Three dimensional coupled modeling systems to understand problems related to ozone and air quality

Georg Grell (GSD)

Steven Peckham(GSD), Stuart McKeen (CSD), J.-W. Bao (PSD)

Many national and international collaborators (PNNL, NCAR,….) for WRF/Chem
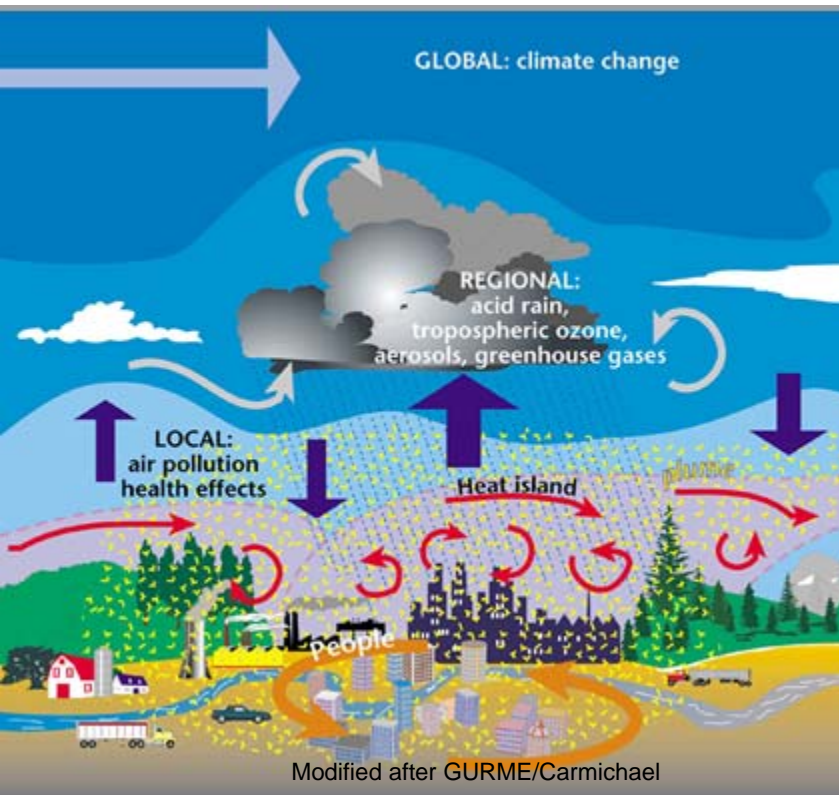
And the ESRL FIM group for FIM

Outline

- Sharpening a tool to study ozone and air quality: WRF/Chem
- Transition to global modeling

Why do we couple models?


Modified after GURME/Carmichael

Many of today's environmental challenges depend on complex interactions of various processes. The modeling of these processes has evolved into separate disciplines, resulting in many different type of models that are only loosely related (the models! Not the real world!). Only recently has it become clear that the interactions of these processes are important

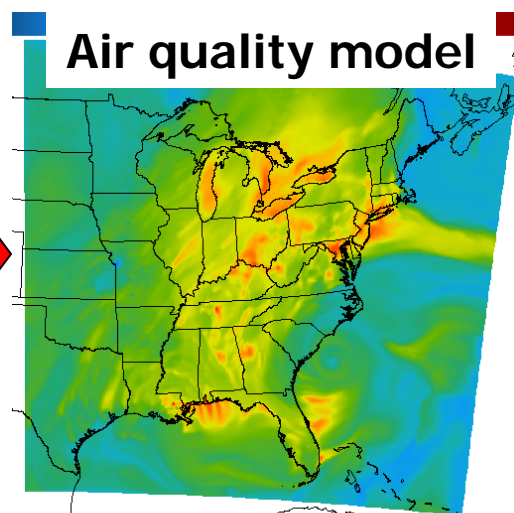ESRL is a great place to develop this type of modeling system: Expertise in both disciplines

Ozone and Air Quality Modeling: The commonly used approach ("offline")

Weather Data Analysis & Assimilation
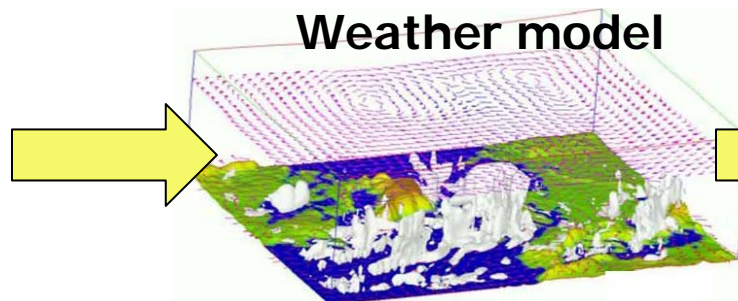
Weather model

Weather-Forecast

Biogenic and Anthropogenic emissions

Air quality model

1Hr Avg Ozone Concentration(PPB) Ending Tue Sep 13 2005 4PM EDT
(Tue Sep 13 2005 20Z)
National Digital Guidance Database
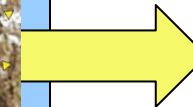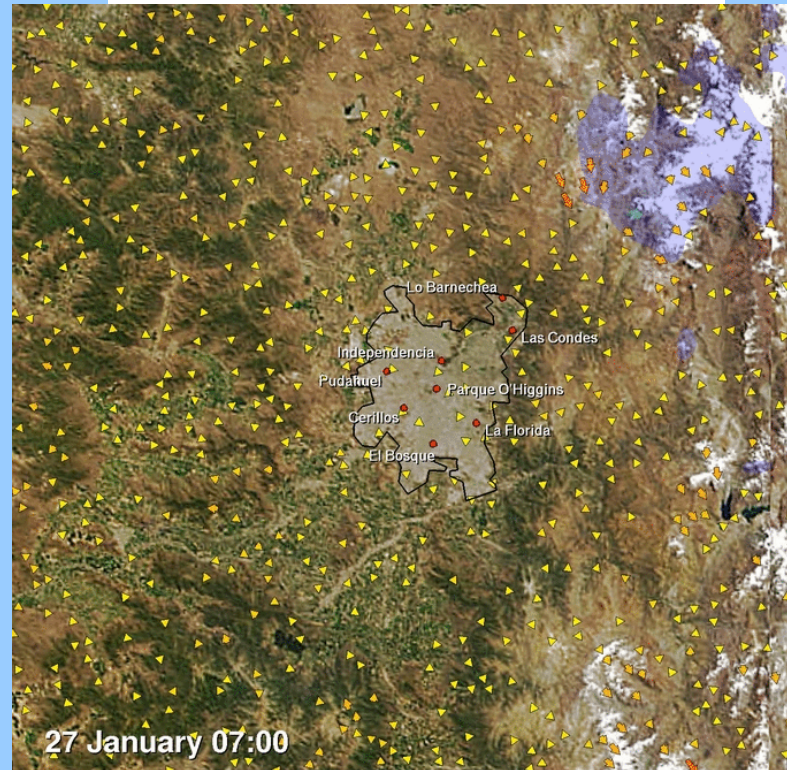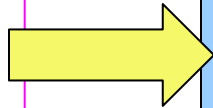12z model run   Graphic created-Sep 13 1:22PM EDT

Removal modules

AQ-Forecast

WRF/Chem: Online coupling of modeling systems

Weather Data Analysis & Assimilation & Emissions

Simultaneous forecast of weather and air quality

27 January 07:00

Weather and AQ-Forecast

Chemistry, Aerosols, radiation, clouds, temperature, winds

Full interaction of meteorology and chemistry

WRF/Chem: widely used nationally and internationally, development led by ESRL

- Automatic generation of chemical mechanisms (the part of the model that treats the interactions of the chemical species with each other),
- Includes aerosol direct and indirect effect,
- Multiple aerosol models (simple to very complex)
- Biogenic emissions from BEIS3.13 and MEGAN
- Coupled with a sophisticated fire plumerise model
- Global to local scale (**Large Eddy Simulation and cloud resolving**) applications, 1- and 2-way nesting capabilities

Many of the chemistry modules are verified by scientists from CSD and PSD

KPP: Kinetic PreProcessor (Damian et al, 2002, Sandu et al, 2003, Sandu and Sander 2006): A useful tool to study ozone chemistry and air quality

- Automatic tool to generate chemical mechanisms with a choice of time integration schemes

- Can also generate adjoints

- Well documented, tested, and widely used

Advantages of KPP tool

- Great flexibility to

  - Update mechanisms by additional equations

  - Adjust mechanism to local conditions

  - Sensitivity studies

- Much less time-consuming than manual coding

- Easy adjoint generation

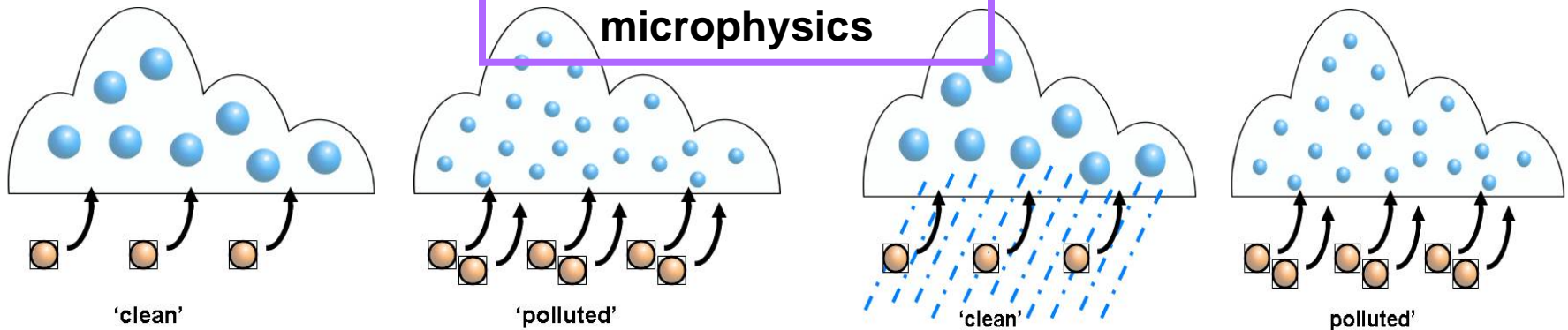# Aerosol effects included in WRF/Chem

Semi-Direct Effect

Direct Interaction with radiation

'clean' 'polluted'
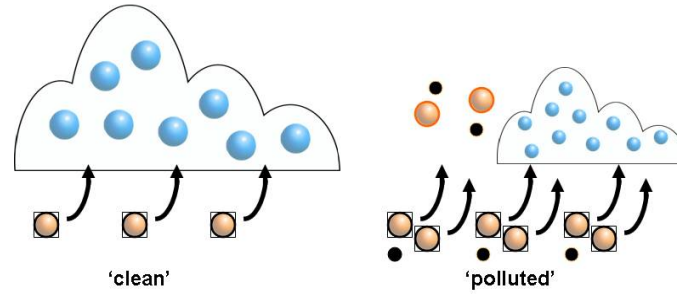
Direct and semi-direct effects are caused through the direct interaction of aerosols with radiation

First Indirect Effect

Second Indirect Effect
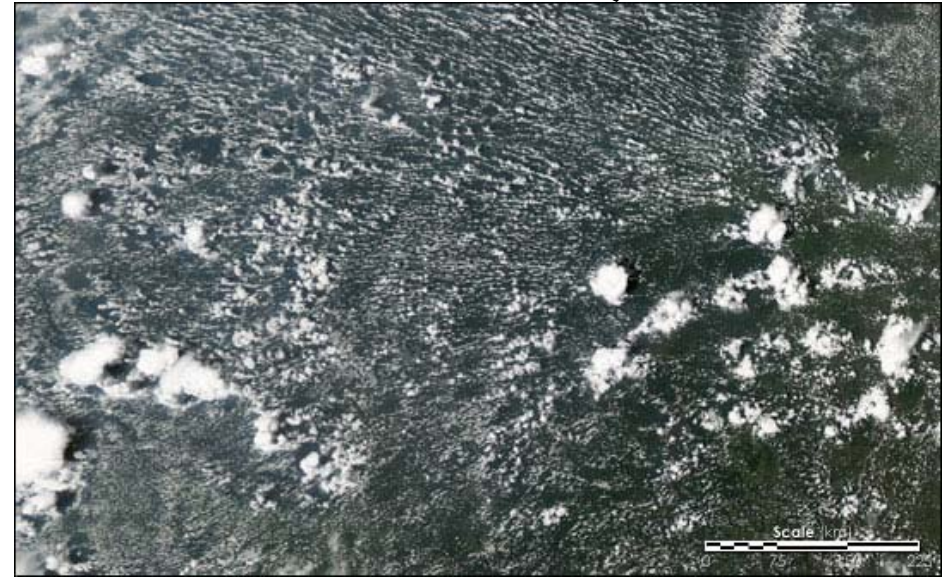
Direct Interaction with microphysics

'clean' 'polluted' 'clean' polluted'

Indirect effects are caused because of the interaction of aerosols with cloud microphysics (through Cloud Condensation Nuclei)

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

Initialized with Satellite data GOES-ABBA and MODIS

Semi-direct and indirect effect caused by biomass burning

Chemical data assimilation

NMM-WRF/Chem forecast

Ozone – RMSE (ppb) vs Hour UTC, Aug 20, 2006

- 3DVAR for Ozone and PM is used to produce optimal initial state of weather/chemistry (at ESRL)

- Adjoint will be developed for data assimilation and research work

- Voices for chemical Observational System Simulation Experiments (OSSE's) are getting louder

  - What should be measured to improve forecasts

  - How should and could effective observational networks be designed

- Research necessary to be able to do OSSE's

  - Need chemical data assimilation system

  - The problem of identical twins is much more complex in chemistry. How different will the models have to be
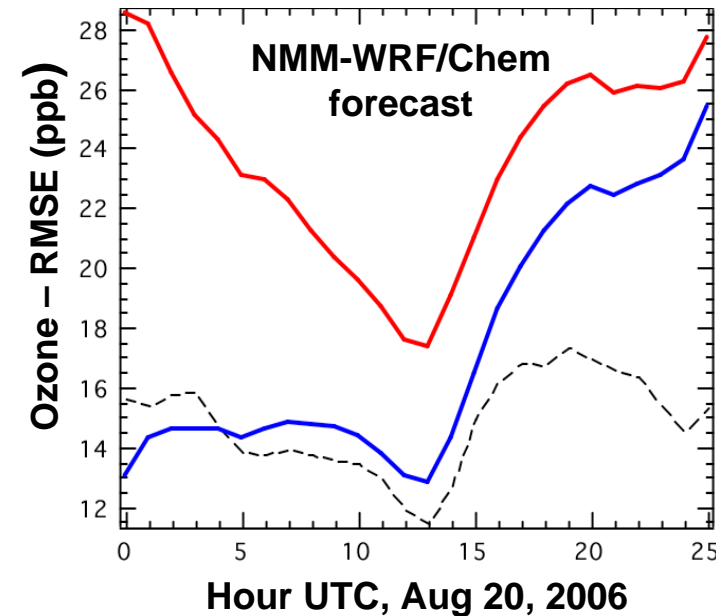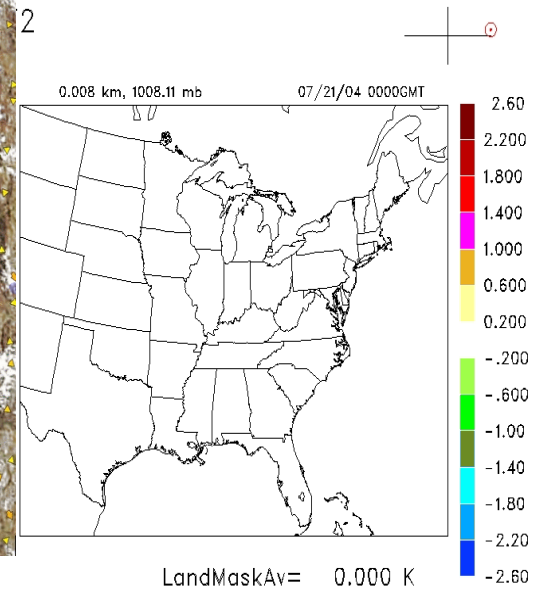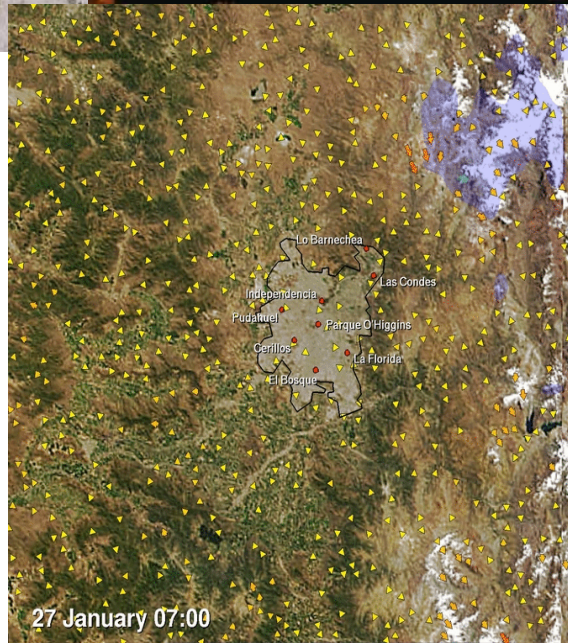
Current possible applications

Weather

Hazardous Release

Air Quality

Global Climate Change

AQ/weather/climate linkage
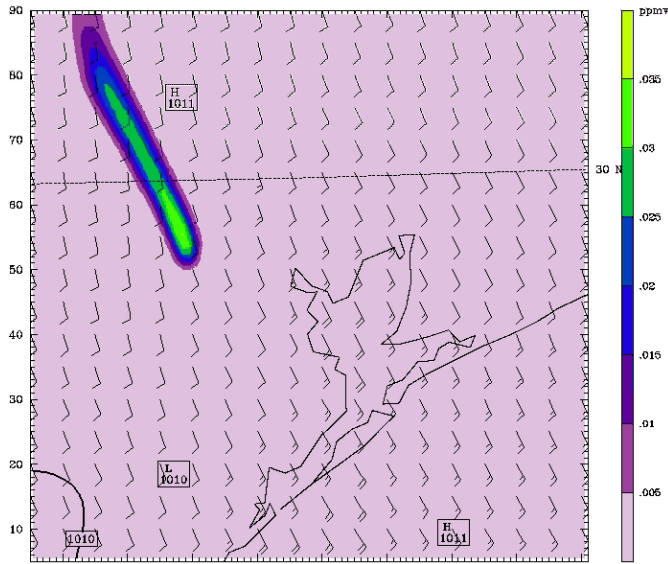
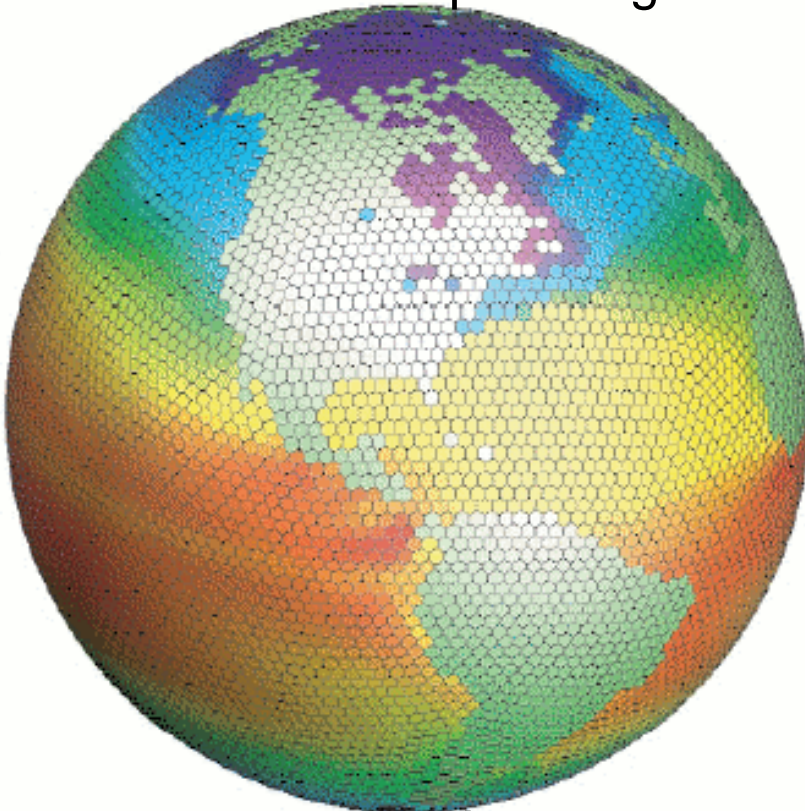# Some news on global model development

FIM: A Global Flow-Following Finite-Volume Icosahedral Model with 3 Unique Features
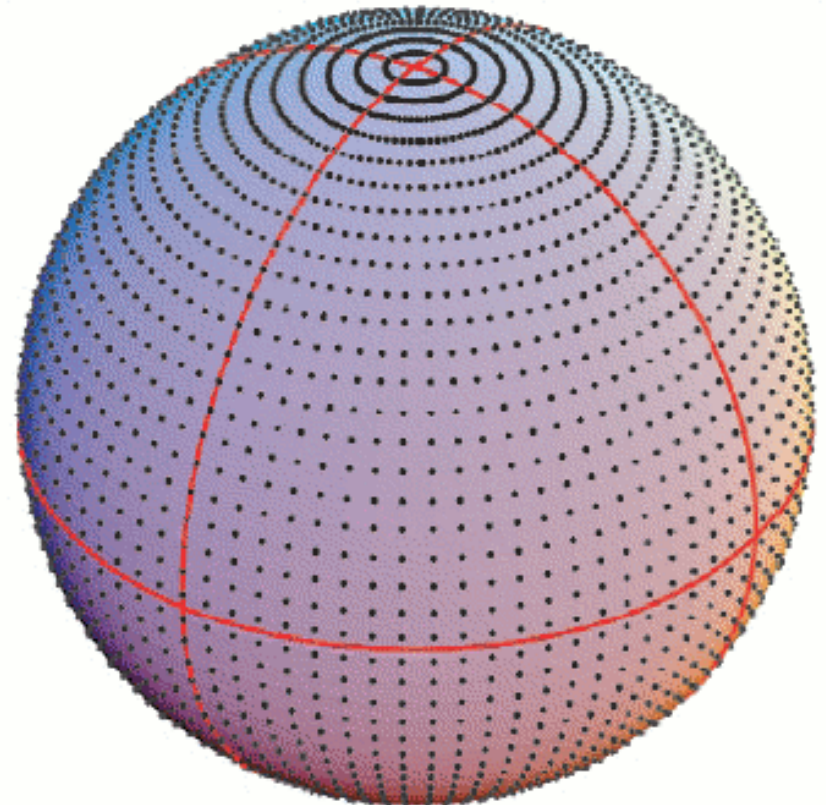
1. <u>Icosahedral grid</u>
    Computational elements are hexagons, with 12 embedded pentagons
    No pole singularities for better representation of circulations in polar regions


Icos grid   Standard lat-lon grid

FIM combines 3 unique features (continued)

2. <u>Adaptive, hybrid-isentropic vertical coordinate</u> (similar to HYCOM ocean model) -- accurate and conservative long-range transport of atmospheric constituents (water vapor, chemical constituents, fine dust particles, etc.

3. <u>Finite-Volume numerical procedures</u> -- conservation of fundamental physical quantities (mass, momentum, water vapor, etc.)
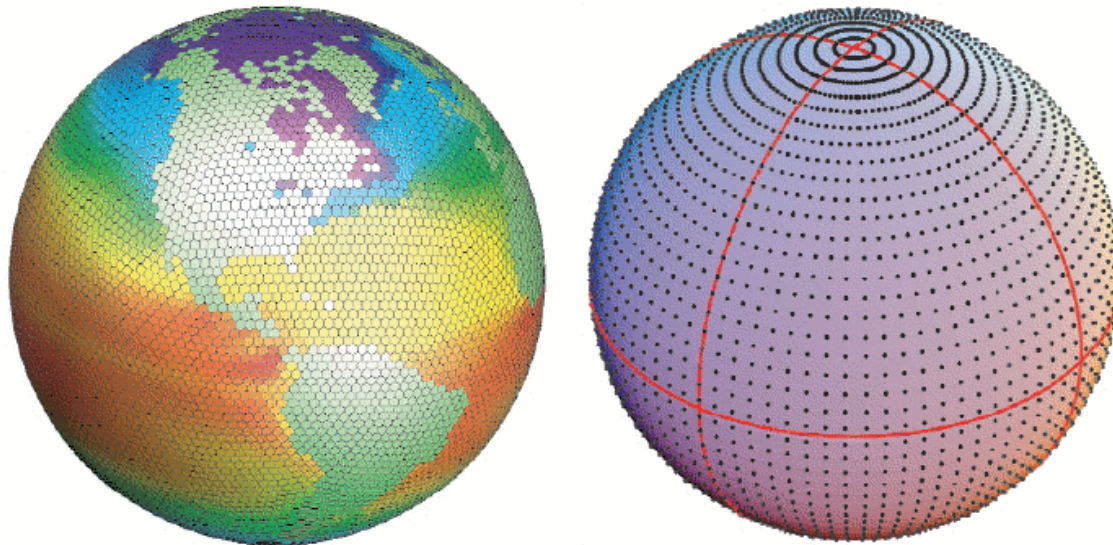
Current developments

- Using WRF/Chem physics and chemistry packages within global models (e.g. FIM)
    - Direct "inline" coupling
    - Create Chemistry or physics components from WRF/Chem and couple to FIM using the Earth System Modeling Framework (ESMF)

Both approaches will be compared here at ESRL

Direct inline coupling

- Because of the modularity within WRF/Chem a direct link can be established between FIM and WRF/Chem - all WRF/Chem functionality will be available

- Future WRF/Chem developments will automatically be available within FIM

Coupling with ESMF

- Components will be created using WRF/Chem:
  - GOCART Aerosols only (dust, sea-salt, black and organic carbon, simple sulfur chemistry, no ozone)
  - CHEM_LITE: GOCART Chemistry and aerosol packages coupled with simple global chemical mechanism for ozone/pm prediction
  - "heavier" packages
  - Possibly similar approach for physics