Grid based calibration of SWAT hydrological models

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Abstract. The calibration and execution of large hydrological models, such as SWAT (soil and water assessment tool), developed for large areas, high resolution, and huge input data, need not only quite a long execution time but also high computation resources. SWAT hydrological model supports studies and predictions of the impact of land management practices on water, sediment, and agricultural chemical yields in complex watersheds. The paper presents the gSWAT application as a web practical solution for environmental specialists to calibrate extensive hydrological models and to run scenarios, by hiding the complex control of processes and heterogeneous resources across the grid based high computation infrastructure. The paper highlights the basic functionalities of the gSWAT platform, and the features of the graphical user interface. The presentation is concerned with the development of working sessions, interactive control of calibration, direct and basic editing of parameters, process monitoring, and graphical and interactive visualization of the results. The experiments performed on different SWAT models and the obtained results argue the benefits brought by the grid parallel and distributed environment as a solution for the processing platform. All the instances of SWAT models used in the reported experiments have been developed through the enviroGRIDS project, targeting the Black Sea catchment area.

1 Introduction

The studies and the predictions of environmental phenomena are based also on complex hydrological models by processing huge spatial data sets in order to obtain high resolution results. Actually, the simulation sessions and the searching for a convergence toward the optimum calibrated model are not trivial processes, and require the use of flexible interactive tools. Sometimes the obtained results are not relevant enough to obtain meaningful predictions, and the processing has to be repeated several times by the user. Better predictions require a great number of simulations, which increase the computation resources needed to process all this data. Moreover, extensive resources are imperatively required by high quality services in a scalable system. The scalability is defined in terms of number of users, number of application instances, number of running models, and number of computation and storage resources.

Grid infrastructure offers such a solution for high power computation and extensive resources, but it involves as well a lot of issues such as the management of interoperable software and hardware platforms, distribution of huge spatial data model over storage nodes, process scheduling, parallel and distributed processing, execution monitoring, load balancing, security, scalability, and many others.

One of the main challenges of the user application is to hide the complexity of grid infrastructure management, and to offer all the main functionality to the specialist user, similar with the case of processing and visualization through a local application, similar with a single user of resources, data protection, and good control of processing. The user must have all the time feedback information about the model status, progression of the task execution, results, quality of processing, and user interaction.

This paper presents the gSWAT application as a web practical solution for environmental specialists to calibrate extensive hydrological models and to run scenarios, by hiding the complex control of processes and heterogeneous resources across the grid based high computation infrastructure. The paper highlights the main objectives of the research work, through which solutions are explored for the basic functionalities of the gSWAT platform, and the possible features

supported by the graphical user interface, in order to provide good usability.

The presentation is concerned with the development of the working sessions (i.e. projects), interactive control of the calibration, direct and basic editing of parameters, process monitoring, and the graphical and interactive visualization of the results. A few practical experiments have been performed on different SWAT models (SWAT, 2012), and the achievements argue indeed the benefits brought by the grid parallel and distributed environment as a solution for the processing platform. The gSWAT application and the SWAT hydrological models used in the reported experiments have been developed through the enviroGRIDS (Black Sea Catchment Observation and Assessment System supporting Sustainable Development), funded by the European Commission (EC) through 7th Framework Programme (FP7) (enviroGRIDS, 2012), targeting the Black Sea catchment area, and particularly the Danube River.

The enviroGRIDS system resources are accessible to the large community of users through the Black Sea Catchment Observation System (BSC-OS) portal that includes the gSWAT application as well as other web applications for data management, satellite image processing, report generation and visualization, and virtual training center (Fig. 1).

The gSWAT platform and application improve the features and the performance by significantly reducing the total calibration time through high storage and computing capabilities due to the grid infrastructure, multicalibration processing, exposure as web application, and interactive results management. Calibration and execution results of the SWAT model could be analysed and visualized over interactive maps, using different image processing algorithms in order to correctly classify the land management practices on water, sediment or agricultural chemical yields. All of these features will be described in the following sections.

The paper is structured as follows: Section 2 presents the works and achievements related with the enviroGRIDS project. Section 3 describes the SWAT hydrological model as the main model used by gSWAT application. Section 4 analyses the requirements of the parallel and distributed processing of SWAT models. Section 5 enumerates the high power computation possible solutions, and concerns mainly on grid infrastructure. The gSWAT solution is described in Sect 6. Section 7 details the graphical user interface and the available features. Section 8 enumerates the user categories related with gSWAT based scenarios. Three experiments are described and analyzed in Sect. 9. The last section sketches the conclusions and the future research directions regarding the hydrological model processing.

2 Related works

The enviroGRIDS project aims to use the SWAT model as a high-resolution (i.e. sub-catchment spatial and daily temporal resolution) water balance model for the entire Black Sea catchment. The model will be calibrated and validated using river discharge data, river water quality data, and crop yield data as in Abbaspour et al. (2007). The Black Sea watershed related hydrological model is very complex due to the highly interconnected and continuously evolving interactions at many spatial and temporal scales, and requires to gather and integrate different sets of environmental data (e.g. physical, chemical, biological) (GEO, 2007). Other European projects aim environmental related subjects (Environment, 2011). IS-ENES project develops the European Network for Earth System Modeling (ENES), which calls together the European climate/Earth system modeling community in order to work on understanding and prediction of future climate change. Many other European projects such as SAW-GEO, CYCLOPS, GDI-grid, GEO-grid, DEEGREE, DORII, and GENESI-DR address the management of spatial data and environmental tools and applications.

The hydrological models can be developed by some similar tools such as SWAT (SWAT, 2012), HSPF (HSPF, 2012), and SHETRAN (Ewen et al., 2000). HSPF (Hydrological Simulation Program – Fortran) is a software application that simulates the hydrological and associated water quality processes on pervious and impervious land surfaces. SHETRAN (Système Hydrologique Européan) models coupled surface and subsurface water flow in river basins. The processing results are visualized by animated graphics. SHETRAN could be used in the analysis of environmental impacts: land erosion, pollution, climate change, or in surface-water and ground-water resources studies.

One of the main goals of the gSWAT application is related to the assessment of the sustainability and vulnerability in the Black Sea catchment. Calibrating the SWAT model becomes an important problem when applying the model on such large watersheds. In these cases the calibration time could take days to complete, even on the finest standalone machines. There are a few approaches and tools that could be used to calibrate the SWAT model. The first one is to execute the calibration process on a single-core machine. An important progress was already established in this direction through the SWAT-CUP (SWAT Calibration and Uncertainty Procedures) application (Abbaspour et al., 2008). SWAT-CUP is a software tool designed to calibrate the SWAT model, based on some input parameters. The tool provides complex capabilities regarding the analysis of the calibrated outputs by charts. This solution supports efficiently small watershed SWAT models. The second solution extends the SWAT-CUP application to work on multicore machines. This significantly reduces the total calibration time, but still could not be applied on large watersheds (e.g. huge Black Sea catchment models), just on small and medium ones. Even though the SWAT-CUP application is used for several years to perform the SWAT model calibration process.

The SWAT-CUP solution simplifies the usage of large distributed infrastructures such as grid and cloud, which offer
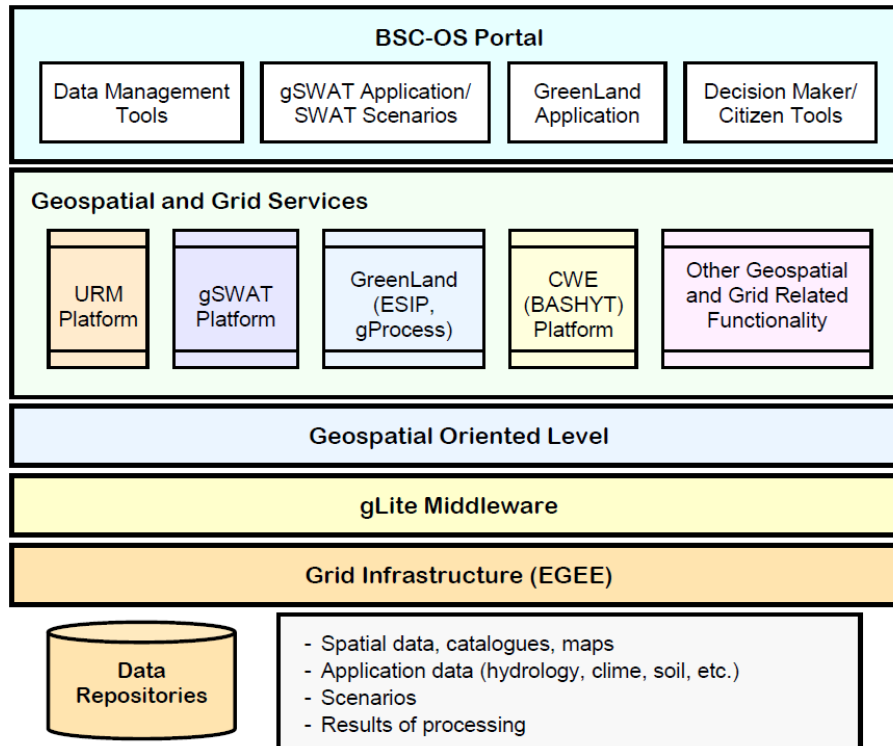
Fig. 1. BSC-OS portal architecture.

high computation and storage capabilities. The main difference between them is that the grid could be used free of charge as long as the user has valid grid certificates, signed by a competent CA (Certificate Authority). Meantime, using the cloud infrastructure, users have to pay for each time they use its services. With proper configuration and scheduling mechanisms of the large scale distributed systems, analysed and experimented in Pop et al. (2008); Simion et al. (2007); Pop (2010), the grid infrastructure could provide significant speed up, regarding the calibration and execution of the SWAT hydrological model. The Experimental results section details all these aspects.

The goal of the DRIHMS project (DRIHMS, 2012) is to systematically build a bridge between the HMR (hydro-meteorological research) and ICT (information and computing technology) communities, and to identify requirements of HMR users and match them to capabilities of the newly developed ICT infrastructure.

The projects EGEE (EGEE, 2010), SEE-GRID-SCI (SEE-GRID-SCI, 2010), and C3grid (C3Grid, 2012) provide solutions for sharing complex spatial and environmental data sets and grid based processing tools and applications. The aim of the C3grid project, for instance, is to create a grid based working environment for Earth system research.

The coordination of the grid infrastructure is now taken over by the European grid initiative (EGI, 2012), which is the future sustainable computing grid infrastructure in Europe.

The new European middleware initiative (EMI) aims to improve and standardize the dominant existing various middleware in order to produce one simplified and interoperable middleware (EMI, 2012). EMI attempts to unify a few grid platforms such as ARC (ARC, 2012), gLite (gLite, 2012), Unicore (UNICORE, 2012) and dCache (dCache, 2012). The EMI platform will empower the EGI infrastructure with more stable, usable and manageable software.

Although a recent survey (Lecca et al., 2011) indicates that grid technology in hydrology has been successfully tested to improve flood prediction and ground-water resources management, only minimal efforts on reduction of computation time have been made in the past for SWAT modeling (Whittaker, 2004).

The enviroGRIDS project gathers solutions and experience from all these mentioned projects in order to approach the particularity of the Black Sea catchment in terms of SDI, platforms interoperability (i.e. geospatial and grid, and software platforms like URM, gSWAT, ESIP, eGLE, etc), high resolution models, processing scalability, user interaction usability, and processing efficiency (Gorgan et al., 2011).

3 Hydrological models

Hydrological models are simplified, conceptual representations of a part of the hydrological cycle and they are primarily used for understanding hydrologic processes and for

hydrologic prediction. One of the main problems that exist when using the hydrological models is that different combinations of parameters or even different model structures yield similar results in terms of a defined performance measure, or objective function. This is a serious problem as it leads to difficulties in interpreting past behavior of the catchment system but also future predictions.

SWAT (Soil and Water Assessment Tool) (SWAT, 2012) is a large scale hydrological model developed to estimate the impact of different land management practices on water quantity and quality, sediment and agricultural chemical yields in large, complex watersheds. It allows a number of physical processes to be simulated in a basin (Yalewa et al., 2010). Basic data requirements for SWAT models include elevation, soil properties, topography, land use, and climate data. Depending on the objective of the model information, the calibration of the model requires river discharge data, water quality information (sediment concentration, levels of nitrate, levels of phosphate, etc.), and agricultural practices (fertilizer application, harvesting, irrigation, etc.). The inputs of SWAT models can be grouped by different levels of detail: watershed, sub-basin, HRU and reservoirs, and the input files can be gathered from different sources and in different formats.

Applying hydrological models and obtaining meaningful predictions requires performing both a good calibration and a good prediction analysis. The need for a model calibration is a major limitation, especially where no stream-flow measurements are available. To calibrate a selected model structure to a large number of catchments, statistical relationships between the parameters and the characteristics of the catchment, such as size, land use or soil types, must be established. These relationships can then be used to derive parameter values for an un-sized (not-calibrated) catchment. In the model calibration process, the parameters are adjusted until the system output and the model output show an acceptable level of agreement, usually measured by an objective function. Manual calibration is time consuming and difficult in the presence of parameter dependence, especially for non-specialist users.

From the hydrological point of view, SWAT model calibration consists of three steps: water balance and stream flow, sediment and nutrients. This process is very expensive, as it is based on the Monte Carlo approach. From the computational point of view, the SWAT calibration is the process of running SWAT iterations several times, using different parameter sets, until the calibration criteria is satisfied (Rodila et al., 2011b). Each such iteration consists of hundred of simulations which are independent one from another.

4   Parallel and distributed execution of SWAT hydrological models

Some large problems can be subdivided into smaller ones, which can run in parallel. There are several forms of parallel

computation, each one dealing with different strategies, such as with instruction, data or task parallelism. For SWAT, the parallelism at instruction level is quite a difficult task. The data parallelism is much easier to accomplish based on the idea of the calibration process. The task parallelism would require splitting the high resolution SWAT hydrological model into smaller components that could be computed in parallel.

The parallel computation can run on various infrastructures, such as multicore machine, cluster, grid or cloud. A multicore machine can offer limited computational resources where the grid or cloud can offer theoretically unlimited resources. In addition, based on the execution requirements, the computational infrastructure could select the best suitable resource.

The calibration process takes, in general, very much time, mainly because of the complexity of the SWAT hydrological models and the necessity to run multiple iterations. In each iteration we need to execute a high number of simulations. To decrease the execution time, we must parallelize the application at some level (simulation, executable or model). The resources needed for calibrating SWAT models are distributed: data on a dedicated storage resource and execution on different computational resources. The easiest way is to parallelize the execution at the simulation level. This parallelization is implicit for the calibration process because each simulation runs independently of the other ones. In this way, we can theoretically execute each simulation on a different processor. We don't need to split the model, we just run each simulation on another machine.

For the gSWAT application, we have chosen this method, parallelization at the simulation level, because it can be used for any SWAT hydrological model, it does not depend on the model itself.

5   High power computation infrastructure

Both the calibration and the execution of SWAT models require a large number of input and output data files. Due to the large set of input and output data and the high number of simulations required for obtaining a good and meaningful SWAT model calibration, there are some basic computational requirements needed to be fulfilled. These requirements can no longer be assured by a desktop computer or a single server; they require a high power computation infrastructure able to offer high computational resources as well as storage resources.

5.1   Multicore architecture

Multicore architectures are based on many processors and associated caches or memories. The multicore executions benefit of all the advantages of a PC and the most important ones are the full control of the job being processed and the easy access to the available resources. This architecture has been

exploited as execution environment for SWAT models calibration (Rouholahnejad et al., 2011) and the obtained results were quite promising compared to desktop execution.

5.2 Cloud infrastructure

The definition of cloud computing, given by the European expert group, is the following: "A cloud is an elastic execution environment of resources involving multiple stakeholders and providing a metered service at multiple granularities for a specified level of quality (of service)". The research interests in the cloud computing area are oriented on solving problems like interoperability, portability, data distribution and protection, automatic management of resources, elastic scalability, etc. In the context of SWAT hydrological models, we are planning to experiment the execution of SWAT calibration over an experimental cloud and to make a comparative analysis for the advantages offered by cloud compared to the grid infrastructure.

5.3 Computer cluster

By computer cluster, we understand a set of connected computers that are working together and from the outside the cluster can be viewed as a single system, or a virtual computer. In such a system architecture, each cluster component, or node, runs its own instance. They are mainly used to improve computational performance and availability. The solution to parallelize the calibration process on computer clusters is somehow similar to the one for the grid infrastructures, but lacking the scalability offered by grid.

5.4 Grid infrastructure

The grid infrastructures are offering both computational and storage solutions for scientific communities. The provided functionality is exposed through a set of services, dealing with security, data management, execution, information, etc. Grid users are grouped under the umbrella of a so-called virtual organization (VO) and are sharing the same resources, data, processors, software components and the hardware infrastructure. Each VO is in particular addressed to a specific scientific community, such as earth science, physics, biology, oceanography, etc.

In order to access the grid resources each user must first be authenticated and authorized. To authenticate, the user must have a grid certificate, which can be viewed as a personal identity card, issued by a certification authority (CA). For each VO the virtual organization membership service (VOMS) allows defining privileges for each user that makes part of that VO (meaning the authorization). The typical entry point in a grid infrastructure is the user interface (UI), which allows the users to perform some operations using a command line interface. For instance, the users can submit jobs for execution, manage their running jobs (cancel the execution, retrieve the output from the completed jobs, view the

status of the running jobs, etc.), manage data, or interrogate the Information System to retrieve information related with available resources. This approach is not suitable for all kinds of users, so in many cases the users access the grid functionality through a graphical user interface that hides some of the complexity of the underlying infrastructure.

A job represents a unit of work and is described by specifying some information such as the name of the program to run, the input files, the output files that are produced and the requirements that must be fulfilled by the machine that will execute the job. Each job will be executed on a worker node (WN), basically the computational resource. To submit jobs, the users interact with a computing element (CE). The CE is a collection of computing resources (WNs) that are localized at a site (similar to a cluster). Each CE has an entry point, which is the generic interface to the computing resources, and a local resource management system, which manages grid jobs.

A user or an application stores data on a storage element (SE), which is a specialised machine that provides uniform access to data storage resources. The data that is stored on a SE is considered read-only, meaning that the data can be changed only by physically removing it or replacing it. The information service (IS) provides information regarding the grid resources used mainly for monitoring purposes. The most important grid middlewares are gLite and Globus. Both of them are offering services related to job and data management, security, monitoring, etc.

In the enviroGRIDS project, we have created a VO called envirogrids.vo.eu-egee.org. Currently we have integrated one CE (ce01.mosigrid.utcluj.ro) and one SE (se01.mosigrid.utcluj.ro). The computational resources consist of 128 physical CPUs, meaning a total of 1024 logical CPUs. The storage capacity is approximately of 13 TB.

5.5 Grid based solution for SWAT calibration

The most important algorithms that could be used for calibrating SWAT hydrological modes are SUFI2 (Sequential Uncertainty Fitting), GLUE (Generalized Likelihood Uncertainty Estimation) and ParaSol (Parameter Solution). SUFI2 can be used for obtaining quick calibration results, but it is not as accurate as GLUE or ParaSol algorithms. It performs uncertainty analysis for the SWAT hydrological model, based on some objective functions, including Chi square, Nasch-Sutcliffe, R2 and bR2. It is the most suitable algorithm for parallelization because each simulation can run independently.

As we already stated, the execution time of the calibration process can be improved by using the computational resources offered by the grid infrastructures. The size of a high resolution SWAT model is quite high (some GBs). For this reason, we are using a SE machine to store the initial SWAT hydrological models and some of the outputs generated by running the simulations.
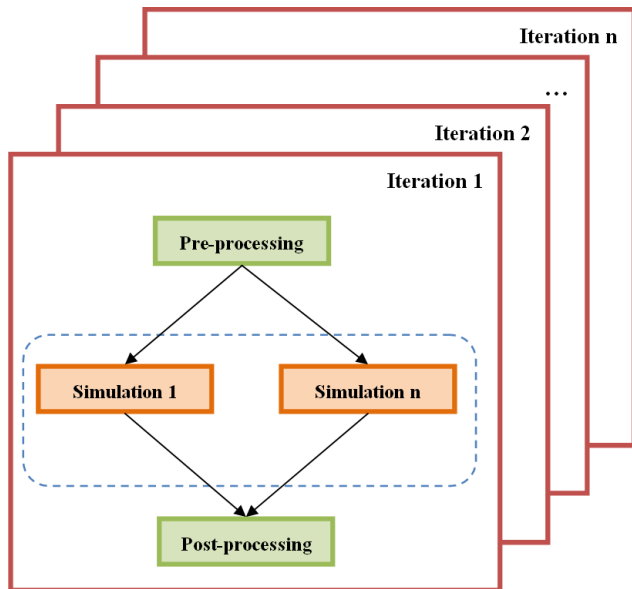
Fig. 2. SWAT model calibration process.

Fig. 3. gSWAT application flow.

The calibration process (Fig. 2) consists of running a variable number of iterations until a calibration goal is fulfilled. For each iteration, we are performing the same steps:

1. pre-processing – we generate the parameter sets for each simulation using the Latin hypercube sampling. Together with the SWAT model, it represents the input data for one simulation;

2. execution of simulations – we execute each simulation on a WN from the grid infrastructure;

3. post-processing – we compute the goal function value for each simulation and we determine new parameter ranges.

The pre-processing and post-processing steps are not so computational intensive so we are executing them on the server side, not in grid. We are submitting only the simulations to be executed on the grid resources. The monitoring of simulations is very important because we need all the simulations to provide some output results. If the execution of one simulation fails then we need to execute again the same simulation.

Depending on the SWAT hydrological model complexity, we reserve a number of WNs to be used to run the simulations. Because the number of simulations will be in general higher than the number of WNs that we are reserving, each WN will execute one or more simulations. For each simulation, we copy the initial SWAT hydrological model from SE, we copy the parameter set that was generated from the gSWAT server, we run the SWAT model and in the end, we collect the results.
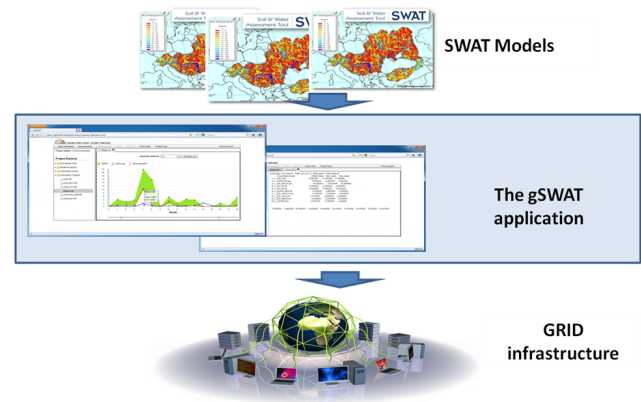
6 gSWAT application

The gSWAT is a client-server platform (Fig. 3) used in the process of calibrating medium and large SWAT hydrological models. Because it is a web-based application, it does not require any kind of installation for which the house-hold user should be concerned. It is a remote application, which could be accessed over the Internet. It is worth mentioning that the implementation of such a system raised several problems, such as processing large volumes of data, security issues regarding data access, implementing simple but powerful human-computer interaction techniques, etc. The following paragraphs will describes these kinds of problems along with their technical solutions.

Another important feature of the gSWAT platform is related to the possibility of creating prediction scenarios (e.g. water-use sustainability, improving irrigation systems, improving crops growth by changing the quantity of nutrients, etc) based on data obtained through the SWAT model. Because this data mainly consist of estimated values, first a calibration algorithm is needed to bring these values as close as possible to measured values for the same watersheds. These estimated values are used mainly in the prediction process (e.g. what impact will have a larger quantity of nutrients on surrounding land crops?) (Pohlert et al., 2007; Zhang et al., 2008).

The link between the user requests and the server-side functionality of the gSWAT platform is based on web services. For a specific request, the graphical user interface waits until a valid or an error response arrives, and then makes proper GUI customizations. The client side is developed using Adobe Flex 4 latest technology. One of the most important reasons for choosing this technology in the gSWAT development stage was the fact that it runs in Adobe Flash Player, supported by all common browsers and operating systems. Also the ease of plotting data charts is another advantage offered by this technology. The java web services that reside on the server side are called from the graphical user
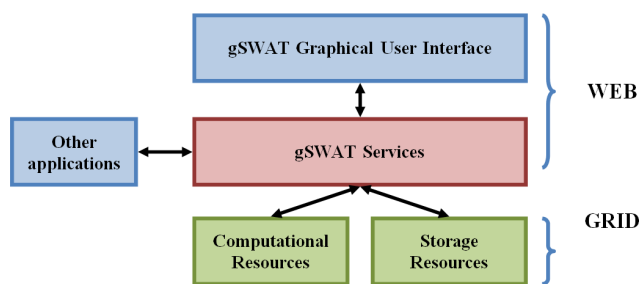
Fig. 4. Functional layers of the gSWAT application.

interface through user requests. The main advantage of the web services are their accessibility and compatibility with all software platforms and programming languages.

This section points out the most important user interaction techniques implemented within the gSWAT application and describes them in a simple and intuitive manner.

6.1 gSWAT based hydrological model processing

In this section, we are presenting the entire flow regarding the SWAT hydrological model integrated in the enviroGRIDS portal. Most of the tools and applications involved in this flow are developed in the frame of the enviroGRIDS project.

SWAT hydrological models are developed using specialized software such as ArcSWAT or AvSWAT. The ArcSWAT application is an ArcGIS-ArcView extension providing a flexible graphical user input interface for developing SWAT models. To be able to define specific scenarios on a SWAT model, the user has to calibrate it. The calibration process requires huge computation resources for high-resolution models (involves the running of hundreds and even thousands of simulations) that can be offered by the grid infrastructures. After the calibration process is completed and the model is calibrated we need to upload the calibrated model to BASHYT (the basin scale hydrological tool) (Manca et al., 2009). BASHYT is a web-based interface that allows to define new scenarios in a flexible manner. New scenarios, which represent new SWAT models, are transferred to the gSWATSim (Bacu et al., 2011) component, which is specialized in executing scenarios. gSWATSim application runs the scenario also on the grid infrastructure and then uploads the execution results to BASHYT. The user has the possibility to visualize reports developed in BASHYT and based on the scenario execution. A report aggregates different information such as maps, charts, tables, images, text, etc.

6.2 gSWAT oriented architecture

The gSWAT application is composed of three different functional layers (Fig. 4):

1. the Graphical User Interface – it is developed in Adobe Flex and allows the users to define the calibration

parameters, to start and monitor the calibration process, to visualize and download the output results;

2. the gSWAT Services – create new calibration projects, upload SWAT models, start new iterations, save finished iterations, delete iterations, upload data to grid in Storage Element, download output data, monitor the execution of the calibrations, update the iteration status;

3. the Computational and Storage resources – are the resources that are used in the calibration process; the users access these resource in a transparent manner, using the graphical user interface. The gSWAT services are exposed as web services and can be used to define other applications or to integrate the calibration functionality.

7 gSWAT graphical user interface

7.1 gSWAT features overview

This application has a simple design that adopts the Nielsen heuristics. This design is divided into three main sections: the menu bar options, the projects list and a user actions dedicated section. The menu provides a set of options that became active based on the user's current operation (e.g. the upload menu item is active only for projects with empty or incomplete uploading statuses). Projects management, grid execution and monitoring capabilities and output visualization are the most important features provided to the user throughout the gSWAT menu module.

It is worth mentioning that each project has a status that reflects its grid calibration progress. The supported statuses are (Fig. 5): Empty project (the project exists in the database only by name, but no physical inputs were attached), incomplete upload (uploading SWAT model inputs failed due to technical inconsistencies), uploading project (uploading input data set in progress), loaded project (all files were successfully uploaded to the server), running iteration (SWAT model calibration is in progress), incomplete iteration (generated by different technical problems, such as grid or network failure), and finished iteration (the calibration process successfully ended for the current iteration). A progress bar is displayed for the projects that have uploading project or running iteration status. This feature estimates the remaining time to complete the action. The projects list contains minimal information about all the users' projects. By default, a project has a private access attribute for all other users.

In order to obtain more details about a project, as presented in Fig. 6, its selection from the project list (by mouse click or by keyboard interaction) is required. This window is also used for other user actions (e.g. create a new project, upload SWAT input files, changing project settings, etc.). If the project has an error status (incomplete uploading for example), a new link will be added into this project information window that offers technical information about this event.
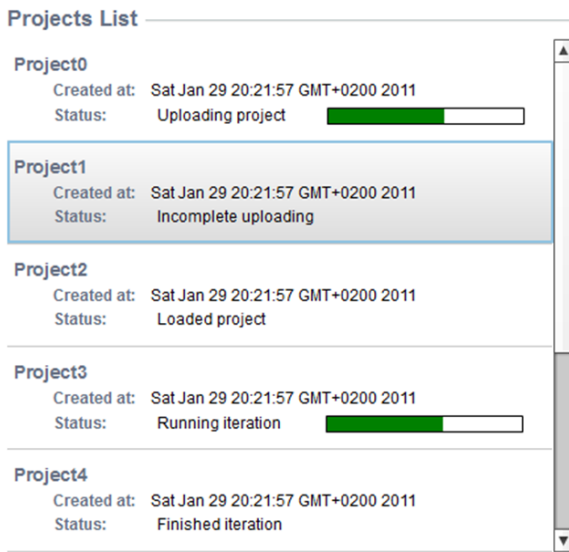
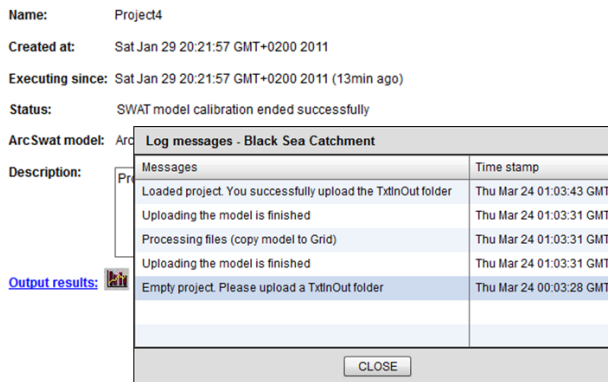**Fig. 5.** User projects list.

Fig. 6. Project information details.

Each action of the user is recorded into the system log that acts like a history mechanism for the users' actions. At each new user's operation, some specific information will be automatically added into this log, along with the project name and the time stamp related to this operation. Error messages are also part of this mechanism in order to increase the recover from error usability.

7.1.1 Search and filter mechanism

When the projects list grows in size, the search and filter system is very useful for the user. The search mechanism allows the finding of projects based on keywords that are contained in the project's name or description. For generality, the search is not case sensitive, meaning that capitalized and lowercase letters could be used with the same effect. The filter mechanism updates as well the projects list in real time. The possible filters are closely related to the project status, but a date filter is also implemented (Fig. 7).
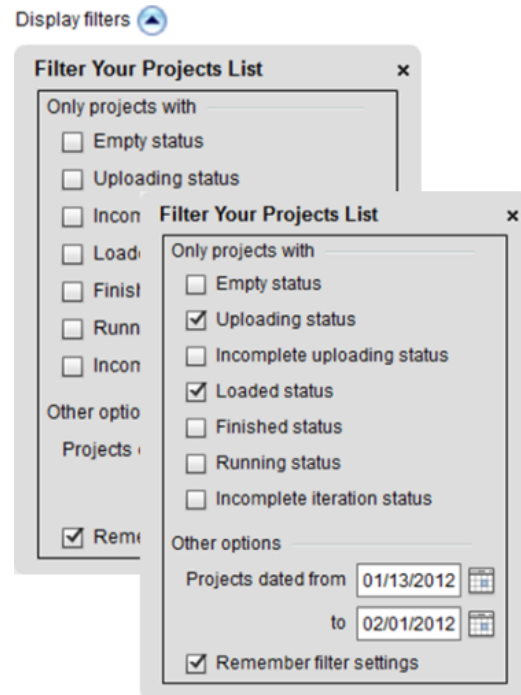

Fig. 7. Filter settings for user projects list.

Taking into account the fact that the user may access the application from different geographical locations or different physical machines, a new mechanism should be implemented in order to apply the same filters, defined by the user, from one session to another. In the gSWAT preloading phase, a web service provides from a centralized database the filter settings for the logged in user. Figure 7 presents the possible list of filters that the user could choose from. For saving these settings, the last check box should be selected.

7.1.2 Input data specification

After creating a new project by using the gSWAT menu features, it's time to assign it with input data (TxtInOut folder from a SWAT model in our case). This action is performed through an upload mechanism integrated within the gSWAT platform. After this stage, the project displays the loaded status. Because the gSWAT application is designed to deal with medium and large watersheds, the TxtInOut folder could reach thousands of files in size. Taking this into account the user is restricted to upload folders archived as zip, rar or tar.gz. The limitation refers only to the files packaging and has no restriction regarding their size. The upload mechanism requires two user related actions:

1. browse the local files and folders structure in order to select the right data inputs (TxtInOut archive in our case);

2. transfer the archive content to the gSWAT application server. At this stage, the database is properly updated
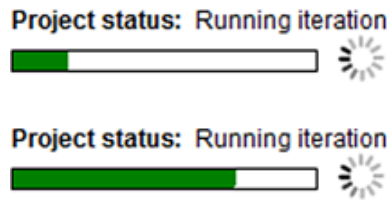
Fig. 8. SWAT calibration in multiple process phases.

with the new incoming information. A progress bar indicates the stage of the upload process. It is worth mentioning that the upload mechanism is highly dependent on the network traffic and bandwidth and on the number of users that simultaneously access the application server.

7.1.3 Starting SWAT calibration process

Using the start calibration menu feature, the user is able to calibrate an already uploaded SWAT model. Before this action, all the internal parameters that could affect the calibration result should be specified. This pre-processing step is done through the text editor module that will be presented in the following paragraphs.

When the SWAT calibration process starts a general timer is activated that periodically interrogates the database. This way the graphical user interface of the gSWAT application is always up to date with the calibration progress on the worker nodes of the grid. It is worth mentioning that all the SWAT calibration processes are done on the grid infrastructure due to its high computation and storage capabilities.

The calibration progress in the gSWAT user interface is represented by a progress bar, that starts from 0 % (initial phase) up to 100 % (at the end of the calibration). As each job finishes its execution this progress bar updates accordingly. Also an animated spinning wheel is placed along with this graphical feature, to give the user an extra execution feedback (Fig. 8). In this step the project displays the running iteration status.

At any time in the calibration process the user is able to stop the grid execution by clicking on a single button, called stop calibration. The actions performed in the background are transparent for the user, and have the effect of cancelling all calibration related tasks.

Before starting a new calibration of the same SWAT model, the user has the possibility to save its previous work. All the saved iterations are accessible to the user in the iteration history folder, placed in the TxtInOut tree structure.

7.1.4 Output results analysis

When creating a new project in the gSWAT application, a predefined folders and files structure as created on the server side. This structure is then loaded into the graphical user interface, where it could be explored by the user.

The gSWAT editor module offers the possibility to edit the files contained in this TxtInOut structure. On double click event on these files, their content is displayed into a text area, readable and editable for the user. This text editor supports multiple files opened at the same time, where each such file is located in a different tab.

The basic operations that exist in any other text editor tools were already implemented into the gSWAT application (save file, save all file, close file, redo, undo, copy and paste etc). When the content of a file is modified by the user, an asterisk (*) appears at the beginning of the file name. This alerts the user that the content inside that tab was not saved. Also, the action of editing large files, with tens of thousands of lines is supported by the editor module.

The output results of the SWAT model calibration processes consists of several data files that contain values of the calibrated parameters. One of these files is extremely important because it could be displayed to the user as an interactive chart, as presented in Fig. 9.

All the data represented in the chart module is parsed from the 95ppu.txt file. The plotted values are not dependable on the number of parameters listed in this file. The example described in Fig. 6 contains only 5 such parameters. This chart defines the best estimated parameters values (obtained during the SWAT calibration process) and the observed ones (measured from station spread across the entire watershed) so that the specialist could make a statistical approximation of the calibration accuracy. An uncertainty analysis could be performed based on this kind of data representation.

The tool tips button displays numerical values for the chart key points. Each inflexion point gives the user the possibility to visualize the best estimated and ground measured values of the SWAT parameters. The x-axis of the chart represents the temporal scale used in the calibration process. The y-axis displays the numerical values for the current selected parameter. The user could also increase or decrease the temporal interval by using an animated slider with two thumbs. Each thumb represents one of the extremities of this interval (e.g. if 17 months data is available, the user could reduce it to display only usable information for the time interval represented by the 12th and 17th month value on the x-axis of the chart).

8 gSWAT user categories

The gSWAT platform is useful in developing use case scenarios, based on calibrated SWAT models. The purpose of these scenarios is the prediction and analysis of different Earth phenomena, in the hydrological domain field. The gSWAT application could be used by specialists in the hydrology and computer science domains, or by non-technical persons who are interested in visualizing the output results of different scenarios created by the specialists.

There are two main user roles related to the sSWAT application. These roles assign different permissions in accessing
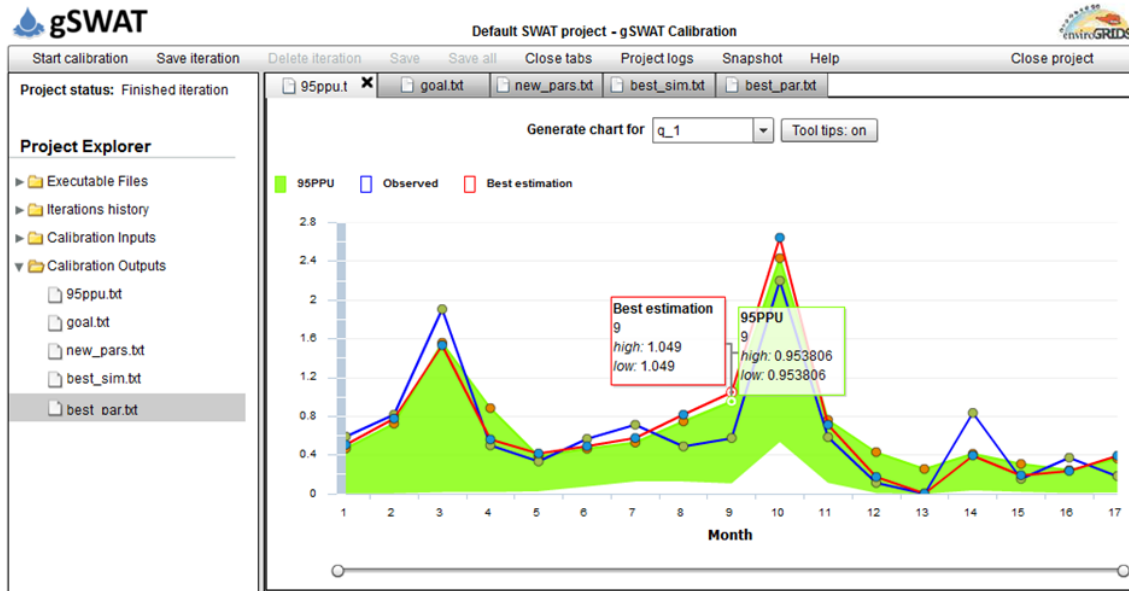
Fig. 9. Detailed visualization of the gSWAT calibration results.

the grid and the web data levels. The first one allows the users the possibility to calibrate SWAT models over the grid infrastructure and to transfer data between the grid nodes and the application server. The second role restricts the users to access only public data, available outside the grid infrastructure. This means that they could only analyze the SWAT calibration outputs, create use case scenarios based on the SWAT calibrated models, perform statistic measurements, etc. At a closer look, the gSWAT user categories could be further divided into data providers, specialists, decision makers and citizens:

- Data providers – this category includes the governmental agencies, hydrology domain field specialists or other persons who are willing to share SWAT models with the gSWAT community. The data confidentiality is assured by the grid certificates and web credentials owned by these users.

- Specialists – they are involved in the SWAT calibration process over the grid infrastructure. The specialists have access to both web and grid data repositories. The main goal of this user category is to provide calibrated SWAT models that could be used in the creation process of use case scenarios.

- Decision makers – these types of users operate only at the web application layer. They analyze the results obtained during the SWAT calibration processes and decide if the models are suited to be used in predicting different Earth natural phenomena.

- Citizens – they can only access results obtained during the scenarios execution process. These results play an informative role regarding the predictions for the simulated Earth phenomena.

9 Grid based experiments

The calibration of SWAT hydrological models has been successfully executed over the grid infrastructure in several experiments performed on different SWAT models and the obtained results were able to sustain the benefits brought by the grid parallel and distributed environment as execution platform. All the instances of SWAT models used in our experiments have been developed by our enviroGRIDS partners from EWAG and they are targeting the Black Sea catchment area.

The Danube River Basin project, described also in Rodila et al. (2011a,b); Rouholahnejad et al. (2011), is a large SWAT hydrological model build using the SWAT 2009 program and covering an area of 801 093 km^2 over a distance of 2826 km – the distance the Danube River flows by. This area was divided into 1224 smaller sub-basins and 69 875 HRUs, based on elevation, climatic information, land use, etc. and the simulation period was set to 5 yr. We have performed experiments based on two instances of the Danube River Basin model and we called them Danube1 and Danube2. These two instances of the model differ from the size point of view, i.e. the number of used parameters, the amount of used data, etc. The Danube2 instance is considerable larger than the Danube1.
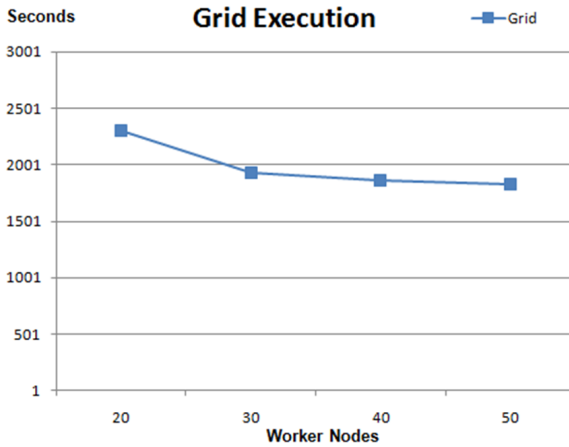
Fig. 10. Danube 1 total calibration time over the grid.

Fig. 11. Danube 2 total calibration time over the grid.

Fig. 12. Danube 2 execution per simulation over the grid.

9.1 Medium SWAT model processing

The first experiment consists in executing the calibration of Danube1 over the grid infrastructure with 48 simulations. We have performed several tests, with a varying number of computing elements (worker nodes in the case of the grid) and we have also made a comparative analysis (Rodila et al., 2011a,b) based on the obtained results and these obtained by our partners (Rouholahnejad et al., 2011) when executing the same model instance on a multicore architecture. The reference point for this experiment is the execution of the model calibration process on a single server, without any parallelization options which took approximately 2 days (1 day, 11 h and 30 min – 127 920 s).

Figure 10 (Rodila et al., 2011a) presents the execution results in seconds obtained for running one iteration with 48 simulations in the process of Danube1 calibration over the grid while varying the number of worker nodes (processing units): 20, 30, 40 and 50 nodes.

The calibration of Danube1 took around 39 min when using 20 processing units and around 31 min with 50 processing units, compared to almost 2 days in which it took to execute the same process sequentially on a single server. These results clearly emphasize the strength of the grid infrastructure in executing large scale processing as well as the successful parallelization of the SWAT calibration process at the simulation level.

9.2 Large SWAT model processing

The second experiment consists in executing the calibration of the Danube2 instance (larger in size than Danube1) with a varying number of simulations: 24, 100 and 500, highlighting the scalability of the grid for large scale applications. To have an idea about the size of the model instance, the number of input files used for calibration is 327 000, grouped in 1.3 GB. All these files have to be backup for execution, obtaining at
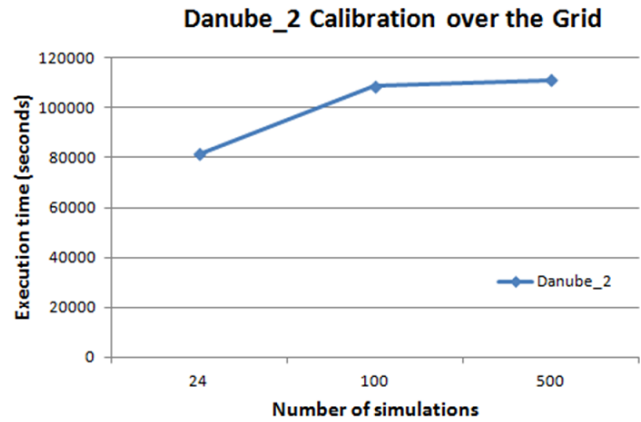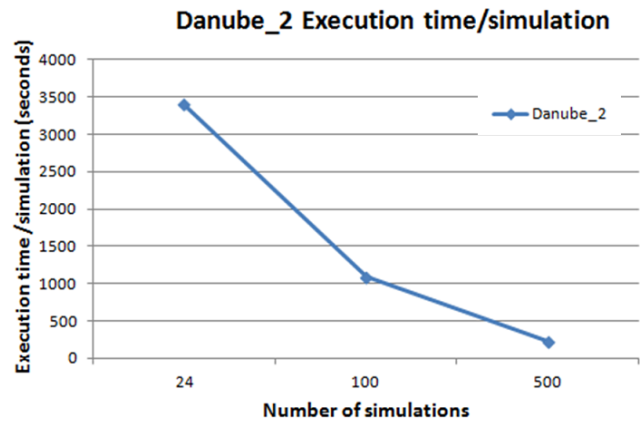
the end, considering also the SWAT executables and default files, an archive of approximately 1.6 GB.

Figure 11 presented in (Rodila et al., 2011a), shows the scalability of the grid infrastructure for executing the calibration of Danube2 as the number of simulations increases. This scalability is assured by the large number of resources available in the grid. The differences in executing the calibration of a large model over the grid with 100 and, respectively, 500 simulations are quite small due to this scalability: approximately 30.18 h compared to 30.85 h.

The time needed to execute one simulation in an iteration decreases considerable as the number of simulations increases: while for 24 simulations the average time for executing one simulation is 57 min, when executing 500 simulations it is 3.7 min – Fig. 12 (Rodila et al., 2011a).

9.3 User scalability

The third experiment shows the influence of multiple users running in the same time some calibration processes. The variables for this experiment were the number of grid WNs that perform the SWAT simulations and the number of users
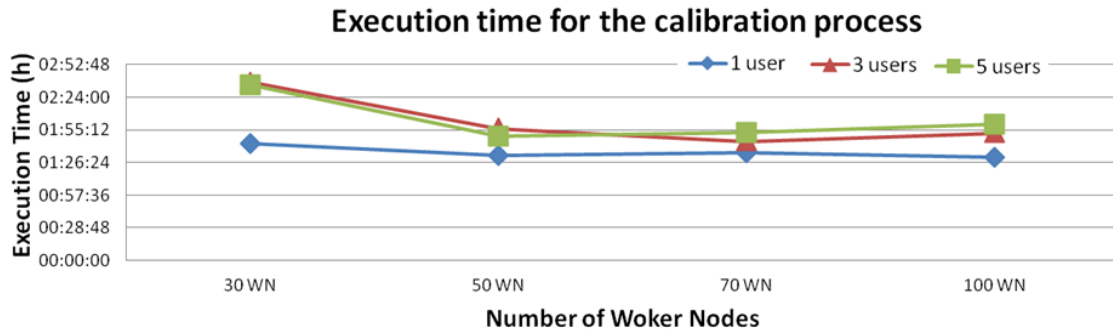
Fig. 13. Calibration time as a function of number of workers and number of current users.

that are running simultaneous iterations using the gSWAT application. We varied the number of grid jobs between 30 and 100. For all experiments, we used the same number of simulations, that is 100. The results of the experiment are presented in Fig. 13. In all cases, the execution time decreases by using more WNs. In some cases, even though the execution time decreases, it is not a good solution to start more WNs because the improvement is not so high (see for example the results for 70 and 100 WNs for one user). Obviously, the execution time depends not only on the SWAT hydrological model complexity, but also on the availability of free WNs. If multiple users are running the calibration process at the same time, the performance of the system is decreasing, mainly because the number of WNs is limited. Another reason for this decrease is that the CE has to manage a higher number of grid jobs.

10 Conclusions

The development of the BSC-OS portal and generally the research through the enviroGRIDS project have revealed a lot of challenges regarding the gathering of data into a dedicated SDI, interoperability between geospatial and grid infrastructures, and interoperability between platforms developed by different partners (e.g. URM, gSWAT, ESIP, gProcess, gLite, BASHYT, and eGLE), huge spatial data sets involved in the development of hydrological models and environmental scenarios (e.g. Danube, Black Sea catchment, Istanbul, and Rioni River in Georgia), security and access management in different platforms, application development in distributed and heterogeneous systems, etc.

Another issue the portal development has to face is the compatibility with new technologies and functional requirements. One main concern is the compatibility with the new European middleware initiative (EMI) that aims to improve and standardize the dominant existing middlewares in order to produce one simplified and interoperable middleware (EMI, 2012). EMI attempts to unify a few grid platforms such as ARC, gLite, Unicore and dCache. The EMI and Globus platforms will empower the EGI (European grid infrastructure) with more stable, useable and manageable software.

We have to develop extended and high resolution models and scenarios, to improve the tool and application functionality, and to improve the user interaction techniques with spatial data models.

The service oriented architecture, multicore, GPGPU based systems, cloud processing are other technologies that we intend to explore in order to extend the functionality, application usability, system efficiency, and to improve the performance of data processing.

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