Proposal n°2010PA3427

Submitted for the assessment cut-off date : Thursday 15 September 2016 at 11:00:00 CEST

General information

Type of proposal: Preparatory type **A – Code scalability testing.**
Start date: 15-December-2016
The start date should be either one and half or two months after the announced date for evaluation cut-off.

Project name: Porting and scalability test of a multiscale online chemical-aerosol weather prediction system: the NMMB/BSC-CTM system
Research field: Earth Sciences and Environment

Template documents for the mandatory final report :
(as described at **http://www.prace-ri.eu/Information-for-PRACE-Awardees**)

- **PRACE - FRF_PC_TypeA.doc**
- **PRACE - FRF_PC_TypeB.doc**
- **PRACE - FRF_PC_TypeC.doc**

Project leader (personal data and contact)

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Organisation with a research activity: **Yes**
Employment contract of the project leader is valid at least 3 months after the end of the allocation period: **Yes**

For commercial companies,

- **Is the head office of the organisation in Europe? –**
- **% of R&D activity in Europe as compared to total R&D activity : –**

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Requested computer systems

Computing center	Machine
BSC *Barcelona Supercomputing Center*	☑ MareNostrum
BSC *Barcelona Supercomputing Center*	☐ MareNostrum Hybrid Nodes
CINECA	☑ Marconi – Broadwell
CSCS *Swiss Swiss National Supercomputing Centre*	☐ Piz Daint
Gauss/FZJ *Juelich*	☐ Juqueen
Gauss/HLRS *High Performance Computing Center Stuttgart (HLRS)*	☐ Hazel Hen
Gauss/LRZ *Leibniz-Rechenzentrum*	☑ SuperMUC

1. Summary of the project *(for Types A, B, C)*

To be published in the PRACE website. Maximum 500 words.

Some of the today's most significant environmental concerns are related to the composition of the atmosphere. The increasing concentration of the greenhouse gases and the cooling effect of aerosols are prominent drivers of a changing climate, but the extent of their impact is still uncertain.
At the Earth's surface, aerosols, ozone and other reactive gases such as nitrogen dioxide determine the quality of the air around us, affecting human health and life expectancy, the health of ecosystems and the fabric of the built environment. Ozone distributions in the stratosphere influence the amount of ultraviolet radiation reaching the surface. Dust, sand, smoke and volcanic aerosols affect the safe operation of transport systems and the availability of power from solar generation, the formation of clouds and rainfall, and the remote sensing.

To address these environmental concerns, there is the need to push further the boundaries of what numerical simulations can provide. The Earth Sciences Department of the Barcelona Supercomputing Center (ES-BSC) is currently developing a new fully on-line coupled chemical weather prediction system for research applications and experimental forecasts at sub-synoptic and mesoscale resolutions on global and regional domains.

The NMMB/BSC-CTM system is based on the Non-hydrostatic Multiscale Model on the B-Grid (NMMB), developed at US National Centers for Environmental Prediction (NCEP). The main feature of NMMB/BSC-CTM is its online coupling of chemistry and meteorology. The new chemical system component solves the gas-phase tropospheric chemistry and the life cycle of the mineral dust, sea salt, black carbon, organic carbon, and

sulphate. The direct effect of non-climatic aerosols on the radiative budget is already implemented and allows to study further mesoscale processes associated with air pollution and its interactions with meteorology, both at high resolution and on a global scale. Furthermore, the model also includes and ensemble-based data assimilation system for aerosols using data from satellites and ground-based observations.

In data assimilation mode, the model is capable of ingesting observations to estimate improved model initial conditions, or analyses, as well as to generate retrospectively consistent analysis datasets over a long period (reanalyses). Reanalyses are key to monitor past state of the atmosphere. In the data assimilation mode multiple (independent) NMMB/BSC-CTM simulations are run to account for model uncertainty in the calculation of the data assimilation corrections. Such ensemble runs make the optimization of the model efficiency even more crucial.

NMMB/BSC-CTM currently benefits of strong collaboration ties between ES-BSC, NCEP, the Technical University of Catalonia, the University of California Irvine and the NASA Goddard Institute for Space Studies. ES-BSC considers porting and evaluating NMMB/BSC-CTM on different high-performance computational platforms a top priority, before making the code generally available to the scientific community.

Initial work on the CURIE system (PRACE Preparatory Access projects 2010PA0419 and 2010PA0627) with an early version of the model pointed out some issues to be addressed before performing scalability tests. Initial results show scalability up to 8000 cores. We aim to finalize the porting and investigate scalability and performance of the NMMB/BSC-CTM model on the MareNostrum, Marconi, and SuperMuc supercomputers. We target a high-resolution configuration reaching the foreseen capabilities of next year's numerical weather prediction systems.

2. Scientific case of the project *(for Types A, B, C)*

Explain the scientific case for which you intend to use the code(s). Maximum 500 words.

Atmospheric composition services have emerged recently, in particular in Europe in the context of the EU-funded Copernicus programme, to monitor and characterise changes in atmospheric composition by ingesting observations into computationally expensive numerical models. Accurate information obtained from such systems helps us to provide reliable information on atmospheric composition past trends and current conditions, and it can contribute to understand why and how the current climate is changing, as well as to issue warnings when well-being or security are threatened. The accuracy of atmospheric composition simulations depends greatly on the way we represent small-scale processes, in particular in the meteorological component. High-resolution simulations, together with a better understanding and representation of small scale features in models, are central to improving the quality of atmospheric monitoring and prediction.

The progress in atmospheric modelling has always been related to advances in computer technology. The unprecedented computer power that is now available allows operational application of horizontal resolutions on the order of 10 km on the global scale. However, the current parallel computer architecture requires that some widely adopted modelling paradigms are reconsidered to productively utilize as much power of parallel processing as possible.

To assess the performance of complex atmospheric models and its abilities to run at higher horizontal resolutions, we propose to port the model NMMB/BSC-CTM to the MareNostrum, Marconi, and SuperMuc supercomputers and profile its scalability. The main configuration tested will be a global configuration with a horizontal resolution of 10 km and 64 vertical layers (HR).

Configuration HR is extremely computationally intensive, requiring resources currently available on a few

supercomputers, including the MareNostrum, Marconi, and SuperMuc clusters. We plan to assess the scalability of NMMB/BSC-CTM by profiling the model in different configurations:

(1) with meteorology component only;
(2) activating mineral dust component;
(3) activating natural aerosols component (i.e. mineral dust and sea salt aerosols).

We expect to identify possible porting issues and performance bottlenecks and characterize the feasibility of runs at high horizontal resolutions.

3. Computer resources requested *(for Types A, B, C)*

Total storage required (Gbyte) (only available during the duration of the preparatory access project)	5 000.00
Maximum amount of memory per core (Mbyte)	1.50

4. Please provide the details listed below for the main simulation application *(for Types A, B, C)*

Name and version	NMMB/BSC-CTM v1.0
Webpage or other reference	http://www.bsc.es/es/earth-sciences/nmmbbsc-project
License If the code is open source please, fill out *open source* for this query.	The NMMB/BSC-CTM configuration used in the present proposal is a research version under development. For that reason it is still not available to general public.

5. Describe the main algorithms and how they have been implemented and parallelized *(for Types A, B, C ; Maximum 250 words)*

NMMB/BSC-CTM is a parallel MPI application designed to run on both global and local scale. It subdivides the domain of operation into horizontal tiles and assigns them to computational units. Thus, the parallelization is addressed on a subdomain basis approach. Since the global latitude-longitude grid deforms toward the pole region, the nodes closer to the poles perform an additional filtering step using fast Fourier transform (FFT) to be applied to keep the integration stable using a time step of decent size. However, the polar filtering based on conventional fast Fourier transform requires transpositions involving further communications and thus limits scaling.

NMMB/BSC-CTM is a coupled model constructed over the Earth System Framework model (ESMF) coupling framework; this implies that in between the execution of each module (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 tendencies, the forward-backward scheme for horizontally propagating fast waves, and an implicit scheme for vertically propagating sound waves. Additionally, the chemistry module applies a Euler-Backward Iterative scheme to solve the ordinary differential equations of the stiff system of gas-phase chemistry.

The I/O strategy of the system is designed for the setup of dedicated writing nodes. These results in a partition between computational and I/O nodes.

6. Current and target performance
(for Types A, B, C ; including the points below. Maximum 250 words)

- Describe the scalability of the application and performance of the application
- What is the target for scalability and performance? (i.e. what performance is needed to reach the envisaged scientific goals)

Initial work on the CURIE system (PRACE Access projects 2010PA0419 and 2010PA0627) with an early version of the model pointed out some issues to be addressed before the performance of scalability tests. The current version has several improvements on the parallelisation and memory routines which should increase the performance of the model. In this respect, some work to analyse the scalability of some significant functions for the chemistry configuration has already been done using BSC performance tools (Extrae and Paraver). Although most of the functions provide good scalability, some of them such as radiation, photolysis, and ODE solver have limited scalability in comparison to the rest, and will need a deeper analysis for their performance to be improved.

As described in the previous section of the document, FFT transformations are applied to maintain the model stable. These routines are communication intense and when running high-resolution configurations with a large number of cells in the mesh, can have an impact on the efficiency of the model. Some tests using the MKL Intel library have been carried out to overcome this bottleneck.

Our target performance is to run the NMMB/BSC-CTM model at a much higher resolution than what it is currently done in operations (up to 10km x 10km) and using up to 8000 cores.

7. Confidentiality *(for Types A, B, C)*

Is any part of the project covered by confidentiality? Yes

If YES, please specify which aspect is confidential and justify:

Until the initial open source release of NMMB/BSC-CTM, the model will be under a full confidentiality clause. This is also the case for the NMMB/BSC-CTM configuration used in the present.

8. Describe the I/O strategy regarding the parameters indicated below *(for Types A, B, C)*

8.a) Is I/O expected to be a bottleneck?

The model uses asynchronous I/O, writing raw binary outputs. This means that the reserved resources are separated to computation and I/O resources. The computation nodes send the corresponding data to the I/O servers to save the files on the hard disk while they continue the computation without being interrupted.

8.b) Implementation: I/O libraries, MPI I/O, netcdf, HDF5 or other approaches:

The resulting binary files are post-processed to NetCDF files. This method is still done in a sequential task

(although we are working on a parallel version to speed-up the model) and is one of the major bottlenecks of the model.

8.c) Frequency and size of data output and input:

Each experiment will include a day simulation (24 hours) on a 3-hourly basis. As a result, each experiment will include eight binary files.

The default output variables have an estimated size of each binary file up to 65GB for case (3) activating natural aerosols.

8.d) Number of files and size of each file in a typical production run:

Results are written periodically according to the configuration set by the user; in a typical scenario they are written every three hours of simulation.

In total, for a day of the simulation, a NetCDF files including the default output variables has an estimated size up to 300GB for case (3) activating natural dust aerosols.

9. Main performance bottlenecks *(for Types B, C. Maximum 250 words)*

Not applicable.

10. Describe possible solutions you have considered to improve the performance of the project *(for Types B, C. Maximum 250 words)*

Not applicable.

11. Describe the application enabling/optimization work that needs to be performed to achieve the target performance *(for Types B, C. Maximum 250 words)*

Not applicable.

12. Which computational performance limitations do you wish to solve with this project? *(for Types B, C. Maximum 250 words)*

Not applicable.

13. Describe the impact of the optimization work proposed? *(for Types B, C. Maximum 250 words)*

- Is the code widely used?
- Would the code be used only within this original research project?
- Would the code be used for other similar research projects with minor modifications?
- Would the code be used in many research projects of the research field indicated in the proposal?
- Would the modification be easy to add to the main release of the software?

Not applicable.

14. Describe the request plans for work with support from PRACE experts *(for Type C only)*

14.a. Describe the level of collaboration with PRACE experts you have planned for and how much effort (person months) have you reserved for this?

Not applicable.

Specify a rough estimate for the amount of person months this work entails :

14.b. Describe the optimization work you expect to be done with the support of a PRACE expert for your project

Not applicable.

14.c. Please specify the amount of PRACE experts person months required to support your project (1-6 PMs): **0.00**

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The users commit to:

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b. Acknowledge the role of the HPC Centre and PRACE in all publications which include the results above mentioned. Users shall use the following (or equivalent) wording in such acknowledgement in all such papers and other publications:

« We acknowledge PRACE for awarding us access to resource [machine name] based in [country] at [site] »

Where technical support has been received the following additional text should also be used:

« The support of [name of person/people] from [organisation name], [country] to the technical work is gratefully acknowledged. »

c. Allow PRACE to publish the mentioned report as of one year from the termination of the allocation period.
d. Commit to collaborate with PRACE, upon its request, in the preparation of dissemination material.
e. The applicant commits to not use the project results for military purposes.