Barcelona Supercomputing Center
Centro Nacional de Supercomputación
RES RED ESPAÑOLA DE SUPERCOMPUTACIÓN

AECT-2020-1-0018 Addressing a key dust model uncertainty: haboob dust storms

1. General Information

Activity Id
AECT-2020-1-0018

a) Activity Title
Addressing a key dust model uncertainty: haboob dust storms

b) Area
Astronomy, Space and Earth Sciences

c) Type of application
Standard Activity for the next 4 months

--- 2. Research Project Description

a) Is this a Test Activity?
No

b) Is this a Long Term Activity that will extend over two application periods?
No

c) Brief description of the Project
The proposed activity will constitute an important part of the ongoing Marie-Skłodowska-Curie Individual Fellowship project "Addressing key uncertainties in mineral DUST EmiSsion modelling to better constrain the global dust cycle" (DUST.ES, grant agreement No. 789630) awarded to the applicant, Dr. Martina Klose. DUST.ES is funded through the European Union's Horizon 2020 research and innovation programme. The objective of DUST.ES is to constrain present-day global soil dust emissions from natural and anthropogenic (agricultural) sources.

Strong winds can lift soil dust particles from the surface into the atmosphere where they can travel long distances. Soil dust is the dominant aerosol type globally in terms of mass. It affects weather and climate through interactions with clouds, radiation, and the carbon cycle. Dust storms can cause road and air traffic incidents, have serious effects on air quality, and the exposure to dust aerosol can harm the human cardiovascular system. To quantify and mitigate dust aerosol and its effects, the representation of dust processes in numerical weather and climate models is critical.

Dust emissions are linked with wind forces through a non-linear relationship. As a result, small errors in modelled wind speed lead to large errors in modelled dust emission. Dust models show moderately good behaviour when dust outbreaks are caused by large-scale weather systems. In contrast, the modelling of moist-convective dust storms ("haboobs") – immense dust storms produced by mesoscale downdrafts from moist-convective systems – remains a challenge, in particular for coarse-grid global models in which moist-convective systems are unresolved. According to a recent field campaign, haboobs are among the most important meteorological dust injection processes in the Sahara in summer, both in terms of cumulative duration and intensity (Allen et al., 2015). Missing the contribution of haboobs in models therefore generates a bias in the estimated global dust aerosol loading.

Only a few attempts have been made to parameterize haboobs in a way that could in principle be used in large-scale models (Miller et al., 2008; Pantillon et al., 2016). The inclusion of haboobs in global models could significantly improve estimates of the amount, spatial distribution, and seasonal and interannual variability of global dust emission. DUST.ES aims to tackle this challenge and to estimate the regional and global relative significance of haboob dust emissions. Research in DUST.ES is conducted by the RES applicant, Dr. Martina Klose, under the supervision of Dr. Carlos Pérez García-Pando, both dust experts working at the Barcelona Supercomputing Center (BSC). Dr. Pérez García-Pando holds an AXA Chair on Sand and Dust Storms: a long-term research programme with the objective to better understand and predict sand and dust storms to be able to better manage their effects and impacts across multiple spatial and temporal scales for the benefit of society. Research in DUST.ES is aligned with and contributes to the goals of the AXA Chair programme.

The proposed activity is also related to other ongoing projects at the BSC, namely the Barcelona Dust Forecast Center (http://dust.aemet.es) and the World Meteorological Organization (WMO) Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) regional center for Northern Africa, the Middle East, and Europe (https://sds-was.aemet.es/). The Barcelona Dust Forecast Center is an initiative under the umbrella of the WMO managed by the Spanish State Meteorological Agency AEMET and the BSC with the main objective to generate timely and quality dust forecasts. The WMO SDS-WAS has the ambition to provide sand and dust storm information to users through an international partnership between research and operational communities. Dust forecasts produced and distributed within the Barcelona Dust Forecast Center and the WMO SDS-WAS Regional Center, with fundamental contributions from the BSC, are followed and used by national weather services, the industrial sector, policy makers and the general public. Innovations that can improve dust forecasting, as we hope to achieve by including haboob dust storms within DUST.ES with RES support, would therefore have a direct and sizeable benefit for a wide community.

d) Grants and funded projects related to this activity

Reference code	Project title		
201800005089	Encomienda para la realización de actividades de desarrollo y mejora de los productos y servicios suministrados por los centros regionales de tormentas de polvo y arena de la Organización Meteorológica Mundial (OMM)		
Starting date	Ending date	Total financing (in EUR)	Financing source
2018-09-10	2021-09-09	500.196,00	National

Reference code	Project title		
789630	Addressing key uncertainties in mineral DUST EmiSsion modelling to better constrain the global dust cycle (DUST.ES)		
Starting date	Ending date	Total financing (in EUR)	Financing source
2018-11-01	2020-10-31	158.121,60	European

Reference code	Project title		
792103 (LCE-11-2017)	Solving water issues for CSP plants (SOLWARIS)		
Starting date	Ending date	Total financing (in EUR)	Financing source
2018-05-01	2022-04-30	11.621.106,50	European

Reference code	Project title		
AXA Chair 2015	AXA Chair on Sand and Dust Storms		
Starting date	Ending date	Total financing (in EUR)	Financing source
2016-10-01	2031-08-31	1.587.906,57	Other

e) Brief description of the Project (if this Activity takes place in the context of a Technology or Industrial Project)

NA

f) Specific Activity proposed

Our goal is to further-develop the haboob paramaterization from Pantillon et al. (2016) and implement it in the Multiscale Online Non-hydrostatic AtmospheRe CHemistry model (MONARCH; e.g. Pérez et al., 2011; Badia et al., 2016; Gonçalves et al., in prep.; see also Section 2g) to simulate moist-convective dust storms in coarse-grid regional and global model runs. The haboob scheme is based on the assumption that the downdraft mass flux from the model's convection scheme spreads out radially as a cylindrical cold pool. By default, MONARCH uses an adjustment rather than a mass flux scheme to parameterize convection. We will therefore modify the haboob scheme such that the haboob radial outflow is estimated based on atmospheric stratification rather than downdraft mass flux.

To further-develop and calibrate the haboob parameterization, comprehensive and statistically sound information on haboob occurrence and properties are needed. We will obtain this information through a combination of high-resolution regional convection-permitting simulations and observations. Using model simulations will provide all geophysical quantities necessary to describe the haboob conditions, which would not otherwise be accessible, while comparison with observations will guarantee that the model simulations and derived quantities are close to reality. Here, we will not only simulate meteorological variables at high resolution, but also include a full representation of the dust cycle to calibrate the dust-coupling of the haboob parameterization. Online dust-computations at high resolution are rare due to the additional computational effort this requires. MONARCH includes a dust module (Pérez et al., 2011; Haustein et al., 2012; Klose et al., in prep.), which solves the mass balance equation for dust taking into account the processes of (1) dust generation and uplift by surface wind forces and turbulence, (2) horizontal and vertical advection, (3) horizontal diffusion and vertical transport by turbulence and convection, (4) dry deposition and gravitational settling, and (5) wet removal including in-cloud and below-cloud scavenging from convective and stratiform clouds.

Specifically, we will conduct MONARCH regional simulations for a domain covering northern Africa and the Middle East, where haboobs occur frequently in summer. Simulations will be conducted with two configurations:

(A) at a moderate horizontal resolution of 0.1 degrees (~10 km) with a combination of explicit and parameterized convection;
(B) at a high horizontal resolution of 0.025 degrees (~3 km) with explicit convection.

Simulations in A will be conducted to test the model setup (e.g. compare results with different input/boundary conditions) and to spin up soil variables, which need longer to adjust than atmospheric variables. The soil conditions after spinup will be used as input for simulations in B. Five years of simulation are planned in A, three years for testing and two years for spinup.

The model runs planned in B will cover one full year of simulation to capture the seasonal cycle and an additional summer season of three months where haboob occurrence is maximum. In both cases, a spinup of two weeks is needed for the dust variables, starting from zero dust loading. Two more months of simulation are estimated to test the final model setup at high resolution and to reproduce simulations in the case of issues (total simulation time 18 months).

Both model configurations will use 60 vertical model layers. This leads to a total of 15.7 million grid points for configuration A and 249.9 million grid points for B for the 3-dimensional domain. To facilitate numerical stability, a small computational time step is needed in combination with the high spatial resolution. Here we are planning to use a time step of 20 s for configuration A and of 5 s for configuration B, which means about 7.9 million computational time steps for the 5 years of simulation planned with configuration A and 9.5 million time steps for the 18 months of simulation with configuration B. Turbulence, surface layer, dust emission, sedimentation and dry deposition routines are called every 4 computational time steps, moist convection, microphysics and wet scavenging routines every 8 time steps, and short- and longwave radiation routines are called every hour (i.e. every 180 time steps for A and every 720 time steps for B). The meteorological fields are re-initialized daily, while dust fields and soil conditions are transferred between the daily runs.

Preliminary tests in MareNostrum4 have been successfully conducted to ensure that such demanding simulations are feasible with MONARCH and to estimate the required resources. Based on these tests, a one-year simulation with configuration A is estimated to require approximately 73 thousand CPU hours and with configuration B about 5.7 million CPU hours (see summary below for more detail).

The following tables summarize the results of the preliminary tests and the planned experiments together with the required resources:

Preliminary experiments:
Config. ... Resolution ... #grid points ... time step ... #cores ... Exec. time per sim. day (CPU hours)
A .... 0.1 deg .... 15.7 mio .... 20 s .... 528 .... 0.38 hrs (201)
B .... 0.025 deg .... 249.9 mio .... 5 s .... 9504 .... 1.65 hrs (15,682)

Planned experiments:
Config. ... Resolution ... #grid points ... time step ... #cores ... Total sim. time ... Total CPU hours
A .... 0.1 deg .... 15.7 mio .... 20 s .... 528 .... 5 years 366,168
B .... 0.025 deg .... 249.9 mio .... 5 s .... 9504 .... 18 months 8,609,198

The full MONARCH hourly output would generate files of about 13TB in size for one year of simulation with configuration A and 217TB for configuration B. As part of the MONARCH workflow, the file size is reduced such that storing only basic post-processed meteorological and dust variables reduces files to about 3TB for a one-year simulation with hourly output using configuration A and 23TB using configuration B. However, a generous buffer is necessary during the run to account for the time needed to execute the file reduction, account for delays in the workflow, etc.

After completion of the simulations, we will identify and track haboob-related winds and dust emissions in the convection-permitting simulations (configuration B) using meteorological criteria such as temperature tendency at the 925 hPa pressure level and vertical velocity at 850 hPa (e.g. Heinold et al. 2013). We will use the extracted properties to further-develop the parameterization of haboobs for use in coarse-grid models. Measurements of dust concentration and meteorological parameters in the Sahel as well as sun photometer and satellite observations in Northern Africa will additionally be used to calibrate the new coupled haboob-dust emission scheme.

Such an ambitious modeling enterprise is only possible with appropriate access to tier-0 computing resources such as those offered through RES. The activities proposed here will be conducted by a team of dust modeling experts, dust observations experts, and computer scientists with vast experience in HPC infrastructure and computing as well as workflow and data management (see Sections 2g and 4c-e). This will ensure that HPC resources assigned to the project are utilized and managed appropriately and that the complex high-resolution simulations proposed here can be completed successfully.

g) Computational algorithms and codes outline

MONARCH is a multiscale modeling system able to simulate the atmosphere including atmospheric constituents such as aerosols or trace gases for global and regional domains. MONARCH is a parallel MPI application designed to run with both regional and global domains. Parallelization of MONARCH follows a subdomain basis approach, i.e. the model domain is divided into horizontal tiles, which are assigned to individual computational units. MONARCH is a coupled model constructed over the Earth System Modelling Framework (ESMF) coupling library. This implies that between the execution of each module (dynamics, physics, chemistry, aerosol), the model executes a coupling step to exchange information. The numerical methods employed within the model are: the Adams-Bashford scheme for horizontal advection, the Crank-Nicholson scheme for vertical advection tendencies, the forward-backward scheme for horizontally propagating fast waves, and an implicit scheme for vertically propagating sound waves. The I/O of the system uses dedicated writing nodes, resulting in a partitioning between computational and I/O nodes.

To run the model, we use the workflow manager Autosubmit (Manubens-Gil et al., 2016) together with the MONARCH-specific extension auto-monarch developed within the Earth Sciences department at the BSC, which facilitates easy management of the model runs as well as pre- and post-processing on high-performance computing platforms, such as MareNostrum4.

MONARCH undergoes continuous development at the BSC on dust processes, atmospheric chemistry, emissions, data assimilation, general structure (I/O, parallelization), workflow management, evaluation, and operational forecasting. The model has been a key tool in several previous PRACE and RES projects (e.g. PRACE eFRAGMENT1, RES AECT-2019-3-0001) and was successfully applied on MareNostrum4. In fact, the Computational Earth Sciences group of the Earth Sciences Department at the BSC, leading members of which are part of the team in the present proposal, are currently starting performance analysis in collaboration with BSC's Computer Sciences Department to improve the model's performance.

MONARCH is used for different applications. For example, the model provides regional daily dust forecasts for Northern Africa, the Middle East, and Europe through the WMO SDS-WAS Regional Center hosted by the BSC, and contributes to the International Cooperative for Aeorosol Prediction (ICAP) Multi Model Ensemble with global forecasts. Currently, MONARCH is a candidate model to be included in Europe's regional forecasting service (CAMS_50) of the European Centre for Medium-Range Weather Forecasts (ECMWF). In recent and ongoing projects, the dust-cycle component of MONARCH was upgraded with (1) a new global representation of natural and anthropogenic dust sources based on satellite data (MODIS Deep Blue) and historical environment reconstructions (HYDE) at 10 km resolution, (2) multiple options to parameterize dust emission, (3) a new drag partition correction for the threshold for dust emission, (4) the ability to run the model with separate mineral tracers instead of bulk dust using a soil mineralogy atlas, (5) a flexible treatment of atmospheric chemistry, and (5) a dust (and aerosol) data assimilation system based on the Local Ensemble Transform Kalman Filter (LETKF). The applicant, Dr. M. Klose, was the main developer of upgrades 1 – 3.

3. Software and Numerical Libraries

Software components that the project team requires for the activity.

a) Applications + Libraries

BLAS, GSL, HDF5, LAPACK, NETCDF, R, TOTALVIEW, GNUPLOT, IMAGEMAGICK, NCVIEW, NCL, NCO, OPENBLAS, INTELMPI

b) Compilers and Development Tools

GCC, INTEL

c) Utilities + Parallel Debuggers and Performance Analysis Tools

CMAKE, PERL, PYTHON

d) Other requested software

DDT, ESMF, CDO, SUNDIALS, SuiteSparse

e) Proprietary software

MONARCH - Multiscale OnliNe AtmospheRic CHemistry model, private webpage

4. Research Team Description

a) Personal Data

Name of Team Leader	Martina Klose
Gender	Female
Institution	Barcelona Supercomputing Center
e-mail	martina.klose@bsc.es
Phone	934134051
Nationality	Germany

b) The employment contract of the activity leader with the research organisation is valid at least 3 months after the end of the allocation period.

Yes

c) Curriculum Vitae of the Team Leader

Dr. Martina Klose holds a diploma and a doctoral degree in Meteorology from the University of Cologne, Germany. Dr. Klose's research goal is to better understand the dust cycle and to advance its representation in models. She pioneered the development of a stochastic parameterization of aerodynamic dust entrainment by turbulence using theory and large-eddy simulation, and implemented the new scheme in the Weather Research and Forecasting model with chemistry (WRF-Chem). Using her own and other dust emission schemes, she conducted regional simulations of dust events. She developed a new method to estimate the contribution of dust devils to the dust budget, which was – for the first time – based on a dust devil population. During a two-year fellowship in the U.S., she gained first-hand experience in the field measurement of aeolian processes. At the BSC, Dr. Klose focuses on developing MONARCH to better constrain natural and anthropogenic contributions to the dust cycle.

Only five years after obtaining her doctoral degree, Dr. Klose's research resulted in 19 publications in peer-reviewed international journals (8 as the lead author; 4 also published as book chapters; citations: 460, h-Index: 13, i10-Index: 14; Google Scholar, 07 Jan 2020), the participation in 25 international and 3 national conferences/workshops, the organization of 1 international workshop, several invited visits/presentations at renowned research institutions around the world, and an invited presentation at the worldwide largest geosciences conference. She has (co-)convened 5 sessions at international conferences. Dr. Klose was awarded individual research fellowships by the German Research Foundation, the Agency for Management of University and Research Grants of the government of Catalonia, and the European Commission. She is a lead author in a recent volume reviewing current knowledge about dust devils and identifying knowledge gaps. She is an associate editor for the international journal Aeolian Research.

Dr. Klose is an experienced HPC user. At the University of Cologne, she conducted regional and very-high resolution (10 m) large-eddy simulations with WRF-Chem using the CHEOPS supercomputer of the Regional Computing Centre Cologne. Currently, she uses MareNostrum4 to conduct global atmosphere/dust simulations with MONARCH and provided more than 50 years of global MONARCH simulations to external partners. As a team member, Dr. Klose contributed to the PRACE project eFRAGMENT1.

d) Names of other researchers involved in this activity

Sara Basart, Barcelona Supercomputing Center, sara.basart@bsc.es
Miguel Castrillo, Barcelona Supercomputing Center, miguel.castrillo@bsc.es
María Gonçalves, Universitat Politècnica de Catalunya/Barcelona Supercomputing Center, maria.goncalves@bsc.es
Francesca Macchia, Barcelona Supercomputing Center, francesca.macchia@bsc.es
Carlos Pérez García-Pando, Barcelona Supercomputing Center, carlos.perez@bsc.es
Kim Seradell, Barcelona Supercomputing Center, kim.serradell@bsc.es

e) Relevant publications

Tintó Prims, O., M. Castrillo, M. C. Acosta, O. Mula-Valls, A. Sanchez Lorente, K. Seradell, A. Cortés, F. J., Doblas-Reyes (2019), Finding, analysing and solving MPI communication bottlenecks in Earth System models, J. Comput. Sci, 36, doi:10.1016/j.jocs.2018.04.015

Badia, A., O. Jorba, A. Voulgarakis, D. Dabdub, C. Pérez García-Pando, A. Hilboll, M. Gonçalves, Z. Janjic (2017), Description and evaluation of the Multiscale Online Nonhydrostatic AtmosphеRe Chemistry model (NMMB-MONARCH) version 1.0: Gas-phase chemistry at global scale. Geosci. Model Dev. 10, 609-638, doi:10.5194/gmd-10-609-2017

Klose, M., B. C. Jemmett-Smith, H. Kahanpää, M. Kahre, P. Knippertz, M. T. Lemmon, S. R. Lewis, R. D. Lorenz, L. D. V. Neakrase, C. Newman, M. R. Patel, D. Reiss, A. Spiga, P. L. Whelley (2016), Dust devil sediment transport: From lab to field to global impact, Space Sci. Rev., doi:10.1007/s11214-016-0261-4

Basart, S., Ll. Vendrell, J. M. Baldasano (2016), High-resolution dust modelling over complex terrains in West Asia, Aeolian Res., 23, 37-50, doi:https://doi.org/10.1016/j.aeolia.2016.09.005

Klose, M., Y. Shao (2016), A numerical study on dust devils with implications to global dust budget estimates, Aeolian Res., 22, doi:10.1016/j.aeolia.2016.05.003

5. Resources

a) Estimated resources required for the Activity for the current Application Period

Requested machine	MareNostrum 4 ((Intel(R) Xeon(R) Platinum 8160, 2.10GHz with Intel(R) Omni-Path / 165888 cores)
Interprocess communication	Tightly Coupled

Typical Job Run				
Number of processors needed for each job		528.00		
Estimated number of jobs to submit		1825.00		
Average job durations (hours) per job		0.38		
Total memory used by the job (GBytes)		800.00		
Largest Job Run				
Number of processors needed for each job		9504.00		
Estimated number of jobs to submit		549.00		
Average job durations (hours) per job		1.65		
Total memory used by the job (GBytes)		17000.00		
Total disk space (Gigabytes)	**Minimum**	50000.00	**Desirable**	60000.00
Total scratch space (Gigabytes)	**Minimum**	200000.00	**Desirable**	220000.00
Total tape space (Gigabytes) (*)	**Minimum**	0.00	**Desirable**	0.00
Total Requested time (Thousands of hours)		8975.37		

If this activity is asking for more than 10Million CPU hours, you need to justify the amount of resources requested for the activity. (max 1000 characters)

INFORMATION: The estimated cost of the requested hours, considering only the electricity cost, is 9603.6459 euros.

The required resources have to be executed in the selected machines, the other architectures do not fit the requirements to execute the proposal.
** this option implies that if no hours in this machine/these machines are available, the acces committee will reject the full application.

6. Abstract for publication

High-resolution, convection-permitting regional simulations of weather and dust aerosol for more than one year over northern Africa will be conducted using the online multi-scale MONARCH chemical weather prediction system. The model simulations will serve as a reference and statistical basis to parameterize “haboobs” - intense dust storms generated by deep convective systems - in global models in which this important process is typically lacking due to the coarse model grid. A better representation of haboobs in models could reduce biases in the quantification of global dust aerosol and its effects, and has the potential to improve dust forecasting to benefit society.

7. Contact with CURES during last year

Information about the RES Users Committee (CURES).

a) User has contacted the CURES during last year

No

b) If not, indicate why you have not contacted the CURES

Because this is my first application to RES.

Usage Terms & Conditions

- The Usage Terms & Conditions have been already accepted.