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Development and evaluation of a new operational Air Quality Forecast Model: GEM-MACH15

Mike Moran
AQRD / STB / EC
Toronto, ON

Louis-Philippe Crevier
AQMAS / MSC / EC
Dorval, QC

RPN Seminar Series CMC, Dorval 30 May 2008

Talk Outline

- Project goals and objectives
- Background
  - Air-quality (AQ) modelling components
  - AQ processes
- GEM-MACH description
- GEM-MACH15 description
- GEM-MACH15 evaluation
  - Some meteorological evaluation results
  - Some AQ evaluation results: ozone (O3)
- Summary and next steps

Initial Project Goal

- To replace CHRONOS, the current EC operational off-line regional AQ forecast model for O_3, NO_2, $PM_{2.5}$, and PM_{10}, with a new GEM-based on-line operational AQFM that includes a science package equivalent to the one in AURAMS

- Project started in Fall 2005
  - See November 2005 seminar for more info

Project motivation

- CHRONOS science needs to be upgraded to improve performance
  - Add new or improve existing processes
  - Add chemical data assimilation

- Technical issues:
  - CHRONOS code is OpenMP'ed but is not MPI'ed
    - Currently just fits in operational window
  - Interpolation between GEM and CHRONOS grids is time-consuming and introduces errors.

Secondary Goals

- To develop an initial chemical library and interface to GEM that could be expanded upon by other projects instead of having to « reinvent the wheel» each time.
- To formalize the links between the EC atmospheric chemistry community and the GEM community
- To formalize the role of the GEM chemistry librarian

Current GEM-MACH "Team"

ARQI

- **Mike Moran**
- Paul Makar
- Wanmin Gong
- Sunling Gong
- Sylvie Gravel
- **Alexander Kallaur**
- Balbir Pabla
- Craig Stroud
- Ping Huang (contractor)
- Alain Robichaud
- (Didier Davignon)

AQMAS

- **Louis-Philippe Crevier**
- **Sylvain Ménard**
- **Donald Talbot**
- Hugo Landry
- Mourad Sassi
- Stéphane Gaudreault
- Samuel Gilbert
- Véronique Bouchet
- David Anselmo
- (Paul-André Beaulieu)

RPN

- Michel Desgagné
- Vivian Lee

Other groups/people involved (or soon to be)

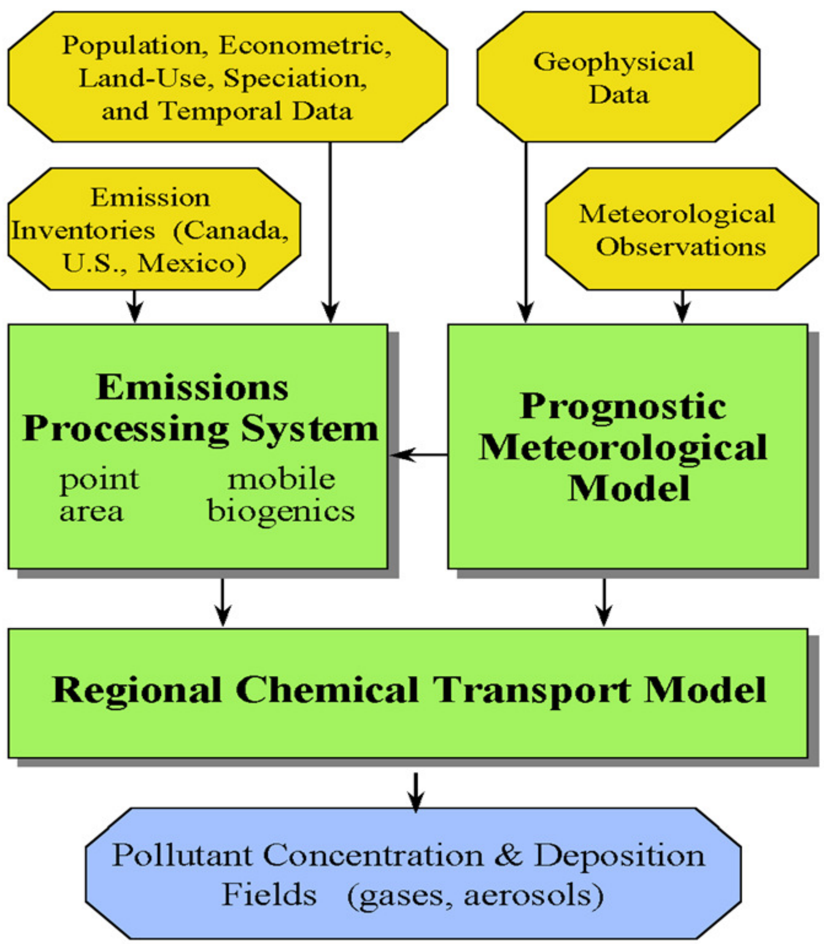
- RPN (Paul Vaillancourt)
- CMDN (Alain Patoine, Amin Erfani), CMDW (Stavros Antonopoulos)
- CMOI, A&P, AQ regional forecasters and science groups

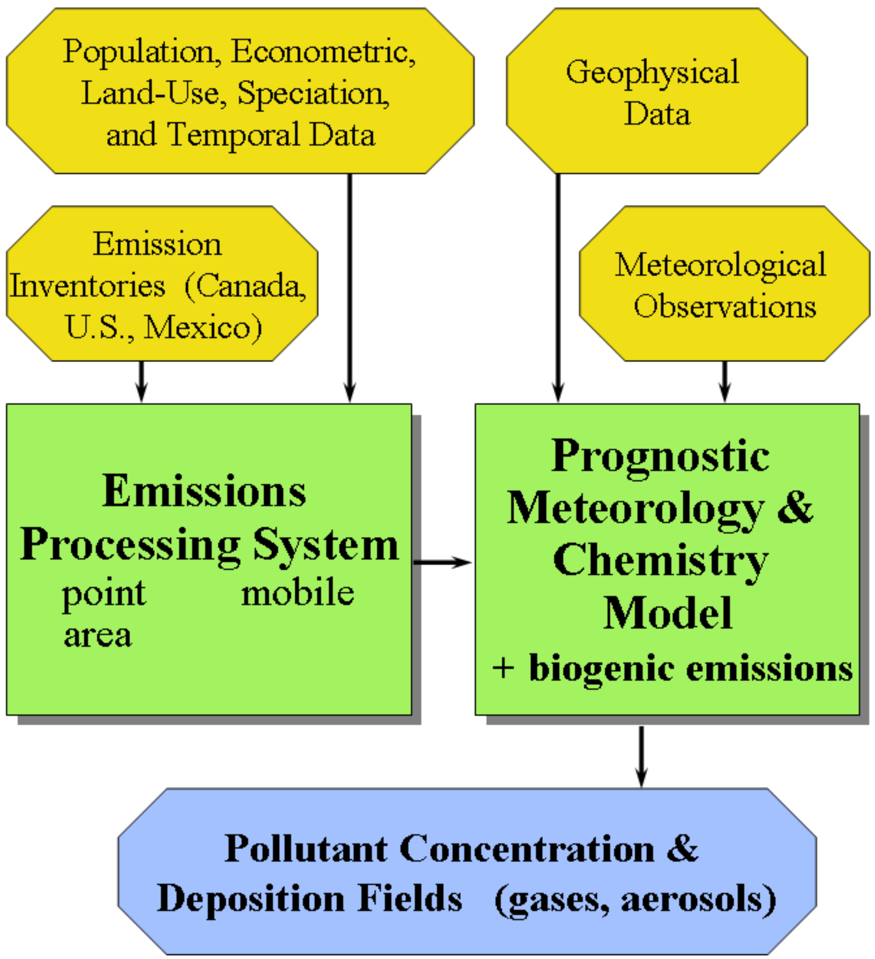
Background

Primary AQ System Components

- To model air quality ("chemical weather"), three primary components must be represented:
  1. emissions of pollutants or their precursors
  2. meteorology and transport & diffusion
  3. transformation and removal processes

AQ Model Data Flow





On-line Treatment of Chemistry

- Allows chemistry calculations
  - on GEM grid and timestep and provides access to all GEM fields, and
  - avoids need for interpolation to another model grid
- Provides better framework for chemical data assimilation
- Gives potential (in future) for chemical feedback to meteorology (e.g., radiation, clouds)
- Increases complexity of the single model

Representation of Emissions (1)

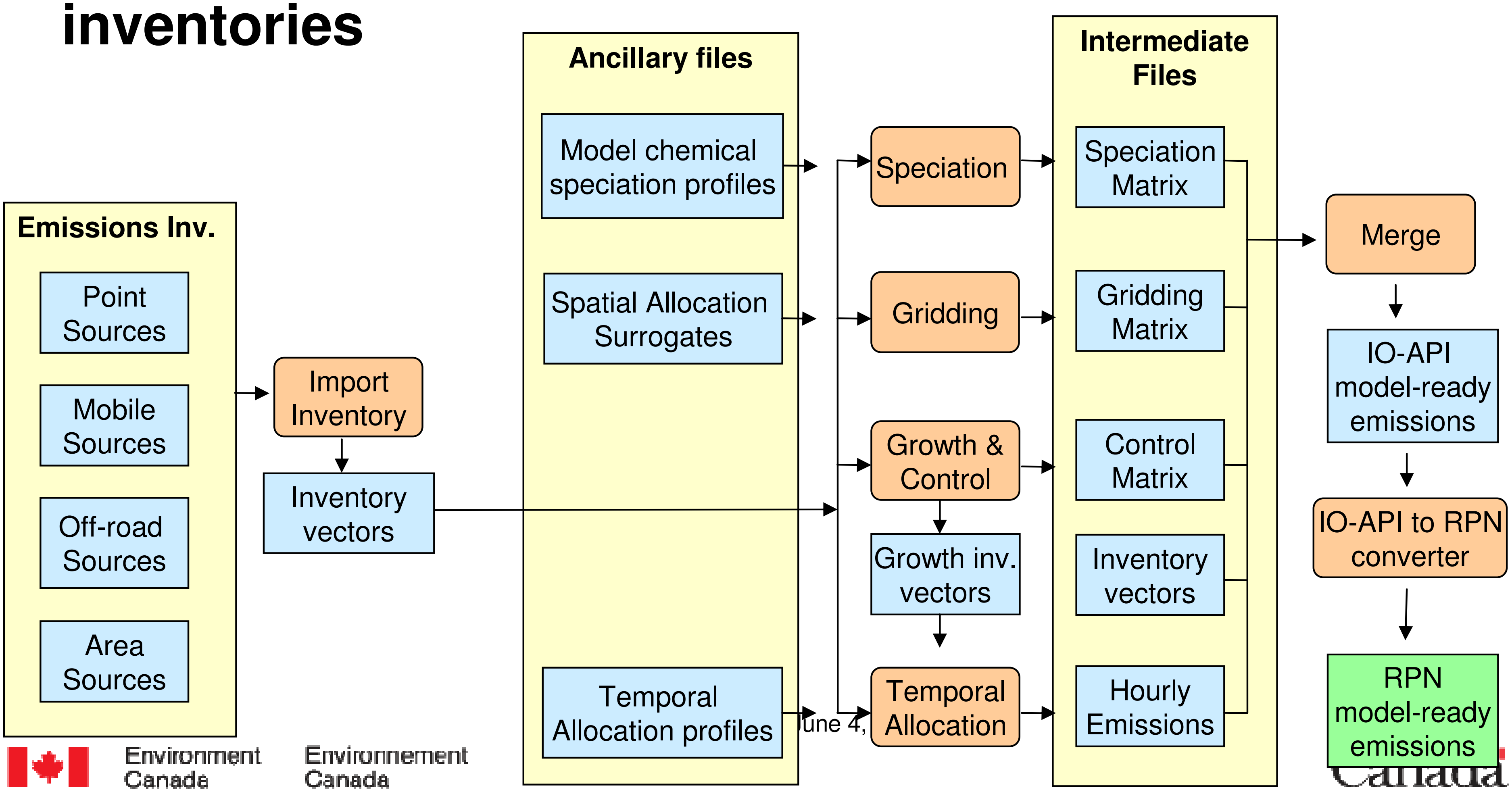
- Important aspect of chemical weather but important source of **model uncertainty**
- Analogous to a set of day-specific, time-varying (hourly!) geophysical fields
- Very difficult to quantify:
  - Strong dependence on human activity (*i.e.,* socioeconomics, technology, geography, legislation, culture, fuel type, season, …)
  - Some dependence on meteorology
  - Must be comprehensive: i.e., all sources must be identified and quantified

Representation of Emissions (2)

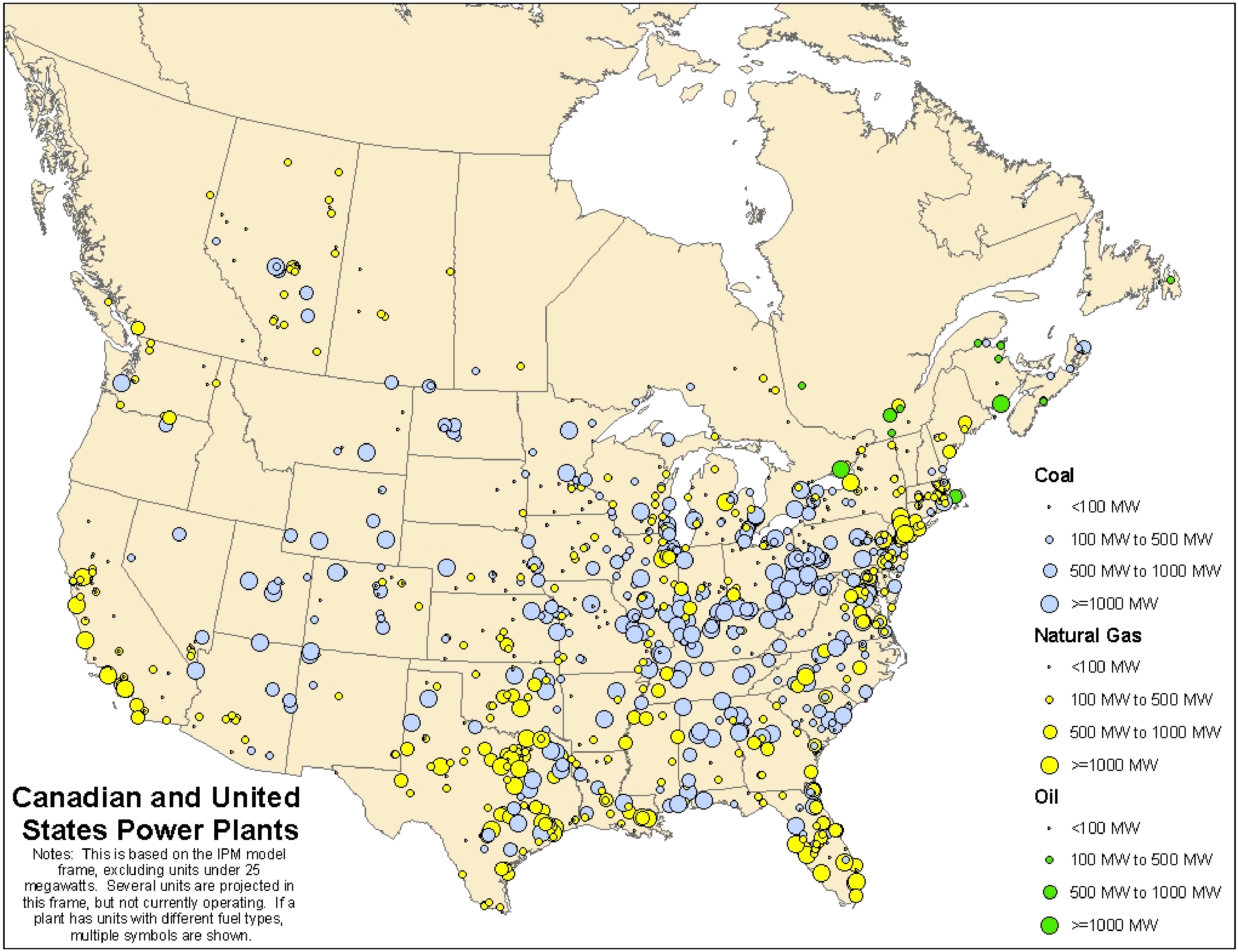
- Primary source types and examples:
  - Point sources
    - Power plants, smelters, factories, incinerators, …
  - On-road mobile sources
    - Car, trucks, motorcycles, buses
  - Off-road mobile sources
    - Construction, agriculture, and mining equipment, locomotives, marine vessels, pleasure craft, aircraft, snowmobiles, …
  - Area sources
    - Small point sources (e.g., houses, lawnmowers, BBQs), painting, fertilizer application, road-paving, crop harvesting, …
  - Natural sources
    - biogenic, biomass burning, geogenic, volcanic, oceanic, lightning

SMOKE (Sparse Matrix Operator Kernel Estimation) Emissions Processing System

- **creates hourly, gridded, speciated "model ready" emission files from annual, jurisdiction-based, criteria-air-contaminant national emission inventories**

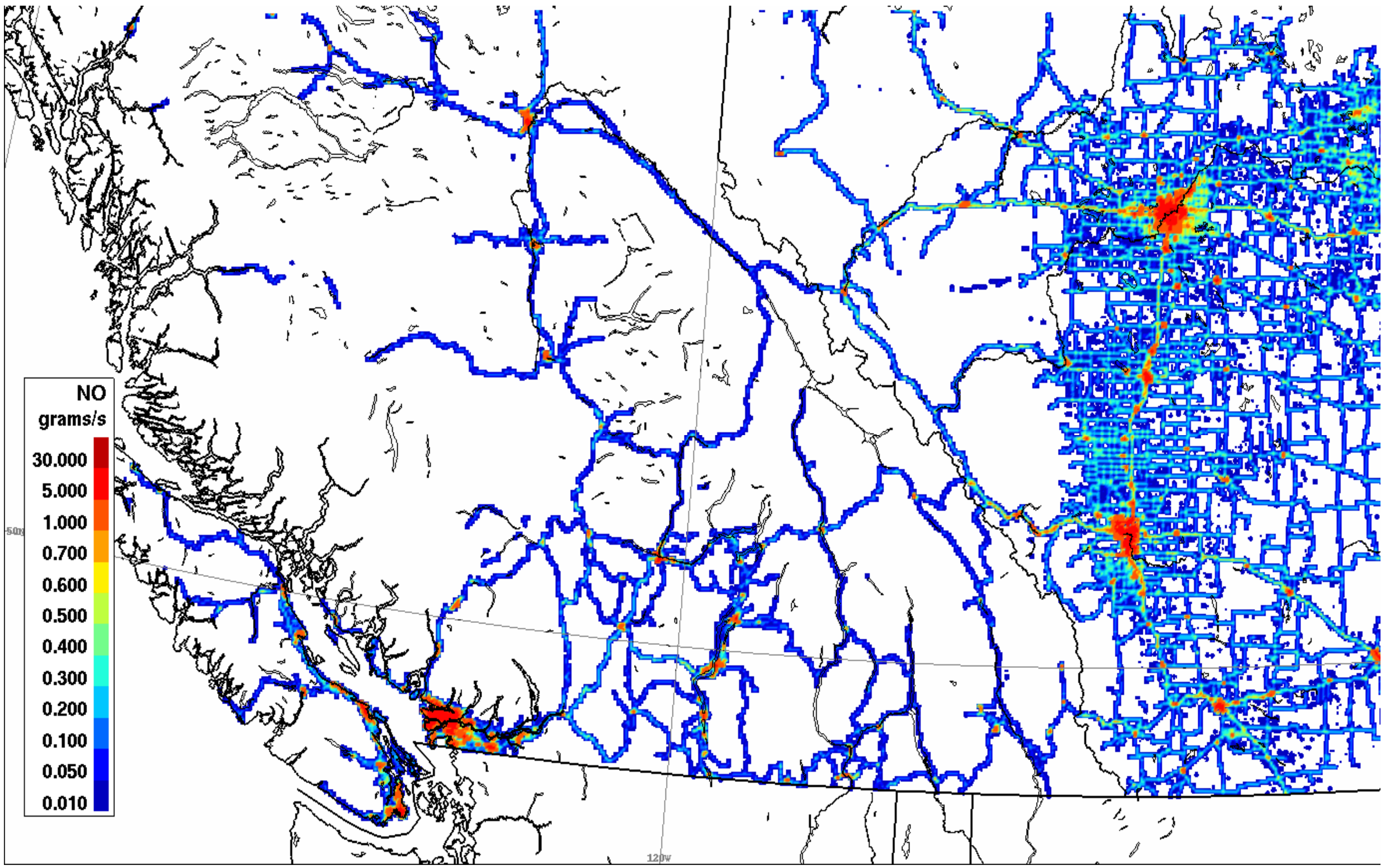


Location of Cdn & U.S. Thermal EGUs



[Src: *2005 Canada-U.S. Emissions Cap & Trading Feasibility Study*]

NO Emissions in Western Canada from On-Road Mobile Sources



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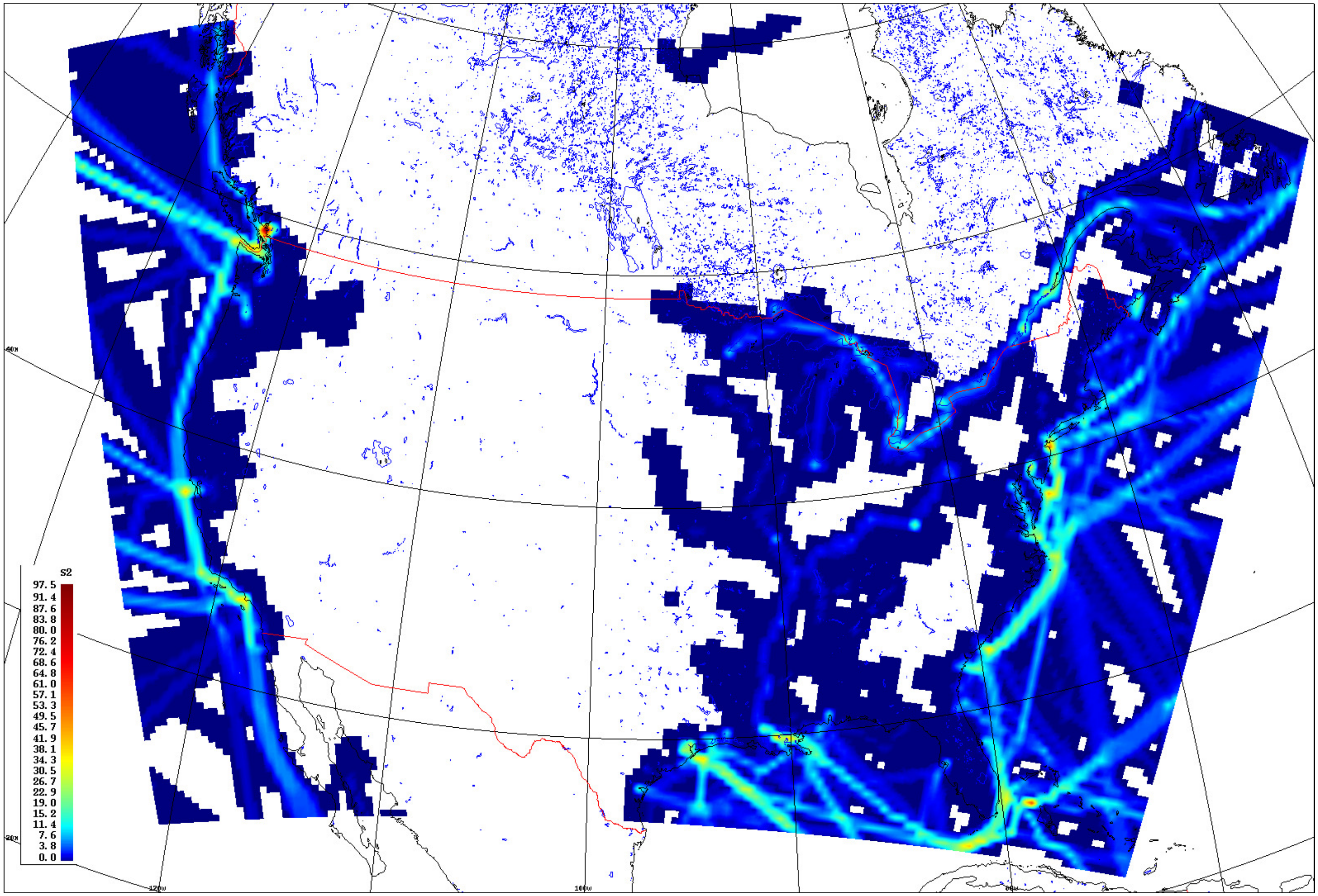
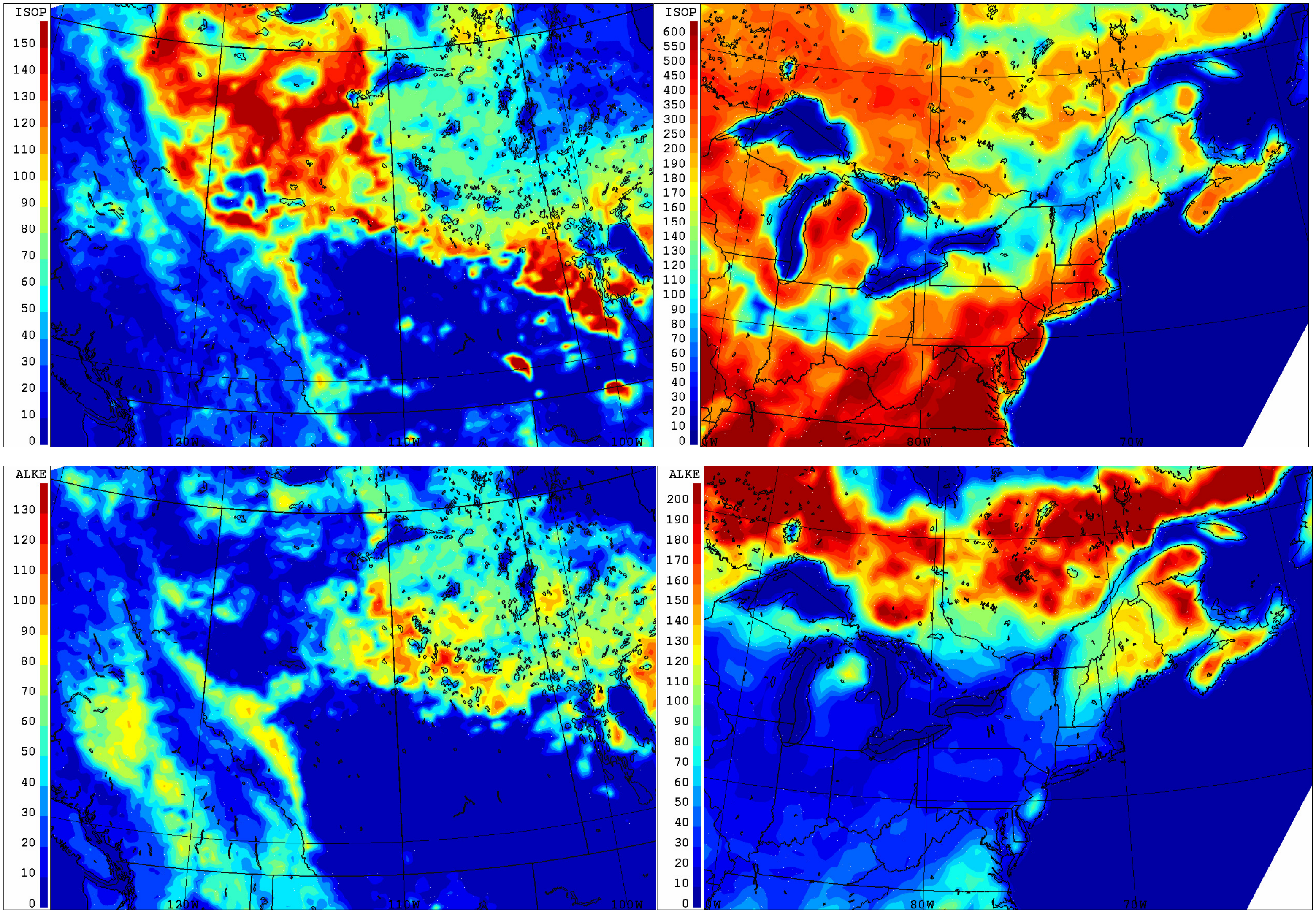
SO_2 Emissions from Commercial Marine Vessels



Sample Multi-day Mean Biogenic Emission Maps for Isoprene and ALKE Emissions (2001 Cdn Forest Inventory & U.S. BELD3 Data)

ISOP

ALKE



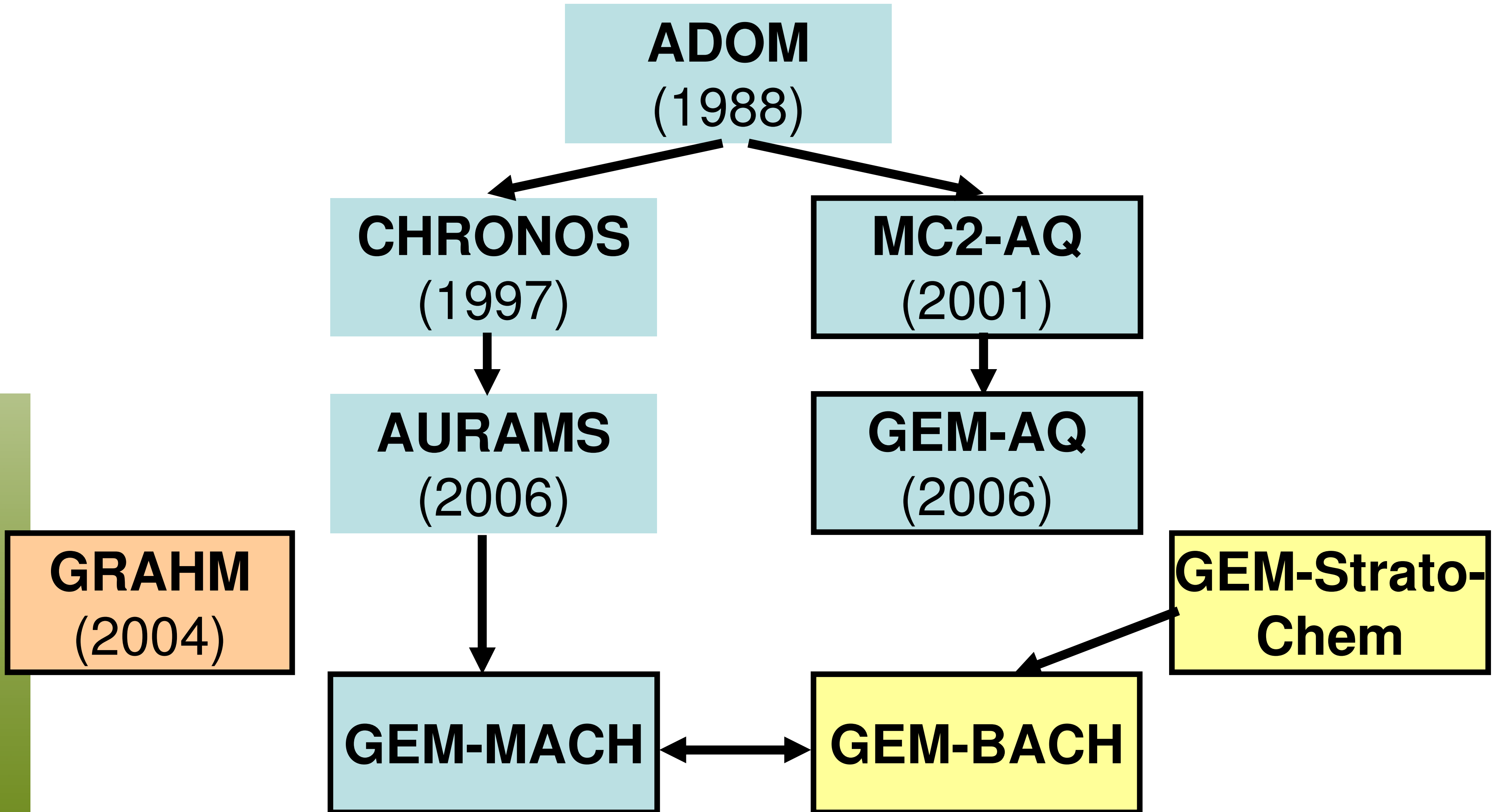
Western Canada

Eastern North America

GEM-MACH Description

GEM-MACH Family Tree

(Colours Denote Chemistry Mechanisms, Heavy Box Outlines Denote In-Line Models, Years Refer to Foundation Publication)



GEM v3.3.0 as an AQ Milestone

GEM v3.3.0 released May 2007

- First official version of GEM to include the new chemistry interface needed by **GEM-MACH**

GEM Chemistry Interface (1)

- Design follows GEM physics interface very closely
- Consists of four chemistry data buses: dynamics, permanent, volatile, entry
- Chemical species abundance fields ("chemistry tracers") are assigned to chemistry dynamics bus, advection handled automatically by GEM

GEM Chemistry Interface (2)

- Call to chemistry follows call to physics
- Interface development was a collaborative effort between AQRD, AQMAS, and GEM developers (M. Desgagné, V. Lee)
- Prototype version of interface was developed for ESA contract (R. Ménard, PI), with subsequent refinements for GEM-MACH

AQ Processes Now Implemented in GEM-MACH (1)

- **acquisition of all required meteorological fields**
- **initialization of chemical species (including cycling of chemical tracers from day to day)**
- **chemical lateral boundary conditions (for LAM)**
- **chemical upper boundary conditions**
- **input and injection of anthropogenic surface emissions and elevated emissions (incl. plume rise)**
- **calculation and injection of biogenic emissions**
- **vertical diffusion of chemical species**

AQ Processes Now Implemented in GEM-MACH (2)

- dry deposition of gaseous species and particles
- wet deposition of gaseous species and particles
- gas-phase chemistry (ADOM-II mechanism)
- secondary organic aerosol formation (IAY scheme)

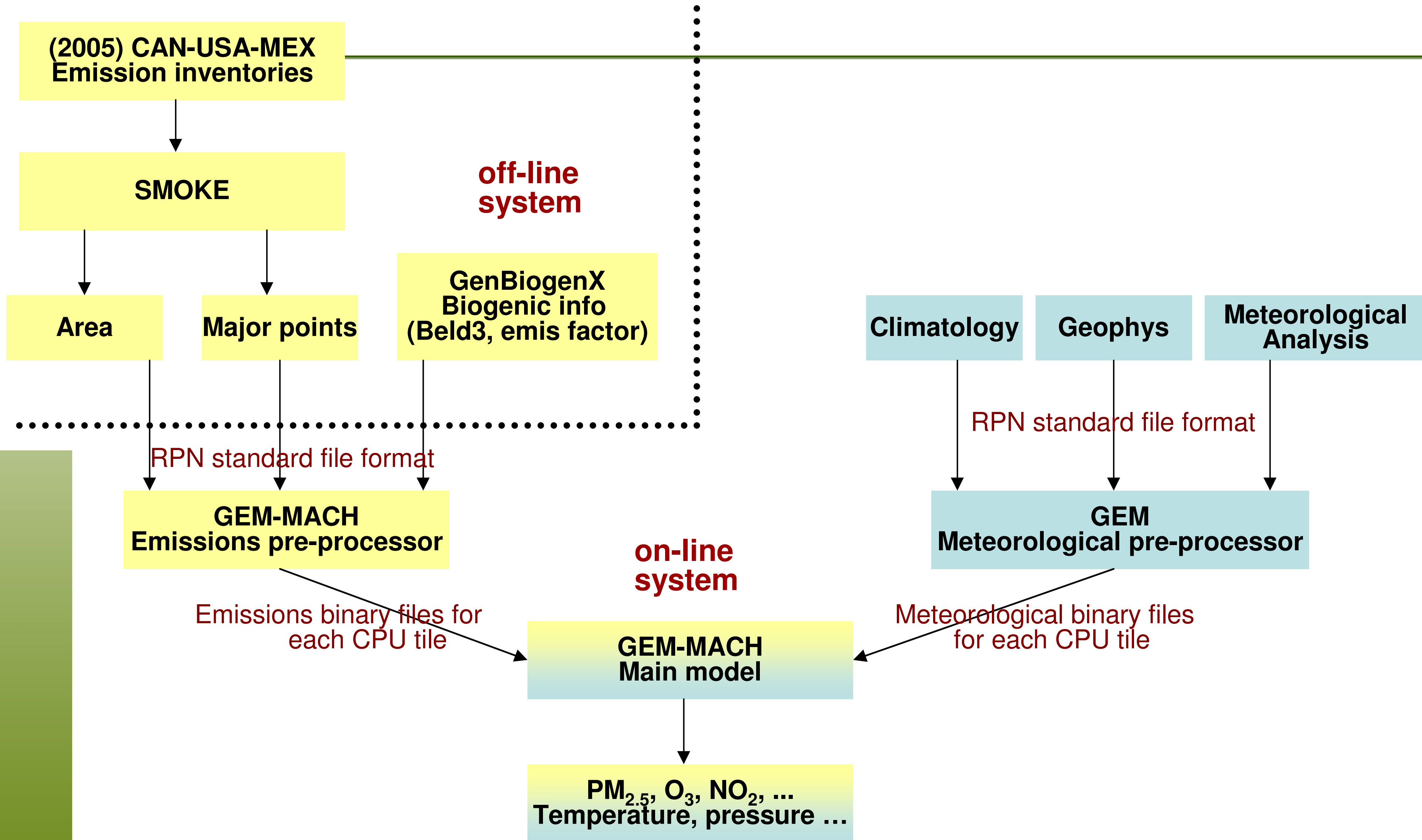
- aqueous-phase chemistry (ADOM scheme)
- heterogeneous inorganic chemistry (HETV scheme)
- variable number of PM size distribution "bins"
- PM size-dependent processes: natural emissions, nucleation, condensation, coagulation, activation, dry deposition, wet deposition

AQ Processes For Consideration

- subgrid-scale convective vertical transport
- wind-blown dust emissions
- North American wildfire emissions
- urban heat island influence on near-surface vertical mixing
- enhanced gas-phase chemistry (incl. CH_4, C_2H_6?)
- improved vertical diffusivity parameterizations
- updates to inorganic heterogeneous chemistry
- cloud ice-phase chemistry
- improved biogenic emissions

- global anthropogenic emissions, including marine vessels
- global biomass burning, wildfires, and volcanoes
- global lightning-generated NO_x
- global oceanic emissions (e.g., DMS)
- undoubtedly others!

GEM-MACH Data Flow



Emissions Entry Program

- Emissions information is needed by GEM-MACH on an **hourly basis** (not a GEM requirement historically)
  - Files of gridded emissions fields are first created off-line using an emissions processing system (SMOKE) modified to work with GEM grid
  - Emissions entry program splits emissions fields into BMF files according to model topology and run parameters
  - During model execution, BMF files are read at appropriate timesteps
  - GEM now has capacity to read non-gridded data for major point sources (Y-grid); also split between tiles, input hourly

GEM-MACH15 Description

CHRONOS Configuration

- Forcast duration/frequency
  - 48-h forecast, twice per day
- Domain:
  - 21-km resolution (polar stereographic projection)
  - 24 Gal-Chen levels to ~6 km
- Emissions:
  - Year 2000/01 Canadian and US inventories
  - Emissions split into four seasonal file sets
- Initialization:
  - Chemical fields are cycled from previous forecast run (12-h forecast)

GEM-MACH15 Configuration (1)

- 48-h forecast, twice per day
- LAM configuration:
  - Points are co-located with Regional 15 km (GEM15) grid core
    - ~about 45% of the number of grid points of GEM15
  - Same 58 vertical levels as current regional model
  - Using GEM v3.3.0, Physics 4.5
    - Physics and dynamic packages are nearly identical to GEM15
    - Hzd_type_S= EXPLICIT for LAM instead of HO for GEM15 (almost no diffusion anyway)
    - Vspng_nutop = 2. in the LAM since Vspng_mf=10. as in GEM15 does not apply to a LAM
  - Piloted hourly from GEM15 forecast
- Initialization:
  - Meteorology initialized with GEM15 0h prognostic fields
  - Surface fields come from analysis
  - Chemistry fields are cycled from previous forecast run (12-h forecast)

GEM-MACH15 Configuration (2)

- Chemistry:
  - ADOM-II gas-phase chemistry, ADOM aqueous-phase chemistry, HETV heterogeneous chemistry, IAY SOA scheme
  - 2-bin sectional representation of PM size distribution with 9 chemical components
- Emissions:
  - Year 2005 Canadian and US emissions inventories
  - Emissions split into 12 monthly file sets
  - Improved biogenic emissions
    - Improved land-use database
    - Improved emission factors
- Timings
  - «Ozone» chemistry only: 75 min @ 64 CPUs
  - Complete model (Ozone + PM): about 75 min @ 192 CPUs (est.)

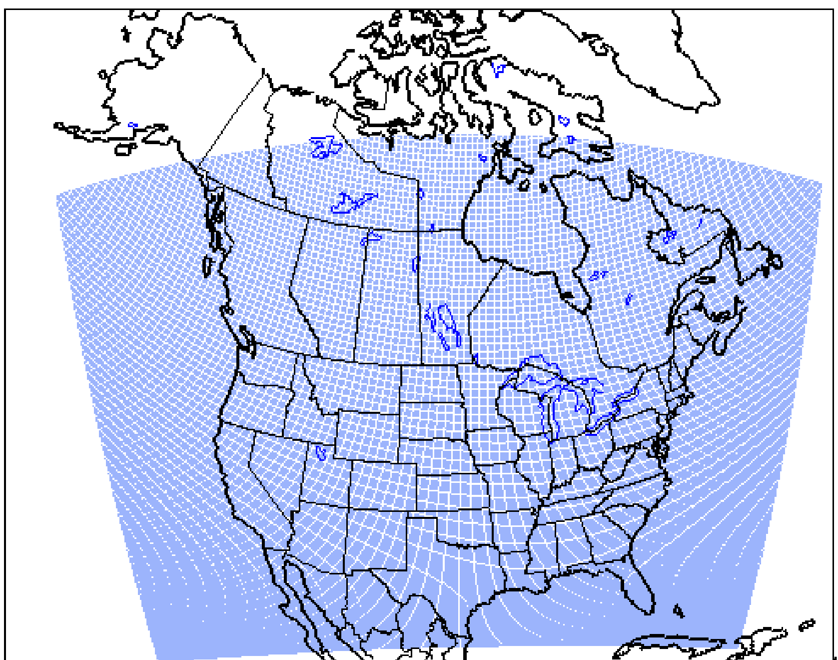
GEM-MACH15 vs CHRONOS Modelling Domains

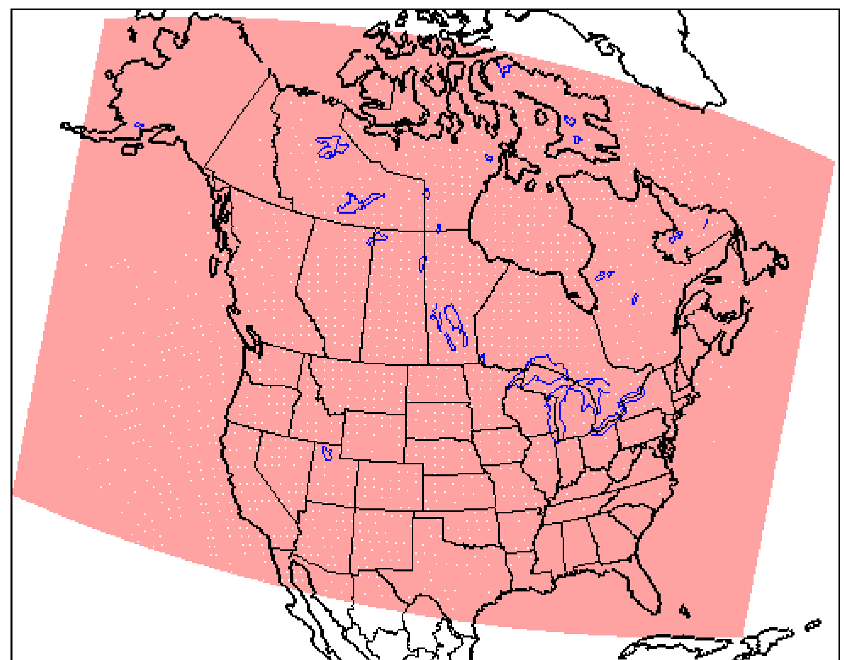
CHRONOS

Resolution:
- 350 x 250 gridpoints, secant PS
- **21 km** horizontally
- **24** vertical levels **up to ~ 6 km**
- Δt = **3600** s

GEM-MACH15

Resolution:
- 348 x 465 gridpoints, rotated LL
- **15 km** horizontally
- **58** vertical levels **up to ~ 30 km**
- Δt = **450** s



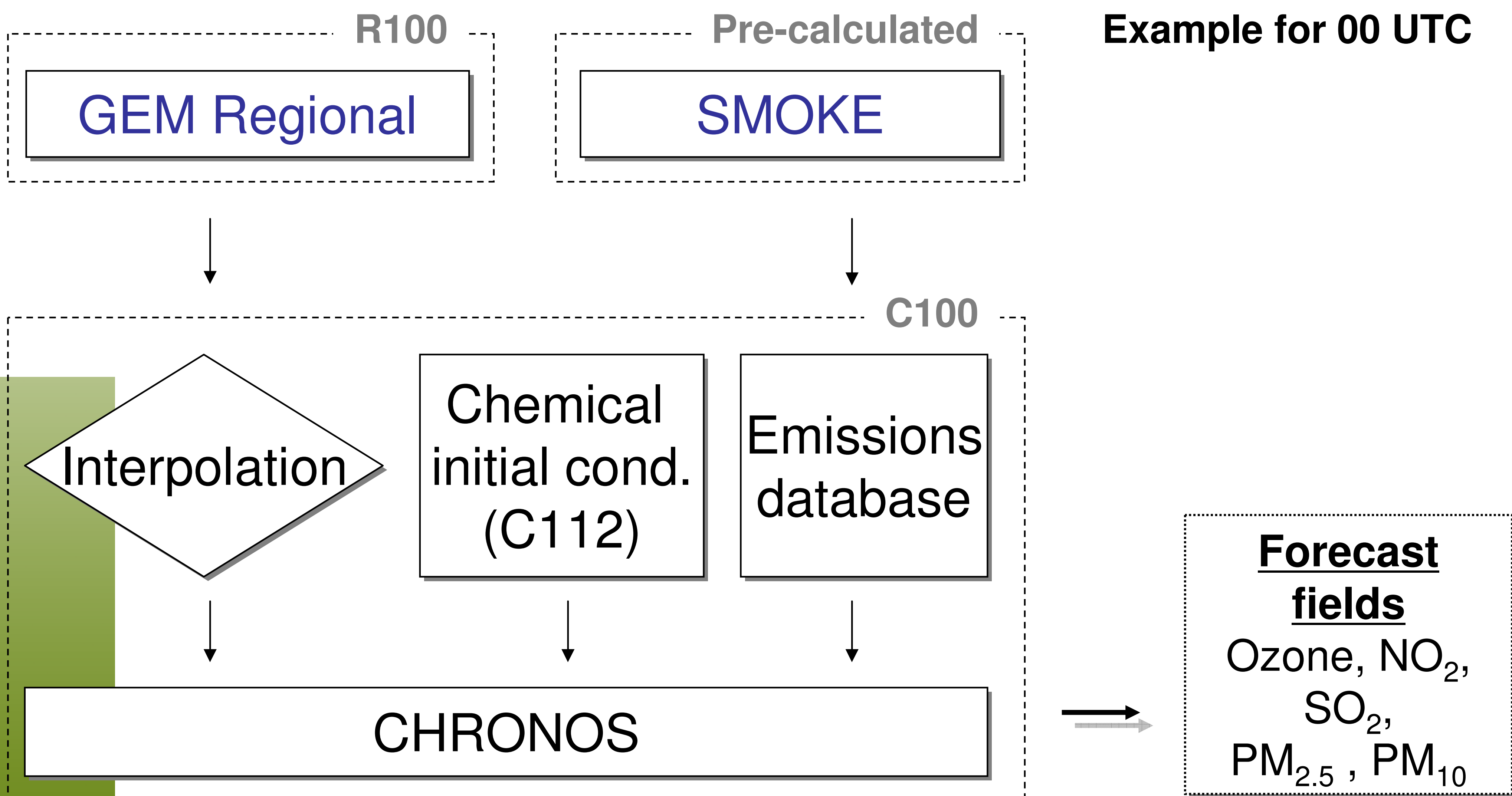


Main Differences in Chemical Processes Between CHRONOS and GEM-MACH15

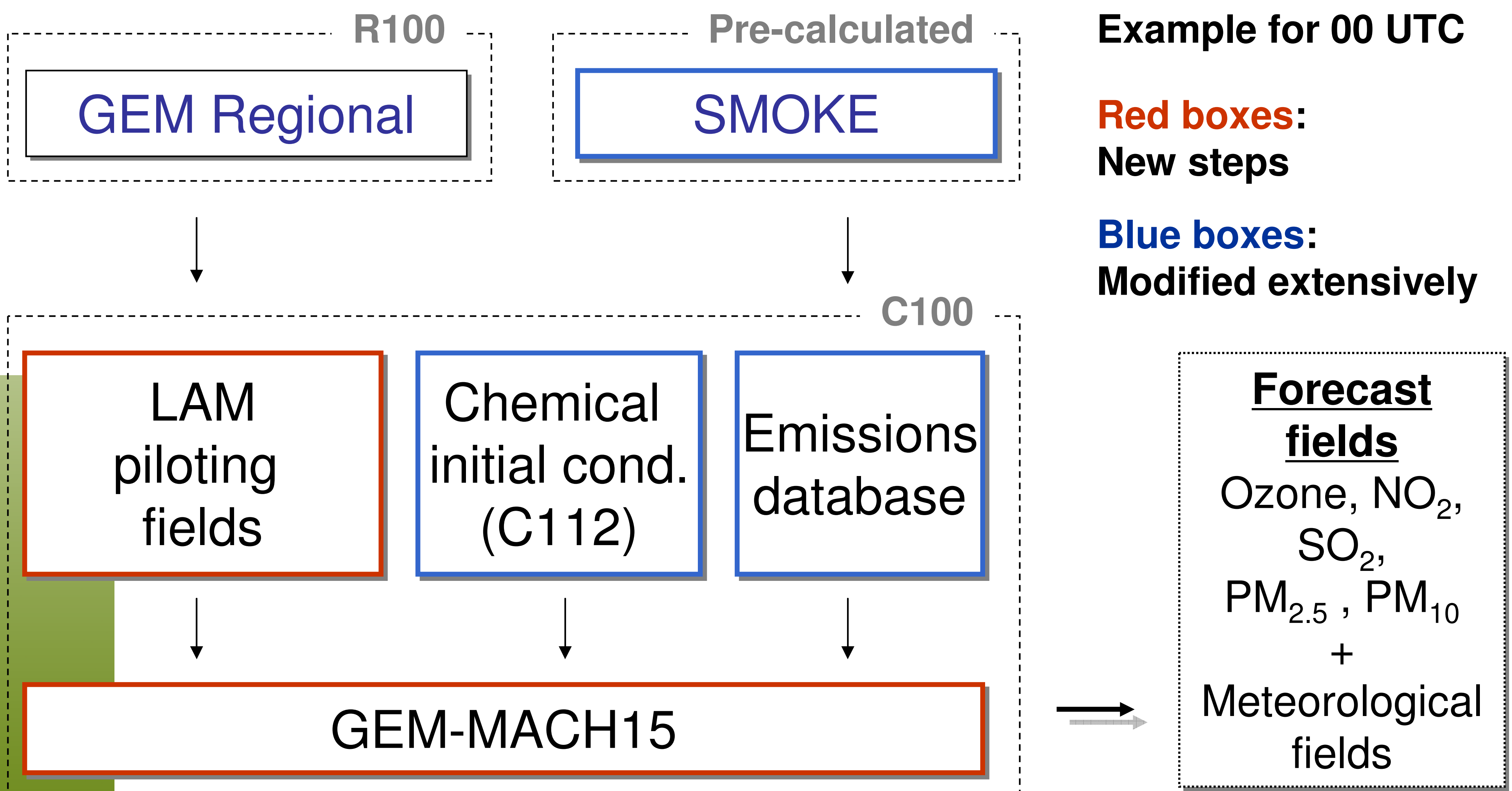
	CHRONOS	GEM-MACH15
Emissions	$PM_{2.5}$ and PM_c primary emissions are assumed to be bulk emissions; 17 gas-phase species emitted	$PM_{2.5}$ and PM_c emissions **speciated to 7 species** by primary source type (point, area, mobile); 17 gas-phase species emitted
Gas-Phase Chemistry Mechanism	ADOM-2 mechanism (Stockwell and Lurmann, 1989); 47 advected species	ADOM-2 mechanism (Stockwell and Lurmann, 1989) with **1) p-SO_4 replaced by H_2SO_4+p-SO_4** 2) **N_2O_5 + H_2O** "heterogeneous nitrate formation" rate enhancement **switch=off.**
Aqueous-Phase Chemistry	None	**ADOM aqueous-phase chemistry**
PM Composition	4 species: sSO_4, sOC, H_2O, primary PM	**9 species**: SO_4, NO_3, NH_4, EC, pOC, sOC, CM, SS, H_2O
Aerosol Dynamics	Sedimentation	Sedimentation, **Nucleation, Condensation, Coagulation**
Secondary Organic (SOA) Yields	Based on Pandis et al. (1992)	**IAY scheme** Based on Jiang (2004)
Wet Deposition	Distribution of LWC is used to calculate the wet scavenging term by applying Sundqvist formulae for the rate of release of precipitation	Transfer of tracers from cloud to rain water based on **precipitation production. In-cloud and below-cloud scavenging of soluble gases and particles (size-dependent) .**
Chemical boundary conditions	Zero-gradient inflow, open boundary out-flow	**climatological profiles** with Davies boundary conditions

Current Operational Air Quality Forecast System

Example for 00 UTC



Operational Air Quality Forecast System with GEM-MACH15



GEM-MACH15 Development Status

- GEM-MACH15 has now been evaluated for **ozone forecasting only**. Implementation of PM forecasting capabilities is being finalized and evaluation is beginning.
- The ozone field is essentially de-coupled from PM chemistry. Only small indirect feedbacks exist between the two.
  - Tests with AURAMS have shown that impact on ozone field of adding PM chemistry is of order of 0.1% bias, r^2 of 0.999
- The modelling setup should not change when PM processes are turned on: that is,
  - same configuration, same input fields
  - extra chemical processes activated by namelist keys

Evaluation Results

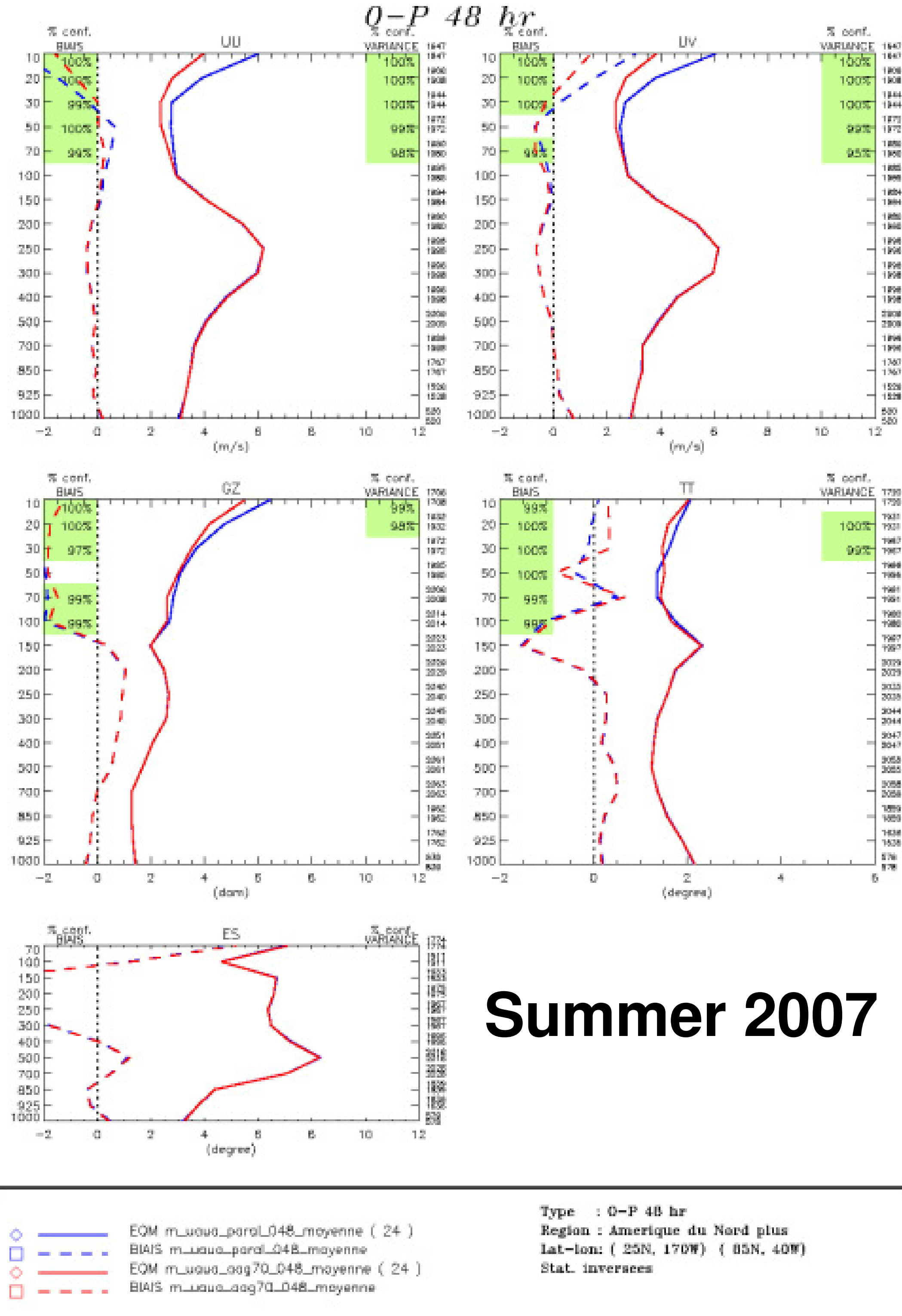
Model Evaluation: Methodology

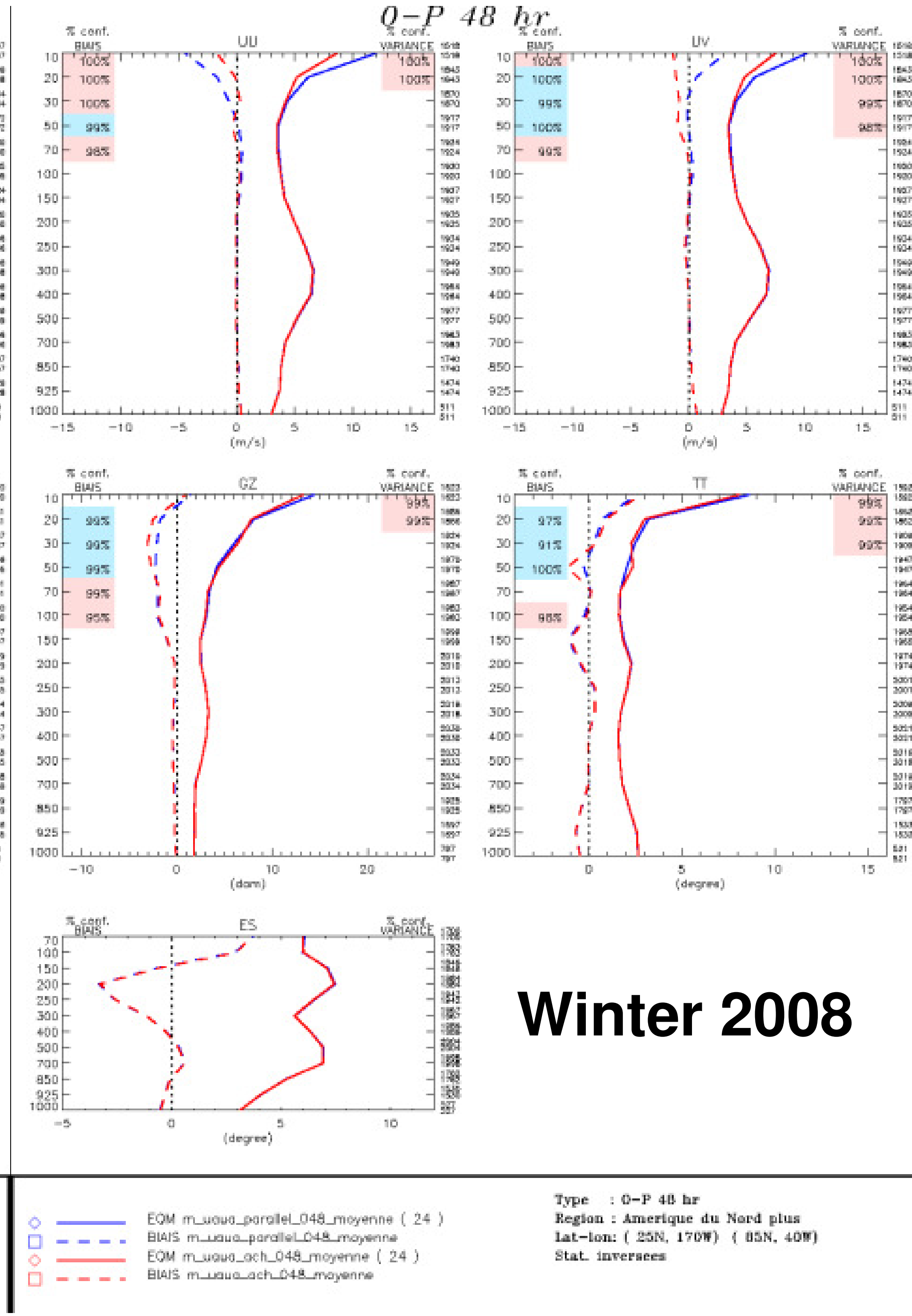
- Initial evaluation of GEM-MACH15 ozone forecasting capacity is completed
- Two forecast series were run for summer and winter conditions (24 cases each, initialized every 36 h)
  - Summer: June 8th, 2007 to July 13th, 2007
  - Winter: February 2nd, 2008 to March 8th, 2008
  - Two-week spin-up period precedes each period
- Results are compared to observations over the entire North American continent for day 1 and day 2 forecasts

Model Evaluation: Meteorology

- The impact on meteorology of having a LAM configuration instead of GV was evaluated
  - ARCAD scores were computed over North America for each period
  - Precipitation objective scores were also calculated for the same domain and periods

- Conclusions:
  - The two models produce nearly identical forecasts for most levels. Near the model top, the LAM configuration seems to show an improved forecast.
  - Impact on precipitation is neutral

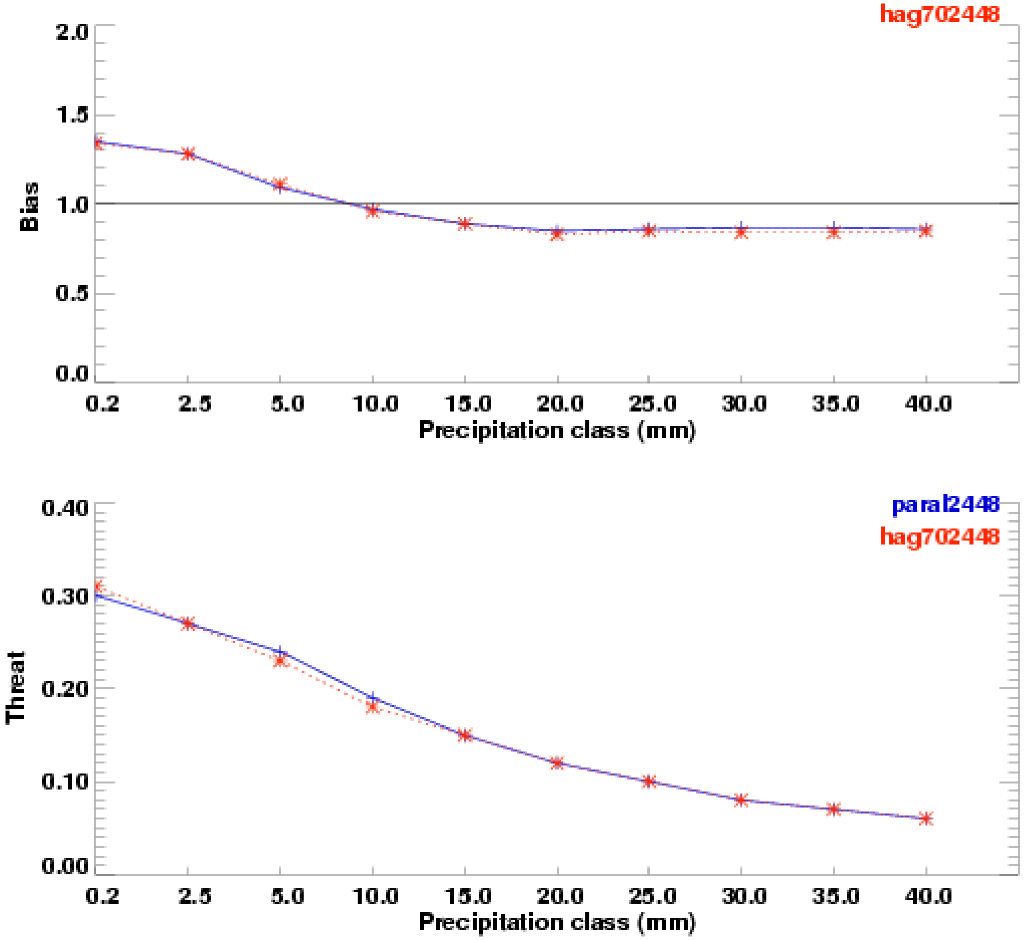

O-P 48 hr
UU
UV
GZ
TT
ES
% conf. BIAIS
% conf. VARIANCE
(m/s)
(dam)
(degree)
Summer 2007
EQM m_uaua_paral_048_moyenne (24)
BIAIS m_uaua_paral_048_moyenne
EQM m_uaua_aag70_048_moyenne (24)
BIAIS m_uaua_aag70_048_moyenne
Type : O-P 48 hr
Region : Amerique du Nord plus
Lat-lon: (25N, 170W) (85N, 40W)
Stat. inversees


O-P 48 hr
UU
UV
GZ
TT
ES
% conf. BIAIS
% conf. VARIANCE
(m/s)
(dam)
(degree)
Winter 2008
EQM m_uaua_parallel_048_moyenne (24)
BIAIS m_uaua_parallel_048_moyenne
EQM m_uaua_ach_048_moyenne (24)
BIAIS m_uaua_ach_048_moyenne
Type : O-P 48 hr
Region : Amerique du Nord plus
Lat-lon: (25N, 170W) (85N, 40W)
Stat. inversees

24 hours precipitation forecast verification against observation

SHEF network data for valid time 12z
24 to 48 hours forecast fm 12Z run only All of USA
12 cas ete 2007

Summer 2007



Number of observation

22321	13545	10783	6820	4634	3303	2344	1752	1354	1039
22321	13545	10783	6820	4634	3303	2344	1752	1354	1039

24 hours precipitation forecast verification against observa

SHEF network data for valid time 12z
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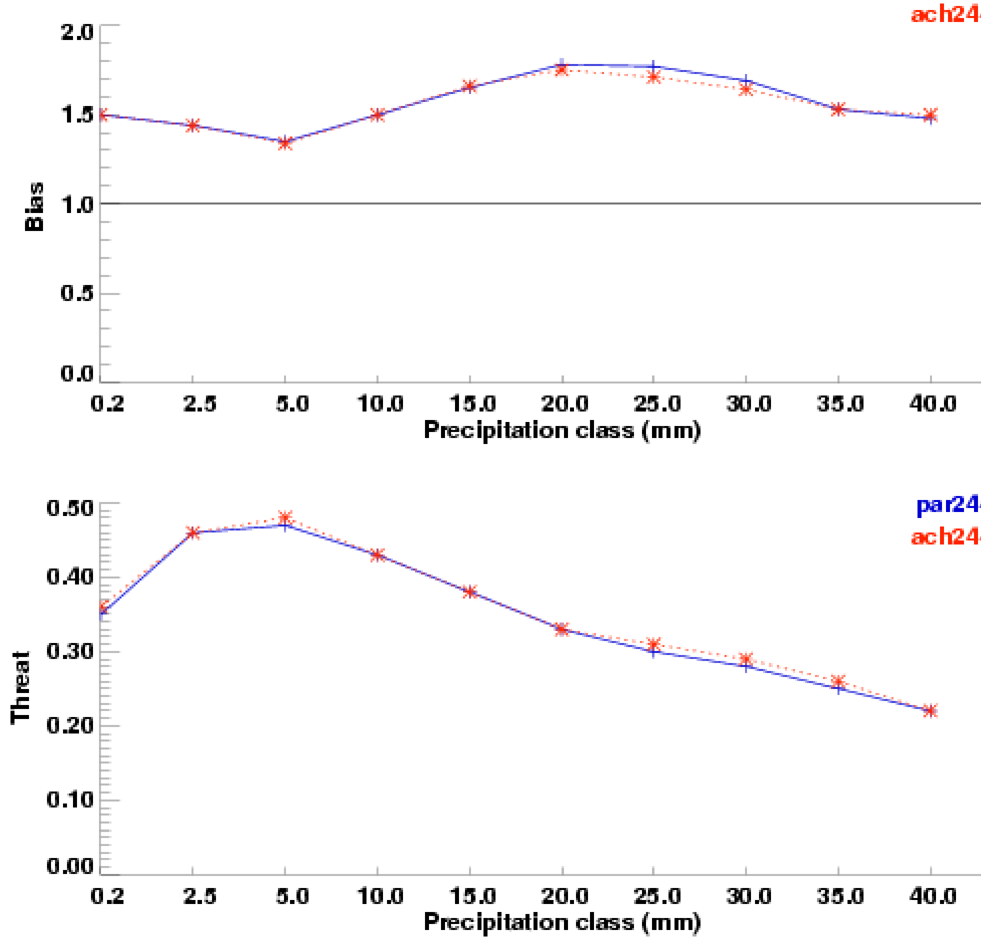
Winter 2008

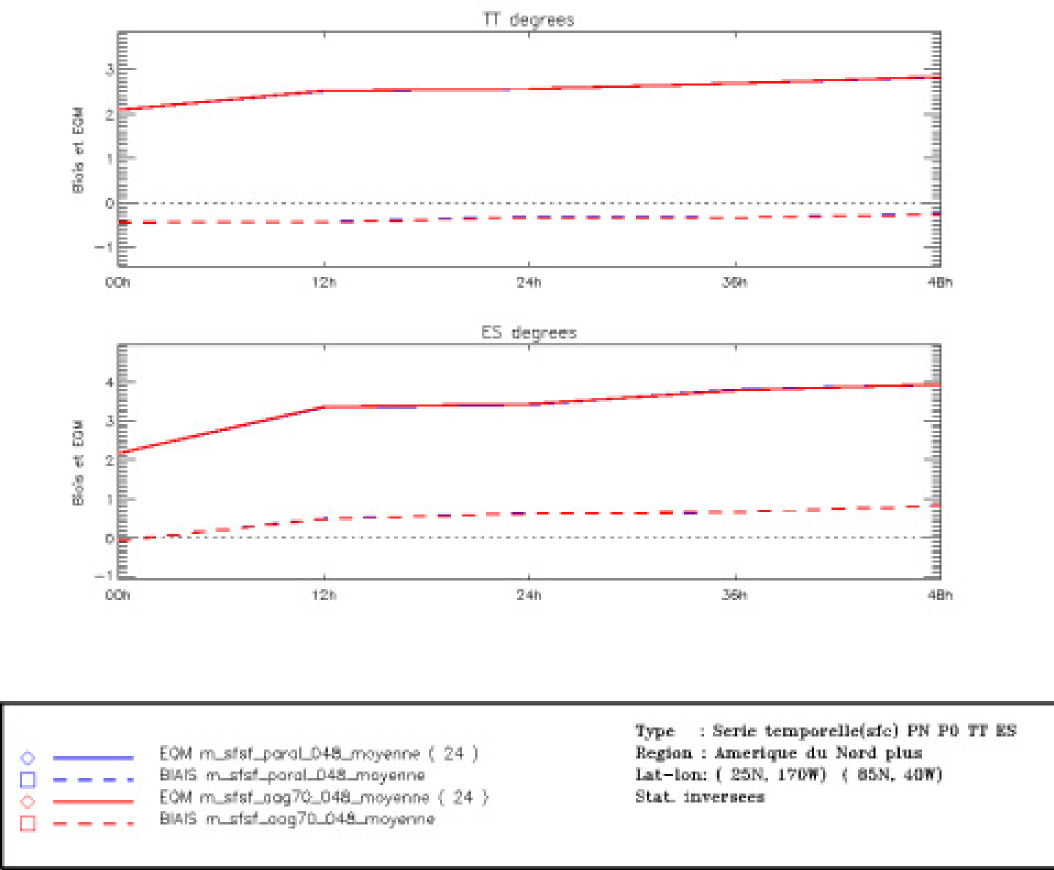


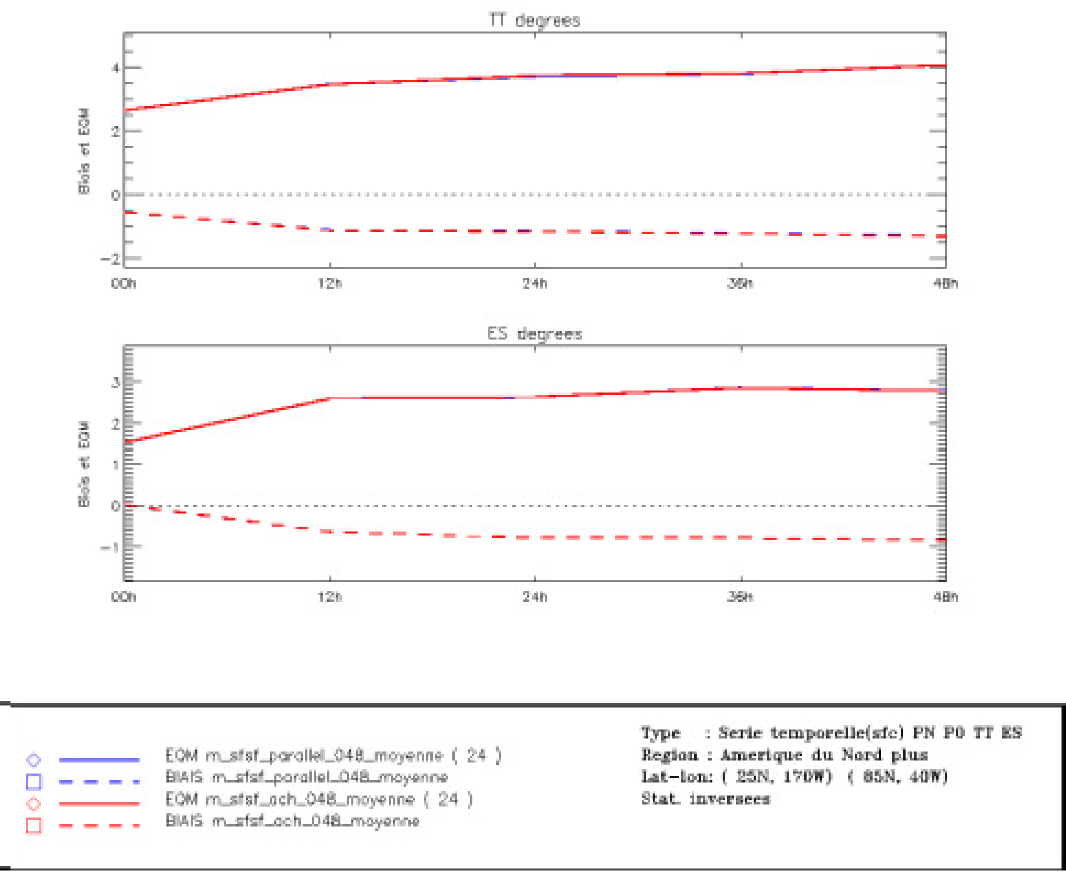
Number of observation

33035	19418	15424	9217	5910	3820	2551	1715	1257	87
33035	19418	15424	9217	5910	3820	2551	1715	1257	87

Summer 2007

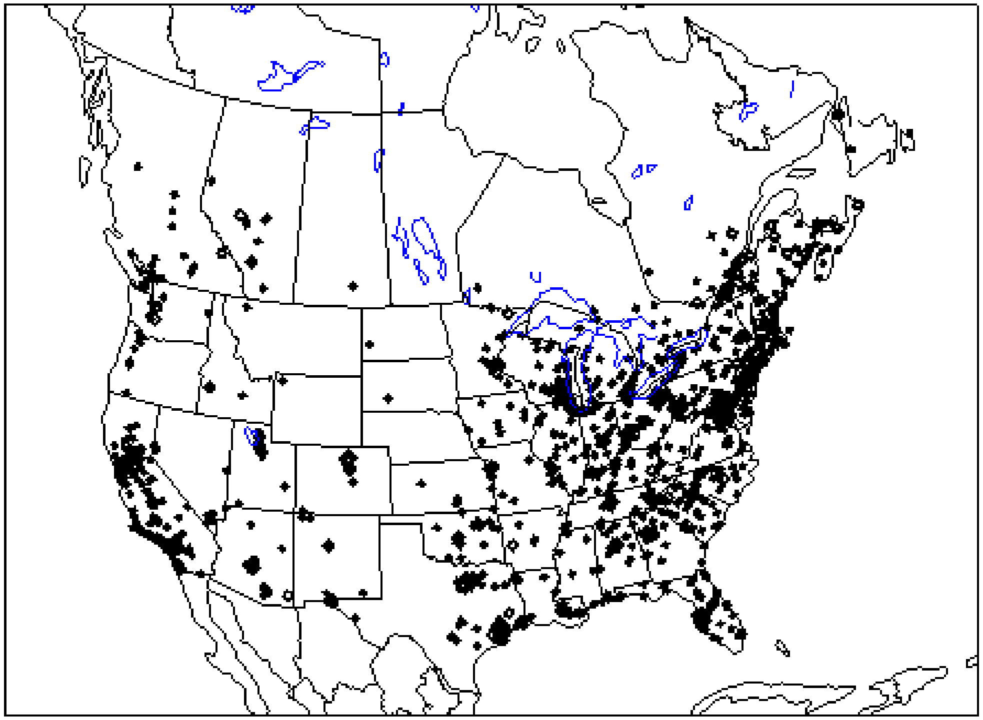
Winter 2008





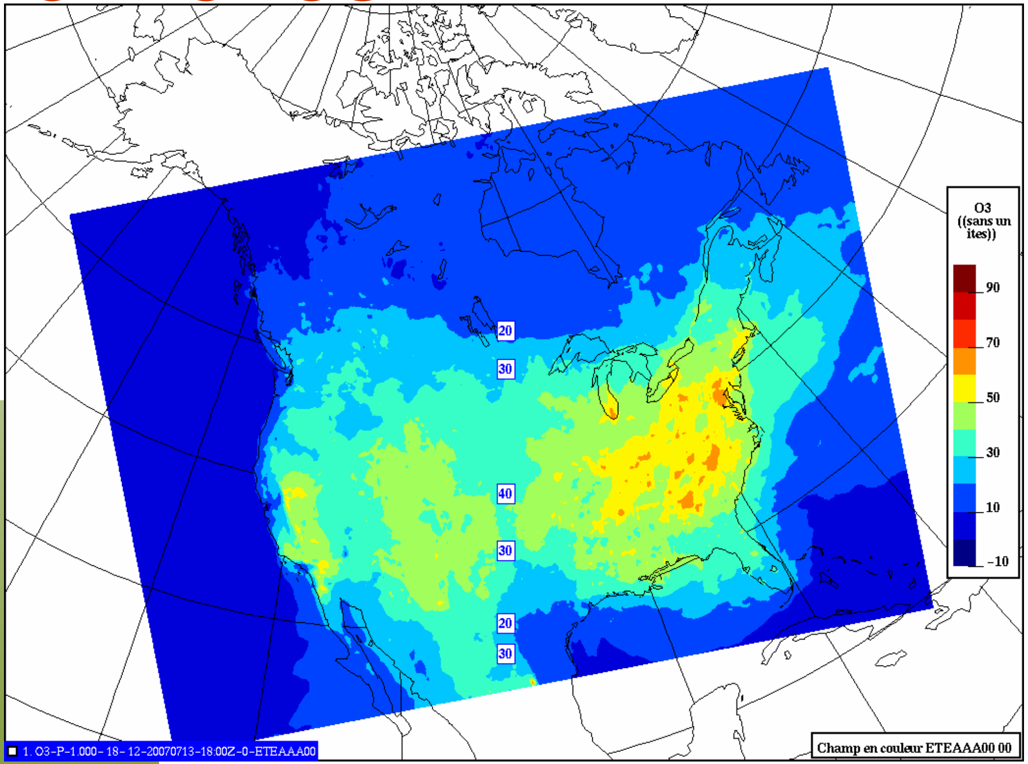
Model Evaluation: Ozone (O_3)

- Results are compared to observations over the whole North American continent for day 1 and day 2 forecasts
  - 1,124 stations in summer
  - 568 stations in winter (some stations shut down in winter)
- Observation network coverage (summer)

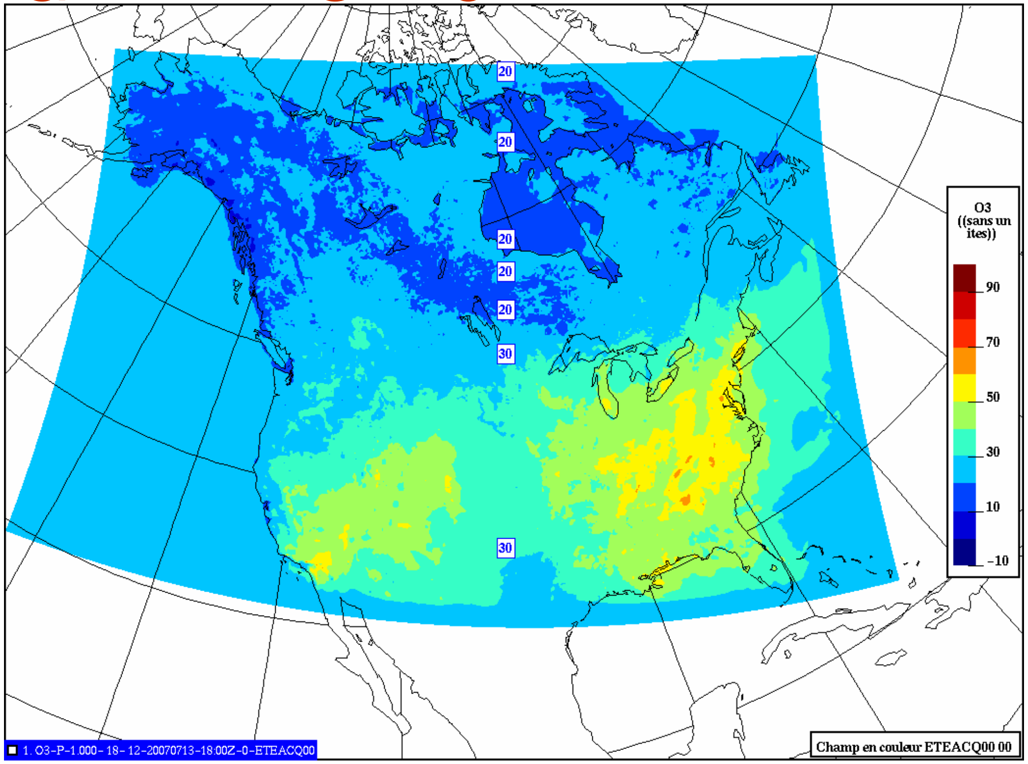


Ozone Forecast Comparison For Summer

CHRONOS

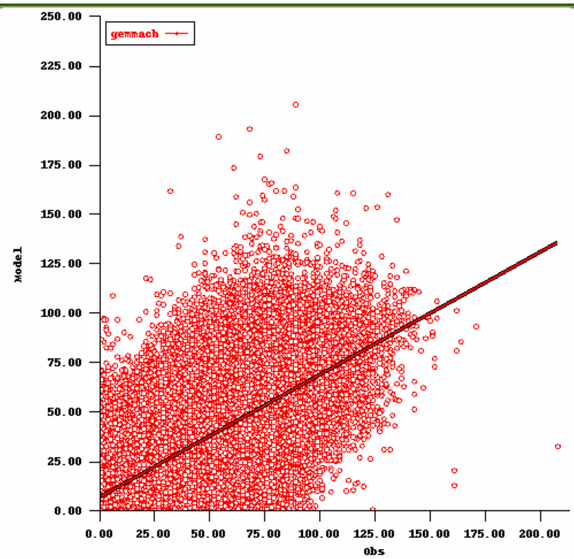


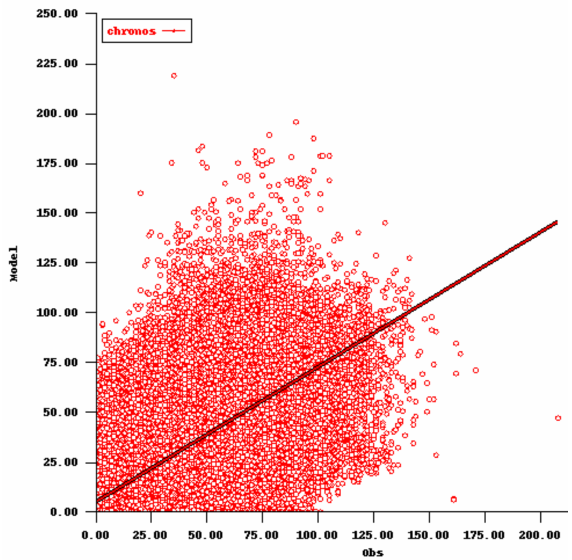
GEM-MACH15



Average ozone pattern of all 12 18-h forecasts from 00 UTC model runs from 2007-06-08 to 2007-07-13

Ozone Verification For Summer





GEM-MACH15

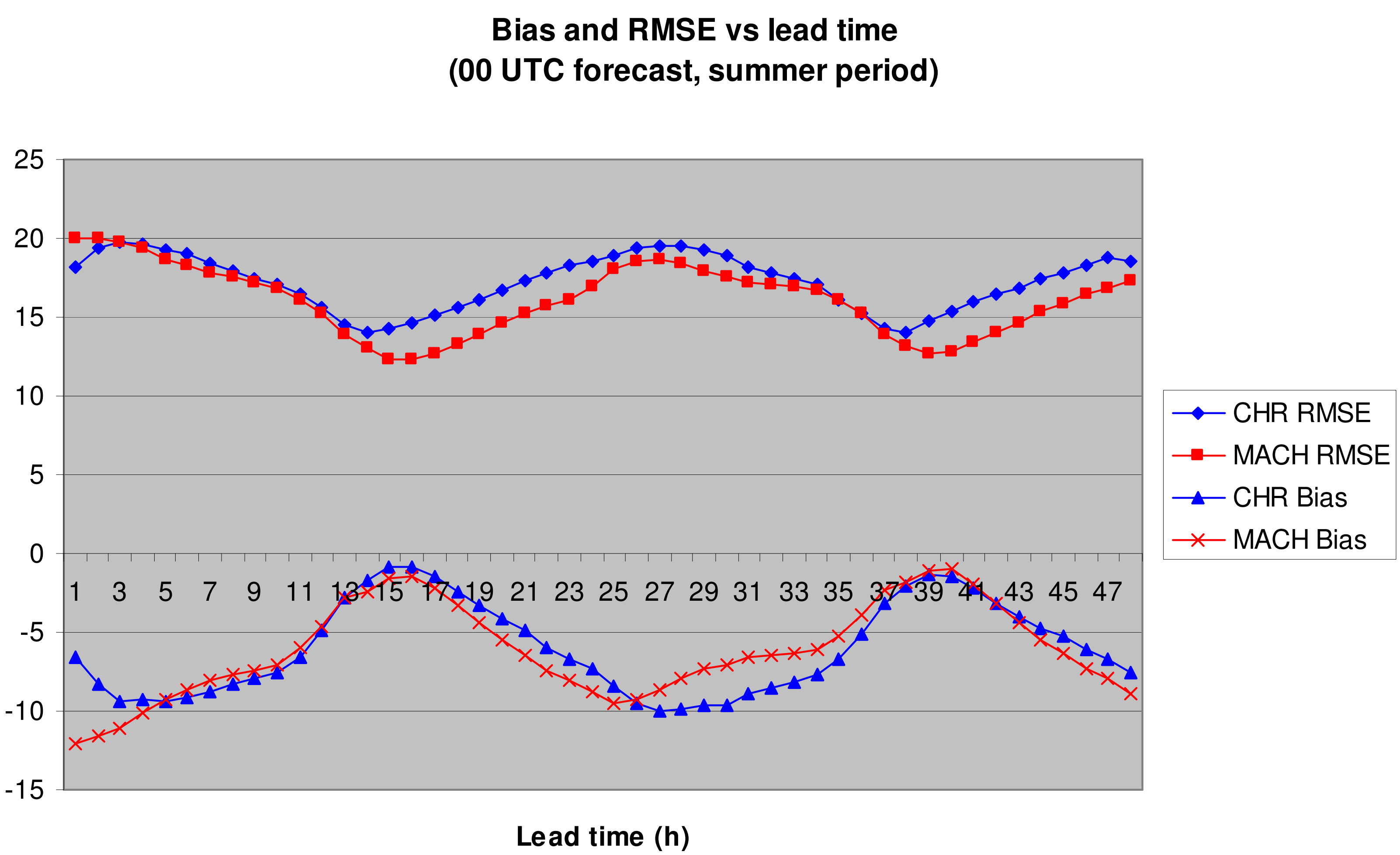
	All	Day 1	Day 2
R^2	0.46	0.47	0.46
Bias	-6.12	-6.17	-6.07
RMSE	16.21	16.16	16.25

24 48h forecasts (00 and 12 UTC)
(2007-06-08 to 2007-07-13)

CHRONOS

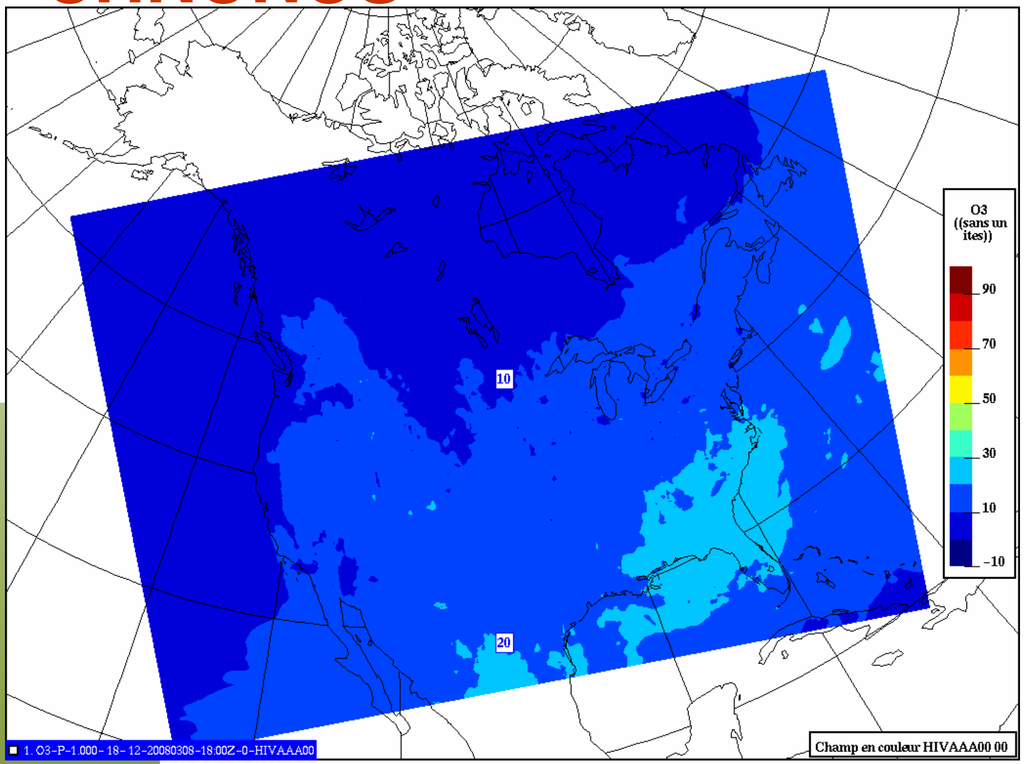
	All	Day 1	Day 2
R^2	0.44	0.45	0.44
Bias	-6.19	-6.09	-6.29
RMSE	17.26	17.19	17.32

Ozone Verification:
Diurnal cycle (summer 00 UTC runs)

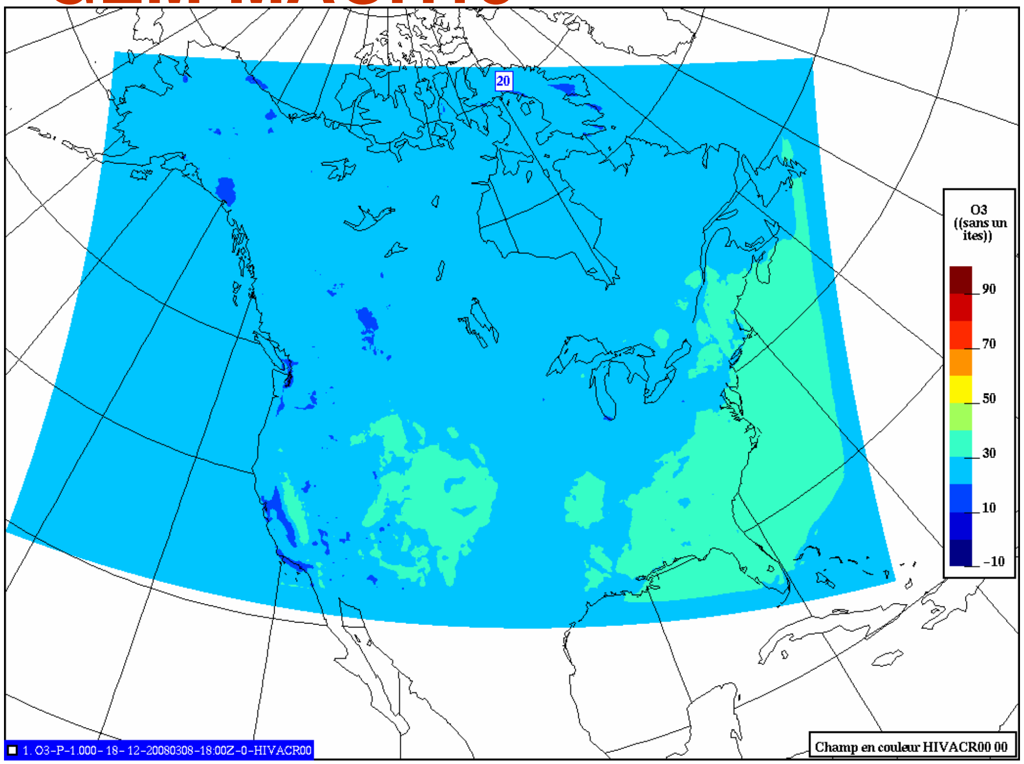


Ozone Forecast Comparison For Winter

CHRONOS

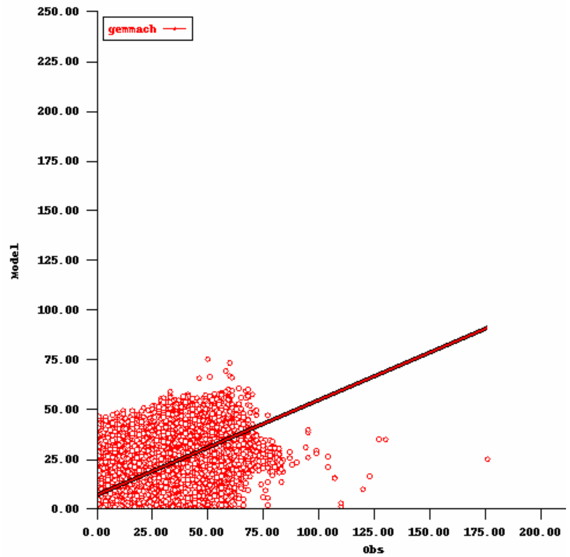


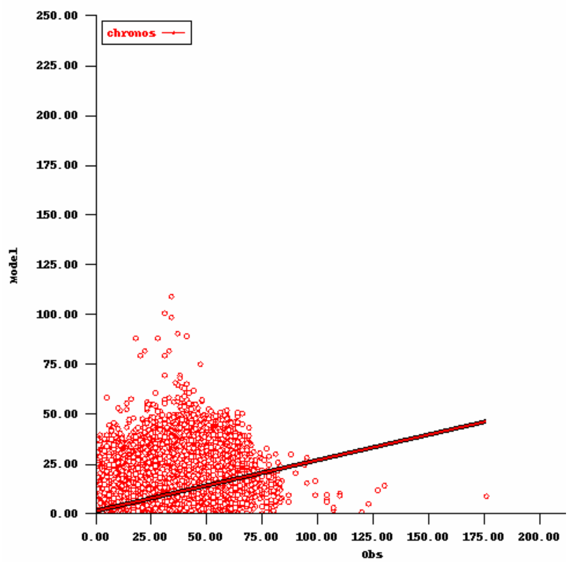
GEM-MACH15



Average ozone pattern of all 12 18-h forecasts from 00 UTC model runs from 2008-02-02 to 2008-03-08

Ozone Verification For Winter





GEM-MACH15

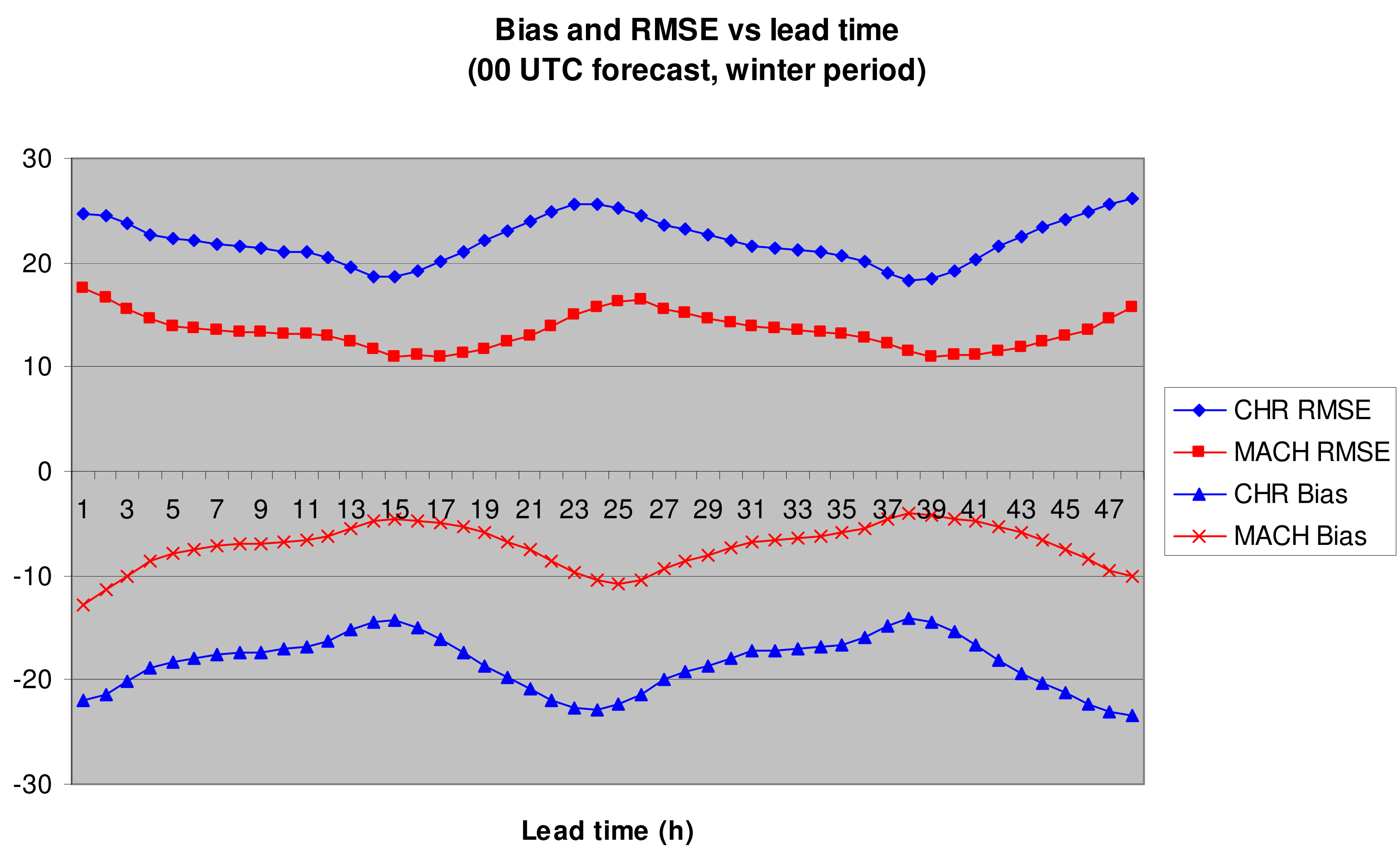
	All	Day 1	Day 2
R^2	0.35	0.37	0.34
Bias	-7.08	-7.24	-6.91
RMSE	13.45	13.40	13.50

24 48h forecasts (00 and 12 UTC)
(2008-02-02 to 2008-03-08)

CHRONOS

	All	Day 1	Day 2
R^2	0.21	0.22	0.20
Bias	-18.39	-18.31	-18.48
RMSE	22.12	21.98	22.26

Ozone Verification:
Diurnal cycle (winter 00 UTC runs)



Summary and Conclusions (1)

- GEM-MACH, a new air-quality forecast model embedded in GEM, has been developed jointly by AQRD, AQMAS, & RPN
- The in-line structure of GEM-MACH has some technical advantages over the current CMC operational AQ forecast model (CHRONOS)
- The GEM-MACH framework offers a flexible long-term upgrade path, can also be used with other chemistry mechanisms and species sets, and is more suitable for chemical data assimilation

Summary and Conclusions (2)

- One configuration, GEM-MACH15, uses a LAM grid congruent with the interior of the regional GEM15 model's core mesh and piloted hourly by the GEM15 forecast
- A version of GEM-MACH15 with full photochemistry has been evaluated for meteorological and ozone forecasts; evaluation is beginning on an advanced version of GEM-MACH15 with PM chemistry
- GEM-MACH15 meteorological performance is equivalent to GEM15; GEM-MACH15 performance for O_3 is comparable to CHRONOS in the summer and better in the winter

Next Steps

- CPOP proposal for gas-phase chemistry experimental run over the summer
  - Forecast ozone over the summer
    - Get feedback from meteorologists
    - Evaluation with A&P and the regions this summer
  - Preparation for implementation is on-going
- Prepare for parallel run of full model this fall
- Objective is to be ready to implement operationally before summer 2009
- Link GEM-MACH15 with UMOS-AQ

Merci pour votre attention!