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Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

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

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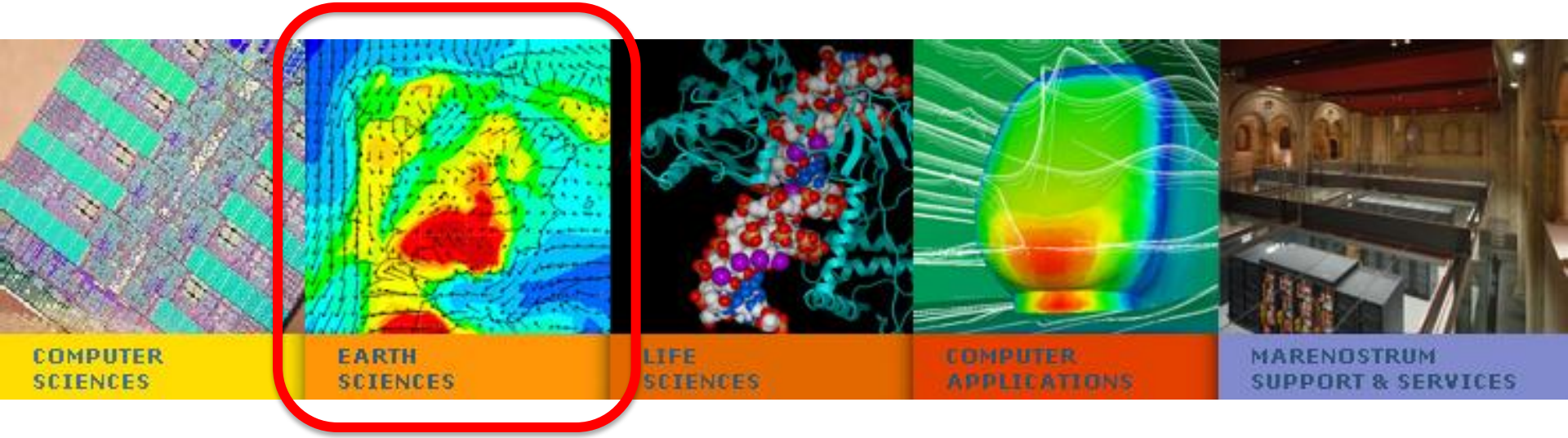
Acknowledgments: Z. Janjic, T. Black, C. Pérez, S. Basart, A. Badia, M. Spada, J.M. Baldasano, D. Dabdub, K. Haustein, M. Carreras, K. Serradell, F. Benicasa

RES Earth Sciences Seminar, Barcelona, May 28, 2014

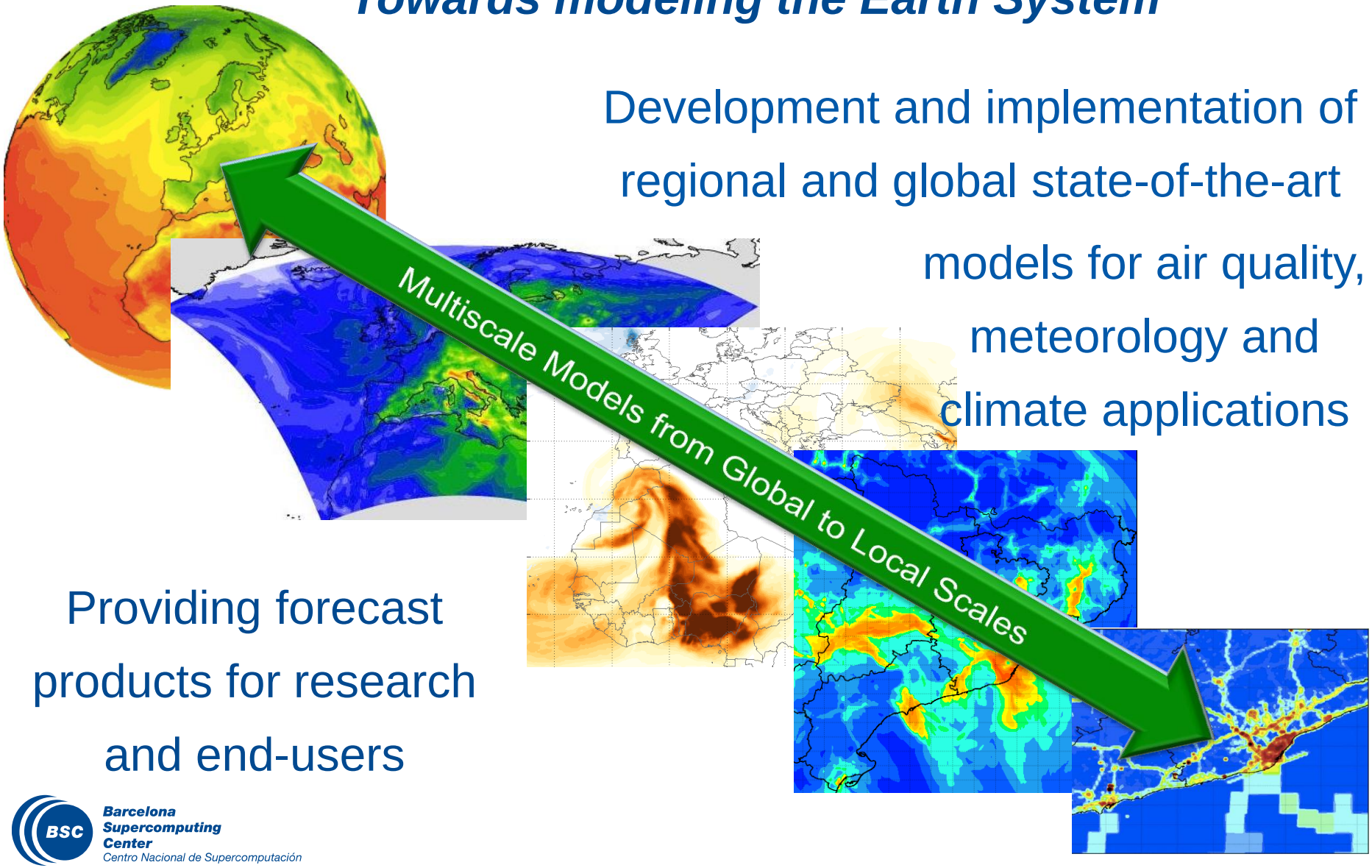
BSC Departments



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

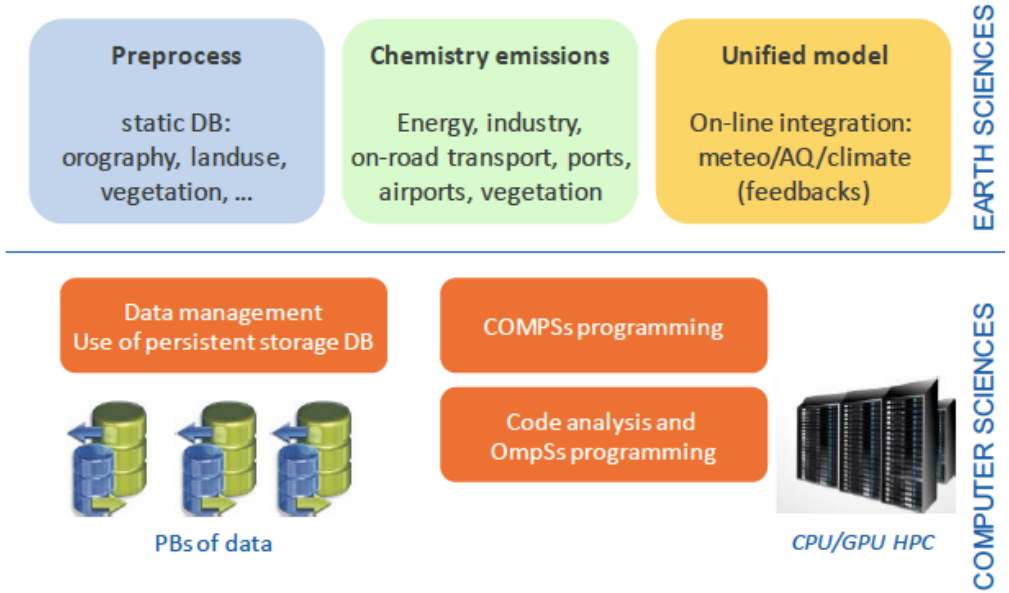
Development and implementation of regional and global state-of-the-art models for air quality, meteorology and climate applications



Providing forecast products for research and end-users

Severo-Ochoa Earth Sciences Application

- 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

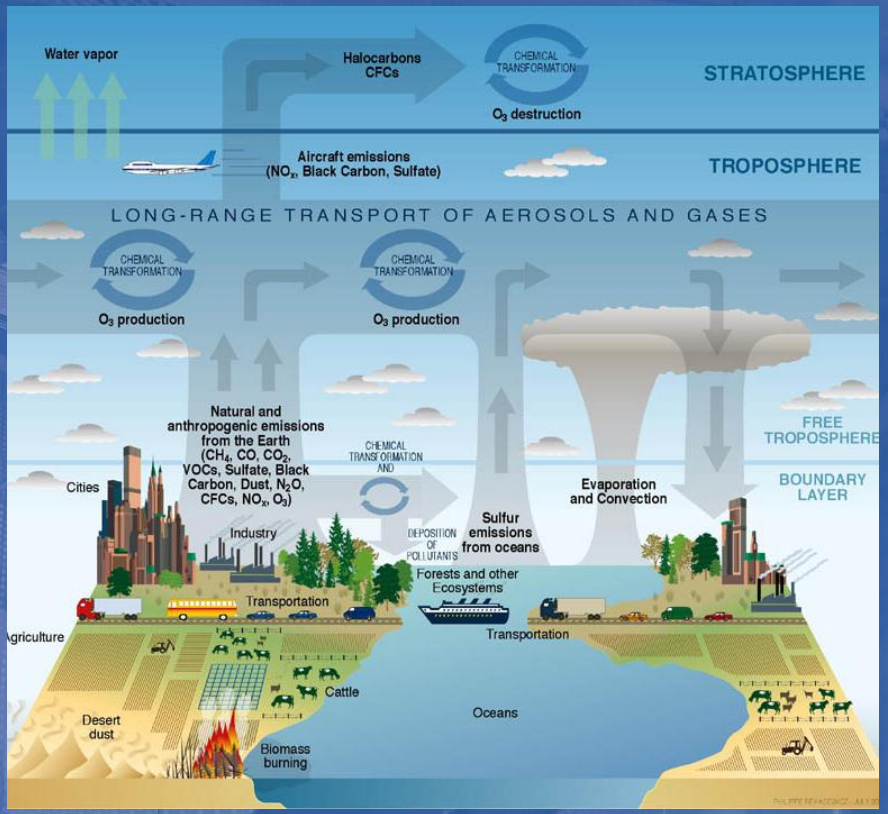
National Centers for Environmental Predictions

Climate
Global aerosols

Goddard Institute Space Studies

Air Quality

Uni. of California Irvine



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NMMB/BSC CHEMICAL TRANSPORT MODEL

NMMB/BSC-Chemical Transport Model (Overview)

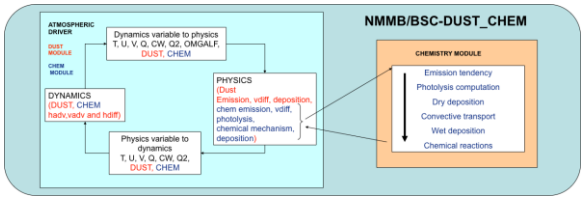
- fully on-line access coupling: feedback processes allowed
- multiscale: global to regional scales allowed

NMMB/ BSC-CTM

Nonhydrostatic Multiscale Model on the B-grid (NMMB)

meteo variables/parameters

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



BSC Chemical Transport Model

(gas/aerosol variables: mass mixing ratios)

GAS-PHASE CHEM (52 species)

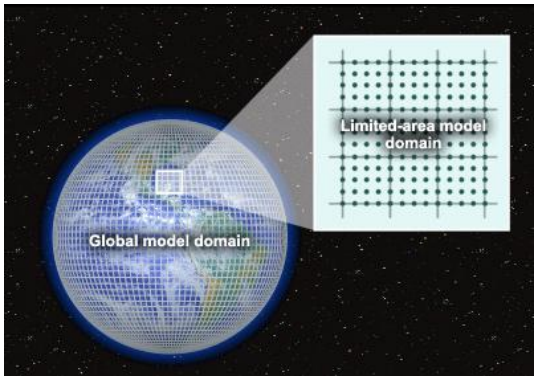
→ Jorba et al. (JGR 2012)
→ Badia and Jorba (AE 2014)

DUST (8 bins)

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

SEA-SALT

→ Spada et al. (ACP 2013)



Model equations

METEOROLOGY CHEMISTRY ON-LINE INTERACTIONS TAKEN INTO CONSIDERATION BY NMMB/BSC-CTM MODEL AND ITS FUTURE DEVELOPMENTS

$$\partial_t Q_{i,j} + (\vec{v}\cdot\vec{\nabla}) Q_{i,j} = \sum_k \frac{dQ_{i,j}}{dt}(u^*, \vec{q}_w, \vec{c}_g, \ldots)\Big|_{aero,k}$$

$$\partial_t \rho_{d,a} + \vec{\nabla}(\rho_{d,a}\vec{v}) = 0$$

$$\partial_t \vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v} = -f\vec{k}\times\vec{v} - \vec{\nabla}\Phi - \frac{1}{\rho_a}\vec{\nabla}p + \frac{d\vec{v}}{dt}\Big|_{turb}$$

$$\partial_t T + (\vec{v}\cdot\vec{\nabla})T = \sum_k \frac{dT}{dt}(I_\lambda, \ldots)\Big|_{diab,k} + \frac{dT}{dt}\Big|_{turb}$$

$$\partial_t q_{w,\eta} + (\vec{v}\cdot\vec{\nabla})q_{w,\eta} = \sum_k \frac{dq_{w,\eta}}{dt}\Big|_{water,k}$$

$$p\alpha = RT$$

$$\partial_t c_{g,\gamma} + (\vec{v}\cdot\vec{\nabla})c_{g,\gamma} = \frac{dc_{g,\gamma}}{dt}(\vec{c}_g, I_\lambda, \ldots)\Big|_{photochem,k} + \ldots$$

$$\frac{dI_\lambda}{dt} = f(I_\lambda, \tau_\lambda^{aero}, \omega_\lambda^{aero}, g_\lambda^{aero}, \ldots)$$

Radiative Transfer Eq.

Resolving the full compressible primitive equations:

Mass conservation

Momentum conservation

Energy conservation

Moisture conservation

Gas – aerosol conservation

NMMB – Nonhydrostatic Multiscale Model on the B grid – Main characteristics
Under development at NCEP (Janjic, 2005; Janjic et al., 2011; Janjic and Gall, 2012)

Unified nonhydrostatic dynamical core (list of features is not exhaustive)

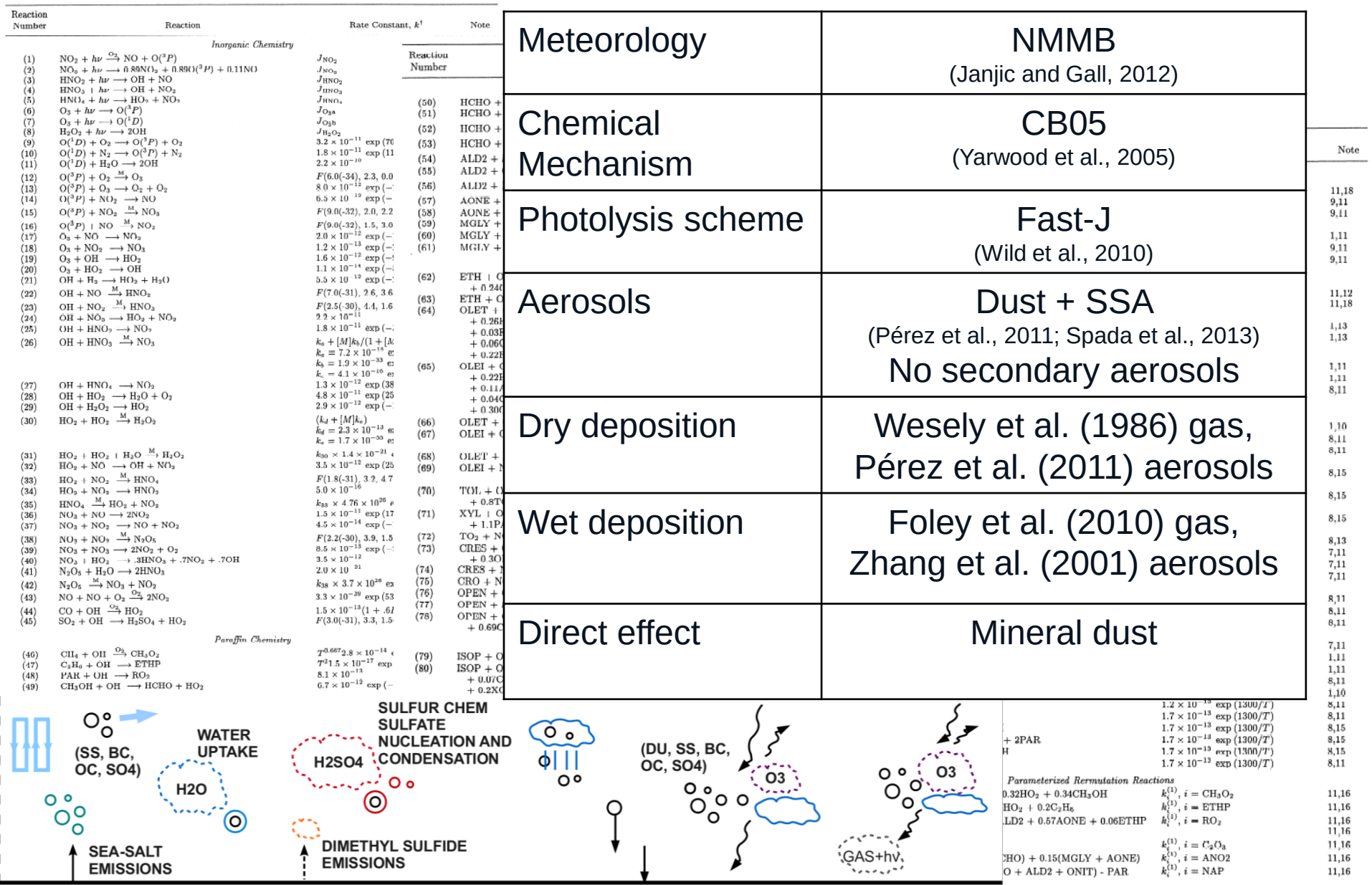
- ✓ Wide range of spatial and temporal scales (from meso to global)
- ✓ Regional and global domains (just a simple switch), nesting capabilities (1-way, 2-way, moving nest)
- ✓ Evolutionary approach,built on NWP experience by relaxing hydrostatic approximation
  - ➢Favorable features of the hydrostatic 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

NMMB/BSC-Chemical Transport Model

- Mineral Dust module – NMMB/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 NMMB – chemistry solved after NMMB 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 NMMB/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



Reaction Number	Reaction	Rate Constant, $k^{\dagger}$	Note
	Inorganic Chemistry		
(1)	$NO_2 + h\nu \xrightarrow{O_2} NO + O(^3P)$	J_{NO_2}	
(2)	$NO_3 + h\nu \longrightarrow 0.89NO_2 + 0.89O(^3P) + 0.11NO$	J_{NO_3}	
(3)	$HNO_2 + h\nu \longrightarrow OH + NO$	J_{HNO_2}	
(4)	$HNO_3 + h\nu \longrightarrow OH + NO_2$	J_{HNO_3}	
(5)	$HNO_4 + h\nu \longrightarrow HO_2 + NO_2$	J_{HNO_4}	
(6)	$O_3 + h\nu \longrightarrow O(^3P)$	J_{O_3a}	
(7)	$O_3 + h\nu \longrightarrow O(^1D)$	J_{O_3b}	
(8)	$H_2O_2 + h\nu \longrightarrow 2OH$	$J_{H_2O_2}$	
(9)	$O(^1D) + O_2 \longrightarrow O(^3P) + O_2$	3.2×10^{-11} exp (70	
(10)	$O(^1D) + N_2 \longrightarrow O(^3P) + N_2$	1.8×10^{-11} exp (11	
(11)	$O(^1D) + H_2O \longrightarrow 2OH$	2.2×10^{-10}	
(12)	$O(^3P) + O_2 \xrightarrow{M} O_3$	$F(6.0(-34), 2.3, 0.0$	
(13)	$O(^3P) + O_3 \longrightarrow O_2 + O_2$	8.0×10^{-12} exp (−	
(14)	$O(^3P) + NO_2 \longrightarrow NO$	6.5×10^{-12} exp (−	
(15)	$O(^3P) + NO_2 \xrightarrow{M} NO_3$	$F(9.0(-32), 2.0, 2.2$	
(16)	$O(^3P) + NO \xrightarrow{M} NO_2$	$F(9.0(-32), 1.5, 3.0$	
(17)	$O_3 + NO \longrightarrow NO_2$	2.0×10^{-12} exp (−	
(18)	$O_3 + NO_2 \longrightarrow NO_3$	1.2×10^{-13} exp (−	
(19)	$O_3 + OH \longrightarrow HO_2$	1.6×10^{-12} exp (−	
(20)	$O_3 + HO_2 \longrightarrow OH$	1.1×10^{-14} exp (−	
(21)	$OH + H_2 \longrightarrow HO_2 + H_2O$	5.5×10^{-12} exp (−	
(22)	$OH + NO \xrightarrow{M} HNO_2$	$F(7.0(-31), 2.6, 3.6$	
(23)	$OH + NO_2 \xrightarrow{M} HNO_3$	$F(2.5(-30), 4.4, 1.6$	
(24)	$OH + NO_3 \longrightarrow HO_2 + NO_2$	2.2×10^{-11}	
(25)	$OH + HNO_3 \longrightarrow NO_3$	1.8×10^{-11} exp (−	
(26)	$OH + HNO_3 \xrightarrow{M} NO_3$	$k_a + [M]k_b/(1 + [M$	
		$k_a = 7.2 \times 10^{-15}$ ex	
		$k_b = 1.9 \times 10^{-33}$ ex	
		$k_c = 4.1 \times 10^{-16}$ ex	
(27)	$OH + HNO_4 \longrightarrow NO_2$	1.3×10^{-12} exp (38	
(28)	$OH + HO_2 \longrightarrow H_2O + O_2$	4.8×10^{-11} exp (25	
(29)	$OH + H_2O_2 \longrightarrow HO_2$	2.9×10^{-12} exp (−	
(30)	$HO_2 + HO_2 \xrightarrow{M} H_2O_2$	$(k_d + [M]k_e)$	
		$k_d = 2.3 \times 10^{-13}$ ex	
		$k_e = 1.7 \times 10^{-33}$ ex	
(31)	$HO_2 + HO_2 + H_2O \xrightarrow{M} H_2O_2$	$k_{30} \times 1.4 \times 10^{-21}$ e	
(32)	$HO_2 + NO \longrightarrow OH + NO_2$	3.5×10^{-12} exp (25	
(33)	$HO_2 + NO_2 \xrightarrow{M} HNO_4$	$F(1.8(-31), 3.2, 4.7$	
(34)	$HO_2 + NO_3 \longrightarrow HNO_3$	5.0×10^{-16}	
(35)	$HNO_4 \xrightarrow{M} HO_2 + NO_2$	$k_{33} \times 4.76 \times 10^{26}$ e	
(36)	$NO_3 + NO \longrightarrow 2NO_2$	1.5×10^{-11} exp (17	
(37)	$NO_3 + NO_2 \longrightarrow NO + NO_2$	4.5×10^{-14} exp (−	
(38)	$NO_3 + NO_3 \xrightarrow{M} N_2O_5$	$F(2.2(-30), 3.9, 1.5$	
(39)	$NO_3 + NO_3 \longrightarrow 2NO_2 + O_2$	8.5×10^{-13} exp (−	
(40)	$NO_3 + HO_2 \longrightarrow .3HNO_3 + .7NO_2 + .7OH$	3.5×10^{-12}	
(41)	$N_2O_5 + H_2O \longrightarrow 2HNO_3$	2.0×10^{-21}	
(42)	$N_2O_5 \xrightarrow{M} NO_3 + NO_2$	$k_{38} \times 3.7 \times 10^{26}$ ex	
(43)	$NO + NO + O_2 \xrightarrow{O_2} 2NO_2$	3.3×10^{-39} exp (53	
(44)	$CO + OH \xrightarrow{O_2} HO_2$	$1.5 \times 10^{-13}(1 + .6P$	
(45)	$SO_2 + OH \longrightarrow H_2SO_4 + HO_2$	$F(3.0(-31), 3.3, 1.5$	
	Paraffin Chemistry		
(46)	$CH_4 + OH \xrightarrow{O_2} CH_3O_2$	$T^{0.667}2.8 \times 10^{-14}$ e	
(47)	$C_2H_6 + OH \longrightarrow ETHP$	$T^{2}1.5 \times 10^{-17}$ exp	
(48)	$PAR + OH \longrightarrow RO_2$	8.1×10^{-13}	
(49)	$CH_3OH + OH \longrightarrow HCHO + HO_2$	0.7×10^{-12} exp (−	
(50)	HCHO +		
(51)	HCHO +		
(52)	HCHO +		
(53)	HCHO +		
(54)	ALD2 +		
(55)	ALD2 +		
(56)	ALD2 +		
(57)	AONE +		
(58)	AONE +		
(59)	MGLY +		
(60)	MGLY +		
(61)	MGLY +		
(62)	ETH + O + 0.24		
(63)	ETH + O		
(64)	OLET + + 0.26 + 0.03 + 0.06 + 0.22		
(65)	OLEI + + 0.22 + 0.11 + 0.04 + 0.30		
(66)	OLET +		
(67)	OLEI +		
(68)	OLET +		
(69)	OLEI +		
(70)	TOL + + 0.8T		
(71)	XYL + O + 1.1P		
(72)	$TO_2 + N$		
(73)	CRES + + 0.3O		
(74)	CRES +		
(75)	CRO + N		
(76)	OPEN +		
(77)	OPEN +		
(78)	OPEN + + 0.69		
(79)	ISOP + O		
(80)	ISOP + O + 0.07 + 0.2X		
	+ 2PAR	1.2×10^{-13} exp (1300/T)	8,11
	H	1.7×10^{-13} exp (1300/T)	8,11
		1.7×10^{-13} exp (1300/T)	8,15
		1.7×10^{-13} exp (1300/T)	8,15
		1.7×10^{-13} exp (1300/T)	8,15
		1.7×10^{-13} exp (1300/T)	8,11
	Parameterized Permutation Reactions		
	$0.32HO_2 + 0.34CH_3OH$	$k_i^{(1)}$, $i = CH_3O_2$	11,16
	$HO_2 + 0.2C_2H_6$	$k_i^{(1)}$, $i = ETHP$	11,16
	LD2 + 0.57AONE + 0.06ETHP	$k_i^{(1)}$, $i = RO_2$	11,16
		$k_i^{(1)}$, $i = C_2O_3$	11,16
	HO) + 0.15(MGLY + AONE)	$k_i^{(1)}$, $i = ANO2$	11,16
	O + ALD2 + ONIT) - PAR	$k_i^{(1)}$, $i = NAP$	11,16

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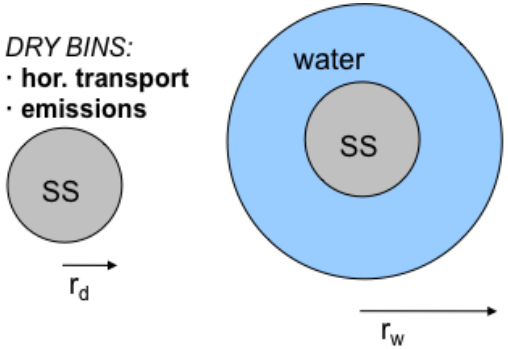
SEA SALT AEROSOL MODULE

The sea-salt module (Spada et al., 2013)

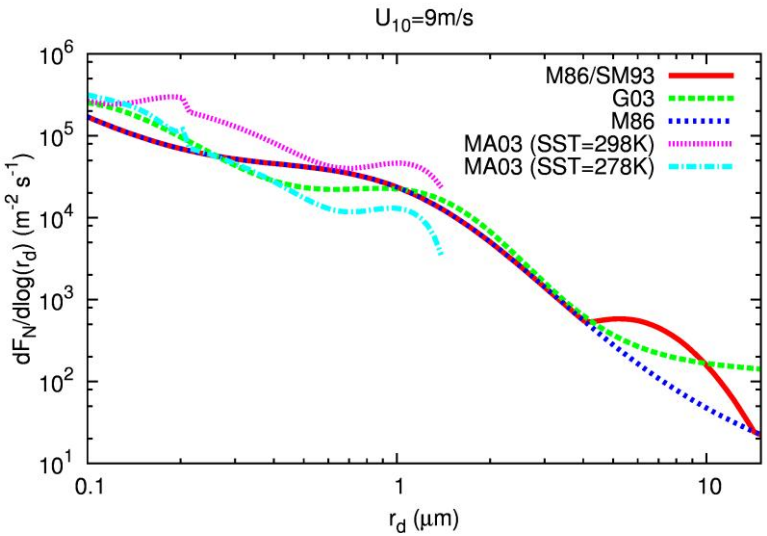
→ emission of ssa aerosol depends on surface wind speed and SST

→ aerosol module extended to wet aerosol



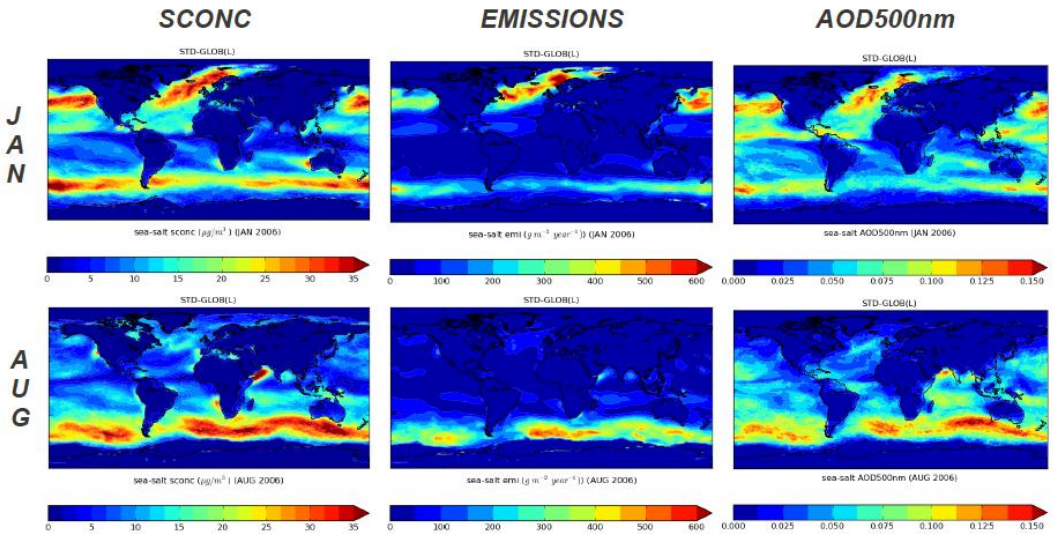
$$r_d \rightarrow r_w = r_d \cdot \Phi(RH)$$

$$\rho_d \rightarrow \rho_w = \rho_d \Phi^{-3} + (1-\Phi^{-3})\rho_{water}$$

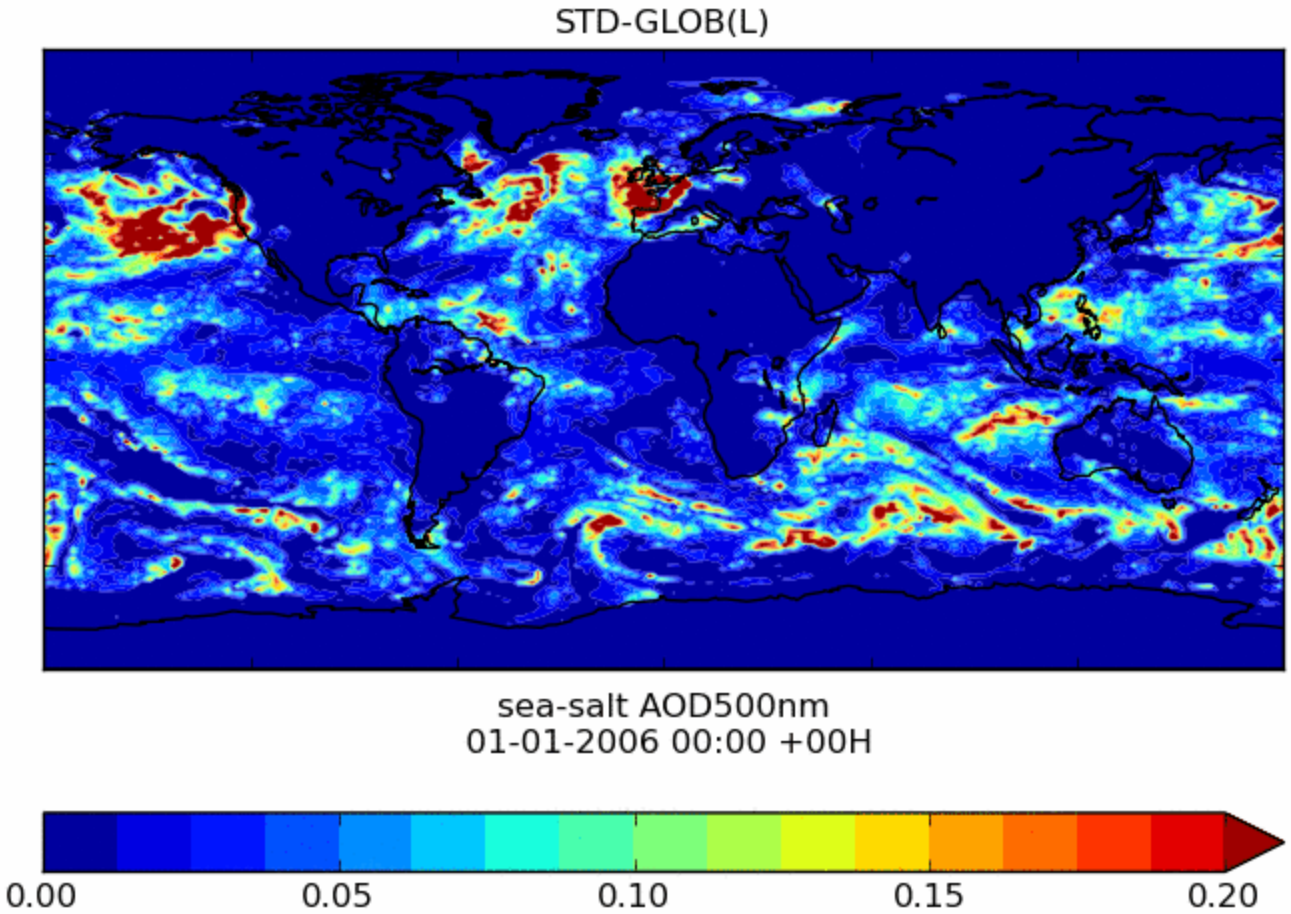


→ NMMB/BSC-CTM, ref year 2006
· emi total: 7307.8 Tg/y
· load: 6.6 Tg
· lifetime 9.56h

– AEROCOM median, year 2000
· emi total: 6212.3 Tg/y
· load: 6.1 Tg
· lifetime 8.64h

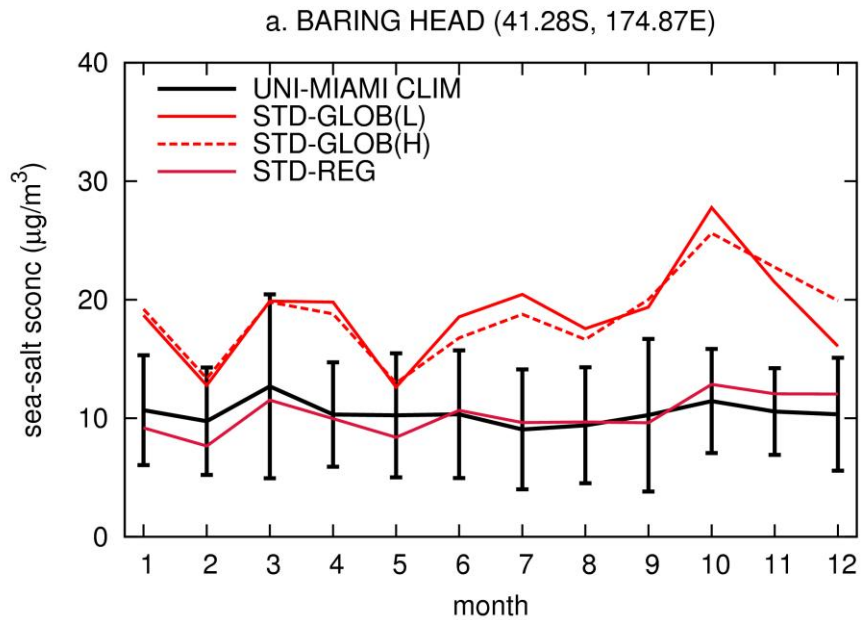


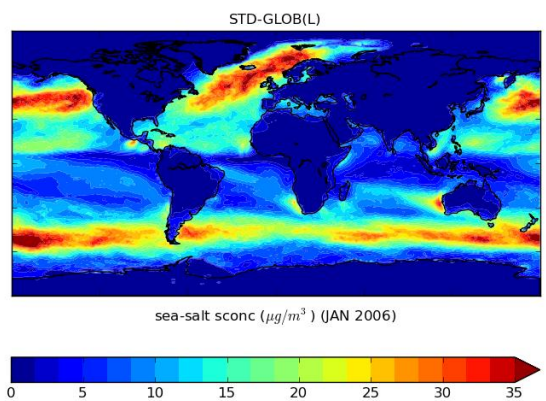
SEA-SALT AOD500nm

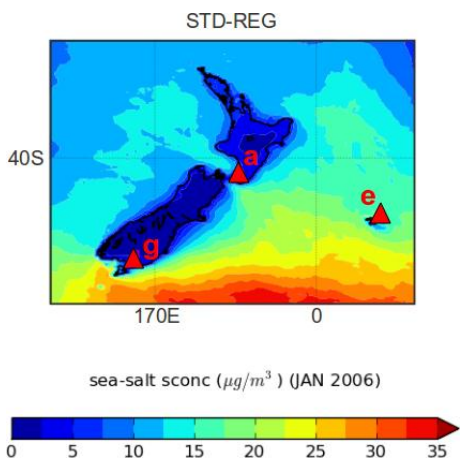


Impact of resolution (Spada et al., submitted)

· 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)

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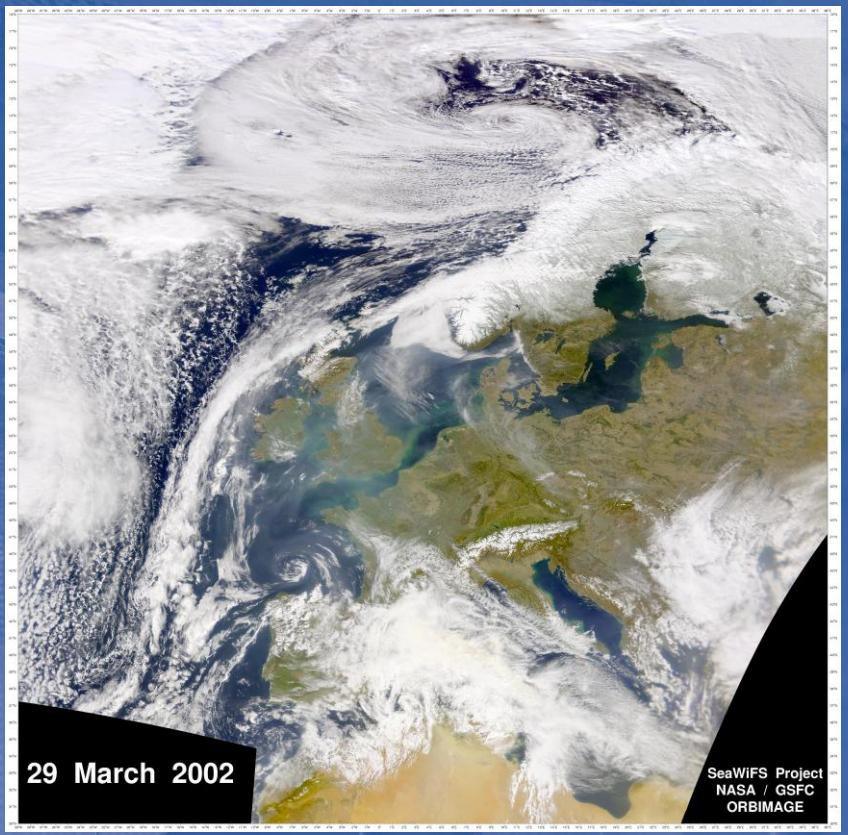
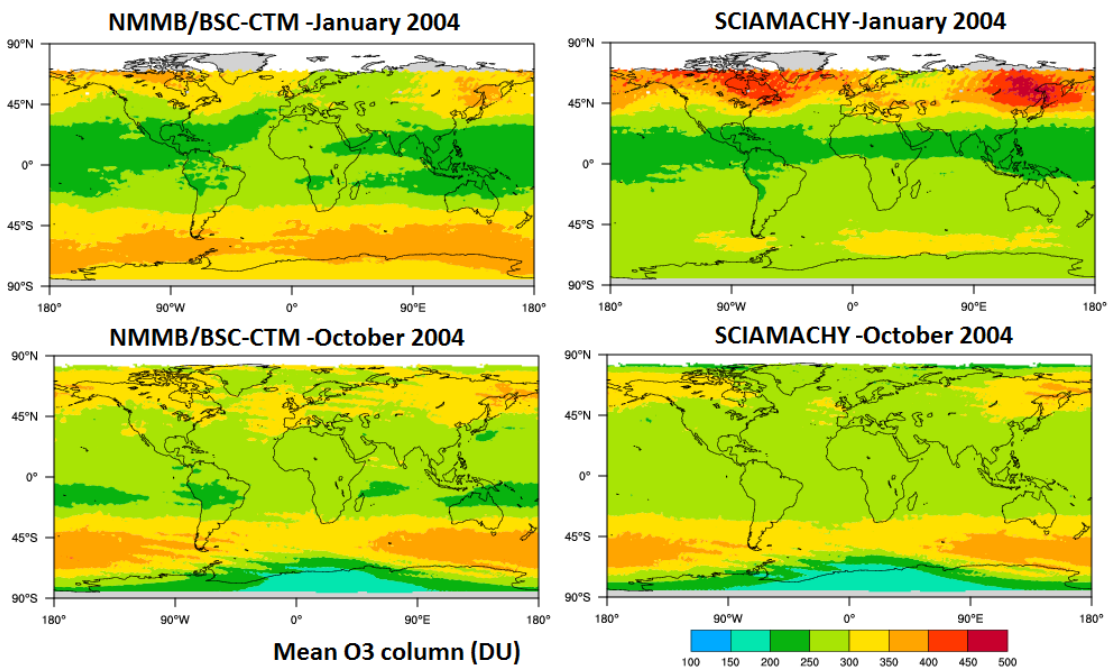


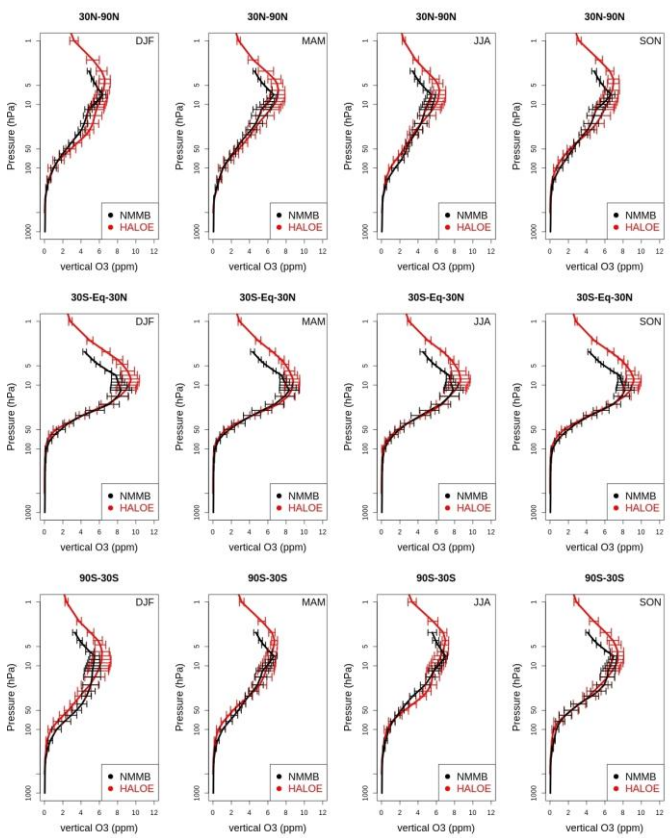
GAS-PHASE MODULE

Model setup

- → Global domain
- → Non-hydrostatic physics
- → 1.4º x 1º horizontal resolution
- → 64 vertical (sigma-hybrid) layers
- → 1º x 1º 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)

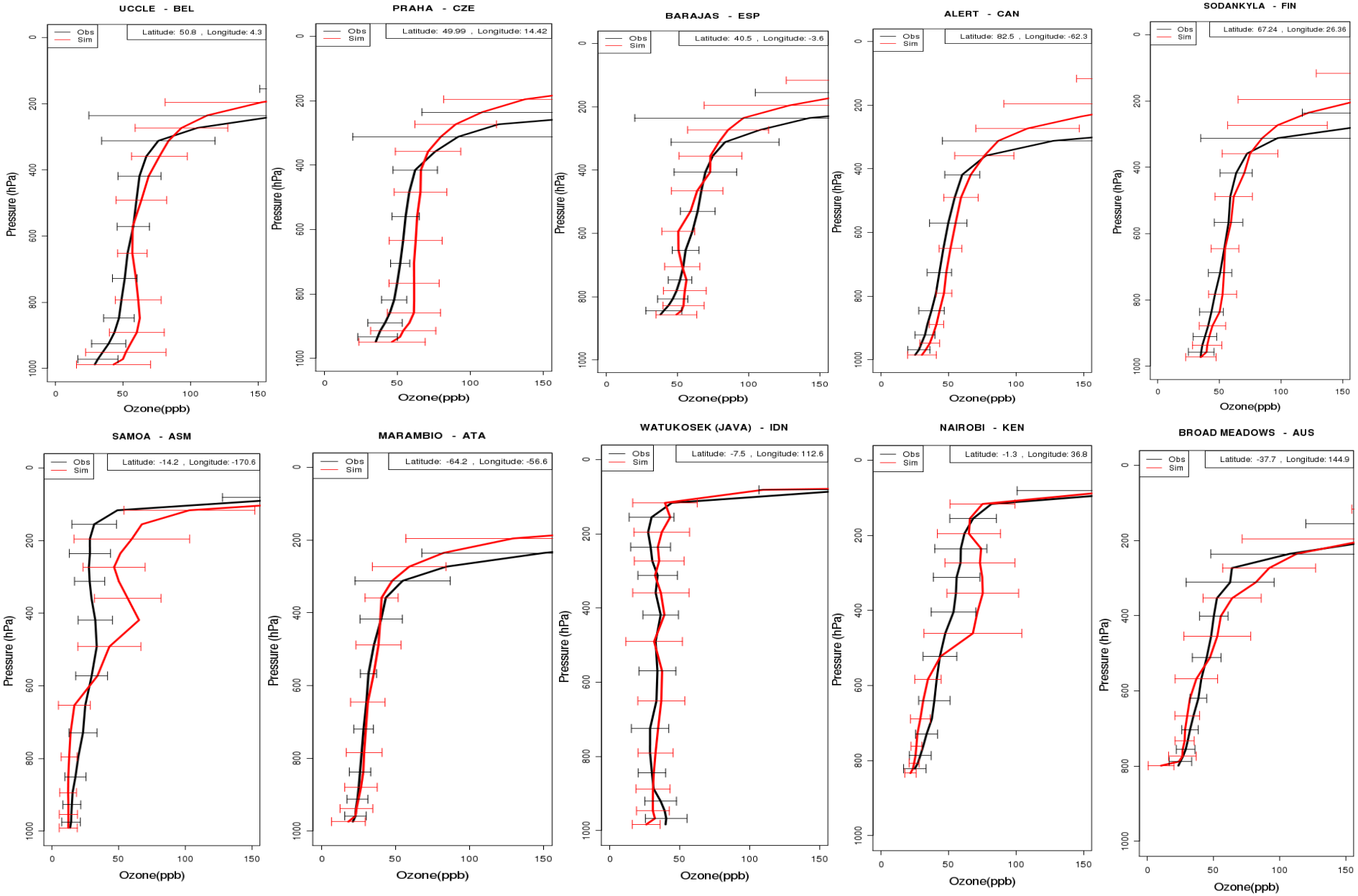




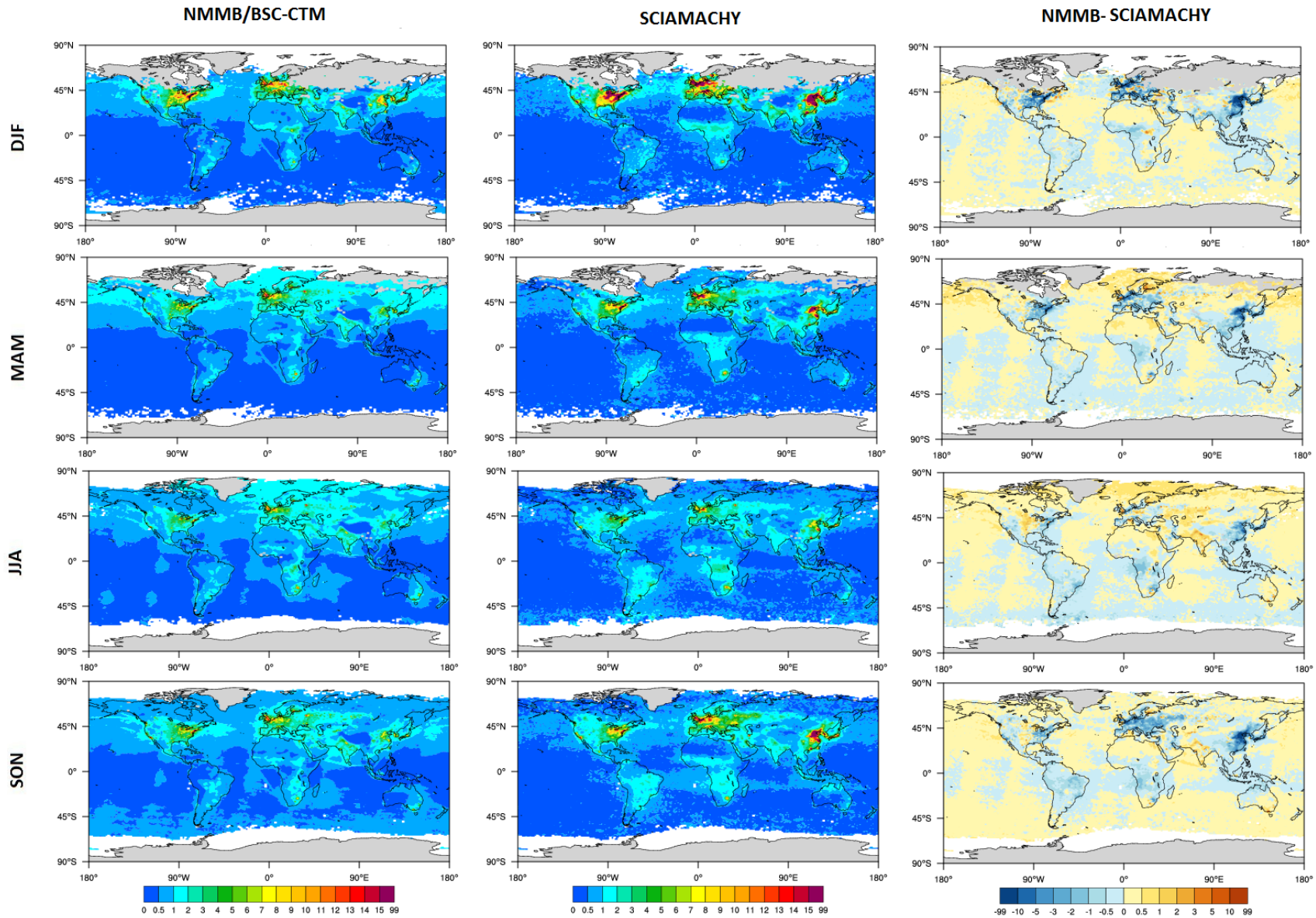
Satellite comparison: SCIAMACHY and HALOE

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

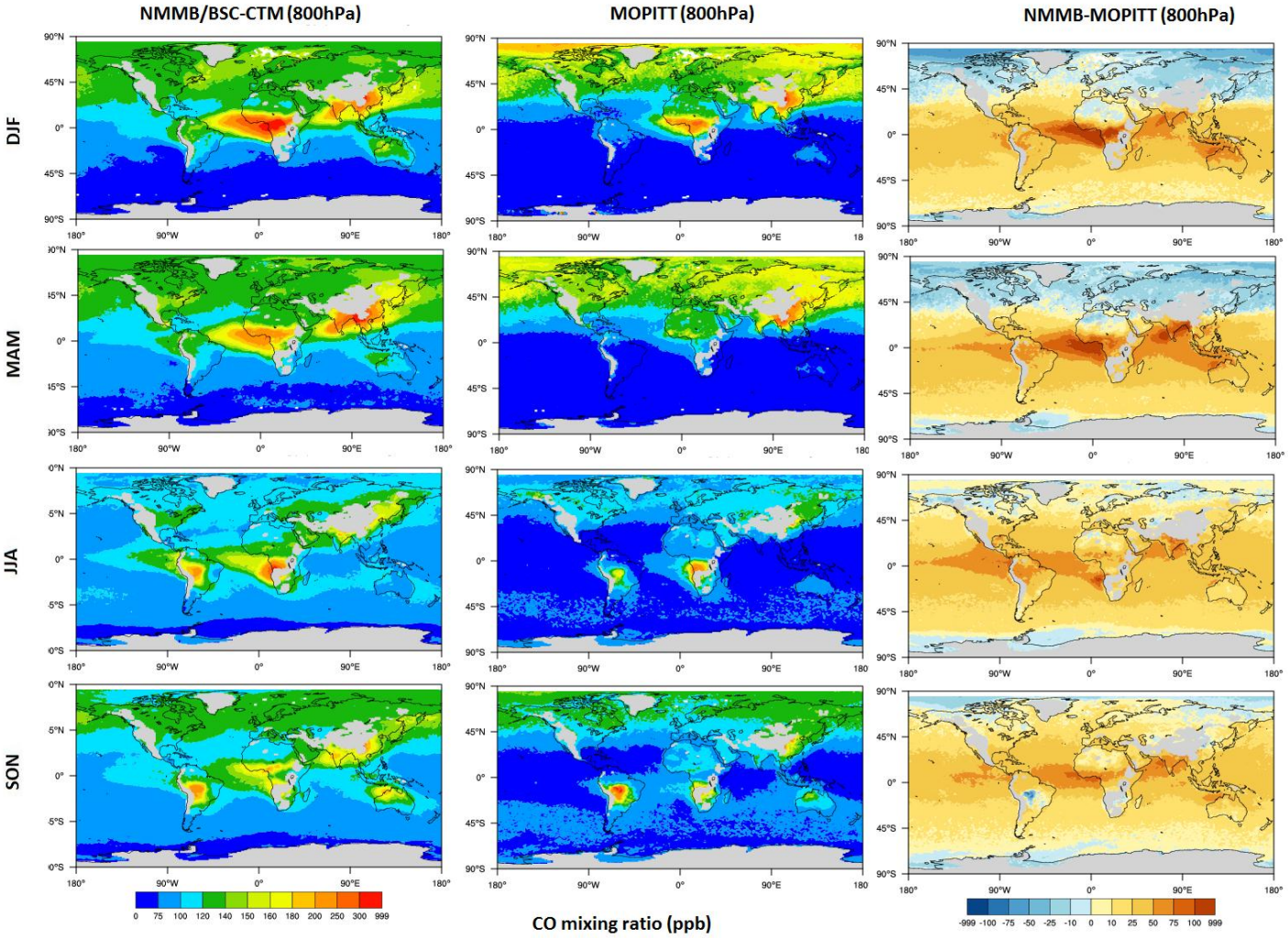
Comparison with Ozonesondes



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

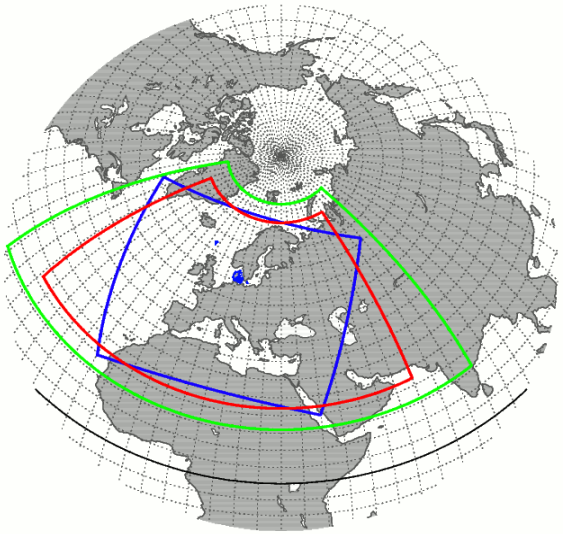
Emissions: TNO-MACC; Biogenics: MEGAN; No Fire Emissions

Horizontal Resolution: 0.2º x 0.2º

Vertical Resolution: 24 (and 48) top 50hPa

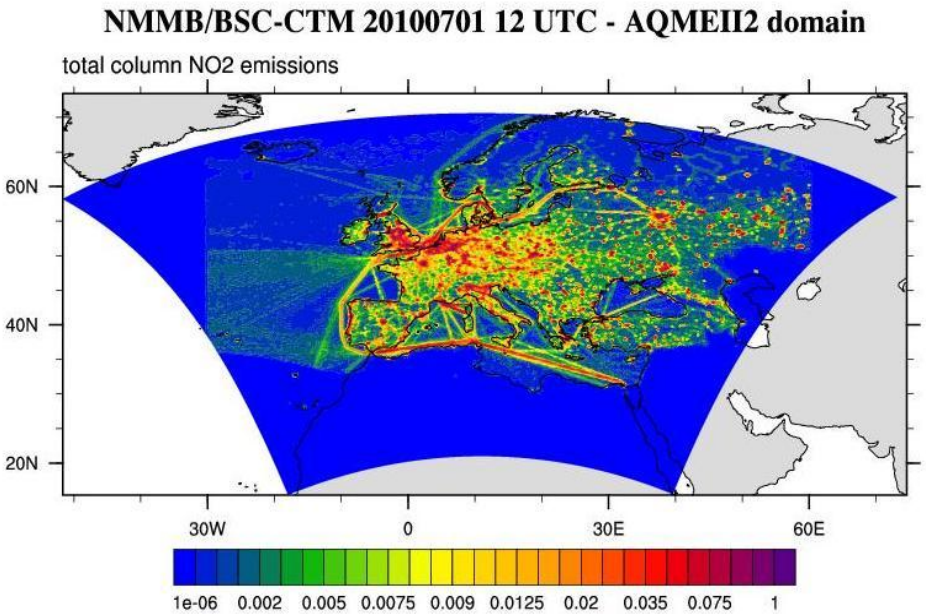
Gas Chemical mechanism: CB05

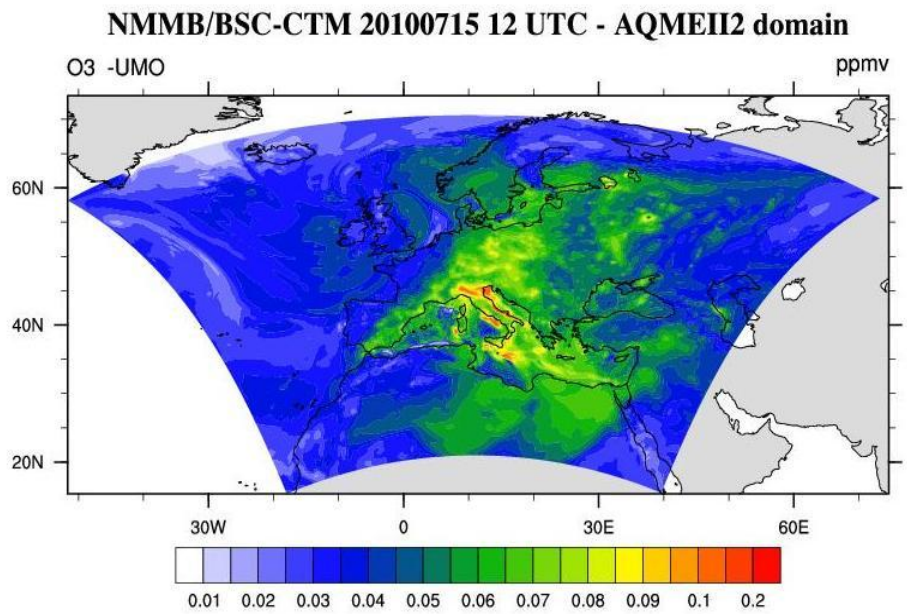
Aerosols: only dust-ssa

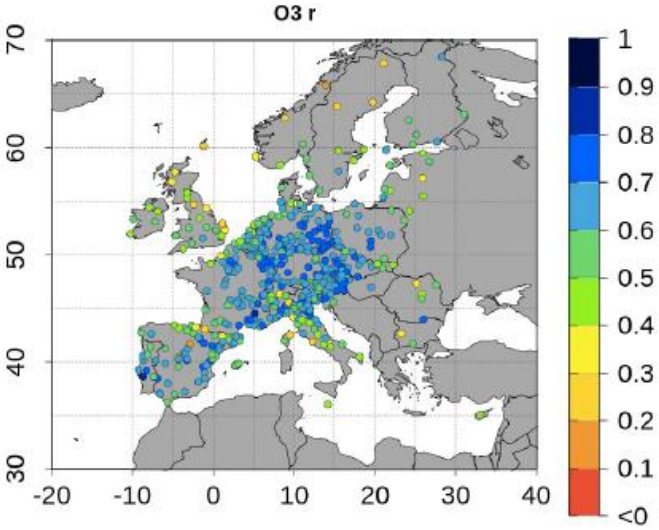


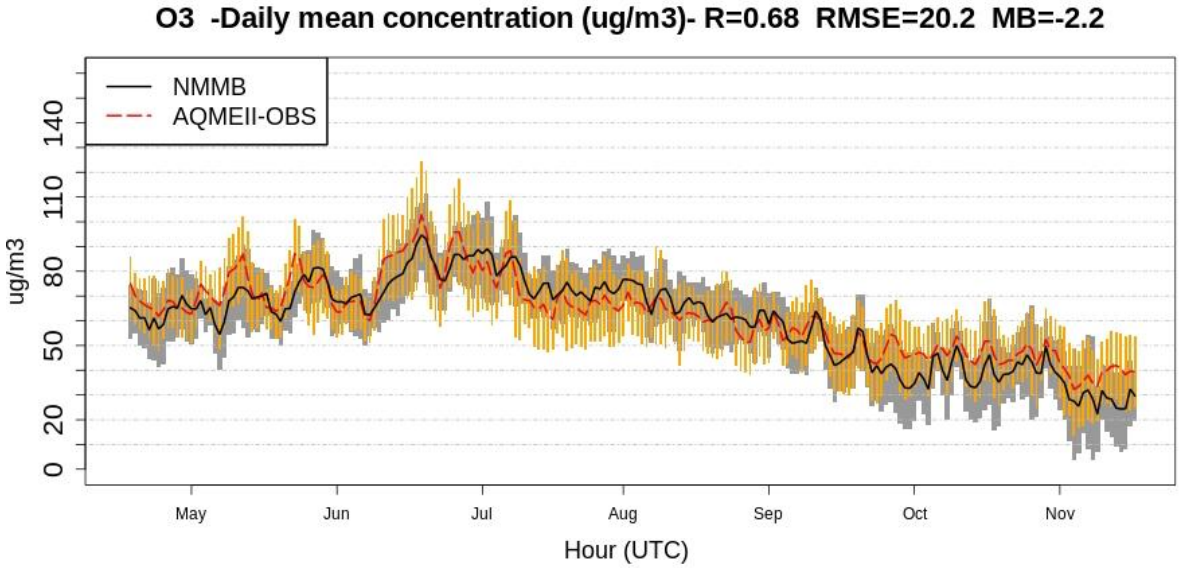
Blue: model domain
Red: AQMEII domain (to submit)
Green: BC domain

Regional run results (Badia and Jorba, 2014)



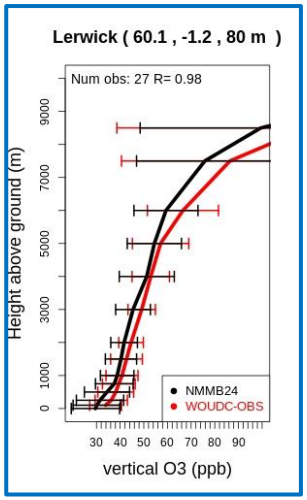


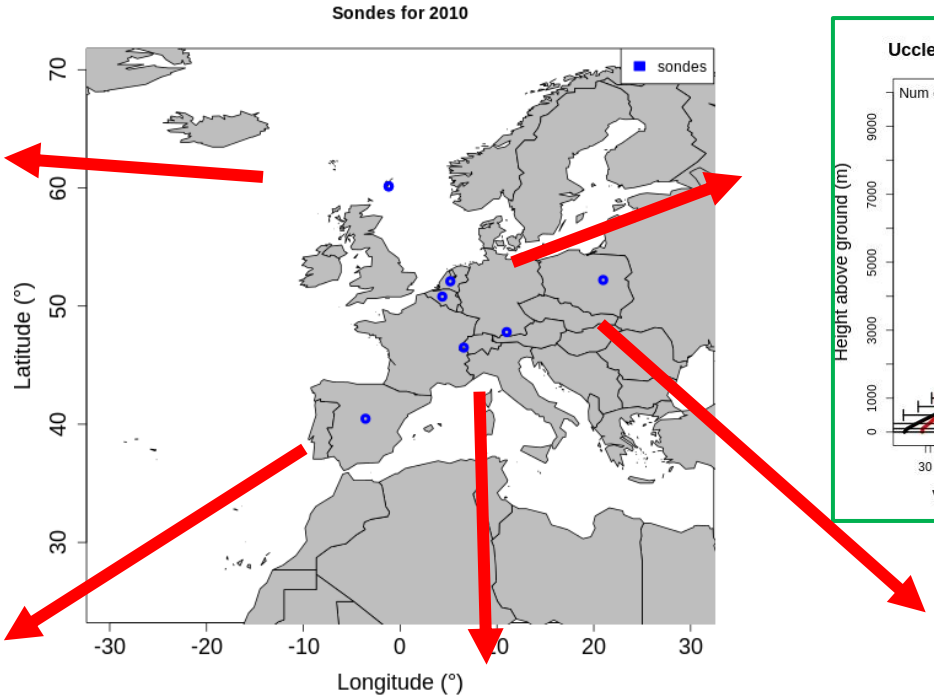


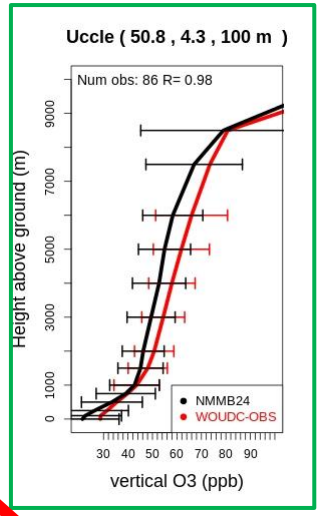


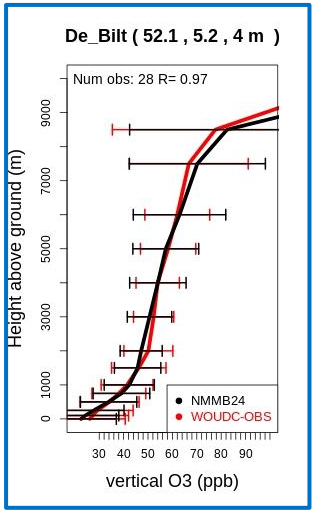
O_3 vertical profiles for each EU station at:

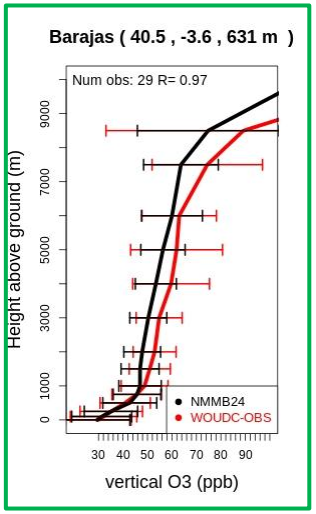
0, 100, 250, 500, 750, 1000, 1500, 2000, 3000, 4000, 5000, 6000, 7500,8500, 10000, 12000, 15000, 18000 m

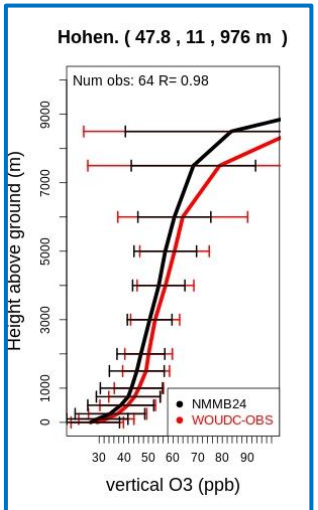


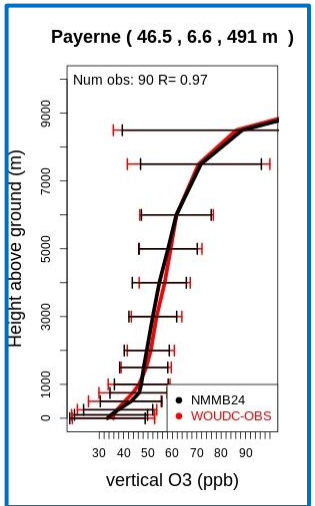


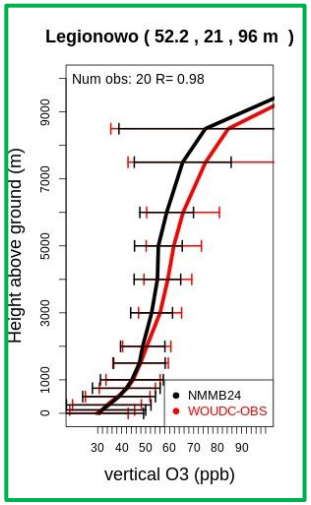












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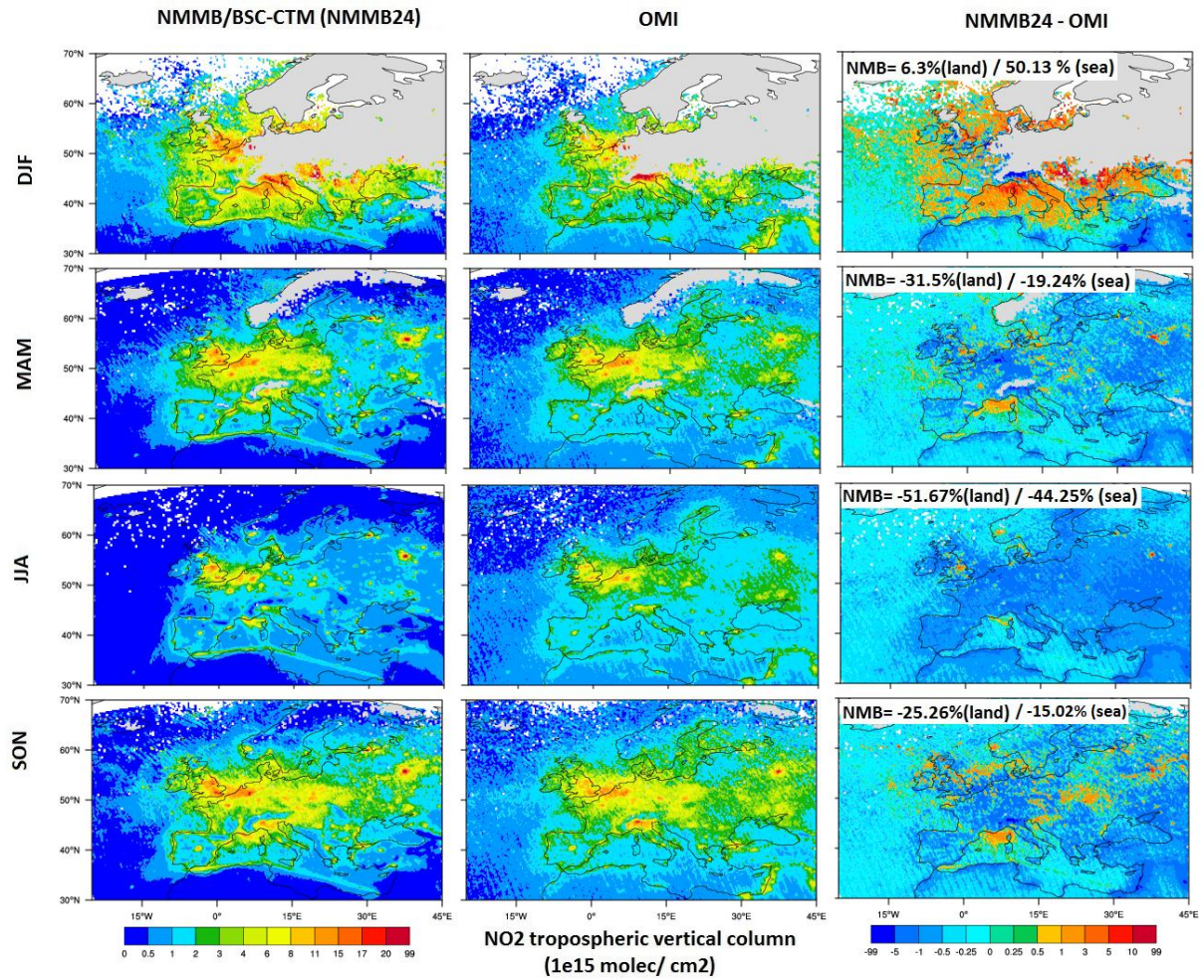
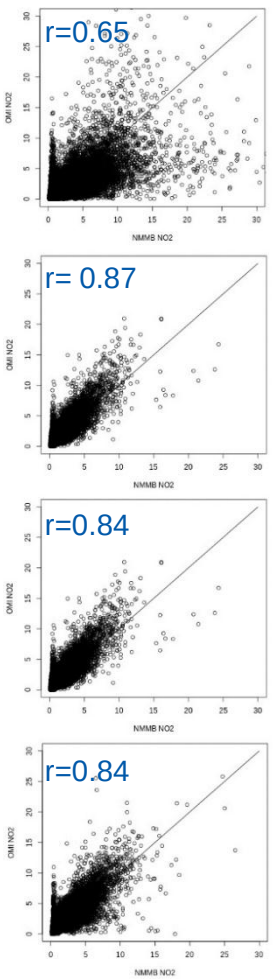
Comparison of modelled NO_2 VTC against satellite data (OMI) for (from top) winter (DJF), spring (MAM), summer (JJA) and autumn (SON)

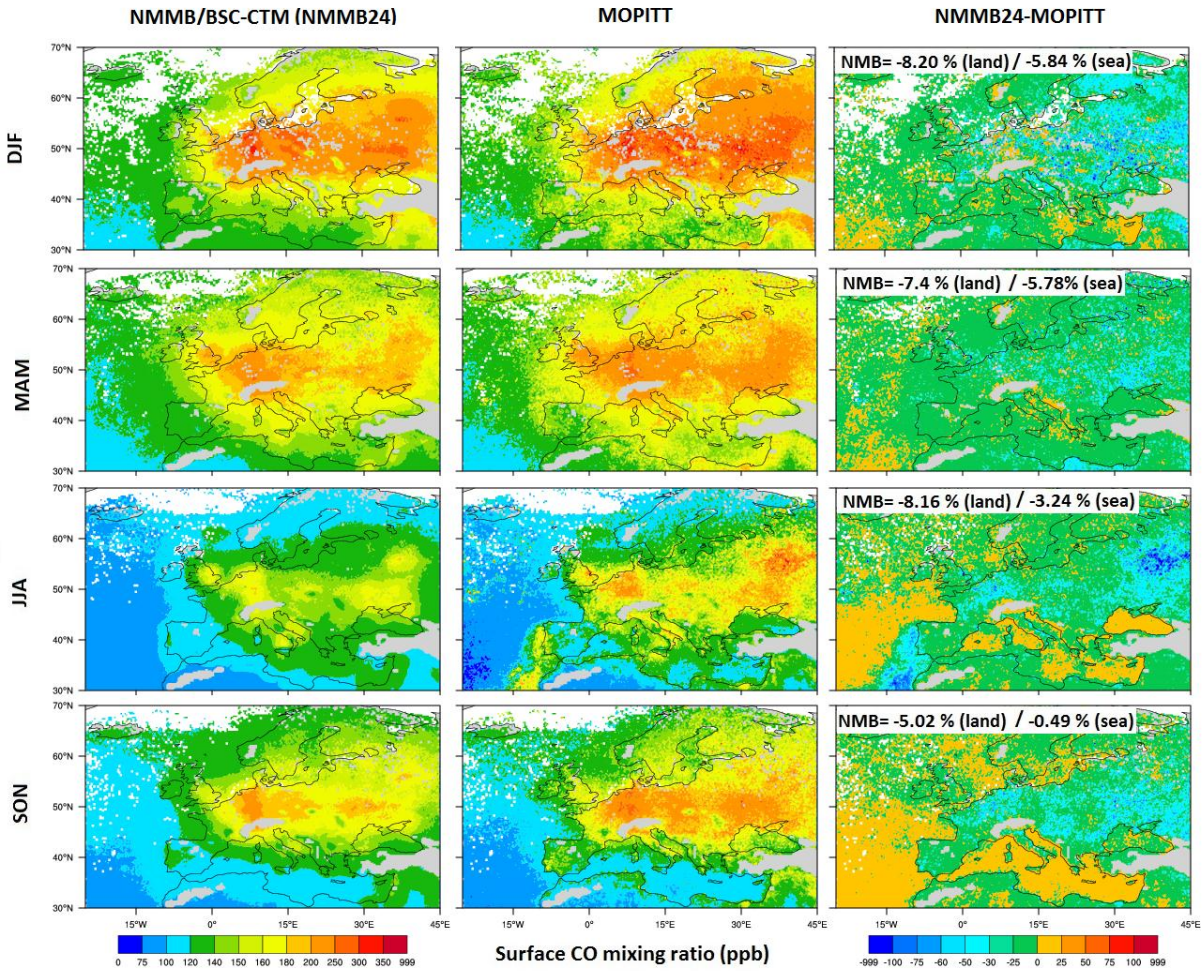


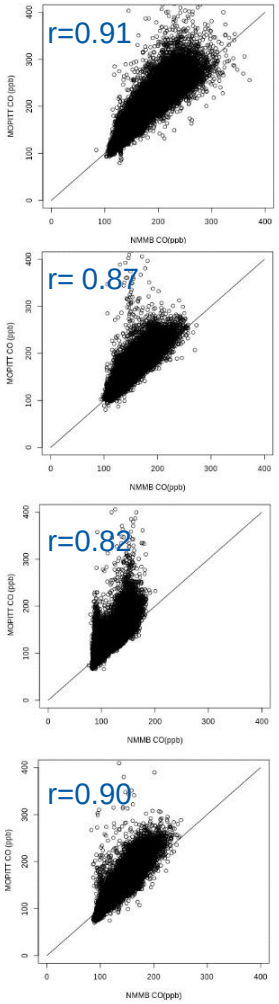


(Badia and Jorba, 2014)

- Capturing higher NO_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?

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





(Badia and Jorba, 2014)

- The pattern of emissions in central EU is well-captured.
- **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)

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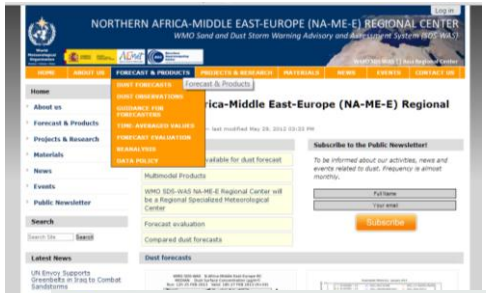
FUTURE WORK

Future Developments

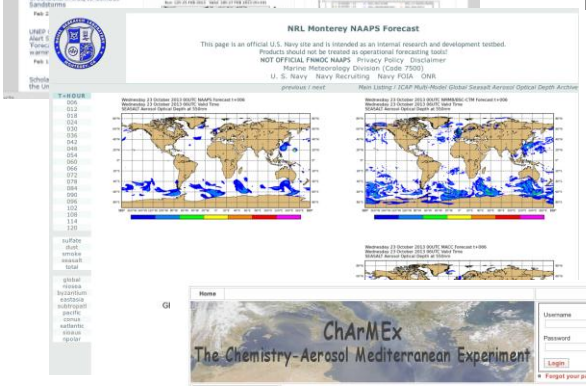
- Coupling of chemistry gas-phase with a secondary aerosol scheme for LAM applications at high-resolutions.
- Implementation of the other global relevant aerosol species, i.e. black (BC) and organic carbon (OC), and sulfate (SO4), in addition to dust (DU) and sea salt (SSA). Implementation of a volcanic 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**

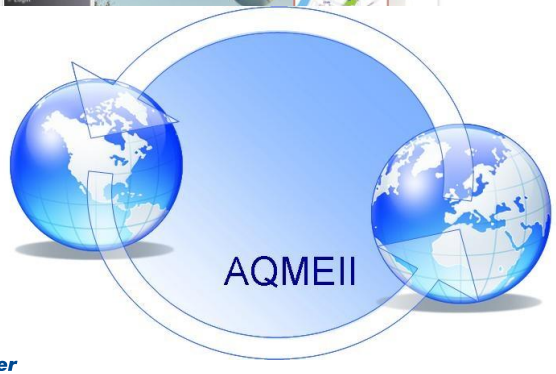
http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast



· **Participate in the ICAP global-model intercomparison project**

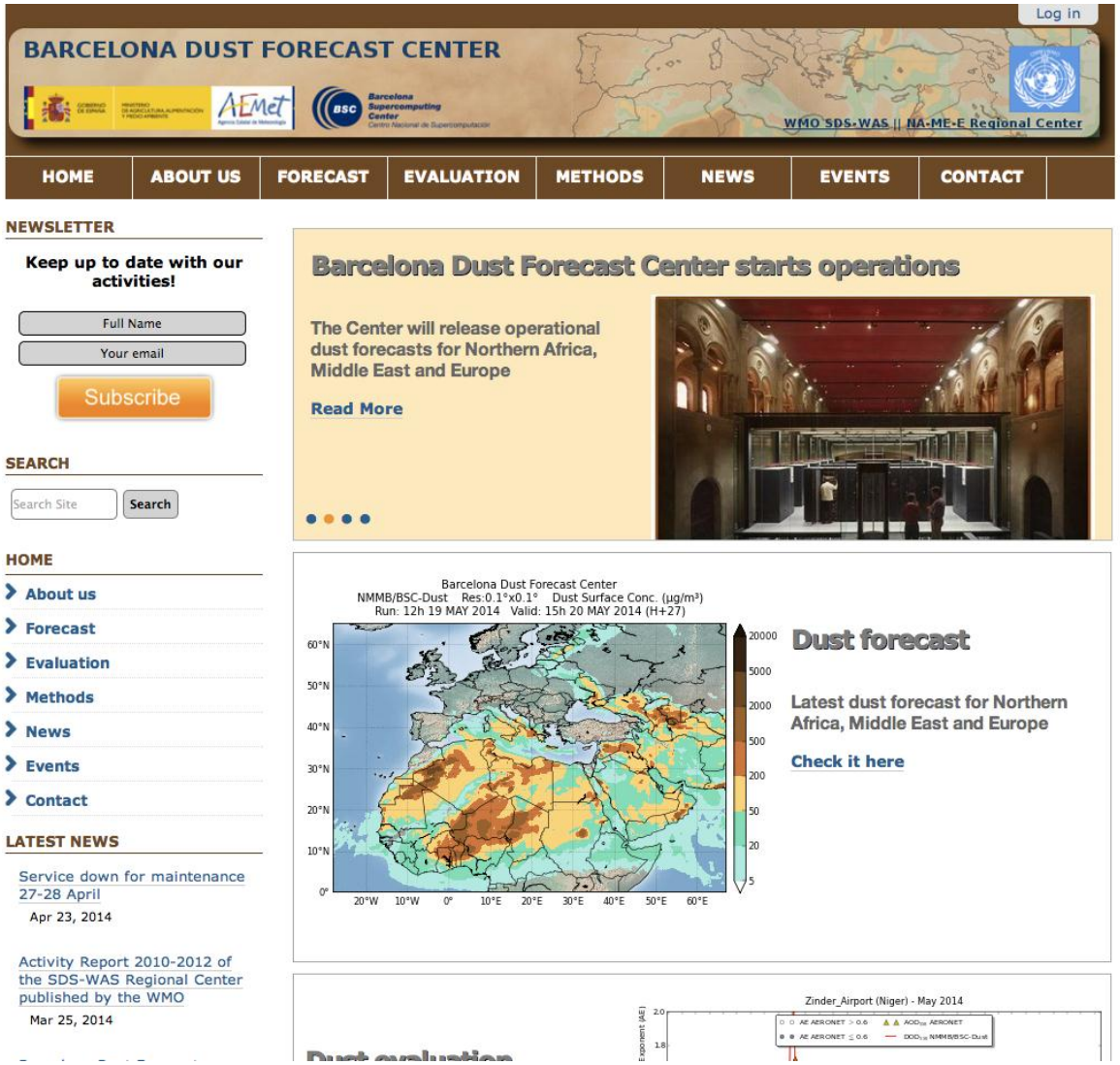
http://www.nrlmry.navy.mil/aerosol/icap.1087.php

· **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

www.bsc.es

EXCELENCIA SEVERO OCHOA

Barcelona Supercomputing Center

Centro Nacional de Supercomputación

Thank you!

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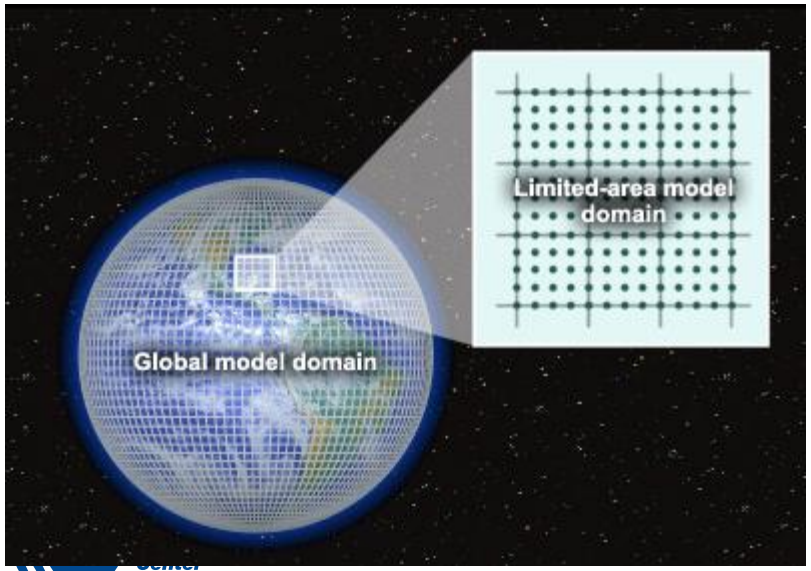
www.bsc.es/earth-sciences

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 1km^2 horizontal resolution)



Source: COMET