Semantic Support for Computational Land-Use Modelling

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***Abstract*— In this paper we explore the use of proposed Semantic Grid standards and methodology through deployment of a land use modelling service. The FEARLUS-G service architecture is presented which allows large scale simulation experiments to be distributed over the Grid. We also discuss ontology support for simulation parameters, hypotheses and results that will facilitate sharing and re-use of such resources among land-use scientists. This leads to a description of infrastructure for semantic data management which integrates Jena2 and the ELDAS data access service.**

I. Introduction

Collaborations between large groups of scientists are increasingly seen as essential to enhance the scientific process. While research has always involved collaboration between individual scientists, there is now even greater necessity for tools to support sharing of knowledge, resources, results and observations. Scientists already rely extensively on computer and communication technologies to bring together different expertise, using the Web as the main vehicle of communication. While the Web does allow access to distributed data, it does not facilitate managed sharing and coordination of computational resources.

For these reasons recent e-science activities [1] have focused on facilitating and promoting collaboration between scientists using advanced distributed information management systems. The vision of e-science is to facilitate large scale science using Grid technologies [2] as a fundamental computing infrastructure to manage distributed computational resources and data. However a major gap exists between current technologies and the vision of e-science. Where Grid technologies overcome some of the limitations of existing Web tools in terms of managing computational tasks, there is still a need for greater ease of use and seamless automation to support truly flexible collaboration. For these reasons the concept of a Semantic Grid [3] has emerged, which integrates Semantic Web [4] and Grid technologies.

According to the vision of the Semantic Grid community, next generation Grids should include knowledge discovery and knowledge management functionality for applications and system management [3]. An emerging research field known as 'Grid Intelligence' studies ways to acquire, integrate, represent and exchange information available on the Grid to produce useful knowledge; such functionality will be encapsulated in so called Grid Intelligence services [3]. Central to the vision of the Semantic Grid is the adoption of metadata and ontologies [5] to describe resources, services and data sources in order to promote enhanced forms of collaboration among the scientific community. Ontologies and metadata facilitate intelligent search mechanisms, one of the key enablers through which such services could be realised.

The FEARLUS-G project, described in this paper, explores the application of emerging Grid and Semantic Grid technologies within the social sciences, through deployment of an existing land-use modelling tool into the Grid context.

The project is one of a number of pilot studies funded by the UK Economic & Social Research Council (ESRC), under their e-social science[1] initiative. FEARLUS [6] is an agent-based model of land-use change developed at the Macaulay Institute in Aberdeen. The system contains objects that represent human decision-makers in the real-world (land managers) and takes into account attributes such as yield from land parcels. Parameters to the modelling environment allow a variety of land-use strategies and their outcomes to be explored. We chose to deploy FEARLUS as a Grid service

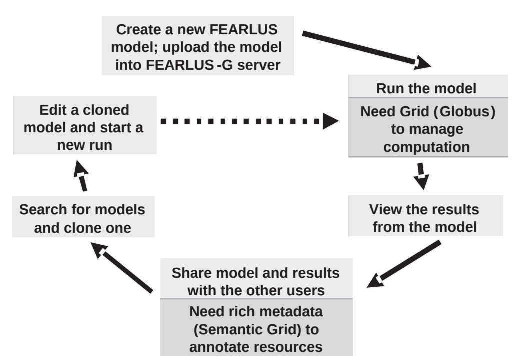

Fig. 1. The FEARLUS-G Experiment Cycle.

for a number of reasons: firstly, the Grid infrastructure allows large simulation experiments to be distributed across the Grid to make use of unused processing power; in fact, a typical FEARLUS experiment already involves running a series of

[1] http://www.ncess.org/

simulations, but on a single machine. Secondly, the use of Semantic Web technologies with Grid infrastructure allows us to create a co-laboratory where land-use scientists can access the FEARLUS-G service and share and reuse results and observations. Figure 1 shows our view of collaboration in the context of a FEARLUS experiment.

The goals of our work are thus as follows:

- annotate FEARLUS models, experiments and hypotheses with relevant meta-data, providing a common vocabulary and shared meaning, so they can be shared;
- describe FEARLUS as a Grid service, so that remote users can discover and invoke it, and obtain interpretable results by making use of the semantic resources;
- manage the Grid service, to control user access and allocation of resources;
- maintain histories of interactions with users, allowing experiments to be replayed and results to be aggregated.

In the remainder of this paper we briefly discuss simulation modelling and in particular the FEARLUS model of land-use simulation. We then describe the FEARLUS-G service architecture presenting its various components. We also introduce an ontology to support description of simulations, hypotheses and experiments. As a contribution to infrastructure for the Semantic Grid we present a solution which provides storage, query and retrieval of semantic data to allow a virtual community of land-use scientists to share and reuse FEARLUS-G experimental results and observations.

II. Simulation Modelling of Land-Use Change

Using computer technologies to study social and economic phenomena is now commonplace [7]. Such processes are often studied via simulation modelling [8]. In such simulations, the model consists of a representation of the structure and behaviour of a particular real world entity which we wish to study. One of the advantages of modelling is that the results obtained are repeatable; this allows models to be shared among the scientific community allowing further analysis and reuse. A simulation consists of running the model under a specific set of circumstances defined by a parameter set and then analysing the outcome. The aim of the simulation is to construct a model where behaviour matches the real entity in at least a significant aspect. By constructing such a model, social scientists aim to develop conclusions that provide insight into the behaviour of real world entities or phenomena; such modelling is often exploratory. Alternatively the simulation may be used to confirm how reliable a predicted behaviour is under certain key conditions which may or may not be under direct control.

There are often many competing models available, and the problem then is how to choose between different types of model in a particular problem context. It may also be difficult to interpret the behaviour from a model even when it has been previously validated experimentally. Ideally a model should be structured in such a way that it is possible to determine if a particular question can be answered using it.

A. The FEARLUS Model

There has recently been a proliferation of computer models of land-use change and water management; many of these are spatially explicit models, in which a set of distinct localities, and spatial relationships between them, are directly represented [9]. As computational resources, and the availability of machine-readable georeferenced data increase, growth in spatially explicit modelling within these domains is likely to continue. Attention is now turning to how such models can most effectively be used, both in management and policy-related applications, and in social and geographical science.

In FEARLUS Model 0-6-5 parameters to the modelling environment allow a variety of land-use strategies and their outcomes to be explored. FEARLUS aims to improve understanding of land use change, particularly as regards rural Scotland. The agent-based simulation component in FEARLUS is implemented using the Swarm system developed at the Santa Fe Institute [10]. Swarm provides an environment that can handle large experiments using agent-based simulation models. A FEARLUS simulation might involve for example, studying the dynamics of imitative[2] and non-imitative approaches to land use selection change under different circumstances, in the context of environments differing in spatial and temporal heterogeneity. This involves an initial set of exploratory studies where the model is run in a simulation with different initial parameters and the outcomes observed. The result of the exploratory study is the formulation of a hypothesis regarding patterns of behaviour of specific aspects of the land use model. Figure 2 shows the graphical output of an interactive run of the FEARLUS model. It uses graphical output to render different aspects of the model in order to facilitate exploratory studies. Using experimental validation it is then possible to check whether the model does consistently show the patterns of behaviour suggested by the exploratory studies. Further details of the FEARLUS model are available [6].

III. FEARLUS-G Grid Service

The FEARLUS-G Grid service extends the existing desktop application by enabling land use simulations to be executed on the Grid.

As mentioned earlier, a typical FEARLUS experiment might involve studying the differences between imitiative and non imitative selection strategies in a specific environment. If a scientist wished to test the hypothesis: “Innovators do better than imitators in environment A” a possible solution would be to run a set of simulations in which innovators compete against imitators in that environment using different random seeds[3]. If in this set of simulations innovators outperformed imitators in a significant number of simulations, the experimental result could be used to support the hypothesis.

Experiments running on a single machine can take a considerable time depending on the number of simulations necessary.

[2] Imitation is a social phenomenon, e.g. land managers may be influenced by other managers owning a neighbouring land parcel.

[3] The random seed is used by the multi-agent system underlying FEARLUS to generate the random behaviour defined in the simulation model.

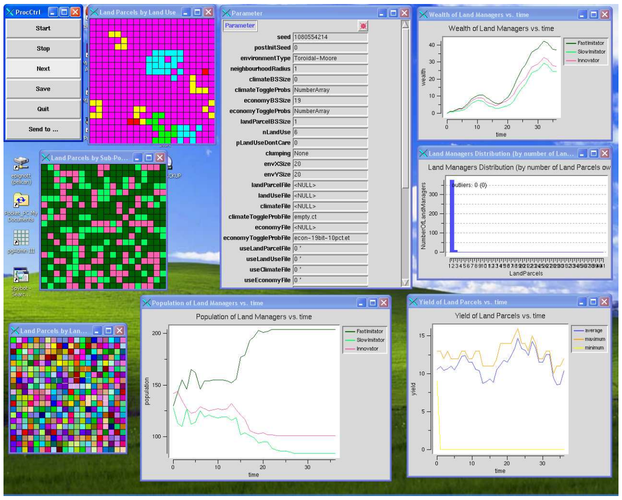

Fig. 2. The FEARLUS Desktop Application.

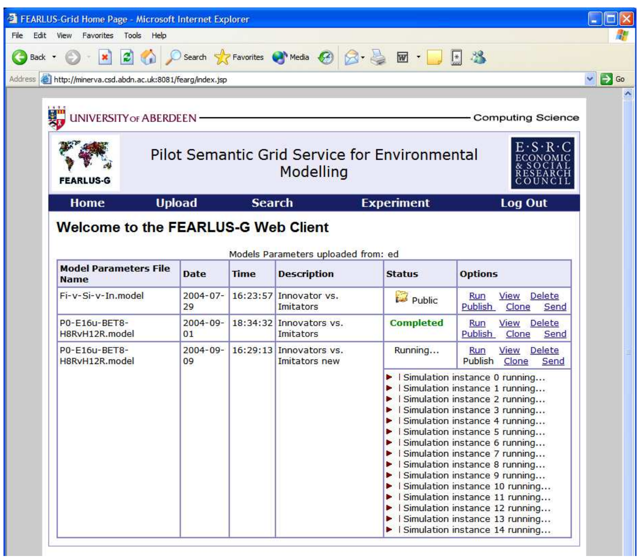

Fig. 3. The FEARLUS-G Web Client.

In our example to reach a statistically significant number of simulations we need to run dozens or even hundreds of simulation instances. FEARLUS-G distributes the load of an experiment across different Grid services depending on the resources available. Figure 3 shows different simulation instances running across the Grid. Furthermore, FEARLUS-G facilitates the reuse of model parameters and experiments using Semantic Web technologies. Ontology support is used in order to maintain histories of interactions with users, allowing experiments to be replayed and results to be aggregated.

Figure 4 presents an overview of the FEARLUS-G architecture, which is built on top of Globus Toolkit 3 (GTK3). The five core components are as follows:

1) **FEARLUS-G Service:** The access point for FEARLUS-G simulations and experiments. This service creates experiment or simulation instances by identifying the components inside an experiment definition.

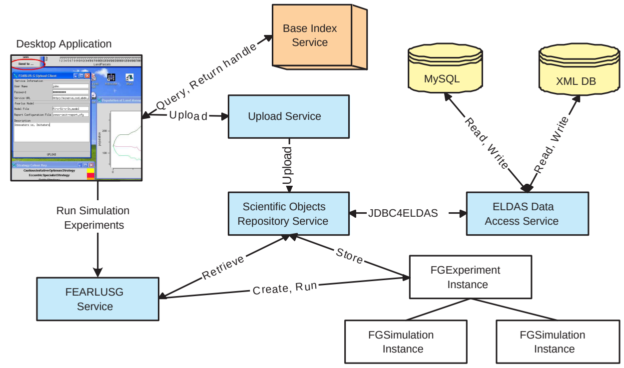

Fig. 4. The FEARLUS-G Service Architecture.

2) **Upload Service:** Allows the client application to upload Scientific Objects to the Grid application. Scientific Objects are defined in RDF [11] using the ontologies described in Section 4 of this paper.
3) **Scientific Objects Repository Service:** Stores and retrieves the model parameters and experiment definitions acquired from the Upload Service into persistent storage. Integrates the management of data and semantic metadata as described in Section 5.
4) **FEARLUS-G Experiment:** Allocates different simulation instances depending on the characteristics of the experiment. This service also collects the results from the various simulations and stores the results.
5) **FEARLUS-G Simulation:** Performs the simulation using FEARLUS model 0-6-5 and stores the results. It creates FEARLUS runs, and store the results in the appropriate simulation instance in the Scientific Objects Repository.

FEARLUS-G uses the Globus base index service to identify available services through their service descriptors. Experiments and simulations can be allocated to different nodes depending on the resources available. In our approach, users provide specifications of the experiments and the initial parameters for the simulation. This information is stored using the Scientific Objects Repository. This can be done by a client application integrated within the FEARLUS desktop client (see Figure 2) or through a Web portal designed for FEARLUS-G (see Figure 3). The FEARLUS-G environment contains the middleware to find resources available and the input data required to perform a specific simulation by making use of a service descriptor associated with the FEARLUS-G service. The service descriptor contains the characteristics of the resources available in the node such as the maximum number of simulations and the simulation instances available. In order to make this possible each distributed node with a FEARLUS-G service instance notifies the base index service whenever there is a change in its status. Grid services or user applications that need a FEARLUS-G service can query the base index service to obtain a handle for an appropiate service depending on the size of the experiment they need to perform.

Once a request to perform an experiment has been allocated

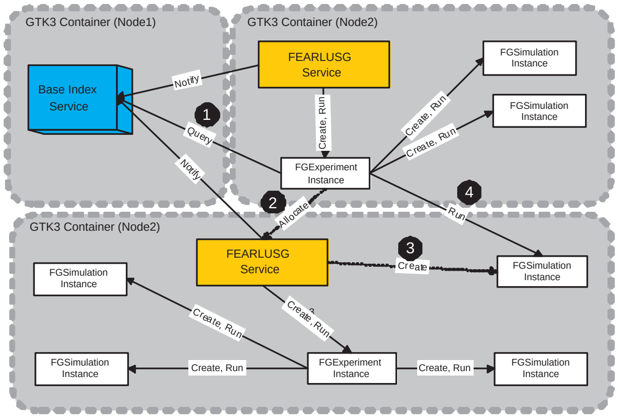

Fig. 5. Allocation of a FEARLUS-G Simulation.

to a FEARLUS-G service, the system allocates simulation instances to perform the various parts of an experiment and collect the results. Figure 5 illustrates how an experiment and its related simulations are allocated in FEARLUS-G:

1) The experiment instance queries the base index service to obtain the location of a FEARLUS-G service with available resources. If resources are available on the same node the experiment instance creates instances of a FEARLUS simulation.
2) If the resources available are on a different node the experiment instance sends a request to the remote FEARLUS-G service instance to allocate a simulation instance;
3) The remote FEARLUS-G service creates the simulation instance and returns the handle to the original experiment instance;
4) The experiment instance then uses the newly created remote simulation instance to run part of its experiment.

As explained earlier, FEARLUS-G aims to facilitate sharing and reuse of models and experiments among the land use scientific community. For this reason the Scientific Objects Repository service can be used to search for and clone existing model parameters and experiments. A social scientist can use the cloned model or experiment to further investigate the specific problem addressed within it. For example, they could use an experiment to disprove a previous hypothesis or reuse a model for a different research problem. Figure 1 shows a typical experiment cycle.

Figure 3 shows the existing FEARLUS-G Web client[4] through which users can perform experiments and share results. The metadata used to describe models, hypotheses, results and experiments within the service environment allows annotations to specify properties of models and experiments, including creator, contributors and supporting evidence (e.g. publications).

IV. Representing Simulations, Hypotheses and Experiments

As described in Section 2, the classical approach to simulation studies is to create a model of a real entity in order to analyse hypothetical behaviours. Simulations are used to generate numerical results representing future states of the model under specific conditions. By testing the numerical results with an appropriate method it is possible to agree or disagree with a hypothesis. In this section we propose a conceptual layer through the definition of an ontology which captures the concepts and relationships important to scientists performing their research activities.

Figure 6 shows the core classes and properties in our ontology. It includes a collection of generic elements that are intended to be applicable to any e-science application, and also elements that are specific to simulation modelling and FEARLUS-G in particular.

Instances generated from the classes in the ontology are of three types: those which need to be created by the user, e.g. the definition of an experiment; those instances created by the Grid service, e.g. the set of simulation run instances associated with an experiment, and the experiment result instance summarizing the results; the third group are instances created to support scientific argumentation, sharing and reuse. For example, an hypothesis can be associated with related publications and experiments.

The key class in our generic representation is the *Hypothesis*, which we consider to be a scientific concept that has not yet been fully verified. An hypothesis is "a tentative explanation that accounts for a set of facts and can be tested by further investigation"[5]. This implies that a scientific community works to support an hypothesis by contributing publications, experiments and other related hypotheses that agree or disagree with the "target" hypothesis. In our vision, the classes *HypothesisObject*, *ExperimentObject*, *SimulationObject* and *Publication* are subclasses of a generic *ScientificObject* class.

We define two properties `agreesWithHypothesis` and `disagreesWithHypothesis` which link any given scientific object to *Hypothesis* instances. Those properties allow us to support scientific argumentation in the FEARLUS context by linking specific evidence (`FearlusExperiment`, `Run`, `FearlusResult`) to hypotheses. The generic scientific object representation can, of course, be adapted for different scientific domains by extending it with more specific subclasses and properties.

We use the Dublin Core[6] ontology to provide basic annotation of *ScientificObject* instances. For example `dc:creator` defines the creator of an hypothesis, publication or experiment, `dc:contributor` the contributor(s). Figure 7 shows an example. We also aim to provide support for refinement of hypotheses; in particular we use `dc:replaces` to represent that a new hypothesis replaces another.

[4]http://minerva.csd.abdn.ac.uk:8081/fearg/

[5]www.pages.drexel.edu/∼bcb25/scimeth/vocabulary.htm

[6]http://dublincore.org/

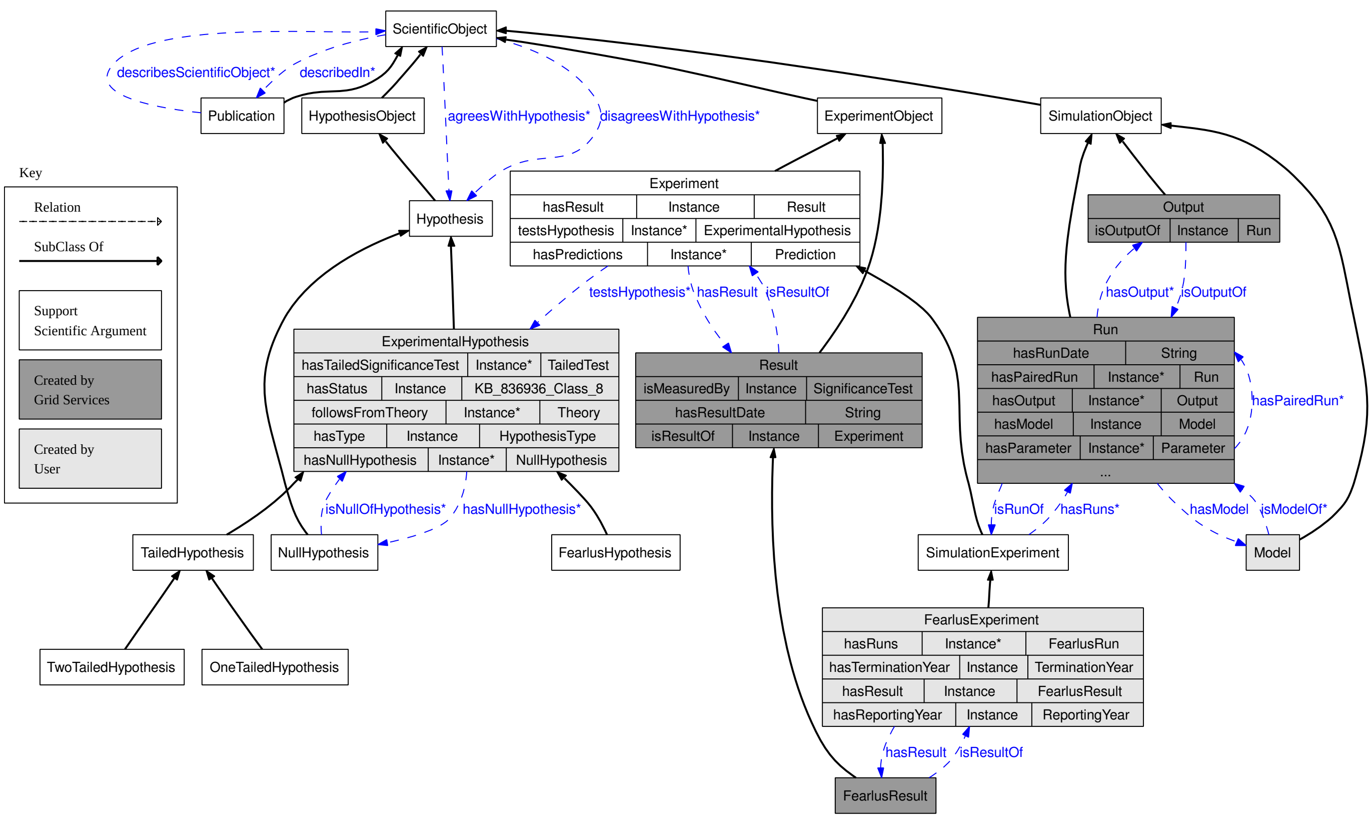

Fig. 6. Part of the FEARLUS-G Ontology Illustrating Hypothesis, Publication, Experiment & Run Concepts.

Another important attribute is `describedIn`. This is used to record that a publication can be used to describe any given scientific object.

An *ExperimentObject* is intended to be any object that defines a real experiment, this includes the experiment definition (class *Experiment*) and the experiment results (class *Result*). We define *FearlusExperiment* as a subclass of *Experiment* to extend our generic ontology to include a FEARLUS experiment. A typical simulation experiment in FEARLUS (class *FearlusExperiment*) compares a number of subpopulations by making them compete in the simulation environment.

In our ontology a simulation experiment includes a set of simulation runs (class *Run*) in a specific simulation model (class *Model*) and the related output (class *Output*). The instances of such classes are generated automatically from the FEARLUS-G grid services and stored in the Repository Service (see Figure 4). This allows the system to recognize if a specific simulation run has already been executed by querying the Repository Service. If a pre-existing run and its associated results are detected, the FEARLUS-G system does not need to perform another simulation but only aggregate existing data.

V. A Grid Enabled Semantic Data Service

In the previous section we introduced a possible ontology starting point for supporting scientific research via the Semantic Grid. We plan to use this ontology in the Grid context to make use of the potential of both technologies by sharing computational and data resources across different hosts, with the semantic metadata providing support for management of these shared resources.

As part of the FEARLUS-G project we are developing an open source reusable semantic data service based on Jena2 [11] and Globus Toolkit 3 [12] to provide semantic data storage, query and retrieval functions. This service uses ELDAS [13] to manage data repositories for RDF models; ELDAS was developed by the UK National e-Science Centre eDIKT project[7].

Jena2[8] is a Java framework for writing Semantic Web applications. It provides programmable access to RDF and OWL sources, ontologies, documents, ontology reasoning and RDF query capabilities [14]. The advantage of enabling Jena2 as a Grid service is that semantic resources can be distributed and used in a dynamic environment. Searching a large collection of RDF resources can be a computationally intensive task; the Grid offers the potential for distributed processing of such queries. The following subsections describe these technologies and how we combine them together.

A. ELDAS Data Access Service

Data access is an important feature in many Grid applications. For this reason the Data Access and Integration Working Group (DAIS-WG) produced the Grid Database Service

[7]http://www.edikt.org
[8]http://jena.sourceforge.net/

```
<ExperimentalHypothesis rdf:ID="hyp_1">
  <hasHypothesisDescription>
    Fast imitators do better that innovators
  </hasHypothesisDescription>
  <dc:creator rdf:resource="#GaryPolhill"/>
  <hyp:replaces rdf:resource="#hyp_0"/>
  <dc:contributor rdf:resource="#NickGotts"/>
  <describedIn rdf:resource="#pub_1"/>
  <hasType rdf:resource="#fearlusType1Hypothesis"/>
  <hasStatus rdf:resource="#hypothesisUnderInvestigation"/>
</ExperimentalHypothesis>

<SimulationExperiment rdf:ID="exp_1">
  <agreesWithHypothesis rdf:resource="#hyp_1"/>
  <testsHypothesis rdf:resource="#hyp_1"/>
  <describedIn rdf:resource="#pub_3"/>
  <hasNumberOfRuns>10</hasNumberOfRuns>
</SimulationExperiment>

<Publication rdf:ID="pub_2">
  <dc:title> Innovative Strategies Comparison</dc:title>
  <dc:contributor rdf:resource="#JohnSmith"/>
  <disagreesWithHypothesis rdf:resource="#hyp_1"/>
</Publication>
```

Fig. 7. Example of *ExperimentalHypothesis, SimulationExperiment* and *Publication* Instances.

specification (GDSS). The GDSS presents a specification for a collection of data access interfaces for relational data resources [15]. The main interfaces described by GDSS provide methods for accessing the data from a Grid service.

ELDAS [13] is an implementation of the GDSS specifications. ELDAS attempts to overcome some of the issues raised while working with application scientists in several disciplines. The main characteristics of ELDAS are:

- implementation using J2EE which is machine independent;
- able to access and integrate data stored in multiple types of data storage system, such as Mysql, Oracle and DB2;
- accessible as both a Grid service and a Web service.

The main advantage of using ELDAS and the GDSS specification is that they make Grid data services available to the scientific community, resolving issues associated with sharing relational data from different database systems.

B. Integrating Jena2 and ELDAS

There are issues surrounding deployment of Jena2 as a Grid service as it was not designed with this in mind. Jena2 does provide a module which extends the RDF model interface so that it is possible to store and retrieve statements using a database. Although this module supports different database servers such as MySql, Oracle and PostgreSQL, it needs direct access to the database server and is not designed to operate in a distributed environment such as the Grid. For these reasons it was necessary to develop a bridge between the Jena2 database module and the ELDAS data access service to allow Jena to communicate with the database across the Grid instead of via a direct connection.

JDBC[9] is a programming interface which allows external access to databases and query operations using SQL. Moreover JDBC allows the integration of database calls with the

[9]http://java.sun.com/products/jdbc/

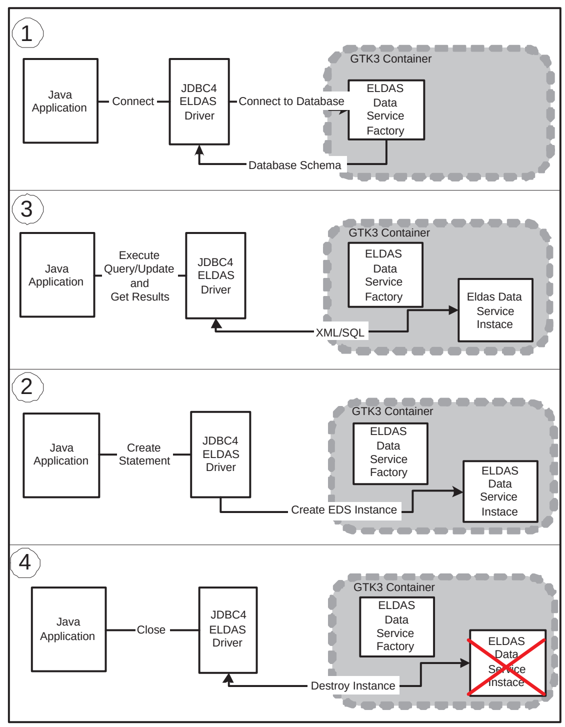

Fig. 8. JDBC4ELDAS Usage Summary.

Java programming environment making database operations simple and intuitive. We have developed a bridging solution, JDBC4ELDAS which allows connections to different databases supported by the ELDAS data access service using standard JDBC library routines. Figure 8 illustrates the use of JDBC4ELDAS.

The JDBC4ELDAS driver[10] enables the Jena2 database mod-

[10]The drivers and associated documentation are available at http://www.csd.abdn.ac.uk/research/fearg/links.php

ule to store models using ELDAS as a Grid data access service. The advantage of using a JDBC bridge driver between Jena and ELDAS is that both applications remain untouched. Moreover the JDBC4ELDAS driver is easily reusable for any Java application that requires Grid data support. We have developed a sample client application using Protégé[11] in order to test the JDBC4ELDAS driver and to explore the potential of Protégé as a visualization/editing tool for the Grid data storage solution. Protégé [16] allows a user to create and edit ontologies and instances which can be stored in a file or in a database using OWL, RDF or Protégé's own application specific format. The input of new instances is performed through customisable forms automatically generated from the ontology. We configured the existing Protégé database module to use JDBC4ELDAS simply by indicating the name of the driver class in a configuration file; using Protégé in this manner we can easily access our existing ontology and instances (see Figure 9).

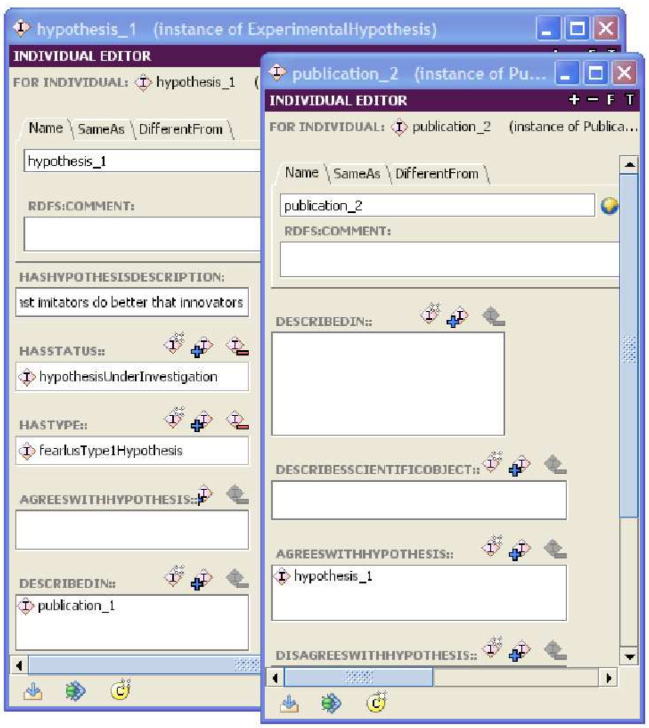

Fig. 9. Example FEARLUS-G Instances Rendered via Protégé.

VI. Related Work

We have identified a number of activities that share important characteristics with FEARLUS-G. The MyGrid project [17] [18] enables biologists to perform and manage *in silico* experiments by providing a problem-solving workbench based on Semantic Grid technologies. User scientists in MyGrid browse a registry and select a workflow template. The system then asks the user to manually select instances of the services associated with the workflow or automatically selects services based on a user profile (user preferences). The MyGrid services collect and co-ordinate data inputs and outputs for the experiment, as well as provenance information about the performance of experiments. MyGrid develops the use of workflow ontologies to capture web-based procedures and provenance ontologies [19] to describe how and why results were produced.

Majithia et. al. [20] propose a system which facilitates automated synthesis of scientific experiment workflows, based on a high-level goal specification. This approach differs from MyGrid as it uses a composition algorithm to adapt available resources on the Grid to high level objectives defined by the user. Moreover, the system makes a distinction between different levels of abstraction of the workflow in order to allow reuse and sharing.

The two systems described above focus on provenance (MyGrid) and workflow abstraction (Majithia) to support sharing and reuse of scientific process information. However, in both systems scientific argumentation is not supported; experiments and results are not associated with hypotheses. In our opinion the FEARLUS-G argument structure approach is likely to be more intuitive to user scientists, reflecting as it does the evidence-based approach widely used within the scientific community.

SemanticOrganizer [21] is a knowledge management system designed to support distributed NASA projects, including multidisciplinary teams of scientists, engineers and accident investigators. SemanticOrganizer provides a semantically-structured information repository that serves as a common access point for all work products related to an ongoing project. The repository not only stores files but also metadata describing domain concepts. The system allows accident investigators to collect and manage evidence, perform different type of analyses that generate derivative evidence, connect the evidence together to support or refute accident hypotheses. SemanticOrganizer is implemented using standard Web services for both the repository and the user interface. This project successfully adopts Semantic Web technologies to support construction of an evidence-based argumentation structure. While this approach does have much in common with the FEARLUS-G solution described in this paper, it does not of course provide support for execution of large-scale experiments.

VII. Lessons Learnt and Discussion

Our Grid service provides scientists interested in land-use phenomena with a means to run much larger-scale experiments than previously possible on standalone PCs, and also gives them a Web-based environment in which to share simulation results. The Grid is clearly a valuable tool for managing the computation involved in running such large-scale experiments. In fact the Globus environment is ideal for simulation modelling because the cost of a simulation run is less that the cost of the communication necessary to run a distributed experiment and aggregate the results. However, the Globus environment is not well-suited for the fine grained exploratory work that the existing FEARLUS desktop application is able to

[11]http://protege.stanford.edu/

achieve. Scientists still want to use the patterns of workflow related to the desktop application. For this reason, we have extended the existing desktop application to be able to upload models to the Grid service, creating a link between the exploratory tool and the Grid experiment platform.

We have defined an initial collection of ontology elements that describe the scientific objects necessary to enable collaboration between members of a community of land-use scientists. Our ontology represents generic scientific concepts such as hypotheses and experiments, as well as more domain-specific concepts tailored to the use of FEARLUS. Social scientists are able to run FEARLUS experiments on the Grid and collect the results; a private interface allows them to manage their activities (experiments, investigations, etc.) while their work is in progress. Scientific resources can also be made public, allowing others to investigate them further.

Not all categories of users require access to the same meta-data. For example, we have exposed FEARLUS model parameters to land-use scientists familiar with the existing FEARLUS application in such a way that the complexity of the Grid services is hidden to them. We provide a Web application which allows users to access and manipulate low-level simulation model parameters needed to run a FEARLUS experiment. However, we also need to provide high-level data to promote accessibility to the wider scientific community. For this reason we provide access to our public interface where resources contain high-level generic properties (e.g. *describedIn*, *agreesWithHypothesis*, *hasDescription*).

Throughout this project we have encouraged computational land-use modellers at the Macaulay Institute to lead the process of engineering the FEARLUS ontology. This important activity forced them to think about what conducting an experiment actually meant. Prior to this project, Perl scripts were used to conduct experiments with FEARLUS and the experimental design was thus hidden. One positive side-effect of the ontology building exercise is that the experimental workflow is now exposed, making its use transparent to other users.

We have engaged a group of “assessors” from the international scientific communities interested in agent-based social simulation, land-use and water management modelling. These assessors have agreed to conduct usability trials using the FEARLUS-G Grid service either in a research capacity (uploading FEARLUS models, comparing results from their own models with those from FEARLUS, checking results in FEARLUS publications, or exploring FEARLUS’s capabilities and limitations as a stage in the process of designing a new model), or as a teaching tool, or both. Evaluation of the FEARLUS-G service is expected to provide more general insight into the effectiveness of current Semantic Grid technologies and methodologies.

Acknowledgment

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