Initialization of aerosols in LIMA scheme for AROME

RC LACE stay report

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Introduction

LIMA (Liquid Ice Multiple Aerosols) scheme is a two-moment microphysical scheme, which was developed in MESO-NH to improve modeling of the complex aerosol–cloud interactions (Vié et al., 2016). For now the scheme has been implemented in AROME model (cy42t1). Because LIMA is a two-moment scheme, its prognostic variables are not only mixing ratio of hydrometeors (r_C, r_R, r_I, r_S, r_G), but also number concentration of aerosols (N_{Free}, $N_{Activated}$) and hydrometeors (N_C, N_R, N_I) in kg^{-1} units. In the first version constant values were set to the aerosol fields, but it is more precise if we use real aerosol fields for initialization.
There are chemical models that can provide this kind of data, for instance MOCAGE, which is the Météo-France multi-scale Chemistry and Transport Model, which covers a range of scientific applications, from the study of climate-chemistry interaction to chemical weather forecasting (Peuch et al., 1999).

The aerosol types and units are different in MOCAGE and LIMA and the resolution of the models is also different, so before we could run forecast with initial aerosol fields, a lot of preparatory work had to be done. For this work pythons scripts were used based on the *epygram* tools (http://www.umr-cnrm.fr/gmapdoc/meshtml/EPYGRAM/index.html).
LIMA uses lognormal size distribution for each aerosol mode, so an important part of the work was to estimate the parameters of the size distribution. It is possible to calculate from MOCAGE fields, because each aerosol type is separated into six bins. The information about the bins can be seen on Table 1.

Table 1: Size characteristics of MOCAGE aerosols

Bin borders [m]	2.00E-9	1.00E-8	1.00E-7	1.00E-6	2.50E-6	1.00E-5	5.00E-5
Bin borders [µm]	0.002	0.01	0.1	1	2.5	10	50

Mean diameter [m]	4.47E-9	3.16E-8	3.16E-7	1.58E-6	5.00E-6	2.24E-5
Mean diameter [µm]	0.00447	0.0316	0.316	1.58	5	22.4

Table 2: MOCAGE aerosol types (grey background indicates the fields used for AROME/LIMA)

	Nr of bins	Name of aerosol species	Short name	Density [kg/m^3]
species 1	6	Desert dust	DESDUS	2650
species 2	6	Black carbon	BLACKC	1000
species 3	6	Sea salt	DYNSAL	2200
species 4	6	Organics (anthropogenic PM)	ORGANC	1000
species 5	6	Sulfates	SULFAT	1000
species 6	6	Nitrates	NITRAT	1000
species 7	6	Ammonium	AMMONI	1000
species 8	6	Sodium	SODIUM	2200
species 9	6	Chlorine	CHLORE	2200
species 10	6	Water	WATERE	1000
species 11	1	Pollens	POLLEN	800

Table 3: LIMA prognostic variables, which has to be initialized

	Name of variables (number concentrations in kg^{-1})	Short name	Initialized values
1	Cloud droplets	N_CLOUD	calculated from mixing ratio
2	Rain drops	N_RAIN	calculated from mixing ratio
3	CCN free 1	N_CCN_F1	SULFAT+NITRAT+AMMONI from MOCAGE
4	CCN free 2	N_CCN_F2	DYNSAL from MOCAGE
5	CCN free 3 (= hydrophilic BC + O → coated IFN)	N_CCN_F3	BLACKC+ORGANC from MOCAGE
6	CCN activated 1	N_CCN_A1	0
7	CCN activated 2	N_CCN_A2	0
8	CCN activated 3 (= hydrophilic BC + O → coated IFN)	N_CCN_A3	0
9	Pristine ice crystals	N_ICE	calculated from mixing ratio
10	IFN free 1	N_IFN_F1	DESDUS from MOCAGE
11	IFN free 2	N_IFN_F2	HBLACK+HORGAN from MOCAGE
12	IFN activated 1	N_IFN_A1	0
13	IFN activated 2	N_IFN_A2	0
14	Coated IFN in crystals (= hydrophilic BC + O)	N_IFNCOAT	0
15	Homogeneous freezing of CCN	N_CCN_FR	0

MOCAGE aerosol fields

Table 2 shows the available MOCAGE aerosol types. We used the first seven species from this list for LIMA scheme. We used a special experiment of MOCAGE, where black carbon and organics were separated into hydrophobic (HBLACK, HORGAN) and hydrophilic types (BLACKC, ORGANC). Later this additional two species was also used in LIMA. This separation is important in LIMA, because one group of cloud condensation nuclei (CCN) is special. These aerosols act first as CCN and then as coated ice freezing nuclei after freezing.
LIMA predicts the number concentration of free and activated aerosols. For initialization, every aerosols were considered as free aerosols and there were no activated particles. So MOCAGE fields were put into the free CCN and IFN fields (see Table 3 right column).

Size distribution

For the determination of the size distribution of aerosols three-month long MOCAGE experiment was used from 6th March 2016 to 31st May 2016. Files were used in three-hour temporal resolution to take into account the diurnal cycle of aerosols. Average aerosol values were calculated for each bin. These values were applied to estimate the parameters of lognormal size distribution.

Computation steps to determine the size distribution

1. Read MOCAGE fields (species 1-7+HBLACK, HORGAN) for each vertical level.
2. Convert the variables from mixing ratio (x) to number concentration (x') with the following formula seen below:

$$x' = \frac{x}{\rho} / \left(\frac{4}{3} \pi \left(\frac{d}{2} \right)^3 \right)$$

3. Calculate the field mean at each vertical level.
4. Plot vertical profile of aerosol types.

Usually the number concentration is close to constant until 30 levels (see Figure 1) so vertical mean value was calculated from the values from level 30 to level 47. We did this for each bin. These mean values were used to estimate the parameters (d_X and σ_X) of lognormal size distribution:

$$n(d_a)\mathrm{d}d_a = \frac{N_X}{\sqrt{2\pi} d_a \ \ln(\sigma_X)} e^{-\left(\frac{\ln(d_a/d_X)}{\sqrt{2}\ln(\sigma_X)}\right)^2} \mathrm{d}d_a$$

Since there are only six bins, the fitting is very difficult, so a fundamental method, the trial and error approach was chosen. Finally, with the help of Benoit Vié the parameters seen in Table 4 were implemented into the model. Figure 2 illustrates the fitted function on the data in the case of IFN_F2.

Table 4: Estimated parameters of lognormal size distribution for LIMA variables

	diameter [μm]	sigma
CCN_F1	0.1	2.7
CCN_F2	0.02	2.2
CCN_F3	0.016	2.5
IFN_F1	0.05	2.4
IFN_F2	0.016	2.5

Figure 1: Vertical profiles of hydrophobic black carbon (left) and sea salt (right) from MOCAGE for each bin

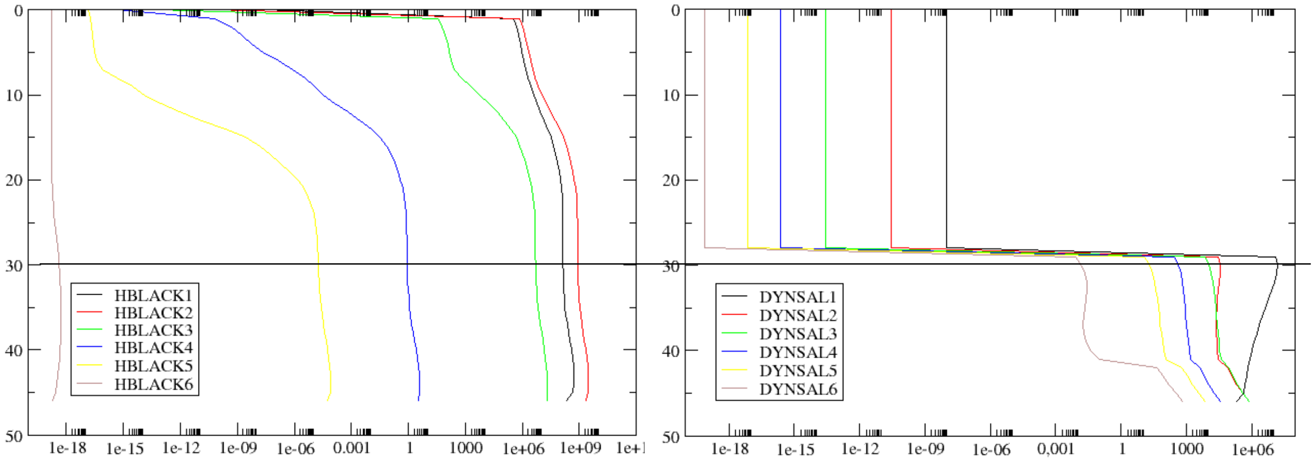
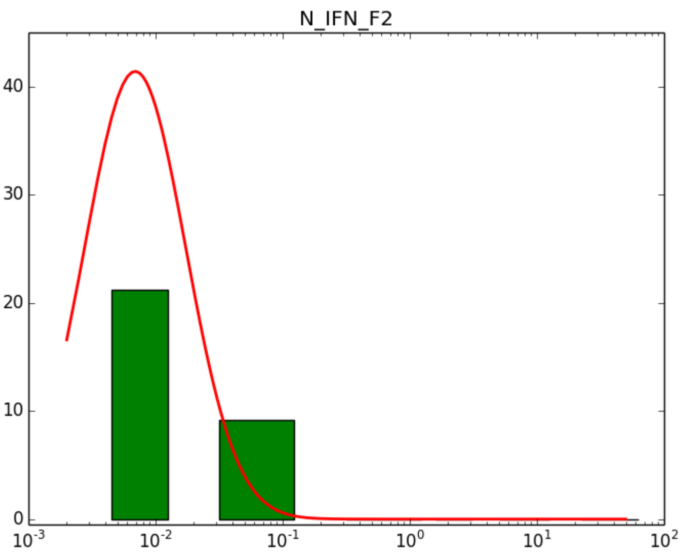


Figure 2: Estimated size distribution (red) based on mean number concentration of IFN_F2 data (green columns).



Conversion of MOCAGE aerosol fields into AROME

For the conversion of MOCAGE aerosols types into LIMA the estimated size distribution was used. It is known that the third moment of the size distribution is proportional to the total volume, so the total mass can be given with the following formula:

$$M = \frac{4}{3}\pi\int \rho(r) r^3 n(r) \mathrm{d}r = \frac{\pi}{6} N \rho d_m^3 \exp(\frac{9}{2}\ln\sigma^2)$$

With this formula mixing ratio can be converted into number concentration. Combining the MOCAGE aerosol types into LIMA types happens easily summarizing the proper converted number concentrations from MOCAGE.

In the next step vertical and horizontal interpolation of the aerosol fields took place. For the vertical interpolation we need the pressure levels in AROME that are easily gained with the help of epygram, as well as the geometry of the fields.

AROME uses a mass-based hybrid pressure terrain-following coordinate, and ICMSH files contains only parameters A and B, so before the vertical interpolation was performed, the model levels of AROME were transformed to pressure values at 90 model levels. In MOCAGE files there are pressure fields at each model level (47 levels).
Since the lowest model level is lower in AROME than in MOCAGE, the values of the lowest MOCAGE level were used at the lowest levels in AROME. As the horizontal model resolution is also different, horizontal interpolation was performed too. The order of the horizontal and vertical interpolation is also relevant. Both orders were tested and in the end, we decided to start with vertical and then horizontal interpolation, because it gives smoother fields over the orography.

Previously a local python library called '*converto*' was used for interpolation, not *epygram*. During the stay former interpolation scripts was rewritten to use *epygram* library instead of *converto*.
After the interpolation, an initial AROME file was ready to run a forecast with 15 species in LIMA scheme.

Case study: 5th April 2016

The modification concerns mainly the microphysics, so 5th April 2016 was chosen, when a great amount of precipitation fell in France. Figure 3 shows the 24-hour accumulated precipitation fields (rain+snow+graupel) for the original ICE3 scheme, the first version of LIMA scheme with 8 species, the actual LIMA experiment with 15 species and observations. Compared the result of LIMA scheme with ICE3 lots of improvement can be seen, but it seems the initialization of aerosols does not affect too much on the precipitation fields, only in Bordeaux region of France and over the Mediterranean sea can be seen more precipitation in the new version.

In this experiment the initial values of number concentration of hydrometeors were set to zero, because the new routine which should have set the number concentrations based on mixing ratios did not work and during my stay the problem was not solved. In December, after debugging the experiment was rerun, but the results were very similar to the one presented here.

As it can be seen a lot of work with the LIMA scheme remained. It was planned to run an experiment where not only the initial file contains the aerosol fields from MOCAGE but also the LBC files. Unfortunately there was no time to perform more experiments during my stay. But the work is continued by Yann Seity.

Acknowledgment

I would like to thank Yann Seity for all his help and guidance during my stay. I found the discussions really useful with him and Benoit Vié.

References

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Vié, B., Pinty, J.-P., Berthet, S., and Leriche, M.: LIMA (v1.0): A quasi two-moment microphysical scheme driven by a multimodal population of cloud condensation and ice freezing nuclei, *Geosci. Model Dev.*, 9, 567-586, doi:10.5194/gmd-9-567-2016, 2016.

Figure 3: 24-hour accumulated precipitation field on 06/04/2016 at 00UTC (initial date: 05/04/2016 00UTC) in case of ICE3, LIMA with 8 species (first version), LIMA with 15 species (new experiment) and RADAR observations.