M.A. Guravage — CWI

RepoSE

An On-Line Repository for Simulation Experiment Descriptions

Maastricht — 21 May 2012

PROBLEMS THAT PLAGUE MODELS

- Same Simulation - Different Results

- Lost Customizations

- Incorrect Initial Values

- Overlooked Procedures

- Broken Functionality

REPRODUCIBLE RESULTS REQUIRE

- Name and version of all the constituent parts

- Detailed description of any changes

- The exact input parameters

- The procedures followed to run the experiment

- List of external dependencies

SPECIFY MINIMUM REQUIREMENTS

- Minimum Information Requested In the Annotation of Biochemical Models (MIRIAM)

- Minimum Information About a Simulation Experiment (MIASE)

- Simulation Experiment Description Markup Language (SED-ML)

RepoSE is the realization of the entire SED-ML schema within a content management system named Plone. Each instantiable UML class in the SED-ML schema becomes a content type.
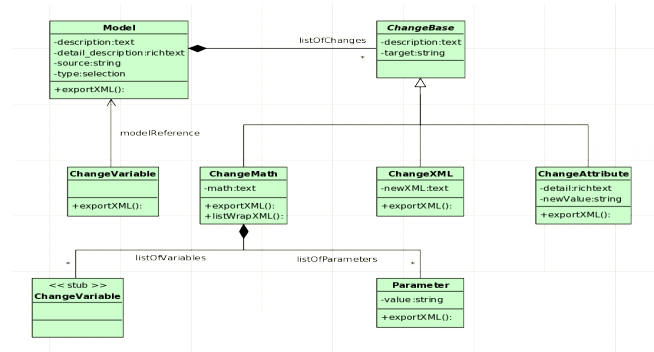
What is RepoSE's goal

- Make SEDs more understandable by pairing SED-ML's formal precision with prose descriptions

- Make SEDs more accessible by giving modelers control over who can see, append to or edit their SEDs

- Make SEDs more reliable by facilitating curation

- Organize SEDs by the judicial application of generic and domain meta-information
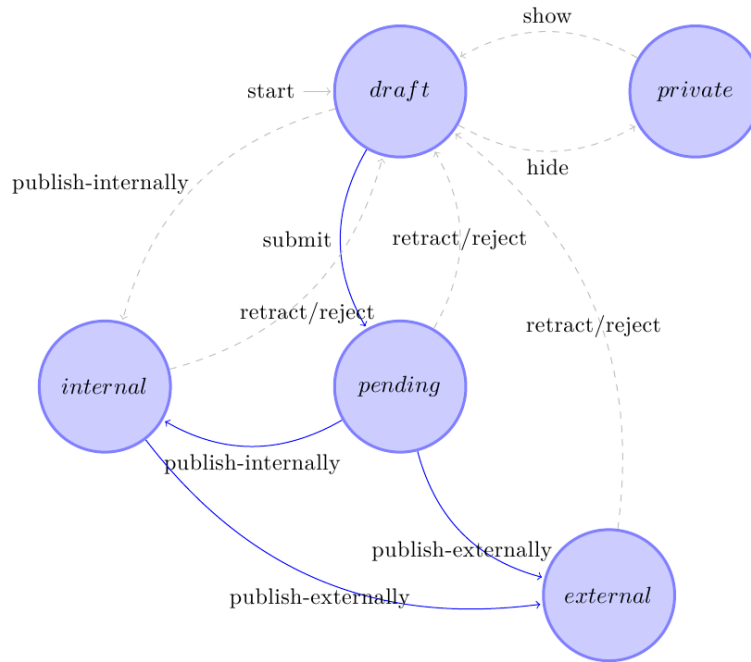
What is a content type

- UI components to create, edit and view data

- Machinery that implements the relationships and cardinality of the UML model

- Machinery that reads and writes data from and to the database

- Machinery that complies with Plone's security and workflow systems

Workflows

Workflows control access and guide curation.

XML based SEDs

- RepoSE exports SED-ML compliant simulation experiment descriptions

- SEDs using, e.g., SBML can be exported and run directly

General Purpose SEDs

- We wanted to investigate whether SED-ML could be used as a way to organize simulation experiments written in general-purpose languages. To date we have several SEDs that describe how to build simulation models of developing plant organs using VirtualLeaf.

- Our experience is that models and simulations implemented in code can be of a very different nature where SED-ML concepts do not apply.

The Future

- Improve the User Interface

- Import existing SED-ML files

- Keep pace with SED-ML development

- Use libSedML to validate and export SED-ML

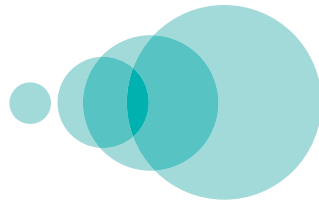- Make general purpose SEDs run autonomously

TRY IT YOURSELF

- You'll find the repository at: http://sed.project.cwi.nl

- Click on the repository tab

- Choose the SED named O2C2

- Click on the `Export This' link at the bottom right of the page

- Upload and run the SED on the SED-ML Web Tools site.

ACKNOWLEDGEMENTS

Thank You

Questions?