Project VI-SEEM – a Regional Virtual Research Environment

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Abstract

In this paper, the H2020 VI-SEEM project and the wind simulation over rugged terrain in its framework of meteorology applications, are discussed. The focus of the paper is twofold. First, the role of VI-SEEM for the creation of a regional virtual research environment offering high computing capacities to research communities is presented. Second, the spatial and temporal scalability of the OpenFOAM software, for resolving Navier-Stokes equations in high performance computing systems in terms of memory and runtime is analysed. Low and medium digital elevation models are used in the process of spatial digitization to shape the relief.

Keywords: VI-SEEM, Wind Simulation, OpenFOAM Scalability.

1. Introduction

The H2020 project VI-SEEM [https://vi-seem.eu/] for creation of a unique Virtual Research Environment (VRE) in Southeast Europe and the Eastern Mediterranean (SEEM) goes as a natural continuation of a 15-years long successful history of regional infrastructure projects focused in networking – SEEREN-1-2, integrated grids – SEE-GRID-1-2-3, and high performance computing (HPC) – HPSEE, funded by European Commission with participation of Southeastern European, Black Sea and Caucasus countries.

The scope of this suite of projects remains the same – offering integrated high computing resources to research communities in the region and promoting the integration into the European Research Area following the path of pan-European related initiatives as GEANT [https://www.geant.org/], EGI [https://www.egi.eu/], PRACE [www.prace-ri.eu/] etc. Firstly the Institute of Informatics and Applied Mathematics (INIMA) of Academy of Sciences of Albania, followed by Polytechnic University of Tirana (UPT), are principal Albanian partners in these initiatives.

A number of applications are considered within the scope of these projects, selected from important research areas as life sciences, environment, physics, and lately cultural heritage. The projects offered possibilities for integration of related applications into the regional infrastructure. VI-SEEM extends the geographical scope including some of Eastern Mediterranean countries, and focuses in applications from life sciences, climate – meteorology, and cultural heritage. In this framework the role of UPT is simulation of wind over rugged terrain as part of meteorology package.

The open source software package OpenFOAM was selected for the spatial – temporal simulation of wind. Simulations are realized in a spatial 3D section of the atmosphere modified following the shape of the relief. A literature review is undertaken to understand problems related with this software in the context of wind simulation. The main scalability

problems to be expected were dependence from the problem to be solved, model size, inter-process communication, etc. [1-13]. In most of the reviewed literature the analysis of scalability was done for concrete problems, without giving details on memory usage, which resulted critical in our experiments confirming the remark of Culpo that "the size of the problems that can be handled on a HPC cluster lies beyond the limitations imposed by smaller in-house clusters" [6].

We used the NASA SRTM Digital Elevation Model (DEM) of the terrain for Albania and surrounding areas from the USGS archive [https://lta.cr.usgs.gov/]. Experiments were carried out in the local parallel system of UPT for the preliminary evaluation of memory and runtime requirements, as a first step before running the models in the VI-SEEM VRE. In a second step we ran the models in parallel systems of Institute of Information and Communication Technologies of Bulgarian Academy of Sciences, an act that simultaneously was promoted from another European project – the COST Action IC1305 NESUS.

2. The VI-SEEM Project

VI-SEEM is a three-year project that aims at creating a unique Virtual Research Environment (VRE) in Southeast Europe and the Eastern Mediterranean (SEEM), in order to facilitate regional interdisciplinary collaboration, with special focus on the scientific communities of Life Sciences, Climatology and Digital Cultural Heritage (Figure 1). The project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 675121. VI-SEEM builds on the success of its predecessor e-Infrastructure projects that have been crucial for enabling high-quality research & ICT developments by providing networking and computational resources, application support and training, in both South East Europe and Eastern Mediterranean, and have supported the European vision of inclusive and smart growth, based on knowledge and innovation, enriching the European Research Area [https://vi-seem.eu/].

The project unifies existing e-Infrastructures into an integrated platform to better utilize synergies, for an improved service provision within a unified Virtual Research Environment to be provided to scientific communities of high impact in the combined South East Europe and Eastern Mediterranean region. VI-SEEM will significantly leverage and strengthen the research capacities of user communities, thus improving research productivity and competitiveness on the pan-European level. Joining, sharing and exploiting the resources across the SEEM region in a common platform will ensure continuity and expansion of the available resources and services that will further propel excellence across the region.

The project goal is to provide scientists with access to state of the art e-Infrastructure as computing, storage and connectivity resources available in the region; and promote the inclusion of additional resources into an integrated Virtual Research Environments. Part of functions are facilitation of data management for the selected Scientific Communities, engaging the full data management lifecycle, link data across the region, and providing data interoperability across disciplines.

The project is bringing high level expertise in e-Infrastructure utilization to enable research

activities of international standing in the selected fields of research, complemented by adequate user support and training programs for the user communities in the SEEM region.

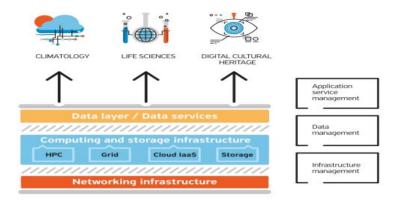


Figure. 1. The concept of the VI-SEEM Virtual Research Environment

The project has six work-packages focused in administrative and technical management; communication, marketing, training and innovation; e-Infrastructure services for the unified underlying e-Infrastructure; data management lifecycle; domain-specific services and support for three target regional communities climatology, life sciences and cultural heritage; and capacity building, open calls and sustainability.

3. The VI-SEEM Infrastructure

The integrated infrastructure of VI-SEEM includes HPC, grid and cloud systems from partner institutions, including 21,500 CPU cores, 325,000 GP-GPU cores and 18,500 Intel Xeon Phi cores of HPC, 2,900 grid cores, 10,500 cloud VM cores, 11 PBytes of storage; with 5-15%, 10-15%, 5% and 10% of respective capacities dedicated for the project.

The local infrastructure in Faculty of Information Technology in UPT includes two systems – HPC and cloud. The HPC system is composed by the Sugon-Dawning blades system, with 24 nodes of 2x4 cores, two gateway servers used to access remotely the system, 4 GB central memory per node, with actually 144 nodes active, 1 GBPS switch, NFS (Network File System), operating system Scientific Linux 6, and middleware MPI & Torque.

The system was from an initiative of Albanian Ministry of Innovation and donated by P.R. of China Government. The system is accessible via secure shell protocol. User directories and the software package OpenFOAM are installed in the gateway sub-system and accessible by all nodes via NFS.

The cloud system is based on the old grid cluster funded by the SEE-GRID projects and Albanian Ministry of Education and Science.

The actual cluster has four nodes with dual core Intel Xeon 1.86GHz, 2GB RAM and 80GB storage per node. One of nodes serves as cloud controller, and the rest of three nodes serve as compute nodes running virtual machines over KVM hypervisor. Each virtual machine has

one VCPU, 512 MB RAM and 30GB external storage, running Ubuntu 14.04. In total there are prepared six virtual machines for the scope of the project. The open source software package OPENSTACK (MITAKA) is used to create the cloud virtual environment, accessible through the web interface that permits users to create and use virtual machines.

4. The VI-SEEM Application in UPT

Selected application for UPT is wind simulation using the software OpenFOAM, a complicated open source package for solving of generalized Navier-Stokes equations [14], already functional in the system HPC SUGON of FTI. The 3D model of atmosphere is defined as a volume of 360x480x10km, which lower border surface is deformed following the terrain (Figure 2) [15-16].

Based on the available SRTM DEM of resolution 3" (100m in equator) we prepared three basic models with mesh cell size 10km for low resolution, 1.0km for medium resolution, and 100m for high resolution.

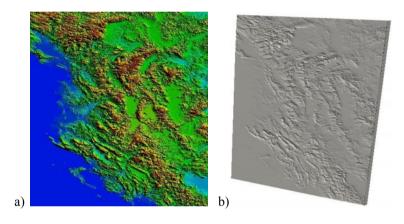


Figure. 2. DEM image (a) and deformed 3D volume of atmosphere (b)

We succeeded to run small and medium resolution models with digitizing grids up to 1km, which is not sufficient in case of Albanian relief where part of valleys have the same typical width. The maximal STRM DEM resolution offered freely from USGS is at the range of 100m, sufficient for conditions of Albanian relief, but requested computing resources for running OpenFOAM were not sufficient for such resolutions (at least until the time of writing this paper).

Memory requirements for basic modules of OpenFOAM – digitizing BlockMesh and the solver IcoFoam are presented in Figure 3. The disk space is given for a single temporal solution, as well as for a case of 100 temporal solutions, necessary to study turbulence phenomena. Central memory requirements for medium size models of resolution 1km mesh is 16GB; and a simple interpolation for the high resolution model of 100m mesh gives for the central memory values at the range of 2TB, practically unreachable.

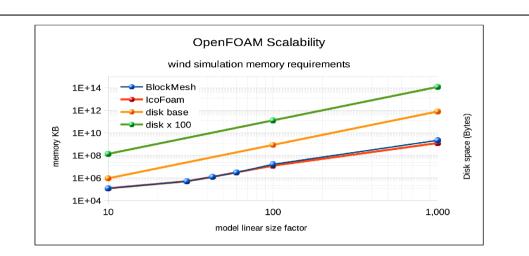


Figure. 3. Memory requirements of OpenFOAM

Disk requirements are variable depending on concrete values of mesh node coordinates, in our case single solution disk space varies around 1.3GB for the medium resolution model and interpolated for the high resolution model 1.0TB.

Runtime scalability is studied from points of view of model sizes and of number of processing cores (processes), presented in Figure 4 and Figure 5. Beside IcoFoam module (the only one that can be run in parallel), digitizing module together with data decomposing and recomposing modules for parallel processes are considered.

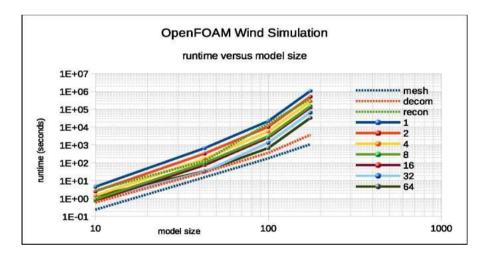
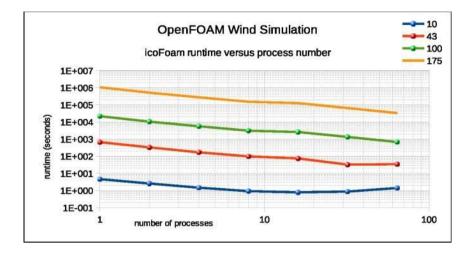


Figure. 4. OpenFOAM scalability versus model size, for 1 ÷ 64 cores

Slow decrease of runtime of the solver IcoFoam is apparent. It is greater than the runtime of preparatory modules for mesh creation and cutting of data for parallel processing, but the module for combination of results chunks from parallel processes into a unified solution



required considerable runtime compared with single process computing of the solver.

Figure. 5. IcoFoam solver scalability versus processing cores, per different model sizes

The decrease of runtime with the increase of number of processes represents a small step when passing from 8 processes in single node in 16 processes in many nodes. Also there is a degeneration of runtime when high number of processes is used for small models.

Some preliminary results of simulations are presented in Fig. 6. The distribution of the speed of the wind in altitude 1,500m in case of difference of pressure North to South is extracted using ParaFoam visualization module. In the figure there are presented the speeds in directions North to South, East to West, and vertical flow of the wind. There are visible the reduced wind speed in closed valleys, strong vertical wind flows in mountain slopes facing North, and some weak traversal flow East – West created because of the oblique extension of principal valleys. Presence of near surface vertical wind flows may create problems for wind farms.

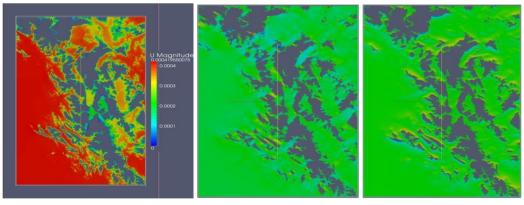


Figure. 6. Wind speed in altitude 1,500m, directions N-S, E-W and vertical.

3. Conclusions

Realization of regional models with high resolution requires huge computation capacities – both memory and runtime, which are impossible in small HPC systems. Medium resolution models were possible in Avitohol parallel system of IICT, Bulgarian Academy of Sciences in Sofia. Preparatory modules of OpenFOAM require the total of central memory, and the study of dynamic turbulent wind simulations require resolution of the model for a suite of time steps, multiplicating the runtime. The increase of spatial resolution must be correlated with the temporal resolution in order to assure the convergence. Integration in the simulations of factors as temperature remains a task for the future.

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