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Grid-enabled Spatial Data Infrastructure for environmental sciences: Challenges and opportunities

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ABSTRACT

Spatial Data Infrastructures (SDIs) are being widely used in the environmental sciences to share, discover, visualize and retrieve geospatial data through Open Geospatial Consortium (OGC) web services. However, SDIs have limited analytical capabilities, an essential task to turn data into understandable information. Geospatial data are typically processed on desktop computers, but their limited power limits the types of analyses that can be conducted given ever-increasing amounts of high resolution data. With the recently introduced Web Processing Service and the availability of large storage and computing facilities offered by Grid infrastructures, new opportunities are emerging within the environmental sciences communities. The enviroGRIDS project, funded by the European Commission "Seventh Framework Programme" (EU/FP7), will target these issues.

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1. Introduction

Understanding the complex, highly interconnected and continuously evolving processes of the Earth-system is a challenging task which requires gathering and integrating different data sets about physical, chemical, biological and anthropic systems [1]. These environmental data sets need to be processed to turn them into understandable information before they can be disseminated to appropriate decision-makers, stakeholders, and the general public.

Environmental data are often spatially referenced and are thus part, in a broader context, of geospatial data. Geospatial data typically describe geographical locations giving through various attributes knowledge about their spatial and/or temporal extents. Geospatial data, also known as geodata, are extremely valuable as users can build spatial relationships between feature and data [2]. If previously geospatial data were mostly presented in the form of paper maps, they are now used and analyzed within a Geographical Information System (GIS). This computer-based system is capable of assembling, storing, manipulating and displaying geospatial

data [3]. A GIS gives the ability to merge existing data from different sources, facilitating collaboration in creating and analyzing them. This collaborative approach highlights the need to have harmonized data sets in digital form to store them in databases that allow easy storage and dissemination, facilitating data exchange, sharing and updating, and finally improving the accessibility for multiple purposes [4,5].

As a result of the previous considerations, the concept of Spatial Data Infrastructure (SDI) was developed to facilitate and coordinate the exchange of geospatial data [6]. A SDI encompasses data sources, systems, network linkages, standards and institutional issues involved in delivering geospatial data and related information from many sources to the widest possible group of potential users [7].

1.1. Geospatial service oriented architecture

Today's effort on the technical development of SDI components clearly focuses on the exchange of geospatial data and processes in a way that ensures interoperability [8] through services that allow efficient access to spatially distributed resources. The shift towards an infrastructure offering services, rather than a stand-alone system allowing one to find, view and analyze geospatial data, and is highlighted by the growing importance of the distributed model based on independent, specialized, and interoperable services [9]. This shift is driven by the increasing role that geospatial data are

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playing in our every day life, the maturity of web technologies, and the need for organizations to work efficiently by reusing data, capabilities and invested effort and capital. Hence, geospatial technologies are evolving from monolithic GIS systems toward Service Oriented Architecture (SOA) [10], an IT architectural approach defined as "a paradigm for organizing and utilizing distributed capabilities that may be under the control of different ownership domains" [11]. The aim of this architecture is to promote loosely coupled, standard-based, protocol-independent distributed computing so that its components can be reused [12,13].

In a SOA, the key components to build applications are services. These services are well-defined sets of self-contained and stateless actions that do not depend on the state of other services. In other words, a service is simply a collection of operations that a user can discover and invoke. In the case of the geospatial domain, an operation can be a simple request to create a map or a complicated geoprocessing routine applied to a remote sensing image. These services are defined in a standard manner, have a published interface, and can communicate with other services to achieve a specific process or task. Therefore, an SOA provides the framework and rules for services description, discovery, interaction, and execution [10]. To support reusable deployment of services a common pattern defines three components: service provider, service requestor and service broker associated with three operations: publish, find and bind. An SOA relates these three components to the three operations allowing automated discovery and use of services. It must be highlighted that such an automated process depends on syntactic conventions used by the service(s) involved (i.e. matching inputs, preconditions and outputs). In a traditional scenario, a service provider hosts a service and "publishes" a service description to a service broker. The service requestor uses a "find" operation to retrieve the service description and uses it to "bind" with the service provider and to invoke the service itself. This approach can deliver more flexible and agile systems that are easier to maintain and adapt to evolving technologies and requirements than stand-alone software. Indeed, most users of GIS systems are using only a small portion of their software functionalities. Consequently, the open and interoperable environment provided by SOA, based on reusable and standardized services, allows application development to be more focused by providing users just the functionality they need [9].

As of today, implementations of SOA application are mostly realized through the use of web services [14,15]. Web services support interoperable application-to-application communication over a network (e.g. Internet) and are based, in general, on a maturing set of open standards that are widely accepted and used like eXtended Markup Language (XML), Simple Object Access Protocol (SOAP), and Web Service Description Language (WDSL) [16]. This broad acceptance provides a common approach to define, publish, and use web services and permits the development of platform and programming language independent services accessible over standard Internet protocols [17,12]. Web services emphasize the necessity that the systems involved must communicate with each other meaning that web services rely on interoperability. The core functionalities of this type of service are: communication with Internet protocols (commonly HTTP) and data exchange with formatted XML documents. In addition, it is generally accepted to describe a service using WSDL and to use SOAP to transport XML documents over HTTP.

At this point, it is important to distinguish between (1) the generic term of web services that refers to any service provided through the web and (2) the specific web services solutions that are services conforming to a well-defined set of specifications. Hereafter we use the second definition.

Within the geospatial community, SOA is the underlying concept for an interoperable environment based on reusability and

standardized components, and thus it is fundamental for SDIs to allow applications and related components to exchange data, share tasks, and automate processes over the Internet [18]. Based on SOA principles, the Geospatial Portal Reference Architecture [19] specifies four classes of services that are required to implement an efficient SDI using related interoperability specifications: (1) Portal services offer an entry point to discover and access data as well as management and administration capabilities; (2) Catalog services provide information about data and services; (3) Portrayal services focus on mapping and styling capabilities; and (4) Data services concentrate on data access and processing.

To deploy these different service classes, the OGC proposes to use web services relying on XML-Remote Procedure Call (RPC), a protocol that uses XML to encode its calls and HTTP as transport mechanism. Indeed, OGC's first specifications were proposed in late 90's and actual standards (like SOAP/WSDL) were not available back then. However, OGC specifications are continuously evolving and they are now defining new approaches to extend their standard capabilities to use SOAP/WSDL [20–23] as well. This is an important requirement so that OGC Web Services (OWS) can be combined with other types of web services and web-based applications (that are not necessarily geo-enabled). Moreover, the SOAP/WSDL layer provides useful information for discovering and chaining services. Thus, it allows users to create and manage workflows much more easily using, for example, Business Process Execution Language (BPEL) standard [24].

In summary, OWS provides an interoperable framework for web-based discovery, access, integration, analysis, processing and visualization of geospatial data and allows users to build new applications to achieve a specific task based on this set of reusable services.

1.2. The need for interoperability

Being interoperable means that two or more systems or components are able to transmit or exchange information through a common system and to use that information. The great advantage of interoperability, and the reason why it is an essential building block for an SDI, is that it describes the ability of locally managed and distributed heterogeneous systems to exchange data and information in real time to provide a service [18].

Following the OGC [18] there are two levels of interoperability:

- syntactic (or technical): when two or more systems are capable
 of communicating and exchanging data. Specified data formats
 and communication protocols are fundamental. Syntactical interoperability is required for any attempts of further interoperability.
- semantic: the ability to automatically and accurately interpret
 the information exchanged to produce useful results as defined
 by the end users of both systems. To achieve semantic interoperability, both sides must defer to a common information exchange reference model, so that what is sent is the same as what
 is understood.

Being syntactically and semantically interoperable can leverage the full potential of interoperability by allowing services to be seamlessly coupled, reusable and available for a variety of applications.

OGC web services share the ability to return an XML document that describes their capabilities (e.g. data available, formats, and functions) using a standard communication method, enabling applications and other web services that implement OGC standards to interoperate. This means that in an OGC-compliant SDI, a user can access data stored in different databases, in different formats, and running on different operating systems.

1.3. The need for processing capacities

Current SDIs are essentially supporting data discovery, visualization and retrieval, but have typically limited analysis capabilities [25]. This means that the processing of geospatial data is donein general on the client's desktop computer which is an inhibiting factor when very large and high resolution data sets must be processed. With the recently introduced Web Processing Service (WPS) and the promises of high storage and computing capacities offered by the Grid [26] and Cloud [27] infrastructures, new opportunities are emerging within the environmental communities [28]. Following Foster et al. [29] a Grid is a parallel processing architecture in which computational resources are shared across a network allowing accessing unused CPU and storage space to all participating machines. Resources can be allocated on demand to consumers who wish to obtain computing power. In other words, a Grid aims to harness resources in a dynamic, distributed environment. Recent studies have exemplified a successful approach to extend Grid technology to the remote sensing community [30,25], as well as to the field of disaster management [31,32] making OGC web services grid-enabled.

In the last years, Cloud computing has increased in popularity. The term Cloud represents the Internet or whatever large networking infrastructures in which data storage and processing are performed directly on distributed resources provided by thirdparty storage and processing facilities [27,33]. According to Foster et al. [29], an evolution from Grid computing gave rise to Cloud computing, which has been a result of a shift in focus from an infrastructure that delivers storage and compute resources (such as Grids) to one that is economy based aiming to deliver more abstract resources and services (such as Clouds). Cloud computing has a business model in which computing resources are packaged as metered services similar to a physical public utility, such as electricity [6]. Popular examples of Cloud infrastructures ran by large companies are the Amazon Elastic Compute Cloud (EC2) and Simple Storage Service (S3), Microsoft Azure platform, and Google App Engine.

Grid and Cloud infrastructures mostly deal with the same issues (manage large facilities, methods to discover and use resources). Nevertheless they differ in different aspects such as security, programming models, business models, computer models, and data-application models [33]. Moreover, the targeted communities are different. The Grid is mainly used within the scientific community that runs large-scale models and resource time-consuming applications (e.g. climate simulations, particle physics, molecular docking) whereas Cloud targets small to medium companies that wish to scale on-demand their web-based applications without the need to invest in a large computational infrastructure [27,33, 34].

Although Clouds user interfaces are typically more user-friendly than standard Grid user interfaces, Clouds cannot satisfy all the needs of Grid users today. Aspects of collaboration, result-sharing in virtual organizations, and complex data management are still not well covered by Clouds. A first attempt to bring an OGC web service into the Cloud has been successfully achieved high-lighting some promises (response time, publish-find-bind pattern not modified, economical aspects) and also some bottlenecks (data allocation, high traffic on servers) [27].

Consequently, Grids and Clouds appear to be promising facilities to extend SDIs capabilities at least for processing large geospatial data sets. In our view, it is therefore too early to consider Cloud computing as a sustainable alternative to access the distributed computing resources within the enviroGRIDS framework.

The aims of this paper are (1) to give from an SDI perspective an overview of the actual status of technologies used to describe, catalog, share and process an ever-growing set of high resolution geospatial data, (2) to discuss promises and challenges offered by the Grid to extend the analytical capabilities of SDIs, and (3) to present the approaches of the EU/FP7 enviroGRIDS project to make SDIs and Grids interoperable.

2. Background

The aim of the EU FP7 enviroGRIDS project (hereafter enviroGRIDS) is to build capacities in the Black Sea region to use new international standards, like those proposed by the OGC and the International Organization for Standardization (ISO), to gather, store, analyze, visualize and disseminate crucial information on past, present and future states of the environment of this region to assess its sustainability and vulnerability (see http://www.envirogrids.net). To achieve its objectives, enviroGRIDS will build a grid-enabled Spatial Data Infrastructure (gSDI) serving data, information and services in global and regional initiatives like the Global Earth Observation System of Systems (GEOSS) [35] and being compatible with both the European directive on Infrastructure for Spatial Information in the European Union (INSPIRE) [36] and the United Nations Spatial Data Infrastructure (UNSDI) [4]. The overarching scientific aim of the enviroGRIDS project is to start building an observation system that will address the nine GEO Societal Benefit Areas (SBAs) (disasters, health, energy, climate, water, weather, ecosystems, agriculture, biodiversity) within a changing climate framework. This observation system will contain an early warning system that will inform in advance the decision makers and the public about risks to human health, biodiversity and ecosystems integrity, agriculture production or energy supply provoked by climate, demographic and land cover changes on a 50 year time horizon. This system will allow systematic monitoring and assessment of GEOSS SBAs in the Black Sea region and aims to serve as a decision-making support tool to assist stakeholders to attain sound decisions in a timely manner based on valid scientific information. To support the development of this observation system, the gSDI (currently under development) will provide interoperable and standardized data storing, discovery, accessibility and retrieval as well as processing capabilities based on the Grid infrastructure of the Enabling Grids for E- SciencE (EGEE) project. Hence, one of the key challenges of the enviroGRIDS project is to bridge the technological gap between SDIs and Grids infrastructures and to make these two infrastructures interoperable.

2.1. Why do we need Grids?

A Grid infrastructure will be important to address several objectives during the four-year timeframe of enviroGRIDS:

- Running a high-resolution (sub-catchment spatial and daily temporal resolution) water balance model will be applied to the entire Black Sea catchment (2.1 million square kilometers) using the Soil Water Assessment Tool (SWAT) [37].
- Adequate sensitivity and uncertainty analysis will be performed on the Black Sea SWAT model. A gridified version of the SWAT-CUP [38] tool will be used for that purpose.
- Access to real time data from sensors and satellites will provide early warning and decision support tools to policy-makers and citizens. These data may be streamlined into the gSDI to ensure fast computation and dissemination of results.
- Because spatial data is very heterogeneous in format and quality across the European community, urgent efforts are needed to organize and standardize spatial data to improve its interoperability. The gSDI will rely on the development of policies, technologies, data, common standards, standard practices, protocols and specifications such as those of the OGC, GEOSS and INSPIRE. Through cataloguing, the Grid infrastructure will help implementing and sharing standardized data sets.

The strong Grid component of the project will foster data interoperability and will certainly trigger new directions of research or alternative ways of analyzing high resolution data sets. In terms of analysis capacities, this will offer the possibility to shift from a traditional single desktop computer to sizable computing resources, allowing environmental scientists to leverage the full potential of high resolution spatio-temporal data sets. Moreover, the large worldwide user community of SWAT may greatly benefit from a gridified version of the software and associated tools. The enviroGRIDS gSDI will be a distributed system built on an SOA paradigm that allows a flexible use of services over heterogeneous components and technologies (OGC and Grid services). The functionality provided by web services could be used anywhere over the computing infrastructure by open standards and communication protocols. Making OGC and Grid services interoperable in an SOA is therefore a key requirement for the project. The enviroGRIDS gSDI should be very innovative due to its implementation in a trans-national framework.

3. Describing and cataloguing geospatial data

Administrations and governments recognize that spatial information is a critical element underpinning decision making for many disciplines [39,6] and must be part of the information infrastructure that needs to be efficiently coordinated and managed for the interest of all citizens [39,40]. Nevertheless, these geospatial data, stored in different places and managed by different organizations, are often poorly documented [41]. Therefore, the vast majority of these data are not being used as effectively as they should due to issues such as the lack of awareness of their availability, poor documentation, and numerous data inconsistencies [2,18].

Nebert [2] highlights that data documentation, commonly known as metadata, is an essential requirement for locating/ evaluating data and associated services. Moreover, Masser [42] reinforces this need by asserting that without appropriate metadata services, an SDI fails its main objective of promoting greater and efficient use of geospatial data. Ideally, each newly created data set (e.g. a map, a single file or a collection of data) must be described by metadata allowing users to determine whether the shared data set is useful to meet their needs [5]. In a networked environment, web-based metadata services can act as gateways to geographic information [42,39,43,44] providing an entry point to SDIs and allowing users to search for a specific data, to know where to obtain it, and to understand access constraints and the history of data capture. This allows one to interpret correctly the information about data, to trust it and eventually to meaningfully integrate it with data coming from other sources.

Describing a geospatial data set through metadata is thus an essential task, but it is not sufficient to ensure wider knowledge and usage [3]. The collected metadata must be accessible, searchable and query-able, which means that metadata must be stored in a catalog system made of a database with an interface that has the required functionalities [4]. In addition, users should not have to individually access different catalogs but rather have the possibility to query from a single entry point collections of metadata stored and maintained in different places. Such capacities could enhance geospatial data access and sharing within and between distributed organizations, avoiding duplication, increasing cooperation and coordination of data collection and, at the same time, preserving data and information ownership [4].

In the geospatial community, international standards such as OGC and ISO form the basis for most catalog implementations [45]. The ISO standard 19115 (Geographic Information—Metadata) defines the schema required for describing geospatial data and services. It provides different information such as identification, spatial and temporal extent, quality, distribution rights or spatial reference system. This standard is complemented by ISO 19139

(Geographic Information - Metadata - Implementation Specification) that defines the XML encoding schema for describing, validating, storing and exchanging georeferenced metadata and by ISO 19119 (Geographic Information-Services) that describes associated geospatial web services. In addition, the OGC Catalog Service for the Web (CSW) specification [26] was developed to define a standard interface to publish, discover, search and query metadata about geospatial data and related services. This specification allows an independent and interoperable access to geospatial metadata [41] defining a set of operations like *GetCapabilities* (retrieves capabilities and characteristics of a service), DescribeRecord (discover the information model and definitions), GetRecords (search the registry and retrieve results) and GetRecordById (retrieve a result by an identifier). In summary, metadata and interoperable catalogs are the basic components of any SDI to facilitate access to data and related resources.

Searching data or related services directly in a search engine like Google is difficult because it will return hundreds of potential documents in response to a simple query like "land cover data". Fortunately, geospatial data (and services) described through metadata can give information through their coordinates, place names, reference date, or capabilities. Such descriptions can therefore give a solution to refine user's queries by offering a common vocabulary that describes data and services that can be used for searching and retrieval [2]. The prerequisite to search geospatial data and services is that metadata must be stored in catalogs that can support functionalities to search, query and access. These functionalities are commonly known as "catalog services" proposed in the OGC Geospatial Portal Reference Architecture [19]. A catalog service and its user interface allow users to query distributed sets of geospatial data or services through their metadata descriptions. A user aiming to locate a specific service needs to access a search user's interface to fill out a search form and to build a query for a service with certain properties. The search is then sent to a gateway that queries one or more registered catalogues. Each of these catalogues manages their own collection of metadata. By using a common descriptive vocabulary provided by standards like ISO19115/19139/19119, a common search and retrieval protocol like OGC CSW, and a registry of metadata collections, an interoperable search across different catalogues is possible. The Global Earth Observation System of Systems (GEOSS) is a good example of such an interoperable system that can query multiple catalogues registered in its system.

Nevertheless, this set of specifications (CSW and ISO19115/191 19/19139), targets essentially data (and related services) discoverability. As of today, processing services based on the Web Processing Service specification (see Section 5) do not require the use any metadata standards, such as ISO19115. GetCapabilities and DescribeProcess operations offer a possibility to access some metadata about the WPS service. In addition, WPS standard recommends including WSDL documentation [46] but such metadata does not specify the content of the input and output data involved in the process [47]. In other words, the lack of adequate service metadata impedes users to discover, evaluate and use WPS processes. Users have to locate a WPS by themselves and then perform GetCapabilities and DescribeProcess requests to determine if a specific service can satisfy their requirements. To overcome this barrier and facilitate WPS discovery, different approaches [46,47] have been proposed to enrich the metadata model of WPS's WSDL document with additional information automatically retrieved from GetCapabilities and DescribeProcess requests. In particular, a process description (e.g. input and output data required) can be directly embedded into the generated WSDL document.

In enviroGRIDS, the approach proposed by Yang et al. [47] for improving WPS discoverability appears to be promising. The authors suggest that clients can get "enriched" WPS's WSDL documents from a catalog service, with process description and data types, allowing them to find appropriate processing service specified constraints (e.g. data type) as search criteria.

4. Accessing and sharing geospatial data

Discovering and evaluating data through their metadata is the first functionality that users can expect from an SDI. Once they know the existence of a specific data set, users want to have the possibility to access it either by direct download or through web services.

Many of the decisions that organizations need to make depend on good, consistent, and readily accessible geospatial data to support decision making processes [25,6,48].

The OGC has specified a suite of standards supporting the data service class of the Geospatial Portal Reference Architecture [19] and two of them are of particular interest for data providers and users: the Web Feature Service (WFS) [20] that provides a web interface to access vectorial geospatial data (e.g. country borders, GPS points or roads) encoded in Geographic Markup Language (GML) and the Web Coverage Service (WCS) [22] that defines a web interface to retrieve raster geospatial data of spatially distributed phenomena such as population maps or digital elevation models. In addition, the Web Map Service (WMS) [21] defines an interface to serve georeferenced map images suitable for displaying purpose based on either vector or raster data. A map served through WMS is only a graphical representation of a geospatial data and does not give access to the data itself. These OWS are invoked using URL and each service supports different sets of standardized operations like GetCapabilities (to describe the service) or GetFeature/GetCoverage/GetMap (to retrieve a selected feature/raster data

EnviroGRIDS aims at building the capacity of scientists of the Black Sea catchment to publish and use data/metdata using OWS. In consequence, the first crucial step is to teach them how to install, configure and publish their data as well as their metadata in an interoperable manner. This will be done organizing workshops along the whole duration of this 4-year project, covering interoperability, hands-on experience with web portals, information access, open source software (GeoNetwork¹ and GeoServer ²) and data/metadata sharing through web services and GEOSS registries.

5. Processing geospatial data

A key feature of OGC-compliant Service Oriented Architecture, as proposed in the Geospatial Portal Reference Architecture [19], is that it provides a set of functionalities composed of independent services allowing dynamic integration and composition [49]. The ability to turn data into understandable information is then dependent on the capacity to acquire data on a specific problem, to apply processing algorithms and then to visualize the result. Chaining web services is the solution envisioned by the OGC to transform raw data into new information by integrating different data sources and different processing steps. As Stollberg and Zipf [48] mentioned, web services orchestration is a central concept of SOA, and it adds great value through the possibility to re-use "simple" services to solve "complex" tasks.

Currently, users can find and evaluate data using SDIs but once they have identified the required data they have to download it on their desktop computer and process it on specific GIS software (like ArcGIS or GRASS). These pieces of software have the ability to process and concatenate data made available either with OGC standards (WFS, WCS, and WMS) or in proprietary formats (like shapefiles). SDIs need to go "one step further" to, first, extend their analysis capacities by providing standardize way

to access GIS calculations and, second, to allow complex chaining and orchestration in order to process data and generate new information [25].

The recently introduced Web Processing Service specification (WPS) [23] aims to close such a gap by offering geoprocessing functionalities in a web service environment [49]. This will allow one to process distributed geospatial data via Internet on remote servers. Through WPS a user can "offer" the possibility to process data to users that do not have such capacities.

Like all OGC standards, WPS provides a set of traditional operations accessible via a URL that allow service description and processes availability (GetCapabilities request), process description and input/output parameters (DescribeProcess request) and finally execution of a selected process (Execute request). The service description request returns a metadata under the form of an XML file that is both readable by humans and machines allowing an automatization of integration procedures using the returned description. After selecting a process that meets the requirements for a specific task, its description interface gives a detailed view of input and output parameters required to execute this process. These parameters could be either complex (like geometries) or literal values. The complex value data type is interesting because it gives the ability to reference remote locations [49] in order to access, for example, a WFS service provided by another organization. Finally, the execution interface allows monitoring the progress of geoprocessing task using simple status message. Once the process is finished, the result can be either returned directly to the client or stored on a

WPS, like any other OGC standards, relies on XML-RPC specification using HTTP as the messaging protocol and XML as the encoding schema to answer. This contrasts with more traditional service-oriented architectures based on SOAP protocol to exchange structured information. This difference leads to an important problem of communication and thus greatly limits the orchestration and chaining capacities of OGC web services [48]. Currently, selection and coordination by a central orchestration engine (semiautomated orchestration) is a widely used approach aiming to provide flexibility and efficiency when building chains of services [49, 50]. Workflows are valuable because real scenarios (e.g. creating an earthquake risk map, analyzing the geographical distribution of species) rarely involve a few simple tasks. Transforming data into information requires, in general, the sequencing and organization of processes. Hence, workflows can be seen as a series of coordinated analytical and processing steps. They can be described as web-based scripts that automate tasks. W3C standards (e.g. SOAP and WSDL) are important for creating and managing workflows using widely accepted standards such as BPEL [7,11]. BPEL is a workflow description language that models the behavior of web services in a process interaction [51,52] and is used by many service-chaining tools such as the Apache Orchestration Director Engine (ODE), Orchestra, EasyBPEL, Kepler, Scientific Dataflow (SciFlo) or Taverna [53]. BPEL defines an XML-based grammar to describe the control logic needed to coordinate the sequence of web services involved in a workflow. It uses WSDL as component model and XML as data model [29]. Despite the fact that Kepler, SciFlo and Taverna are engines natively designed to support Grid services, recent studies [54–56] applied a successful approach, using the Web Service Resource Framework (WSRF), to extend BPEL capabilities to orchestrate Grid and non-Grid services. This appears to be a promising approach to orchestrate OGC services and Grid services [57,58].

Another problem is that XML does not support raw binary data, which implies that WCS cannot be directly integrated into SOAP messages [49]. Different approaches have been identified to overcome these problems and to try to successfully orchestrate OWS [33,59] by encapsulating them into a SOAP message.

¹ http://geonetwork-opensource.org.

² http://www.geoserver.org.

During the second half of enviroGRIDS project time frame, once scientists are sufficiently comfortable using OWS, we will propose new workshops to show them the possibilities offered by workflow engines building chains of services to create customized solutions for solving specific analysis tasks. Following the incremental approach proposed to progressively implement OWS as Grid services (see Section 7) we will first use "non-grid" orchestration engines like Apache ODE. "Grid specific" engines (e.g. SciFlo) will then follow when more and more OWS as Grid services are implemented. To reach the project's objectives we will rely on a continuous cycle of enhancement by which enviroGRIDS is evaluated (e.g. quality of service, usability, performance) and validated according to user needs. These improvements are based on results of research activities, taking into account developments and constraints in the areas of standardization, technologies, and policies.

Processing high resolution distributed data on a networked environment raises the issue of computational performance, especially when working on a single instance of a single server causes an important decrease in calculation speed and provokes high latencies. Thus, to leverage the full potential of OWS and related processing capabilities, a high performance computing environment is required. Grid and Cloud computing [60,33,26] appear to be interesting candidates to empower SDIs.

Environmental sciences are a data-intensive domain in which applications typically produce and analyze a large amount of geospatial data. For example, the recently accessible Digital Elevation Model (DEM) from ASTER [61] covers the world at 30 m resolution and is composed of 22,600 tiles for a total size of 1.2 TB. Analyzing such a data set at global scale (e.g. running a global flood model) is currently impossible with a single desktop computer due to, first, the huge computation time required to run such a model and, second, the size of the data set itself that cannot be assimilated by current GIS software. Therefore, distributed computing infrastructures like a Grid can be helpful. In the case of a global flood model, the possibility to split this DEM in tiles and run the model on each individual tile through independent jobs can speed up the process of analysis and allow consuming this data set in an efficient manner.

Another good example where Grid computing can be useful is the computation of risk map on natural hazards. Modeling risk at the global scale requires to access and process a large number of data (DEM, population, economical) distributed all around the world in different data centers. Experiences acquired from the development of such data sets in the context of the Global Assessment Report on Disaster Risk Reduction,³ showed that covering nine types of hazards (cyclones and related storm surges, droughts, earthquakes, biomass fires, floods, landslides, tsunamis and volcanic eruptions) requires about 6000 CPUhours of computation (i.e. about 250 CPU-days) on a single desktop computer. These risk maps (and related data sets such as vulnerability and exposure) need to be easily updated when new events occur (e.g. updating the risk map on earthquake after major events). Without access to distributed computing facilities, these data sets can currently only be updated once a year. This negatively influences the timely access to reliable and up-to-date information, which is mandatory for efficient and effective responses required in emergency situations.

6. Benefits and challenges to use Grids within SDIs

In the previous section, we have seen that OGC web service specifications provide standards to implement interoperable and distributed geospatial data systems following the OGC Reference Model [24], but at the same time they do not provide secure mechanism to share computing resources to process data. To access a Grid infrastructure, users belonging to different administrative organizations are typically grouped into a specific user community, called a Virtual Organization (VO). A VO is therefore defined as a group of people who share a data-intensive goal. This group of users wants to share geographically distributed resources in a secure way. Users as well as resources must be authenticated by a certification authority before acceptance in the VO (for users) or in the Grid infrastructure (for resources). The acceptance in a VO authorizes users to access resources based on the policies of the VO. Security and confidentiality is of great importance in that context. In environmental sciences, complex data policies typically govern the access to data. As an example, local or regional data concerning the water management may be very sensitive. In their current form, most Grids use encryption and advanced authentication mechanisms, such as public key certificates and different user roles in the VO, to protect data confidentiality [62]. Thus, the Grid paradigm appears to be the ideal candidate to fill this technological gap allowing SDIs to access high performance computing resources.

The main challenge is to be able to use secure sharing and processing mechanisms provided by Grids while using widely adopted OGC interfaces and services within the geospatial community. As Di et al. stated [63], it is difficult to connect Grids and SDIs without extensions and customizations. These authors highlight different reasons for that: first, geospatial data differ significantly from other disciplines (e.g. complexity, diversity and volume). Second, there are already widely adopted sets of standard within the geospatial community. Finally, Grid technology focuses on sharing computational resources thus it is not calibrated well for SDIs' requirements. Two possibilities are envisioned to combine Grid and SDI technologies. The simplest approach is to encapsulate the required OGC Web Service and to use Grids only as a backend for processing or accessing resources. The main advantage of this solution is that existing geospatial services are unchanged, the gridification process is easy and implementation is independent of the underlying Grid middleware [60]. The second approach is the full integration of OGC services in a Grid environment, creating a gridded SDI. It requires extending the Grid's middleware capabilities to support geospatial data characteristics and requirements. Several studies have already successfully implemented such an approach to benefit from distributed processing and data accessing tasks [63,32,64, 65]. All these studies highlight the fact that such a gridification process is not easy to implement, is always middleware-dependent, and is dependent on a broker to allow compliance with the OGC web services. Typical implemented architectures use Grid infrastructures as a foundation for SDIs [66,32]. They integrate the web service approach in the upper functional layers allowing easy communication with other systems based on web-oriented technologies (e.g. SDIs, e-Government) and Grids as the lower functional layer to support data-intensive computation and large data sets storage. The main objective is to hide the complexity of the Grid while preserving OGC interfaces and thus allowing OGC-compliant clients to access and process geospatial data in a Grid environment.

Following Yanfeng et al. [65], the Open Grid Services Architecture (OGSA) is promising and of high interest to combine SDIs and Grids. Indeed, OGSA aims to make different Grid systems interoperable by introducing the Service Oriented Architecture and related web services concepts (based on SOAP protocol) into Grids [67]. Through OGSA-DAI (Data Access and Integration) and OGSA-DQP (Distributed Query Processor), a standardized and uniform service interface is provided allowing data access and integration over a Grid deployment. Padberg and Kiehle [68] provide an overview of actual incompatibilities between Grids and SDIs. For these authors, service description, service interfaces, service states and security differ on many points. Especially, Grid infrastructures are

 $^{^{3}\ \} http://www.preventionweb.net/english/hyogo/gar/.$

based on SOAP to invoke operations and WSDL to describe services while OWS are based on HTTP-GET/POST and XML-RPC. This means that without support for SOAP protocol and automated creation of WSDL description document, integration in a Grid workflow could be problematic. Moreover, OGC services are stateless and thus cannot give any information on their state. WPS is the only standard that supports SOAP and could partially send information about its state. Finally, OGC specifications do not include security mechanisms, a key requirement in Grid architectures. Hence, these limitations must be overcome to leverage the full benefit of Grids to the geospatial community and WPS standard appears as an interesting candidate to be grid-enabled. Recognizing these limitations, the OGC and the Open Grid Forum (OGF) have signed in late 2007 a Memorandum of Understanding to collaborate on the integration of WPS specification into Grid environments and workflow management tools, as well as on the integration of federated catalogs/data repositories with Grid data movement tools like GridFTP [26].

6.1. Grid-enabling catalogs of geospatial data

In Grid infrastructures, middleware like gLite or Globus Toolkit have their own metadata catalog to describe and localize the distributed data generated by Grid applications. In general, these catalogs associate simple descriptive attributes to the files and suppose a hierarchical, file-based data model. As such, they do not cover the requirements of a geospatial data catalog service in terms of spatial, temporal, and other parameters for data discovery [63]. This means that Grid metadata catalogs appear to be inadequate to deal with geospatial metadata [69] and their functionalities need to be extended to support more complex data types and relationships. Different solutions have been explored to grid-enable geospatial metadata catalog, ranging from a simple wrapper to extend Grid metadata catalog capabilities [69] to a full integration of CSW standard and ISO schema as a Grid Service [63]. The last solution seems promising as it converts a web service into a Grid service, while preserving interfaces as well as request and response messages of the OGC CSW specification. Nevertheless, this approach still requires a lot of development to overcome the barriers mentioned previously and to make geospatial metadata catalogs grid-enabled. An interesting work done by Sandoval [70] has shown a great potential in linking GeoNetwork geospatial metadata catalog with AMGA⁴ (ARDA Metadata Grid Application) used in gLite middleware. This author has successfully extended traditional XML schema used in GeoNetwork [70] to take into account a Grid's specific information such as Logical File Name (LFN) or Grid Unique IDentifier (GUID) used to localize data in Grid environment. Sandoval [70] has also shown the benefits of Grid environment to store and process satellite images.

6.2. Grid-enabling geospatial data services

Currently, no Grid services are equivalent, in terms of functionalities, to WFS and WCS specifications [63]. Moreover, data Grids appear to be an interesting approach [71] to deal with large amounts of distributed data, benefiting from secure controlled sharing and management capabilities offered by a Grid. Padberg and Greve [28] have grid-enabled OGC data services using OGSA-DAI data store implementation allowing users to invoke OGC-compliant WFS and WCS services and accessing data stored inside a Grid infrastructure. Di et al. [63] have applied the same approach they used for grid-enabling CSW to successfully access

OGC-compliant data sources over a Grid, making them traditional Grid services. In terms of performance, these authors noticed that the Grid services offer a performance overhead compared to the Web services, due principally to the authentication cycles [28] and the size of the request and associated response payload. Mazzetti et al. [32] have also grid-enabled WCS specification extending gLite middleware functionalities and they highlighted benefits both in term of scalability (capacity to deal with multiple requests, sending multiple jobs in parallel) and interoperability (between OGC WCS and gLite middleware).

By its distributed nature and characteristics, the Grid environment is potentially an interesting choice for a data management system [64]. It offers robustness (distribution storage and data replication capabilities), efficiency (data stored as close as possible to components that access them) and transparency (hiding Grid complexity from users). In addition, data moving protocols like GridFTP are interesting as well. Indeed, one possible bottleneck when dealing with large data sets is that data access strategy in SDIs is not location-based. This means that current SDIs have limited replication and data transfer capabilities to minimize the access time to a selected data set. Often, geospatial data providers do not offer possibilities to have different replicas distributed in several data centers. Therefore, users must access data directly at its source, which implies that network distance and a potential large number of concurrent accesses can impede users from retrieving data in an efficient way. Moreover, if a geospatial data source disappears, data access to this source is definitively lost if data replication was not enforced. In summary, data replication mechanisms proposed by Grids are promising to avoid single points of failure, to enhance data availability [72-74], and to ensure that data will be as close as possible to the worker nodes (avoiding high latencies produced by the movement of large size data before the beginning of a processing task).

6.3. Grid-enabling geospatial processing services

The Memorandum of Understanding between OGC and OGF primary focuses on the integration of WPS into Grid environments aiming to make high-performance computing available to a wider community [75]. Proofs of concept of such implementations have already been made in different Grid middleware such as Unicore [37], Globus Toolkit [63,28] and gLite [32]. These different studies have shown clear improvements in processing performance and speed, by dividing a given task into smaller subtasks that can be processed in parallel and merged together at the end. Werder and Krüger [75] stated that the real processing benefit of Grids comes from the development of efficient strategies to parallelize tasks. Indeed, not all environmental models can be parallelized (e.g. climate models) due to their high interdependence and process logic, and are better deployed through supercomputers. For these authors, other factors like system architecture, tiling strategies and orchestration [57] could influence the overall result of a geoprocessing task and must be taken into account. Particular attention must also be payed to time investment for parallelizing a specific process. Padberg and Kiehle [68] highlight the importance to define a "break-even-point" where the gain in computational speed outweighs the overhead induced by Grid technologies and implementation. A promising approach in gridenabling WPS is proposed by Padberg and Greve [28]. First, they try to address the differences described previously between OWS and Grid services (service description, service interface, statefulness and security) and, second, to preserve the traditional WPS interface when connecting to a Grid. The gridification is made at the level of the process ensuring that WPS requests are not modified. For that purpose, the authors suggest to split a WPS process into

⁴ http://amga.web.cern.ch/amga/.

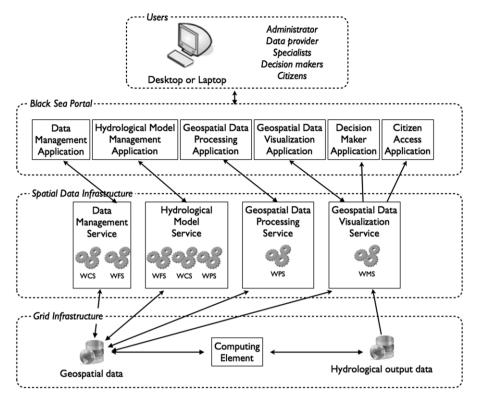


Fig. 1. EnviroGRIDS gSDI components supporting web portals.

two parts, one inside the Grid infrastructure (containing the process logic, methods and functions) and one through a traditional WPS interface (that only invokes the Grid service). Another possibility to grid-enable WPS is represented by the encapsulation of Grid processing services within a standard WPS request [76] by encoding directly Job Submission Description Language (JSDL) to describe job and resource requirements (disk space, CPU and other parameters) directly into the *Execute* request of WPS interface. All these approaches have shown that grid-enabling WPS is feasible and could increase processing capabilities of SDIs.

7. EnviroGRIDS approaches to interoperability between SDIs and Grids

Interoperability is a great challenge for the successful implementation of the enviroGRIDS gSDI. Such a technology can significantly reduce problems associated with archiving, manipulating, analyzing, and utilizing large volumes of geospatial data at distributed locations. EnviroGRIDS gSDI is a distributed system built on a SOA that allows a flexible use of services over heterogeneous architectural components and technologies. The OGC Web Services and the gLite middleware must be able to communicate and interact with each other in order to combine the complex specialized geospatial functionalities with the computation capacities of the Grid.

In the enviroGRIDS project, several applications are intended to be ported on the grid, through a so-called "gridification" process. This process aims to generate a Grid application that can be defined as "software that interacts with Grid services to achieve requirements that are specific to a particular VO or user". The gSDI will be the core of the Grid activities within enviroGRIDS. The different components of the gSDI (Fig. 1) will be implemented throughout the project, and it is likely that many challenges will emerge that are not foreseen at this early stage of the project. The need for sustainable access to the Grid infrastructure stems from

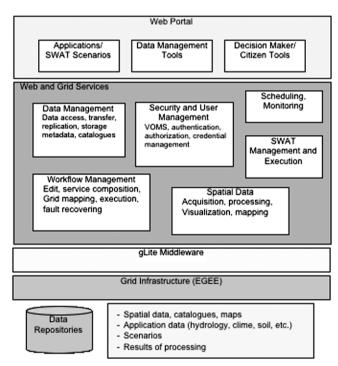


Fig. 2. EnviroGRIDS functional layers [10].

the need of a continuous offering of web and Grid services, and for the future EG web portal(s).

EnviroGRIDS architecture consists of three main functional layers (Fig. 2): data layer, Grid layer and service layer.

(1) Data layer: consists of stored data (data repositories) and functionalities required to manage the repositories. They store raw data (e.g. geospatial data) as well as processed data (e.g. output data such as maps or tables). They also store application

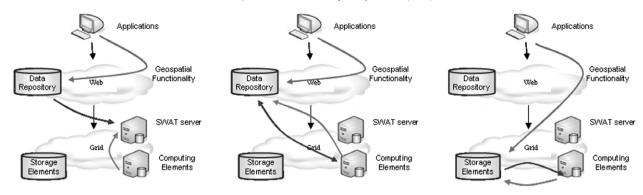


Fig. 3. Scenarios to implement SDI/Grid interoperability in the enviroGRIDS project.

data, which are specific for each application type and instance (e.g. hydrology, climate, soil, etc.). The register stores metadata catalogs that support the searching, discovering and using of distributed data by the user applications, and processing services.

- (2) Grid layer: provided by the EGEE infrastructure and the gLite middleware and giving access to the basic resource management and data processing services available over the Grid infrastructure as secure and persistent services and over the Web as stateless services. The services encapsulate the basic functionality provided to user applications:
 - Data Management: provides the basic operation on data repositories (e.g. data access, transfer, replication, metadata storage).
 - Security and User Management: provides the functionality needed to work with VOMS database, to support user authentication, authorization, and credential management as well as the implementation of particular policies for data access and use.
 - Scheduling: provides optimal resource allocation and sharing through static or dynamic load balancing.
 - Monitoring: supports evaluation of the execution performance, and statistical analysis.
 - SWAT Management and Execution: provides the functionality to control the execution over the Grid of the SWAT modules and related data.
 - Workflow Management: supports the graph description of the processing, service composition, Grid mapping, workflow interpretation and execution, and fault recovering.
 - Spatial Data Acquisition: supports the working with sensors by supervising sensor status, data acquisition and transformation, store, and processing.
 - Visualization and GIS Mapping: supports data visualization in graphical user interfaces.
- (3) Services layer: The enviroGRIDS Portal will expose to the user a set of tools and applications of which functionality is composed of the services (data management, geospatial functionality, security and user management, scheduling, monitoring, SWAT related management and execution, workflow management, spatial data acquisition, and visualization) provided by the below level. There are four types of interactive applications and tools available through the enviroGRIDS Portal:
 - Applications/ SWAT Scenarios Development Tools: the user may develop various scenarios/workflows for natural phenomena and use cases, perform their execution over the Grid, and finally visualize the results and analyze statistical data.
 - Data Management Tools: data administrators and providers may access, upload, update, and organize spatial data.

- Decision Maker Tools: provide the possibility to develop and execute various scenarios on different data series, in order to analyze and make predictions on the phenomenon evolution.
- Citizen Tools: provides the citizen, as an Internet visitor, the ability to execute a given set of scenarios by limited set of data, and graphical visualization of the results.

EnviroGRIDS applications will be in the Web domain while data repositories and resources management and processing services will be progressively implemented in the Grid following an incremental approach enabling communication between the SDI and Grid infrastructures (Fig. 3) [10].

- (1) The first scenario is a file-based communication between SDI and Grid infrastructures. A user sends a request to the portal application that forwards the request to a proxy server. The proxy server identifies the different calls (for SDI calls it executes OGC services directly to extract required data from the data repository, for Grid calls it uses Ganga⁵ functionalities to submit the job to the Grid). Finally, the proxy waits for the results from the SDI and Grid environments, merges the final result and sends it to the client.
- (2) The second scenario is an extension of the first one where the data repository is still in the SDI but Grid accesses data directly using modified OGC web services (grid-enabled) that replace the proxy of the first scenario. This allows Grid services to extract data using WFS or WCS that are outside the Grid.
- (3) The third scenario is where data repositories are not in the SDI part but directly integrated in the Grid infrastructure. Geospatial applications (e.g. geoportals, GIS software) search and use data through Grid services that are compliant with OGC specifications.

In such an incremental approach, complexity will increase following the level of adaptation of OGC and Grid services (e.g. modifications of the Grid middleware and OGC's implementation). In the first scenario, no modification of OGC standards is required. What needs to be done is to write a proper proxy component that can divide SDI and Grid calls, to manage Grid security, and to merge the results obtained under Grid and SDI environments. In the second scenario, different solutions have already been presented in the previous section (grid-enablement of OGC services) and as of today the 52North⁶ implementation appears to be a promising one. The last scenario needs a lot of adaptation, as this requires extending gLite middleware capabilities to make it spatially aware. In other words, specific libraries need to be written and added directly into the middleware. Such an implementation is under

⁵ http://ganga.web.cern.ch/ganga/.

⁶ http://52north.org/maven/project-sites/wps/52n-wps-site/.

development within the gLite-OWS (G-OWS) working group.⁷ Indeed, in the first two scenarios Grids are only used as a backend to process large data sets (both in term of data size and computation time required) provided by a SDI through OGC web services. In the last scenario, data repositories are completely part of the Grid infrastructure and they can benefit from Grids high level of performance and reliability (e.g. data replication, data security). By making geospatial data and related services available in the Grid environment, this can potentially pave the way to the development of innovative workflows involving large data sets obtained from different disciplines. As an example, we can mention the very promising idea of linking environmental data with genetic data [30,77].

Following Mazzetti et al. [32] the major benefits of making Grid technology spatially aware consist of:

- Scalability: the grid infrastructure provides high processing and storage capabilities to: (1) improve output data resolution, (2) improve model complexity, (3) widen the covered area (from local to national/global scales), (4) improve the time-of-response (from hours to minutes), and (5) time-of-response is almost independent of resolution/coverage.
- Flexibility and interoperability: the geospatial service layer allows one to (1) integrate new and heterogeneous input data, (2) integrate outputs in a higher level application chain, (3) facilitate the model's interoperability and composition, and (4) be interoperable with other standard based infrastructures (e.g. GEOSS).

7.1. EnviroGRIDS use-case: satellite image processing

Remote sensing gives the opportunity to have access to continuous data collection. In the context of this project, satellite images will be useful to monitor changes and trends in the Black Sea region/watershed (e.g. land use, deforestation, water quality). Monitoring of land cover/land use is an important element for quantifying land surface characteristics for environmental management. Processing high-resolution/high volume of remotely sensed data requires high computation resources and massive data storage capacity. The main processing consists of imagery classification that can be defined as a search of information through various combinations of multispectral bands. The data exploration, analysis, and interpretation are a multivariable process considering satellite image types (e.g. MODIS, Landsat, and QuickBird), geographical areas, soil composition, vegetation cover, and context (e.g. clouds, snow, and season). All these specific and variable conditions require flexible tools and friendly user interfaces to support an optimal research for the appropriate solutions.

The following user requirements have been highlighted: (1) satellite image visualization tool (search images in a database, zoom in/out, scale, metadata), (2) flexible description and execution of complex processes (workflows), (3) satellite image processing with simple algorithms (indices calculation, map algebra), (5) output visualization (pseudo color rendering, classes), (6) save images in different formats, (7) crop images to an area of interest, (8) display information about the image.

To answer enviroGRIDS user needs, the proposed solution for satellite image processing will be based on the Environment oriented Satellite Data Processing Platform (ESIP) [78] that has been developed through the South East Europe-GRID-eInfrastructure for regional eScience⁸ (SEE-GRID-SCI) project. ESIP is a suite of interactive toolset supporting the flexible description, instantiation,

scheduling and execution of the processing over the Grid infrastructure. ESIP layer is built on top of the gProcess platform, a collection of Grid services and tools providing the functionalities mentioned previously and allowing the development and execution over the Grid of workflow to process remotely sensed images. It supports the exploration of optimal solutions for Grid processing and information searching in multispectral bands of the satellite images. The architecture of gProcess is based on a client-server model developed for the gLite middleware. The services exposed by the server side supports the access to Grid infrastructure resources and distributed databases, while the client side (web and desktop applications) accesses the services of gProcess through SOAP web services. The set of implemented operators can be used in the definition of various vegetation or water indices or other satellite image processing algorithms. The current operators work on GeoTiff images and operate on 512×512 tile dimension. Images are processed by dividing them into smaller pieces, applying the desired operator and then reconstruct the final image by merging all of the smaller pieces.

EnviroGRIDS offers new possibilities to further refine the ESIP platform as well as implementing the support to OGC web services to get an interoperable access to data coming from different sources. Finally, this will give partners the possibility to test some already existing geospatial-oriented grid services and to become familiar with building processing workflows.

8. Conclusions and outlook

In our everyday life, geospatial data have taken a remarkable place allowing us to continuously access a large amount of data ranging from a car's position using a GPS to results of complex simulations (such as climate models). In other words geospatial data are omnipresent. One of the challenges we are facing today is to make sense of this vast amount of data in order to turn them into understandable information to support decision-making processes. This requires analysis capabilities that current Spatial Data Infrastructures cannot fully provide. Moreover, the increasing spatial and temporal resolution of geospatial data causes a tremendous challenge for their computation, with which traditional SDIs cannot cope. To address these challenges, the environmental science community is looking with interest to Grid computing infrastructures because these can satisfy the increasing need for processing power and storage capacity, can improve accessibility to distributed storage and computing resources, and can provide a reliable and secure infrastructure. In other words, Grids have the potential to underpin SDIs services and resources.

To achieve the goal of linking Grids and SDIs, interoperability appears to be a key requirement and an important and challenging task. In particular, the implementation of SOAP messaging protocol into OGC standards is a necessity. This will greatly enhance the gridification process of OGC Web Services as well as allow easier workflows integration using orchestration engine to combine OWS and Grid services [57].

Using Grid as a computational backend represents only a first step, and currently there is no agreed and common solution to gridify OGC Web Services while remaining OGC compliant [60,27]. The integrative approach proposed by the G-OWS Working Group is very promising, extending gLite middleware capabilities with OGC specifications and thus making Grid infrastructures based on gLite spatially aware. This will allow SDIs users to rely on existing standards while hiding the complexity of the Grid. Such a gridded SDI approach could provide a benefit to both environmental science and Grid communities by enhancing discoverability, accessibility, processing and retrieval of geospatial data. As a result, new opportunities and collaborations could emerge.

⁷ https://www.g-ows.org/.

⁸ http://www.see-grid-sci.eu/.

Invoking grid-enabled OWS through mainstream desktop GIS application like ArcGIS⁹ or GRASS¹⁰ would also be a major achievement allowing users to access seamlessly different resources depending on their needs (e.g. data retrieval, processing or map making).

The first generation of SDIs, based on a product model, gave way to a second generation at the beginning of the year 2000 that is characterized by a process model [79–81]. For Masser [42] this evolution emphasizes the shift from the concerns of data producers to those of data users and the shift from centralized structures to decentralized and distributed networks. In our view, connecting Grids and SDIs could potentially mark the advent of a third generation of SDIs extending their capacities to, and benefiting from, Grid infrastructures. These grid-enabled SDIs have the potential to become a powerful tool within the multi-disciplinary field of environmental sciences, empowering researchers to explore new venues to better understand the vast complexity of the interactions between anthropic and natural systems.

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