Overview of the WRF/Chem modeling system

Georg Grell

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

Earth System Research Laboratory
SCIENCE, SERVICE & STEWARDSHIP

Structure of talk

- WRF/Chem: short overview and future activities
- Evaluation and verification with test-bed data sets

WRF/Chem

Community effort

Largest contributing groups: ESRL, PNNL, NCAR

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

Weather Research and Forecasting (WRF) Model

WORKING GROUP 11: ATMOSPHERIC CHEMISTRY

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Mary Barth, *NCAR*
Saulo R. Freitas, *Centro de Previsao de Tempo e Estudos Climaticos, Brazil*
Daewon W. Byun, *University of Houston*
Greg Carmichael, *University of Iowa*
Jerome Fast, *PNL*
John McHenry, *Baron Advanced Meteorological Systems*
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Jeff McQueen, *NCEP*
Jon Pleim, *EPA*
Kenneth L. Schere, *EPA*
Bill Skamarock, *NCAR*
Rainer Schmitz, Univerisyt of Chile, Chile, *University of Chile*
Doug Westphal, *USN Research Lab*
Steven Peckham, *NOAAESRL/GSD*
Julius Chang, *National Central University, Taiwan*

Mission

The mission of the atmospheric chemistry working group is to guide the development of the capability to simulate chemistry and aerosols — online as well as offline — within the WRF model. The resulting WRF/Chem model will have the option to simulate the coupling between dynamics, radiation and chemistry. Uses include forecasting chemical-weather, testing air pollution abatement strategies, planning and forecasting for field campaigns, analyzing measurements from field campaigns and the assimilation of satellite and in-situ chemical measurements.

Interaction with other WRF Groups

The initial development of WRF/Chem is involved with the Numerics and Model Dynamics (WG1), Model Physics (WG5), and Land Surface Modeling (WG14).

Community Involvement

2007 WRF workshop information - Meeting minutes and mini-tutorial presentations

2006 WRF workshop working group 11 meeting minutes

Known issues with the WRF model.

Known issues with the WRF/Chem model.

Email WRF/Chem help with question regarding WRF/Chem model.

WRF/Chem related announcements. Updated 16 July 2008

WRF/Chem version 3.0 Users Guide Updated 22 July 2008

WRF/chem

- Online, completely embedded within WRF
- 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 versions of HIRLAM
  - Is being implemented now into FIM global model (icosahedral in horizontal, vertical adaptive coordinates

Chemistry packages: biogenic emissions modules

- 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)
  - Model for Emissions of Gases and Aerosols from Nature (MEGAN)

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
- ***K***inetic ***P***re***P***rocessor (KPP)

Available Aerosols modules

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

Aerosol direct and indirect effect has been implemented for the Goddard radiation scheme and the Lin et al. microphysics

Processes in the GOCART ***aerosol*** *and* ***chemistry modules***

- Simple chemistry (gas-to-particle conversion)
- Dry deposition and settling
- Wet deposition
- Hygroscopic growth for black and organic carbon as a function of RH

GOCART ***dust and sea-salt modules***

- Dust:
  - Global – Calculated as a function of fraction of erodible area (currently 1x1 degree resolution), porosity, 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
- 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)

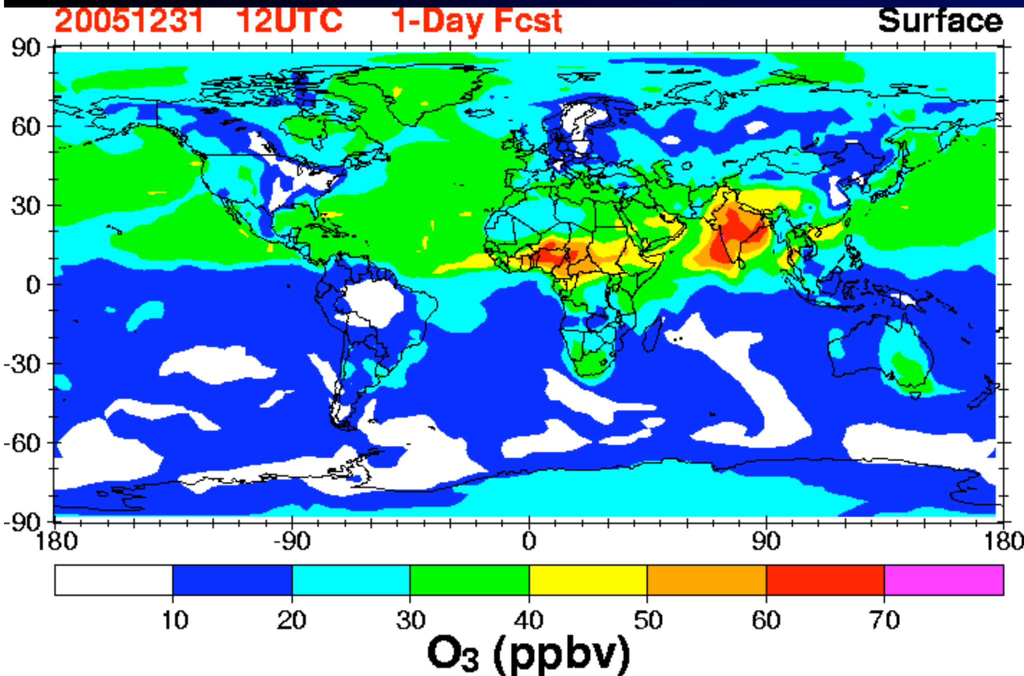
GOCART Global PM Emissions Data set for WRF/Chem (excluding historic volcanic and biomass burning emissions)

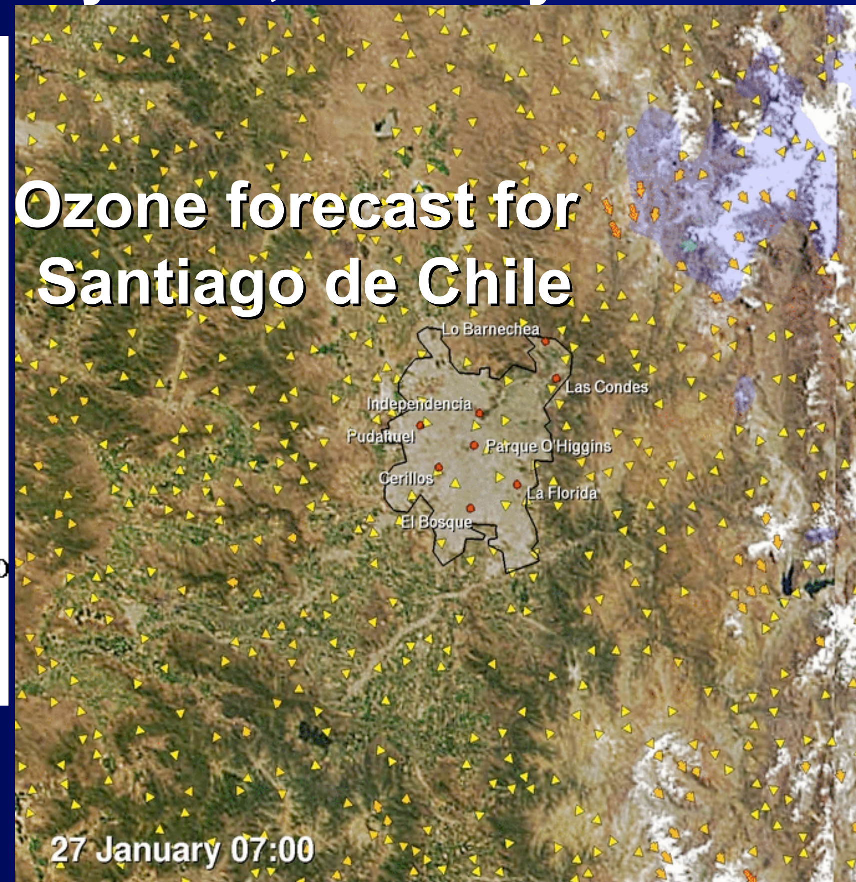
- Anthopogenic (SO_2, BC, OC):
  - Global - IPCC 2000, seasonal variations
  - Asian region – most recent emission work from Streets et al 2002
- Biogenic:
  - DMS (dimethyl sulfide) from the ocean)
  - OC from vegetation (terpene)

Photolysis Packages – all coupled to aerosols and hydrometeors

- Madronich Photolysis
- Madronich F-TUV code also available, in V3 release, but not well tested
- Fast-j photolysis scheme

Use of chemical data from Global Chemistry Model (GCM) for boundary conditions, or 1-way nest, or 2-way nest





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

<u>Now also available for MOZART, RAQMS, CHASER, and of course WRF/Chem</u>

Provided by Rainer Schmitz and Mark Falvey, Univ. Of Chile

dgf

Improved non-resolved convective transport

1. 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
   - **<u>Can be used as 3-d scheme for smooth transition to high resolution</u>**
2. Connected to photolysis and atmospheric radiation schemes
3. Working on ensemble approach for (2) and and aerosol connection

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

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial z} = \gamma g B - \frac{2\alpha}{R} w^2 \quad \begin{cases} \gamma = \frac{1}{1+[\text{redacted}]} & [\text{redacted}] \\ \gamma = \frac{1}{1-[\text{redacted}]\mu} & [\text{redacted}] \end{cases}$$

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

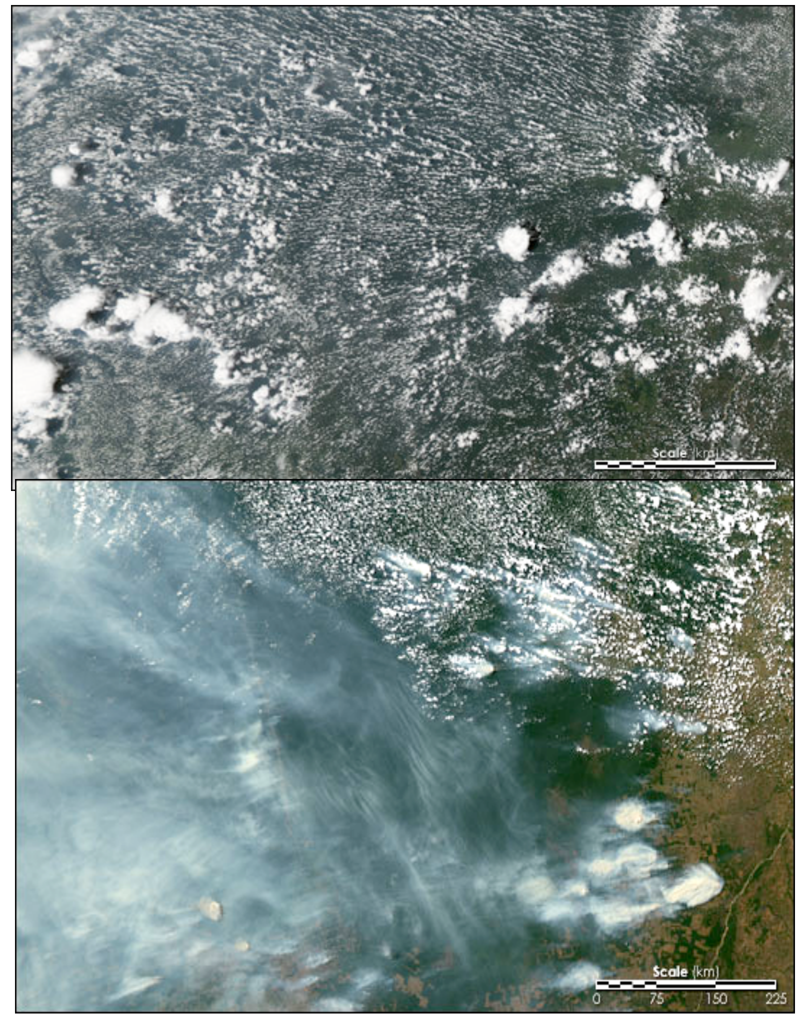
$$\frac{\partial r_v}{\partial t} + w\frac{\partial r_v}{\partial z} = -\frac{2\alpha}{R}|w|(r_v - r_{v,e}) + \left(\frac{\partial r_v}{\partial t}\right)_{microphysics}$$

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

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

$$\left(\frac{\partial \xi}{\partial t}\right)_{microphysics} (\xi = T, r_v, r_c, r_{rain}, r_{ice}), \quad sedim$$

bulk microphysics:
- Kessler, 1969
- Ogura & Takahashi, 1971
- Berry, 1967



WRF/Chem real-time forecast now with wildfires (dx=27km on CONUS grid)

from http://wrf-model.org/WG11

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Model Information

WRF/Chem Public Domain Notice

Current Status of WRF/Chem

Anthropogenic Emissions Available for WRF/Chem

Model Evaluation

Publications related to WRF/Chem

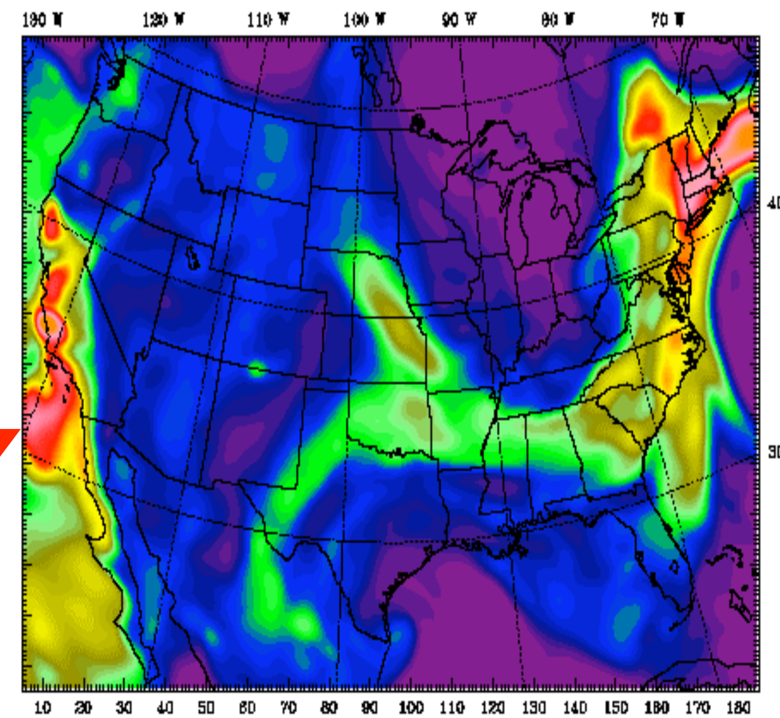
Future Plans

WRF/Chem FAQs

Real-time Air Quality Forecasts using WRF/Chem

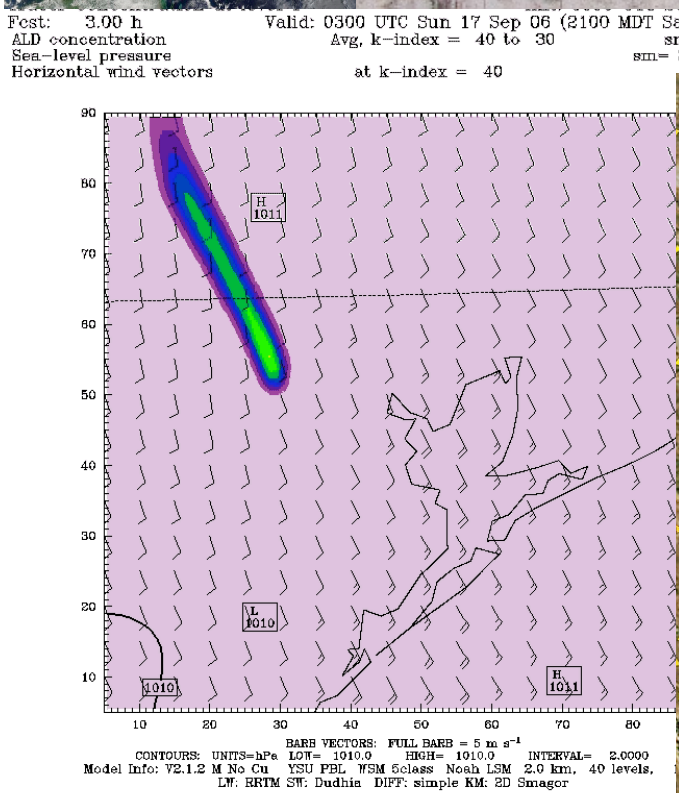
27 km CONUS grid

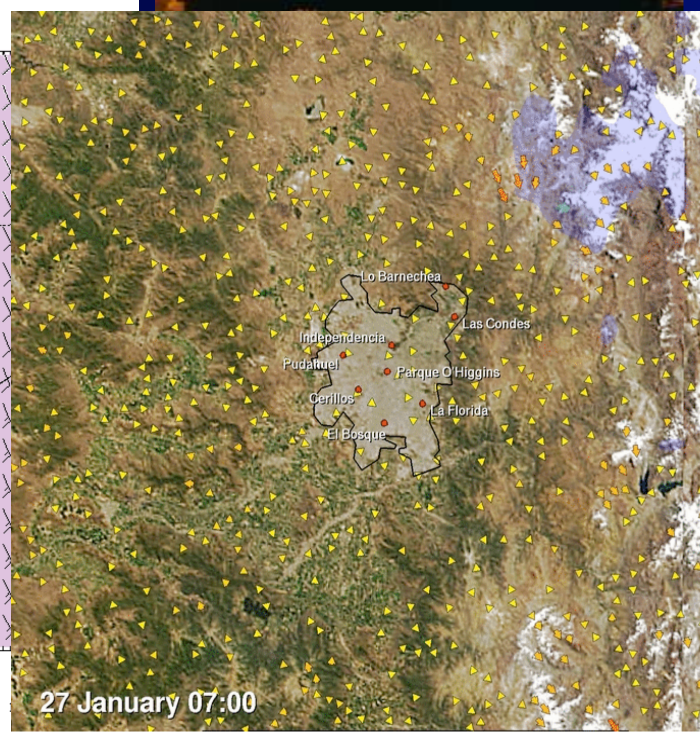
July 24, 00Z

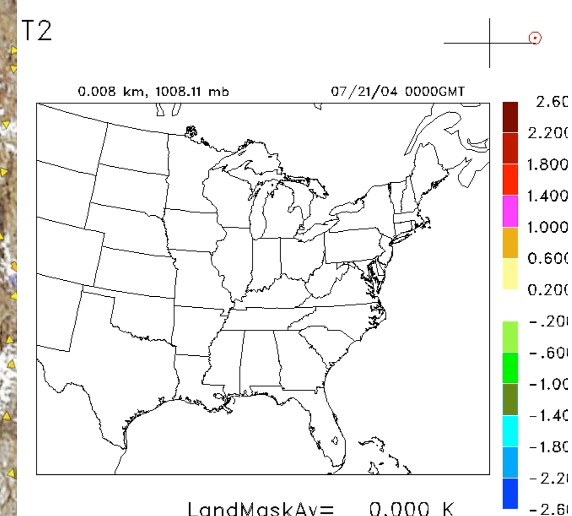


Current possible applications

AQ/weather/climate linkage







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

- More aerosol modules
- Chemical data assimilation
  - 4dvar work in collaboration with Greg Carmichael and Hans Huang using WRF-var
  - Will create adjoint of WRF/Chem
  - 3dvar work at ESRL using GSI
- More choices for "interactive" parameterizations
  - CAMS radiation package
  - Various microphysics packages
  - GD convection parameterization

WRF/Chem Aerosol related work

- Graham Feingold and Hailong Wang (ESRL/CSD): Implementation of TelAviv sectional microphysics that includes CCN activation, condensation/evaporation, stochastic collection, and sedimentation
- Graham Feingold and Hailong Wang (ESRL/CSD): Implementation of double moment bulk microphysics scheme (Feingold et al. 1998)
- Gordon McFiggans (U of Manchester, UK), implementing their multicomponent aerosol approach
- Laura Fowler and others from CSU, implementing some of the RAMS microphysics routines into WRF
- Karla Longo and Saule Freitas (CPTEC, Brazil) looking at aerosol direct effect with BRAMS and WRF/Chem
- Source oriented approach from UC Davis (Mike Kleeman) was talked about

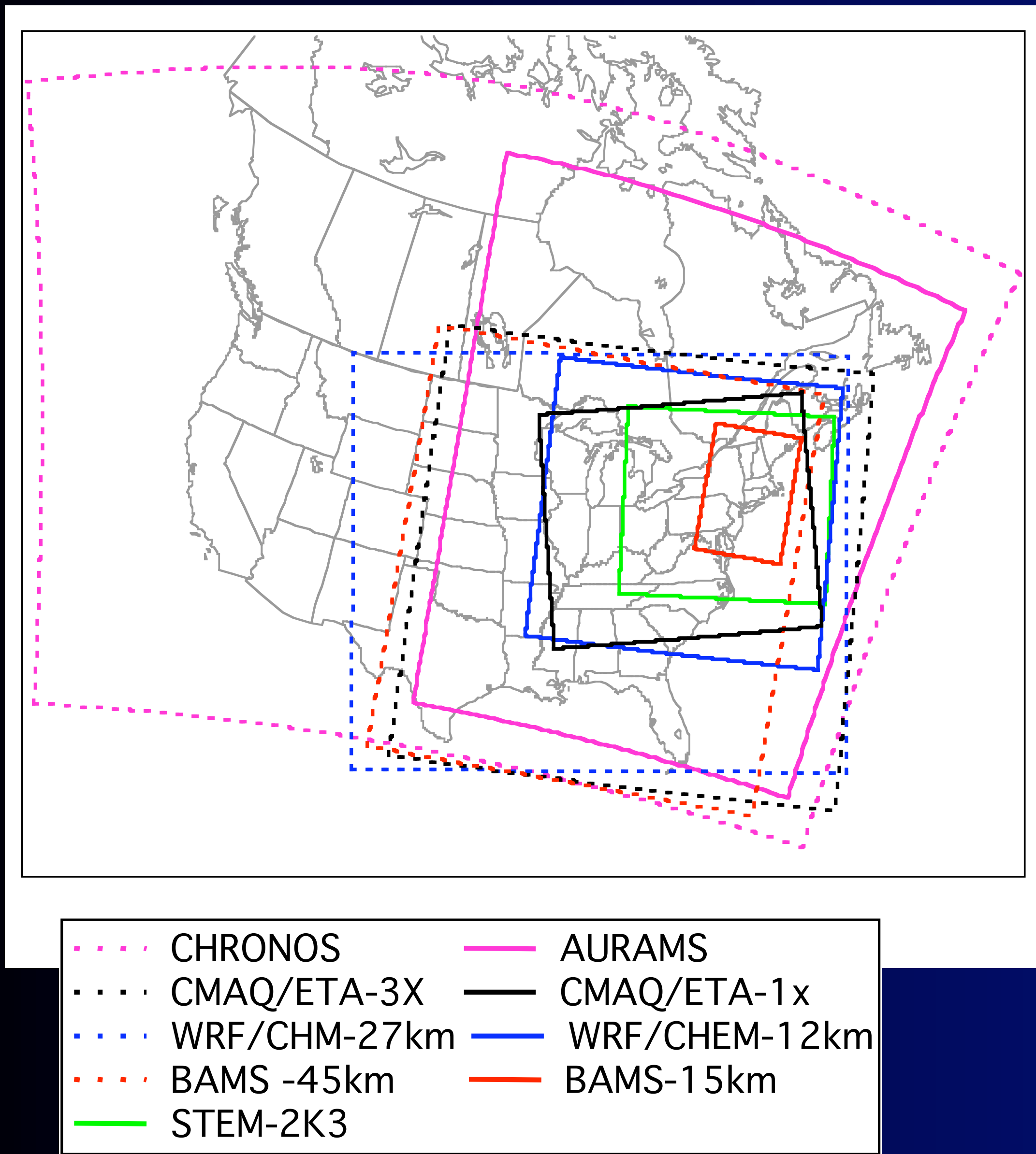
Evaluation of the WRF/Chem model within ESRL/CSD

Stu McKeen, Si-Wan Kim (ESRL/CSD and CU/CIRES)

Evaluation: WRF/Chem in weather/air-quality forecast mode

- Evaluations using data from ICARTT/NEAQS-2004 and TEXAQS 2006
- Surface Network for O_3 and $PM_{2.5}$
- Ronald H Brown Ship data in the Gulf of Maine
- NOAA WP-3 aircraft measurements - detailed chemistry
- NOAA DC-3 Ozone lidar measurements

Models Used in the ICARTT/NEAQS Evaluations



Model:	Anthropogenic Emission Inventory:
AURAMS - 42km CHRONOS - 21km	Canadian National Inv. (1990, 1995)
CMAQ/ETA(1x) - 12km CMAQ/ETA(3x) - 12km(*) BAMS - 45km BAMS - 15km	NEI-99, 2001, grown to 2004
WRF/CHEM-1 - 27km	NET-96
WRF/CHEM-2 - 27km WRF/CHEM - 12km(*) STEM(2K3) - 12 km	NEI-99

Red indicates PM2.5 forecasts available
(*) Indicates a retrospective run

Model variables available for Comparison with NOAA Aircraft and Ron Brown data

gas phase chemistry

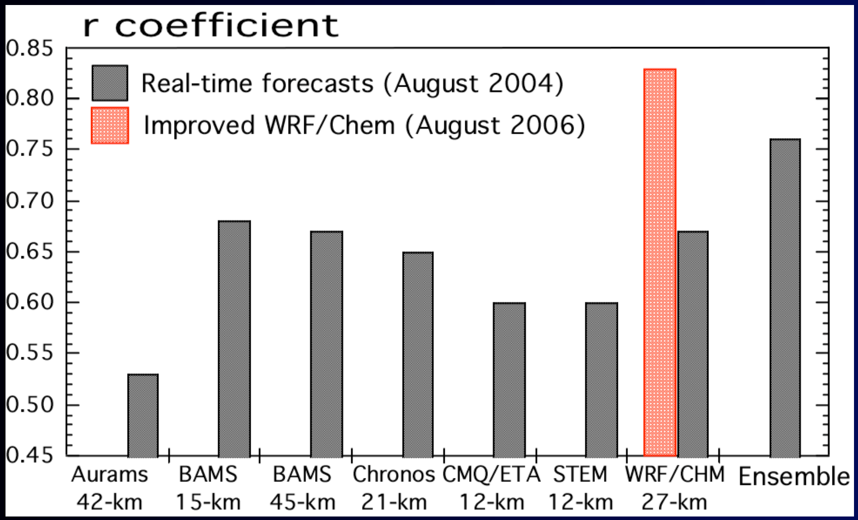
	AURAMS	CHRONOS	STEM	WRF-2
O_3	√	√	√	√
CO			√	√
NO	√	√	√	√
NOx	√	√	√	√
NOy	√	√	√	√
PAN	√	√	√	√
Isoprene	√	√	√	√
SO_2	√	√	√	√
NO_3	√	√		√
N_2O_5	√	√		√
CH_3CHO	√			√
Toluene		√		√
Ethylene	√	√		√
NH_3				√

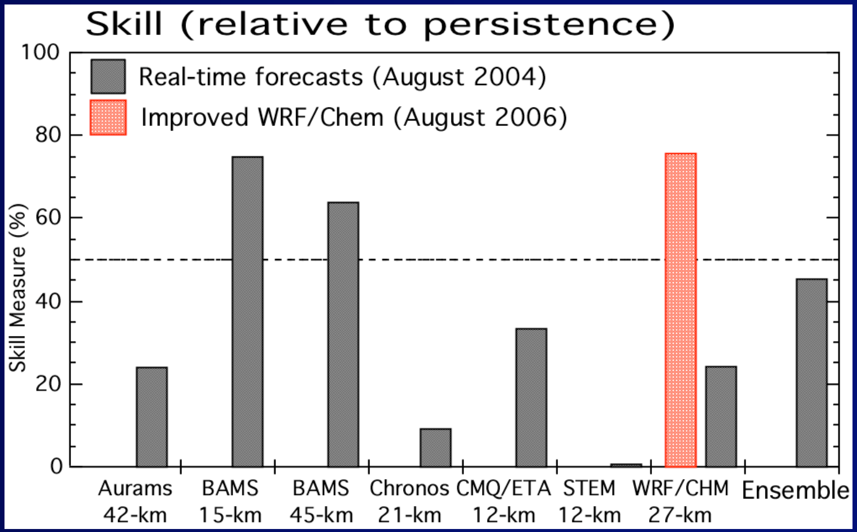
aerosols, radiation, meteorology

	AURAMS	CHRONOS	STEM	WRF-2
PM2.5	√	√	√	√
Asol SO_4	√	√	√	√
Asol NH_4	√			√
Asol OC	√	√	√	√
Asol EC	√		√	√
Asol NO_3	√			√
JNO_2				√
T	√	√	√	√
P	√		√	√
H_2O	√	√	√	√
winds	√	√	√	√
SST	√			√
Radiation				√

http://www.al.noaa.gov/ICARTT/modeleval/

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

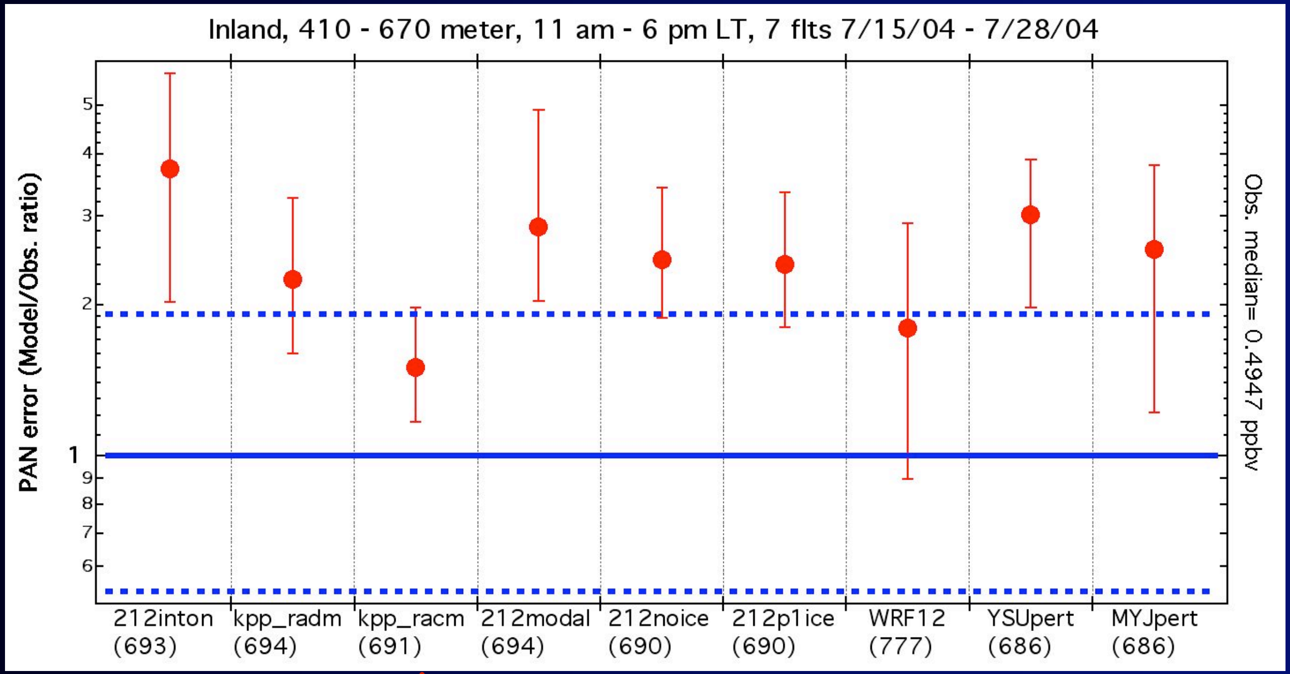




Maximum 8 hour averages
352 O_3 monitors - eastern U.S. and Canada
53 days (July and August 2004)

For WRF/ChemV3: r=.85, skill=83

Comparison of PAN Forecast with NOAA -P3 aircraft data



*

WRFV2.2

Key:

212inton - V2.1.2, Pegasus - CBMZ, no convective subgrid transport

Kpp_radm - V2.1.2, RADM2, subgrid convection on, subgrid photol. reduc. On ice contribution to photolysis reduction in resolved clouds (1. cloud equiv)

Kpp_racm - V2.1.2, RACM, subgrid convection on, subgrid photol. reduc. On ice contribution to photolysis reduction in resolved clouds (1. cloud equiv)

212modal - V2.1.2, RADM2, subgrid convection off, subgrid photol. reduc. off

212noice - V2.1.2, RADM2, subgrid convection on, subgrid photol. reduc. off no ice contribution to photolysis reduction in resolved clouds

212p1ice - V2.1.2, RADM2, subgrid convection on, subgrid photol. reduc. off ice contribution to photolysis reduction in resolved clouds (.1 cloud equiv)

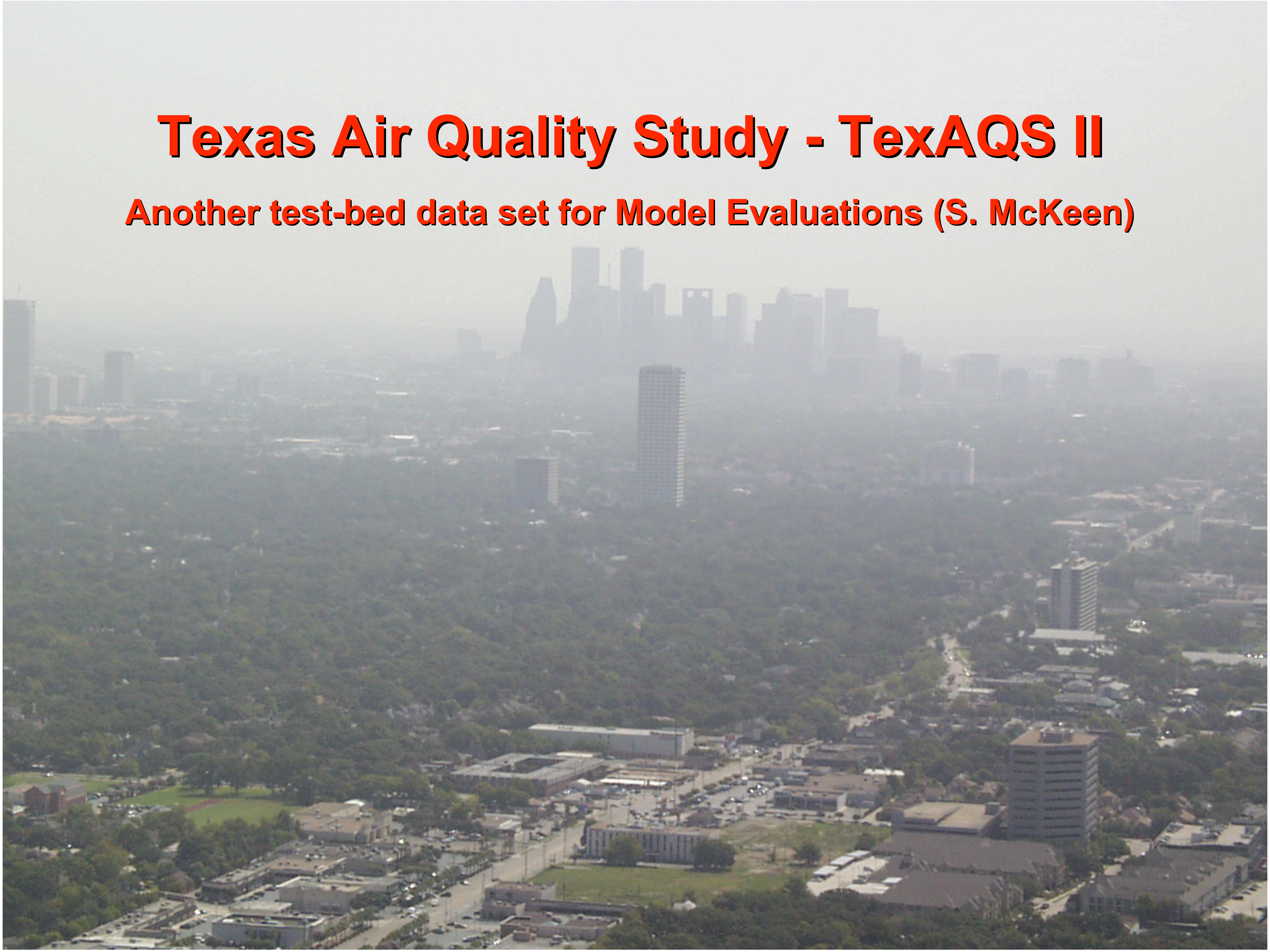
WRF12 - V2.0.3, RADM2, 12 km res. YSU PBL (convection on, no subgrid photol reduc.)

YSUpert - V2.0.3, RADM2, 27km res., YSU PBL scheme (“ “ “)

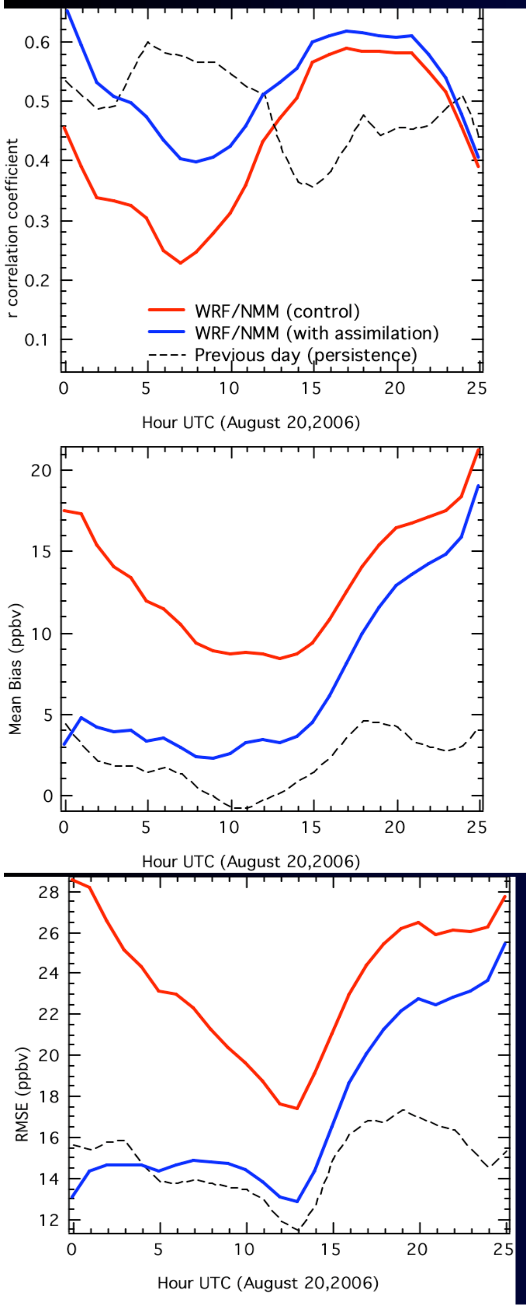
MYJpert - V2.0.3, RADM2, 27km resolution, MYJ PBL scheme (“ “ “)

Texas Air Quality Study - TexAQS II

Another test-bed data set for Model Evaluations (S. McKeen)



Chemical Data Assimilation – 3DVAR and 4DVAR



Initial experiments with 3DVAR chemical data assimilation show that even ozone forecasts can be improved significantly (using GSI and NMM-WRF/Chem)

- For ozone this is somewhat surprising (because of strong dependence on time of day, sunlight, and chemistry
- Work has started with ARW-WRF/Chem and PM assimilation
- Adjoint development will start in collaboration with Greg Carmichael