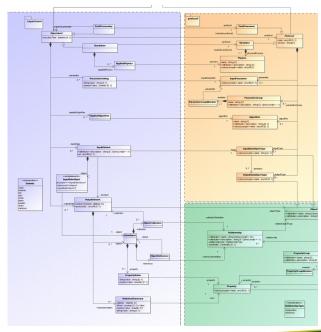


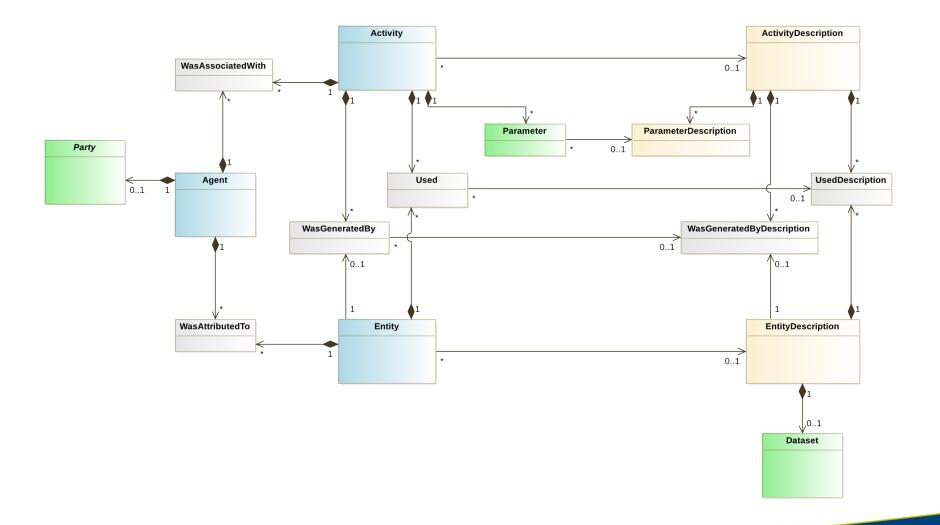
SimDM and ProvenanceDM Asterics Technology Forum, 22-23. March 2017 Provenance Discussions Kristin Riebe

Simulation Data Model (SimDM)

- Data model for structuring metadata for simulations
- Contains some provenance aspects
- See also talk by David Languignon in Dec. 2016
- Extract from SimDM class diagram:



ProvencenDM - overview



Links between SimDM and ProvenanceDM

• also see latest Provenance Working Draft for some examples

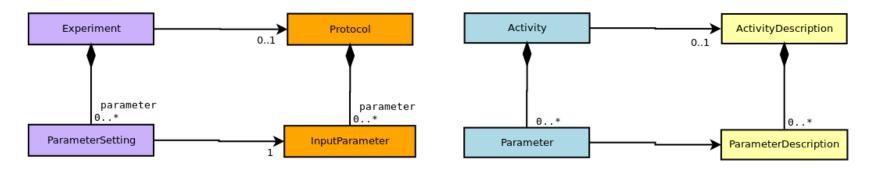
(Table 12):

Simulation DM	Provenance DM	Comment
Experiment	Activity	
Experiment.name	Activity.label	human readable name; name attribute in SimDM is inherited from Resource-class
Experiment.executionTime	Activity.endTime	end time of the execution of an experiment/activity
Experiment.protocol	$Activity.description_ref$	reference to the protocol or description class
Protocol	ActivityDescription	
Protocol.name	ActivityDescription.label	human readable name
Protocol.referenceURL	ActivityDescrip- tion.doculink	reference to a webpage de- scribing it
ParameterSetting	Parameter	value of an (input) parameter $% \left({{\left({{{{\bf{n}}_{{\rm{m}}}}} \right)}_{{\rm{m}}}}} \right)$
InputParameter	ParameterDescription	description of an (input) parameter
Party	Agent	responsible person or or- ganization
Party.name	Agent.label	name of the agent
Contact	WasAssociatedWith	
Contact.role	WasAssociatedWith.role	role which the agent/- party had for a cer- tain experiment (activ- ity); SimDM roles con- tain: owner, creator, publisher, contributor
Contact.party	Was Associated With.agent	reference to the agent/- party

Experiment and Activity

SimDM

ProvenanceDM



- Experiment, Protocol \rightarrow Activity, ActivityDescription
- ParameterSetting, InputParameter \rightarrow Parameter, ParameterDescription
- SimDM offers additionally:
 - (Applied)Algorithm, (Applied)Physics
 - \rightarrow used for characterising the datasets/experiments
 - \rightarrow not expressed in ProvenanceDM
 - \rightarrow could be included as parameters

Experiment and Activity

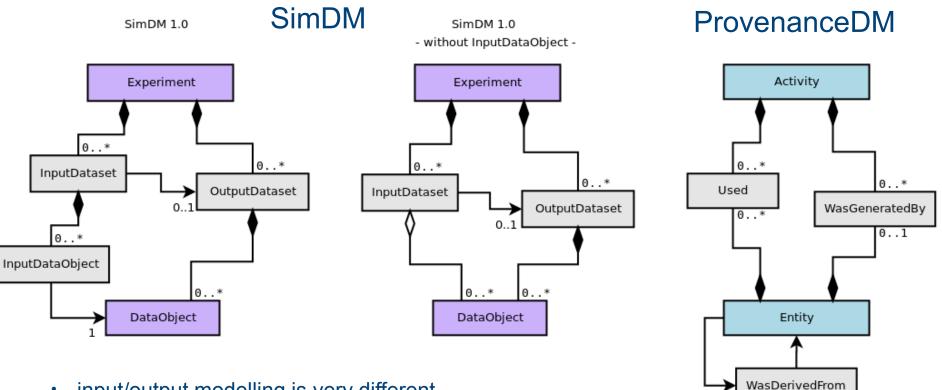
- Attributes:
 - Experiment.name → Activity.label
 Protocol.name → ActivityDescription.label
 - in SimDM a label is a SKOS concept (e.g. Experiment.label)
 → useful for Provenance as well?
 - Experiment.executionTime \rightarrow Activity.endTime
 - Experiment, Activity etc. are *Resources* → inherited attributes:

name, description, created, updated datetime, status

Parameters and Protocols

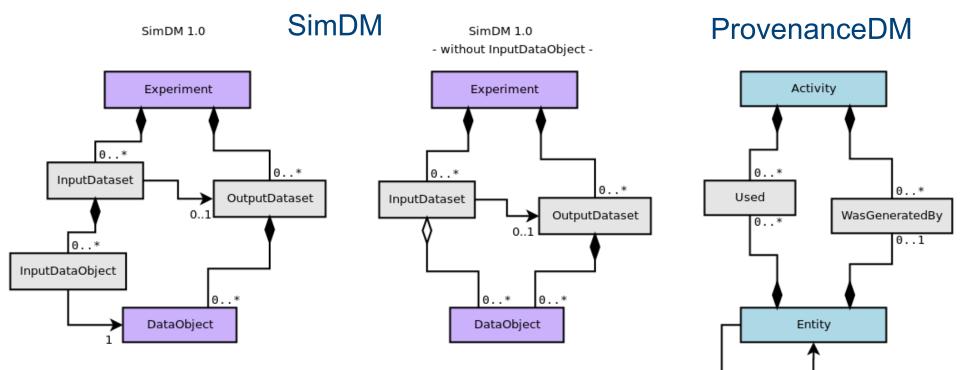
- very similar in SimDM and ProvenanceDM
- in SimDM: InputParameter inherits properties from abstract class "Field"; SKOS label as UCD
- ParameterValue can be int, char, float etc. => not known beforehand
- SimDM: define different protocol for each code (and code version; especially if there are different parameters for each code)
 - e.g. different simulation codes may require different parameters
 - each parameter is attached to exactly 1 protocol (even if the same meaning, e.g. boxsize)
- Protocol.type can be used to group all simulation codes of the same kind, (should use vocabulary list for this)

Datasets



- input/output modelling is very different
- DataObjects are physical objects with properties (e.g. halos from halo catalog, particles from a simulation snapshot)
- in Provenance: entity can be file, database table etc., physical content not so important

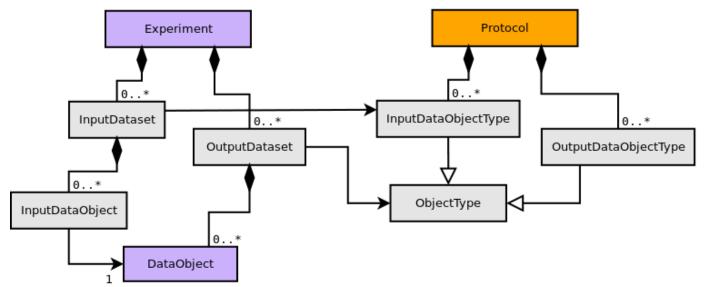
Datasets



WasDerivedFrom

- used.role is hidden in InputDataset.description
- no role for wasGeneratedBy in SimDM

DataObject and -Type



- each InputDataset has an InputDataObjectType (which is linked to Protocol)
- OutputDataset points to ObjectType, can be Target or OutputDataObjectType
- SimDM offers Property and PropertyValue classes
 - · similar to parameters, but for datasets, not experiments

Party, Contact and Agent

- SimDM/Party -> ProvenanceDM/Agent
- SimDM/Contact is used for relations between:
 - Party -> Experiment
 - = wasAssociantedWith in ProvenanceDM
 - Party -> Protocol
 - = people responsible for a code (version),
 - not (yet) included in ProvenanceDM

SimDM implementation

- Expanded django web application with prov_simdm app, see https://github.com/kristinriebe/provenance-cosmosim/
- Many parts of SimDM implemented for CosmoSim metadata, (cosmological simulations with post-processing steps)
- Enable querying by SimDM metadata (search form)

- Provenance endpoints (entities, activities) using SimDM metadata
- a few SimDAL endpoints (datasets, protocols) implemented as well, returning simple VOTABLE

Provenance from SimDM

- Provenance from SimDM
 - export provenance information from SimDM implementation
 - need mapping of classes, attributes
 - make provenance-related classes and attributes required?

- Which "endpoints" etc. should a provenance service provide?
 - Full "workflow" information, also in Prov-N or similar, for using tools from W3C/Southampton suite
 - Search for version, dataset history, but also: derived data

Open for discussions