Welcome!

Mexico City WRF/Chem tutorial, August 2009
Tutorial Program

Wednesday Morning

- 9:00 General overview of WRF/Chem (Georg Grell)
- 9:30 Gas-phase chemistry (Rainer Schmitz)
- 10:00 Introduction to aerosol modeling with WRF/Chem (Rainer Schmitz)
- 10:30 Coffee Break
- 11:00 Setting up and running WRF/Chem (Steven Peckham)
- 11:45 Practical session I: WRF/Chem Basics (Steven Peckham, Georg Grell, Rainer Schmitz, Marcelo Mena)
- 13:00 Lunch

Thursday

All practice (basics in the morning, continuing with special topics in the afternoon)
Overview of WRF/Chem V3.1.1

Georg Grell

Steven E. Peckham, Stuart A. McKeen + others from NOAA/ESRL

Jerome Fast, William Gustafson jr., + others from PNNL
+ Rainer Schmitz (University of Chile)

+ Saulo Freitas, Karla Longo (CPTEC, BRAZIL)

+ Christine Wiedinmyer, Xue-Xi, Gabi Pfister, Mary Barth and others from NCAR

+ many more national and international collaborators

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

• What is WRF/Chem – V3.1.1
• Evaluation, verification, and a few applications
• Future developments
WRF/Chem

Community effort

Largest contributing groups: ESRL, PNNL, NCAR

Other significant contributions from: University of Chile, MPI Mainz, CPTEC Brazil, CDAC India
WRF/chem

• Online, completely embedded within WRF CI
• 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)
• Very modular approach
  – Chemistry subdirectory has been implemented in version of HIRLAM
  – Is being implemented now into FIM global model (icosahedral in horizontal, vertical adaptive coordinates)
Dispersion and Air Quality Modeling: The commonly used approach ("offline")

Weather model

Weather Data Analysis & Assimilation

Biogenic and Anthropogenic emissions

Air quality model

Time averaged or snapshot values!!

AQ-Forecast

Removal modules
WRF/Chem: Online coupling of modeling systems

Simultaneous forecast of weather and air quality

Chemistry, Aerosols, radiation, clouds, temperature, winds

Full interaction of meteorology and chemistry

Weather Data Analysis & Assimilation & Emissions

Weather and AQ-Forecast
Why Online?

• In models, with increasing horizontal resolution, the variability of the vertical velocity becomes extremely important.
• Offline might introduce a large error in estimate of vertical mass transport.
• If dependent on offline, power spectrum analysis should be performed to determine necessary offline frequency.

![CO Mixing ratio graph]

Black is online
Green is 1hr offline
Biogenic emissions

- 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
  - BEISv3.13 (offline reference fields, online modified)
Implementation of the Model of Emissions of Gases and Aerosols from Nature MEGAN in WRFV3/Chem (Courtesy of Christine Wiedinmyer and Alex Gunther from NCAR, also Serena Chung, and Jerome Fast)
Gas Phase Chemistry Packages

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

See talk later by Rainer Schmitz
Available Aerosols modules

1. PM advection, transport, emissions and deposition only
2. GOCART
3. Modal approach (MADE/SORGAM)
4. Sectional approach (MOSAIC)

See talk later by Rainer Schmitz
Aerosol modules comparison

(1) Modal

(2) Sectional

composition
sulfate
nitrate
ammonium
chloride
carbonate
sodium
calcium
other inorganics
organic carbon
elemental carbon

(3) GOCART: Sections for dust and sea salt, otherwise total mass only
GOCART aerosols, GOCART chemistry and other sea-salt and dust parameterizations

- Very simple GOCART chemistry routines (not for Ozone prediction), for black carbon, organic carbone, so2/so4 conversion, dms emissions, and msa production
- GOCART is also coupled to other chemical mechanisms
GOCART Dust and Sea-salt

• Dust:
  – Global – Calculated as a function of surface topographic depression, surface wetness, and surface wind speed (Ginoux et al. 2001)
  – Asian region – also including the recent desertification areas in the Inner Mongolia province in China (Chin et al. 2003)
  – Total 5 size bins 0.1 – 10 µm, erodible fraction map with 1x1 degree resolution
  – New higher resolution “erodible fraction” map is in testing (.25x.25 degree)

• Sea-salt:
  – Calculated as a function of surface wind speed (Gong et al., 2003)
  – 4 size bins 0.1 – 10 µm (1 submicron, 3 super micron)
Aerosol effects included in WRF/Chem

Aerosol direct effect

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

First Indirect Effect

Second Indirect Effect

Indirect effects are caused from the interaction of aerosols with cloud microphysics (through Cloud Condensation Nuclei)
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
How is the meteorological forecast affected by aerosol?

• In general, large importance for climate simulations is recognized (when integrating models over 100’s of years, small differences in the earth’s energy budget are extremely important)

• How about weather forecasting for only a few days?
Direct Effect

Instantaneous Aerosol Radiative Forcing
Noon, August 31, 2000

Average Aerosol Radiative Forcing
August 28 - 1 September, 2000

- Impact of sulfate from power plant
- Impact of organic and elemental carbon from urban and industrial sources

largest impact north of industrial corridor

lines = major highways
dots = major industrial sources

\( \Delta x = 1.3 \text{ km} \)

120 km
(typical GCM \( \Delta x = 100 \text{ km} \))

Paper by Fast et al. 2005
Semi-Direct Effect

Short Wave Radiative Flux Difference
(With Aerosol/Radiation interaction minus Without)

07/22/04 1500 GMT

W/m²

ESRL

15 hr forecast
Indirect Effect: Stratocumulus-Aerosol Interactions

Cloud Effective Radius over Southeastern Pacific: October 2006
Average at 12 UTC

Mean MODIS Cloud Droplet Effective Radius October 2006
(from Matthew Wyant (UW))

(full chemistry run more consistent with satellite data)
Photolysis Packages – all coupled to aerosols and hydrometeors

- Madronich Photolysis
- Madronich F-TUV
- Fast-j photolysis scheme
Use of chemical data from Global Chemistry Model (GCM) for boundary conditions, also 1-way and 2-way nesting.

Now available for versions of MOZART, RAQMS, CHASER, and WRF/Chem.

CHASER output available in real-time, thanks to Takigawa from Frontier Research Center in Tokyo, Japan.

Ozone forecast for Santiago de Chile provided by Rainer Schmitz and Mark Falway, Univ. Of Chile.

27 January 07:00
Improved non-resolved convective transport

- Ensemble approach (based on Grell/Devenyi parameterization)
  - Uses observed or predicted rainfall rates as met-input
  - Ensemble of entrainment/detainment 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 (G3 Scheme as cu_phys=5 for meteorology)**

- Aqueous phase chemistry module called from within convective routine, CMAQ module (not tested and released yet)
- SO2 to SO4 oxidation included
- Connected to photolysis and atmospheric radiation schemes (set cu_rad_feedback=.true.)
A model within a model: Fire Plumerise (Collaboration with Saulo Freitas from CPTEC in Brazil)

1-D Plume model

\[
\frac{\partial w}{\partial t} + w \frac{\partial w}{\partial z} = \gamma g B - \frac{2 \alpha}{R} w^2
\]

\[
\gamma = \frac{1}{1 + 0.5}
\]

Simpson & Wiggert, 1968

\[
\frac{\partial T}{\partial t} + w \frac{\partial T}{\partial z} = -w \frac{g}{c_p} \frac{2 \alpha}{R} (T - T_c) + \left( \frac{\partial T}{\partial t} \right)_{\text{microphysics}}
\]

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

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

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

**bulk microphysics:**

Kessler, 1969

Ogura & Takahashi, 1971

Berry, 1967

\[ (\xi = T, r_v, r_c, r_{\text{rain}}, r_{\text{ice}})_{\text{sedim}} \]

Initialized with GOES-ABBA and MODIS
Alaska 2004 objective: Fire impacts on Weather

Wildfires initialized with:

- Remote sensing satellite information (real-time or historic)
  - MODIS
  - WFABBA (Wildfire Automated Biomass Burning Algorithm)
- Alaska Interagency Coordination Center (AICC), using various sources of ground and aerial surveys, also remote sensing (MOD14)

Model calculates injection heights online

Cloud resolving simulations with full chemistry/physics
How far can you go in real-time?

- **dx=3km over western US**
  - (700x700 grid points, 6-hourly cycle)

  For comparison purposes this was run with and without chemistry.

In the future: Experimentally run Rapid Refresh (dx=13km) for NAM domain with chemical data assimilation, wildfires, and GOCART aerosols for visibility forecasts, AQ forecasts, improvement of chemical and meteorological data assimilation.
Chemical data assimilation: ARW-WRF/Chem and PM2.5

2 months worth of WRF/Chem runs:
1. New England 2004 to estimate background error covariances and lengthscales
2. Houston 2006 for evaluation

PM2.5 - RMSE

PM2.5 - correlation
Current possible applications

Weather

Hazardous Release

Air Quality

Global Climate Change

AQ/weather/climate/weather modification linkage
Some on ESRL/CSD WRF/Chem activities (McKeen, Ahmadov, Kim, Lee):

Focus:
Model evaluation, also

Sensitivity of PM$_{2.5}$ forecasts to physical and chemical parameterizations within WRF/Chem
• PM$_{2.5}$ deposition
• Cloud Phase Oxidation mechanisms
• Emissions (WRF/Chem upgraded to NEI-2005)
• Boundary Layer Parameterizations
• SOA mechanisms

Data-sets used for evaluations:
NOAA WP-3D aircraft (ICARTT-2004, TexAQS-2006)
NOAA Twin Otter - O$_3$ lidar (TexAQS-2006)
AIRNow surface PM2.5 Network (2006)
Model variables available for Comparison with NOAA Aircraft and Ron Brown data

gas phase chemistry

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aerosols, radiation, meteorology

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http://www.al.noaa.gov/ICARTT/modeleva/
Future line-up for WRF/Chem, with various groups working on these issues

- Aerosol interaction with radiation and microphysics as well as more aerosol modules (GOCART now also available for direct effect)
- Chemical data assimilation
  - 4dvar, collaboration with Uof Iowa, U of Colorado, ESRL/GSD, maybe more using WRF-var
  - 3dvar and EnsKF work at ESRL using GSI
- More choices for “interactive” parameterizations
- Lightning NOx parameterization, currently being evaluated (NCAR, Mary Barth)
- Aircraft emissions will be added, also pre-processor for MEGAN (NCAR)
- MOZART chemistry with GOCART aerosols (NCAR, Gabi Pfister)
- Shallow convection (ESRL/GSD)
- NMM-WRF/Chem will become available (mass conservation was fixed, Z. Janjic)
- Offline version is still on the shelf
- Effects of volcanoes will be included (Ash fall as well as emissions important for air quality (Arctic Research Center, ESRL, and CPTEC))
WRF/Chem Aerosol related work – PNNL planned release: next March

- Inclusion of a driver that enables modular and interoperable dry deposition schemes for both MADE/SORGAM and MOSAIC. 4 deposition schemes are included: 2 from MADE/SORGAM, 1 from MOSAIC, and another based on Zhang et al., Atmos. Environ. (2001).
- Cloud-aerosol interactions will be expanded to work with Morrison and Thompson microphysics schemes
- SOA will be added to MOSAIC
- new aerosol model is planned (MOSAIC-ext), that simulates the evolution of the transition between internal and external aerosol mixing states
- Ice-aerosol interactions will be included
Aerosol Modeling Testbed: What are we Trying to Accomplish?

Create a computational framework, the **Aerosol Modeling Testbed**, that streamlines the process of testing and evaluating aerosol process modules over a range of spatial / temporal scales.

- **Systematically and objectively** evaluate aerosol process modules
- Provide **tools** that facilitate science by minimizing redundant tasks
- **Document** performance and computational expense
- Better **quantify uncertainties** by targeting specific processes
- Build an **internationally-recognized capability** that fosters collaboration
For more information about the AMT...

On ~August 1, more information will be available at:

http://www.pnl.gov/atmospheric/research/aci/aci_proj_testbed.stm

Contacts:

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WRF/Chem Aerosol current and future work – ESRL/GSD and/or CSD

• GSD and CSD: Coupling GOCART aerosol to atmospheric radiation schemes
• Graham Feingold, Hailong Wang, Jan Kazil (ESRL/CSD): Implementation of double moment bulk microphysics scheme (Feingold et al. 1998), LES simulations of POC’s, coupling of MADE/SORGAM to the double moment bulk microphysics scheme
  – Coupling WRF/Chem/KPP gas phase chemistry with aqueous phase chemistry and aerosol microphysics
  – Coupling of the double-moment accumulation mode aerosol, and dissolved gas phase species with the Feingold 1998 double moment microphysics scheme (using it for LES simulations to see how these changes will affect the CCN population, drizzle, and POC's).
  – New nucleation scheme (neutral and charged nucleation of H2SO4/H2O based on CSD laboratory measurements)
Aerosol Effects on Cloud Morphology via Drizzle

**Albedo**

Closed-cell
Albedo $\sim 0.6$
(non-precipitating)

**Onset of drizzle results in transition to open-cell convection**

WRF Model
+ 2-moment $\mu$physics;
60 km domain;
$\Delta x = \Delta y = 300$ m
$\Delta z = 30$ m

Open-cell
Albedo $\sim 0.2$
(precipitating)

**high aerosol**

Garay et al. 2004, MISR

**low aerosol**

Wang and Feingold, 2008
Chemical data assimilation – ongoing work at ESRL

- Incorporation of available observations into a modeling system to produce optimal initial state of weather/chemistry

- 3D variational analysis for Ozone and PM2.5 is used within the Grid Point Statistical Interpolation system (GSI)

- Comparison of Ensemble Kalman Filter (EnKF) with 3DVAR results next inline
Running the RR and HRRR with GOCART: Very large domain, semi-operational runs in real-time. Less than a factor of 2 more expensive than met runs, including chemical data assimilation.

RR: dx=13 km

HRRR: dx=3 km
Direct inline coupling of WRF/Chem chemistry/physics packages into FIM

- 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
FIM: A Global Flow-Following Finite-Volume Icosahedral Model with 3 Unique Features:

* Icosahedral grid, adaptive hybrid isentropic coordinates, finite volume numerics

Will run with global aerosols/dust/biomass burning and volcanoes on dx of about 30 or 50km. Since it uses same chem and physics as WRF/Chem, it will be ideally suited for BC's.
FIM: A Global Flow-Following Finite-Volume

Near Surface PM2.5

Saharan Dust mid-level
Resources

- **WRF project home page**
  - [http://www.wrf-model.org](http://www.wrf-model.org)

- **WRF users page (linked from above)**
  - [http://www.mmm.ucar.edu/wrf/users](http://www.mmm.ucar.edu/wrf/users)

- **On line documentation (also from above)**
  - [http://www.mmm.ucar.edu/wrf/WG2/software_v2](http://www.mmm.ucar.edu/wrf/WG2/software_v2)

- **WRF users help desk**
  - [wrfhelp@ucar.edu](mailto:wrfhelp@ucar.edu)

- **WRF/Chem users help desk**
  - [wrfchemhelp.gsd@noaa.gov](mailto:wrfchemhelp.gsd@noaa.gov)