Supporting Collaborative Use of Scientific Instruments: an MMC Case Study

Line Pouchard, Jim Rome
Computer Science and Mathematics
Oak Ridge National Laboratory

Omer Rana, David Walker
School of Computer Science and Welsh e-Science Centre
Cardiff University

Materials Microcharacterization Collaboratory

MMC: a DOE2000 pilot project

http://tpm.amc.anl.gov/MMC/HomePage.html

What is the MMC?

- Materials Microcharacterization Collaboratory
- Geographically dispersed expertise and resources:
  - electron microscopes, diffractometry instruments (neutron beam line, x-rays)
  - Instrument specialists
- Coordination and control of remote instruments
- Visualization platforms
- Data repositories
- Remote data analysis
- ORNL has user facilities participating in the MMC:
  - Diffraction, Thermo-Physical properties, Microscopy

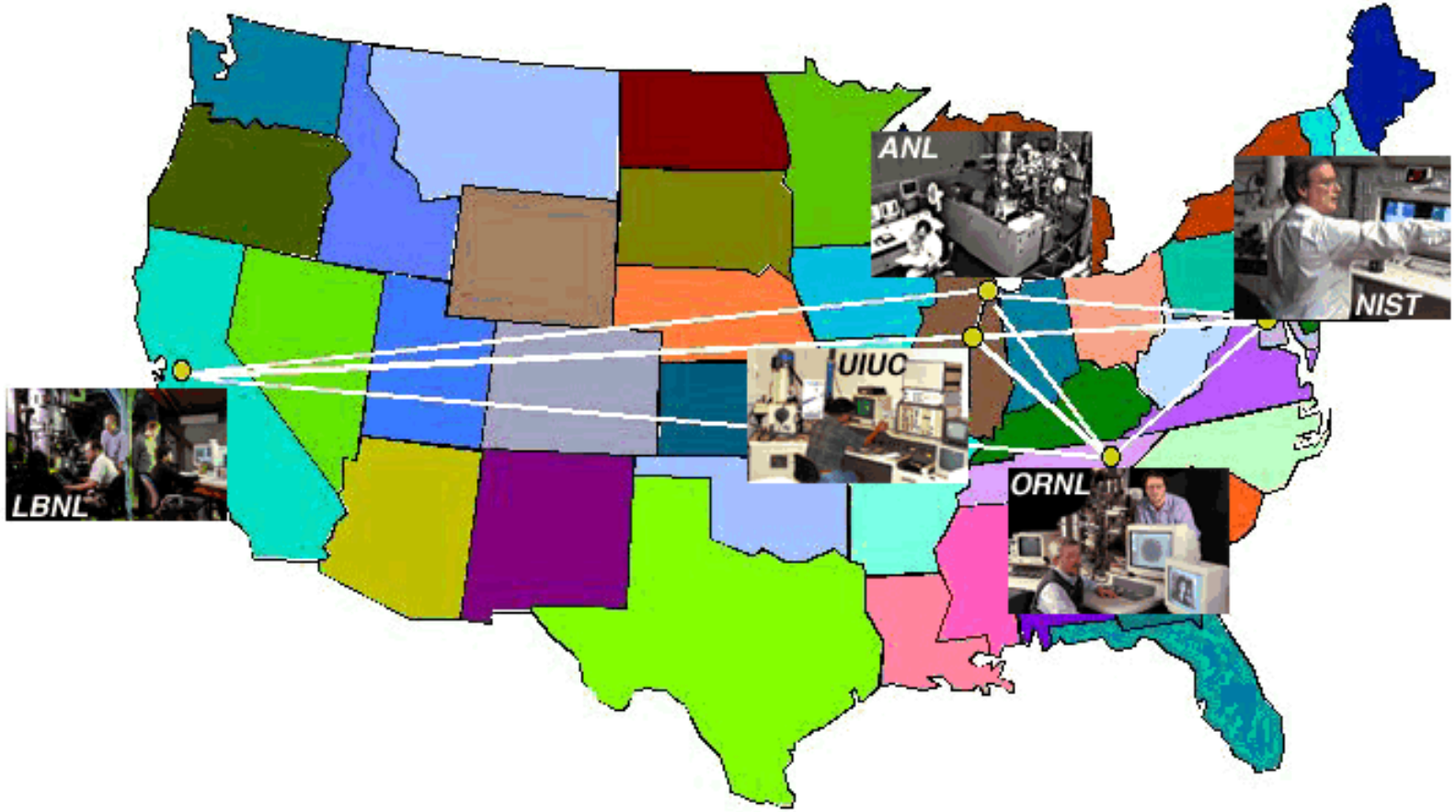
Two Aspects

- User Support
  - Allocating time on instrument
  - Checking credentials of requestor
- Remote Access
- Tools for remote access
- Integration of tools with instrument properties

Using the Grid and issues

- QoS issues
  - What should be remotely accessible
  - Support for multiple (event) channels
  - Fully duplex, real time control (not possible right now)
- Security issues
- User interface components
  - Some standard panels which could be customised
- Identification and limitations of existing middlware
- Common interfaces for connecting instruments (Rick McMullen)
- Integration with data and compute resources – Rick McMullen (workflow engines would be useful to achieve this)

MMC



Materials Microcharacterization Collaboratory Participants

ARGONNE National Laboratory

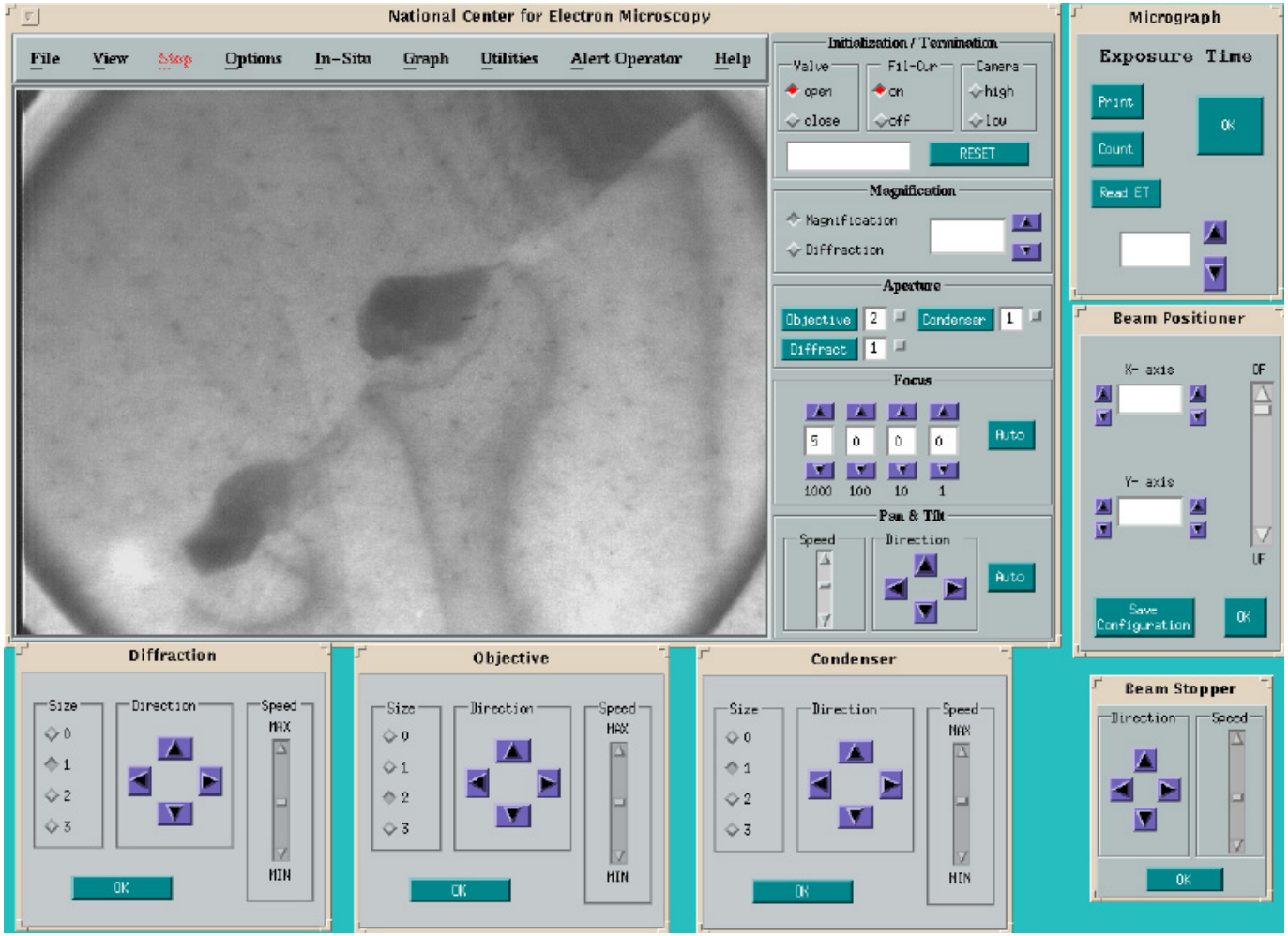
BERKELEY LAB

NIST

ornl

University of Illinois Urbana-Champaign

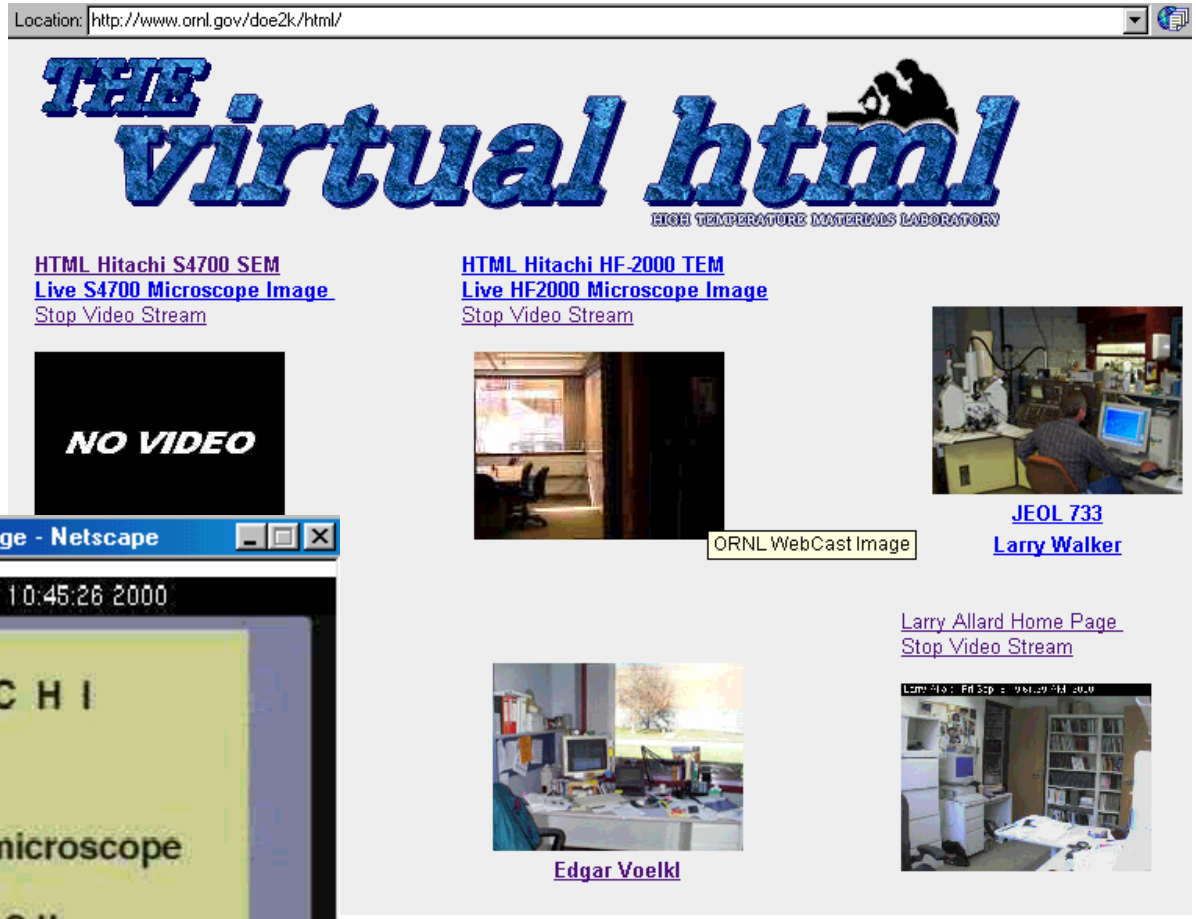
Remote Operator Interface (LBNL)



Standard Remote Operator Interface configured for the Kratos EM-1500 HMEV

The main interface window (a) contains the live 640x480 NTSC image and controls for magnification, aperture selection, focus and specimen tilt.
Other pop-up windows control aperture positions (b), plate camera (c), beam position (d) and beam-stop position (e).

Existing MMC collaboration techniques: WebCast of microscope images



http://www.ornl.gov/doe2k/mmc

Prior to AccessGrid days – this kind of work would now be done via AG software

Instrument Selection

Instrument Directory

File

Name	Type	Location	HostName	On-Line
CM300	TEM	Berkeley	sundog.lbl.gov	Yes
LSMR	Optical	Berkeley	lsmr3.lbl.gov	Yes
Zeiss	SEM	U.Illinois	cmm_sun.m...	No
XL30	SEM	OakRidge	mms39.ms....	No
CM12	TEM	OakRidge	mms39.ms....	No
HVEM	TEM	Berkeley	seer.lbl.gov	Yes
SIMULATOR	SW	Berkeley	vision.lbl.gov	Yes

Device: SIMULATOR

Type: SW

Location: Berkeley

Host: vision.lbl.gov

On-Line: Yes

Info

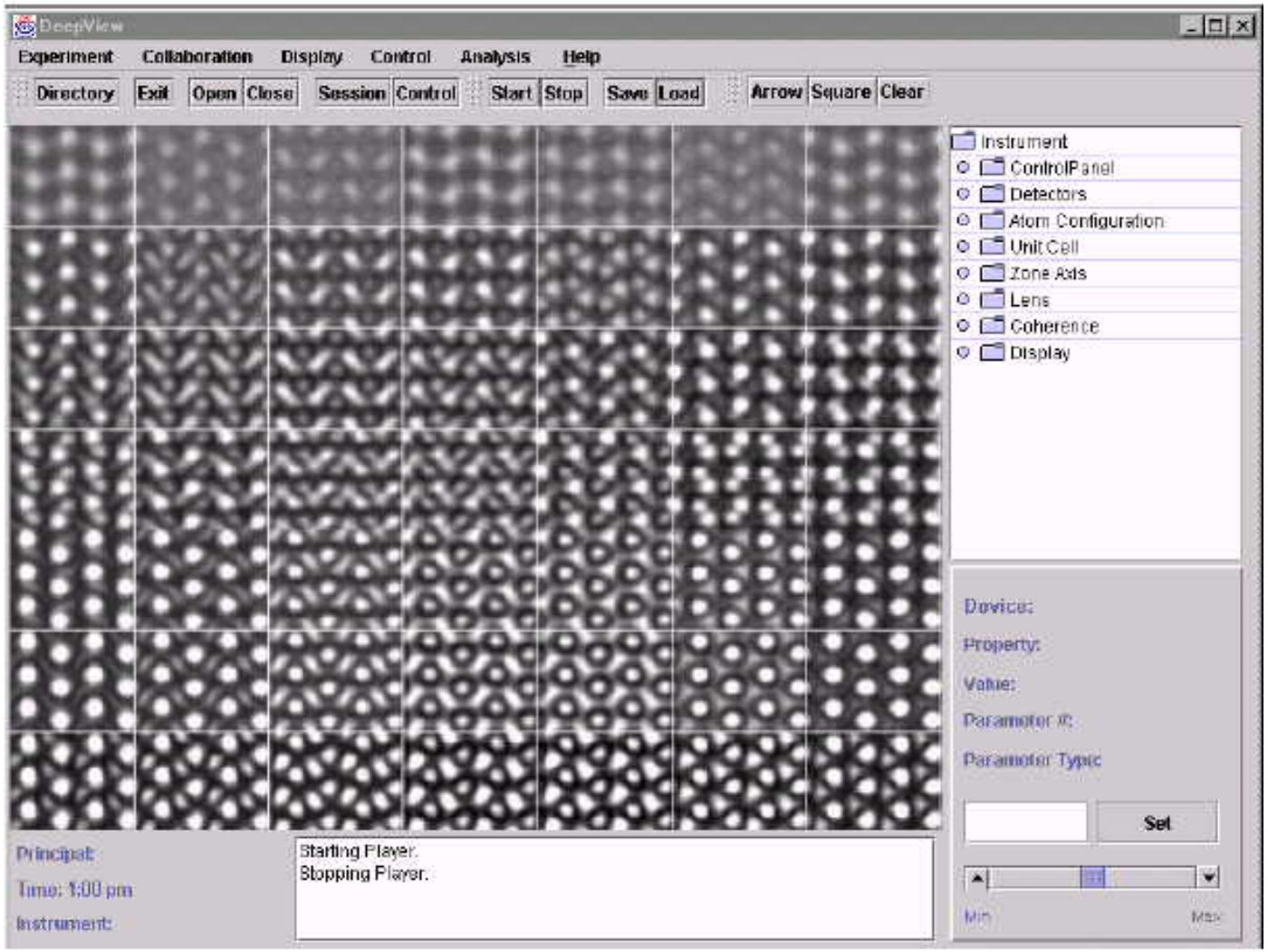
Join

Dismiss

Users View of the Microscopy Channel

Use of a common Naming convention For instruments

DeepView Interface (B. Parvin et al. (LBNL))



Rationale for enhanced collaboration tools

- Attract new users from industry and academia
- Retain current ones
- Offer supporting tools that promote efficient and effective use of resources
- Automate some tasks preliminary to actual use of instrument and site visit
  - facilitate user proposals and information requests
  - facilitate scheduling on an instrument
  - administer safety and security training
- Ensure access control, authorization, and authentication

Scientific Lifecycle for MMC users

- Proposal cycle
  - proposal forms filled and submitted by external users in cooperation with staff scientists
    - 3 months, email and phone calls
  - proposal reviewed by staff scientists
    - establishing a test matrix for review
    - one month
- Formal approval and authorization
  - scheduling scientists and users' time on an instrument
  - security authorizations for site visit
  - safety training, possibly radiation training
  - set-up computer accounts

Scientific Lifecycle for MMC users...

- On-site visit:
  - one-two weeks visit
  - one or two users per institution
  - some collaborators remain at home
  - process and data recording and analysis
  - use of electronic notebooks
- Post-experiment
  - extensive communication with scientists
  - use of electronic notebooks
  - joint publications

Needs for enhanced collaboration tools

- Automating some tasks preliminary to the actual use of instrument and site visit
  - information requests, user proposals, and proposal reviews
  - scheduling on an instrument
  - administer safety and security training prior to visit
- Ensuring access control, authorization, and authentication
- Timely and synchronous visualization of partial results during an experiment on site and at home institution
- Enhanced communication tools for face-to-face and voice interaction during an experiment
- Offering support tools that promote efficient and effective use of resources

Proposed Agent Services

⌘Benefits of using agents

- Integration of existing heterogeneous, distributed, high level components in a single architecture
- Execution on client machines for some agents (except control and instruments)
- Scalable (may add users and instruments)
- Extensible (may add agents)
- Can encode behaviour rules (or constraints)
- May be implemented using a number of different kinds of middleware (e.g CORBA)

⌘An agent-based resource allocation system

- Dynamic scheduling
- Query handling
- Training
- Authentication and access control

ISE: a multi-agent system using intelligent software agents

- Integration of existing heterogeneous, distributed, high level components in a single architecture
- Execution on client machines for some agents (except control and instruments)
- Scalable (add users and instruments)
- Extensible (add agents)

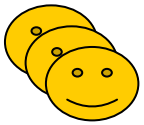
A Controller Agent (CA)
authorizes users to access other agents

A Proposal Agent (PA)
distributes proposals to experts

A Query Agent (QA)
answers user questions

A Training Agent (TA)
administers remote tutorials

User Agents (UA)
represent individual users



Instrument Agents (IA)
schedule users on individual instruments

Expert Agents (EA)
represent experts

Proposal Form available on the Web

ORNL MMC–User Proposal Form2: Experiments and Instruments

Experiment (ExperimentType, InstrumentNeeded, ExpertStaff)

Field required: 9

One of the following is also required: 10 or 11 or 12 or 13 or 14

9	ExperimentType		Thermophysical Properties
10	InstrumentNeeded	Microcharacterization	Tecnai20 CM200 CM30 XL30 APFIM
11	InstrumentNeeded	Materials Analysis	Hitachi S800 SEM Hitachi HF 2000 AEM Hitachi S 4700 SEM Hitachi FB2000 FIB Hitachi HD 2000 STEM
12	InstrumentNeeded	Diffraction	High Temperature X–ray Room Temperature X–ray Neutron Powder diffraction 1600C vacuum furnace 1200C tube furnace
13	InstrumentNeeded	ThermoPhysical Properties	Differential Scanning Calorimeter Dilato Bilayer Dilato Dual Push Rod

ORNL MMC–User Proposal Form3: Sponsoring and Impact

15, 17, 18 are required fields

15 RelatedTo (Is this proposed effort related to another ORNL program or user facility?)

no Go to 17 yes Go to 16

16 NameRelatedTo Go to 17

17 FundingSource

Agency NSF Other A foundation

Funding Office Example: Office of S

Type of Funding SBIR Other a funding type not

18 Research Impact

ResearchImpactEconomic

energy savings
improved processes
improved products

Other Example: new materi

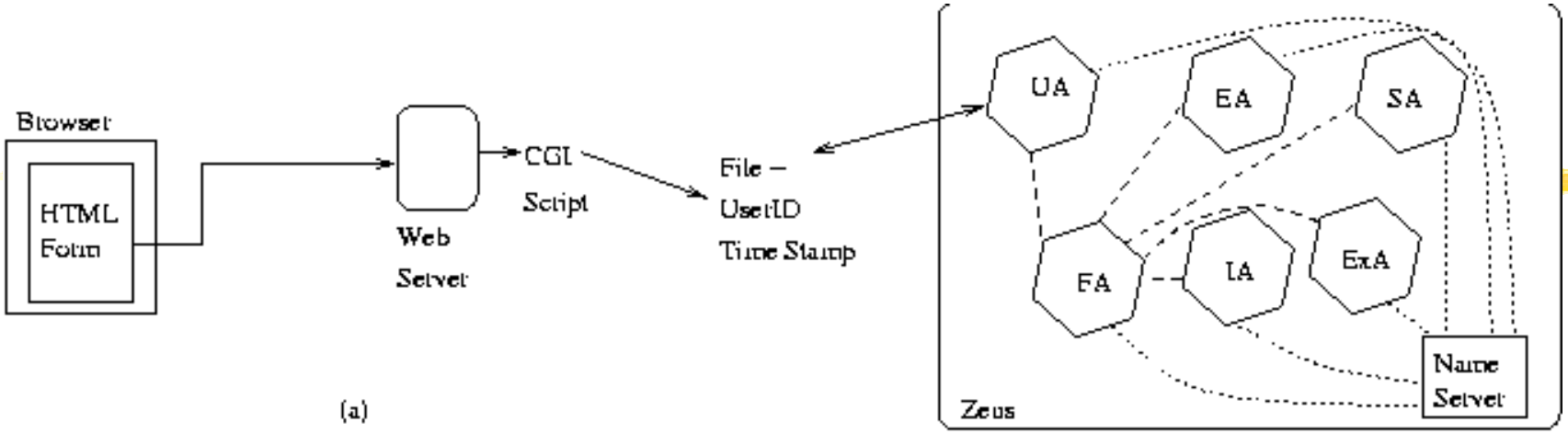
ResearchImpactAcademic

Master Thesis
PhD Dissertation

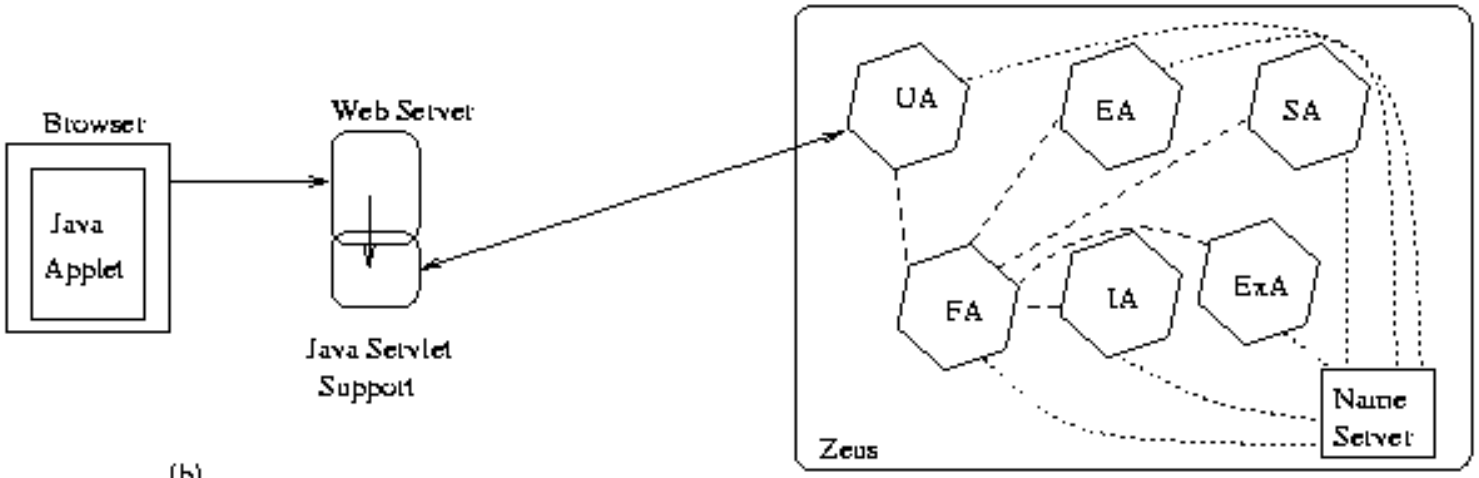
17 IntentToPublish PublicationTitle PublicationType PublicationDate

Journal of Microscop

Journal



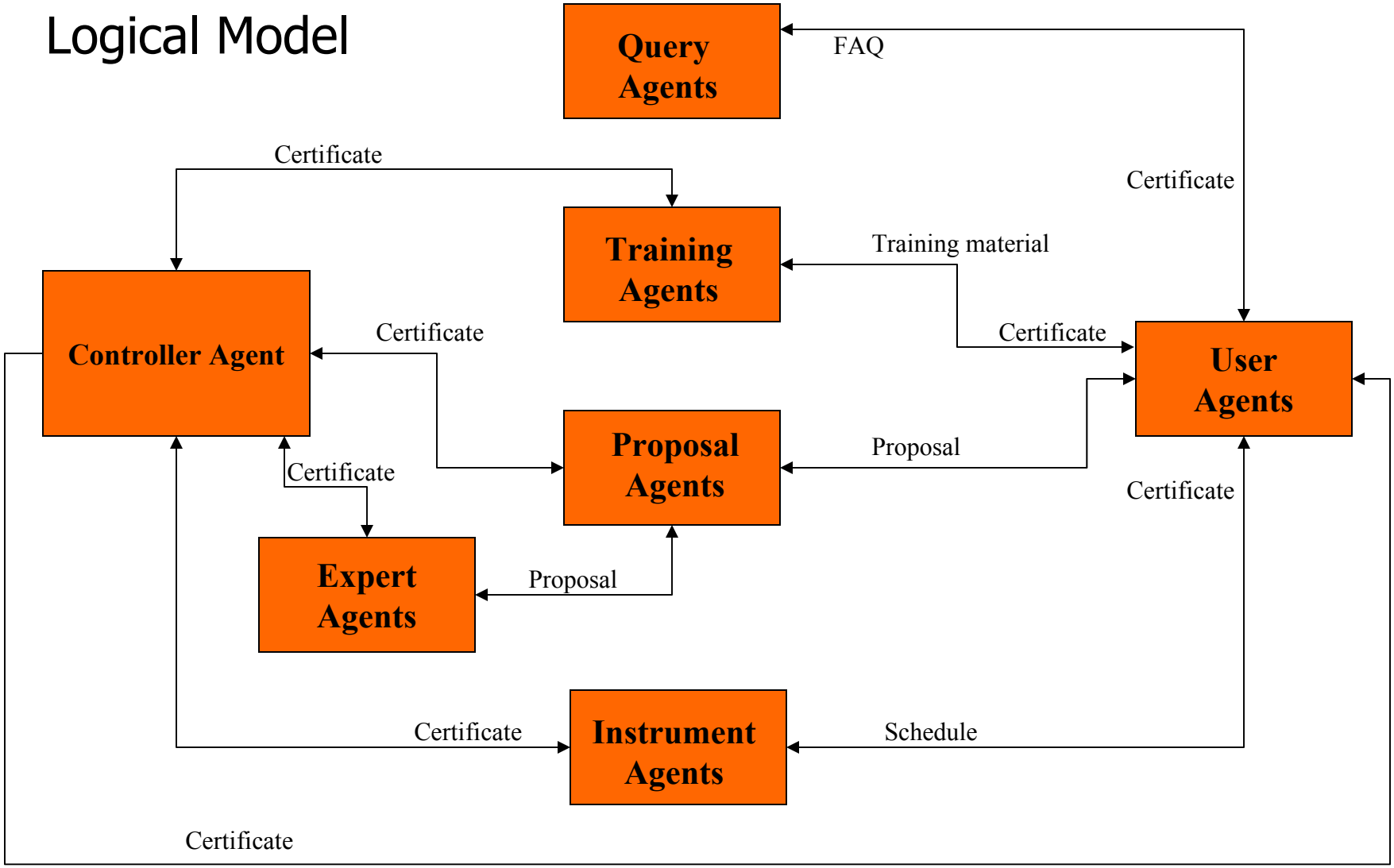
(a)



(b)

UA: User Agent, EA: Expert Agent, SA: Scheduling Agent, FA: Facilitator Agent, IA: Instrument Agent and ExA: Experiment Agent

Logical Model



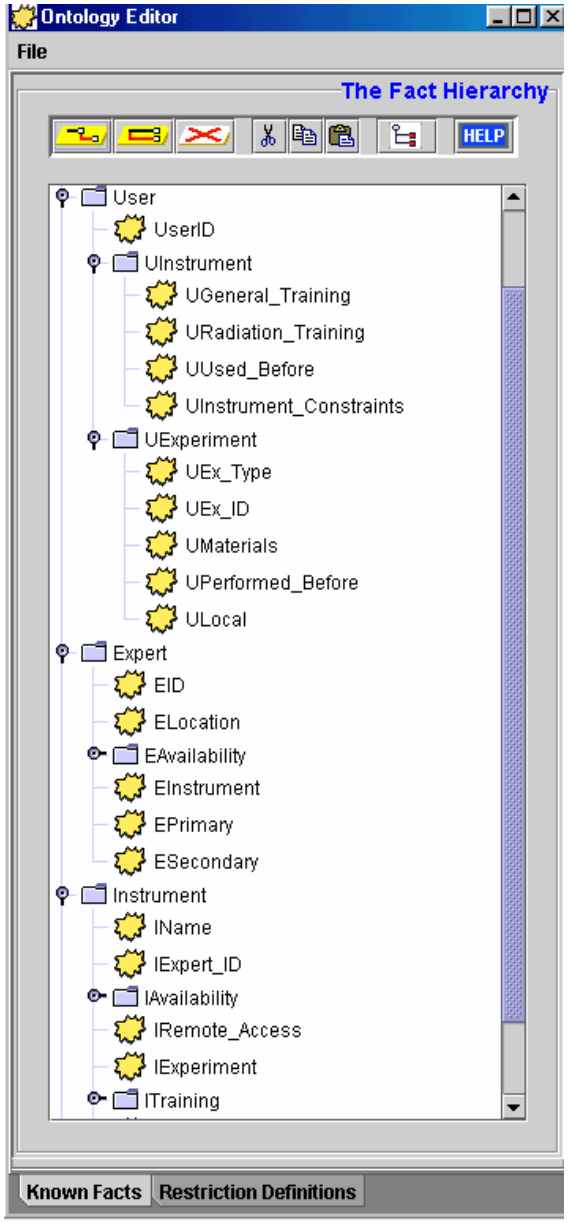
Design

- Five agents for user support
  - Controller, Query, Training, Proposal Agents
  - Additional agent that manages access to DeepView
- Resource agents
  - Instrument, Expert Agents
- Agent roles and responsibilities
  - Key role for the Controller Agent
  - Use of certificates under evaluation
- Technologies
  - FIPA Agent Communication Language
  - XML-tagged data for databases queries

Prototype and ontology

(Implemented using Zeus Agent Kit (from BT Labs))

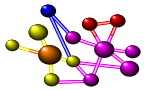
- Some facts in the ontology



- Agents roles in the prototype

An Expert Agent (EA)
authorizes users to access other agents

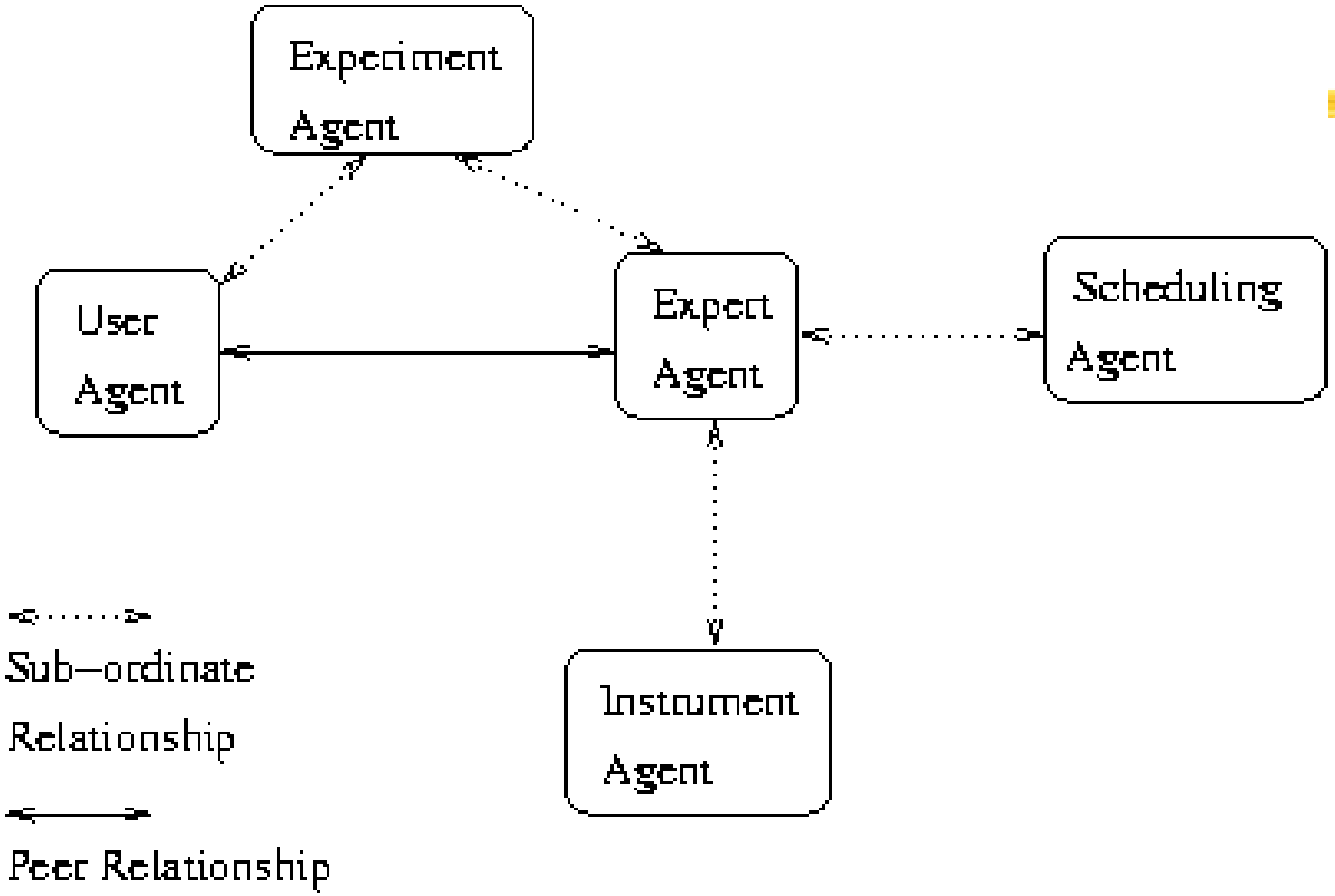
A User Agent (UA)
represent individual users



An Experiment Agent (ExA)
distributes proposals to experts

A Scheduling Agent (SA)
administers remote tutorials

An Instrument Agent (IA)
schedule users on individual instruments


Experiment Agent
User Agent
Expert Agent
Scheduling Agent
Instrument Agent
Sub–ordinate Relationship
Peer Relationship

- Experiment
  - Start Time
  - End Time
  - Start Date
  - End Date
  - Material
    - Type
    - Safety
    - Preparation
  - Requestor
    - Previously Requested
    - UserID
  - Instrument Type
  - Approved
  - Properties
    - Temperature
    - Environment
  - Impact
    - Industry
    - Academic

- Expert
  - ID
  - Location
  - Availability
    - Start Date
    - End Date
    - Start Time
    - End Time
  - Instrument ID
  - Expertise
    - Primary
    - Secondary

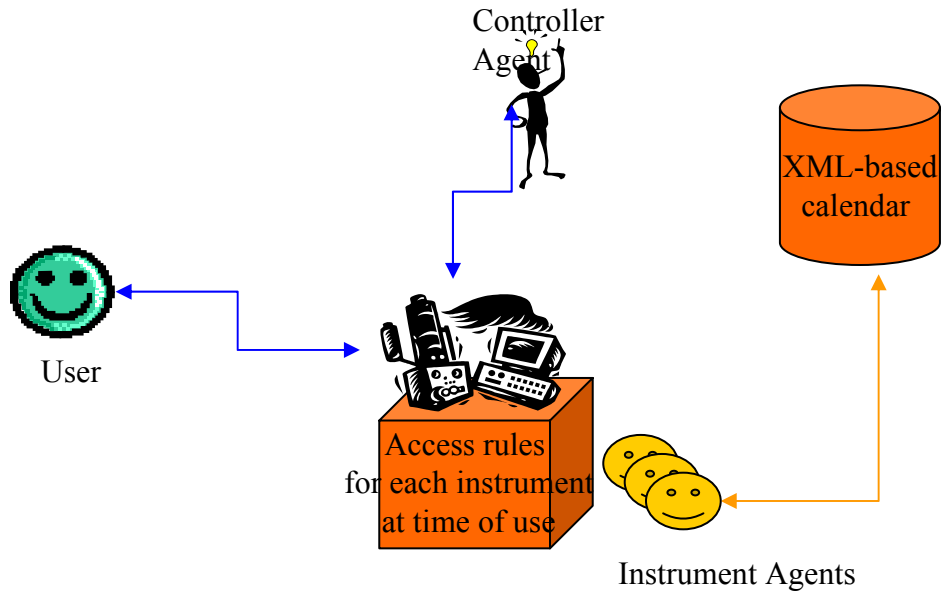
- Instrument
  - Name
  - Expert ID
  - Availability
    - Start Time
    - End Time
    - Start Date
    - End Date
  - Properties
    - Operating Temperature
    - Phase ID
  - Remote Access
  - Experiment ID
  - Training
    - Radiation Training
    - General Training
  - Location

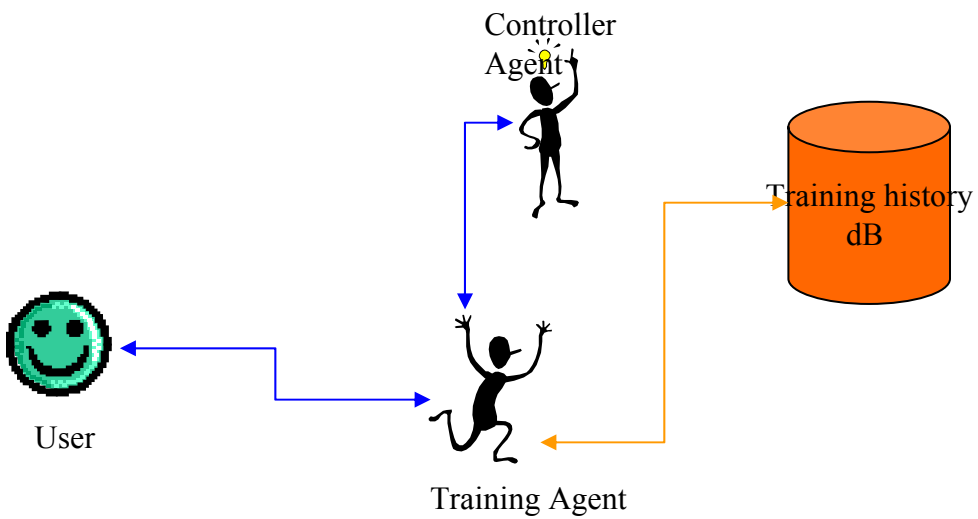
- User
  - Experiment
    - Type
    - ID
    - Materials
    - Performed Before
    - Local/Remote
  - Instrument
    - Trainingg
      - General
      - Radiation
    - Used before
    - Constraints
  - User ID

Interaction Models

- The Controller Agent allows other agents to perform tasks on users' behalf according to:
  - user profile -- affiliation, experience
  - training
  - paid fees
- The Training and Query Agents interact with XML-tagged web pages and databases
- A DeepView agent to enable interaction with the instrument – this is an extension of the user agent

Interaction Model for Scheduling
(right)



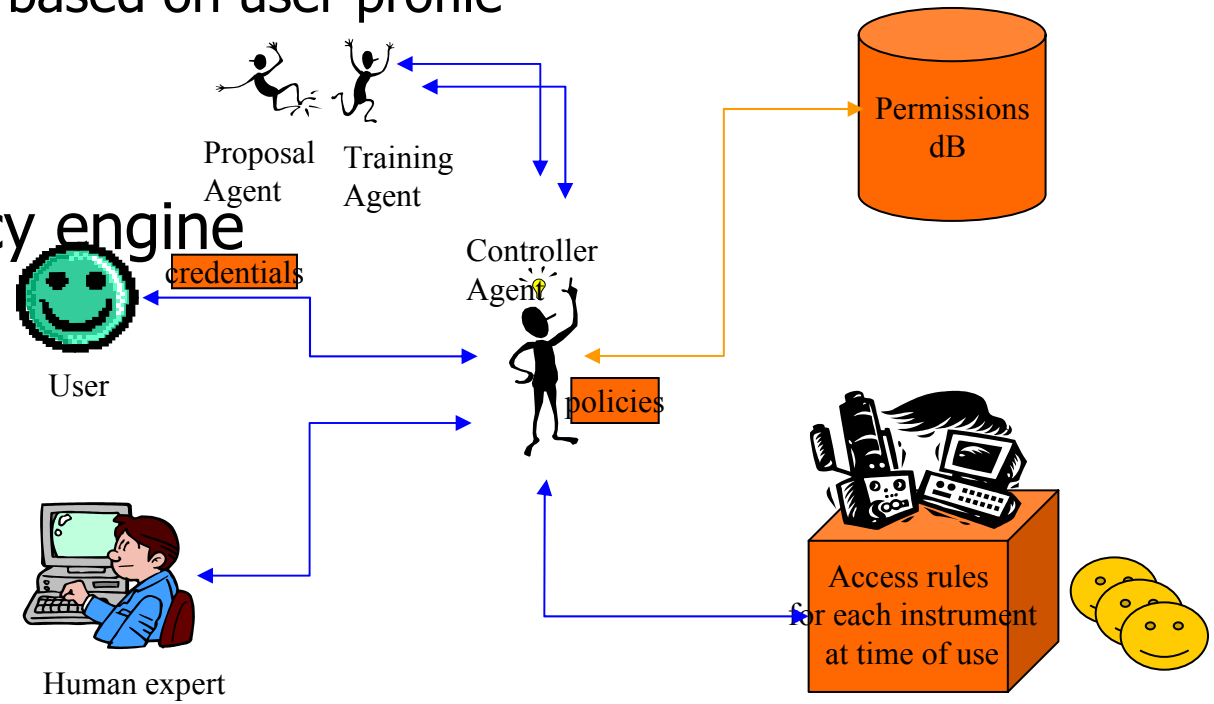


Interaction Model for Training Agent
(left)

The Controller Agent

- X 509.3 user identity certificates
  - user attributes — based on user profile
  - use conditions for instruments
- Requires a policy engine

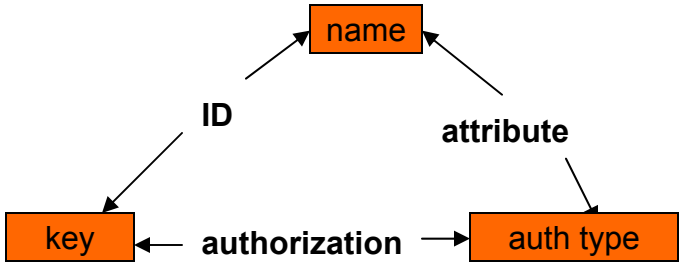
Interaction Model for the Controller Agent



Deep View agent

- *Conventional in site experiments require local operator to make routine adjustments – specimen orientation (tilt), position, illumination conditions, microscope focus, and occasionally magnification (based on video signal from imaging system)*
- Offer the same look-and-feel for remote users (subject to network delays)
  - Use of local automated corrections
  - Have control over: incident-beam illumination, objective lens focus, etc
  - Output from DeepView interface sent to User Agent

Certificate requirements



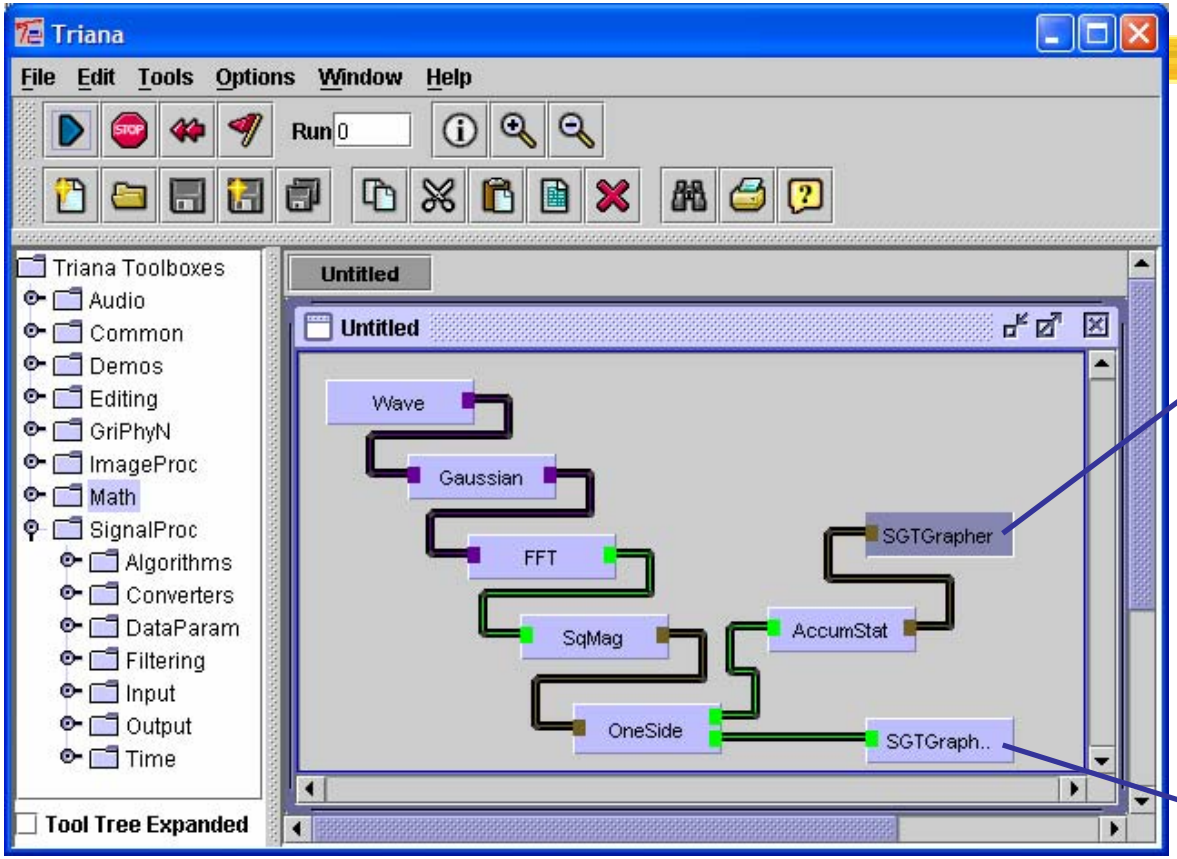
- Fast access to certificate servers
  - Certificates must be checked
- Policy engines must check authorization
- Reliability. If the servers are not up, the user is denied access

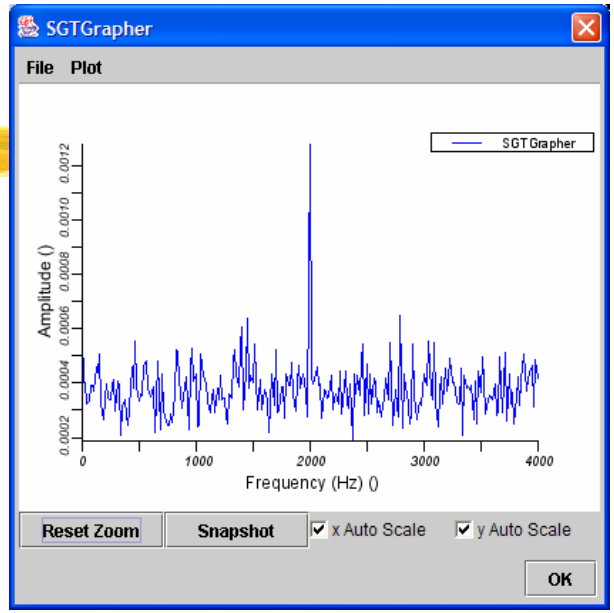
There can be a significant amount of overhead to set up a circuit for a short transaction

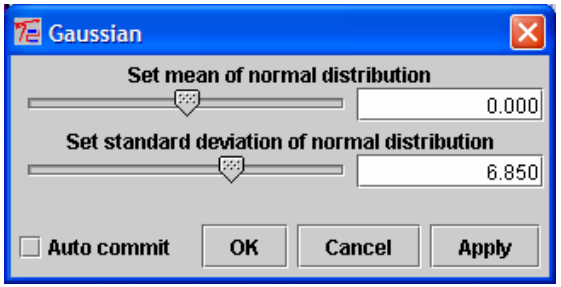
http://mmc.ciit.y12.doe.gov/jar/MMCCerts.html

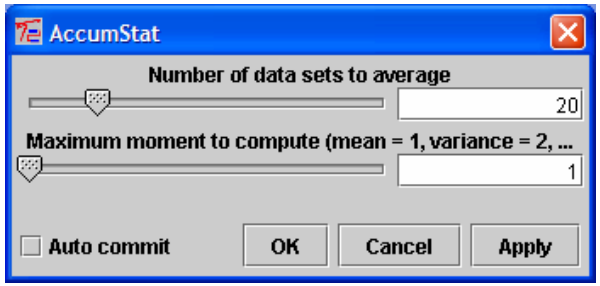
http://www.triana.co.uk/

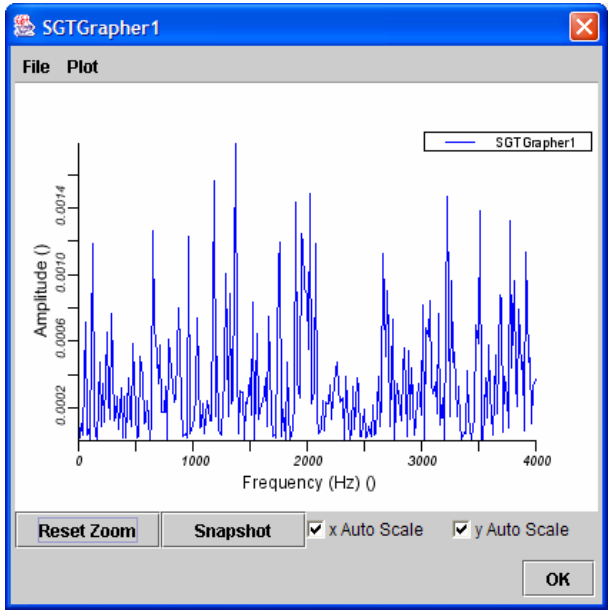
http://www.gridlab.org/





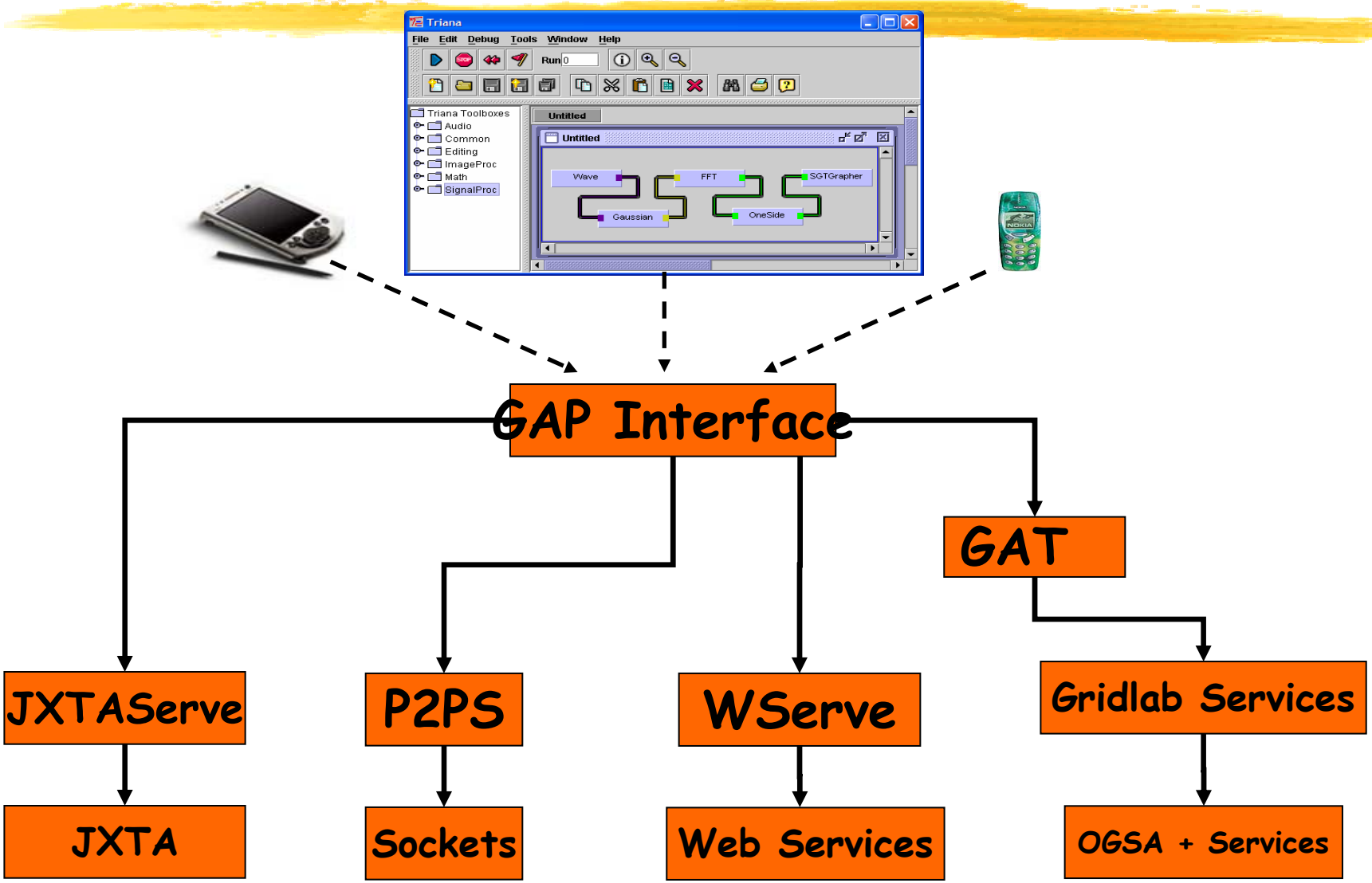






Current GAT Implementations

http://www.trianacode.org/



Summary

- A multi-agent system for supporting users in a scientific environment (real-world problem)
- Integration with the DeepView collaborative framework
- Can be applied to other collaboratories and collaborative problem-solving
  - May use some of this experience in e-HTPX project (led by Colin Nave at Daresbury Lab)
- Integrate intelligence in agents for helping scientists with domain problems (image recognition and feature extraction)
  - present alternative solutions
  - execute alternative solutions

Read more at:

- DeepView: A Channel for Distributed Microscopy and Informatics,
  B. Parvin, J. Taylor, G. Cong, M.A.O'Keefe, and M.H.Barcellos-Hoff, Proceedings of Supercomputing 99, Portland, US

- An Ontology for User Support in The Materials Microcharacterization Collaboratory
  Line Pouchard, Omer Rana and David Walker, Proceedings of Workshop: Ontologies in Agent Systems, at 5th ACM International Conference on Autonomous Agents, Montreal, Canada, 2001

Government Disclaimer

This research was supported in part by the Material Microcharacterization Collaboratory. Pouchard and Rome's work was supported in part by the U. S. Department of Energy, Office **of Science of the Oak Ridge National Laboratory, managed for the U. S. DOE by UT-Battelle, LLC, under contract No. DE-AC05-00OR22725. Accordingly, the U.S**. Government retains a non-exclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.