SHARING SIMULATION MODELS AND TOOLS WITHIN A COLLABORATIVE RESEARCH PROJECT

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ABSTRACT

Our research aims at developing and building a generic collaborative environment to support a research and development process, in which heterogeneous (in formalism and format) models are being shared, reused and executed on distributed heterogeneous tools via the Internet. In this paper we briefly describe the implementation of the environment in its current state and consider the functionality of our environment with respect to sharing simulation models and tools.

1. Introduction

Research and development in multidisciplinary collaborative projects is characterised by a number of particularities. The multidisciplinary teams are distributed geographically, they are free in their choice of research tools and their knowledge domains differ substantially. As the result, there exists significant variety of formats, in which the data and models are being developed by the collaborators. It also means that in order to perform any meaningful actions with such heterogeneous data formats, collaborators have to access the respective tools and have the expertise beyond their research domains to deal with technical idiosyncrasies of those tools.

Our research addresses the needs for a seamless integration of various simulation tools and seamless representation and manipulation of models in different formats and formalisms. The goal of our project is a generic collaborative "different place and different/same time" environment for sharing models and simulations. The environment is intended to support running web-accessible models on distributed heterogeneous tools, as well as piping and linking simulations and other applications according to user specifications, herewith tackling semantic differences in model formalisms and in interfaces between different simulations. The final generic system is to be adjusted to cover any concrete situation at hand (i.e., any concrete collaborative research project with its specific research tools).

In this paper we present the functionality of the current prototype with respect to sharing models and simulation tools. The paper is organised as follows. Section 2 briefly describes the architecture and the implementation of the environment. In section 3 we provide an overview of the functional abilities of the environment. Finally, section 4 concludes the paper with final remarks.

2. Architecture and Implementation

The proposed environment is based on a three-layer architecture: (i) front-end layer (high-level front-ends), (ii) middle layer (controller), and finally, (iii) back-end layer (distributed heterogeneous hardware and software resources). For more information we refer the reader to [1].

The front layer consists of a number of client-side *front-ends*. They provide users with a high level GUI to the system and enable them to operate in the environment (as is shown in section 3). Currently, this layer consists of agent-like software components: trader and mediator agents. Applied to our situation, the *trader agent* maintains a database with metadata on the available models and offers users a mechanism to search it. A *mediator agent* is positioned between (distributed) model sources (at remote hosts) and users. Tasks that are associated with mediation are, for instance, accessing, merging models from different locations and supporting abstraction, generalisation and representation of the underlying model.

The middle layer of the environment consists of one central persistent *controller* written in Python [2]. There are a few aspects characteristic to the controller. First of all, the core of the controller is a run-time system for a small process-interaction simulation language. The former is referred to as Process Oriented Kernel (POKer), and the latter as POKer language [3]. The language is used to model a resource-centric view on the tools in the environment. Each resource in the model represents a logical view on an actual scientific tool in the back-end. In order to configure a new

Element	Meta Name	Description
PUBLISHER	Project Name	An entity responsible for making the model available
TITLE	Model Title	A name given to the model
SUBJECT	Subject	The topic of the content of the model
DESCRIPTION	Description	Short description of the model
CREATOR	Author	The author primarily responsible for making the content of the model
CONTACT	Contact	E-mail address of the CREATOR or PUBLISHER
LINK	Project Homepage	Project Homepage
ACCESS	Access Methods	Access Methods
HOST	Host	Address of the remote machine hosting the model
FILE	Main File	Location of the main model file in the file system of the host
USES	Other Files	List of other files the model depends on
FILTER	Associated solver	ARV name for the solver associated with the model
FORMAT	Format	The physical or digital manifestation of the resource
ARVOUT	Output ARV Class	ARV class for the output produced by the model

Table 1: Elements required for registration

tool into the environment, one has to (1) create a new resource in the controller's model, and (2) configure the resource's parameters. The most important of the resource's parameters are the current capacity of the resource (it shows whether the resource can still serve more simultaneous clients) and the FIFO queue of delayed client's requests. Based on the capacity state of the resource in the model, the controller synchronizes user access to the respective object in the back-end. Only one client per moment can use the object associated with the resource. If necessary, blocking occurs. For more details on the controller, see [4].

The back-end layer consists of a number of applications distributed over the networks that are accessible via the Distributed Object Technology system to the controller (in the middle-layer). The Distributed Object Technology system, we have chosen for the time being is Pyro (PYthon Remote Objects) [5], which closely resembles Java's Remote Method Invocation [6]. Each scientific tool (e.g. the numerical package MatLab) on one of the servers is registered to Pyro Naming Service (NS) as server object. There is always a controlled number of application instances (per object registered to the NS) running for each tool registered to the controller. Though Pyro is rather basic when compared to such general systems as, for example, CORBA, it is small, simple to set up (especially if the rest of the system is being developed with Python), free and provides sufficient services, which makes Pyro an attractive alternative for fast prototyping of distributed systems.

3. Functional Overview

In this section we consider the abilities of the environment to support sharing models and simulations. In order to deal with heterogeneity of models and tools, the environment employs meta-concepts. Throughout this paper two types of metadata will be referenced: Metadata for Resource Discovery (MRD) and Abstract Resource View (ARV). The former is a manifestation of the model's attributes and is based on Dublin Core Metadata Element Set (DCMES) [7]; the latter is an encapsulation of low-level details pertaining to the execution of the model and its respective solver [8].

The functionalities provided by the environment can be divided into three major services:

Registration: whenever a user would like to share a model[1], he sends a registration message to the trader agent. The purpose of this message is to provide metadata for the model's MRD and ARV records, which will be used by the system in the other services. MRD elements (fields) in the message (see Table 1) are a subset of DCMES. Figure 1 shows the web page used for registration. A user needs either to provide the URL-address of the file with the registration message, or fill in the on-line form. As the result of the registration, the metadata about the model (but not the model itself) is stored as MRD and ARV records (see respectively Table 2 and Table 3) in the trader agent's database (it's a special database that stores only metadata about the models).

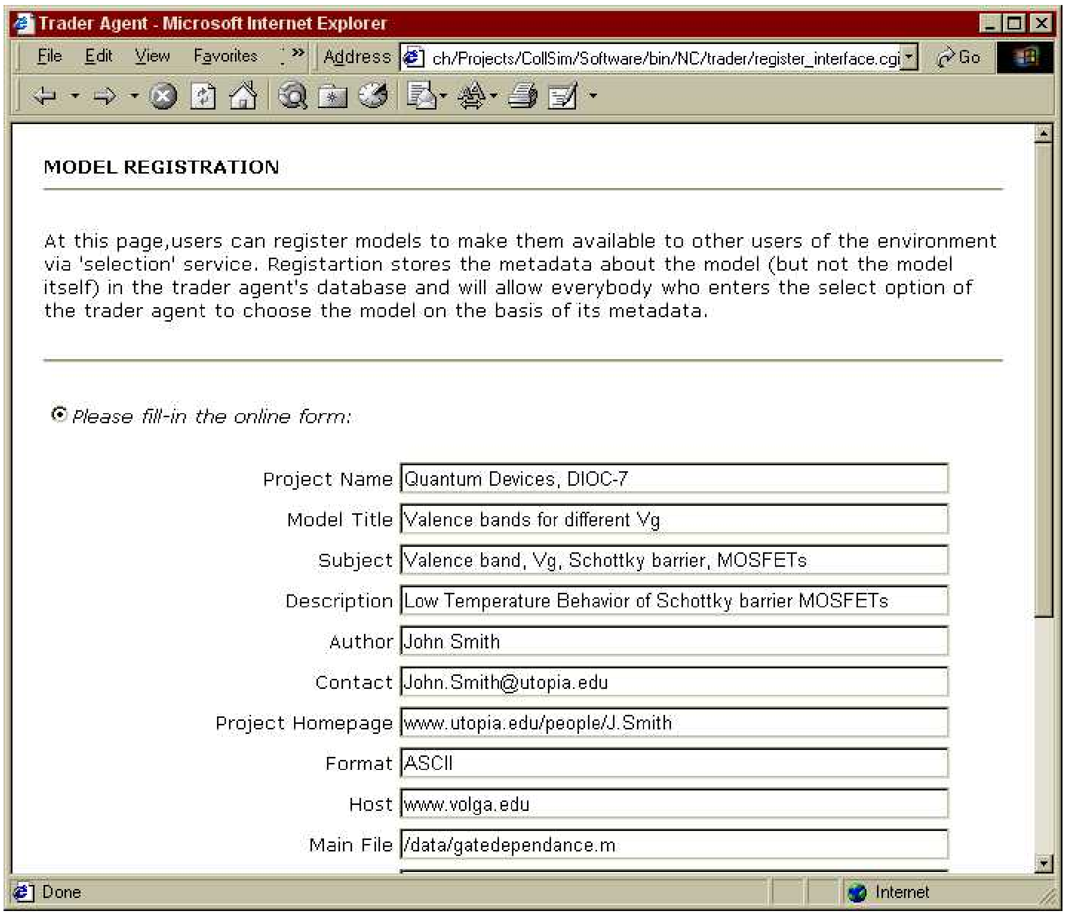
Element	Value
PUBLISHER	Quantum Devices, DIOC-7
TITLE	Low temperature Schottky barrier transistor
SUBJECT	Low Temperature Behavior of Schottky barrier MOSFETs
DESCRIPTION	Abstract
CREATOR	John Smith
CONTACT	John.Smith@utopia.edu
LINK	www.utopia.edu/people/J.Smith

Table 2: Metadata for Resource Discovery

Element	Value
ACCESS	HTTP
HOST	www.volga.edu
FILE	/data/gatedependance.m
USES	/data/sbtparameters.m /data/sbtsetup.m /data/calculatebc.m /data/simpsonint.m /data/poissonzerotemp.m
FILTER	MatLab
TYPE	Model # default
FORMAT	ASCII
FILEOUT	# to be provided for execution
ARVOUT	matlabMAT

Table 3: Metadata for Abstract Resource View

[1] We consider everything (i.e., models in various formalisms, data files in various formats, documents, etc.) as models.


Trader Agent - Microsoft Internet Explorer
File Edit View Favorites
Address ch/Projects/CollSim/Software/bin/NC/trader/register_interface.cgi
Go
Done
Internet

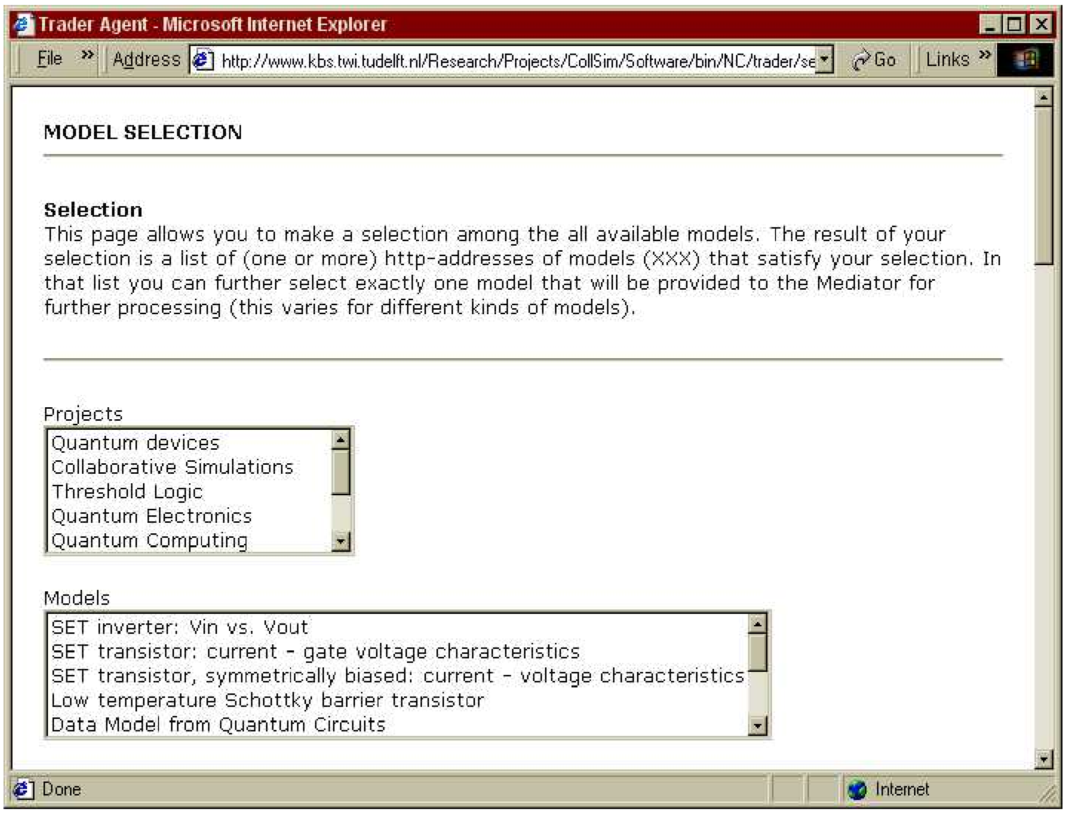
MODEL REGISTRATION

At this page,users can register models to make them available to other users of the environment via 'selection' service. Registartion stores the metadata about the model (but not the model itself) in the trader agent's database and will allow everybody who enters the select option of the trader agent to choose the model on the basis of its metadata.

[✓ *Please fill-in the online form:*]

Project Name	Quantum Devices, DIOC-7
Model Title	Valence bands for different Vg
Subject	Valence band, Vg, Schottky barrier, MOSFETs
Description	Low Temperature Behavior of Schottky barrier MOSFETs
Author	John Smith
Contact	John.Smith@utopia.edu
Project Homepage	www.utopia.edu/people/J.Smith
Format	ASCII
Host	www.volga.edu
Main File	/data/gatedependance.m

Figure 1: Model Registration page


Trader Agent - Microsoft Internet Explorer
File
Address http://www.kbs.twi.tudelft.nl/Research/Projects/CollSim/Software/bin/NC/trader/se
Go
Links
Done
Internet

MODEL SELECTION

Selection
This page allows you to make a selection among the all available models. The result of your selection is a list of (one or more) http-addresses of models (XXX) that satisfy your selection. In that list you can further select exactly one model that will be provided to the Mediator for further processing (this varies for different kinds of models).

Projects
- Quantum devices
- Collaborative Simulations
- Threshold Logic
- Quantum Electronics
- Quantum Computing

Models
- SET inverter: Vin vs. Vout
- SET transistor: current - gate voltage characteristics
- SET transistor, symmetrically biased: current - voltage characteristics
- Low temperature Schottky barrier transistor
- Data Model from Quantum Circuits

Figure 2: Model Selection page

Selection enables users to discover and deference any model registered in the collaborative projects by standard *search criteria*. This service relies on Resource Discovery Metadata and uses a search mechanism. To use this service, a user surfs to the 'selection' web page. There he can search all the available models by the values of their elements in the MRD record. Currently, the user is given a summary of all the existing (no duplication) values for each element. The meta-information about all the available models is presented on the page as pairs of keywords (corresponding to the elements in the record) and their values. The latter are presented as *'select boxes'* and the former as descriptions of the respective boxes. Figure 2 shows the 'selection' web page with selection boxes (only 'Projects' and 'Models' boxes fit into the screenshot). The user can specify the search criteria by selecting values from different 'boxes'. The result is the inclusive-OR of all the selected values. Submitting the values will return the list of models that fit into the search criteria at least by one keyword.

Processing service allows users to perform various meaningful actions with selected models. In doing so, it uses the ARV metadata from the selected models and a library of small scripts, called transformations that constitute the spectrum of actions available in this service. What can be done with a concrete model, depends on what actions (transformations) are associated with the model's ARV. There is always at least one transformation: 'open', which for all different types of models means execution on the associated solver. For example, 'open' on a MatLab model will execute it with MatLab. 'Opening' a 'flat' data file will open the software associated with it (e.g., Gnuplot) and process the data (e.g., according to the transformation, the data is converted into an image).

In order to illustrate the current environment's functionalities, we consider a number of example sessions to demonstrate what a user can perform within the environment. All the examples will start off from the model selection service. Subsection 3.1 shows how data models are handled in the environment. In subsection 3.2, we consider simulation of MatLab models, followed by a demonstration with a real model from Quantum Physics domain.

3.1 Manipulation on Data Model

The user selects '*Quantum Devices'* from the box with the list of projects, and clicks the "Submit" button to request the trader agent to return a list of the available models, that have '*Quantum Devices'* as value for keyword '*Project'* in their metadata.

After a user has selected the model he wants to examine, its ARV-record becomes the input for the mediator agent. Based on the value of the element '`FILTER`' of the model's ARV, the agent automatically associates a number of actions applicable to the selected model, The valid actions are listed on the action bar above the main frame. Typically, at least the following actions are available: 'Open' and 'Details'. The user clicks the 'Open' button to view the model.

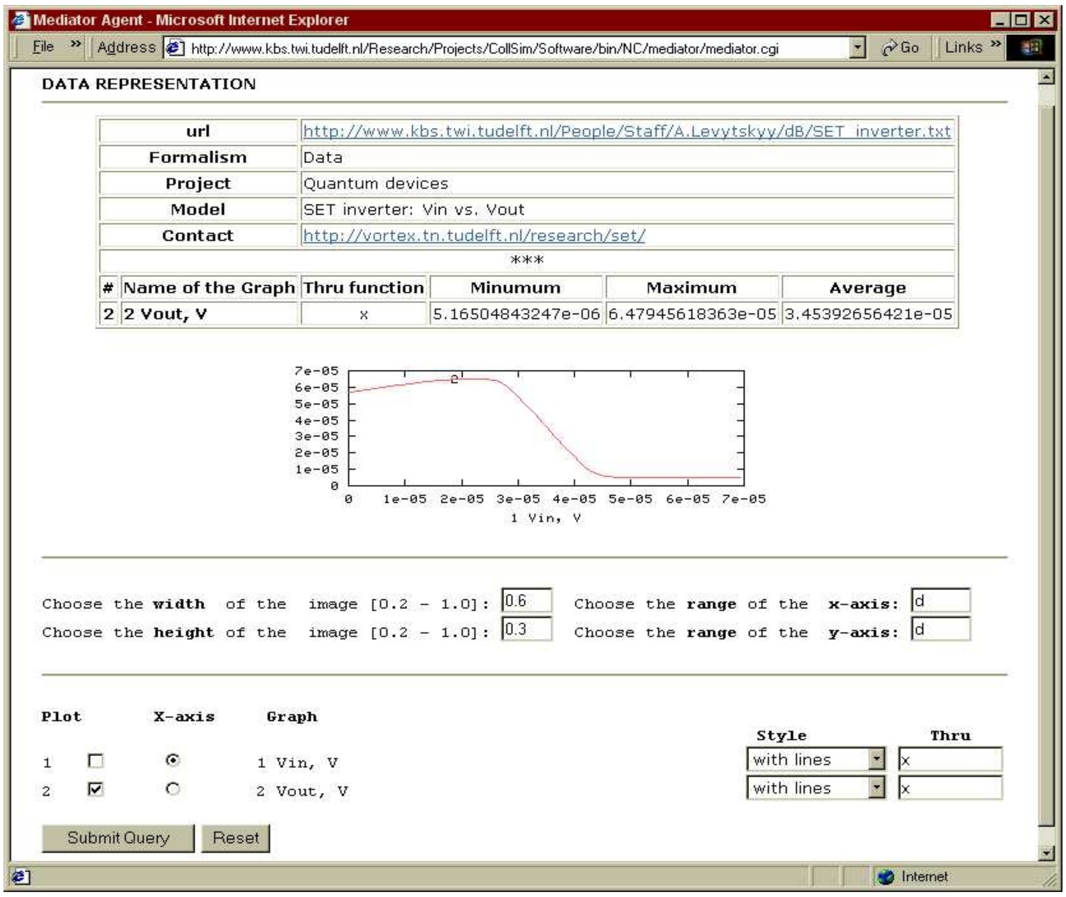
At this point, the mediator agent receives a command to execute the model. To do this, the agent uses the Abstract Resource View (ARV) of the model and respective 'open' transformation. In our case, the "open" transformation uses application *Gnuplot* (as it is indicated in the model's ARV by the element '`FILTER`') to create a graph of the model's data. The mediator agent retrieves the data model from its location and executes the transformation (at this point the controller synchronizes access to the actual tools). This transformation loads the model into Gnuplot and creates the graph with default parameters. The resulting picture is included into a web page that also provides a web-based interface to Gnuplot (see Figure 3). Besides the graphical representation itself, this page provides the user with meta-information on the data and statistics (the table above the image). Beneath the picture, a number of widgets are available to allow the user to customize the look of the graph according to his preferences. The user can:

- change the size of the graph;
- zoom-in/zoom out on a particular part of the graph;
- choose a data column for the x-axis;
- choose data columns to be plotted;
- pipe data of a column through a function, before plotting;
- customise graph styles for columns (solid line, dashed line, or impulses).

On the basis of the user preferences, the transformation script is updated and used by Gnuplot to redraw the graph. The mediator agent includes this updated graph into the HTML document, which is returned to the user. For example, the user may alter the range ([2e-05 : 5e-05]), select impulse in place of line chart, etc. Pressing the "Submit" button returns a new web page with user preferences being applied to the graphical representation for the same data model.

3.2 Manipulation on MatLab model

The user selects '*MatLab'* in *'Solvers'* box. As the result, user gets a number of models enlisted on the new web page. Now the user can either go back to change the search criteria, or make a final selection and confirm it by pressing "Submit". If the latter happens, the user can select an action on the model. For instance, the user clicks "open" the model. The agent extracts the value of element '`FILTER`' and de-references the target file. It can be the application itself, or the associated ARV. In case of MatLab, it is an ARV for a script (a custom MatLab wrapper) that knows the location of MatLab, how to invoke and interact with it. The next step is to de-reference '`FILE`' and '`USES`'. After this everything is ready to 'open' the file transparently for user. The model is downloaded from a remote location and transferred into the temporary directory on the machine where MatLab is installed. Then the MatLab wrapper is executed and locates the MatLab via the Pyro NS, and interactively executes transformation commands. In the following we demonstrate an execution of example MatLab model from Quantum Physics Domain.


Mediator Agent - Microsoft Internet Explorer
File
Address
http://www.kbs.twi.tudelft.nl/Research/Projects/CollSim/Software/bin/NC/mediator/mediator.cgi
Go
Links
7e-05
6e-05
5e-05
4e-05
3e-05
2e-05
1e-05
0
1e-05
2e-05
3e-05
4e-05
5e-05
6e-05
7e-05
1 Vin, V
2
Internet

DATA REPRESENTATION

url	http://www.kbs.twi.tudelft.nl/People/Staff/A.Levytskyy/dB/SET_inverter.txt
Formalism	Data
Project	Quantum devices
Model	SET inverter: Vin vs. Vout
Contact	http://vortex.tn.tudelft.nl/research/set/

***

#	Name of the Graph	Thru function	Minumum	Maximum	Average
2	2 Vout, V	x	5.16504843247e-06	6.47945618363e-05	3.45392656421e-05

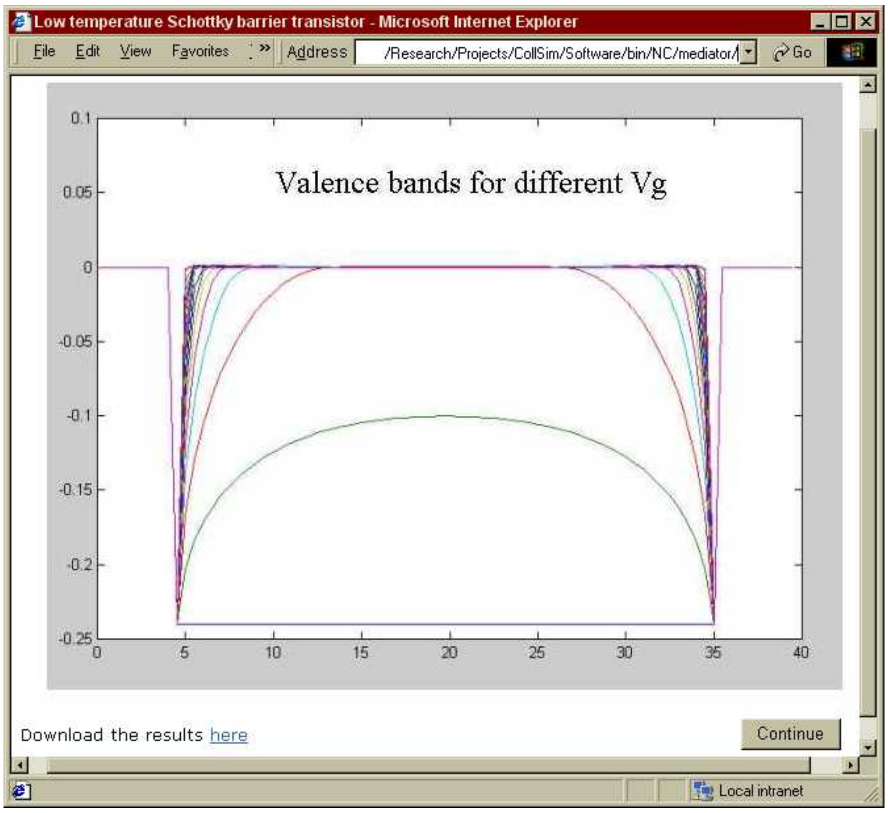
Choose the **width** of the image [0.2 - 1.0]: 0.6 Choose the **range** of the **x-axis**: d

Choose the **height** of the image [0.2 - 1.0]: 0.3 Choose the **range** of the **y-axis**: d

Plot		X-axis	Graph	Style	Thru
1	☐	⦿	1 Vin, V	with lines	x
2	☑	○	2 Vout, V	with lines	x

Submit Query Reset

Figure 3: Display of a data model


Low temperature Schottky barrier transistor - Microsoft Internet Explorer
File
Edit
View
Favorites
Address
/Research/Projects/CollSim/Software/bin/NC/mediator/
Go
Valence bands for different Vg
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.25
0
5
10
15
20
25
30
35
40
Continue
Local intranet

Download the results here

Figure 4: Result of MatLab simulation

Example Application in Quantum Physics

Let us assume that the user selects a model with a title '*Low temperature Schottky barrier transistor'* and by clicking "Submit", starts up the Mediator agent. This agent automatically associates a number of actions applicable to the selected model. The valid actions are listed on the action bar above the main frame. Typically, at least the following actions are available: 'Open' and 'Details'. Next, the user clicks the 'Details' button to get a web page that provides the summary about the chosen model. After familiarizing him with the descriptions of the model (see Table 2), the user clicks on 'Open' button to simulate the model.

At this point, the mediator agent receives a command to execute the model. To do this, the agent uses the Abstract Resource View (ARV) of the model and a transformation. The former encapsulates the details about heterogeneous models and their solvers (see Table 3). The latter is a high-level function that implements an action on the model. In our case the transformation is to "open" a model with the application MatLab (as it is indicated in the model's ARV by the element 'FILTER'), and reads as follows (see Example 1). Argument 'FILE' is the main model file and 'FILEOUT' is a temporary filename for the output (for the purpose of demonstration let's name it "output.mat")

```
openMatlab (FILE, FILEOUT, path='c:\ml\temp'):
{
   SOFTWARE: MatLab
   Begin
     clear
     addpath path
     FILE
     save FILEOUT
   End
}
```

Example 1: "Open" Transformation

The next step is to de-reference the application MatLab itself. Element 'SOFTWARE' of the transformation points to name "MatLab". First of all, the agent assumes that it is the name of the ARV for that application and attempts to look for it in the ARV library. If this fails, an assumption is made that "MatLab" is a program. In our case the search returns an ARV (see Table 4).

Element	Value
NAME	MatLab
ACCESS	HTTP
HOST	www.dnepr.edu
FILE	/bin/tools/ml.cgi
TYPE	Tool

Table 4: An Example of "MatLab" ARV

From this ARV the location of MatLab (actually it is a script that creates a MatLab client object) is extracted, started up and the related input files ("sbtparameters.m", "sbtsetup.m", "calculatebc.m", "simpsonint.m", "poissonzerotemp.m" and "gatedependance.m" as is indicated in the model ARV - see Table 3) are passed to it. The wrapper carries out the following tasks: (1) it finds the MatLab server object (via the NS) and creates a client proxy object for it, (2) it makes the model files accessible to MatLab, and (3) it executes MatLab commands in a generic way on the proxy object. The commands are defined in the transformation body (between the 'begin' and 'end'). In this way, it becomes very easy to create many transformations for MatLab and MatLab models that are based on the same wrapper, but perform different actions: simulation, data processing, visualization, etc.

As the result, application MatLab in accordance to the transformation: (1) clears the workspace and sets up the working directory to that where the files are copied, (2) loads and executes script "gatedependance.m" (value of 'FILE'), which also loads up the rest of the scripts; and (3) saves the resulting workspace into file "output.mat" ('FILEOUT').

Next, the wrapper transfers the output file to the web server and associates an instance of *matlabMAT* ARV with it (as it is indicated in the ARV of the model). *matlabMAT* is an ARV class for MatLab matrixes. This instance is initialized with the new location of the output filename "output.mat". Such 'post-processing' allows the system to interpret the newly created file correctly and associate a number of useful transformations with it ('actions' in the terms of the user interface), for example: *displayMAT* and *registerMAT*. The first transformation allows the data model to be presented graphically; the other assists the user to register the data model to the trader agent's database.

Let us continue our session with the visualisation of the output data. In this case, "Display" action is selected by the user, which executes the *displayMAT* transformation on the output model's ARV. The latter is similar to that in Table 3 (notice that 'FILE' is now "output.mat"); and the former is given in Example 2.

```
displayMAT (FILE, FILEOUT, result,
            path ='c:\ml\temp'):
{
   SOFTWARE: MatLab
   Begin
      clear
      addpath path
      load    FILE
      surf    (result)
      print   -djpeg -f1 -r100 FILEOUT
   End
}
```

Example 2: "Display" Transformation

Within this concept, the same MatLab wrapper (de-referenced via the 'SOFTWARE' element of the transformation) is invoked and interactively manipulates the MatLab server according to the body of the transformation. As the result, MatLab (application) receives commands to (1) load a matrix from the input MAT-file ("output.mat"), (2) visualise it as a graph using 'surf' function, and (3) print the graph into an output file ('FILEOUT'). Finally, the output file is transferred to the web server temporary directory and is inserted into the data representation page (see Figure 4). This page also allows users to download (save to a local machine) the model in question.

After seeing the graphical representation, the user continues with registration of "`output.mat`" into the database. She or he surfs back to the original data model (from which the graph has been created) by clicking the "Back" button of the web-browser and selects "Register" from the list of available actions associated with the model (that is "Display" and "Register"). This action automatically executes the *registerMAT* transformation with the ARV instance for "`output.mat`".

The *registerMAT* transformation passes the metadata from the ARV as CGI variables to the CGI script that implements the user interface for the registration process. The user is provided with a CGI-form, which fields cover all the metadata elements needed for the Resource Discovery Metadata and the Abstract Resource View (see Figure 1). As the matter of fact, all the fields related to the ARV come already with filled-in values (extracted from the temporary ARV that was automatically created with "`output.mat`"). The user can add to and edit the content of the form to his likening. To finish the registration, the user clicks 'submit' button, which sends all the registration information to the executable, which implements the registration function of the trader agent. If the supplied information is valid, the registration is complete and the data model becomes available to the other users in the environment.

4. Final Remarks

Our research aims at developing and building a generic collaborative environment to support research and development process, in which heterogeneous (in formalism and format) models are being shared, reused and executed on heterogeneous distributed tools via the Internet. In this paper we have demonstrated how users can transparently share and execute models regardless of their locations and types, and have outlined the environment's implementation in the current state. Future work will concern further development of the used meta-concepts in order to accommodate more complex simulation scenarios and extending the functionality of the environment with a modelling service. On the implementation side, we plan to move from Pyro as the platform for distributed calculations to CORBA or HLA [9]. In particular the latter is very promising due to its inherent services with support for distributed simulation.

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