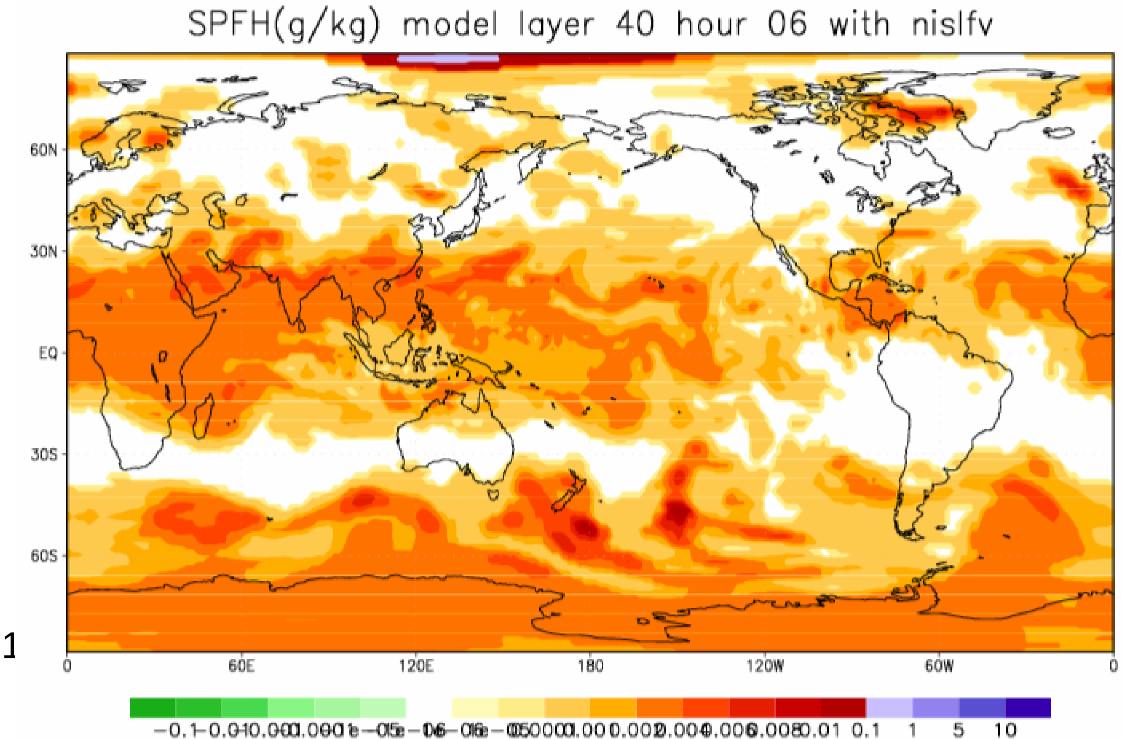
24 h
72 h
nislfv
control
CLW(g/kg) zonal mean hour 24 with nislfv
CLW(g/kg) zonal mean hour 24 control
CLW(g/kg) zonal mean hour 72 with nislfv
CLW(g/kg) zonal mean hour 72 control
10
5
1
0.1
0.01
0.008
0.006
0.004
0.002
0.001
0.0001
1e−05
1e−06
−1e−06
−1e−05
−0.0001
−0.001
−0.01
−0.1
5
10
15
20
25
30
35
40
45
50
55
60
60S
30S
EQ
30N
60N

control



06h fcst specific humidity
at model layer 40

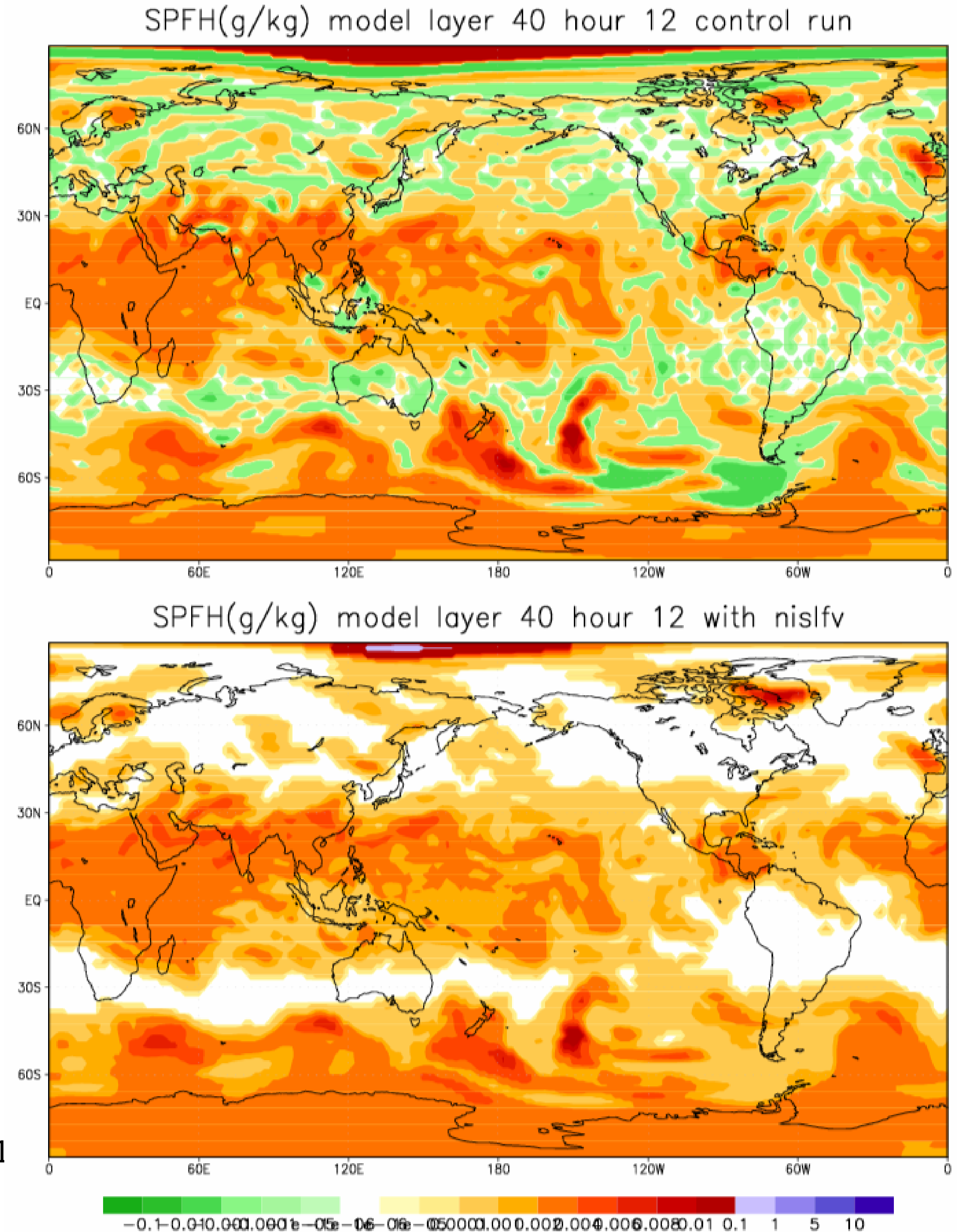
nislfv



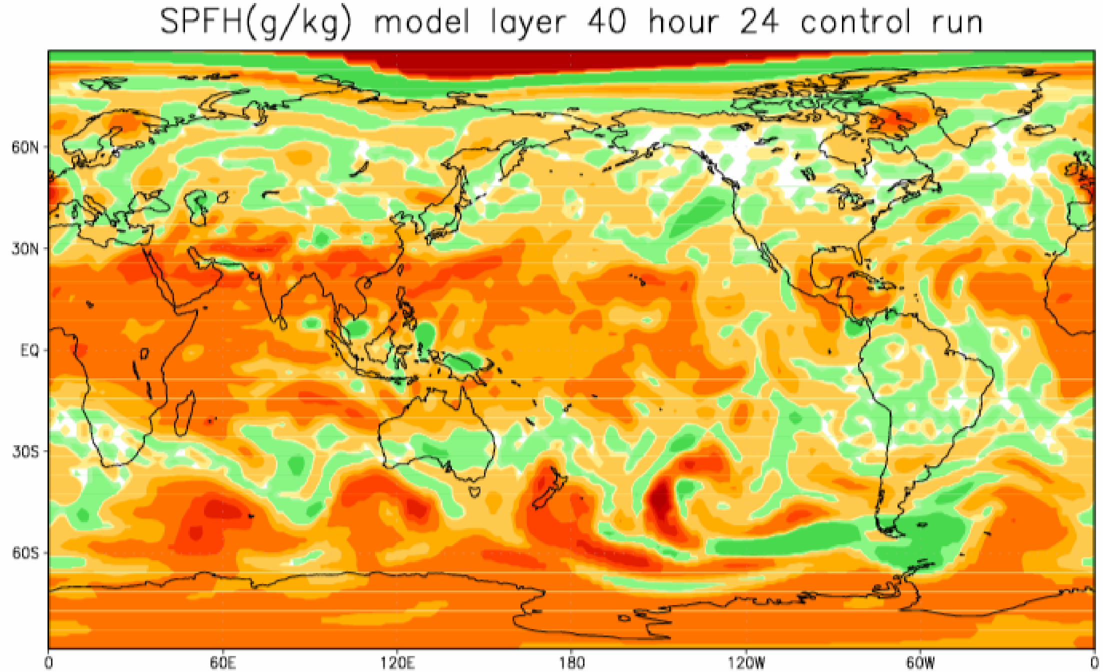
control

12h fcst specific humidity
at model layer 40

nislfv

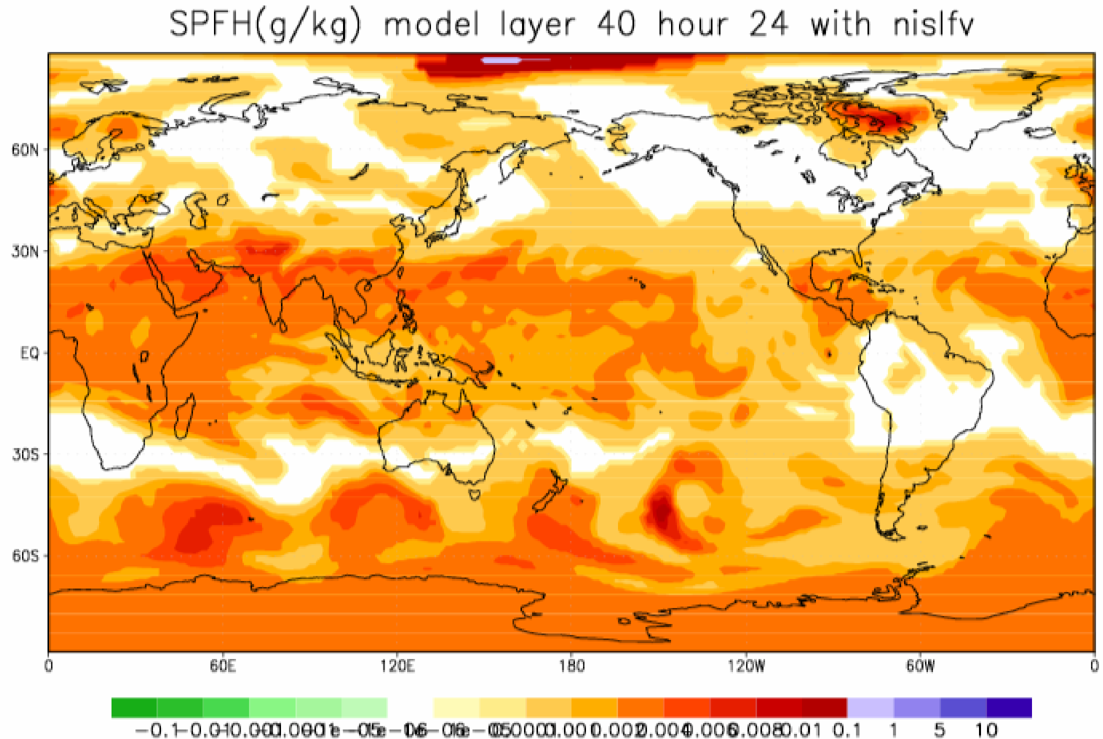


control

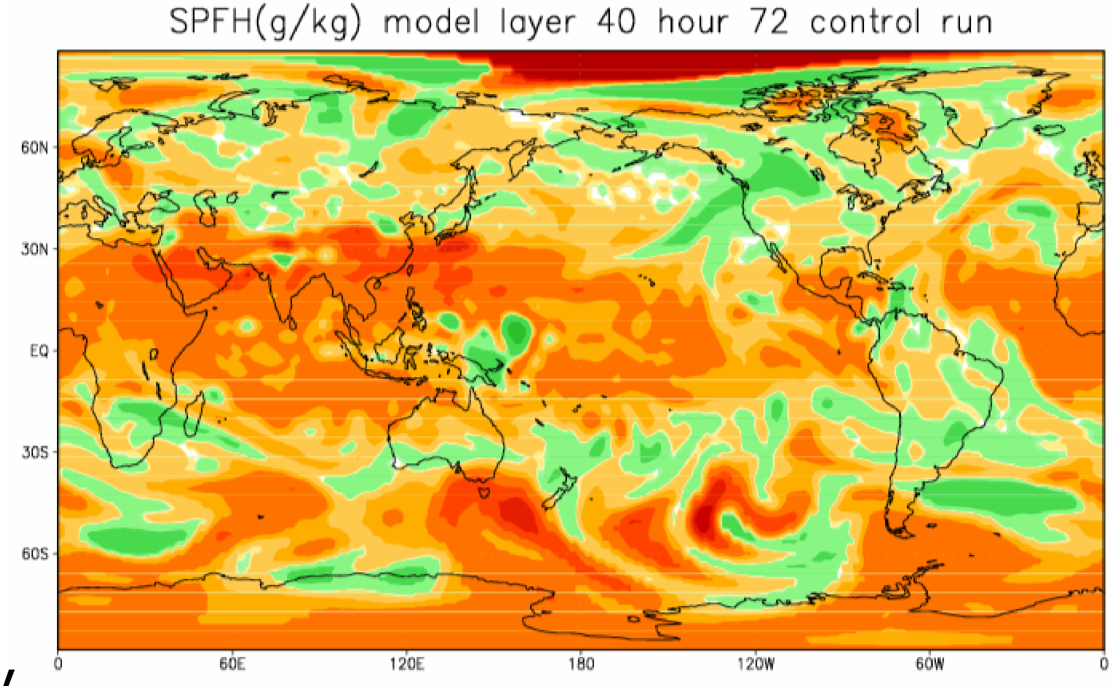


24h fcst specific humidity at model layer 40

nislfv

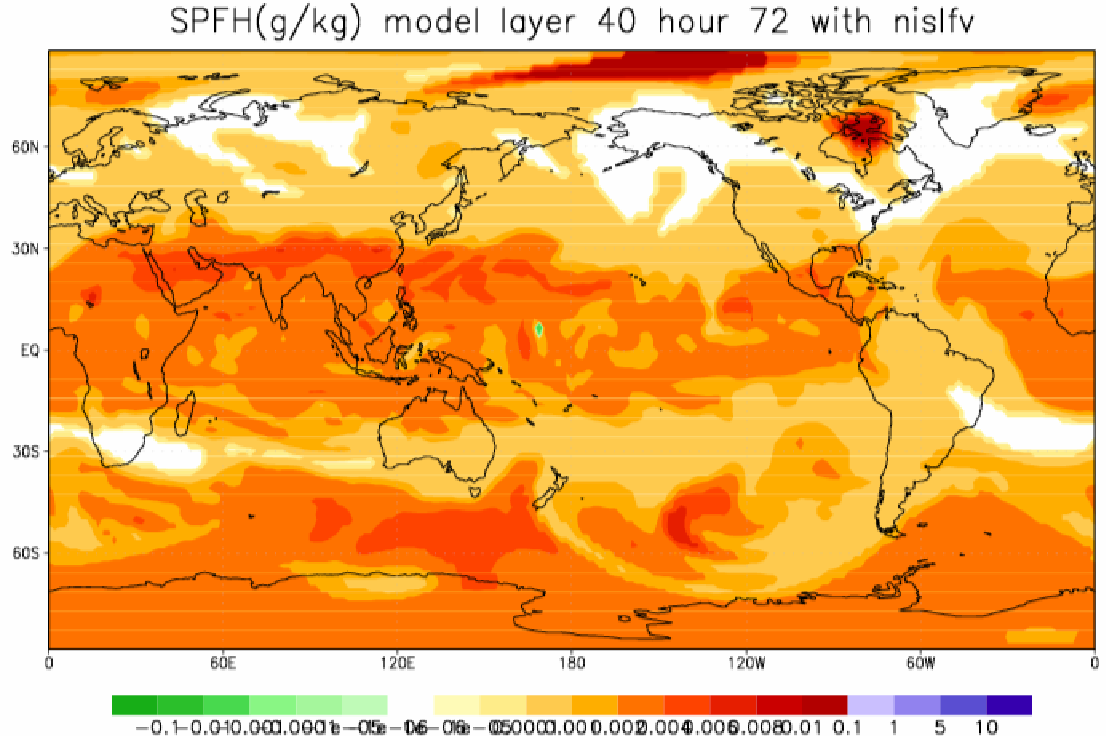


control



72h fcst specific humidity
at model layer 40

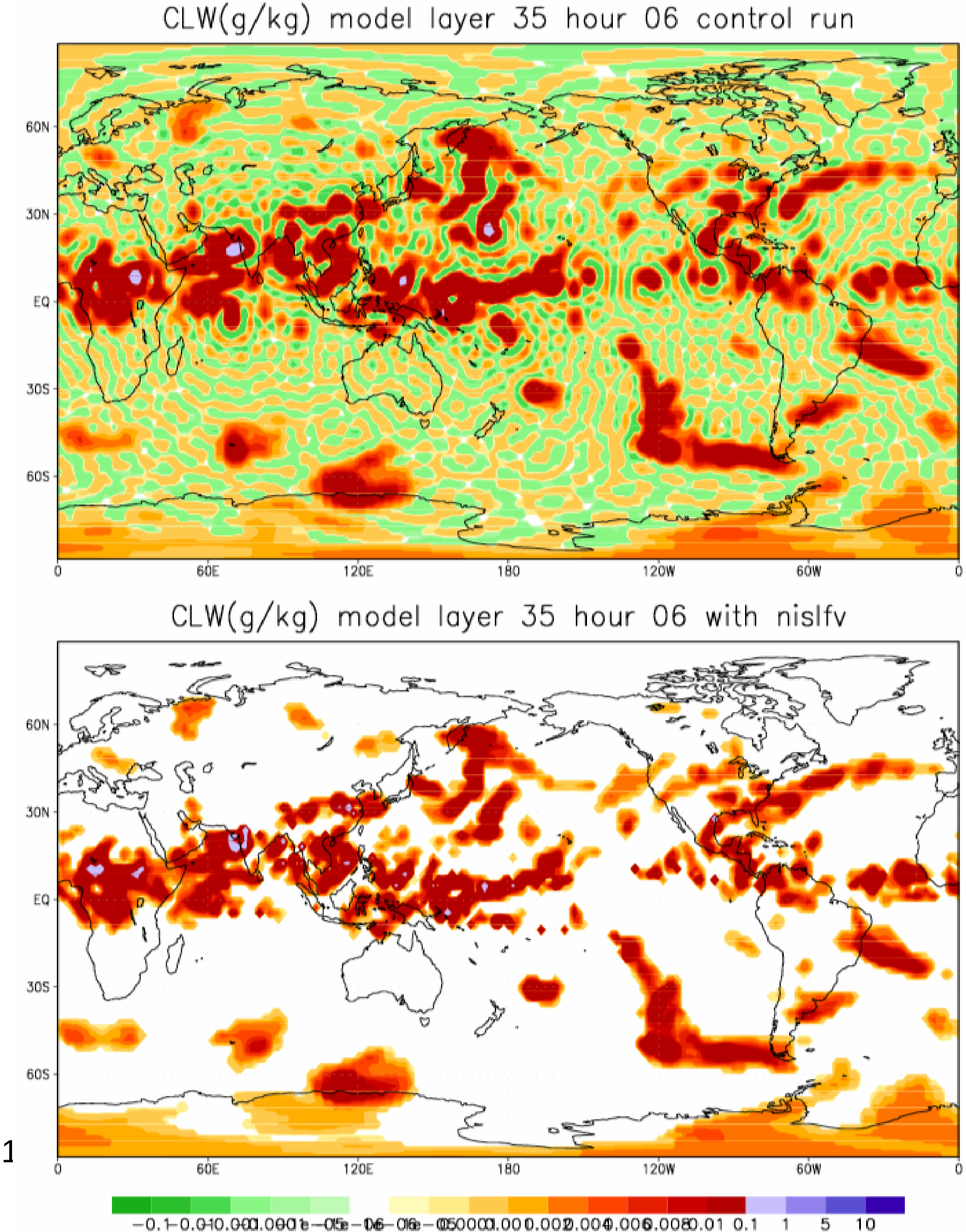
nislfv



control

6hr fcst cloud water at model layer 35

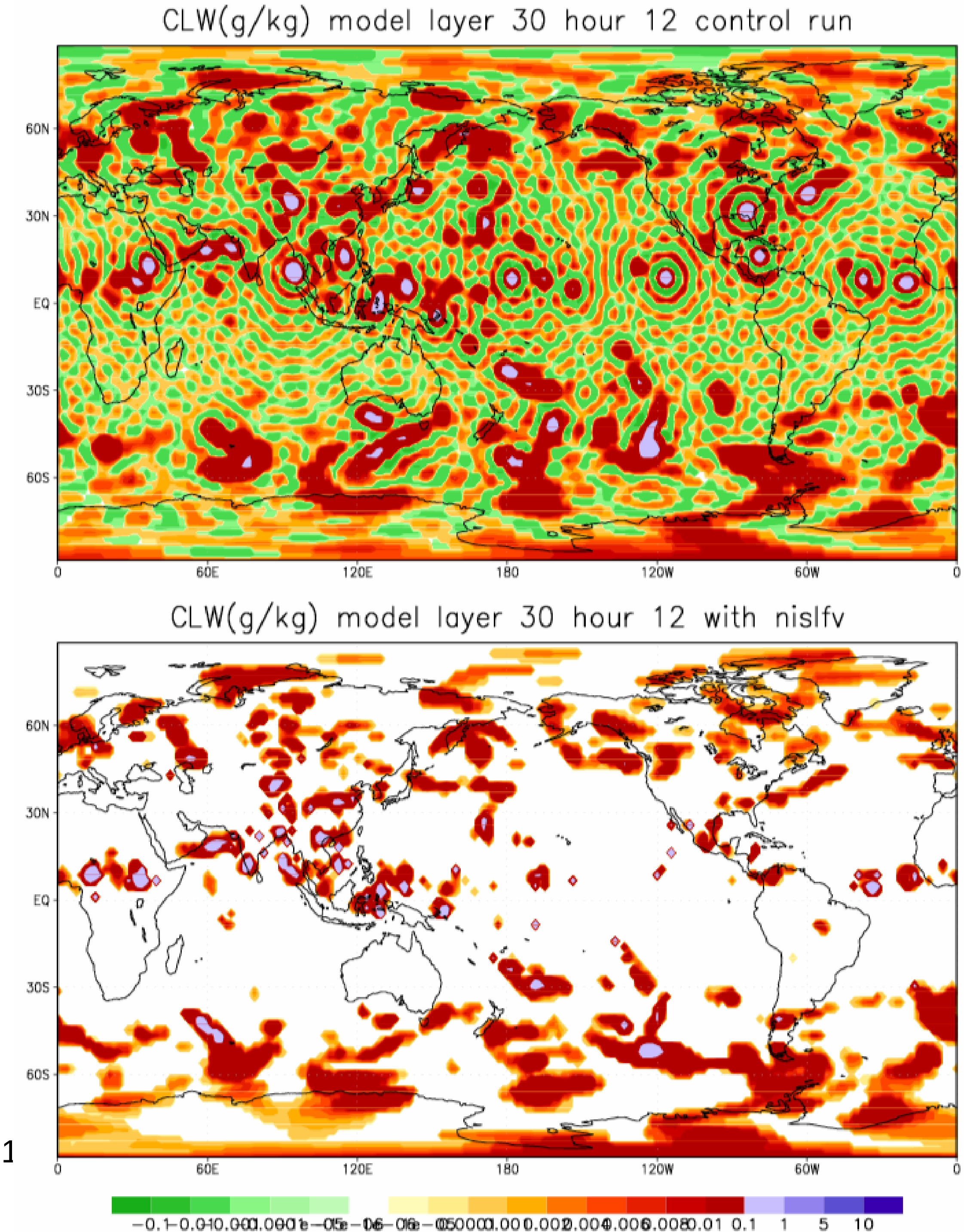
nislfv



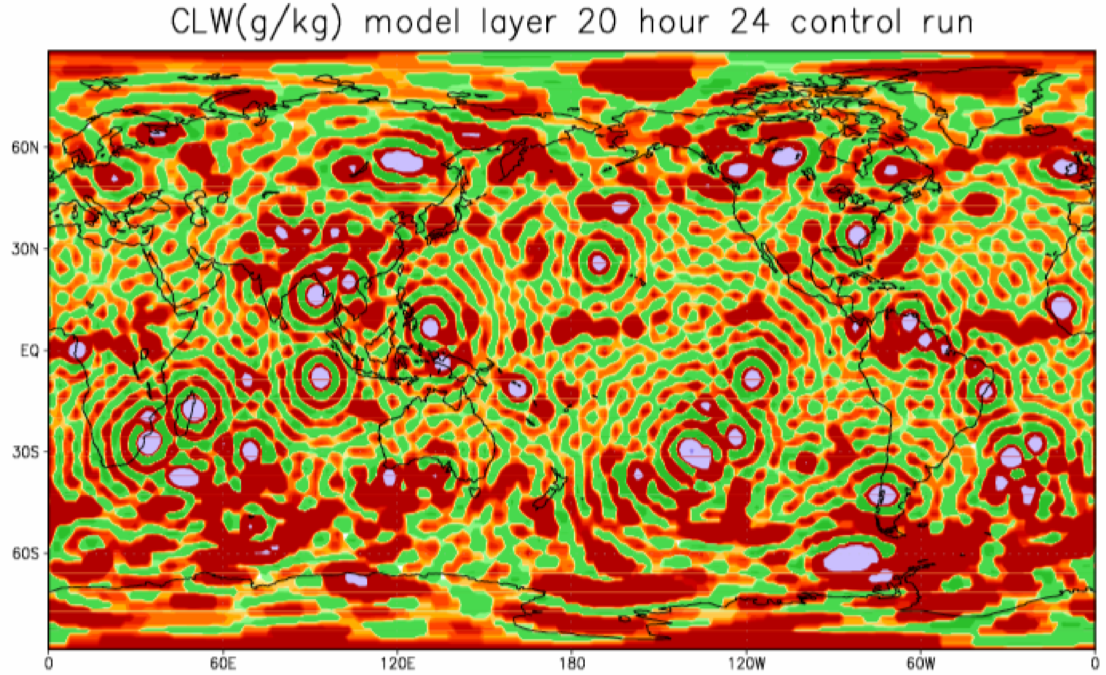
control

12hr fcst cloud water at model layer 30

nislfv

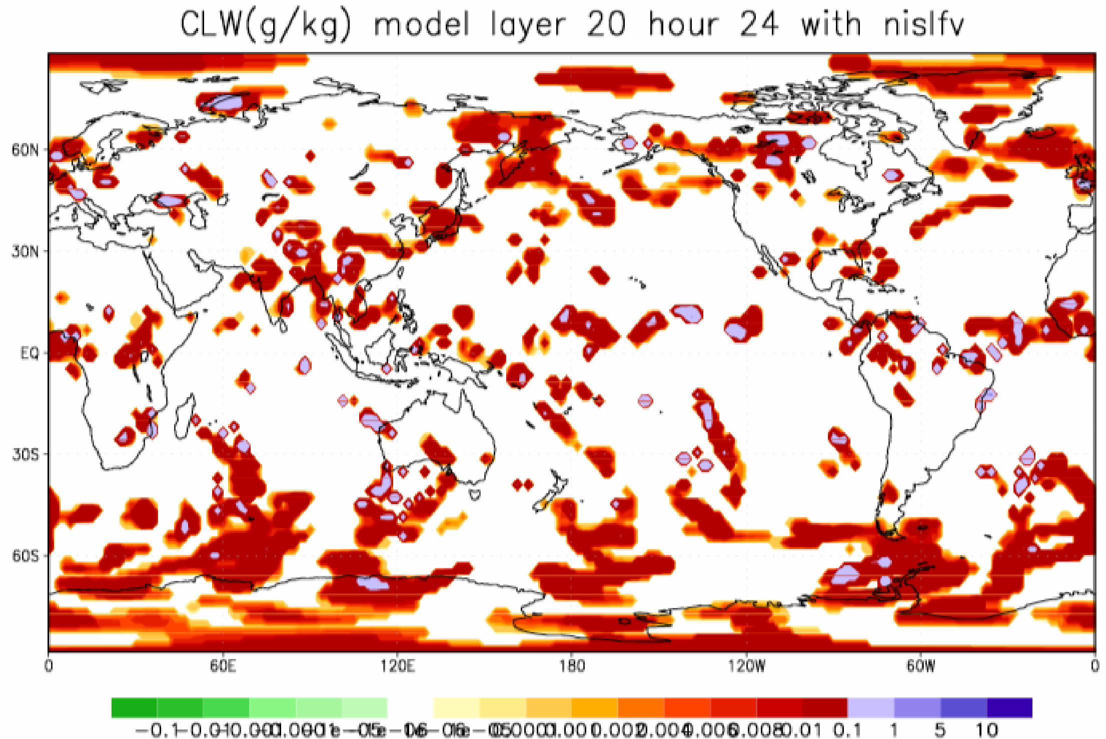


control



24hr fcst cloud water
at model layer 30

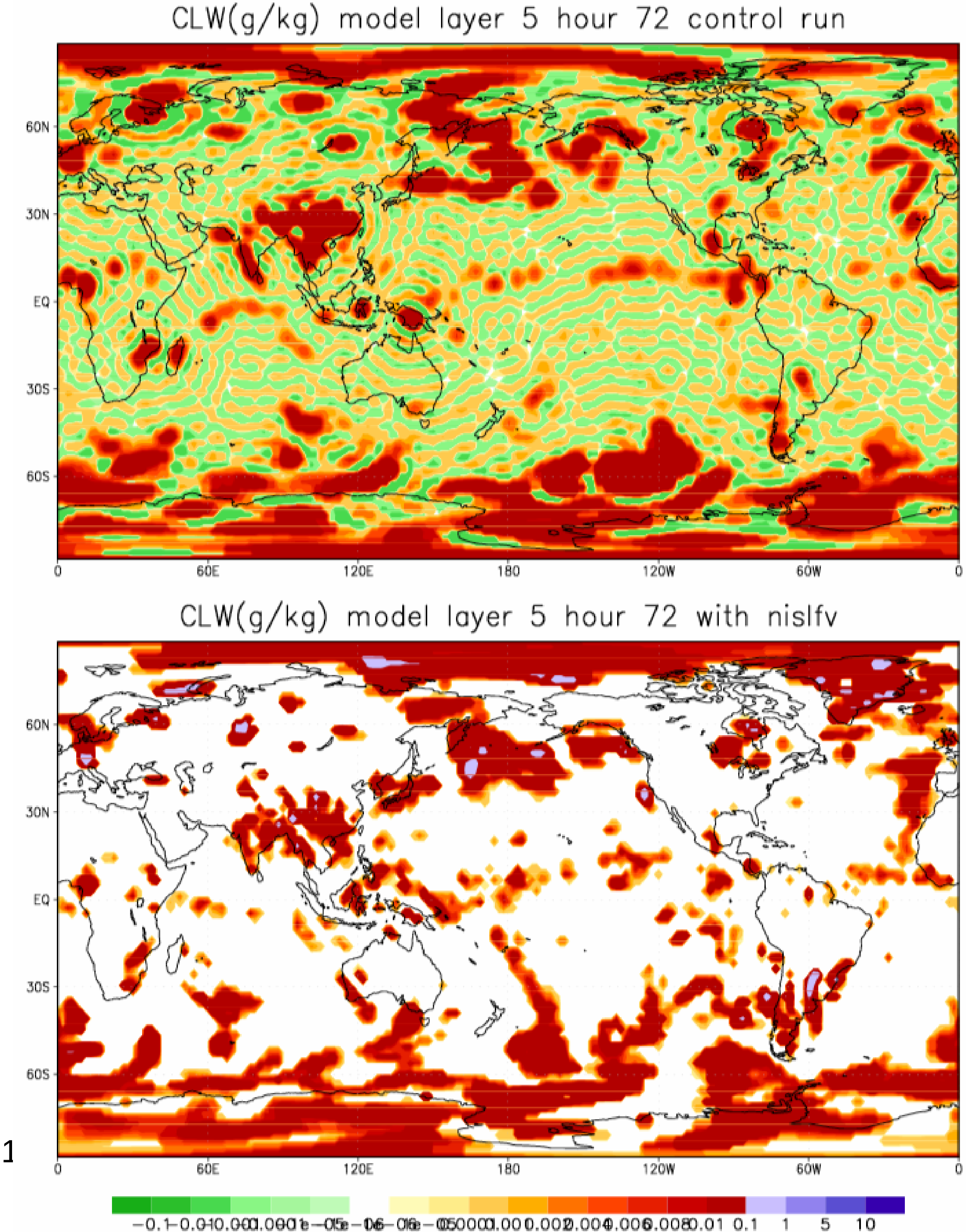
nislfv



control

72hr fcst cloud water at model layer 5

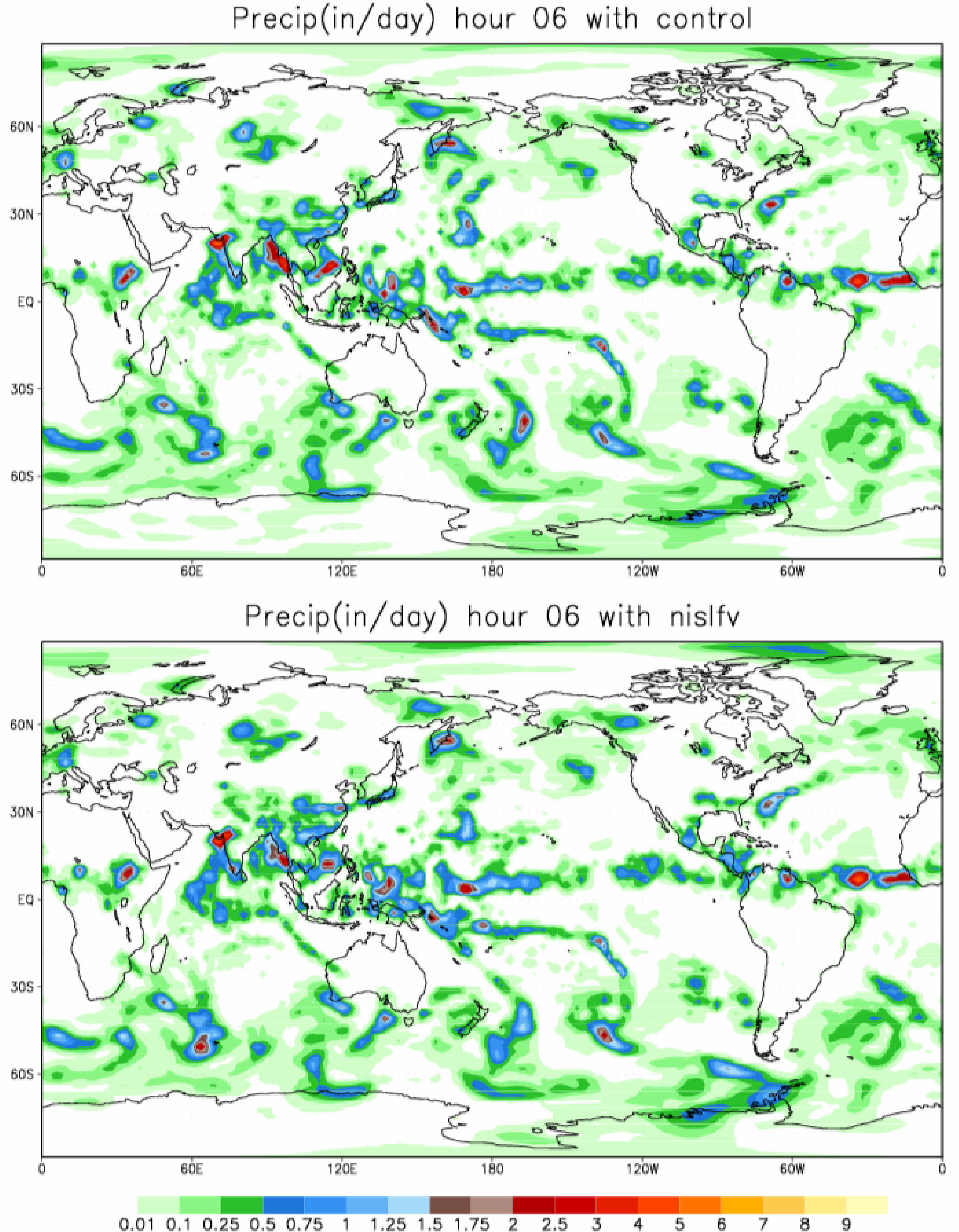
nislfv



control

6hr fcst precipitation

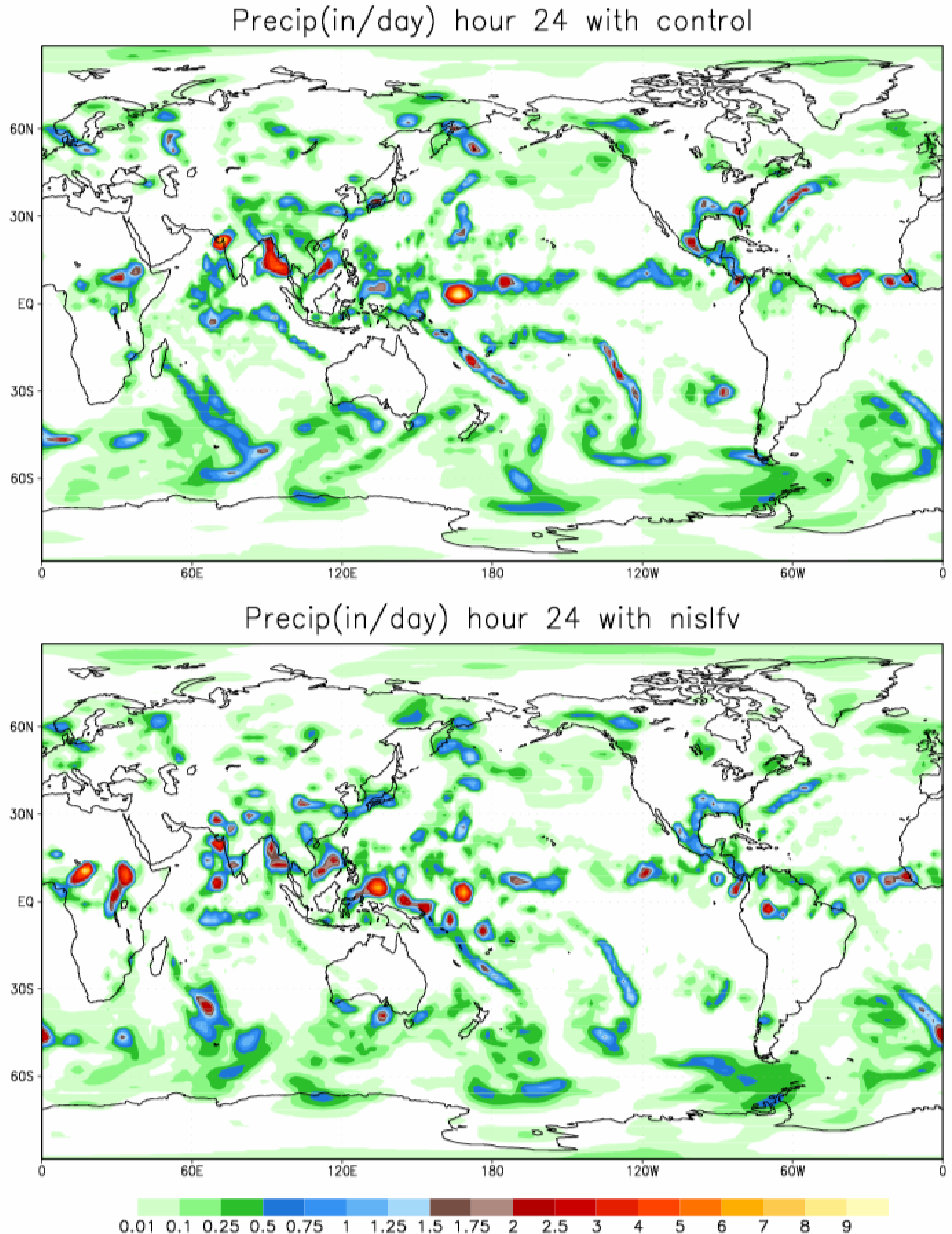
nislfv



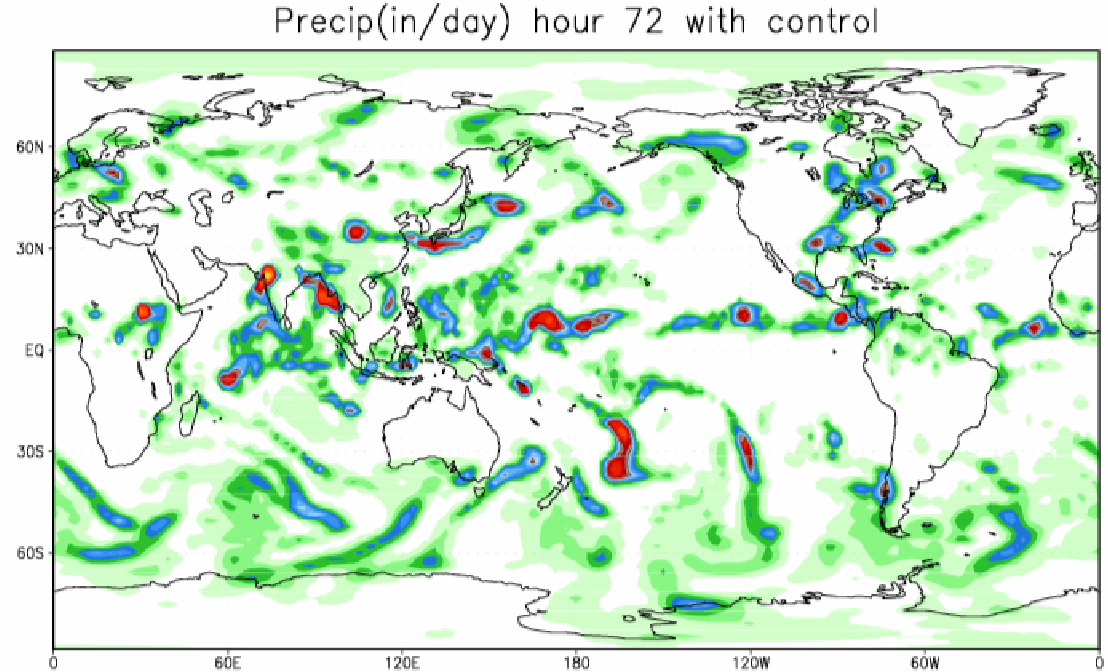
control

24hr fcst precipitation

nislfv

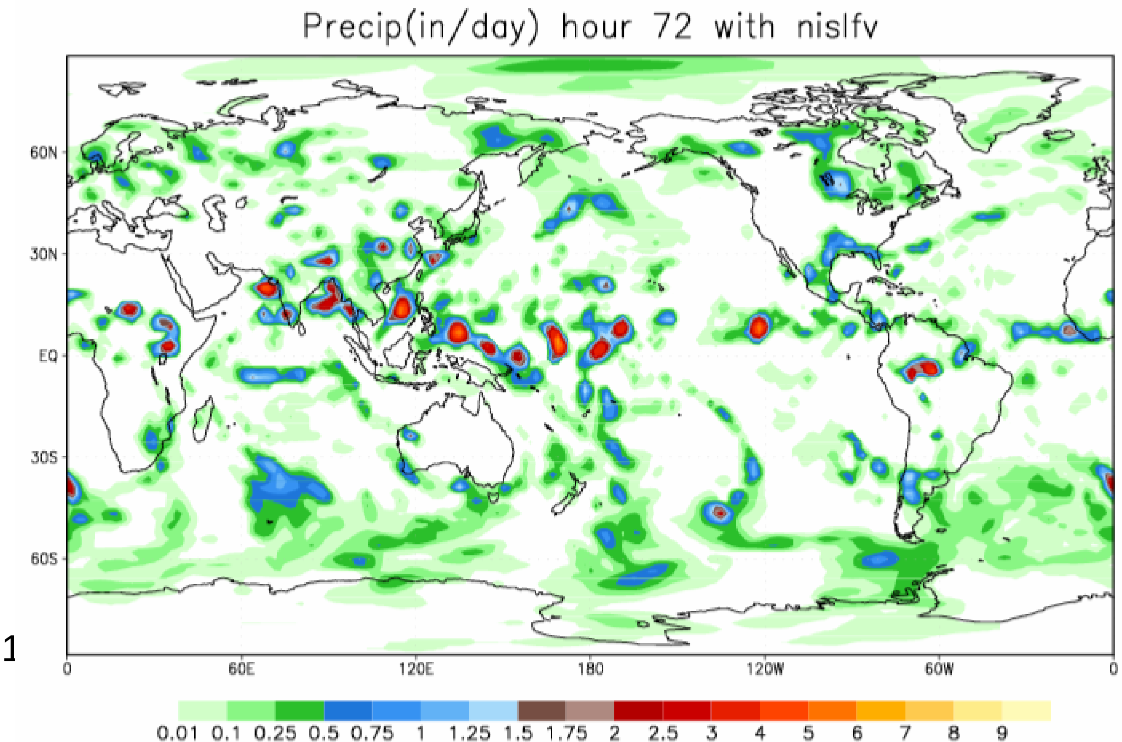


control



72hr fcst precipitation

nislfv



Conclusion & Future Work

- Modified traditional semi-Lagrangian without iteration to locate mid-/departure-points, but require interpolation and remapping with temporal and spatial split computation.
- Mass conserving is included with consideration of semi-Lagrangian for divergence.
- Positive definite is applied with monotone piecewise parabolic method (PPM) for interpolation/remapping.
- Due to spatial split, no halo is required since all required data for computation are all in the partial domain through transpose. Since no halo, there is no extra memory request, but it may have more data in communication than the method with halo and small number of cpu.
- Implement all prognostic variable, not only tracers, to have larger model time step to save integration cost.