Development of a multiscale online atmospheric-chemistry model: from global to regional experiments

Oriol Jorba
Earth Sciences Department
Barcelona Supercomputing Center


RES Earth Sciences Seminar, Barcelona, May 28, 2014
The Earth Sciences Department is devoted to the development and implementation of regional and global state-of-the-art models for air quality, meteorology and climate applications.
Towards modeling the Earth System

Development and implementation of regional and global state-of-the-art models for air quality, meteorology and climate applications.

Providing forecast products for research and end-users.
Development of Unified Meteorology/Air Quality/Climate model
- Towards global high-resolution system for global to local assessments

- Extending NMMB/BSC-CTM from coarse regional scales to global high-resolution configurations
- Extending short-term applications to climate scales

International collaborations:

Meteorology
NCEP
National Centers for Environmental Predictions

Climate
Global aerosols
NASA
Goddard Institute Space Studies

Air Quality
Uni. of California Irvine
nmmb/bsc chemical transport model
NMMB/BSC-Chemical Transport Model (Overview)

- fully on-line access coupling: feedback processes allowed
- multiscale: global to regional scales allowed

**Nonhydrostatic Multiscale Model on the B-grid (NMMB)**

*meteo variables/parameters*

**BSC Chemical Transport Model**

*(gas/aerosol variables: mass mixing ratios)*

→ Janjic and Gall (NCAR/TN 2012)
→ Janjic and Vasic (EGU2012)
→ Janjic et al. (MWR 2011)
→ (…)

**GAS-PHASE CHEM**

(52 species)

→ Jorba et al. (JGR 2012)
→ Badia and Jorba (AE 2014)

**DUST**

(8 bins)

→ Pérez et al. (ACP 2011)
→ Haustein et al. (ACP 2012)
→ Spada et al. (ACP 2013)

**SEA-SALT**
Resolving the full compressible primitive equations:

- **Mass conservation**

- **Momentum conservation**

- **Energy conservation**

- **Moisture conservation**

- **Gas – aerosol conservation**
Unified nonhydrostatic dynamical core (list of features is not exhaustive)

- Wide range of spatial and temporal scales (from meso to global)
- Regional and global domains (just a simple switch), nesting capabilities (1-way, 2-way, moving nest)
- Evolutionary approach, built on NWP experience by relaxing hydrostatic approximation
  - Favorable features of the hydrostatic formulation preserved
- The nonhydrostatic option as an add–on nonhydrostatic module
- No problems with weak stability on mesoscales
- Conservation of important properties of the continuous system
- Arakawa B grid (in contrast to the WRF-NMM E grid)
- Pressure-sigma hybrid
- Improved tracer advection: Eulerian, positive definite, mass conservative and monotonic
- NMMB regional became the next-generation NCEP mesoscale model for operational weather forecasting in 2011
NMNM/BSC-Chemical Transport Model

Mineral Dust module – NMNM/BSC-Dust (Pérez et al., 2011; Haustein et al., 2012)
- Evolution of the BSC-DREAM8b model (Nickovic et al., 2001; Pérez et al., 2006)
- Implementation of all common on-line dust modules for global and regional simulations
- Current DREAM dust emission scheme upgraded to a physically based scheme (explicitly accounting for saltation and sandblasting)
- New high resolution database for soil textures and vegetation fraction
- Direct radiative effect implemented

Gas phase chemistry (Jorba et al., 2012)
- Integrated implementation within NMNM – chemistry solved after NMNM physics
- Consistent advection and diffusion schemes with meteorology
- Feedback interactions aerosols-photolysis allowed
- Processes implemented online: emission, chemistry, dry and wet deposition each time-step. Online biogenic emissions from MEGAN

Global relevant aerosol module (Spada et al., 2013)
- Complementing NMNM/BSC-DUST mineral dust aerosols
- Same numerics like dust implementation
- Inclusion of Sea Salt, BC, OC and sulfate
- Implementation of feedbacks forseen
Chemistry processes and model characteristics

### Meteorology

**NMMB**  
(Janjic and Gall, 2012)

### Chemical Mechanism

**CB05**  
(Yarwood et al., 2005)

### Photolysis scheme

**Fast-J**  
(Wild et al., 2010)

### Aerosols

**Dust + SSA**  
(Pérez et al., 2011; Spada et al., 2013)

No secondary aerosols

### Dry deposition

Wesely et al. (1986) gas, Pérez et al. (2011) aerosols

### Wet deposition

Foley et al. (2010) gas, Zhang et al. (2001) aerosols

### Direct effect

Mineral dust

---

### Table: Base Constants and Reaction Numbers

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Base Constant, $k^2$</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Reaction Number} )</td>
<td>( \Delta H )</td>
<td></td>
</tr>
<tr>
<td>(1) ( \text{NO}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 5.9 \times 10^{-11} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(11) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 7.3 \times 10^{-11} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(23) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 9.5 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(26) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 1.2 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(29) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 1.5 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(32) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 1.8 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(33) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 2.1 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(34) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 2.4 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(35) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 2.7 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(36) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 3.0 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(37) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 3.3 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(38) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 3.6 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(39) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 3.9 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(40) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 4.2 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(41) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 4.5 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(42) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 4.8 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(43) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 5.1 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(44) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 5.4 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(45) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 5.7 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
<tr>
<td>(46) ( \text{H}_2 \text{O}<em>2 \oplus \text{h}</em>\oplus \text{O}_3 \oplus \text{NO}_3 \oplus \text{O}_3 )</td>
<td>( 6.0 \times 10^{-10} \text{exp} )</td>
<td></td>
</tr>
</tbody>
</table>
SEA SALT AEROSOL MODULE
The sea-salt module (Spada et al., 2013)

→ emission of ssa aerosol depends on surface wind speed and SST

→ aerosol module extended to wet aerosol

\[ r_d \rightarrow r_w = r_d \cdot \Phi(RH) \]

\[ \rho_d \rightarrow \rho_w = \rho_d \Phi^{-3} + (1-\Phi^{-3})\rho_{\text{water}} \]
SEA-SALT AOD500nm

STD-GLOB(L)

sea-salt AOD500nm
01-01-2006 00:00 +00H
Impact of resolution (Spada et al., submitted)

- GLOB(L) and GLOB(H) resolutions seem to give quite similar results, although...

→ at smaller scales (REG = 0.1 x 0.1) the model becomes able to resolve steep topographies

→ in these cases (such as for the New Zealand domain), the observed SCONC climatologies are reproduced

→ obvious but not trivial: smaller scales (≈0.1deg) effects may affect larger scales (>1deg)
GAS-PHASE MODULE
→ Global domain
→ Non-hydrostatic physics
→ 1.4° x 1° horizontal resolution
→ 64 vertical (sigma-hybrid) layers
→ 1° x 1° NCEP/FNL analysis for meteorological initial conditions
→ Chemistry initial conditions from MOZART
→ Anthropogenic emissions: ACCMIP
→ Biogenic emissions: MEGAN online model
→ No lightning emissions
→ 1 year year spin-up
→ 2004 simulation
Ozone atmospheric column (Badia et al., under preparation)

Satellite comparison: SCIAMACHY and HALOE

- COPCAT (Monge-Sanz et al., 2011) linear model for stratospheric ozone
- Coupled with the tropospheric mechanism of the CTM
Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes

Comparison with Ozonesondes
NO$_2$ Vertical Tropospheric Column
CO at 800 hPa: comparison with MOPITT (v5)

- Strong overestimations over fire regions.
- Good agreement over polluted areas.
- Need to implement attenuation of radiation due to aerosols in photolysis scheme.
Regional Experiment configuration – AQMEII-Phase2

**Period:** Run one year simulation (2010).

**Domain:** European simulations: 30W- 60E, 25N-70N

**Chemical BC:** MACC (IFS-MOZART)

**Meteorological BC:** NCEP/FNL 1ºx1º

**Emissions:** TNO-MACC; Biogenics: MEGAN; No Fire Emissions

** Horizontal Resolution:** 0.2º x 0.2º

**Vertical Resolution:** 24 (and 48) top 50hPa

**Gas Chemical mechanism:** CB05

**Aerosols:** only dust-ssa

Blue: model domain
Red: AQMEII domain (to submit)
Green: BC domain
Regional run results (Badia and Jorba, 2014)
O$_3$ vertical profiles for each EU station at:
0, 100, 250, 500, 750, 1000, 1500, 2000, 3000, 4000, 5000, 6000, 7500, 8500, 10000, 12000, 15000, 18000 m
Comparison of modelled NO\textsubscript{2} VTC against satellite data (OMI) for (from top) winter (DJF), spring (MAM), summer (JJA) and autumn (SON)

- Capturing higher NO\textsubscript{2} over the most polluted regions.
- **Over land**: Overestimate in big cities and underestimate in rural regions.
- **Over sea**: Overestimation in Mediterranean (Italy) and North seas – shipping emissions or stability of marine boundary layer?

(Badia and Jorba, 2014)
Comparison of modelled CO mixing ratio against satellite data (MOPITT) for (from top) winter (DJF), spring (MAM), summer (JJA) and autumn (SON)

- The pattern of emissions in central EU is well-captured. (Badia and Jorba, 2014)
- **Over land:** satellite evaluation confirms that there is a general trend to underestimate surface CO
- Summer underestimation due to no fires emissions (important fires in Russia and Portugal)
FUTURE WORK
Future Developments

- Coupling of chemistry gas-phase with a secondary aerosol scheme for LAM applications at high-resolutions.

- Implementation of the other global relevant aerosol species, i.e. black (BC) and organic carbon (OC), and sulfate (SO4), in addition to dust (DU) and sea salt (SSA). Implementation of a volcanic ash module (Fall3D model, Folch et al., 2008) within the modeling system.

- Implement effects of aerosols on meteorology

- Nesting capabilities among global-regional-local domains

- Explore methodologies for aerosol data assimilation
Providing forecast products for

- Mineral dust forecasts for SDS-WAS North Africa, Middle East and Europe portal

- Participate in the ICAP global-model intercomparison project

- Participate in the Charmex Chemistry-Aerosol Mediterranean experiment

- Participate in the AQMEII on-line Air Quality model intercomparison project
Barcelona Dust Forecast Center: http://dust.aemet.es/

First Specialized Center for Mineral Dust Prediction of the World Meteorological Organization

Numerical forecasts based on the NMMB/BSC-CTM model developed at BSC
Thank you!

oriol.jorba@bsc.es

Work partially funded by grants CGL2006-11879, CGL2008-02818, CGL2010-19652, CSD00C-06-08924 and Severo-Ochoa grant of the Spanish Government

www.bsc.es/earth-sciences
Main model framework

- The Nonhydrostatic Multiscale Meteorological Model on the B grid (NMMB)
- Developed at National Centers for Environmental Prediction (NCEP)

Multiscale (global to regional) and Nonhydrostatic (up to 1km² horizontal resolution)