Ensembles for Air Quality and Atmospheric Composition Prediction

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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

- Forecast Initial Condition (i.e. Aerosol Mass Concentration, meteorology)
- Data Assimilation (including Aerosol analysis)
- Initial Condition Uncertainty
- Model Uncertainty: - Physics - Meteorology - Emissions
- Forecast Uncertainty (remains unquantified)

MODEL RUN

Deterministic Forecast

Credits: Juli Rubin
The Ensemble Perspective

Forecast Initial Condition
(Aerosol Mass Concentration)

Aerosol Analysis
(Data Assimilation)

Perturbations in ICs
across ensemble
members
or Multiple Members

Different physics,
numerical
methods, inputs
etc. across
ensembles

Range in Forecast
Outcomes:
Probabilistic
Information for Users

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

> 450 “power users” downloading daily air quality information
• 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

Ensemble is usually the top performer.
Performance of individual members can be substantially different, depending on focus variables.

NRT / on-line evaluation
CAMS European air quality approach exported to China

• 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

http://www.marcopolo-panda.eu/
International Cooperative for Aerosol Prediction (ICAP)

ICAP is an unfunded, international forum for aerosol forecast centres, 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 protocol and near-real-time observing systems to support forecasting, the aerosol community is only beginning to organize. Information and data protocols need to be developed between operational centres in order to fully support this emerging field.

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/
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)
ICAP Multi-Model Ensemble products

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

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

African Dust reaching DC, June 23, 2015

1. Ensemble Mean
2. AOT Contour (0.8)
3. Dust Warning Product
4. Normalized Ensemble Standard Deviation

Used by WMO Sand and Dust Storm Warning System (SDS-WAS)
https://sds-was.aemet.es/forecast-products/dust-forecasts/sds-was-and-icap-ensemble-forecasts

Credits: Peng Xian (NRL)
Southeast U.S. case

2013 Regional AOT Fields

Synopsis: The SEAC4RS mission occurred during a highly active biomass burning year. Consequently, the SEUS was impacted by a combination of regional pollution and transported biomass burning events. Nevertheless, 2013 was a “median year” for PM2.5 and regional AOT.

Credits: Peng Xian and Jeff Reid (NRL)
AOT Validation with AERONET

- 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)
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.

Credits: Peng Xian and Jeff Reid (NRL)
WMO Sand and Dust Storm Warning Advisory and Assessment System

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 (*)

FORECAST AND PRODUCTS
• Data exchange
• Joint visualization
• Common forecast evaluation
• Generation of multi-model products
• Calculation of monthly evaluation metrics
• New sources of data for model evaluation
• Sharing model output data files
• Time-averaged products

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

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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

DOD at 550nm from 6-Apr-2016 12:00 to 9-Apr-2016 00:00

Credits: Sara Basart, BSC
Even larger discrepancies in surface concentrations related to differences in emissions and treatment of surface winds and boundary layer.
Generation of multi-model products

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 0.5ºx0.5º grid mesh. Then, different multi-model products are generated:

CENTRALITY: median and mean

SPREAD: standard deviation and range of variation

Credits: Sara Basart, BSC
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.

Evaluation using AERONET

https://aeronet.gsfc.nasa.gov/

Credits: Sara Basart (BSC)
Perturbed Parameter Ensembles for Aerosol Prediction and Assimilation
• 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
Ensemble-Based Data Assimilation at BSC

- **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).

Credits: Enza Di Tomaso, BSC
• 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.
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).
Ensemble-Based Data Assimilation at BSC

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

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).
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

IC_{1,t} → NAAPS_1 → [Mass,AOT]_{1,t+h}

IC_{2,t} → NAAPS_2 → [Mass,AOT]_{2,t+h}

... → ...

IC_{80,t} → NAAPS_{80} → [Mass,AOT]_{80,t+h}

NAVGEM Met Ensemble 1-80 (u,v,T,P,q…)
Emission Inventory Anthropogenic, biogenic aerosol
Fire Emissions FLAMBE (fire size, emissions, duration)
Dust Inputs Erodibility Maps, Threshold Friction Velocity

Credits: Juli Rubin, NRL
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

**Credits:** Juli Rubin, NRL
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.

Credits: Juli Rubin, NRL
Saharan dust event case study on August 2, 2013

**EAKF**: captures dust front shape (not magnitude).

**NAVDAS-AOD 2D-VAR**: observationally driven, produces large DA corrections

**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.
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