Barcelona Supercomputing Center
Centro Nacional de Supercomputación

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

AECT-2018-3-0012 Ammonia—Secondary Organic Aerosol Interactions in the NMMB-MONARCHv1.0 model

1. General Information

Activity Id
AECT-2018-3-0012

a) Activity Title
Ammonia—Secondary Organic Aerosol Interactions in the NMMB-MONARCHv1.0 model

b) Area
Astronomy, Space and Earth Sciences

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
This project falls under several initiatives related to the ongoing development of the online multi-scale NMMB-MONARCHv1.0 chemical weather prediction system:

- H2020: Marie Skłodowska-Curie Individual Fellowship (project number 747048) ACRoNNIM: Aerosol and Climate Response to NH3 in the NMMB/BSC Inter-Scale Model. This project is being coordinated by Dr. Oriol Jorba and executed by Dr. Matthew Dawson, both at the Barcelona Supercomputing Center (BSC), in collaboration with IDAEA-CSIC and researchers at the University of California, Irvine, US. Funding for this project comes from the European Commission's H2020 program.

- COPERNICUS: CAMS Regional Production System (CAMS_50; project number pending) The CAMS Regional Production System provides numerical data and mapping products for air quality and atmospheric composition at the European scale. The Multiscale Online Nonhydrostatic Atmosphere

CAMS_50 multi-model ensemble comprising eleven state-of-the art regional models. The participation of NMMB-MONARCHv1.0 in the CAMS_50 project is being lead by Dr. Oriol Jorba, with funding from the European Commission's Copernicus project.

The development of accurate treatments for aerosol chemistry and physics for use in large-scale regional and global chemical transport models (CTMs) is critical to efforts to predict air quality and climate, and to evaluate the potential impact of proposed emissions scenarios. The oxidation of volatile organic species to form low-volatility products is an important source of aerosol mass in the global atmosphere. Because of the climate, health and visibility effects of particulate matter, inclusion of this so-called secondary organic aerosol (SOA) into regional and global CTMs is the focus of on-going research. Complicating these efforts are the large number of species and oxidation pathways involved, their seasonally, spatially, and diurnally varying importance, and the complex physical processes controlling their phase partitioning. Models generally under-predict SOA mass in the atmosphere compared with field measurements, suggesting the presence of as-yet unidentified sources or unaccounted-for physical processes (Volkamer et al., 2006).

As modelers work to incorporate existing treatments of SOA into global CTMs, laboratory and field researchers continue to identify new precursors and routes to SOA formation. Recently, ammonia has been identified as a potentially important species in the formation and aging of SOA. However, the reactions of ammonia with gas- and aerosol-phase organic species are complex, affecting both SOA yields (Na et al., 2006) and aerosol optical properties (Bones et al., 2010), with implications for air quality and climate. The goal of the ACRoNNIM project is to answer the following questions: How does ammonia affect aerosol mass loading and optical properties on regional and global scales? And, what impact do these effects have on air quality and climate? This is being accomplished by the incorporation of an advanced treatment for SOA into the online multi-scale NMMB-MONARCHv1.0 chemical weather prediction system, followed by the development and implementation of a treatment for the effects of ammonia on organic aerosols into the SOA scheme, as described in more detail below.

Improvements to the treatment of SOA in the NMMB-MONARCHv1.0 model also are within the scope of the CAMS_50 initiative. In addition to a focus on the ongoing incorporation of results from research activities of each of the participating teams into their respective models, as a new member NMMB-MONARCHv1.0 is also required to attain specific quality targets within the grant period, which will likely be facilitated by advancements in the treatment of aerosol processes, including those related to SOA.

d) Grants and funded projects related to this activity

Reference code
747048

Project title
ACRoNNIM: Aerosol and Climate Response to NH3 in the NMMB/BSC Inter-Scale Model

Starting date
2017-09-12

Ending date
2019-09-11

170.121,00

Financing source
European

Reference code
pending

Project title
COPERNICUS PROJECT: CAMS_50 Regional Production

Starting date
2018-10-01

Ending date
2021-06-30

Total financing (in EUR)
91.466,00

Financing source
European

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

The activity does not take place in the context of a Technology or Industrial Project.

f) Specific Activity proposed

As computational ability has improved, global chemical transport models (CTMs) have begun incorporating more complex treatments of SOA that until recently had only been accessible to smaller-scale models. These include, e.g., the re-evaporation of semi-volatile species (equilibrium partitioning), aqueous-phase SOA production, and variations of the Volatility Basis Set (VBS) model to account for SOA aging (Tsigaridis et al., 2014). The Caltech Atmospheric Chemistry Mechanism (CACM) coupled with the Model to Predict the Multiphase Partitioning of Organics (MPMPO) is one of the most advanced treatments of SOA available for box and regional-scale modeling (Griffin et al., 2002, 2005). It has been developed over the last 15 years to accurately predict SOA formation over a wide range of conditions, both urban and remote. CACM/MPMPO is a lumped model that uses the Equilibrium Partitioning scheme of Pankow and co-workers, and utilizes a fully coupled mixed-phase aqueous/organic aerosol scheme. However, its complexity has precluded its inclusion in large-scale high-resolution regional/global models to date. The 2017 upgrade of the MareNostrum supercomputer at BSC and resulting improvements in performance have made feasible the incorporation of such a complex treatment of gas- and aerosol-phase chemistry and physics into a large-scale high-resolution CTM.

Collaborators at the University of California, Irvine (UCI) are currently investigating the role of ammonia

gas-phase species, aerosol composition and optical properties, towards the goal of developing an updated aerosol chemistry and physics model that accounts for the role of ammonia in SOA processes. Their current and on-going observations of ammonia-related SOA chemistry and physics will be incorporated into CACM/MPMPO and then the updated SOA module will be implemented into the online multi-scale NMMB-MONARCHv1.0. The NMMB-MONARCHv1.0 is a chemical weather prediction system maintained by the Earth Sciences Department of BSC and includes modules for dust, sea salt, sulphate, and primary organic aerosol, along with a 2-product SOA module. The NMMB-MONARCHv1.0 is based on the Nonhydrostatic Multiscale Model on the B Grid (NMMB) from the National Center for Environmental Prediction (NCEP) and is a fully coupled, online chemical/meteorological model that is replacing the CALIOPE modeling system as the primary weather and air quality model at BSC, and operates as part of the International Cooperative for Aerosol Prediction Multi-Model Ensemble (ICAP-MME).

The updated NMMB-MONARCHv1.0-CACM/MPMPO will be deployed with a regional (Spain) domain to evaluate the role of ammonia in SOA formation and aging, and its effects on air quality and climate. Collaborators at IDAEA-CISC have recently completed a field campaign in the city of Vic (north of Barcelona), an area known for high gas-phase ammonia concentrations and SOA formed from precursors emitted in the Barcelona area. The campaign employed a suite of gas and aerosol measurement techniques, results from which will be used in evaluating the model output. Thus, NMMB-MONARCHv1.0 will be configured with a 4 km x 4 km resolution using emissions calculated using the HERMESv3 model, and following the general procedure used for regional (Spain) simulations in the CALIOPE model (Pay et al., 2010). The NMMB-MONARCHv1.0 model in various configurations has been extensively tested and run in MareNostrum 4 as part of previous and ongoing projects. Simulations will be performed for a 1-year period encompassing the campaign dates.

g) Computational algorithms and codes outline

The NMMB-MONARCHv1.0 is a parallel MPI application designed to run with both regional and global domains. The operational domain is divided into horizontal sub-sections, which are assigned to individual computational units. Thus, parallelization is accomplished using a sub-domain-based approach. The NMMB-MONARCHv1.0 is a fully coupled model constructed on the ESMF coupling framework, wherein between the execution of each module (e.g., dynamics, physics, chemistry, aerosol) the model performs a coupling step to exchange information. The numerical methods employed within the model are: the Adams–Bashforth Scheme for horizontal advection, the Crank–Nicholson scheme to compute vertical advection, the forward–backward scheme for horizontally propagating fast waves, and an implicit scheme for vertically propagating sound waves. The original chemistry module (CB-5; Yarwood et al., 2005) applies an Euler-Backward-Iterative scheme to solve the stiff set of ordinary differential equations associated with gas-phase chemistry. The updated chemistry and SOA partitioning model (CACM/MPMPO) is being built on the framework of the Part-MC model (Riemer et al., 2009), to provide flexibility in the gas- and aerosol-phase chemistry and partitioning mechanism, and employs the SUNDIALS Backward-Differentiation Formulas (BDF) solver.

3. Software and Numerical Libraries

a) Applications + Libraries

BLAS, GSL, HDF5, LAPACK, NETCDF, R, OPENMPI, OPENBLAS, INTELMPI

b) Compilers and Development Tools

GCC, TOTALVIEW, INTEL, GDB

c) Utilities + Parallel Debuggers and Performance Analysis Tools

CMAKE, PYTHON, VALGRIND, GNUPLOT, NCVIEW

d) Other requested software

ESMF
CDO
SUNDIALS
SuiteSparse

e) Proprietary software

4. Research Team Description

a) Personal Data

Name of Team Leader	Matthew Dawson
Gender	Male
Institution	BSC
e-mail	matthew.dawson@bsc.es
Phone	934134051
Nationality	United States

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. Matthew Dawson received a Bachelor of Science degree in Chemistry from the University of Pittsburgh (PA, USA; 2009) and a PhD in Chemistry from the University of California, Irvine (CA, USA; 2014) where he performed laboratory-based experiments on atmospheric aerosol nucleation mechanisms. He then performed post-doctoral research in the Department of Mechanical and Aerospace Engineering at the University of California, Irvine (2014–2016) where he incorporated incorporated recently identified chemical processes related to the oxidation of aromatic species into the UCI-CIT regional air quality model and developed an aqueous-phase cloud chemistry module for the stochastic model of aerosol and cloud formation in emission plumes, Part-MC. He is currently performing post-doctoral research in the Atmospheric Composition group of the Barcelona

and aerosol chemical mechanism and secondary organic aerosol (SOA) partitioning scheme in the NMMB-MONARCHv1.0 global/regional chemical weather prediction model. These efforts are focused on improving the representation of SOA in the NMMB-MONARCHv1.0 model and investigating the role gas-phase ammonia interactions with organic aerosol. Dr. Dawson has received several awards from non-profits and industry, including a Metrohm Young Chemist Award (www.metrohm.com) and an ARCS Scholarship (www.arcsfoundation.org), and is currently performing research on a Marie Skłodowska-Curie Individual Fellowship.

d) Names of other researchers involved in this activity

Oriol Jorba (BSC; oriol.jorba@bsc.es)
Vincenzo Obiso (BSC; vincenzo.obiso@bsc.es)
Kim Serradell (BSC; kim.serradell@bsc.es)

e) Relevant publications

Griffin, R.J., Dawson, M.L., Dabdub, D., Simulated sensitivity of secondary organic aerosol in the South Coast Air Basin of California to nitrogen oxides and other chemical parameters, Aerosol Sci. Technol., 52 (6), 679–672 (2018).

Dawson, M.L., Xu, J., Griffin, R.J., Dabdub, D., Development of aroCACM/MPMPO 1.0: A model to simulate secondary organic aerosol from aromatic precursors in regional models, Geosci. Model Dev., 9, 2143–2151 (2016).

Dawson, M.L., Varner, M.E., Perraud, V., Ezell, M.J., Gerber, R.B., Finlayson-Pitts, B.J. Simplified mechanism for new particle formation from methanesulfonic acid, amines, and water via experiments and ab initio calculations. PNAS 109, 18719–18724 (2012).

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

Obiso, V. and O. Jorba. Aerosol-radiation interaction in atmospheric models: Idealized sensitivity study of simulated short-wave direct radiative effects to particle microphysical properties. J. Aerosol Sci. 115, 46–61, 2018.

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		1032.00		
Estimated number of jobs to submit		365.00		
Average job durations (hours) per job		1.20		
Total memory used by the job (GBytes)		80.00		
Largest Job Run				
Number of processors needed for each job		1032.00		
Estimated number of jobs to submit		730.00		
Average job durations (hours) per job		3.00		
Total memory used by the job (GBytes)		80.00		
Total disk space (Gigabytes)	**Minimum**	5500.00	**Desirable**	21000.00
Total scratch space (Gigabytes)	**Minimum**	500.00	**Desirable**	500.00
Total tape space (Gigabytes) (*)	**Minimum**	0.00	**Desirable**	0.00
Total Requested time (Thousands of hours)		2712.00		

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 2901.84 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

Recently identified reactions between gas-phase ammonia and secondary organic aerosol (SOA) will be assessed for their impact on air quality and aerosol optical properties using the online multi-scale NMMB-MONARCHv1.0 chemical weather prediction system. As part of an H2020: Marie Skłodowska-Curie Individual Fellowship (ACRoNNIM) and the COPERNICUS: CAMS_50 Regional Production project, an advanced treatment for SOA (CACM/MPMPO) will be incorporated into NMMB-MONARCHv1.0 and used to evaluate the impacts of ammonia–SOA reactions in conjunction with results from field measurements.

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.

Barcelona Supercomputing Center, 2016