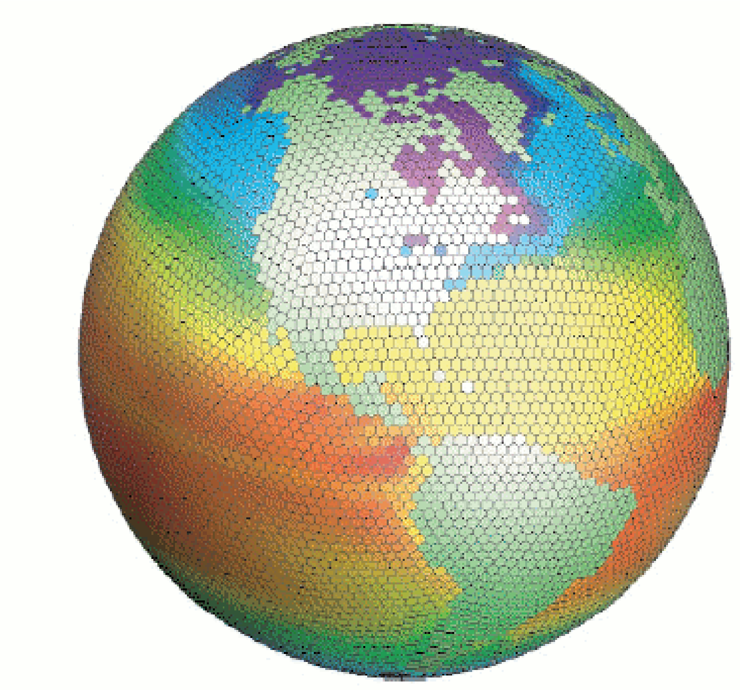
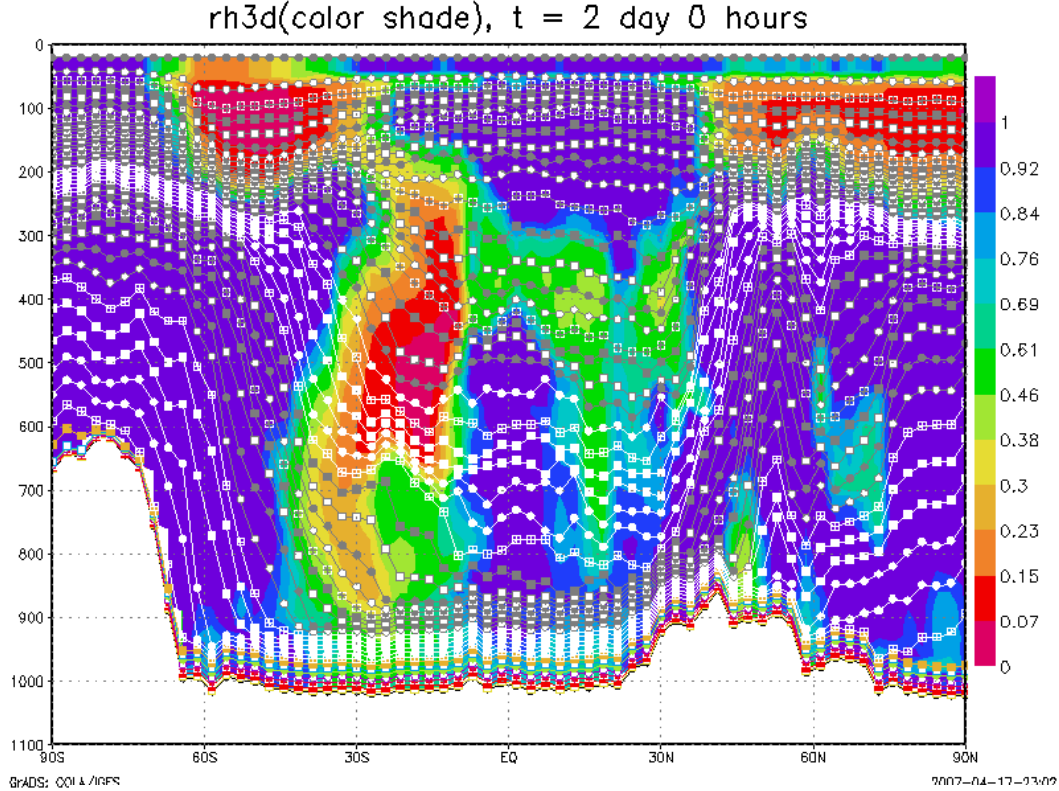
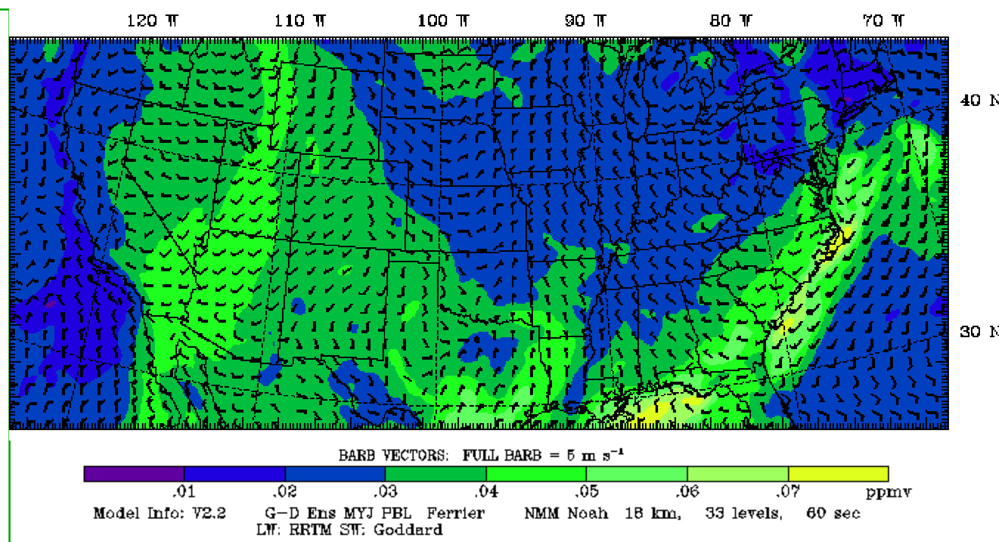





# ESRL Chemistry/ Atmospheric Model (a work in progress)

Stan Benjamin, Jin Lee,
Georg Grell




8m O3 fcst valid 00z 11 Oct 07

# Chemistry component - WRF/chem

Already applied to

- RUC
- WRF-NMM
- WRF-ARW
- MM5
- RAMS
- HIRLAM (European regional model)

Planned/possible applications of WRF/Chem package

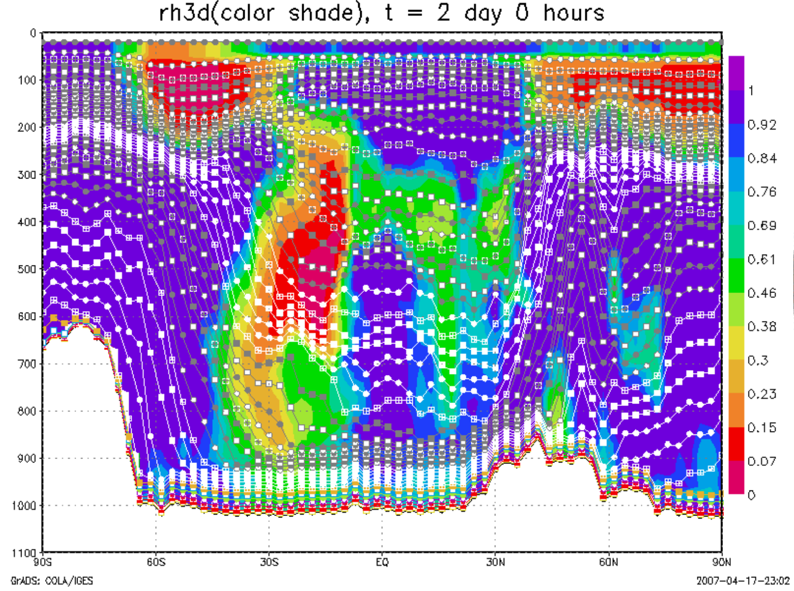
- FIM global model developed at ESRL
- OAR global non-hydrostatic model (GFDL, ESRL, AOML)
- WRF global model
- Simple version in future NCEP Rapid Refresh (aviation-vis)
- ESMF coupling with other components
- OASIS coupling (in Europe)

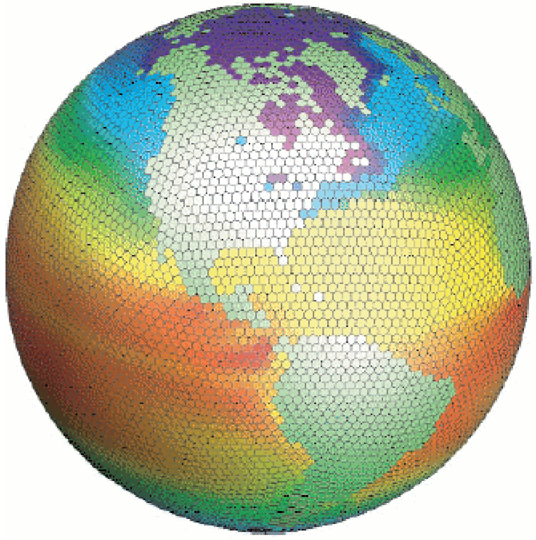
**NOAA/ESRL**

# Flow-following-finite-volume Icosahedral Model

## FIM

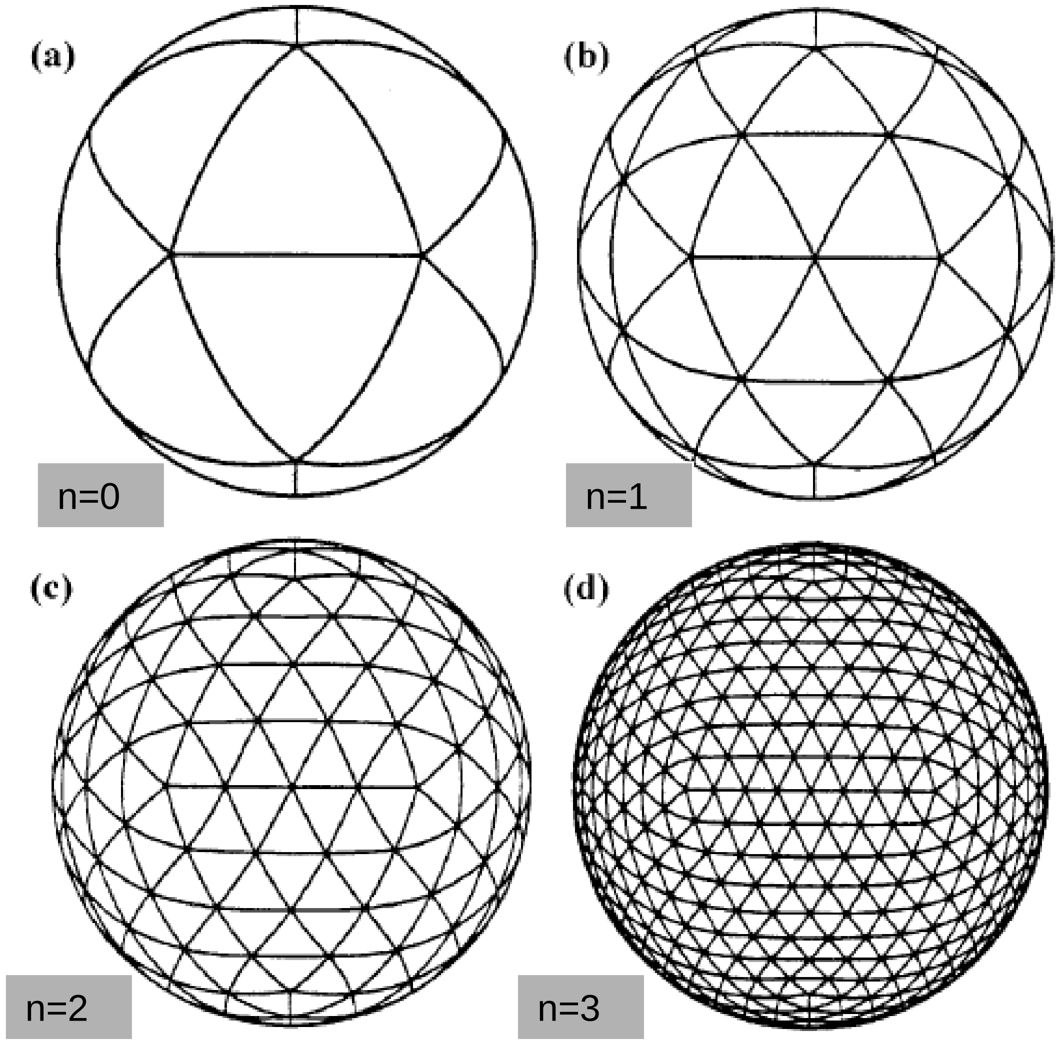

**Jin Lee**
Sandy MacDonald
Rainer Bleck
Stan Benjamin
Jian-Wen Bao
John M. Brown
Jacques Middlecoff
Ning Wang

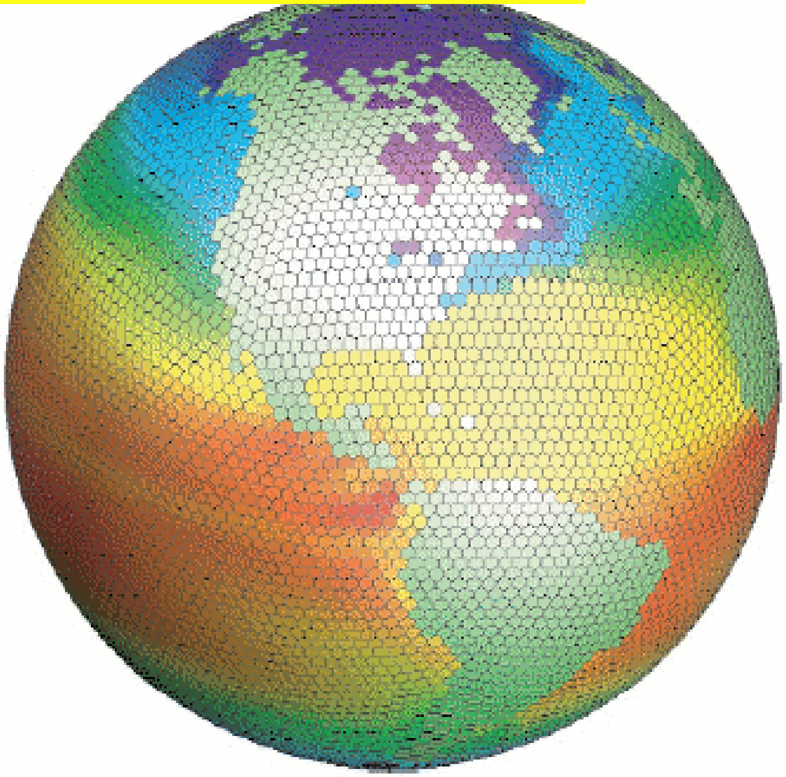
- Applied in real-data cases down to 15km resolution
- MPI implemented with non-structured horizontal grid via ESRL Scalable Modeling System
    - Scaling efficiency from 120→240 procs (98%)
    - 240→480 procs (87%)  (for 30km FIM)
- Allows variable number of prognostic tracer variables (suitable for air chemistry)

# Icosahedral Grid Generation




N=((2**n)**2)*10 + 2 ; 5th level – n=5 → N=10242 ~ 240km;  max(d)/min(d)~1.2
6th level – n=6 →N= N=40962 ~ 120km;  7th level  – n=7→N=163842    ~60km
8th level – n=8→N=655,362   ~30km;     9th level – n=9→N=2,621,442  ~15km

240km icosahedral grid
Level-5 – 10242 polygons



Lat-lon grid

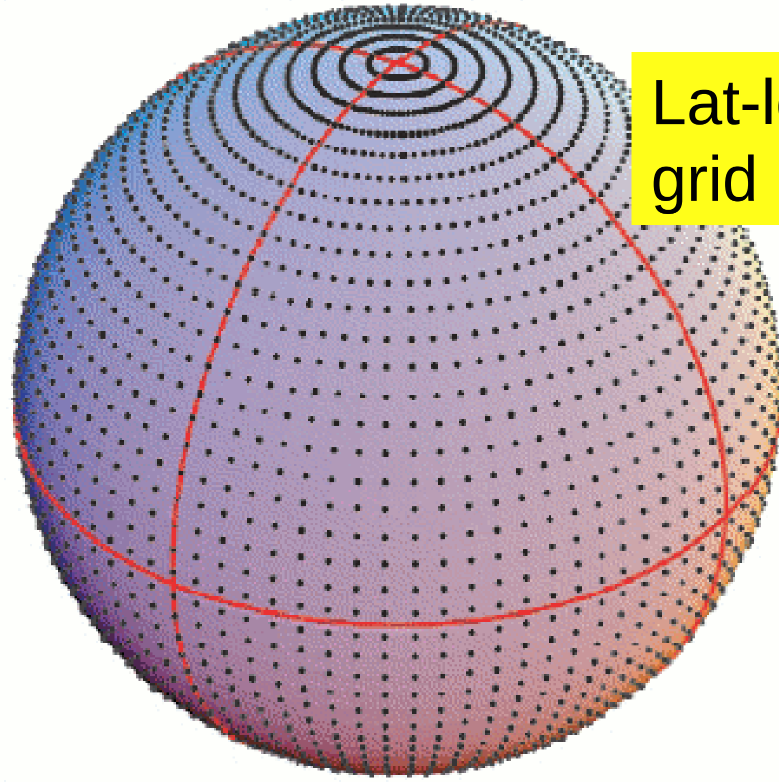


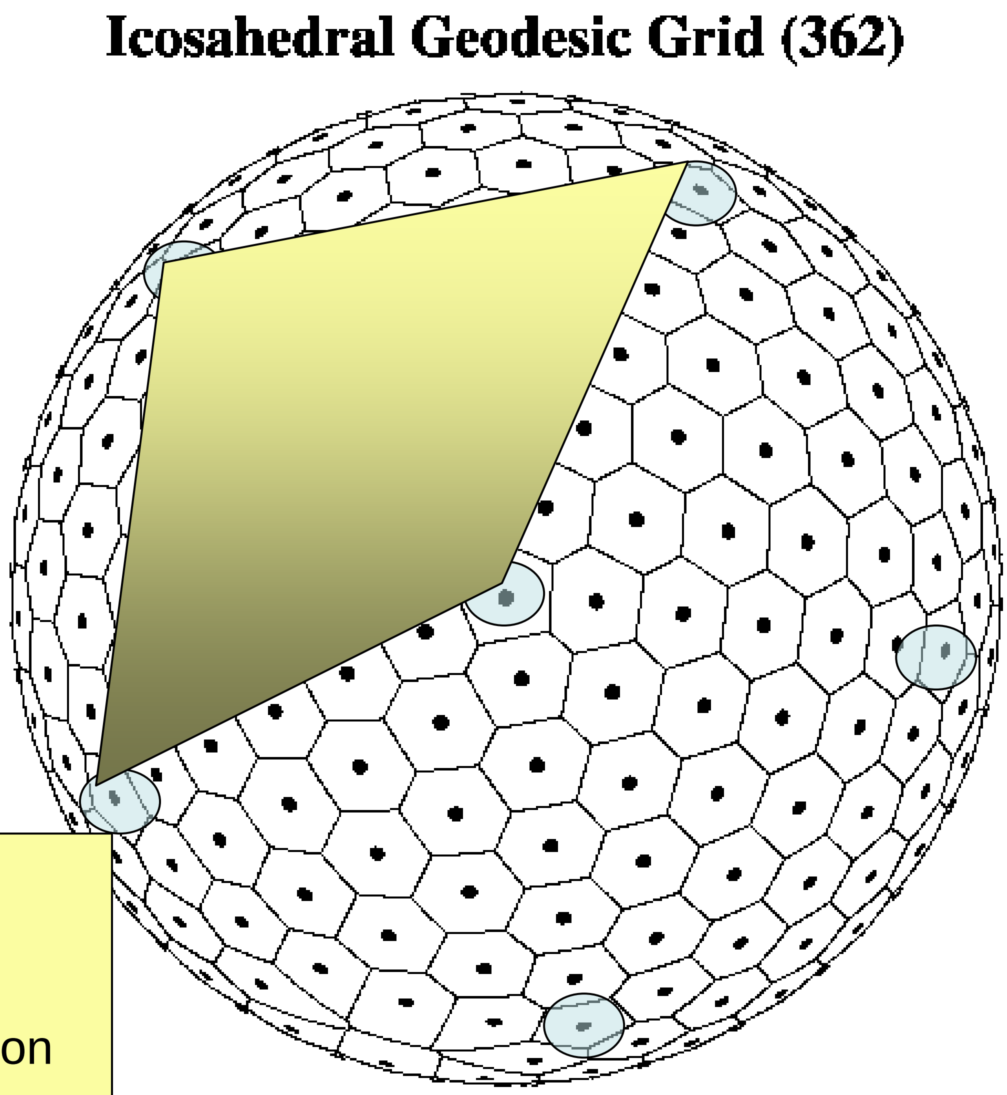
Figure 1. An example of a geodesic grid with a color-coded plot of the observed sea-surface temperature distribution. The continents are

Figure 2. An example of a latitude–longitude grid. A pole is at the top. The black dots represent grid cell centers that are equally spaced in longitude

**Diagrams - Randall et al. – Colorado State University**
http://kiwi.atmos.colostate.edu/DOE_Cooperative_Agreement/pdf/CISE.pdf

<u>Icosahedral grid</u>

- 10 rhombi covering sphere
- All point volumes - *hexagons* (except 12 points at rhombi corners - pentagons)
- **Map-scale factor variation – 0.95**
- Grid resolution example - level-5 icosahedral grid – 240km resolution)




((2**n)**2)*10 + 2 = no. cells

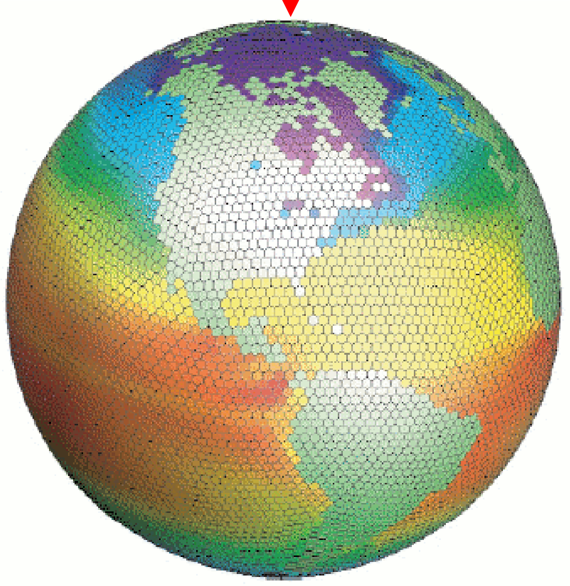
5th level -
(32**2)*10 + 2 = 10242 ~240km resolution
6th level – 40962 cells ~120km resolution
7th level – 163842 cells ~60km resolution
8th level – 655,362 cells ~30km resolution
9th level – 2,621,442 cells ~15km resolution

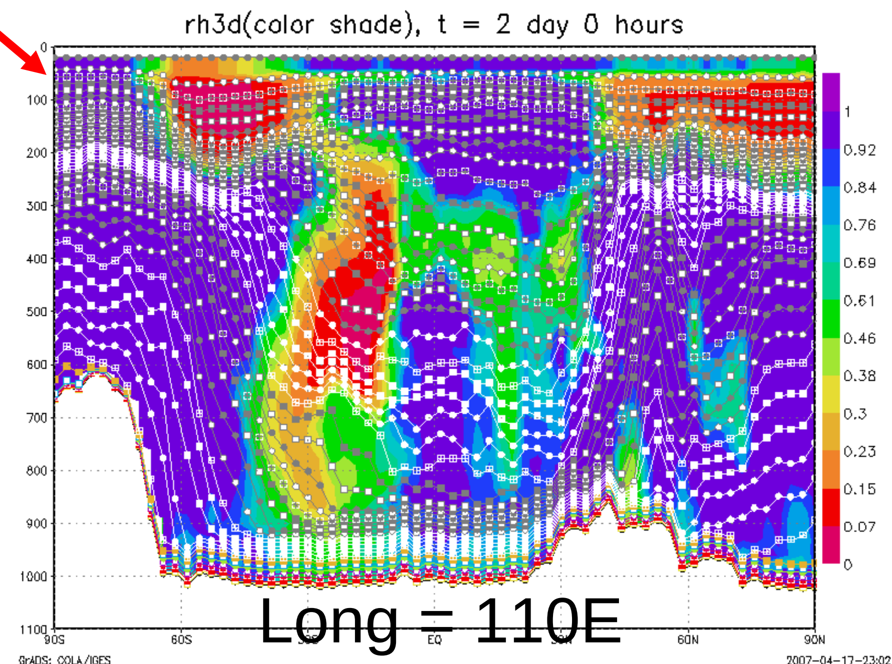
# FIM Dynamic Core

**Finite volume**, flux form equations in horizontal

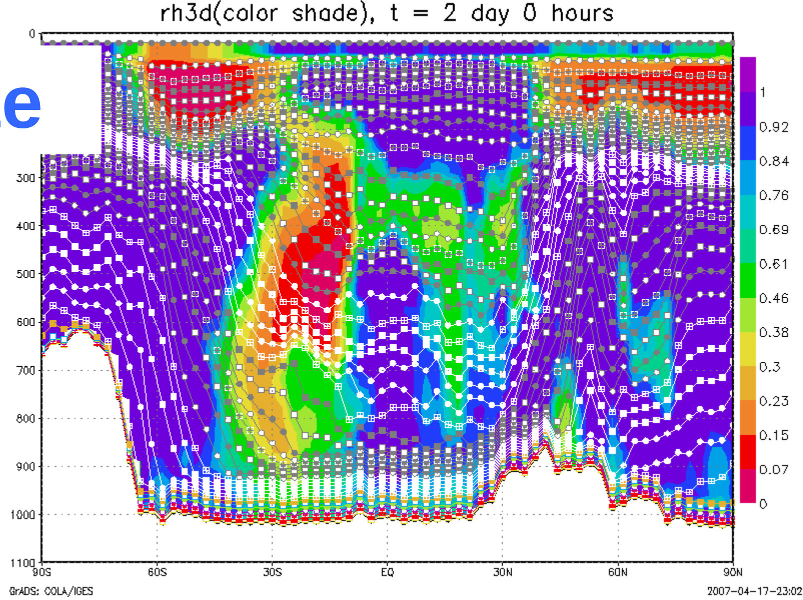
Hybrid isentropic-sigma ALE vertical coordinate
(arbitrary Lagrangian-Eulerian)
- **Flow-following**

**Icosahedral** grid, with spring dynamics implementation





# FIM design – vertical coordinate




**Hybrid (sigma/ isentropic) vertical coordinate**

- Used in NCEP Rapid Update Cycle (RUC) model (Bleck/Benjamin)

- Used in HYCOM ocean model (Bleck)

- Option in upcoming WRF repository branch (Zangl - NCAR and German DWD)

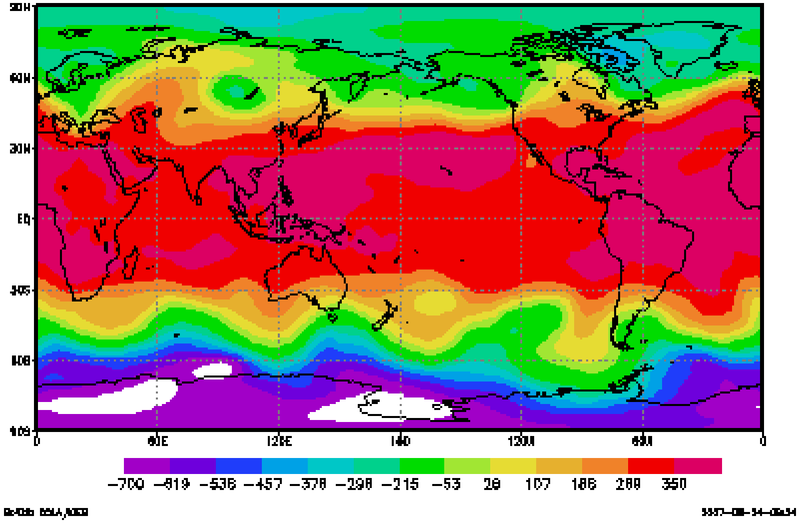
Improved transport by reducing numerical dispersion from vertical cross-coordinate transport, **improved stratospheric/tropospheric exchange.**

Applicable down to 1-km non-hydrostatic scale by using larger-scale 3-d isentropic variation as part of FIM target coordinate definition (e.g, Zangl, 2007 - MWR)

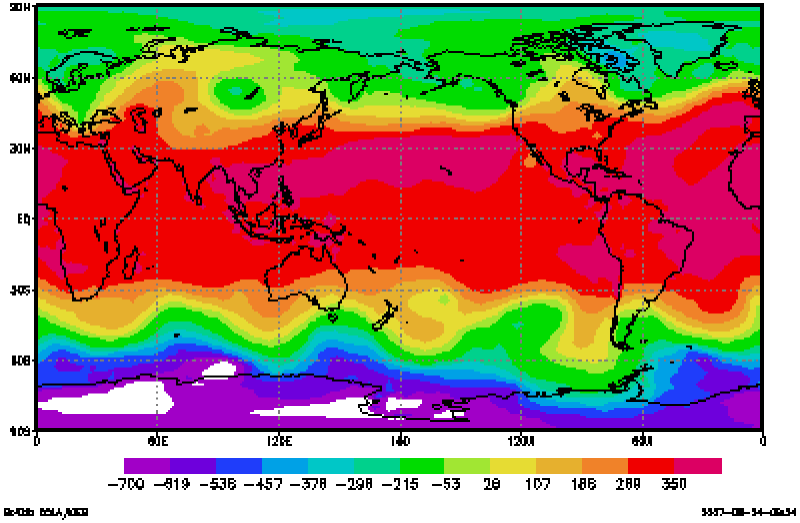
# 500hPa comparison between NCAR/NCEP Reanalysis and FIM (G8~30km) - initialized 9 October 2003

**Initial time @ 00z,10/09/2003**

**NCAR/NCEP reanalysis 500 mb height anomaly**




**FIM forecast 500 mb height anomaly**

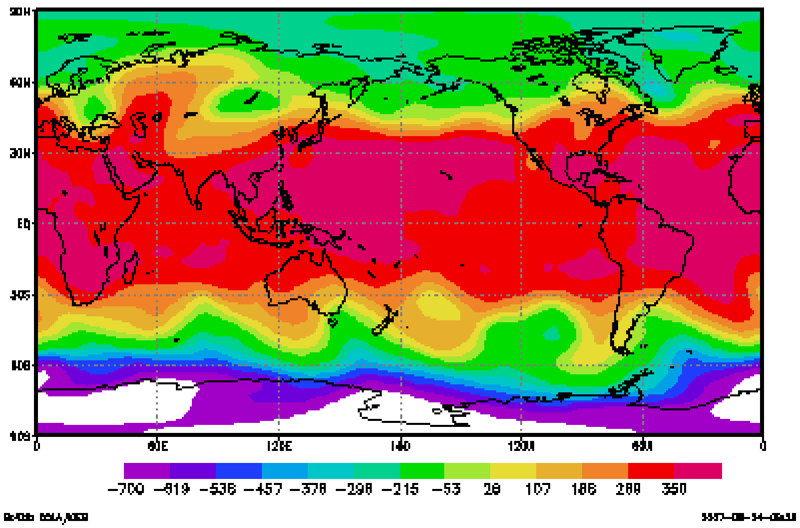



**500mb-mean removed**

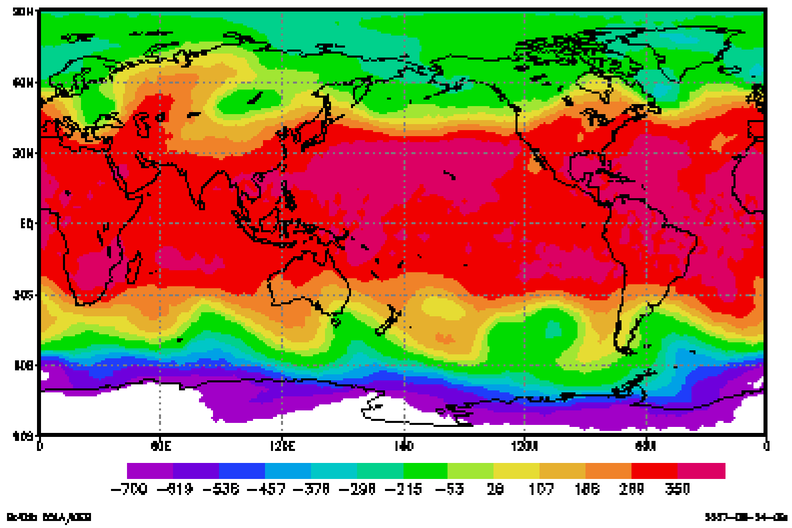
# 500hPa comparison between NCAR/NCEP Reanalysis and FIM (G8~30km) - initialized 9 October 2003

## 1-day fcst verified @ 00z,10/10/2003

**NCAR/NCEP reanalysis 500 mb height anomaly**



**FIM forecast 500 mb height anomaly**

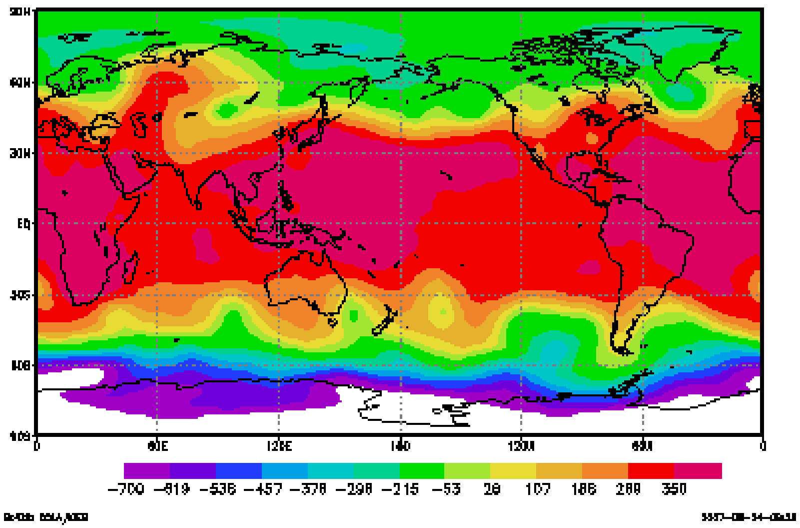


## 500mb-mean removed

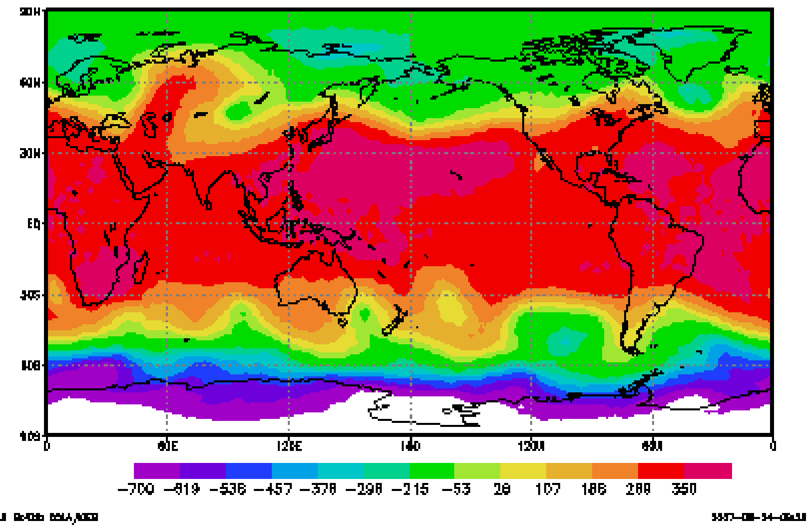
# 500hPa comparison between NCAR/NCEP Reanalysis and FIM (G8~30km) - initialized 9 October 2003

## 2-day fcst verified @ 00z,10/11/2003

**NCAR/NCEP reanalysis 500 mb height anomaly**




**FIM forecast 500 mb height anomaly**

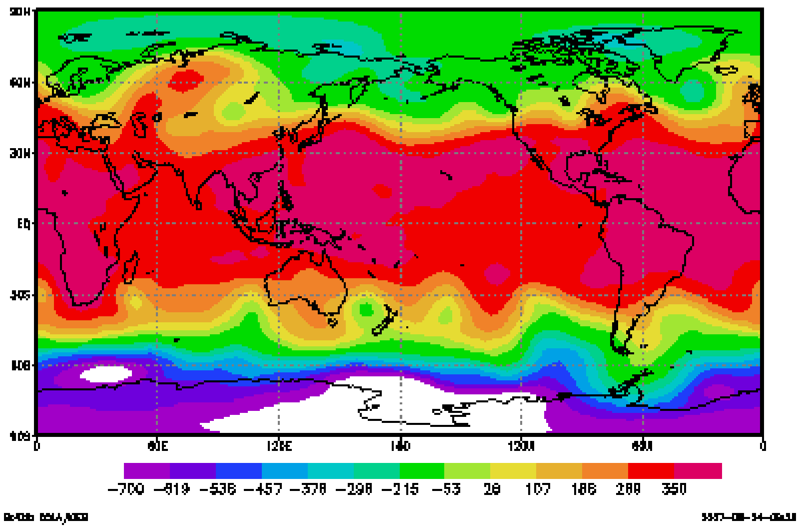



## 500mb-mean removed

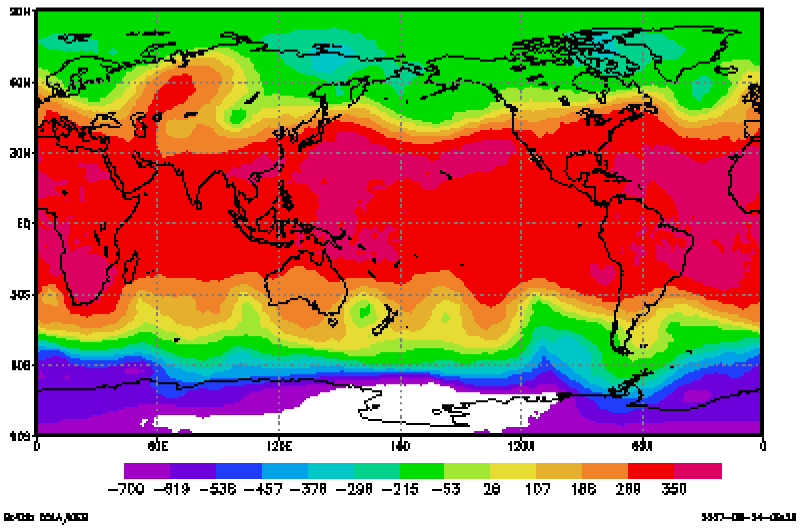
# 500hPa comparison between NCAR/NCEP Reanalysis and FIM (G8~30km) - initialized 9 October 2003

## 3-day fcst verified @ 00z,10/12/2003

**NCAR/NCEP reanalysis 500 mb height anomaly**




**FIM forecast 500 mb height anomaly**

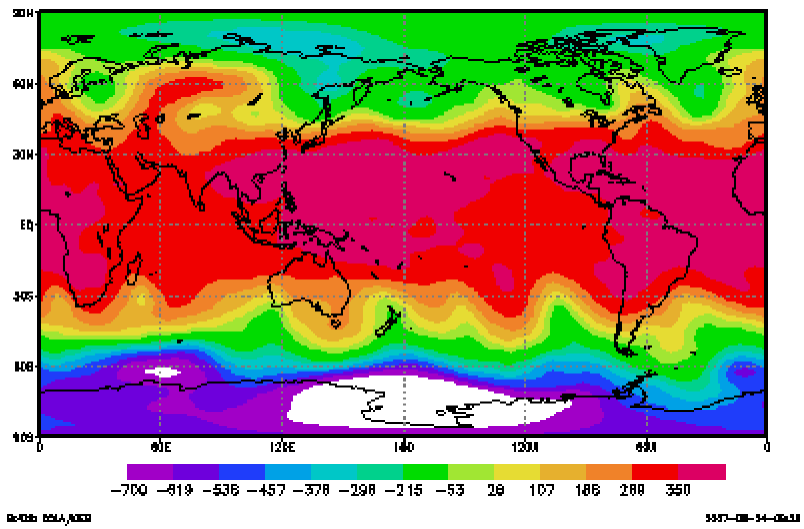



## 500mb-mean removed

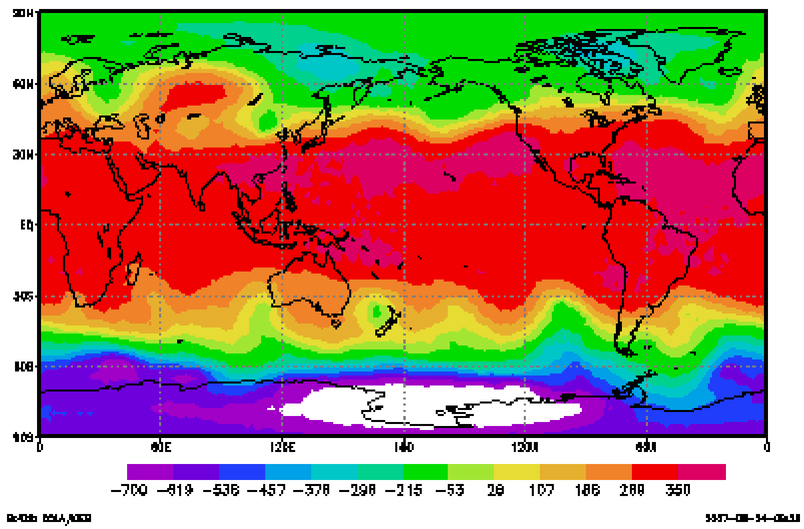
# 500hPa comparison between NCAR/NCEP Reanalysis and FIM (G8~30km) - initialized 9 October 2003

## 4-day fcst verified @ 00z,10/13/2003

**NCAR/NCEP reanalysis 500 mb height anomaly**



**FIM forecast 500 mb height anomaly**

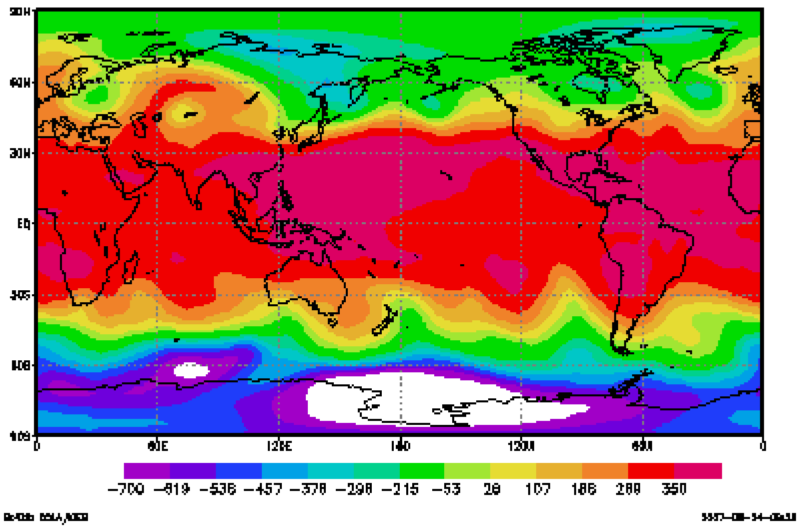


## 500mb-mean removed

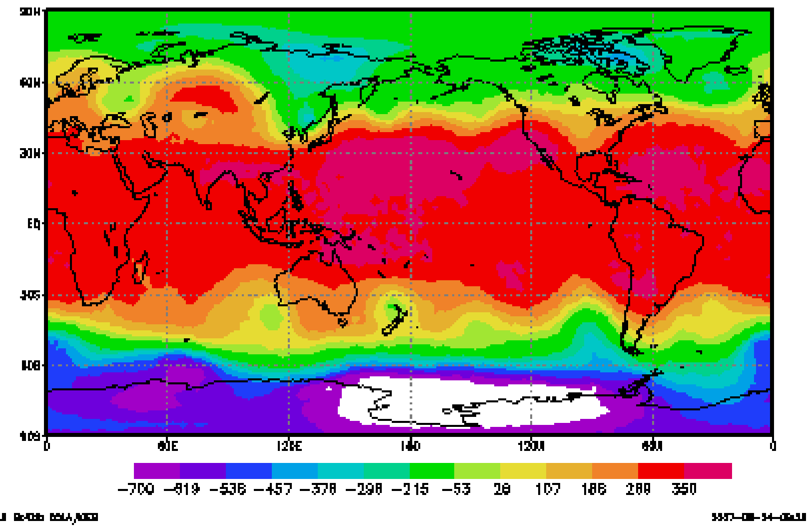
# 500hPa comparison between NCAR/NCEP Reanalysis and FIM (G8~30km) - initialized 9 October 2003

## 5-day fcst verified @ 00z,10/14/2003

**NCAR/NCEP reanalysis 500 mb height anomaly**

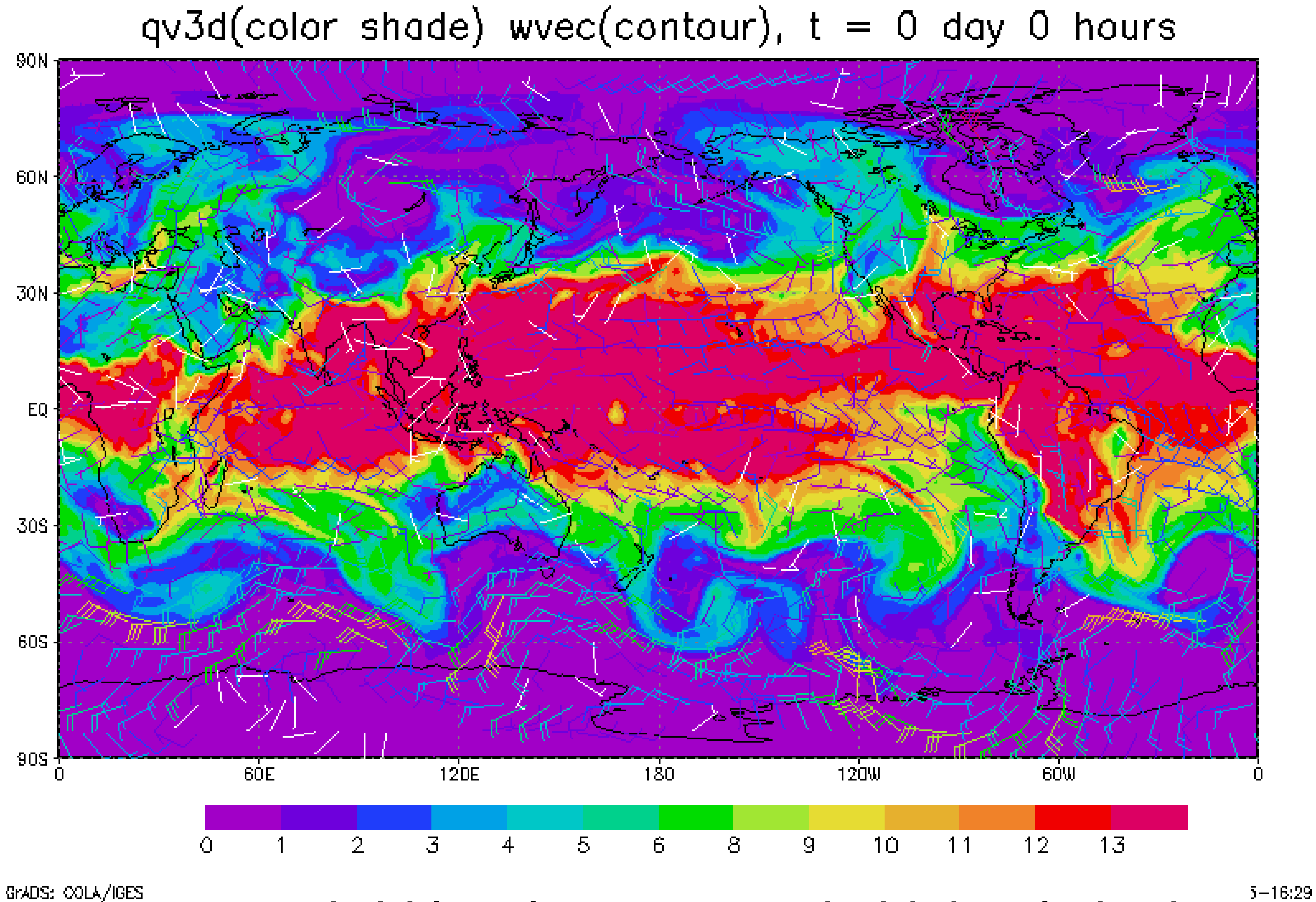


**FIM forecast 500 mb height anomaly**



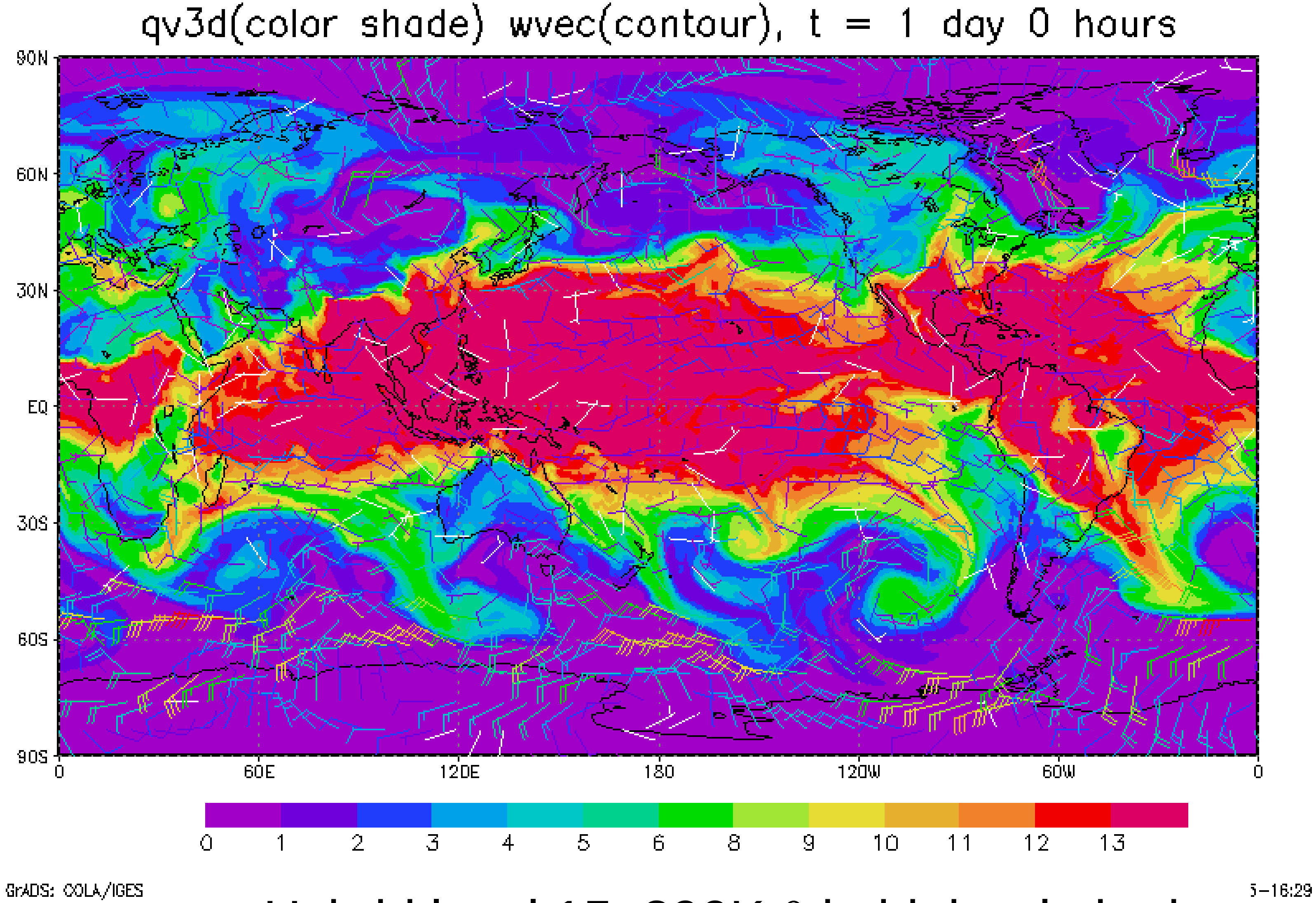
## 500mb-mean removed

# FIM initial condition @ 00z,10/09/2003



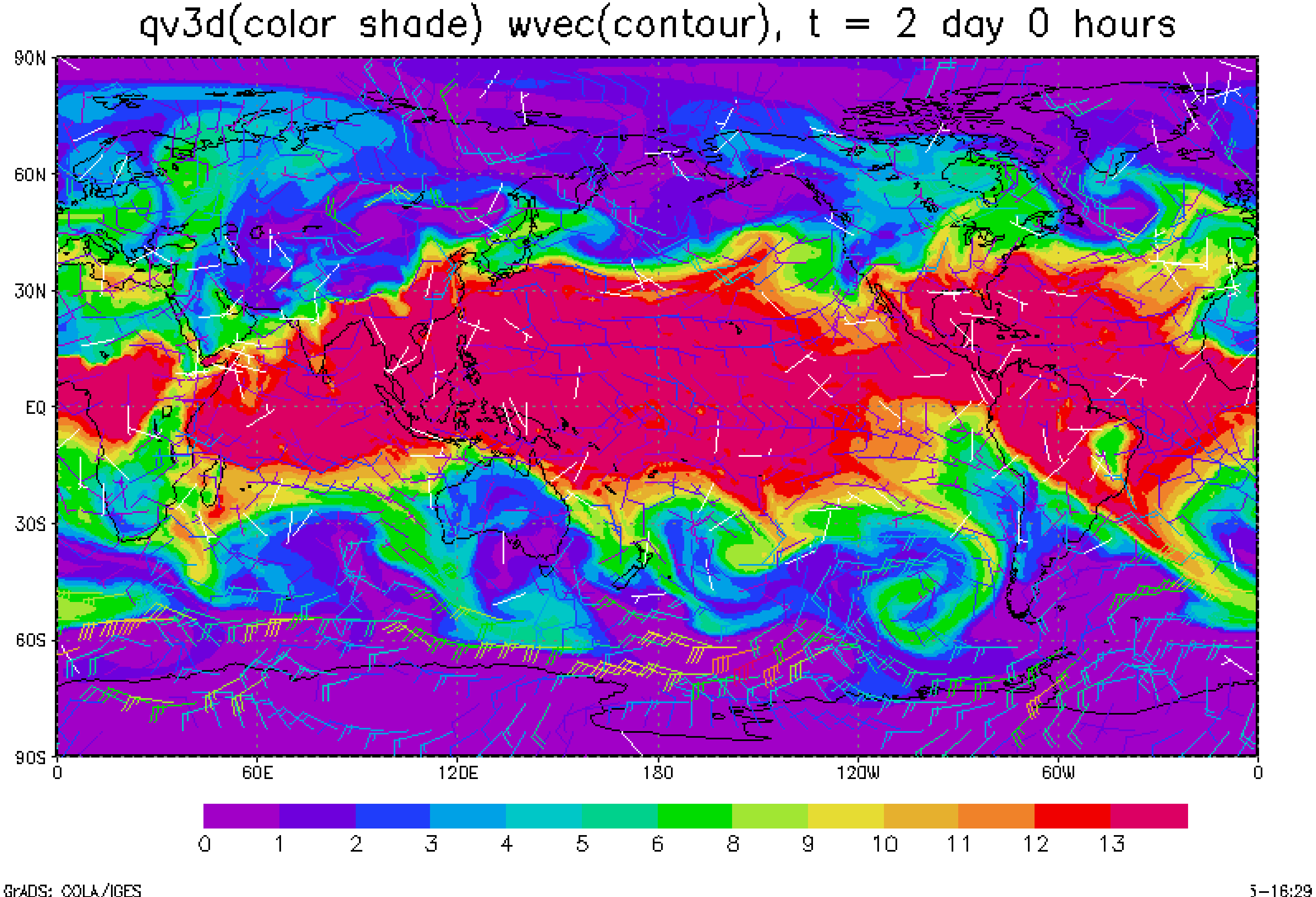

Hybrid level 15, 290K θ in higher latitudes

# 1-day fcst



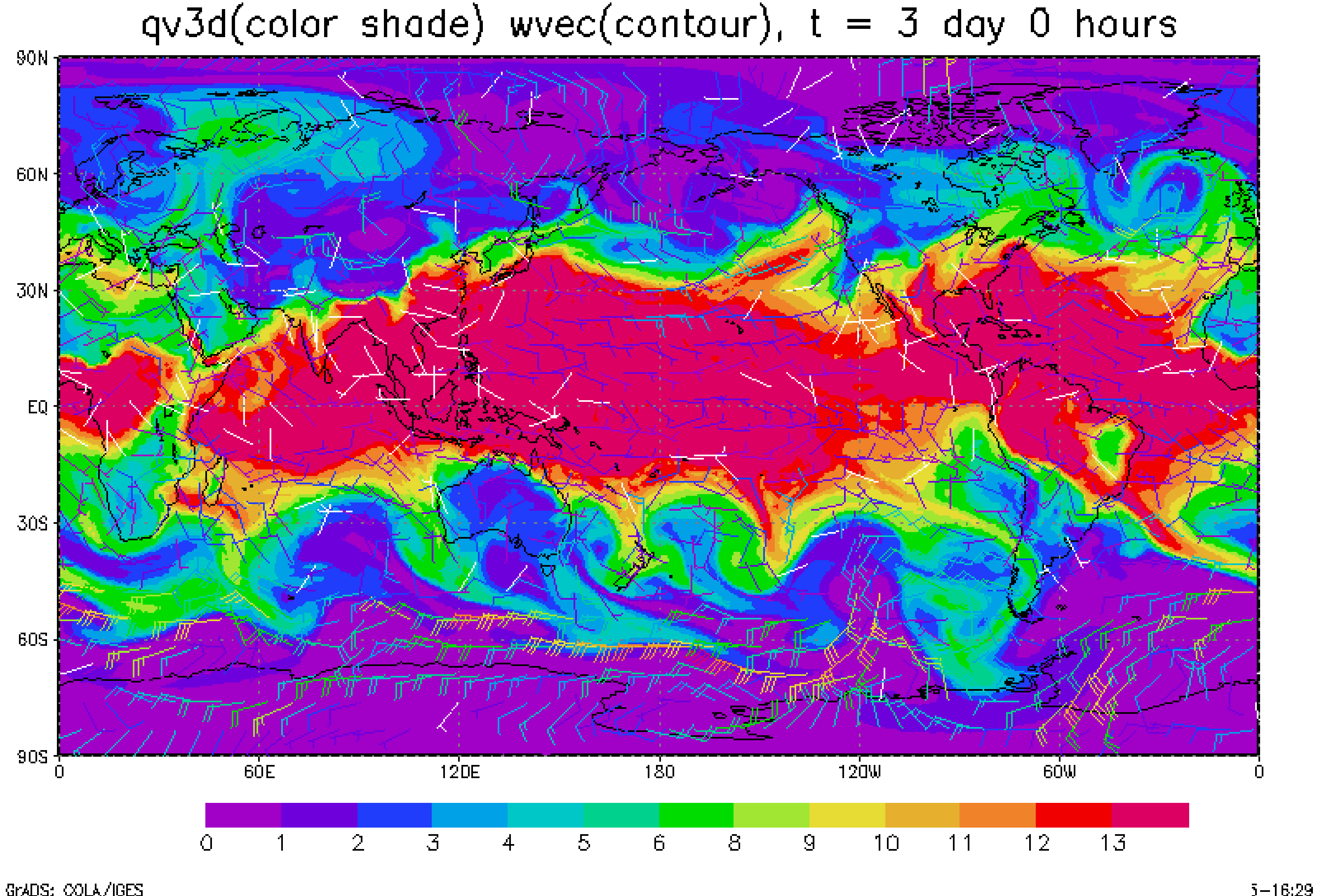

Hybrid level 15, 290K θ in higher latitudes

# 2-day fcst



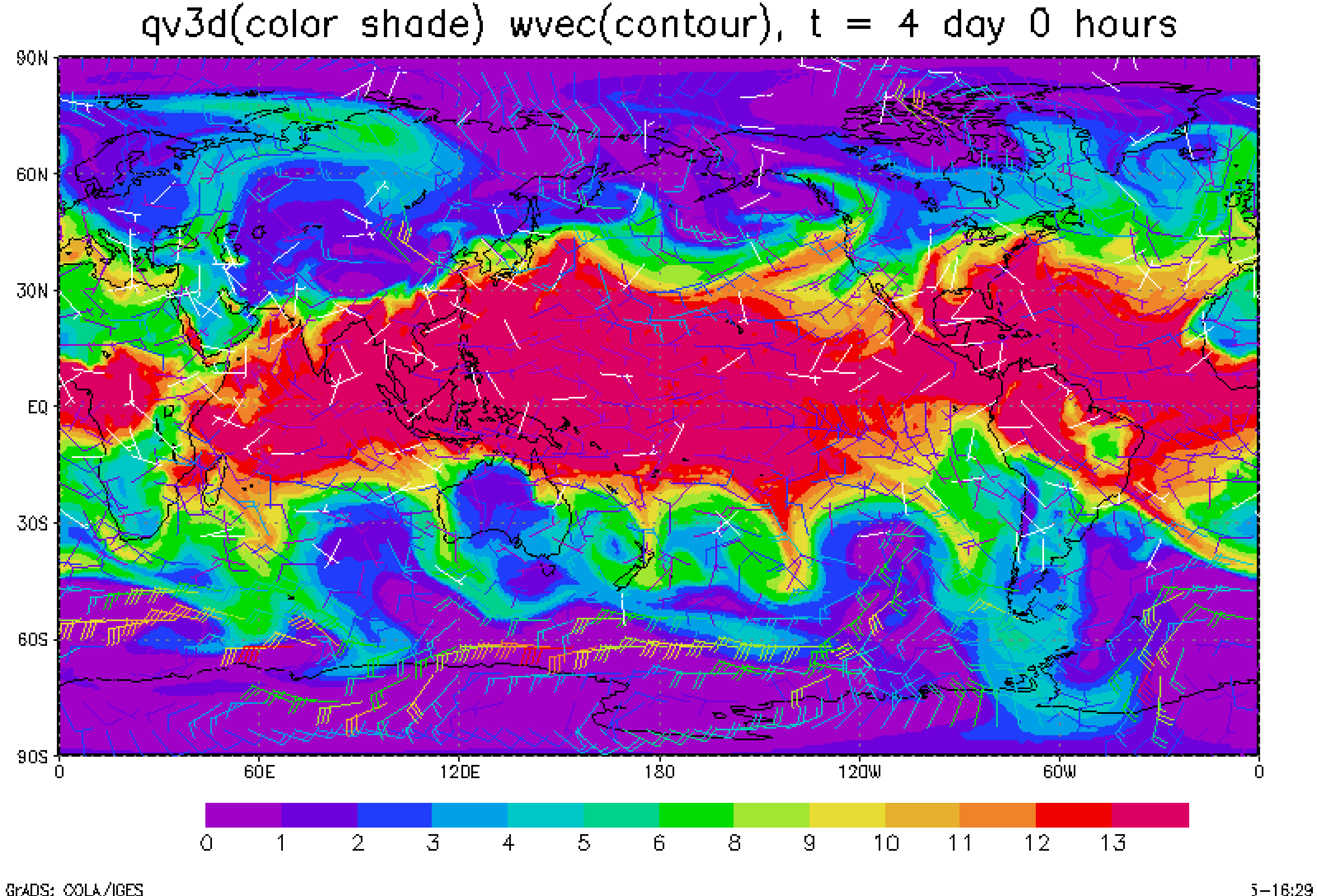

Hybrid level 15, 290K θ in higher latitudes

# 3-day fcst



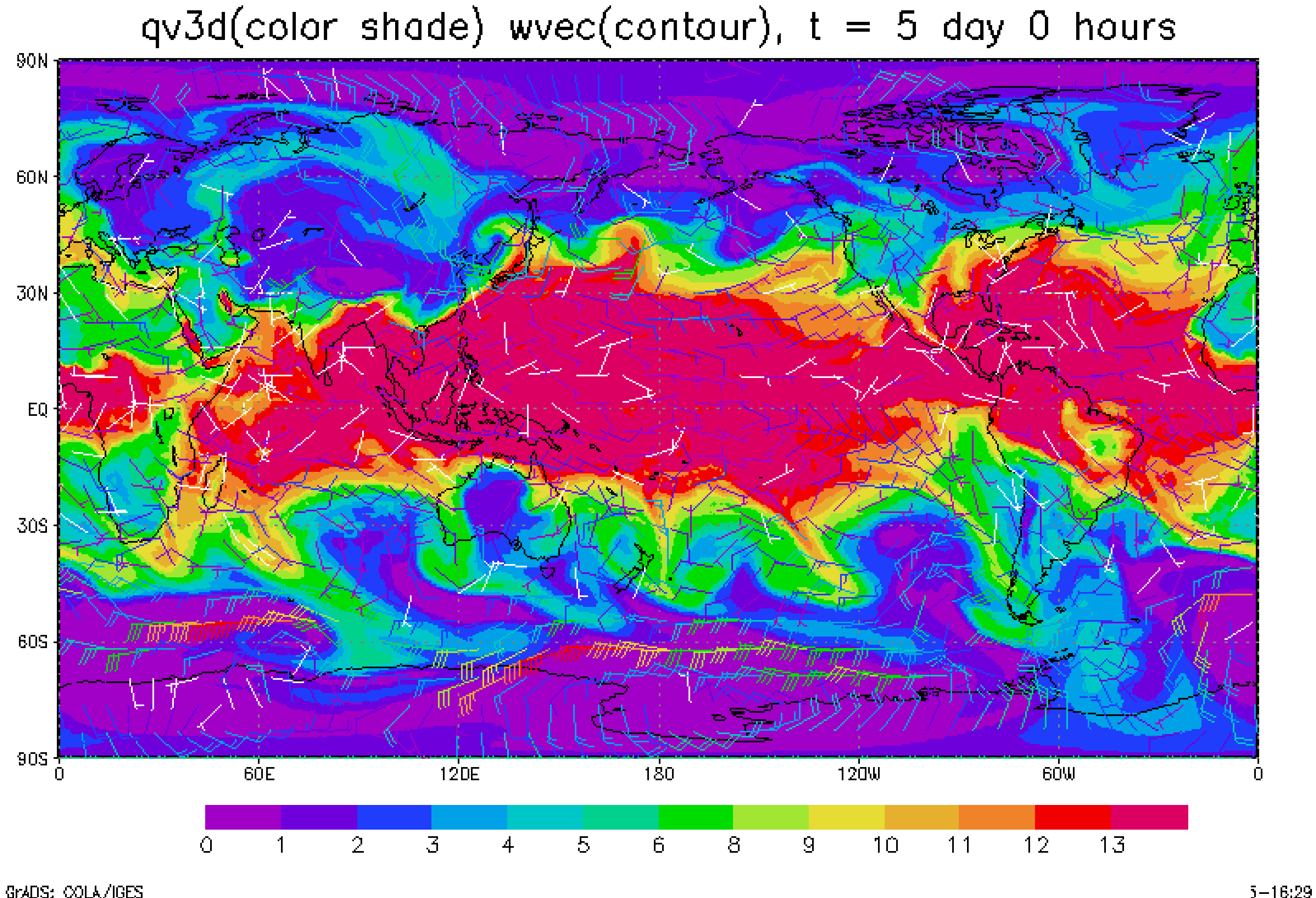

Hybrid level 15, 290K θ in higher latitudes

# 4-day fcst



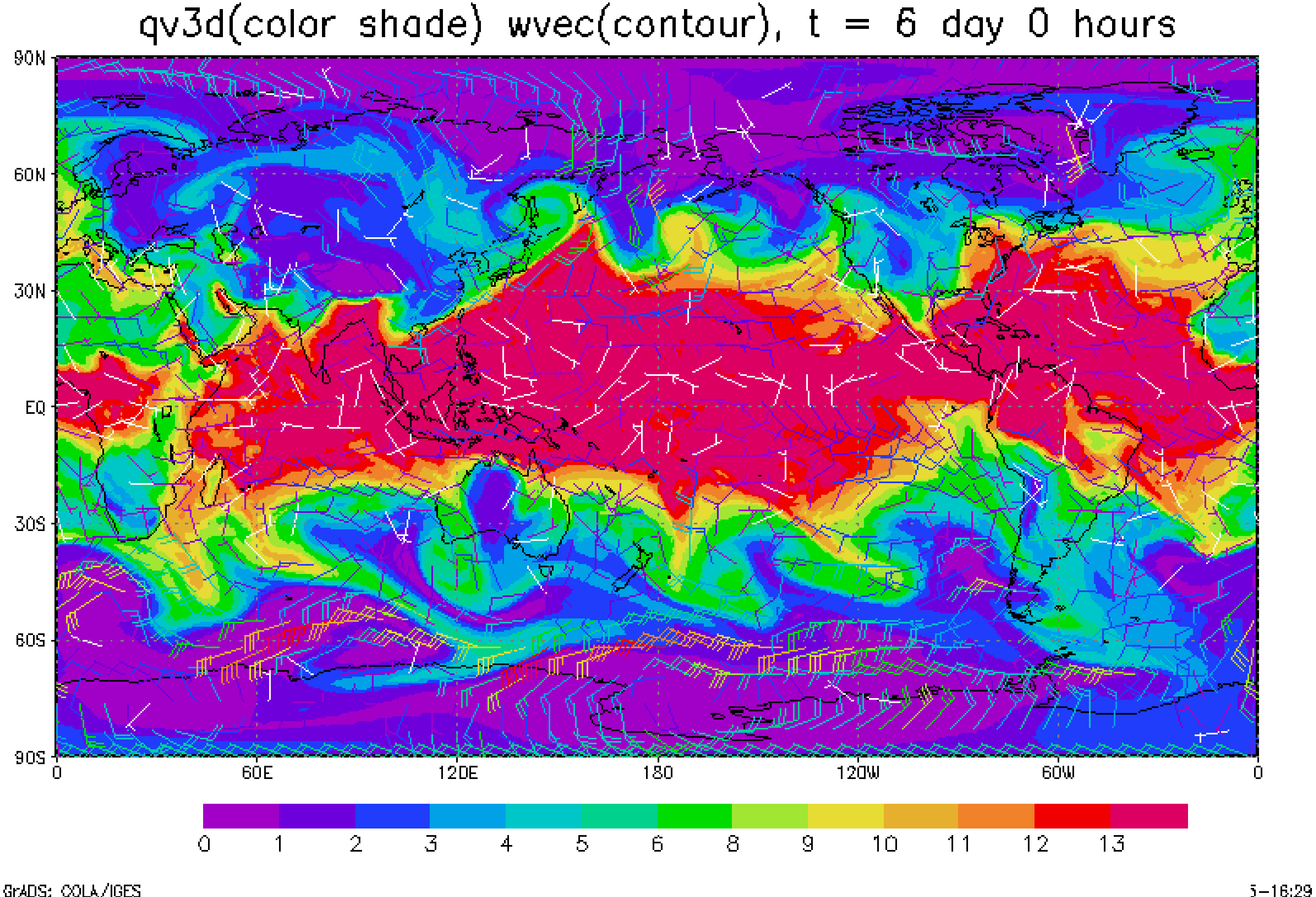

Hybrid level 15, 290K θ in higher latitudes

# 5-day fcst




Hybrid level 15, 290K θ in higher latitudes

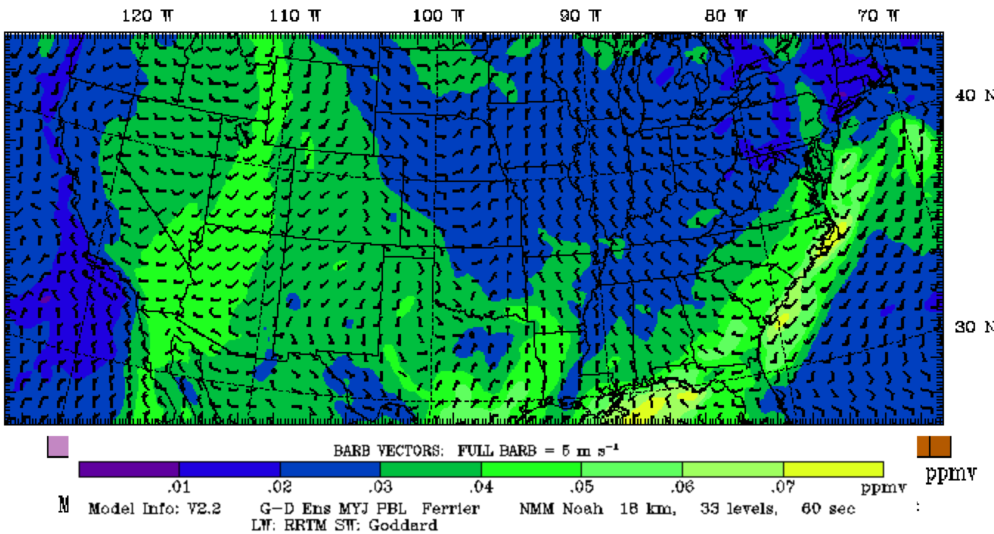
# 6-day fcst



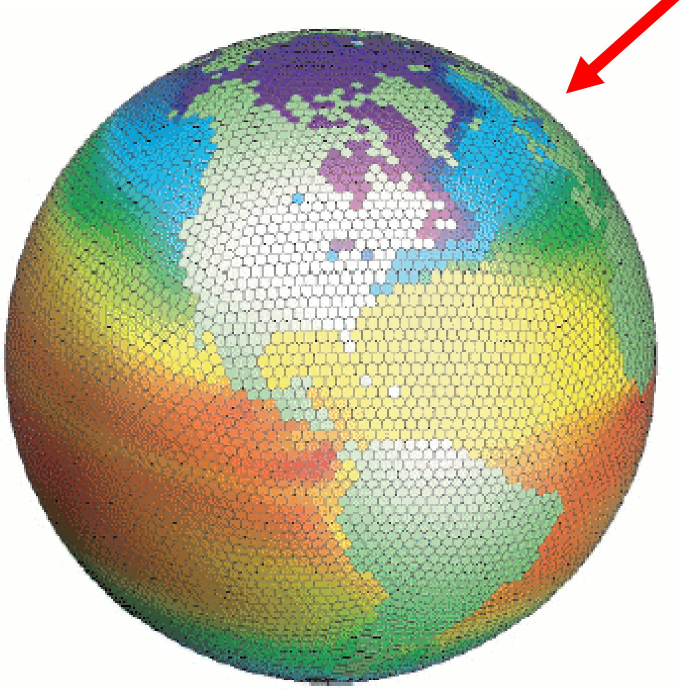

Hybrid level 15, 290K θ in higher latitudes

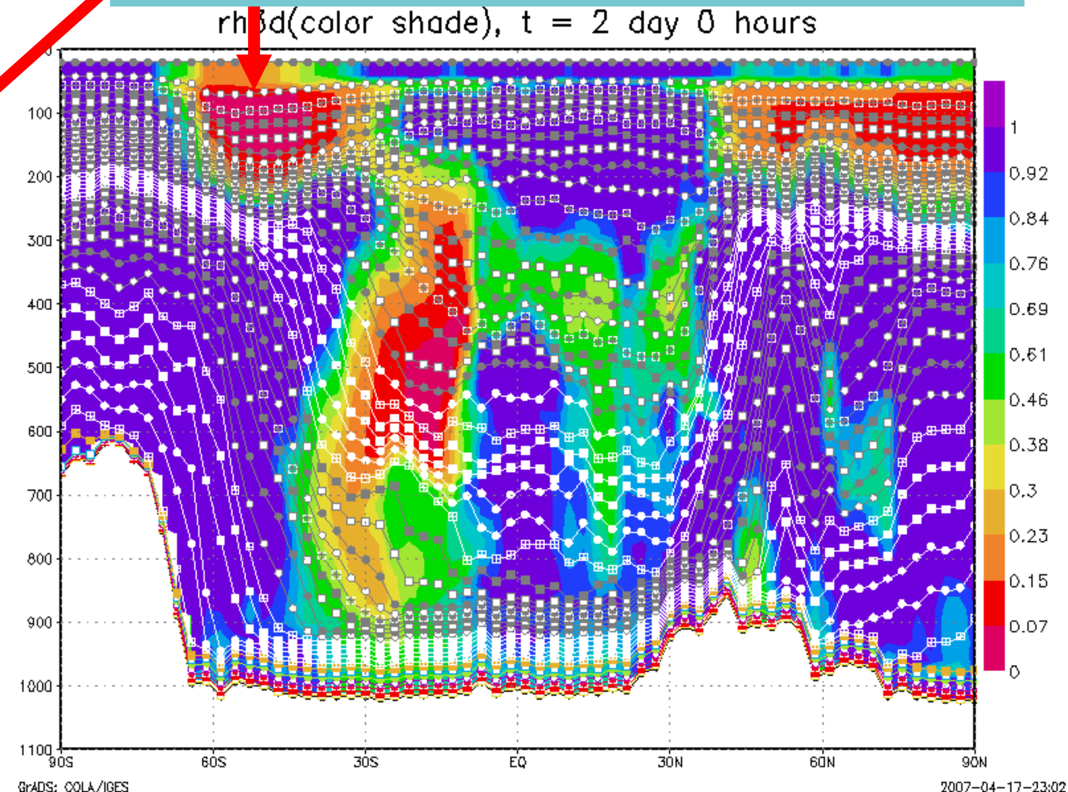
# WRF-Chem package for ESRL global model

Georg Grell




8m O3 fcst valid 00z 11 Oct 07





# Online Chemistry developed for WRF/Chem: An extractable package for ESRL global model, others

Georg Grell

**+ many national and international collaborators**

WRF/Chem web site - http://wrf-model.org/WG11

# Structure of talk

- What is WRF/Chem
- Evaluation
- Future developments

# WRF/Chem

***Community effort lead by ESRL***

***Largest contributing groups: ESRL, PNNL, NCAR***

***Other significant contributions from: Other NOAA  Labs, MPI Mainz, CPTEC Brazil, CDAC India, U of Chile***

# Non-hydrostatic Model Solvers within WRFV2.2 Common Infrastructure

- Eulerian flux-form mass coordinate (Advanced Research WRF, ARW core)
- NMM model (Non-hydrostatic Mesoscale Model, NCEP's core)

# WRF/chem

- Online, completely embedded within WRF computer infrastructure
- Very modular approach
  - Chemistry subdirectory has been implemented in versions of HIRLAM and RAMS
  - May be extracted for other models (e.g., FIM)
- Consistent: all transport done by meteorological model
  - Same vertical and horizontal coordinates (no horizontal and vertical interpolation)
  - Same physics parameterization for subgrid scale transport
  - No interpolation in time
- Easy handling (Data management)

# Deposition/Biogenic Emissions

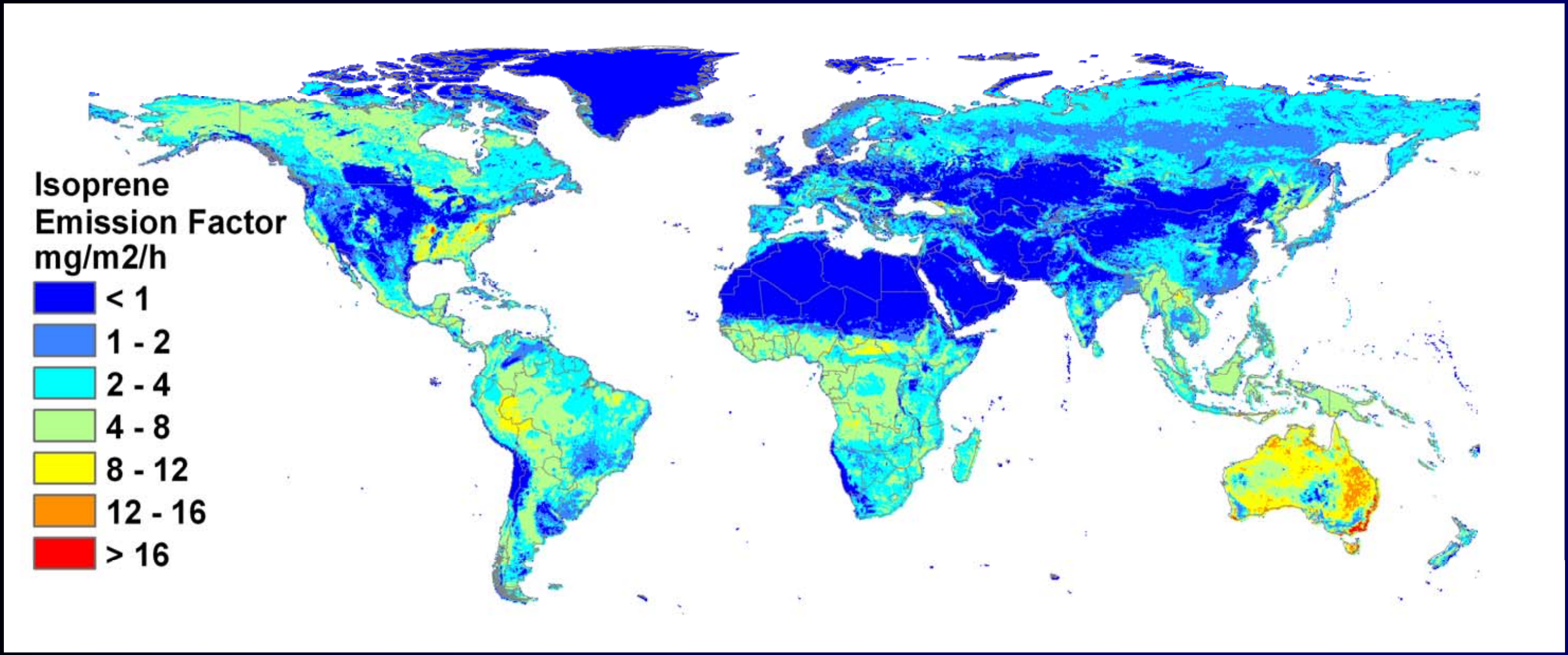
- Dry deposition (coupled with soil/veg scheme, "flux-resistance" analogy)
- Simplified wet deposition by convective parameterization (scavenging factor of .6 for aerosols, no aqueous-phase chemistry involved)
- Biogenic emissions (as in Simpson et al. 1995 and Guenther et al. 1994), include temperature and radiation dependent emissions of isoprene, monoterpenes, also nitrogen emissions by soil
    - May be calculated "online" based on USGS landuse
    - May be input
    - BEISv3.11 (offline reference fields, online modified)

# Implementation of the *M*odel of *E*missions of *G*ases and *A*erosols from *N*ature MEGAN in WRFV2-Chem (Courtesy of Christine Wiedinmyer and Alex Gunther from NCAR with help from Serena Chung and Jerome Fast)

Code is available will officially be released with V3 in March of 2008

# MEGAN: Model of Emissions of Gases and Aerosols from Nature

- Global biogenic emissions model
  - 1 $km^2$ spatial resolution
  - Predicts emissions of > 50 VOC



# Gas Phase Chemistry Packages

1. Chemical mechanism from RADM2 (Quasi Steady State Approximation method with 22 diagnosed, 3 constant, and 38 predicted species is used for the numerical solution)
2. Carbon Bond (CBM-Z) based chemical mechanism, and the

**3.** **K**inetic **P**re**P**rocessor (KPP)

# KPP: Kinetic PreProcessor (Damian et al, 2002, Sandu et al, 2003, Sandu and Sander 2006)

- **Automatic tool to generate chemical mechanisms with a choice of time integration schemes**
- **Can also generate adjoints**
- **Well documented, tested, and widely used**

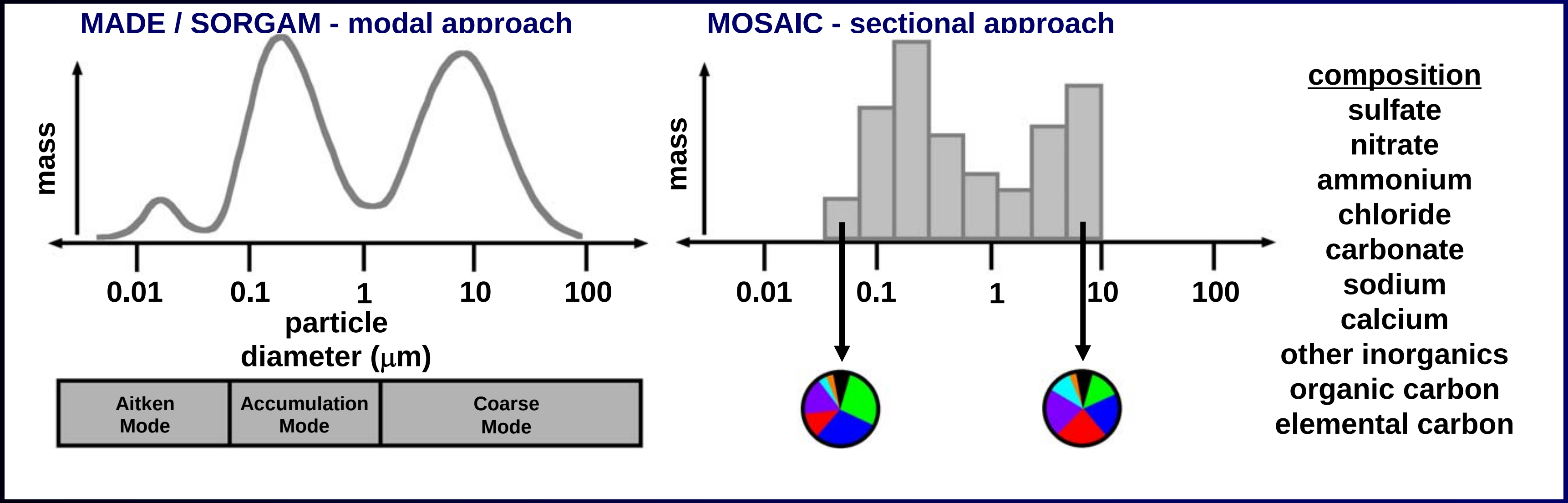
**Thanks to Marc Salzman from the MPI Mainz**

# Available Aerosols modules

1. Modal approach (MADE/SORGAM)
   - Based on Modal Aerosol Dynamics Model for Europe (MADE, Ackermann et al. 1998)
   - Modified to include Secondary Organic Aerosols (SOA), (Schell et al. 2001)
   - Extra transport: total number of aerosol particles within each mode as well as all primary and secondary species for Aitken as well as Accumulation mode
2. Sectional approach (MOSAIC)
3. PM advection, transport, emissions and deposition only

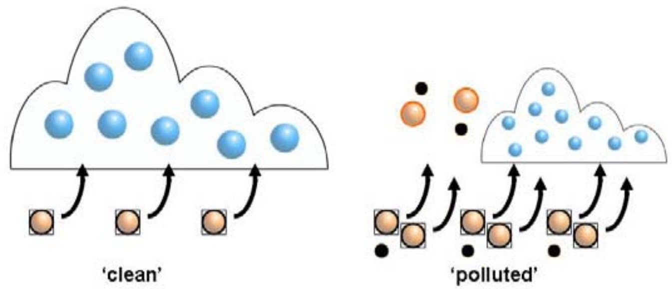
# MOSAIC

- Sectional size distribution; moving-center or two-moment approach for the dynamic equations for mass and number; 112 prognostic species
- Mixing rule for activity coefficients of various electrolytes in multi-component aqueous solutions [*Zaveri et al., JGR, 2005*]
- Thermodynamic equilibrium solver for solid, liquid, or mixed phase state of aerosols [*Zaveri et al., In Press JGR, 2006*]
- Dynamic integration of the coupled gas-aerosol partitioning differential equations [*Zaveri et al., In preparation*]



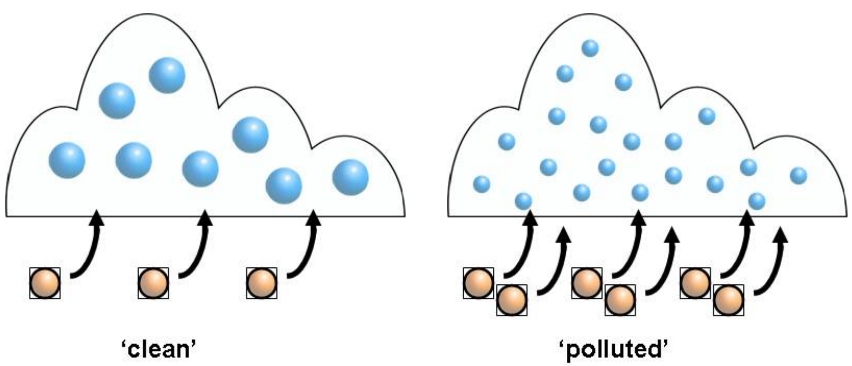
# Aerosol effects included in WRF/Chem in addition to direct coupling to atmospheric radiation

## Semi-Direct Effect



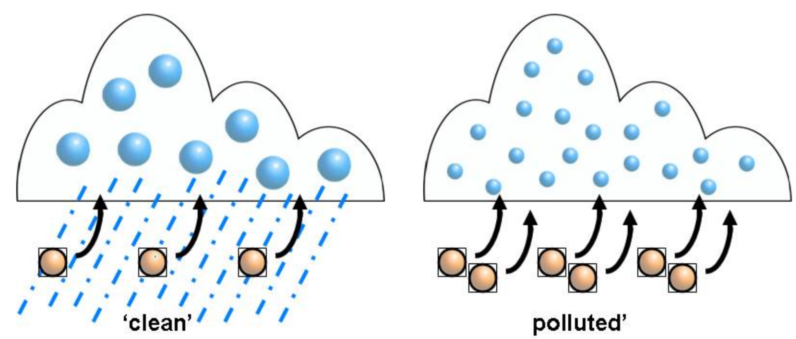

- Influence of aerosol absorption of sunlight on formation and evaporation of clouds

## First Indirect Effect




- Influence of cloud optical depth through impact on effective radius, with no change in water content of cloud

## Second Indirect Effect



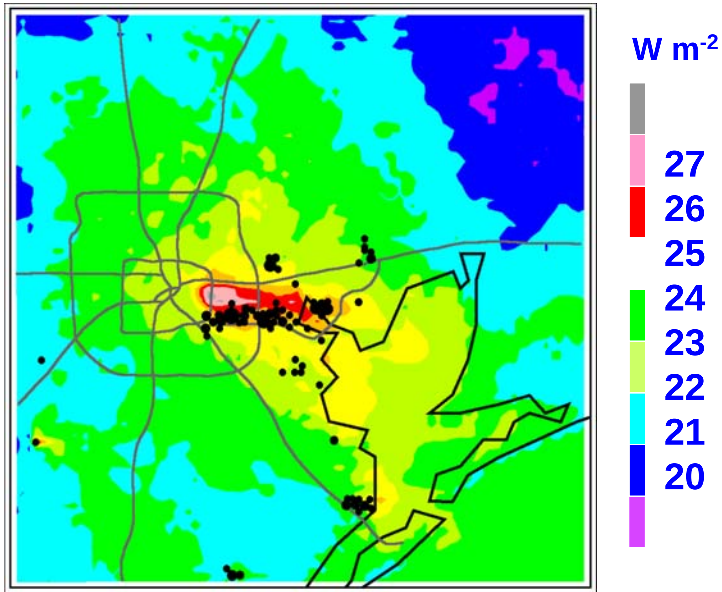

- Influence of cloud optical depth through influence of droplet number on mean droplet size and hence initiation of precipitation

# Aerosol Interactions Not Treated Yet

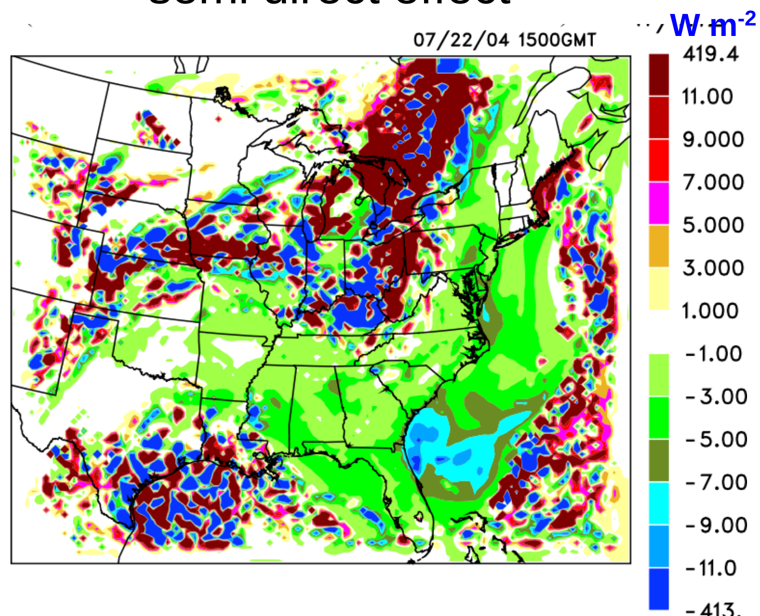
- **First Dispersion Effect:** Influence on cloud optical depth through influence of *aerosol on dispersion of droplet size distribution*, with no change in water content of cloud
- **Second Dispersion Effect:** Influence on cloud optical depth through influence of *aerosol on dispersion* and hence *initiation of precipitation*
- **Glaciation Indirect Effect:** Influence of *aerosol on conversion of haze and droplets to ice crystals*, and hence on cloud optical depth and initiation of precipitation

## Example of direct effects

Dry run – direct effect



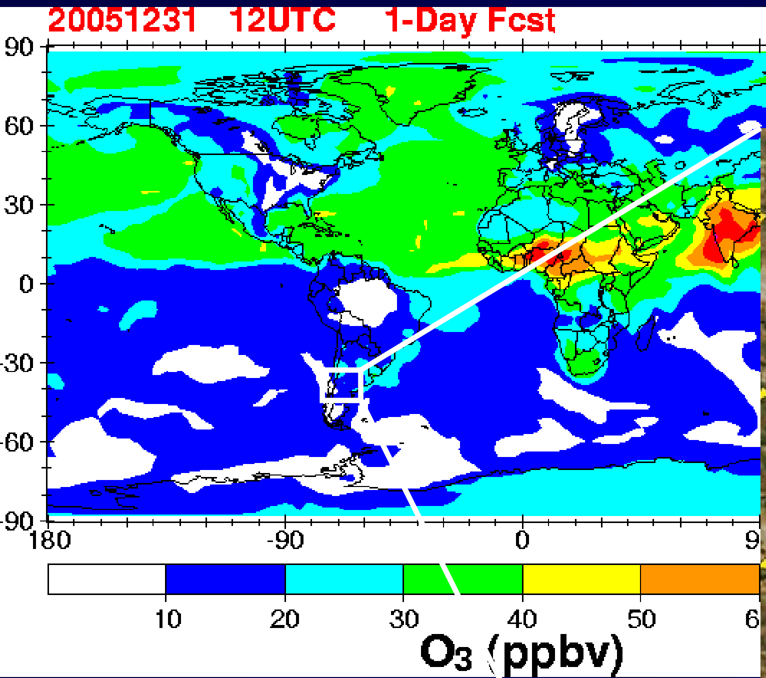

semi direct effect



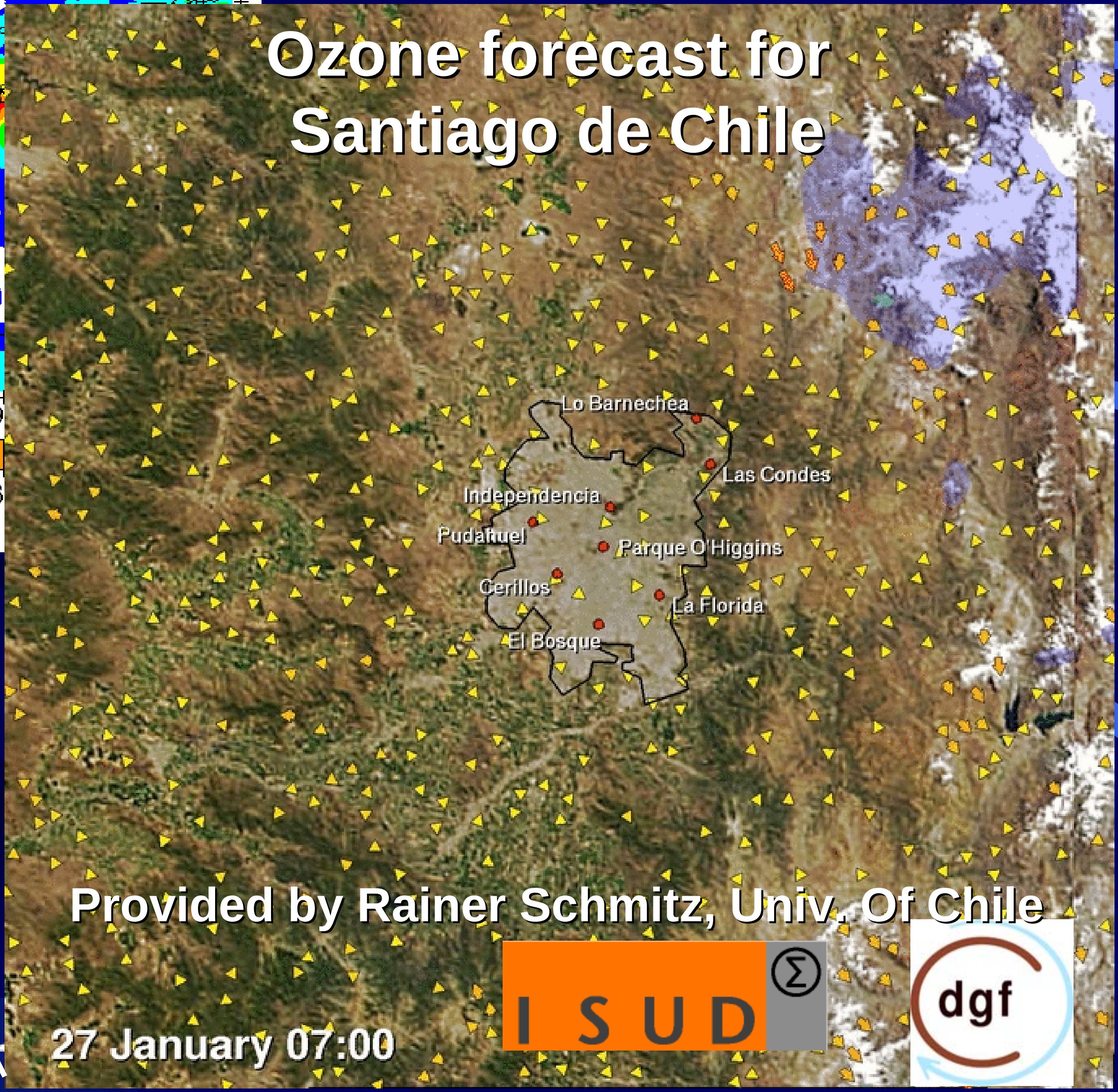
# Photolysis Packages – all coupled to aerosols and hydrometeors

- Fast-j photolysis scheme
- Madronich Photolysis
- Madronich FTUV code available , official release with WRFv3)

# Use of chemical data from Global Chemistry Model (GCM) for boundary conditions




Global forecast by Max-Planck-Instiute, Mainz, Germany (Lawrence, 2003)




Now also available for MOZART and RAQMS and of course WRF/Chem

# Improved non-resolved convective transport

- Ensemble approach (based on Grell/Devenyi parameterization)
  - Uses observed or predicted rainfall rates as met-input
  - Ensemble of entrainment/detrainment profiles and/or downdraft parameters to determine vertical redistribution of tracers
  - Ensembles may be weighted to determine optimal solution
  - Can be used as 3-d scheme for smooth transition to high resolution
- Aqueous phase chemistry module called from within convective routine, CMAQ module (not tested and released yet)
- Connected to photolysis and atmospheric radiation schemes

# A model within a model : Fire Plumerise (Collaboration with Saulo Freitas from CPTEC in Brazil)

***Initialized with GOES-ABBA and MODIS***

## 1-D Plume model

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial z} = \gamma g B - \frac{2\alpha}{R} w^2 \quad \begin{cases} \gamma = \dfrac{1}{1+0.5} & \textit{Simpson\&Wiggert, 1968} \\ \gamma = \dfrac{1}{1-2\mu} & \textit{Siebesma et al, subm. JAS} \end{cases}$$

$$\frac{\partial T}{\partial t} + w\frac{\partial T}{\partial z} = -w\frac{g}{c_p} - \frac{2\alpha}{R}|w|(T - T_e) + \left(\frac{\partial T}{\partial t}\right)_{microphysics}$$

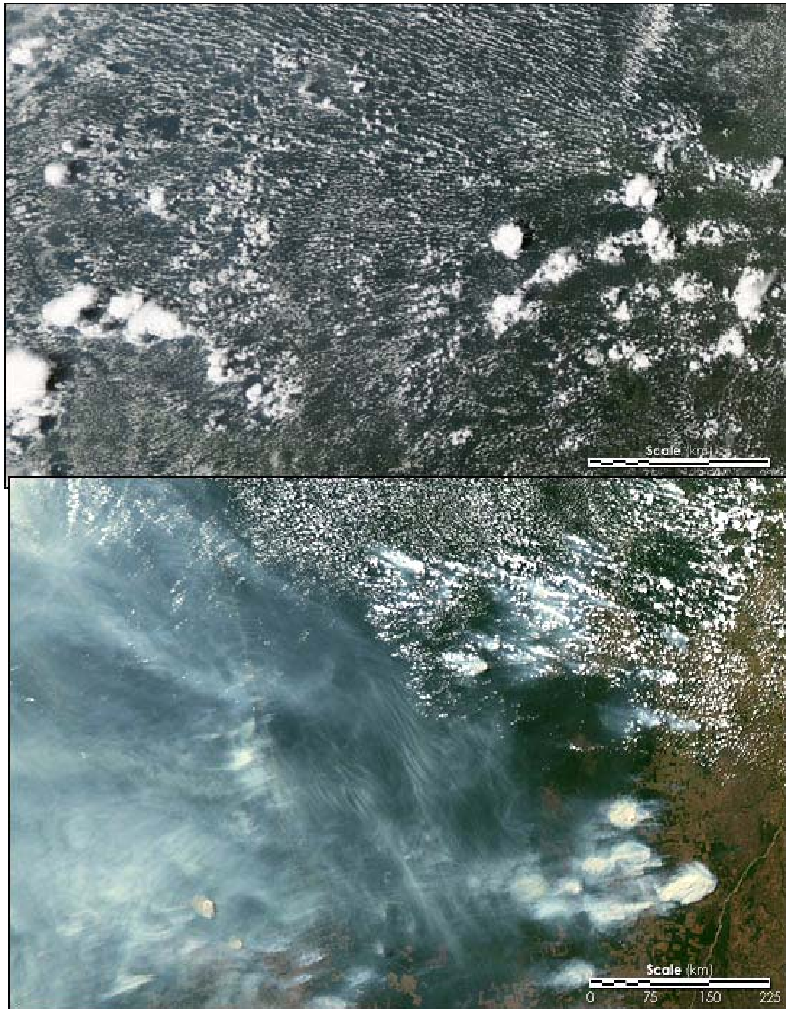
$$\frac{\partial r_v}{\partial t} + w\frac{\partial r_v}{\partial z} = -\frac{2\alpha}{R}|w|(r_v - r_{ve}) + \left(\frac{\partial r_v}{\partial t}\right)_{microphysics}$$

$$\frac{\partial r_c}{\partial t} + w\frac{\partial r_c}{\partial z} = -\frac{2\alpha}{R}|w| r_c + \left(\frac{\partial r_c}{\partial t}\right)_{microphysics}$$

$$\frac{\partial r_{ice,rain}}{\partial t} + w\frac{\partial r_{ice,rain}}{\partial z} = -\frac{2\alpha}{R}|w| r_{ice,rain} + \left(\frac{\partial r_{ice,rain}}{\partial t}\right)_{microphysics} + \text{sedim}$$

$$\left(\frac{\partial \xi}{\partial t}\right)_{microphysics} (\xi = T, r_v, r_c, r_{rain}, r_{ice}), \quad \text{sedim} \begin{cases} \textit{bulk microphysics:} \\ \textit{Kessler, 1969} \\ \textit{Ogura \& Takahashi,1971} \\ \textit{Berry,1967} \end{cases}$$

## Semi-direct (?) effect caused by biomass burning



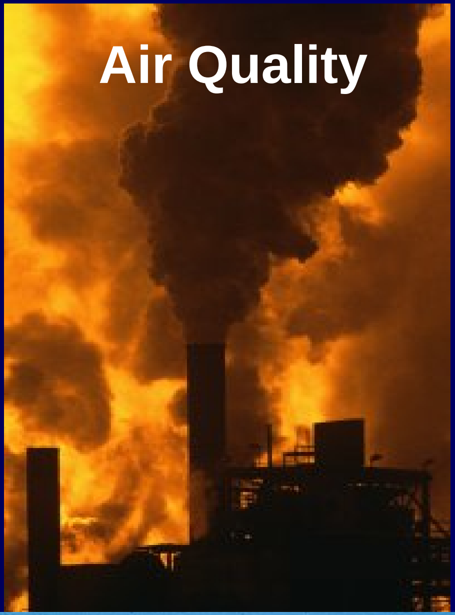
# Near future (for release WRFv3 in March)

- Global WRF/Chem
  - KPP equation file for global gas-phase mechanism from MPI Mainz
  - RETRO or EDGAR anthropogenic emissions data set
  - Global fire emissions from GOES-ABBA and MODIS
  - Other global versions at NCSU and PNNL with different chemical mechanisms, but not for V3 release
- Sea salt parameterization (courtesy of M. Sofiev)
- Coupling of modal aerosol approach with radiation schemes (J. Fast)
- Offline version (Indo-US project)

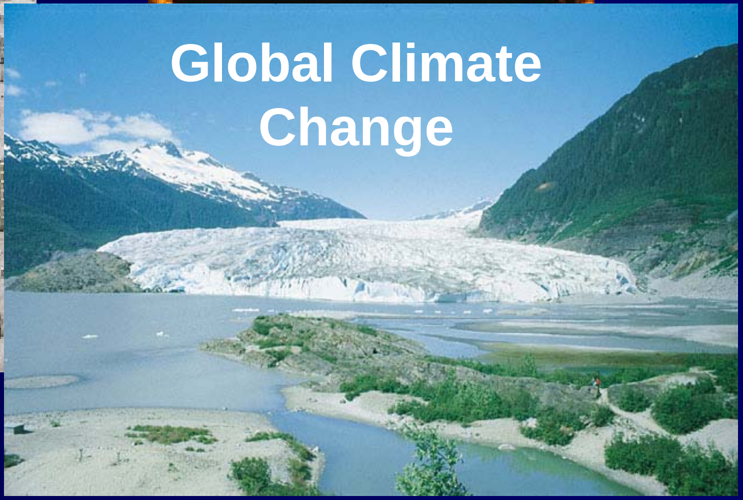
# Near future (maybe for release WRFv3 in March 2008, not guaranteed)

- Dust parameterizations
- Aerosol modules from GOCART

# Current possible applications using different levels of WRF-chem options

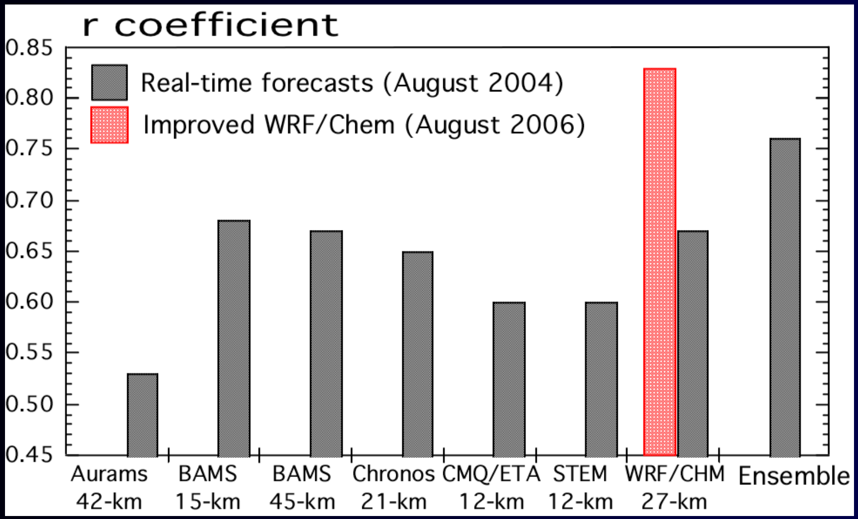


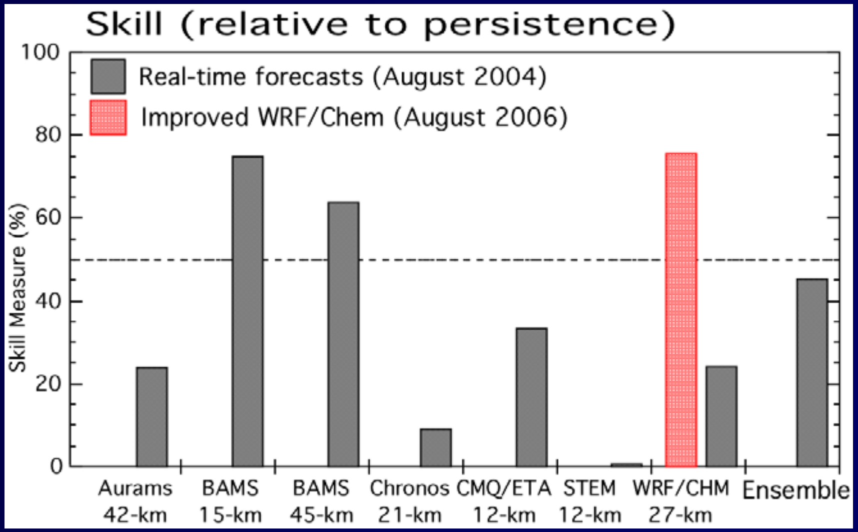


# Current possible applications using different levels of WRF-chem options

- Dispersion-lite: 1 tracer – almost no additional cost
- Dispersion-heavy: ensemble of tracers
  - up to 1.2x meteorology-model CPU cost)
- WRF-Chem very lite: To be determined (simple KPP ozone mechanism, GOCART aerosols) – 1.5-2.0x
- WRF-Chem lite: RACM-KPP and PM advection (full physics intereactions) : 2-3x
- WRF-Chem medium: RACM, Modal aerosols
- WRF-Chem heavy: Up to 450 prognostic variables (currently)
- More granularity in chem options (CPU cost) in future

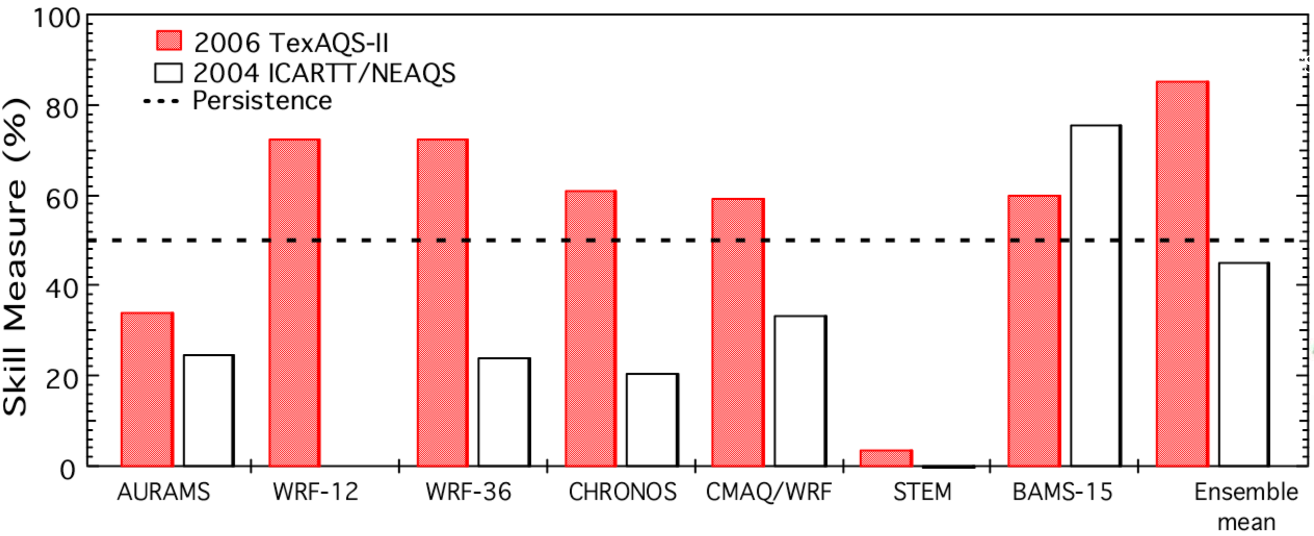
## Improvements in WRF and WRF/Chem from 2004 to 2006: comparisons with AIRNow surface $O_3$ data

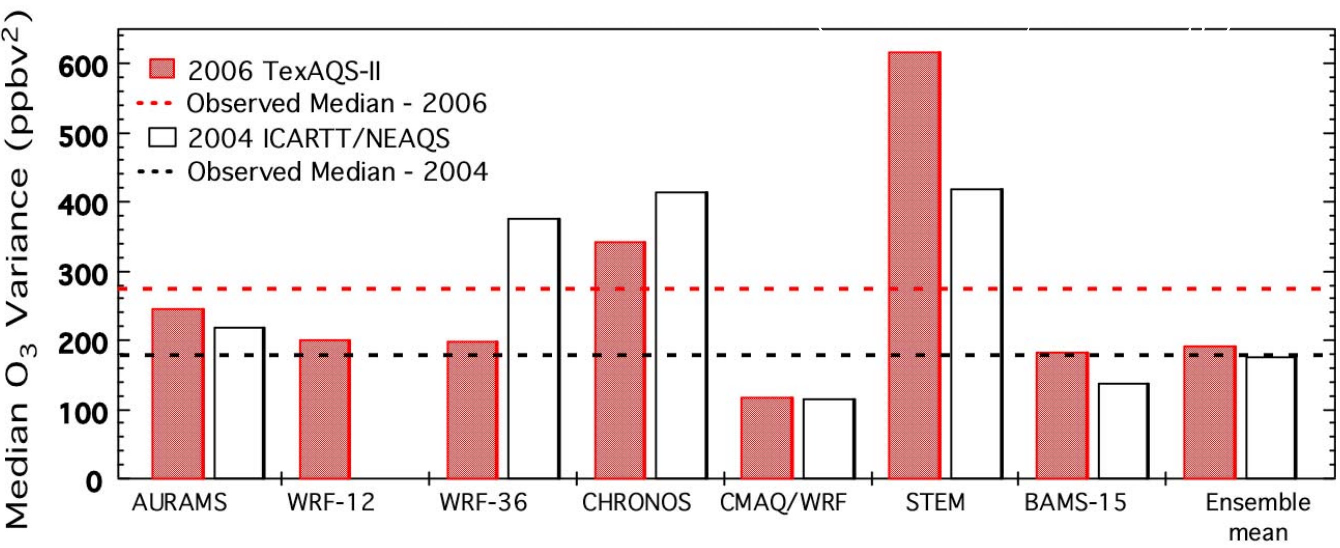


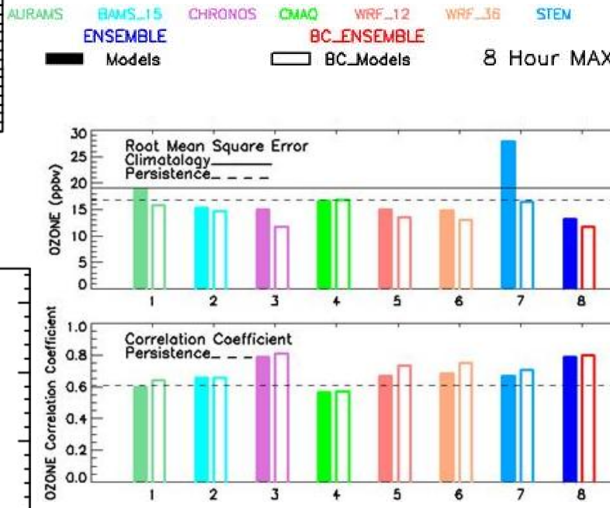




Maximum 8 hour averages
352 $O_3$ monitors - eastern U.S. and Canada
53 days (July and August 2004)

# Texas 2006 versus 2004 surface $O_3$ statistics (no bias corrections)



# Next in line-up for inclusion into WRF/Chem (ARW and NMM)

- CMAQ modules: for compatibility with EPA's CMAQ model: Carbon Bond 5 chemical mechanism, and MADRID sectional aerosol module (collaboration with NCSU, Yang Zhang)
- SMOKE emissions model

# Distant line-up for WRF/Chem, with various groups working on these issues

- More aerosol modules
- Chemical data assimilation
  - 3dvar work here at ESRL using GSI
  - 4dvar work in collaboration with Greg Carmichael and Dale Barker using WRF-var
- More choices for "interactive" parameterizations
  - CAMS radiation package
  - Various microphysics packages
  - GD convection parameterization

# Current FIM FY2008 Goals

- Extensive real-time testing
- Work with EMC on incorporating FIM dynamic core into ESMF model framework suitable as alternative dynamic core
- Incorporate WRF physics options and WRF/chem into ESRL version of FIM
- Introduce target coordinate from WRF hybrid $\theta$-$\sigma$ (Zangl, MWR)
- Design non-hydrostatic extension for FIM

# FY2009 plans

- Acceptance by NCEP/EMC for ESMF-based global ensemble
- Initial testing as global, fully-coupled atmospheric chemistry model for ESRL research
- Initial testing in global data assimilation cycle using GSI

(straightforward interpolation of GSI analysis *increment* to icos/hybrid coordinate)

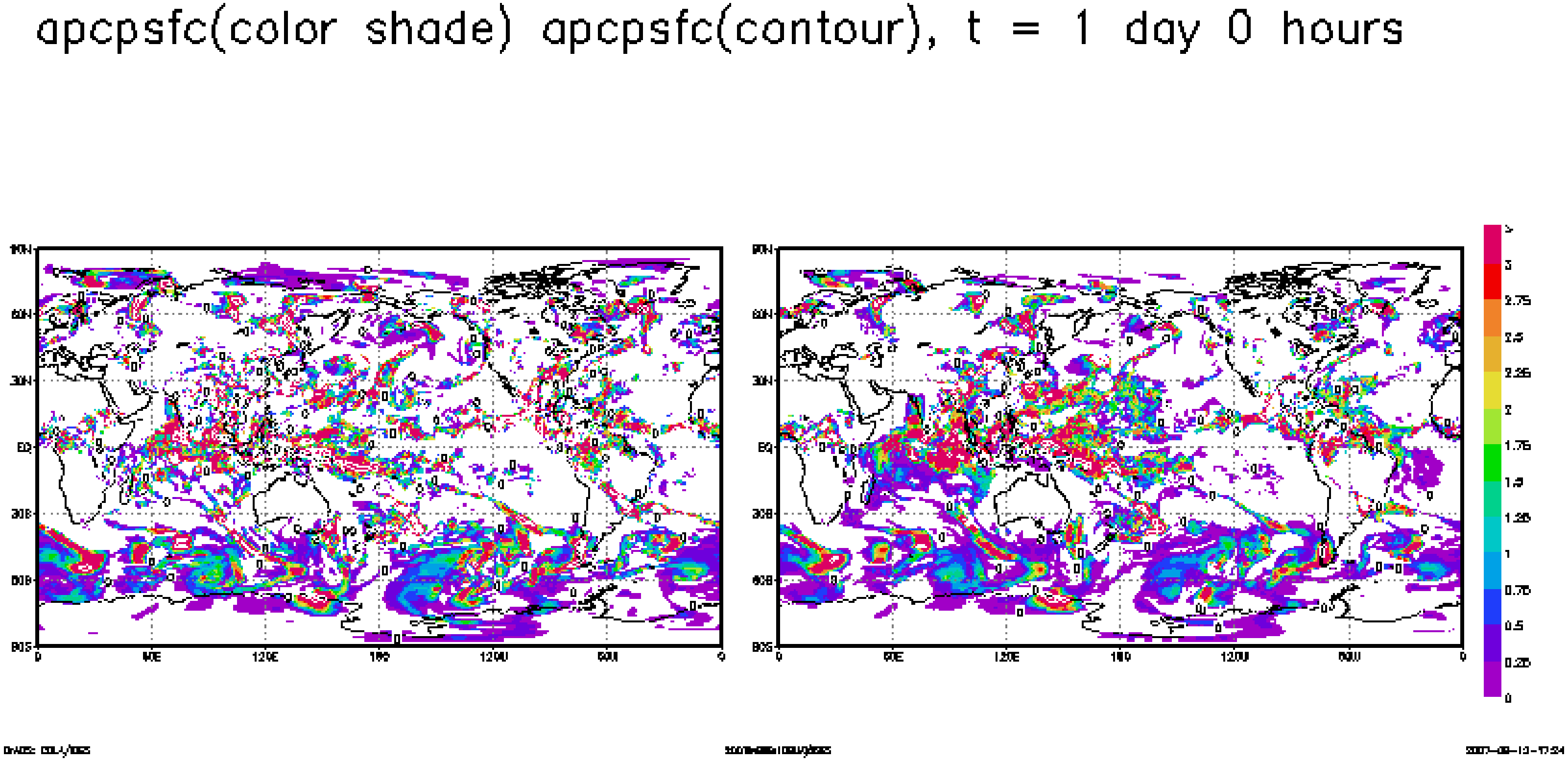
## Among the planned chemistry model applications at ESRL including different versions of WRF/Chem package

- WRF (or ESMF successor with WRF dynamic core options)
  - Possibly including simple chem in future version of NCEP Rapid Refresh for improved visibility/cloud forecasts (Aviation emphasis for Rapid Refresh)

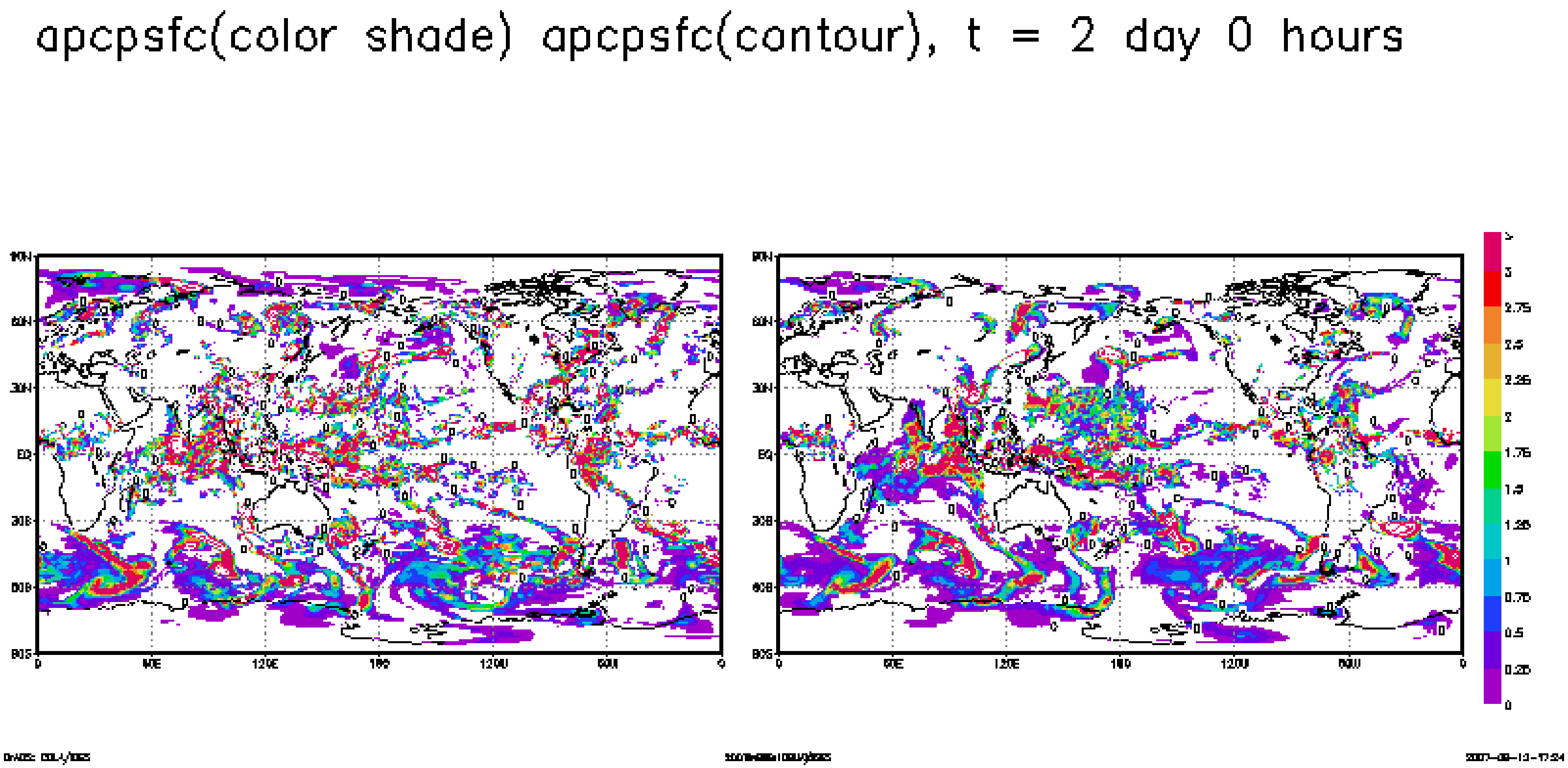
- FIM - currently hydrostatic

- OAR community non-hydrostatic model
  - GFDL, ESRL, AOML
  - components from AM3, FIM, WRF/Chem, others

# Global precipitation comparison between GFS and FIM_sig (G8~30 km) - initialized 9 October 2003



# Global precipitation comparison between GFS and FIM_sig (G8~30 km)



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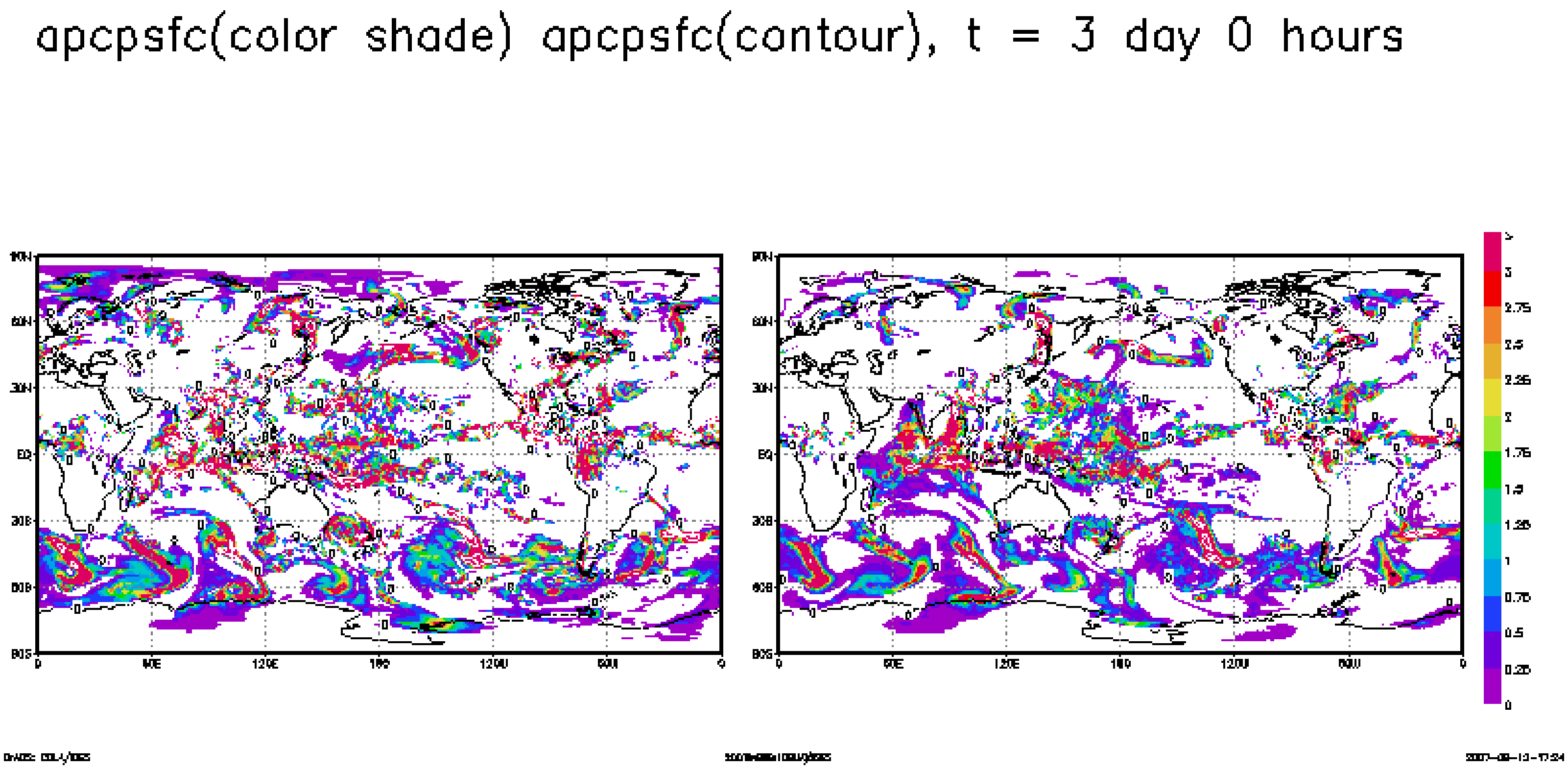
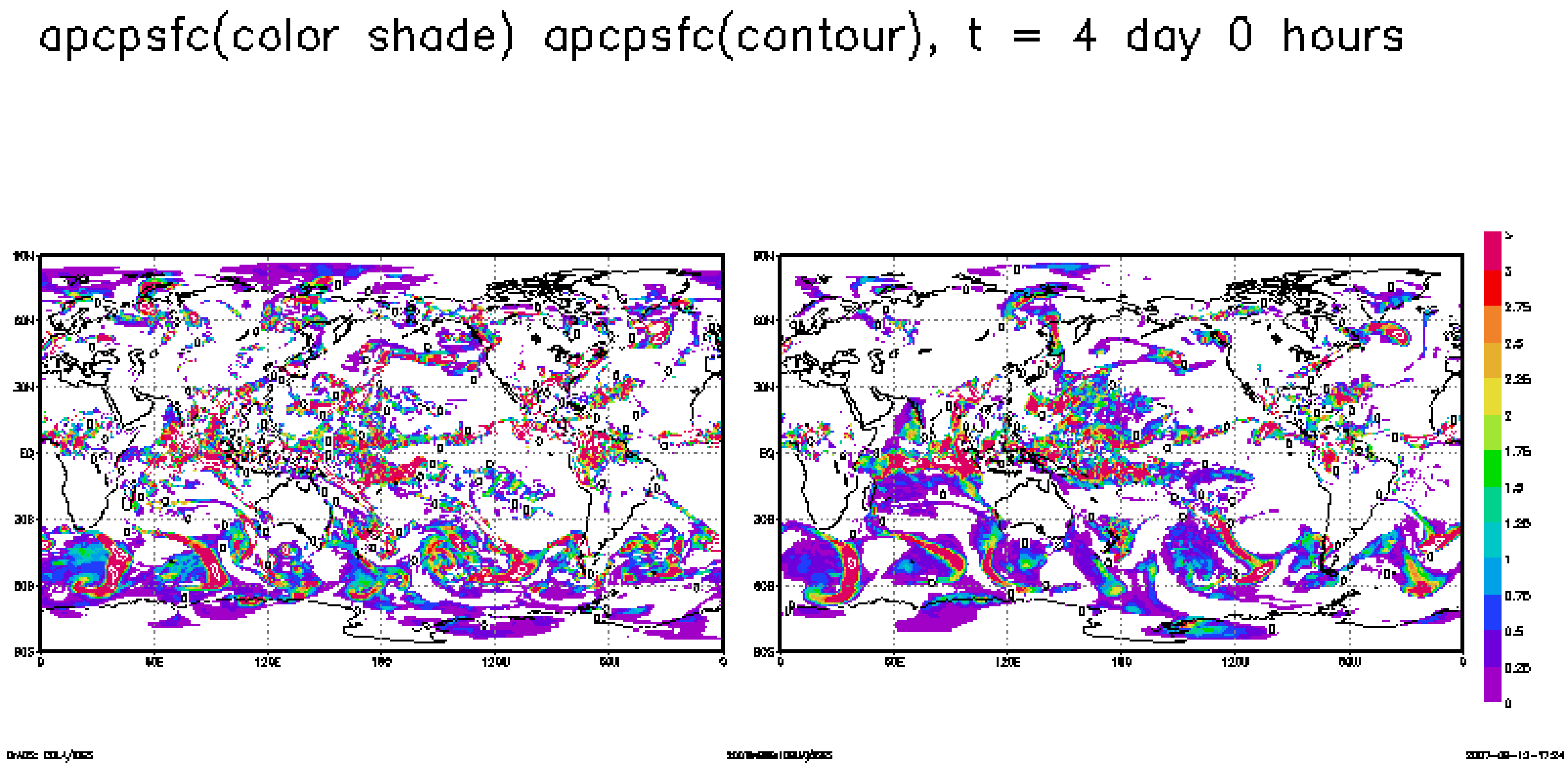


# Global precipitation comparison between GFS and FIM_sig (G8~30 km)



# Global precipitation comparison between GFS and FIM_sig (G8~30 km)