Ensembles for Air Quality and Atmospheric Composition Prediction

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With contributions from: Juli I. Rubin (NRL, Washington D.C.), Peng Xian, Jeffrey Reid, James Hansen, Jim Peak, Doug Westphal (NRL, Monterey), Jeff Anderson (NCAR, Boulder), Enza Di Tomaso, Sara Basart, Enric Terradellas, Francesco Benincasa, Carlos Péréz Garcia-Pando (BSC, Barcelona), Richard Engelen, Vincent-Henri Peuch, Frédéric Vitart (ECMWF)

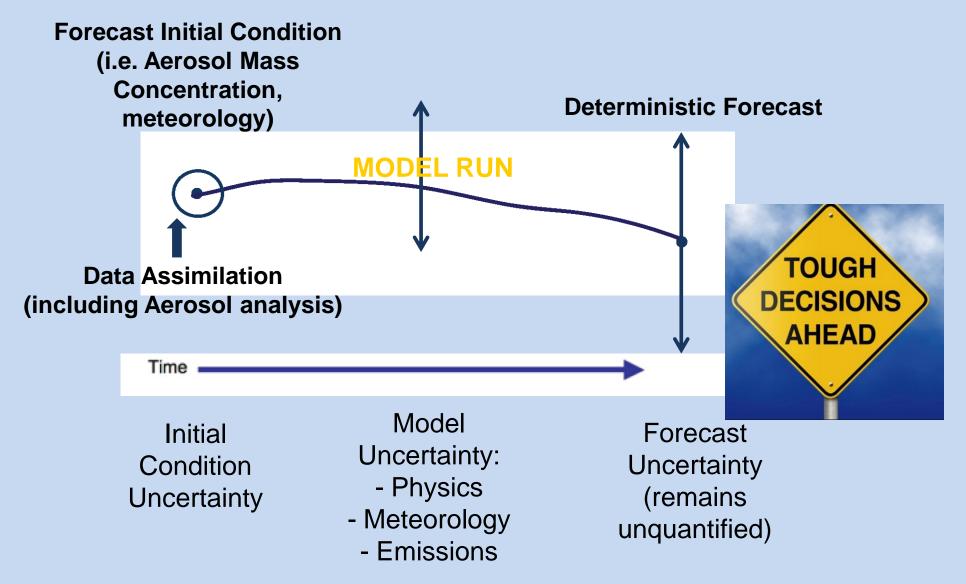


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Outline

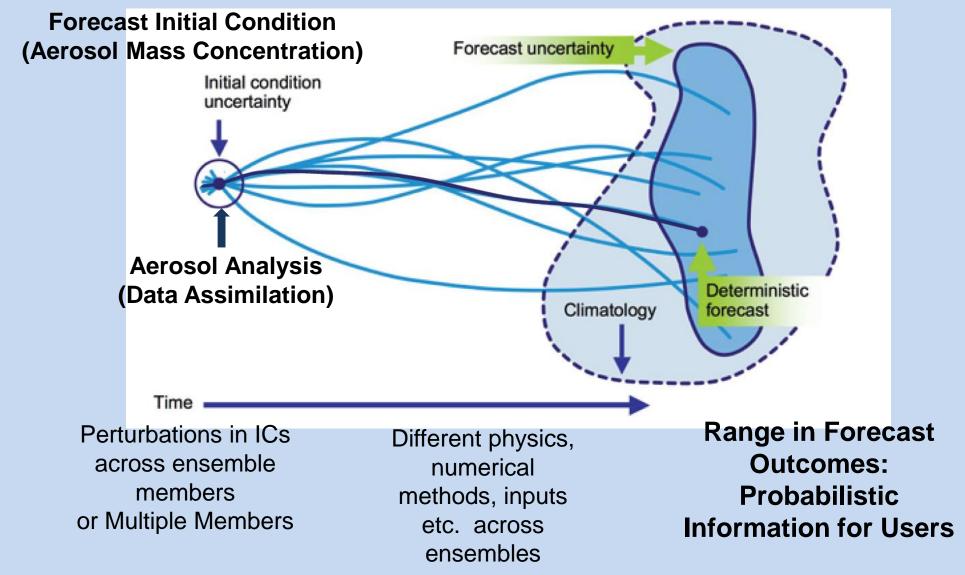
- Background: multi-model ensembles
- The Copernicus Atmosphere Monitoring Service Multi-model ensemble
- for European Air Quality
- Other multi-model examples of AC ensembles (focusing on aerosols)
 - International Cooperative for Aerosol Prediction multi-model global ensemble
 - WMO-Sand and Dust Storm warning and assessment system
- Background: perturbed physics ensembles
- Examples of ensemble prediction and assimilation systems for AC
- Conclusions

The Single-run Perspective



Credits: Juli Rubin

The Ensemble Perspective



Credits: Juli Rubin

Background: Multi-Model Ensembles

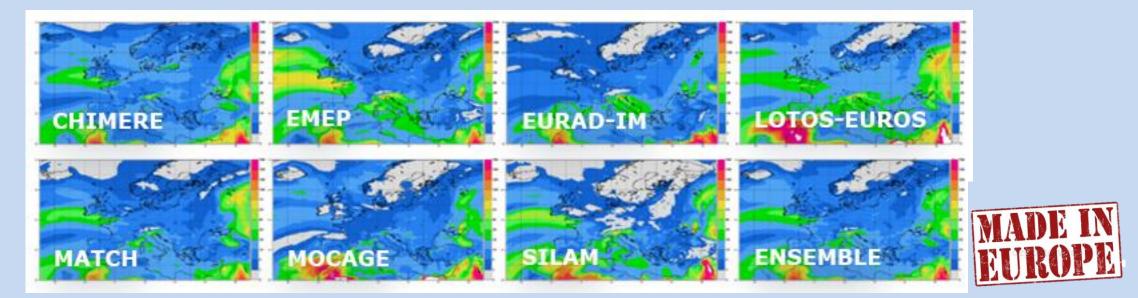
- Different modelling groups around the world represent physical processes in different ways in their models. As a result, there are differences in the forecasts. This is a source of uncertainty known as structural error.
- In order to address this source of uncertainty, the idea of generating multi-model ensembles (MMEs) has been adopted in several communities (for example the climate community) leading to probabilistic predictions.
- A MME is distinct from a Perturbed Physics Ensemble (PPE), in that it emphasises structural errors between different models rather than initial condition or parameter errors within a single model configuration.
- PPEs are commonly used for extended-range weather predictions and data assimilation while MMEs are increasingly used in combination with PPEs for various type of projections including seasonal forecasts, climate change, malaria modelling and air quality, to mention a few.
- For a review of the relative merits of MMEs, see for example Tebaldi and Knutti (2007)

Background: Multi-Model Ensembles (ii)

- The skill of the multi-model system is overall better than the skill of any individual model. Over specific regions, combining several models leads to better forecasts than the best individual model even when number of ensemble members is small
- Different methods to weigh the various members of a MMEs have been proposed in the literature
- Those range from simple mean/median to more sophisticated methods based on reliability of the individual members
- Some argue that excluding poor performing members might bias the outcome and lead to undersampling of the PDF of the forecast.
- Simple averages are sensitive to outliers, while median values provide a more robust estimate.
- For air quality and atmospheric composition applications, both the median and mean approach are used. For operational reliability, however, preference is given to the median approach since it is not uncommon that any given single member may show very poor performance or not provide the forecast in a timely manner.

Multi-Model Ensembles for Air Quality and Aerosol Prediction

An operational multi-model ensemble: the Copernicus Atmosphere Monitoring Service (CAMS) European air-quality forecasts



- Developed as prototype in 2005 during the projects GEMS and follow-on MACC, the CAMS regional forecasting service provides daily 4-day forecasts of the main air quality species from 7 state-of-the-art atmospheric chemistry models and from the ENSEMBLE median.
- Boundary conditions are provided by a global run performed at ECMWF
- This was the first multi-model ensemble system for regional air quality applications ever to be established world-wide.

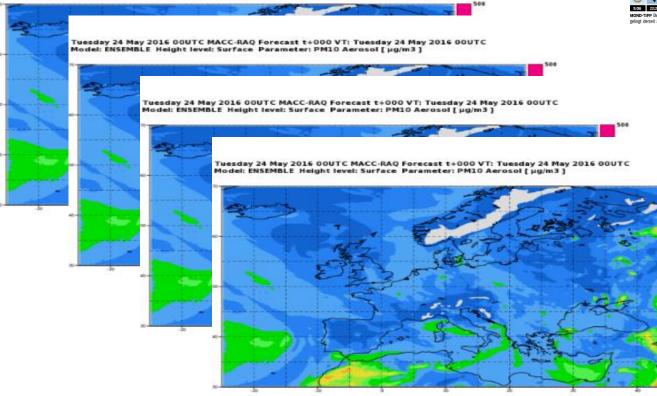
Source: http://atmosphere.copernicus.eu/documentation-regional-systems

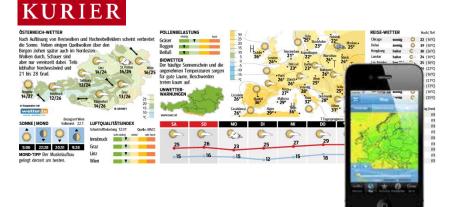


European Air Quality

Europe-wide, ~15 km, hourly outputs to +96h

Tuesday 24 May 2016 00UTC MACC-RAQ Forecast t+000 VT: Tuesday 24 May 2016 00UTC Model: ENSEMBLE Height level: Surface Parameter: PM10 Aerosol [µg/m3]



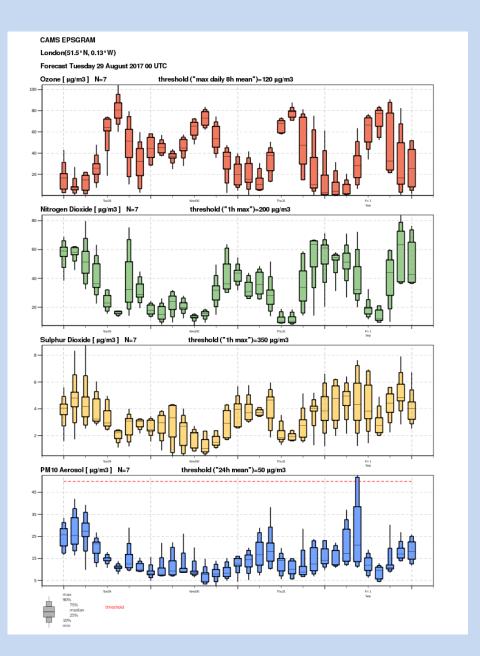


> 450 "power users"
 downloading daily air
 quality information

150



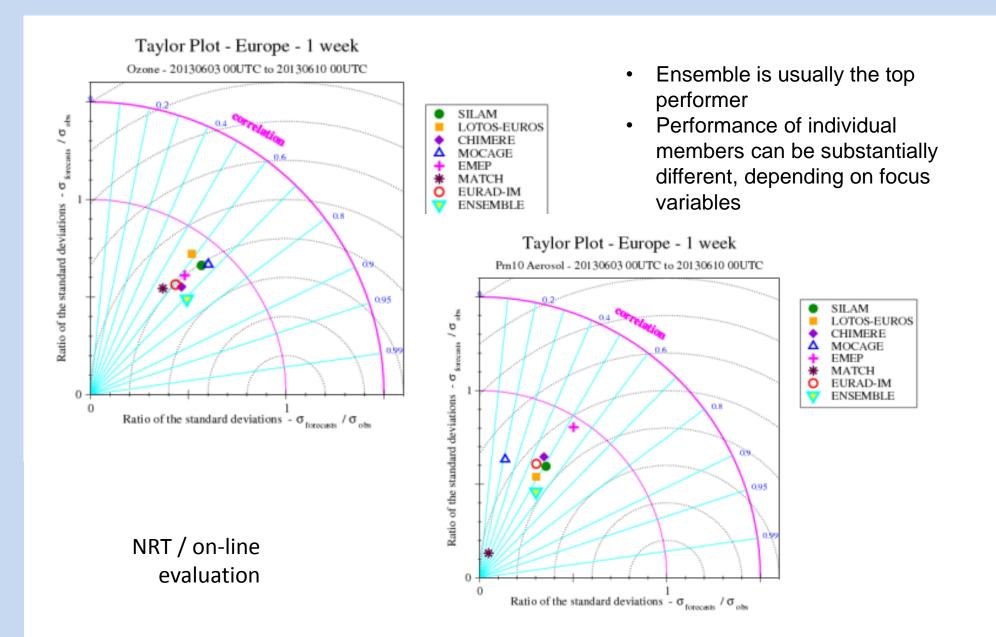
EPSGRAM for air quality parameters



- Same approach used for the ENS meteograms for meteorological variables but applied to pollutants such as ozone, NO2, SO2 and PM10.
- Multi-model spread used as a measure of forecast uncertainty
- Products provided over the major European cities
- Used to forecast the probability of AQ threshold exceedances which are fined by the European Commission (monetary value)

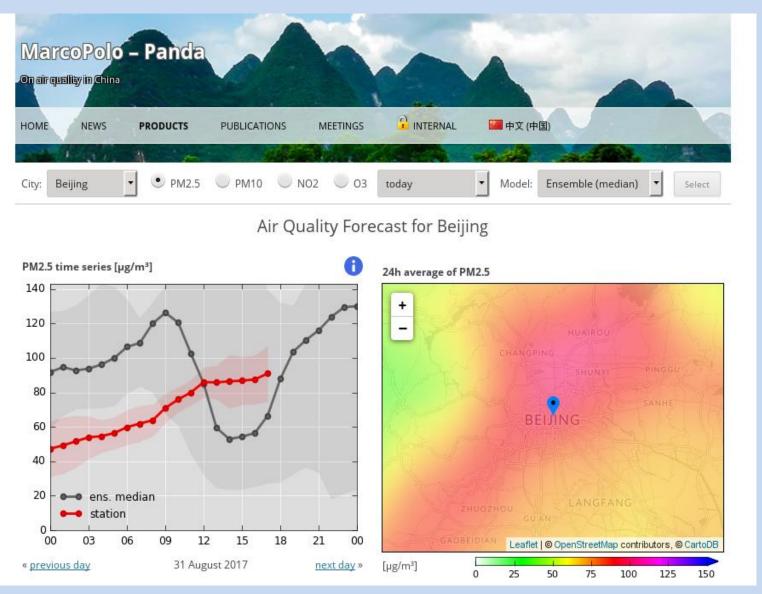


European Air Quality Verification





CAMS European air quality approach exported to China



http://www.marcopolo-panda.eu/

 Within EU-funded FP7 projects PANDA and MarcoPolo,
 Chinese and European partners co-operated to study the air quality in
 China by using space observations and modelling.

- The MACC/CAMS approach was exported to China
- Several modelling groups were involved to provide AQ forecasts
- Ensemble products were generated





International Cooperative for Aerosol Prediction (ICAP)





International Cooperative for Aerosol Prediction (ICAP/AEROCAST)

ICAP is an international forum for aerosol forecast centers, remote sensing data providers, and lead systems developers to share best practices and discuss pressing issues facing the operational aerosol community. While the dynamical meteorology community has a well developed protocols and near real-time observing systems to support forecasting, the aerosol community is only beginning to organize. Infrastructure and data protocols need to be developed between operational centers in order to fully support this emerging field.

ICAP 9th Working Group Meeting: Radiative Transfer and Impacts of Aerosol Radiative Forcing on Numerical Weather Prediction: June 26 - 28, 2017, University of Lille, France

Inquiries: Oleg Dubovik, Jeff Reid, Peter Colarco

The purpose of the 9th working group meeting of the International Cooperative for Aerosol Prediction (ICAP) is to assess the current state of the art and capabilities of radiative transfer models and techniques as applicable to remote sensing of aerosols in the Earth system and use in numerical weather prediction (NWP) models. Recent progress in aerosol remote sensing has placed a considerable demand on radiative transfer forward modeling capabilities in order to close the observation problem, including the use of polarimetric and multi-angle measurements and additional consideration of the surface BRDF. Data assimilation approaches for aerosol prediction models are increasing dependent themselves on forward modeling observed quantities (i.e., radiance) from the model fundamental parameters of aerosol mass and composition, including as well how the aerosol radiances potentially impact the radiance simulation for traditional NWP meteorological data assimilation (e.g., temperature). Further, the inclusion of aerosol radiative transfer inline in NWP models permits radiative forcing of the aerosols to feed back on the NWP solution itself. We will review the current state of the art and current capabilities of the ICAP and other modeling centers, share recent progress, and plan for the future. <u>Meeting PDFs</u> • ICAP is an unfunded, international forum for aerosol forecast centres, remote sensing data providers, and lead systems developers to coordinate efforts and share best practices.

- ICAP organizes yearly meetings to discuss pressing issues facing the operational aerosol community.
- It also coordinates the first global multi-model Ensemble for aerosol forecasts (described in Sessions et al 2015, ACP)

http://icap.atmos.und.edu/

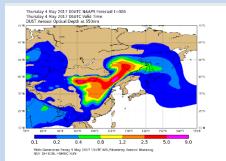


ICAP MME

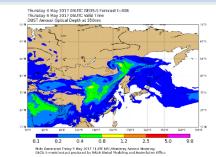


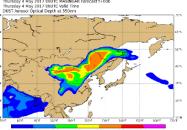
- Participating members are: BSC, Copernicus/ECMWF, US Navy/FNMOC, NASA/GMAO, JMA, NCEP, UKMO, and MeteoFrance (FMI to join soon)
- Aerosol Optical Thickness consensus of deterministic models from 8 centres out to 5 days
- New parameters in future, including surface concentrations
- It helps to identify problem areas for aerosol modeling.
- Ensemble is the top performer (Sessions et al 2015)
- Provides reliable forecast guidance and serves as a research/reference dataset (e.g. TIGGE NWP)
- Public website with ensemble aerosol charts https://www.nrlmry.navy.mil/aerosol/
- Maintained by NRL, Monterey (credits: Peng Xian)

Example: East Asian dust case: May 4, 2017

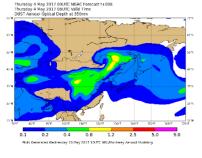


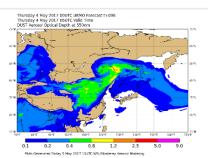


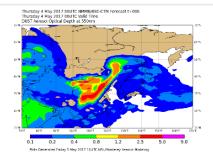


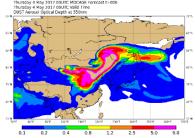






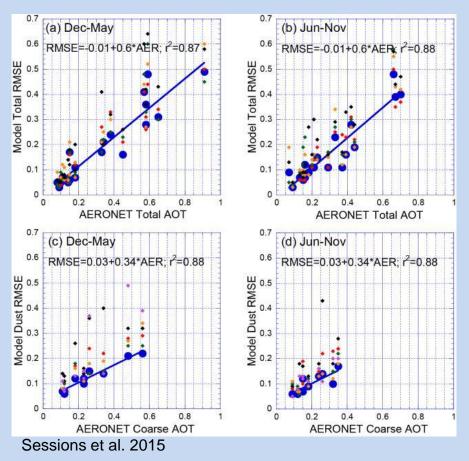






ICAP Multi-Model Ensemble products

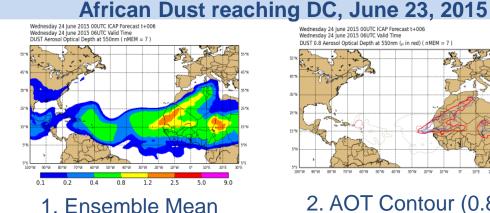
https://www.nrlmry.navy.mil/aerosol/



Used by WMO Sand and Dust Storm Warning System (SDS-WAS)

https://sds-was.aemet.es/forecast-products/dust-forecasts/sds-was-andicap-ensemble-forecasts Credits: Peng Xian (NRL)

- First MME for global aerosol prediction
- Probabilistic products with independence among ensemble members.
- Ensemble mean is the top performer (large blue dots)



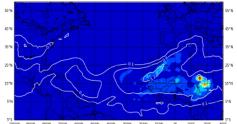


2. AOT Contour (0.8)

Nednesday 24 June 2015 00UTC ICAP Forecast t+006 Wednesday 24 June 2015 06UTC Valid Time OUST AOD Warning Area (>50% members above 0.8) (nMEM = 7)

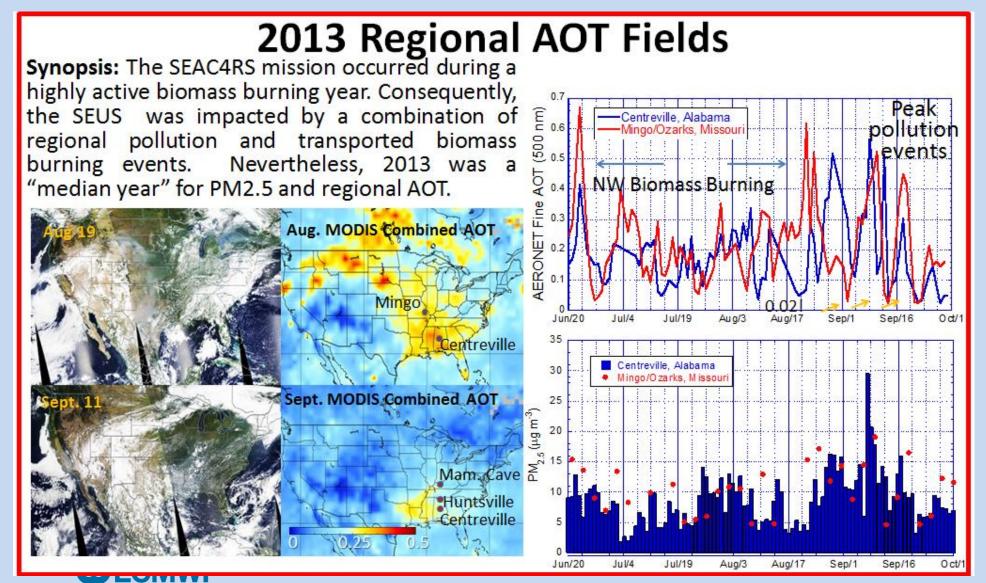
3. Dust Warning Product

Wednesday 24 June 2015 00UTC ICAP Forecast t+006 Wednesday 24 June 2015 06UTC Valid Time OUST Mean AOD at 550nm (white) with Nrml Spread (fill) (nMEM = 7)



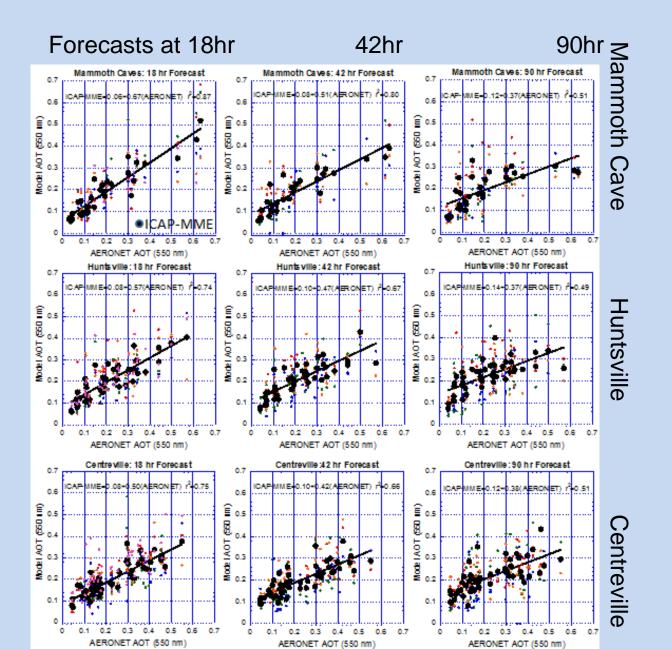
4. Normalized **Ensemble Standard** Deviation

Southeast U.S. case



Credits: Peng Xian and Jeff Reid (NRL)

AOT Validation with AERONET

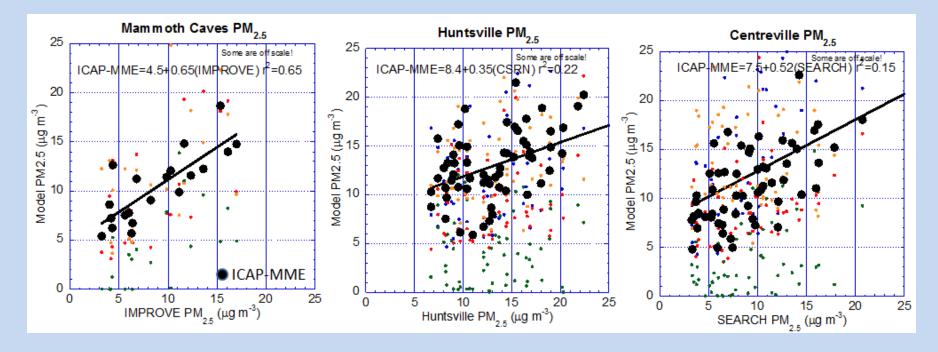


Bold black = ICAP-MME Colored points = individual members.

- Models do well at AOT with solid scores out to 4 days.
- This can be attributed to the fact that in this case AOT distributions are dominated by synoptic meteorology and transport.
- There is stronger bias with forecast range as expected.
- ICAP MME is the top performer among all the models.

Credits: Peng Xian and Jeff Reid (NRL)

18hr PM2.5 forecast



- While all ICAP-MME members did well in predicting AOT, PM2.5 prediction was marginally skillful. PM2.5 is much scattered compared to AOT validation and PM2.5 correlation is only 0.15 for Centreville.
- Models did perform better in the Ohio River Valley (Mammoth Cave), with its high industrial emissions. However in regions with high biogenic emissions the models showed almost no skill (eg. Centerville).
- This is connected to the fact that the near surface environment is often decoupled from the upper levels. Surface PM2.5 recovers much more quickly than AOT after precipitation events.
- Interestingly, the ICAP-MME performed best overall.

CECMWF

WMO Sand and Dust Storm Warning Advisory and Assessment System

	World Meteorological Organization Weather • Climate • Water				
About us Governance	HOME CONTACT US LIGT OF TOPICS LINKS CLIMATE STATISTICS FAC World Weather Research Programme (WWRP)	Related iter			
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rogrammes FCS eetings	and Assessment System	2013 Calendar			
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emes acancies sitors' info	The SDS-WAS programme at WMO	World Weathg Open Stience Confer 17-23 August 21			
arch	SDS-WAS was established in 2007 in response to the intention of 40 WMO member countries to improve capabilities for more reliable sand and dust storm forecasts. Research forecasting products from atmospheric dust models may substantially contribute to risk reduction in many areas of societal benefit. It will rely on real-time delivery of products. More than 15 organizations currently provide daily dust forecasts in different geographic regions. The SDS-WAS integrates research and user communities (e.g. medical, aeronautical, agricultural users). SDS-WAS is established as a federation of partners organized around regional nodes. At the moment two nodes are established: the Northern Africa-Middle East- Europe Node (hosted by Spain) and the Asian Node (hosted by China). The SDS-WAS mission is to achieve comprehensive, coordinated and sustained observations and modeling capabilities of sand and dust storms in order to improve the monitoring of sand and dust storms to increase the understanding of the dust processes and to enhance dust prediction capabilities.				
	Scientific background and modeling of sand and dust storm events				
	SDS-WAS Implementation Science and Implementation Plan	Sand & Dust Storms			

OBJECTIVES:

- Identify and improve products to monitor and predict atmospheric dust by working with research and operational organizations, as well as with users
- Facilitate user access to information
 - Strengthen the capacity of countries to use the observations, analysis and predictions provided by the WMO SDS-WAS project

THREE REGIONAL NODES:

- North Africa-Middle East-Europe Node, managed by BSC/AEMET
- Asian Node, managed by CMA
- Pan-American Node, managed by CIHM

SDS-WAS (http://www.wmo.int/sdswas)

SDS-WAS NA-ME-E Regional Centre (*)

World Meteorological Organization wave - Grant + New	Encelease Supercomputing Center Carter Macard an Supercomputation	and the first of the second
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Materials	ANALYSIS VTA POLICY Vailable for dust	 Joint visualization
News Events	Multimodel Products WMO SDS-WAS NA-ME-E Regional Ce	Common forecast evaluation
Public Newsletter	be a Regional Specialized Meteorolog Center	
Search Search Site	Forecast evaluation Compared dust forecasts	• Generation of multi-model products
Latest News	Dust forecasts	 Calculation of monthly evaluation metrics
UN Envoy Supports Greenbelts in Iraq to Combat Sandstorms Feb 25, 2013	WMO SDS-WAS N Africa-Middle East-Europe MEDIAN Dust Surface Concentration (µg/m Run: 12h 25 FEB 2013 Valid: 18h 27 FEB 2013 (60*N	 New sources of data for model evaluation
UNEP Global Environmental Alert Service releases 'Forecasting and early warning of dust storms'	50°N 40°N 30°A	 Sharing model output data files
Feb 18, 2013 Scholarship on desert dust at	20%	 Time-averaged products

http://sds-was.aemet.es

(*) Jointly managed by Barcelona Supercomputing Center and AEMET

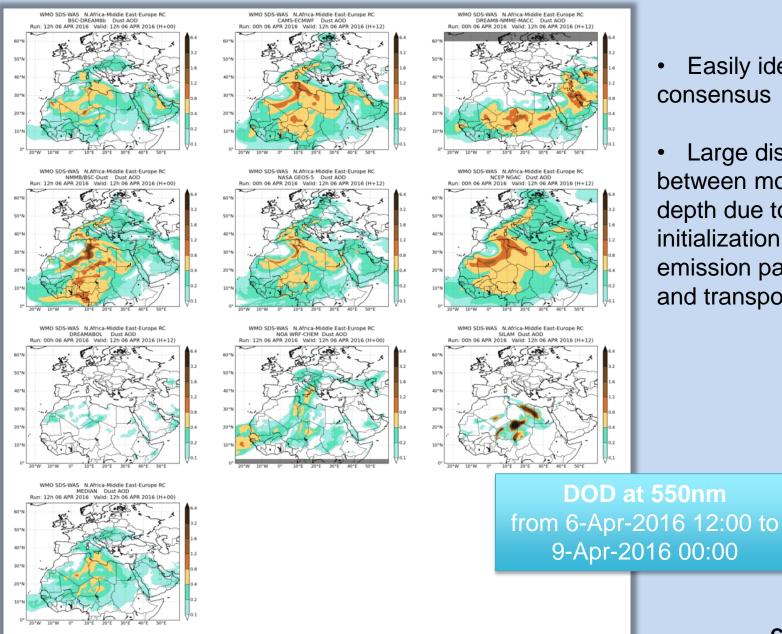
SDS-WAS NAMEE Dust Forecasts

10 (+3 in the pipeline) dust prediction models provide 72 hours (at 3-hourly basis) of dust forecast (AOD at 550nm and surface concentration) covering the NAMEE region.

	Barcelona Supercomputing Center Centro Nacional de Supen	MODEL	RUN TIME	DOMAIN	DATA ASSIMILATION
LMD		BSC-DREAM8b v2.0	12	Regional	No
\bigcirc	Opernicus	CHIMERE	00	Regional	Νο
		LMDzT-INCA	00	Global	No
LSCE		CAMS-ECMWF	00	Global	MODIS AOD
Met Office		DREAM8-NMME	00	Regional	CAMS analysis
		NMMB/BSC-Dust	12	Regional	No
		MetUM	00	Global	MODIS AOD
NASA	AND CONTENS FOR EMVIRONMENTAL AREA	GEOS-5	00	Global	MODIS reflectances
		NGAC	00	Global	No
ISAC		EMA REG CM4	12	Regional	No
		DREAMABOL	12	Regional	No
		NOA WRF-CHEM	12	Regional	No
and arthousand and		FMI-SILAM	12	Global	No

FINNISH METEOROLOGICA

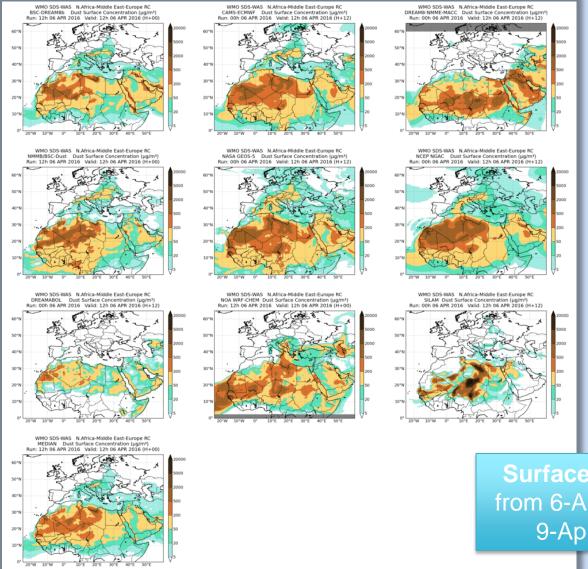
Dust Optical Depth joint visualization



- Easily identifiable areas of consensus
- Large discrepancies
 between models in dust optical
 depth due to difference in
 initialization, dust
 emission parameterizations
 and transport

Credits: Sara Basart, BSC

Surface concentration joint visualization



• Even larger discrepancies in surface concentrations related to differences in emissions and treatment of surface winds and boundary layer.

Surface concentration from 6-Apr-2016 12:00 to 9-Apr-2016 00:00

Credits: Sara Basart, BSC

Generation of multi-model products

WMO SDS-WAS N.Africa-Middle East-Europe RC MEAN Dust Surface Concentration (µg/m³) MEDIAN Dust AOD MEAN Dust AOD MEDIAN Dust Surface Concentration (µg/m³) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) 50°N 40°N WMO SDS-WAS N.Africa-Middle East-Europe RC WMO SDS-WAS N.Africa-Middle East-Europe RC WMO SDS-WAS N.Africa-Middle East-Europe RC RANGE Dust Surface Concentration (µg/m³) WMO SDS-WAS N.Africa-Middle East-Europe RC STDEV Dust Surface Concentration (µg/m³) STDEV Dust AOD RANGE Dust AOD Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00) Run: 12h 06 APR 2016 Valid: 12h 06 APR 2016 (H+00

Surface concentration

DOD at 550nm

from 6-Apr-2016 12:00 to 9-Apr-2016 00:00

Model outputs are bi-linearly interpolated to a common 0.5^ox0.5^o grid mesh. Then, different multimodel products are generated:

CENTRALITY: median and mean

SPREAD: standard deviation and range of variation

Credits: Sara Basart, BSC

Evaluation using AERONET



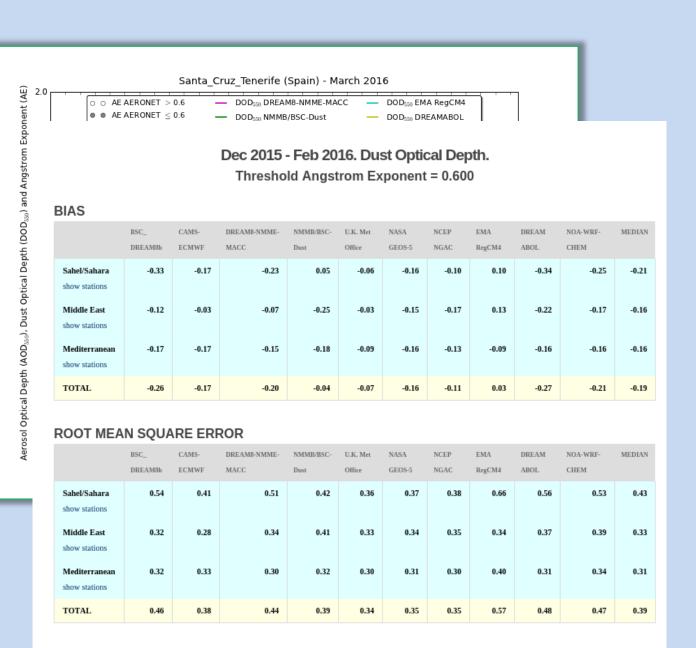
A set of evaluation metrics are selected: *Bias, RMSE, correlation coefficient and Fractional Gross Error*

AERONET observations of Aerosol Optical Depth are filtered to isolate the dust contribution

Calculations evaluation metrics are done for:

- monthly/seasonal/annual
- sites and regions

Ensemble median is not top performer in bias and rms for all regions relative to AOD (UK Met Office is), better performance of the median in surface concentrations



Credits: Sara Basart (BSC)

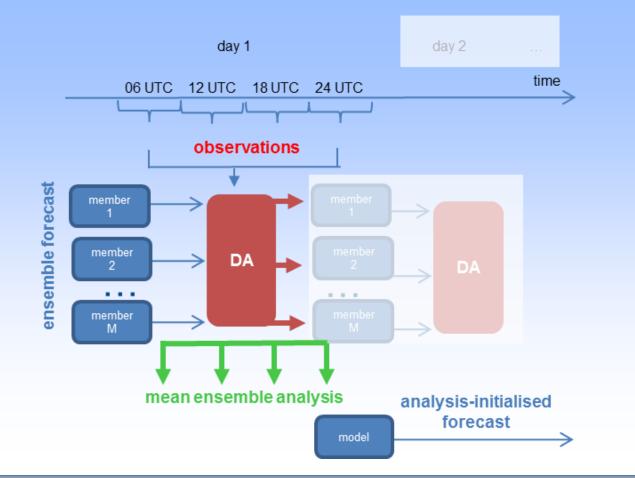
Perturbed Parameter Ensembles for Aerosol Prediction and Assimilation

Background

- Perturbed Physics Ensembles are used at many centres for extended-range weather predictions and other applications
- Ensemble data assimilation is also a growing application for initialization and model error characterization both based on Ensemble Kalman Filter methods or Ensembles of 4D-Var analysis (as it is at ECMWF)
- PPEs for atmospheric composition prediction have also been tested and developed, with assimilation as the main focus
- The problem of how to perturb the initial conditions is common to the meteorological ensembles
- An additional complication is represented by having to also perturb the boundary conditions (i.e the emissions of aerosols/CO2/chemical species)
- Different solutions have been found, but this is still an active area of research
- Very recent experimentation with online systems has included the use of existing meteorological ensembles for extended-range Atmospheric Composition prediction

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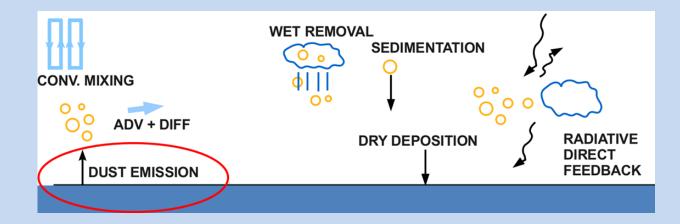
- Dust ensemble forecasts are used at BSC to estimate flow-dependent forecast uncertainty, which is used by data assimilation to optimally combine prior information (forecast) with observations
- The DA scheme is the LETKF (Hunt et al 2007) where the analysis performed locally (particularly suited for aerosol observations which have limited spatial correlations)



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- The implementation of the ensemble forecast is based on known uncertainties in the physical parametrizations of the dust scheme (imperfect model scenario assumption)
- In dust modelling, the emission source term is a particularly large contributor to model error (Huneeus et al., 2011). Hence each ensemble member is run with a different perturbation of uncertain model parameters in the emission scheme.

Modelled dust processes



Barcelona Supercomputing Center

The ensemble forecast has been designed considering model uncertainties with respect to:

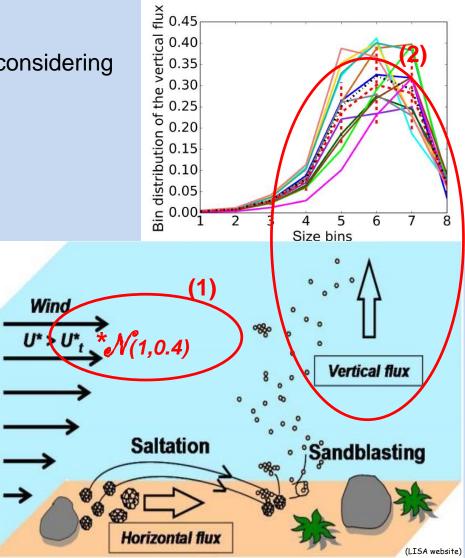
- surface winds,
- soil humidity,
- vertical flux distribution at sources,

by perturbing:

(1) the threshold friction velocity

which is soil moisture-dependent, and determines the velocity above which the soil particles begin to move in horizontal saltation flux;

(2) the vertical flux of dust in each of the eight dust size bins imposing some physical constraint (correlated multiplicative noise across the bins; unimodal distribution).



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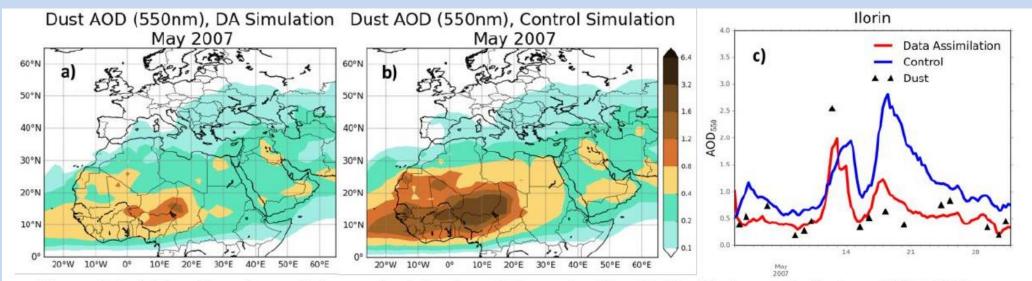


Figure 9.2 a) Monthly values of dust optical depth at 550 nm for May 2007 with the assimilation of MODIS Deep Blue and Dark Target. b) Same as in a), but without data assimilation. c) Comparison between the model simulations in a) and b) and AERONET observations in Ilorin (Niger). Simulations are based on the NMMB/BSC-Dust model. Extracted from Di Tomaso et al. (2016).

- Data assimilation is able to reduce errors in the control simulation
- The agreement with independent dust observations at llorin is much improved

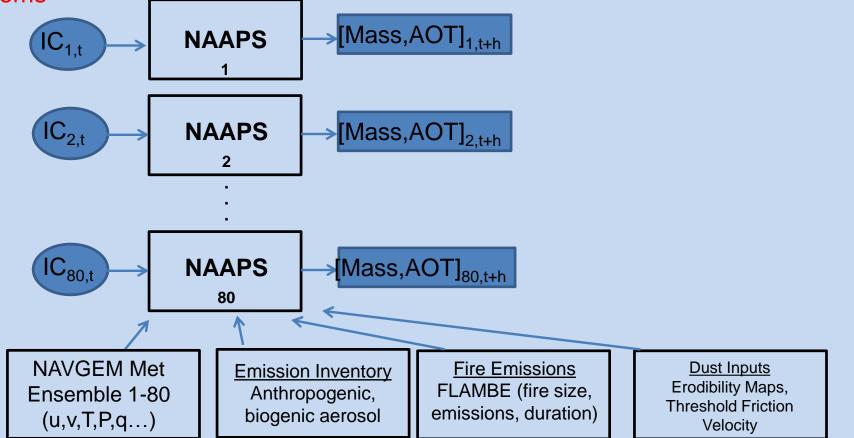


Navy Global Aerosol Prediction: Ensemble NAAPS

Accounts for uncertainty with 20-80 ensemble members in:

- 1. Initial conditions (aerosol mass)
- 2. Meteorology (NAVGEM ensemble)

3. Emissions (perturbed emissions across members) – specific to air quality/aerosol forecasting systems

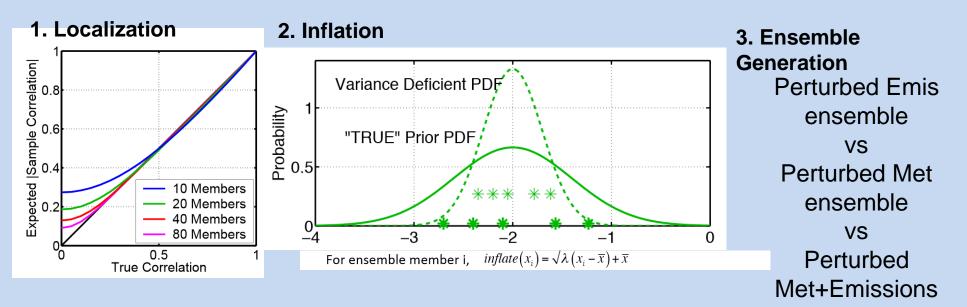


Credits: Juli Rubin, NRL

Navy Global Aerosol Prediction: Ensemble NAAPS + EAKF

Development Efforts have focused on data assimilation:

- 1. ENAAPS coupled to an EAKF data assimilation (DART) to take advantage of flow-dependent forecast errors.
- 2. Ensemble system was optimized to minimize error and produce representative ensemble spread.
- 3. Need for localization decreases with ensemble size

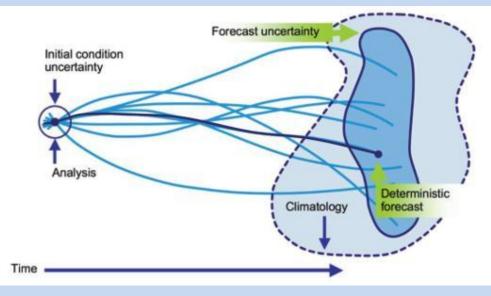


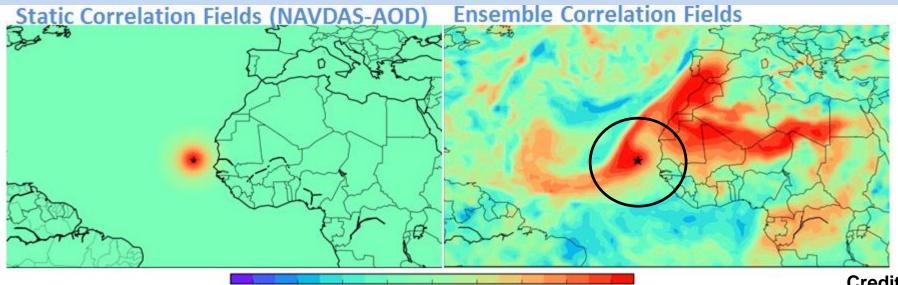
Rubin et al. 2016, ACP



Flow-Dependence: Making better use of observational information

- Ensembles provide a means for representing flow-dependent forecast uncertainty that varies in space and time.
- Flow-dependent representation of uncertainty results in a better analysis.





 $-0.75 \ -0.50 \ -0.20 \ 0.00 \ 0.10 \ 0.30 \ 0.50 \ 0.70 \ 0.90$

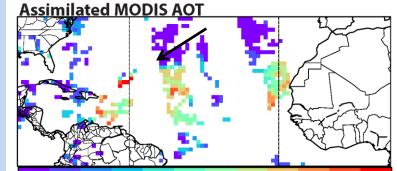
Credits: Juli Rubin, NRL



Ensemble Kalman Filter vs 2D-VAR

Saharan dust event case study on August 2, 2013





MODIS RGB Worldview

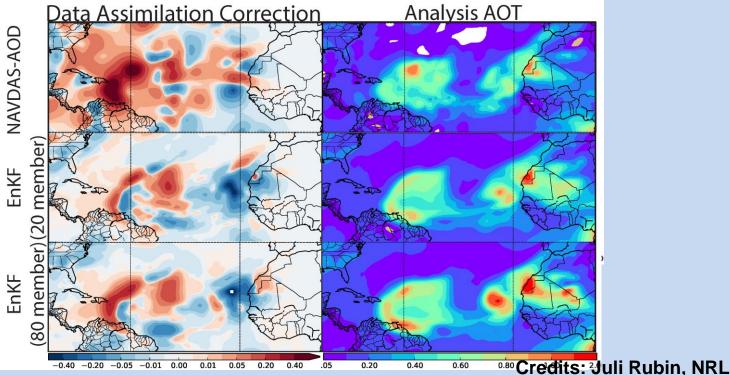
NAVDAS-AOD 2D-VAR:

observationally driven, produces large DA corrections

EAKF: captures dust front shape (not magnitude).

Significant improvement with 80 members in magnitude and position

Rubin et al. 2016, ACP



Ensemble Aerosol Forecasts at ECMWF

• Early attempts involved running the Ensemble of Data Assimilation (EDA) system out to day 5 with prognostic aerosols turned on

• Aerosol perturbations were generated by perturbing satellite aerosol observations of Optical Depth (similarly to what is done for other observations)

 Interesting results were obtained including a sea-salt(*) plume off the coast of Iceland, associated with the 2010 eruption of the Eyjafjallajökull (*no volcanic source was included)

• The EDA has been more recently used to create background error statistics for CO2, aerosols and chemical tracers (Massart, private communication)

• Challenges associated with the perturbations of the emission sources are still being addressed

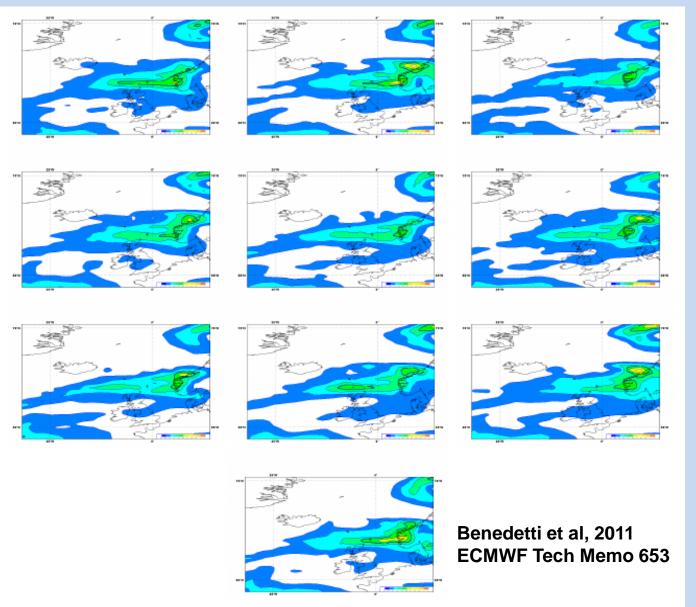
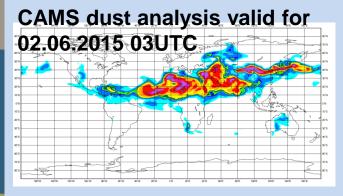
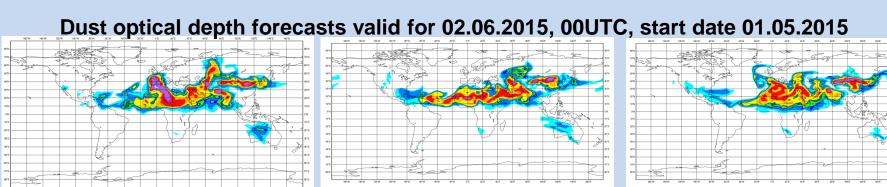


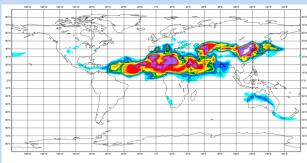
Figure 9: Sea salt plume off the coast of Iceland on April 20, 2010 at 000UTC from ensemble forecasts initialized at 00UTC on April 19, using the analyses from the ECMWF Ensemble of Data Assimilation system.

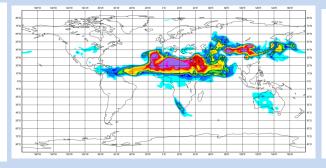
Ensemble Aerosol Forecasts at ECMWF

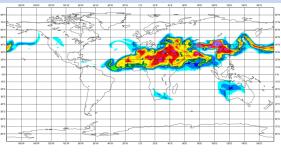


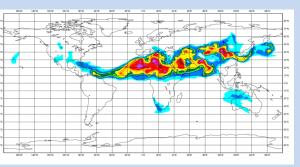
- Recent efforts have involved running the coupled Ensemble Prediction System with prognostic aerosols (CAMS model)
- Ensemble forecasts only have perturbed meteorology
- Aerosol fields differ in the ensemble members as a result of perturbed transport
- For natural aerosols, such as dust, whose emissions depend on wind, sources are indirectly perturbed
- First ever attempt to produce a sub-seasonal prediction of aerosols

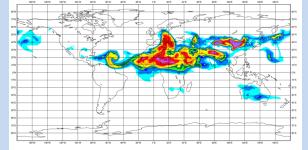


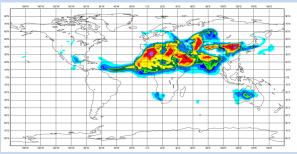














Summary and future outlook

- Ensemble/probabilistic prediction is becoming prominent also for air quality/ atmospheric composition applications
- Various coordinated efforts rely on Multi-Model Ensembles to provide
 - air quality over Europe and China (CAMS, PANDA/MarcoPolo)
 - global aerosol forecasts (ICAP)
 - regional dust forecasts (WMO SDS-WAS)
- Perturbed physics ensembles have also been developed mainly for assimilation applications
- Promising results for ensemble aerosol sub-seasonal to seasonal (S2S) prediction
- The issue of cost could possibly be addressed with reduced precision
- Interest in probabilistic outputs from various stakeholders (i.e. air quality forecasters, aviation industry etc) is likely to increase over time
- Need to promote the use of ensemble products to the wider user community