An Ontology for User Support in The Materials Microcharacterization Collaboratory

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ABSTRACT
We describe the experience of building an ontology for use in an agent-based system in support of the Materials Microcharacterization Collaboratory (MMC). The ontology expresses facts related to users of scientific instrumentation such as electronic microscopes and a neutron-beam line. The users, experts and types of experiments are also described. The Zeus Agent Toolkit ontology editor was used.

Keywords
Ontologies, Agent-based systems.

1. INTRODUCTION AND BACKGROUND
The Materials Microcharacterization Collaboratory (MMC) is a joint project between national laboratories, academia, and industrial collaborators across the US supported under the DOE2000 effort[1]. The purpose of collaboration within the MMC is to characterize the microstructure of material samples using techniques such as electronic microscopy, and x-ray and neutron diffraction. Observation, data acquisition, and analysis are performed using instruments such as transmission and scanning electronic microscopes, and a neutron beam line. An important aspect of the MMC project is the computer co-ordination and control of remote instrumentation, data repositories, visualization platforms, computing power, and user access to expertise that are distributed over a national scale. In the first phase of the MMC, instruments operational at individual laboratories with varying capabilities were brought online and broadcast on the Web; synchronous observation and data analysis can be performed over the Internet [2]. Remote control of instruments is also provided through the DeepView framework [3].

The second phase of the MMC focuses on facilitating user access to the collaboratory by automating various logistics tasks that must be performed before users can access the facilities on-site or remotely. An important aspect of facilitating this access has been designing a resource allocation and distribution system for instruments and for scientists' expertise [4]. In particular, a prototype is being designed that automates the distribution of user proposals to the relevant expert and accelerates the review process granting users permissions to use the facilities. Previously, users manually filled out a proposal after much consultation with expert scientists.

2. AN ONTOLOGY FOR USER SUPPORT
The domain ontology contains entities necessary to represent tasks performed by users and scientists in the access phase of a project. It also contains knowledge pertaining to scientists' expertise as well as instrument parameters. The ontology is used by a prototype system built upon a community of agents. The agent-based system has been designed using the Zeus Agent Toolkit made available on open source by British Telecom [5]. Agents in the system exchange messages structured on FIPA ACL and use the domain ontology to request information from each other. Five main agents were designed based on the stakeholders in the MMC: a User agent, an Expert Agent, an Instrument Agent, an Experiment agent, and a Scheduling Agent. In addition Name Server and Facilitator agents were provided by the Toolkit [6].

One challenge in designing the ontology has been acquiring and formalizing knowledge obtained from the scientists who will review the proposal. An existing proposal form served as the basis for designing the ontology. Interviews with scientists and direct observation were also used. Scenarios were also written to determine tasks performed in the system and verify facts in the ontology. The system takes advantage of the Zeus Ontology editor provided by the Zeus Agent Toolkit. This editor includes the ability to design a classification of terms, as well as rules for constraining the use of these terms. Entities in the ontology are called Zeus Facts. The Zeus Ontology editor does not provide a tool for proving the consistency and completeness of the ontology, nor does it require writing term definitions in formal logic. Mechanisms for re-use of existing

ontologies through pointing to ontology repositories are not directly supported. Re-use of existing ontologies entails translations to Zeus Facts. Some agent tasks such as modifying the value of attributes defined in the ontology may be directly performed through Zeus.

Ontologies pertaining to the support of the complex scientific instruments and experiments available through the MMC were not found. For this reason and the limitations of the toolkit, the ontology for the prototype was entirely created for the prototype.

4. CONTENT OF THE ONTOLOGY

Four main frames in the domain ontology were designed: User, Expert, Instrument, Experiment. The User frame for instance specifies details of the experiment to be performed, properties of the instrument on which the experiment is requested and a unique user identifier issued previously. The Instrument frame specifies the Expert who owns control over the instrument, availability, instrument properties, location, access methods, and the kind of training required to use the instrument (see Figure 1).

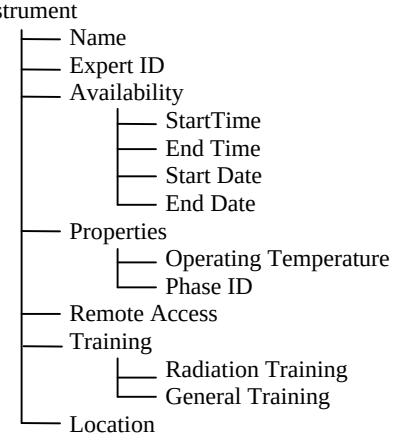

Figure 1: Instrument Frame

The Experiment frame specifies properties related to the proposed experiment, in particular properties of the sample to be examined (Material), the instrument requested for the experiment, properties pertaining to the environment in which the experiment is to be performed (temperature, radiation), and the estimated impact of the proposed experiment on the field (see Figure 2).

3. CHALLENGES AND FUTURE WORK

Eliciting knowledge from the domain-area scientists has constituted the major difficulty in designing this ontology. In particular, the criteria under which proposals are reviewed are qualitative rather than quantitative. These criteria include economic factors (i.e. the industrial impact of the experiment is likely to have), technical factors (i.e. the types of materials to be characterized in the experiment), and credibility factors (user publications and why the experiment is being requested). It was decided that a system serving as a decision-support tool facilitating the presentation of relevant information to the scientist would be designed, rather than automate the decision to accept or reject a proposal.

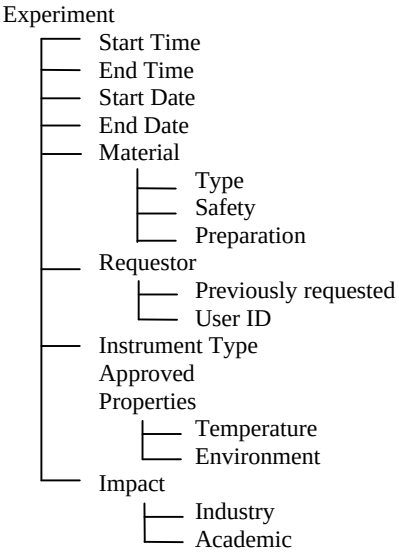

Figure 2: Experiment Frame

Future work involves granting security certificates to users based on a Certificate Issuing Authority. This is to be implemented as an additional agent service. The User frame of the domain ontology will be extended accordingly.

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