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EXCELENCIA SEVERO OCHOA

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Global Aerosol Modeling at the BSC: Activities and developments

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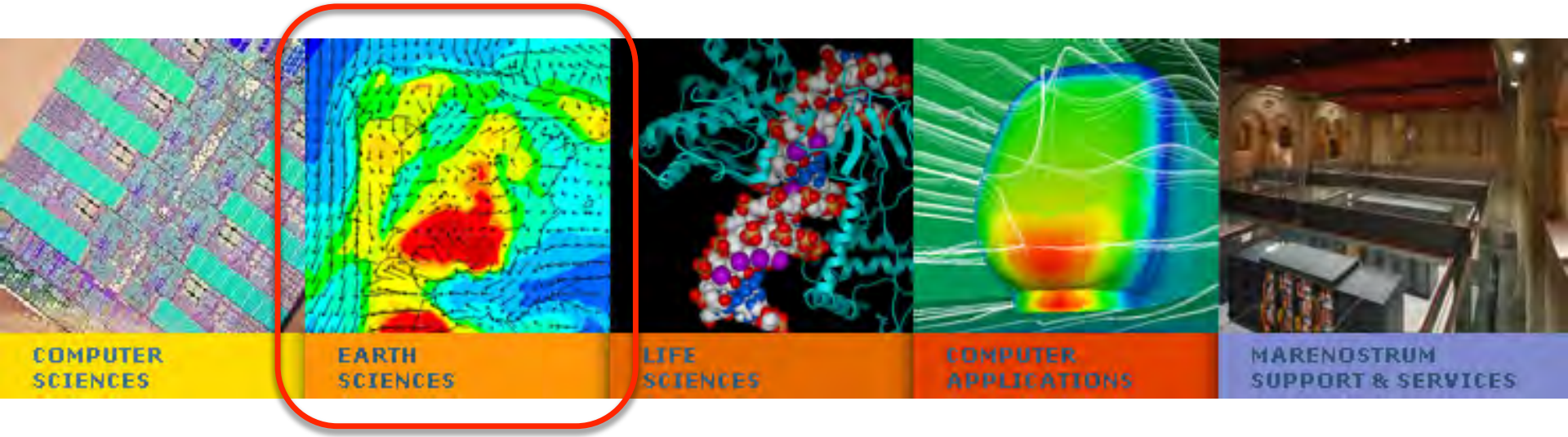
Barcelona Supercomputing Center

6th ICAP meeting, Boulder, Colorado, USA, 21-24 October 2014

The BSC-CNS (www.bsc.es)



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

Earth Sciences Activities

- Research lines:
  - Air Quality
  - Mineral Dust
  - Atmospheric Modeling
  - Climate Modeling
- New on-line Chemistry-Meteorology model:
  - **NMMB/BSC-CTM**
- Dust daily forecast:
  - **BSC-DREAM8b**

    http://www.bsc.es/projects/earthscience/BSC-DREAM/
  - **NMMB/BSC-Dust:**

    http://www.bsc.es/projects/earthscience/NMMB-BSC-DUST/
  - **Mineral dust database:** Files download

    http://www.bsc.es/earth-sciences/mineral-dust/catalogo-datos-dust/

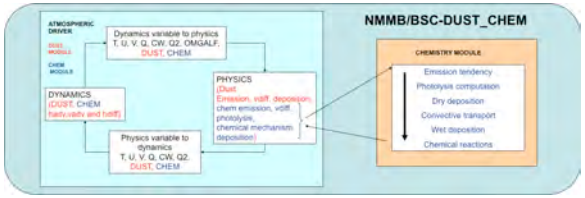
NMMB/BSC-Chemical Transport Model (Overview)

- 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)*
→ *(...)*



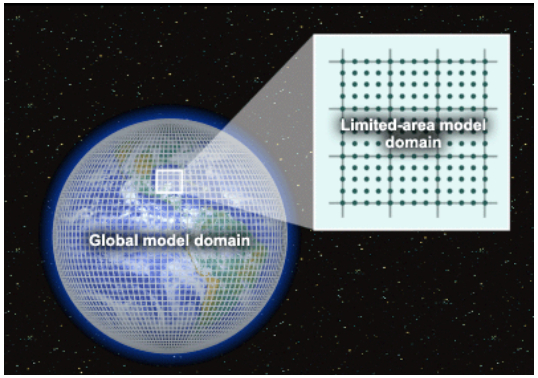
BSC Chemical Transport Model
(gas/aerosol variables: mass mixing ratios)

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 (8 bins)
→ *Spada et al. (ACP 2013)*

BC/OM/SO4



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

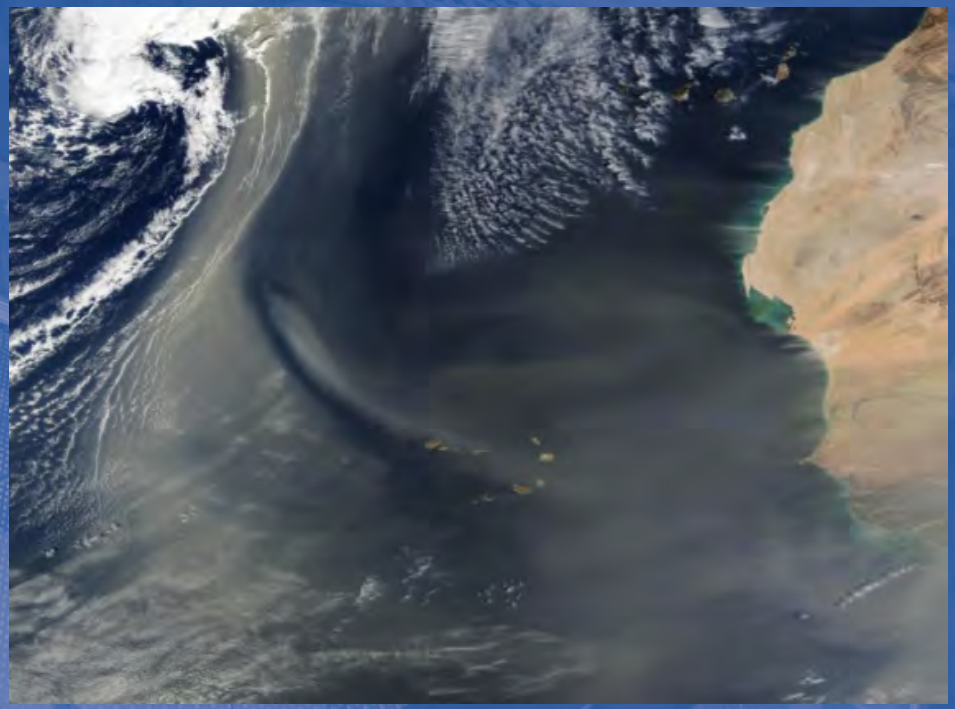
✓ Conservation of important properties of the continuous system

✓ 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



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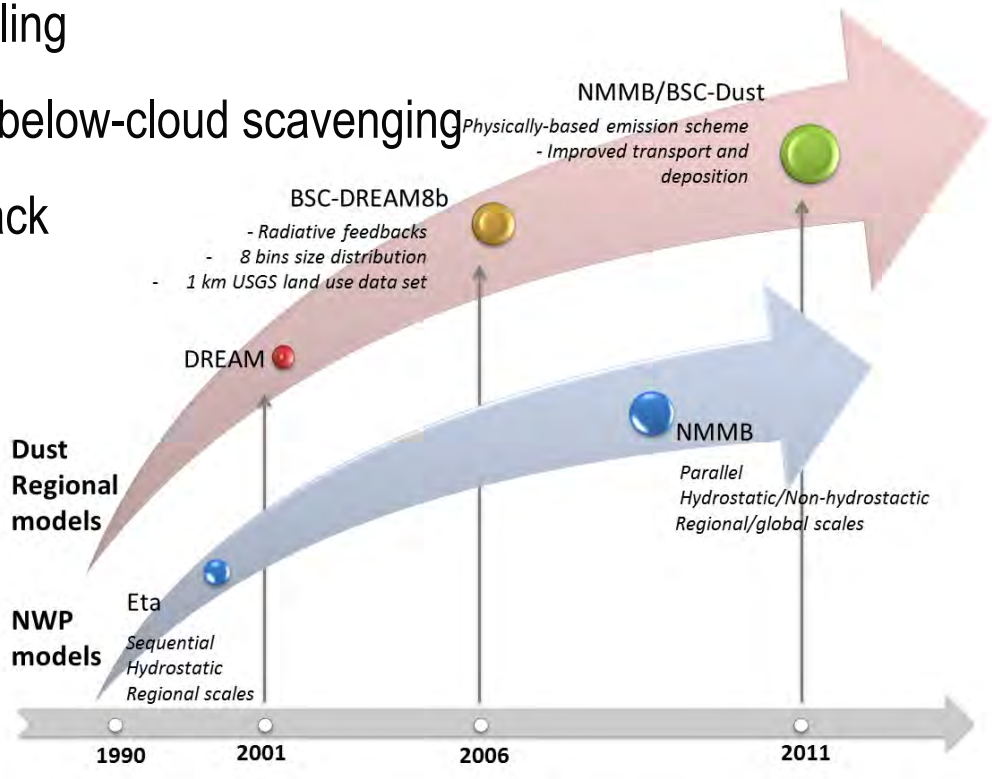
MINERAL DUST MODULE

The NMMB/BSC-DUST model

NMMB/BSC-DUST is embedded into the NMMB model and solves the mass balance equation for dust taking into account the following processes:

- Dust generation/emission by surface wind
- Horizontal and vertical advection
- Vertical transport/diffusion by turbulence and convection
- Dry deposition and gravitational settling
- Wet removal including in-cloud and below-cloud scavenging
- RRTM SW/LW dust radiative feedback

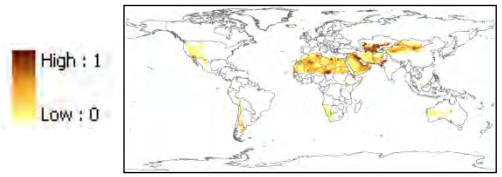
Evolution from
Nickovic et al. (2001)
Pérez et al. (2006ab)



NMMB/BSC-Dust (Pérez et al. 2011)

EMISSION SCHEME

- Source function: includes update land databases (vegetation fraction, land textures, soil types and albedo) and a preferential "topographic" source mask
- Physically-based emission scheme which includes saltation and sandblasting



$$\delta = USGS \cdot PREF \cdot (1 - VEGFRAC) \cdot (1 - SnowCover)$$

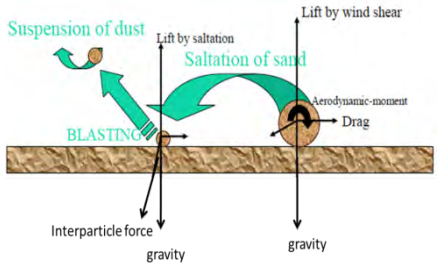
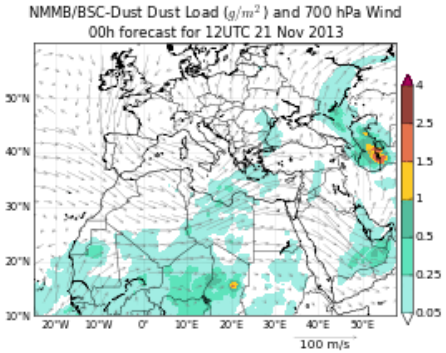
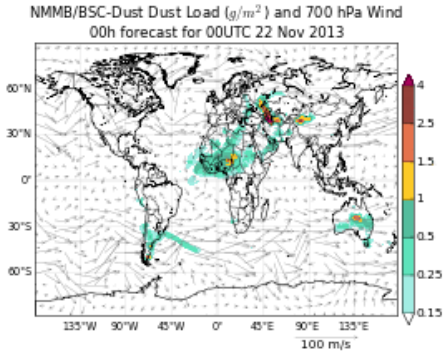


Image from Carlos Pérez

DAILY OPERATIONAL DUST FORECAST AT BSC

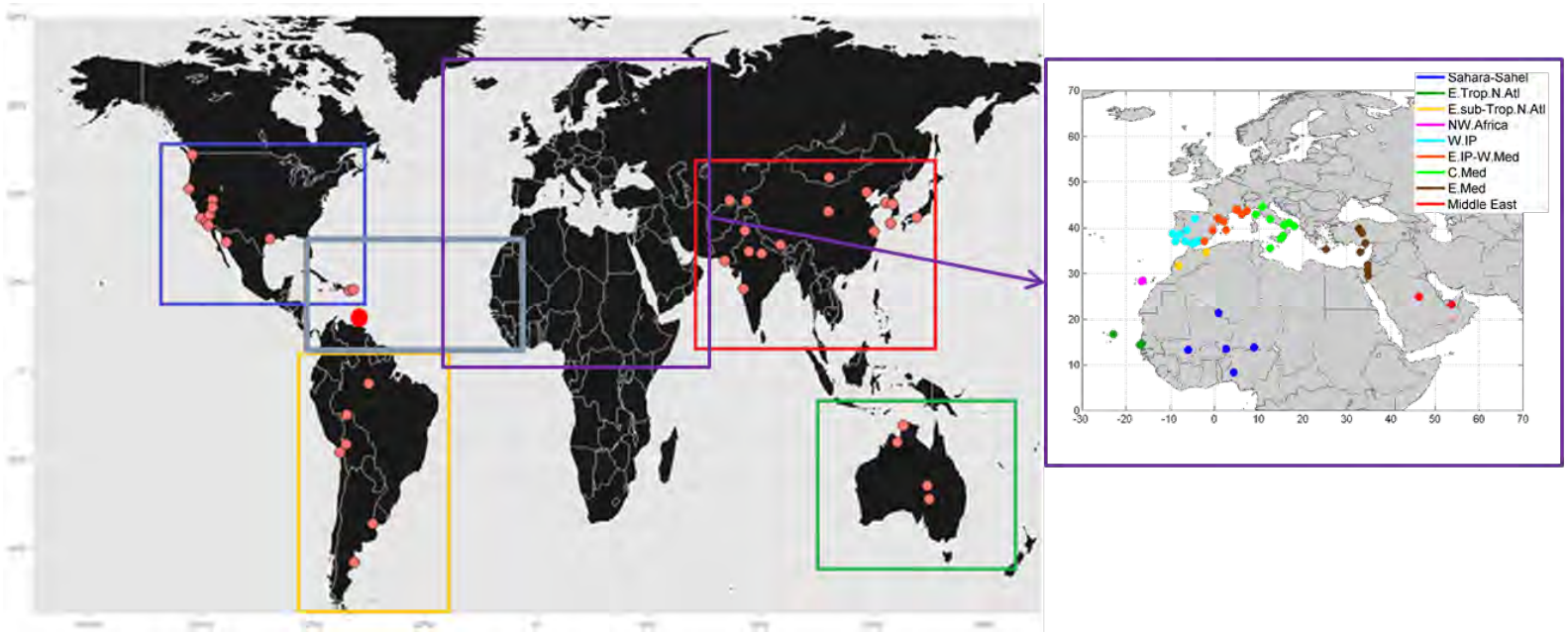




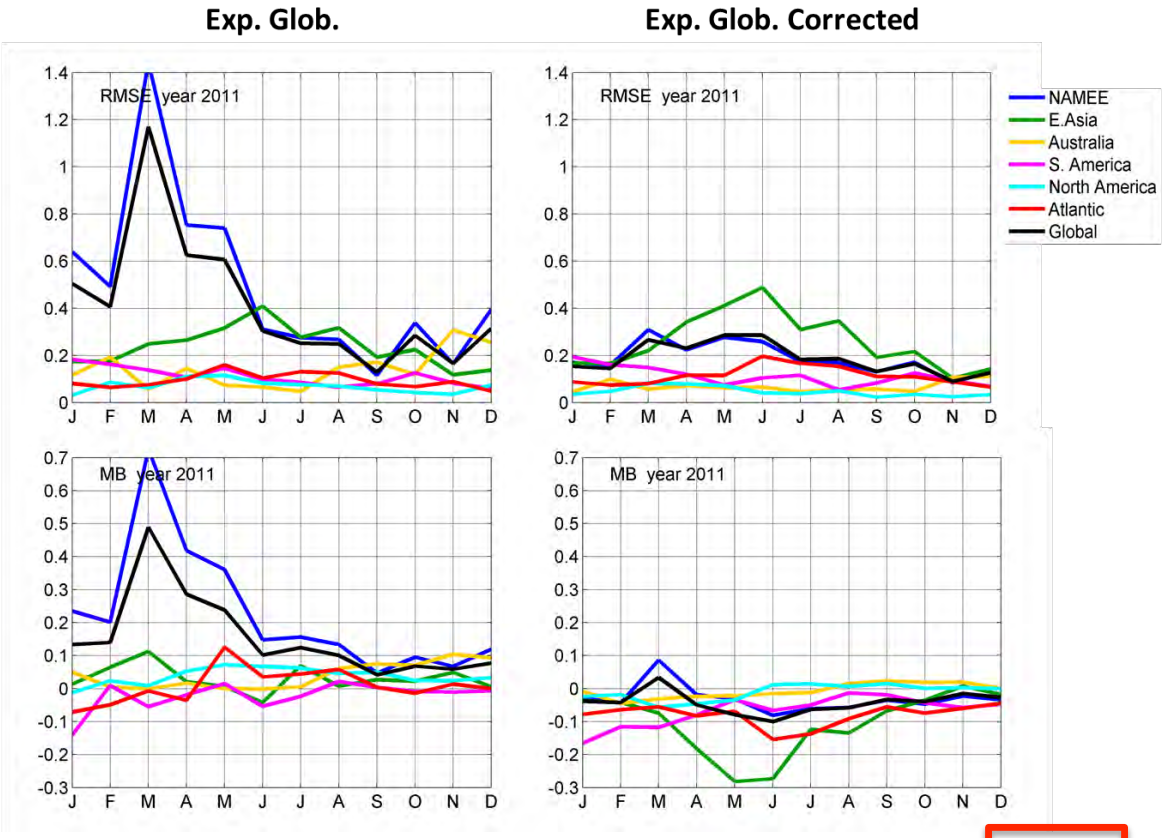
http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast/

Evaluation methods

- Column-integrated AOD at 550 nm from AERONET Level 2.0
- Spectral Deconvolution Algorithm providing AODfine and AODcoarse
- Filter applied to the AERONET observations
  - AE<0.75 is considered in the calculations
  - AE>=0.75 not dust contribution, not considered for calculations
- RMSE, MB, correlation



Improvement of Global dust calibration factor

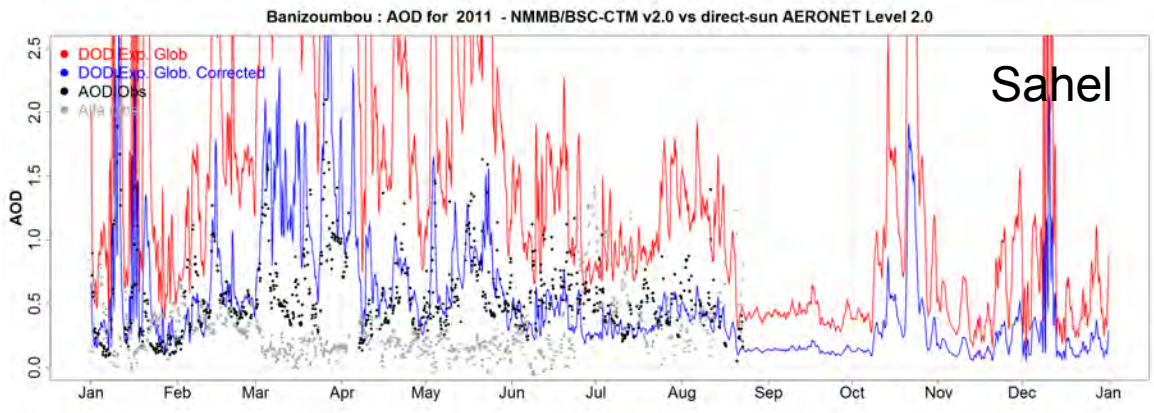


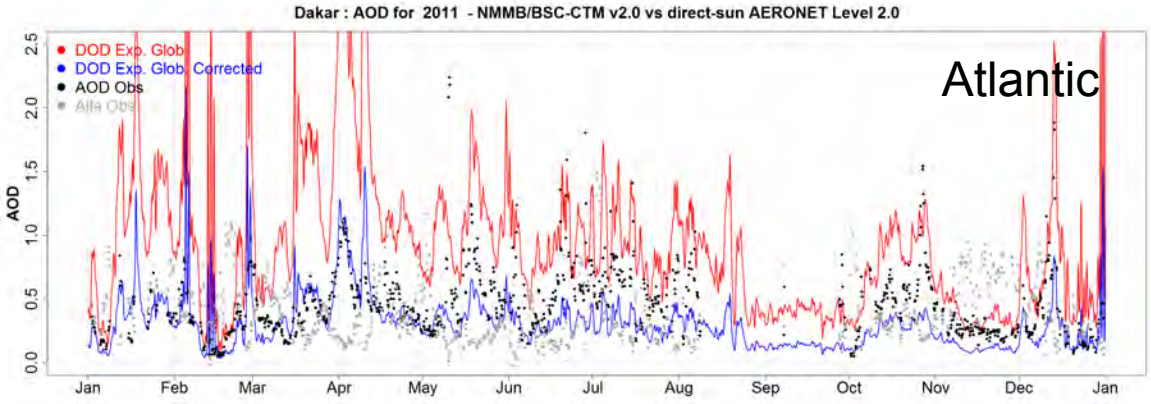
Exp. Global standard calibration factor of Pérez et al. (2011)

Exp. Global Corrected calibration factor same as Regional NAMEE domain

NMEE	Exp. Glob.				Exp. Glob. Corrected			
Regions	*NDATA*	*r*	*RMSE*	*MB*	*NDATA*	*r*	*RMSE*	*MB*
NAMEE	29316	0,70	0,59	0,22	29316	0,70	0,20	-0,03
East Asia	6931	0,61	0,26	0,03	6931	0,61	0,30	-0,12
Australia	2259	0,11	0,17	0,05	2259	0,11	0,07	0,00
South America	1401	0,22	0,11	-0,02	1401	0,22	0,11	-0,05
North America	3366	0,49	0,08	0,04	3366	0,49	0,05	-0,01
Atlantic	2033	0,70	0,10	0,00	2033	0,70	0,12	-0,08
Global	***45306***	***0,65***	***0,49***	***0,16***	***45306***	***0,65***	***0,20***	***-0,05***

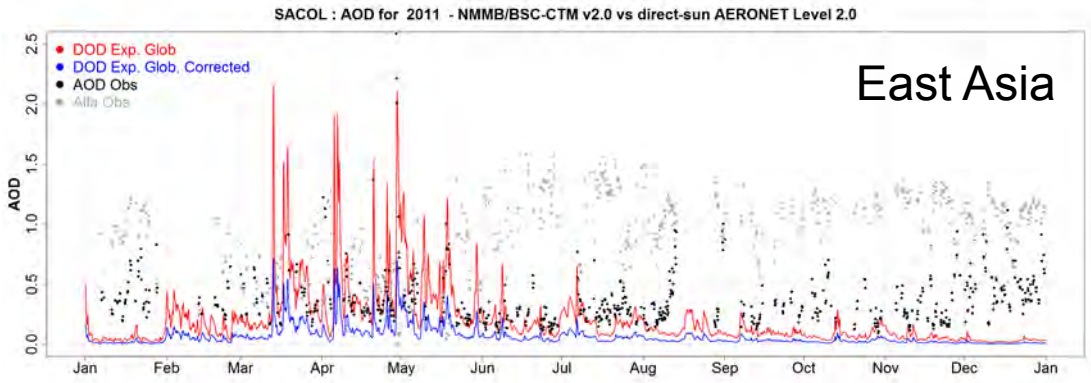
AERONET comparison

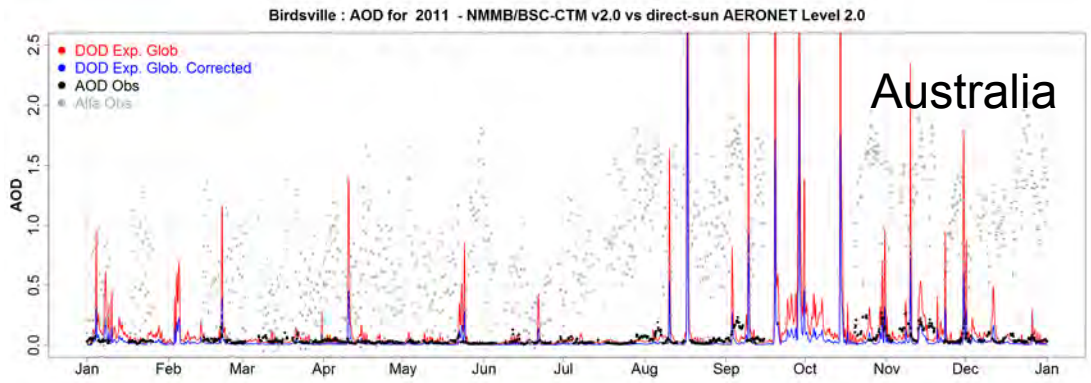


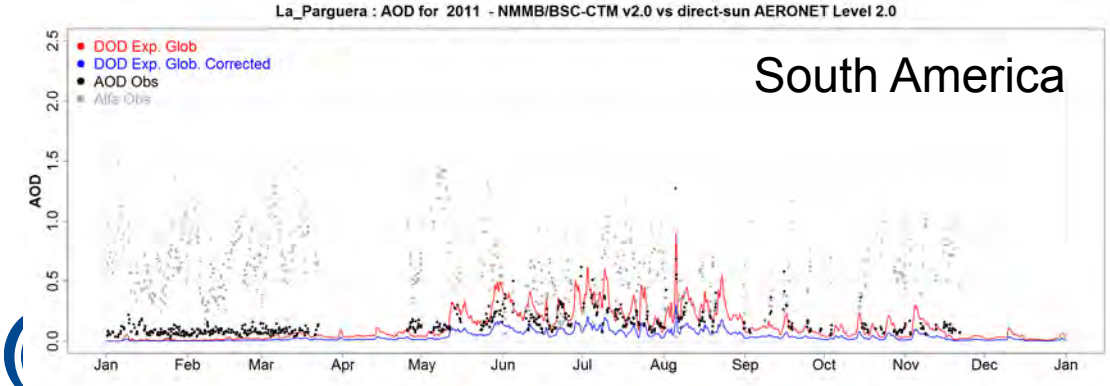


- Clear improvement of the bias near the sources, Sahel-Banizoumbou station, and Dakar-Atlantic.
- The model reproduces the annual cycle, and the daily variability.
- The strong decrease in dust AOD from end of August to October is under investigation. It could be related with the meteorological IC from NCEP/GFS analysis.

AERONET comparison







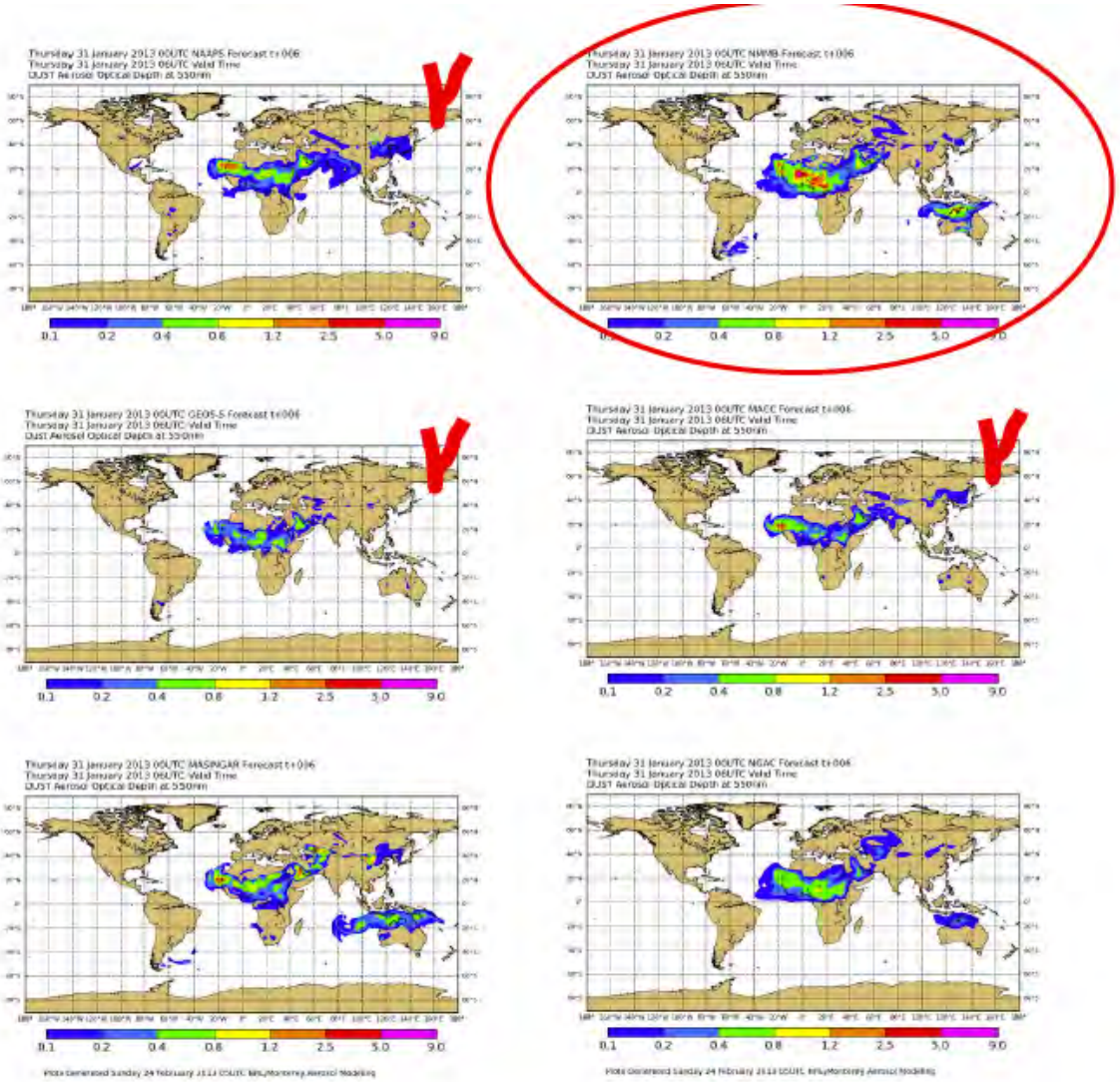
- Now the expected underestimation is present with the new calibration. In regions affected by other aerosols, the dust contribution has been reduced.

- East Asia maximums during Spring well reproduced.

- Australia maximums during fall-winter well reproduced.

- South America during summer well reproduced.

ICAP models with DA



Current global systems with data assimilation for aerosols

Working to include this capability in NMMB/BSC-CTM

✓ = data assimilation

Data Assimilation for NMMB/BSC-CTM: Mineral Dust

- Enhancement of NMMB/BSC-CTM model with data assimilation using an ensemble technique: the **Local Ensemble Transform Kalman Filter** (LETKF)
  - it is particularly suited to high-performance computing applications: it allows a parallel computation of the analysis;
  - it uses flow-dependent background errors: the background error covariance is generated and propagated by the filter, using model dynamics;
  - it is easy to code: it does not require the development of adjoint code.

- Using a smoothed localisation of the observations:
  - observation influence decays gradually towards zero as their distance from analysis location increases.

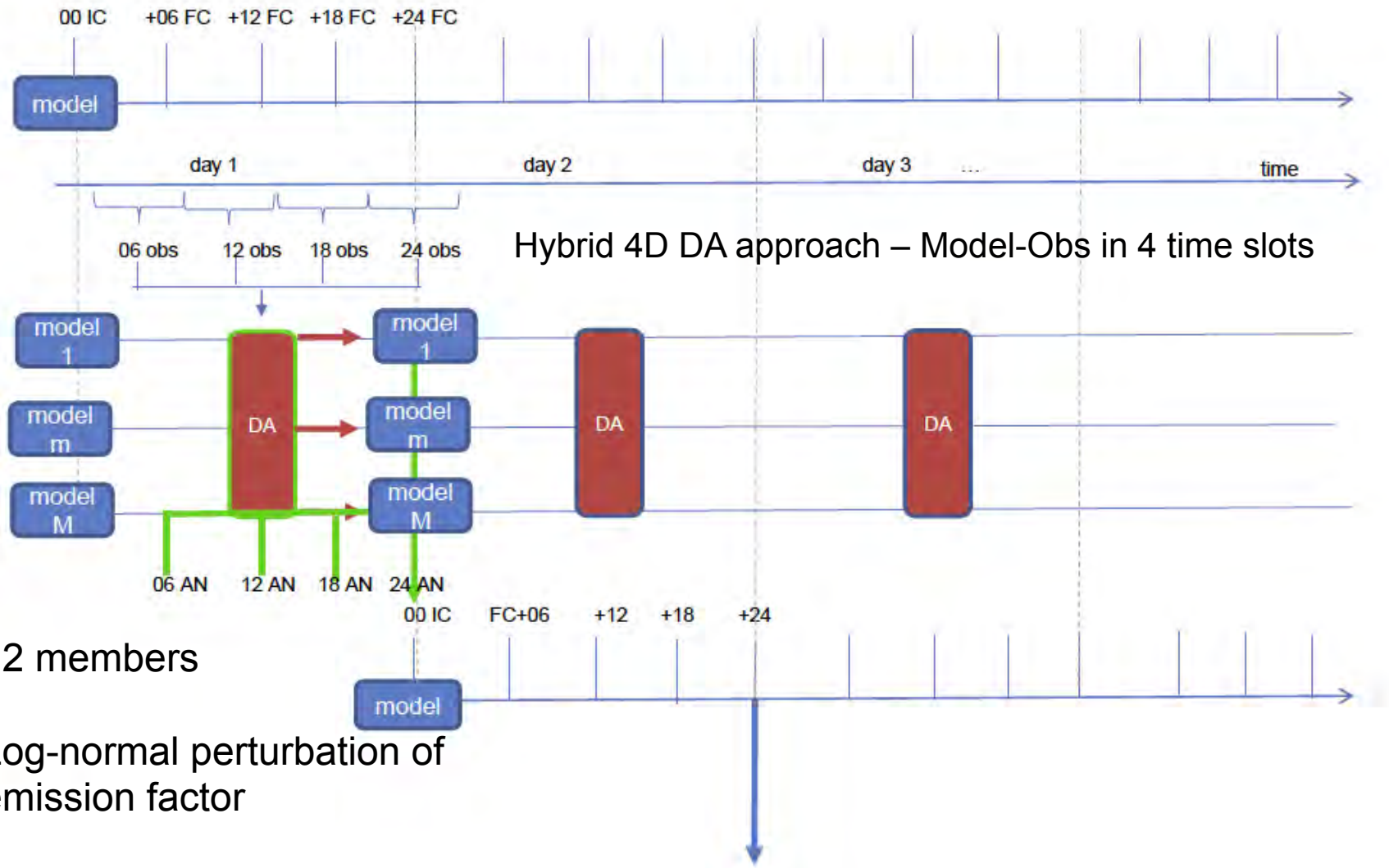
- Testing the assimilation of NRL MODIS AOD:
  - a Level 3 filtered, corrected, and aggregated product, with a retrieval error also provided.

- The following preliminary tests are focused on mineral dust and on low resolution runs of our global model.

Vertical mass flux of dust into a transport bin k

$$F_k = C\,S\,(1-V)\,\alpha\,H \sum_{i=0}^{3} m_i\,M_{i,k} \qquad k = 1, \cdots, 8$$

Data Assimilation Flow



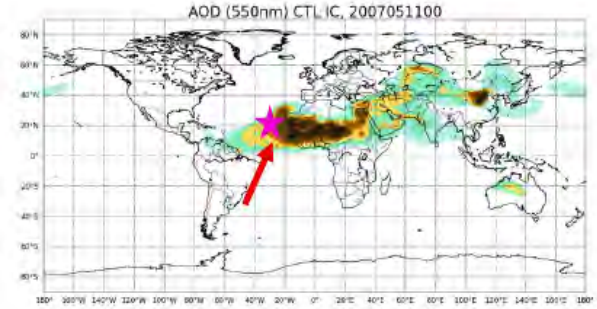
12 members

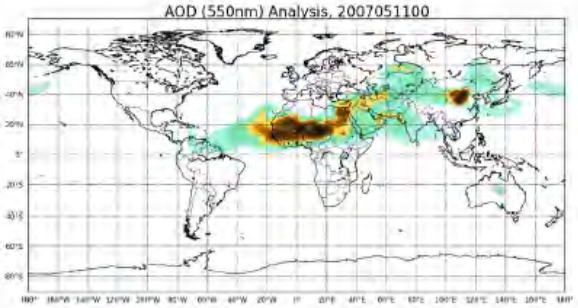
Log-normal perturbation of emission factor

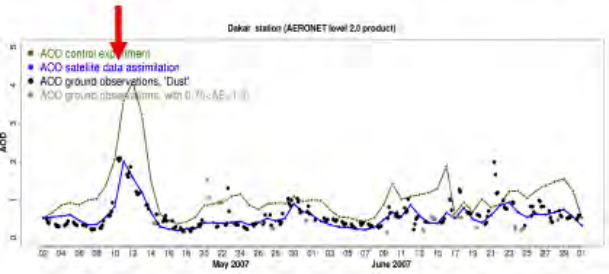
Experiments use a spin-up of 1 month w/o DA

Validation against independent observations

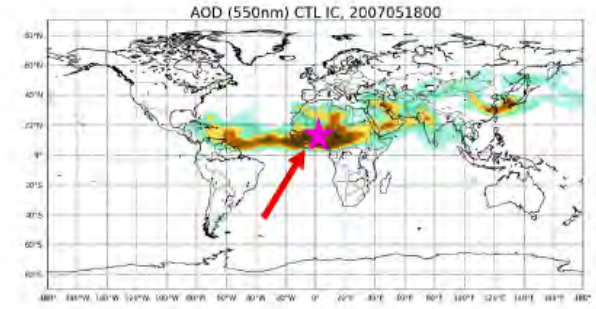
Short-range transport

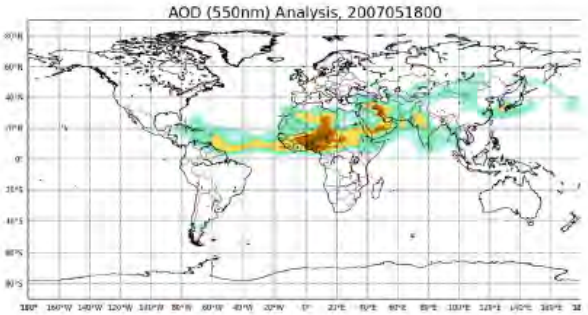


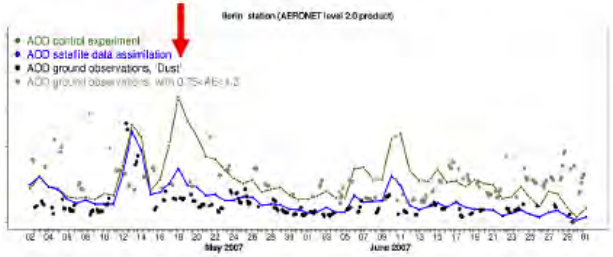




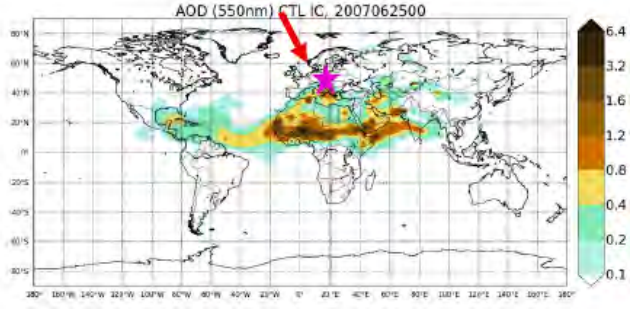
Near sources

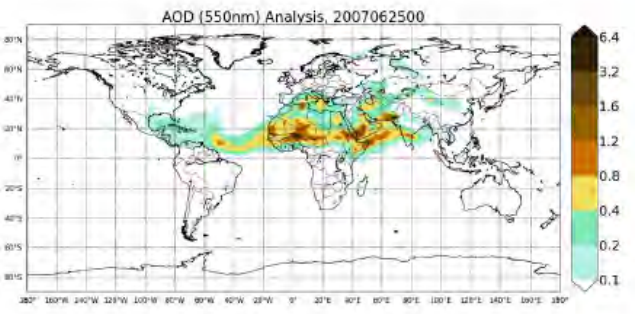


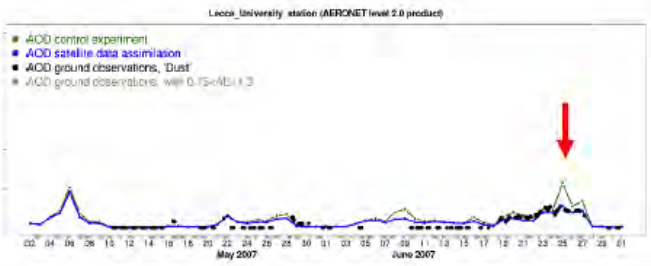




Long-range transport





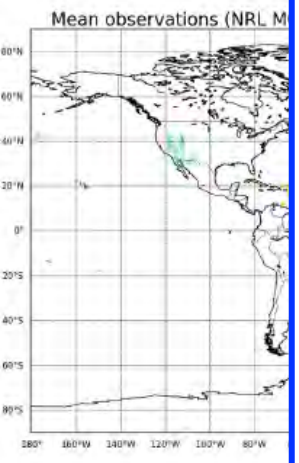


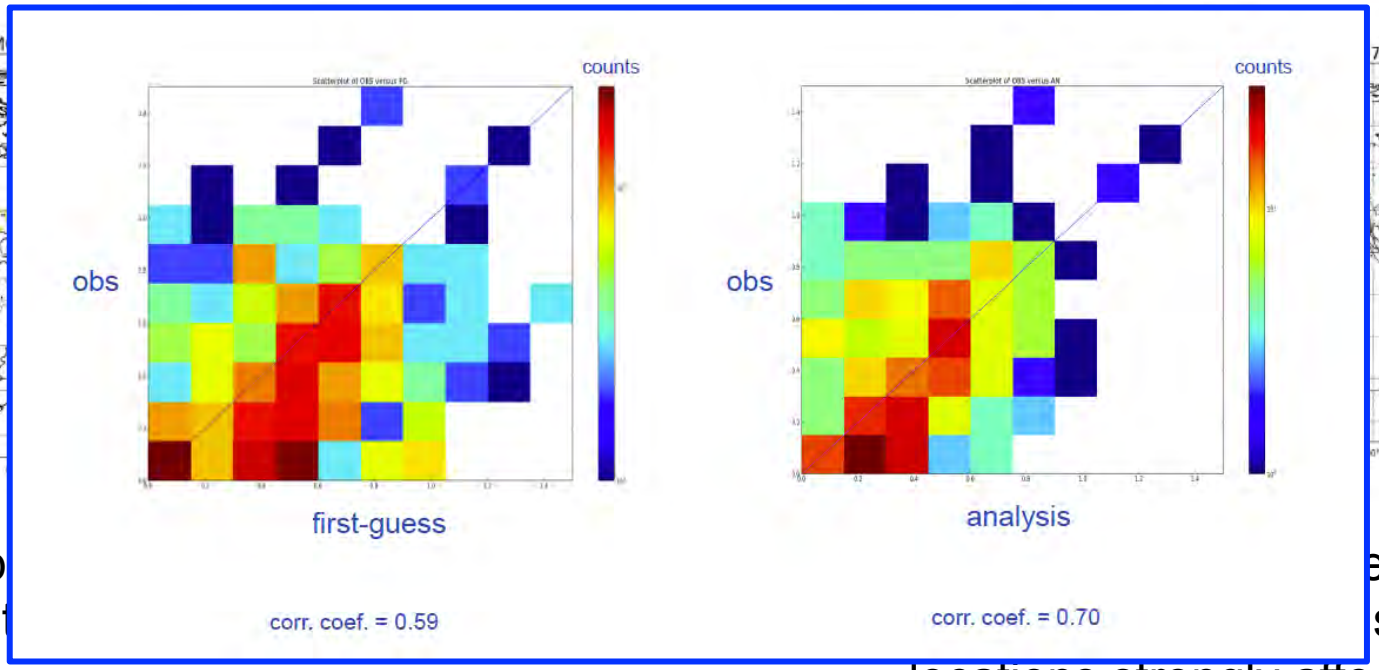
AERONET stations
Black dot → dust AOD AE<=0.75 ;
Grey dots → uncertain type of AOD with 0.75<AE<1.3

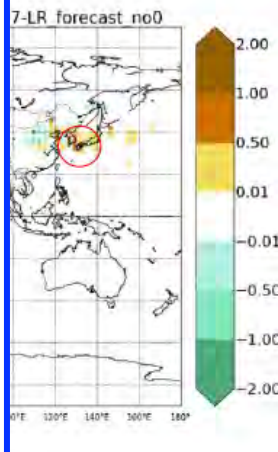
Quality control on the observations

6 hour NRL MODIS AOD are selected according to:

land:	sea:
AE<0.75 from daily MODIS Aqua or Terra products	if AOD>0.2, **FF<0.5** from 6 hour NRL MODIS
AND	if AOD<=0.2, **0.4<FF<0.5** from 6 hour NRL MODIS
AI>1.5 from daily OMI product	**AND**
	AI>1.5 from daily OMI product

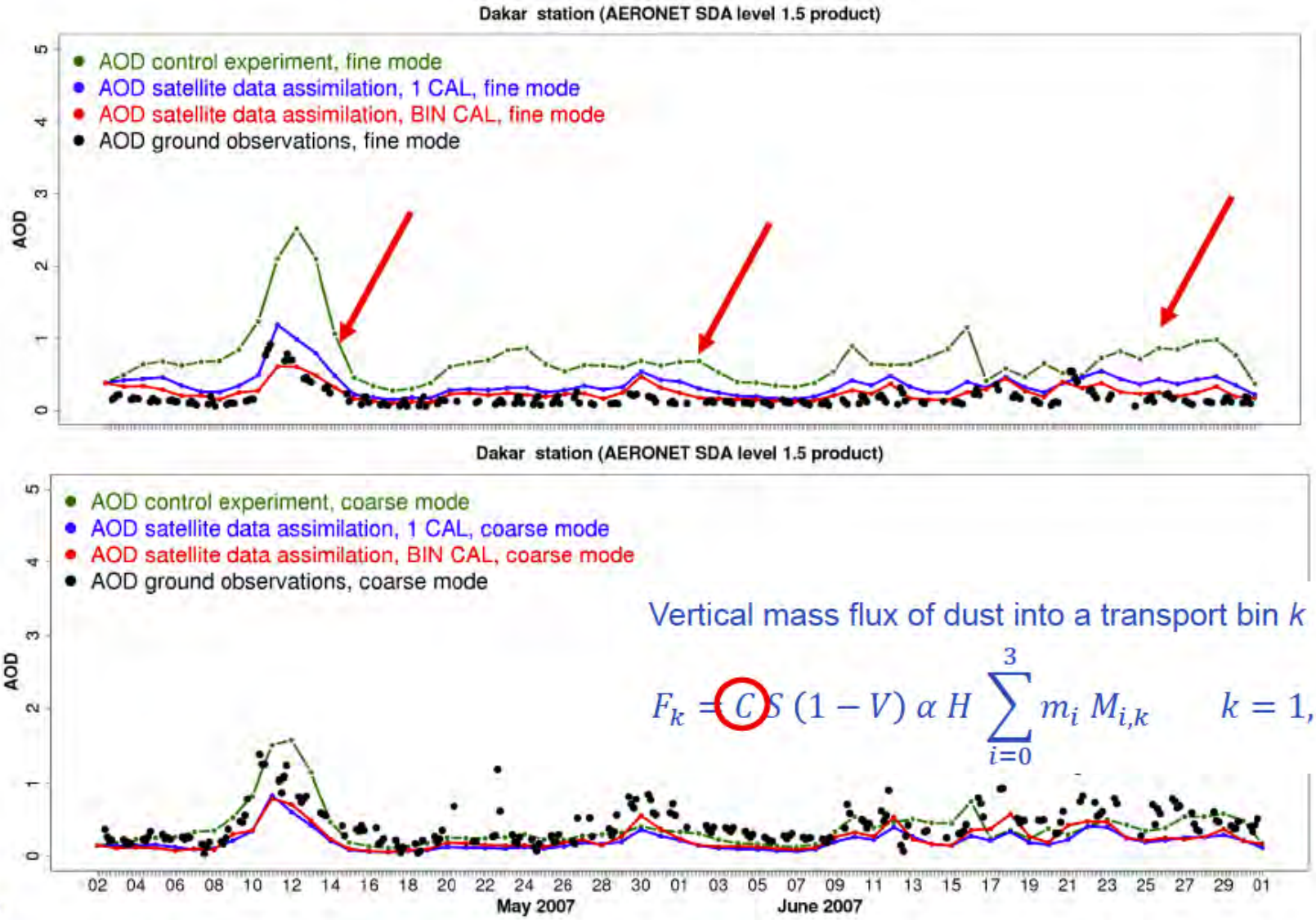






Mean ob es. Still
the qualit some
locations strongly affected by
other types of aerosols.

Impact of calibration factors per bin



Vertical mass flux of dust into a transport bin k

$$F_k = C\,S\,(1-V)\,\alpha\,H \sum_{i=0}^{3} m_i\,M_{i,k} \qquad k = 1,\cdots,8$$

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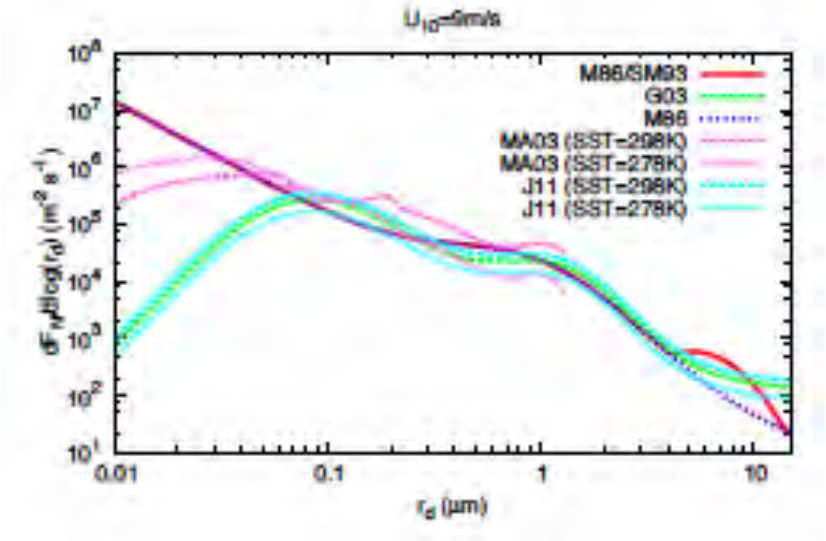
SEA SALT AEROSOL MODULE

SEA-SALT MODULE (emissions)

dF/dr = f(r, **ξ**)

M86 → ξ = U10 (bubbles)
G03 → ξ = U10 (bubbles, spume?)
M86/SM93 → ξ = U10, U_T=9m/s (bubbles, spume)
M86/SM93/MA03 → **ξ** = (U10, U_T, SST) (bubb., sp.)
J11 → **ξ** = (U10, SST) (bubb., sp.)

Monahan et al. (OW 1986)
Gong et al. (GBC 2003)
Smith et al. (RMS/QJ 1993)
Martensson et al. (JGR 2003)
Jaeglé et al. (ACP 2011)



criteria:
· whitecap method
· simplest (low number of parameters)
· bubbles and spume mechanisms

(M86, G03 and J11 extended up to 15μm)

→ **strong differences**
for r_d>5μm (spume)
and for 0.1μm<r_d<1μm (bubbles)

SSA evaluation: sconc and AOD

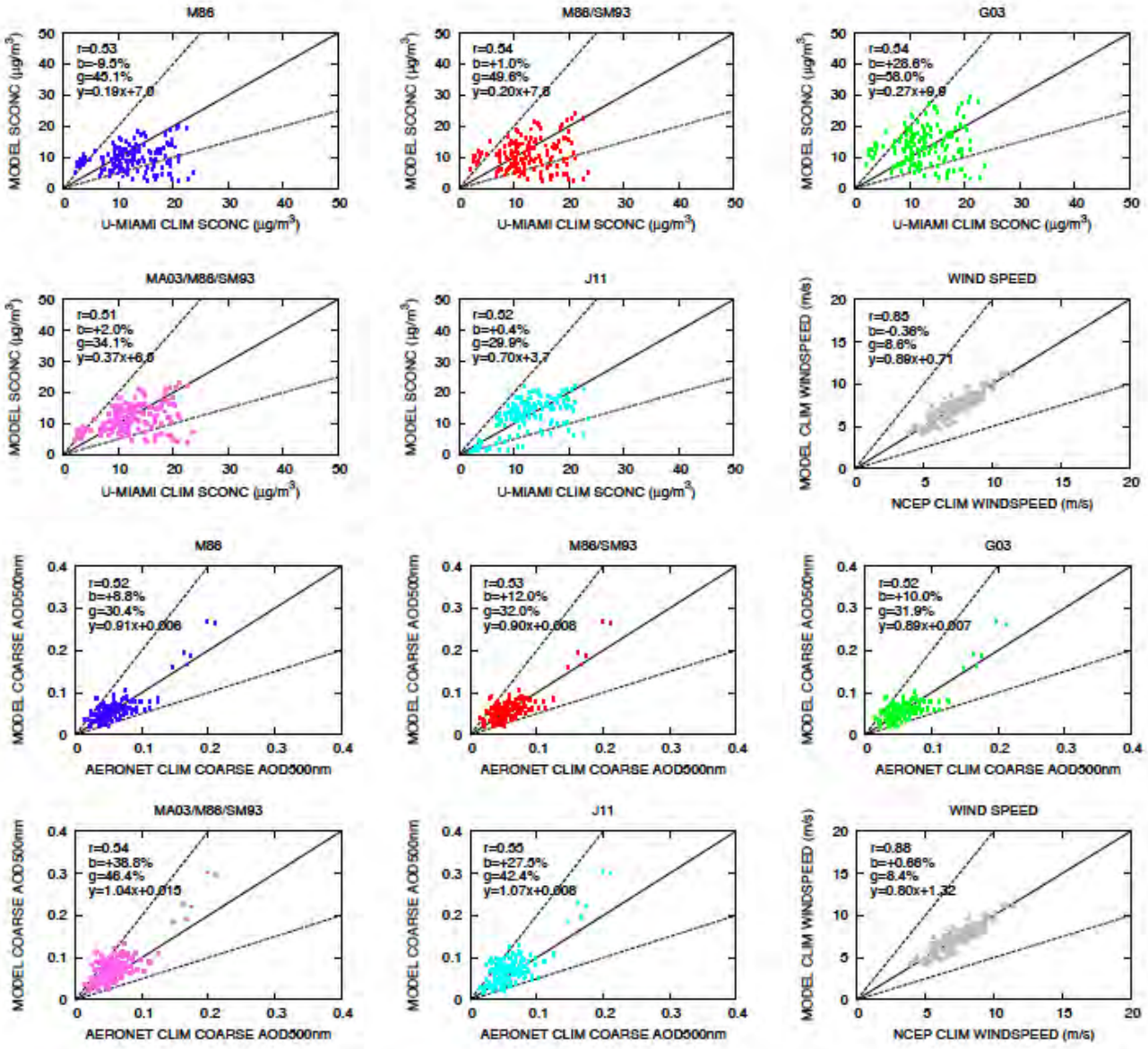
→ Surface monthly mean concentrations from U. Miami network

→ 2002-2006 runs with dust+ssa

→ Monthly mean AOD

→ 2002-2006 runs with dust+ssa

→ Best agreement J11



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BC/OM/SULFATE MODULE

NMMB/BSC-CTM: Global Aerosols

previous version (until 2014):

- DUST (8 mass bins) ←Perez et al., 2011 (ACP)
- SEA-SALT (8 mass bins) ←Spada et al., 2013 (ACP)

new implementations (2014):

- BC (2 mass bins, phob/phil)
- POM (2 mass bins, phob/phil)
- SOA (4 mass bins → 2-product mechanism OR 1 bin → prescribed production, all phil)
- SO4 (1 mass bin, all phil)

related gases:

- SO2, DMS, H2O2, ISOP, TERP, ISOP-P1, ISOP-P2, TERP-P1, TERP-P2 (transported)
- OH, O3, HO2 (off-line climatologies from NMMB/BSC-CTM full gas-phase simulations)

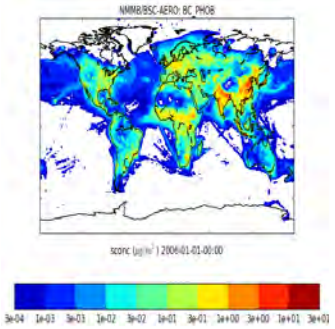
emissions:

- anthro: AEROCOM-ACCMIP emissions ←Lamarque et al., 2010 (ACP)
- DMS: AEROCOM EXP-I ← Dentener et al., 2006 (ACP)
- volcanic: AEROCOM-HC ← T. Diehl
- fires' injection height: under investigation...

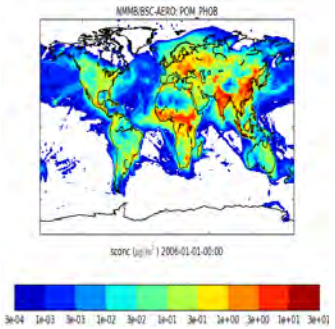
AOD calculation (we have a total AOD now):

- *GADS optical properties*
- *water-uptake depending on RH*

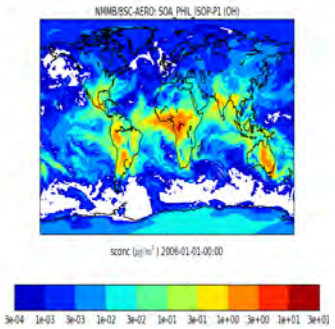
BC_PHOB



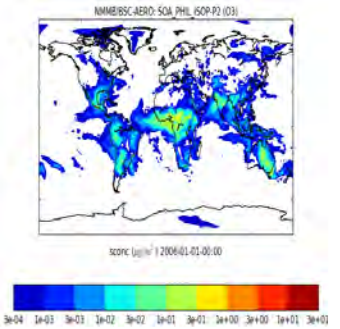
POM_PHOB



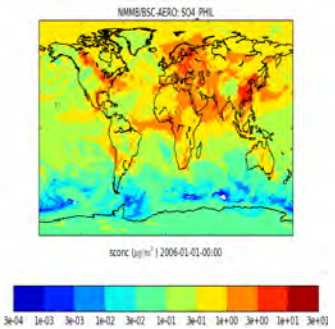
SOA_ISOP-P1



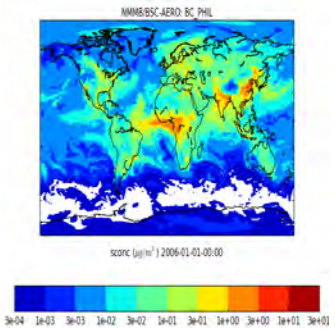
SOA_ISOP-P2



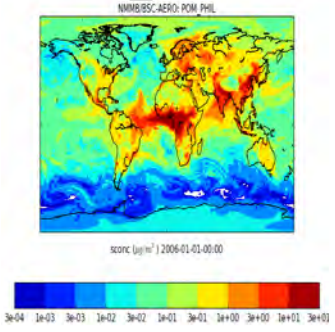
SO4_PHIL



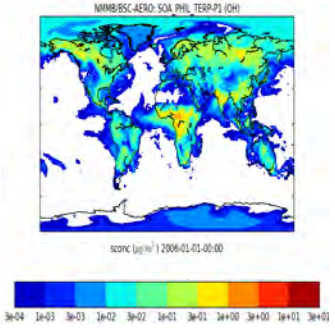
BC_PHIL



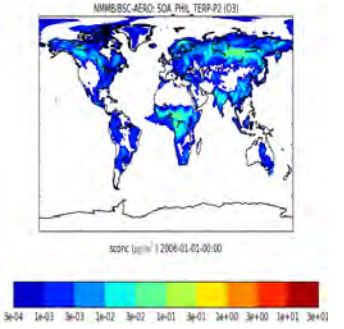
POM_PHIL



SOA_TERP-P1



SOA_TERP-P2



Surface conc. [μg/m^3]

transported gases:

-	-	ISOP-P1, TERP-P1	ISOP-P2, TERP-P2	SO2, DMS, H2O2

clim gases:

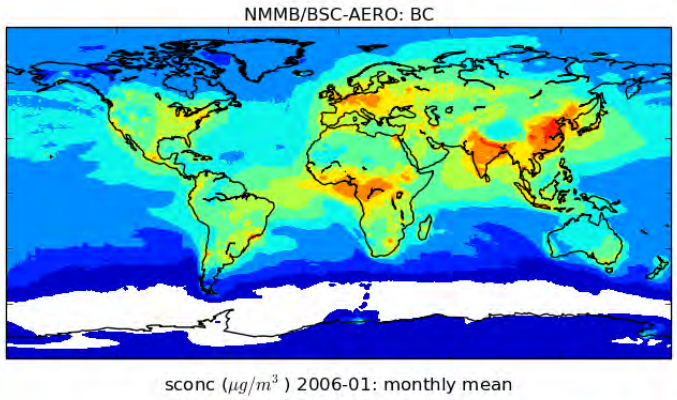
-	-	OH	O3	OH, O3, HO2

emi phob/phil=0.8/0.2 phob-to-phil conv 1.2 days	emi phob/phil=0.5/0.5 OM/OC=1.6 phob-to-phil conv 1.2 days	MEGAN online emissions 2-products SOA mech ← Tsigaridis and Kanakidou, 2003 (ACP)	Sulfur chem (gas and aqueous phases) from MECCA mech (simplified) ← Sander et al., 2011 (GMD)

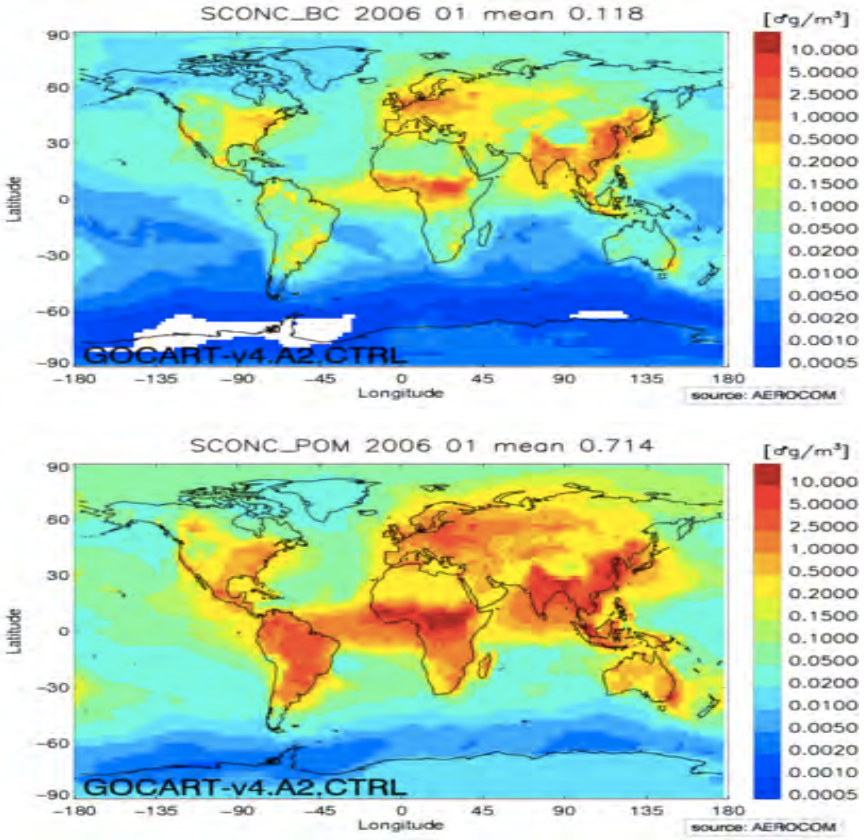
Preliminary RESULTS

JANUARY 2006 SCONC (monthly means)

NMMB/BSC-CTM



GOCART (AEROCOM EXP-II)



BC

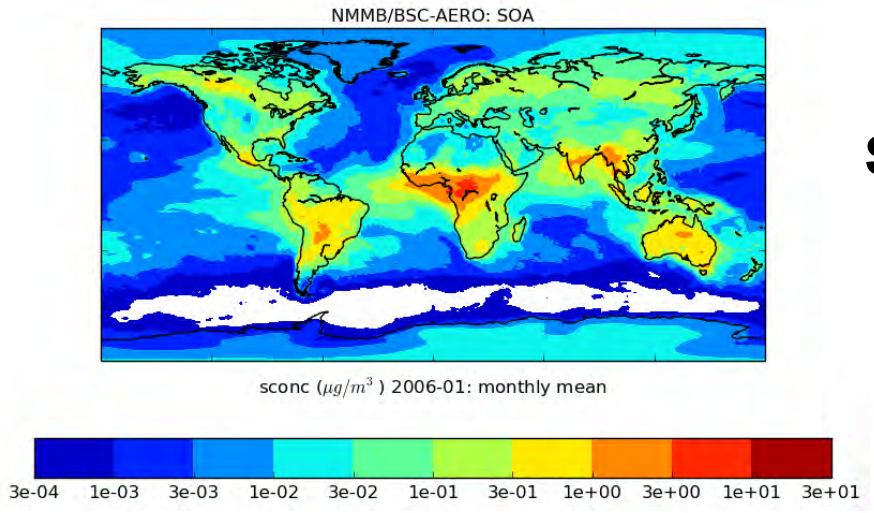
POM

Note: scales are not exactly the same

Preliminary RESULTS

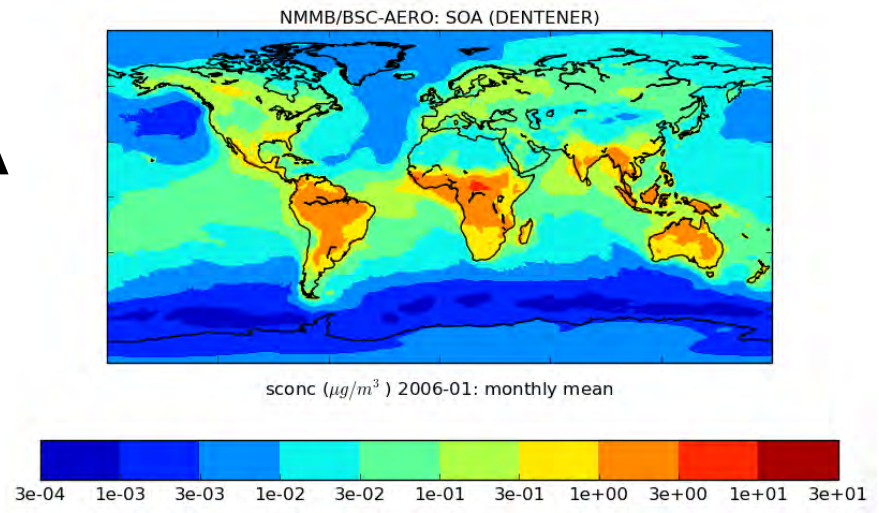
JANUARY 2006 SCONC (monthly means)

NMMB/BSC-CTM (2-PRODUCTS SOA)

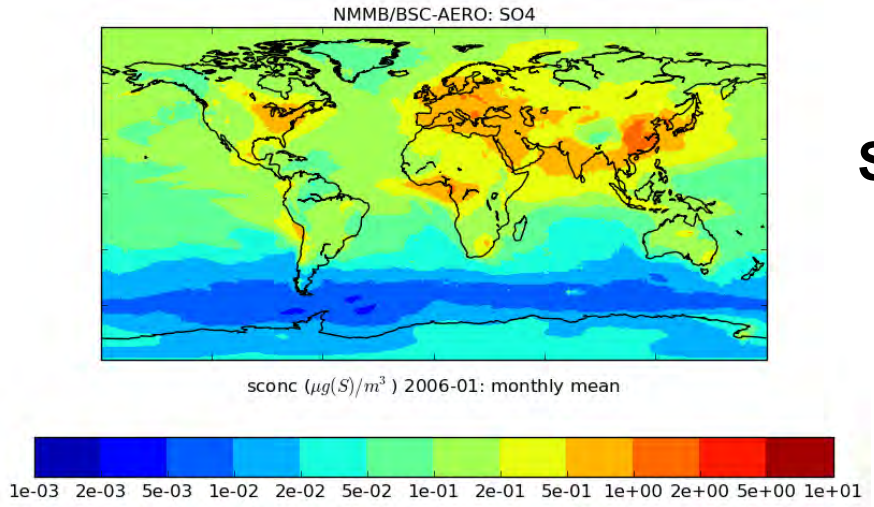


SOA

NMMB/BSC-CTM (DENTENER SOA)

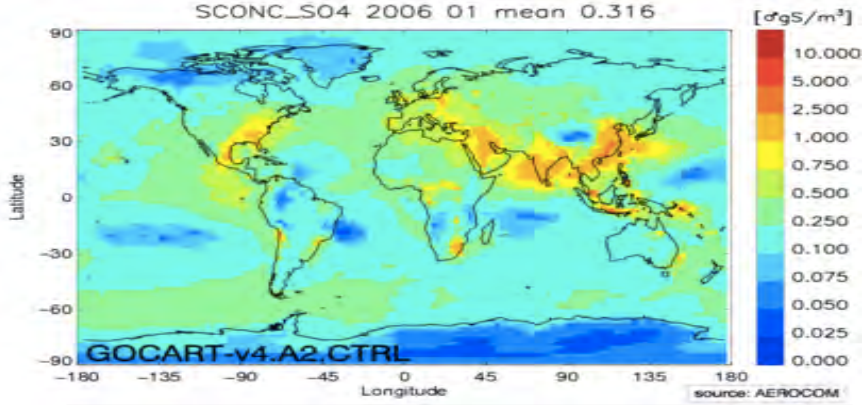


NMMB/BSC-CTM



SO4

GOCART (AEROCOM EXP-II)

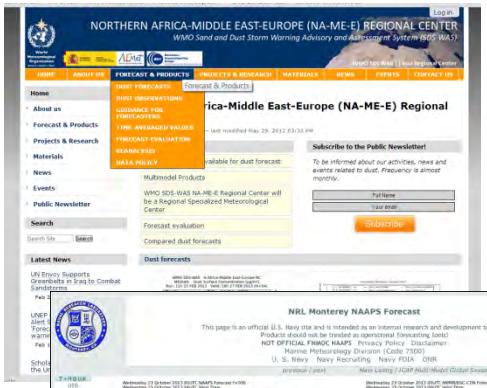


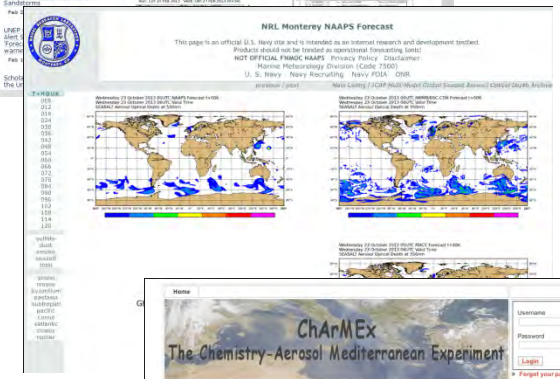
Note: scales are not exactly the same

Future NMMB/BSC-CTM updates in ICAP

- Recalibration of the dust module
- Sea salt scheme based on Jaeglé et al. (2011)
- Data assimilation of MODIS AOD L3 product for mineral dust analysis
- Extending to all aerosol components (BC/OM/Sulfate) to provide smoke and sulfate components

BSC aerosol forecasting collaborations





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

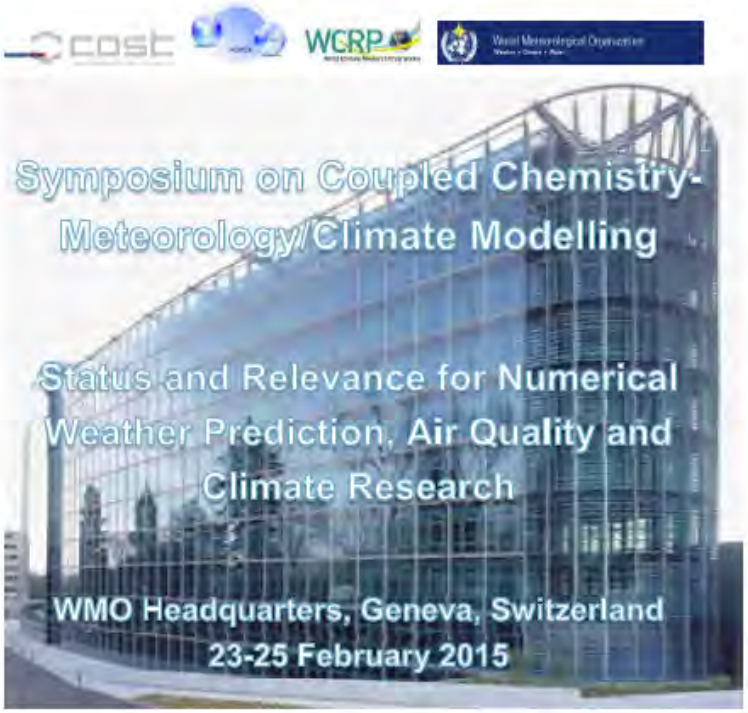
http://sds-was.aemet.es/

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

· **Participate in the Charmex Chemistry-Aerosol Mediterranean experiment**

· **Participate in the AQMEII on-line Air Quality model intercomparison project**

Next Aerosol events



1st Announcement

Key Dates

Deadline for Abstracts	10th Nov. 2014
Notification of acceptance	1st Dec. 2014
Registration (max. 100 participants)	http://eumetchem.info/
Abstract Submission (<1 page)	http://eumetchem.info/

Topics

- Coupled chemistry-meteorology (weather and climate) modelling (CCMM): approaches and requirements;
- Key processes of chemistry-meteorology interactions and their descriptions;
- Aerosol effects on meteorological processes and NWP;
- CCMM for air quality and atmospheric composition;
- CCMM for regional and global climate modelling;
- Model validation and evaluation;
- Data requirements, use of observations and data assimilation;
- Outlook and future challenges.

Organizing Committee and Programme Committee

Alexander Baklanov (WMO), Jose M Baldasano (ES), Veronique Bouchet (CN), Dominik Brunner (CH), Greg Carmichael (US), Renate Forkel (DE), Saulo Freitas (BR), Stefano Galmarini (JRC, EU), Michael Gauss (NO), Georg Grell (US), Christian Hogrefe (US), Øystein Hov (NO), Sylvain Joffre (FI), Rohit Mathur (US), Nicolas Moussiopoulos (GR), Vincent-Henri Peuch (ECMWF), S.T. Rao (US), Michel Rixen (WCRP), K. Heinke Schlünzen (DE), Christian Seigneur (FR), Peter Suppan (DE), Bernhard Vogel (DE)

Venue

The CCMM Symposium will take place at the WMO Headquarters in Geneva. The airport and main train are in easy reach by public transport and offer excellent traffic links to the whole world.

Initiated and supported by

European Cooperation in Science and Technology (COST) Action ES1004: http://www.eumetchem.info/, World Meteorological Organization (WMO) Commission for Atmospheric Sciences (CAS) and World Climate Research Programme (WCRP).

www.bsc.es

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Barcelona Supercomputing Center

Centro Nacional de Supercomputación

Thank you!

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