



Metadata in Problem Solving Environment for Stereology Based Modeling

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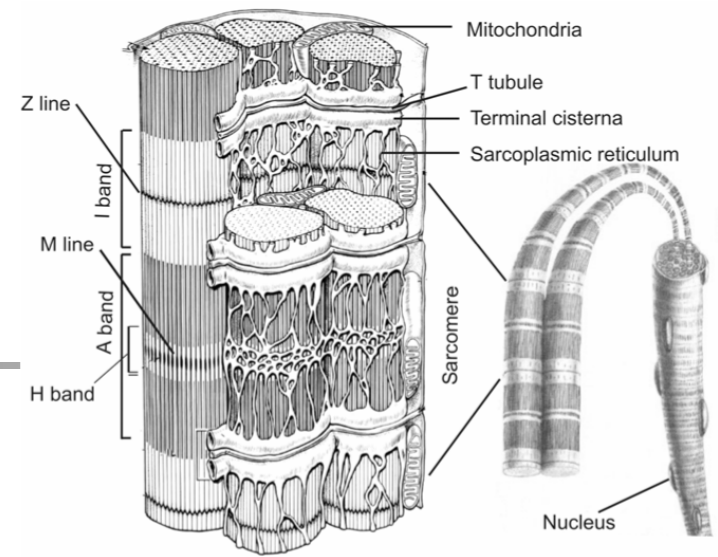
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(3) Institute of Molecular Physiology and Genetics, Slovak Academy of Sciences, Slovakia

(4) Austrian Academy of Sciences, Austria

Main goal

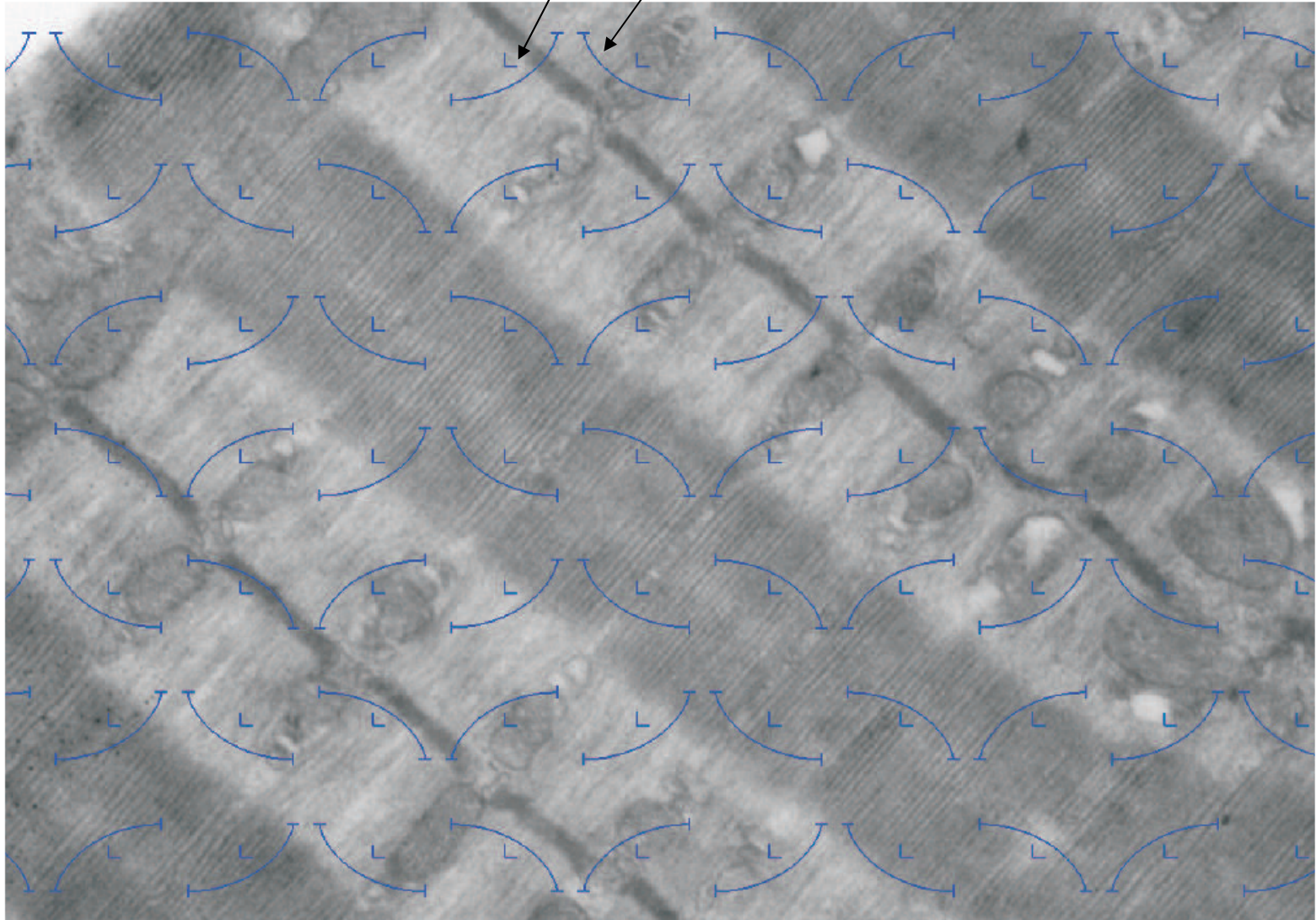
- To create environment that would enable users to
 - **Create** muscle cell models by means of a specialized model description language
 - **Verify** these models according to volume and surface densities (VSDs) of basic cell components - organelles
 - **Visualize** these models



Measurement of VSDs

on real cells

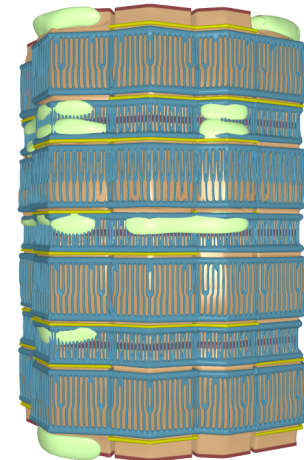
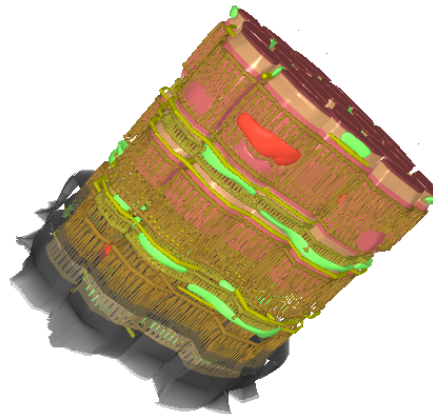
L-type points – Volume density
Cycliods – Surface density





Reverse modeling

- In order to use muscle cell models for testing and simulations, they should meet the requirements for VSDs established by measurements of electron microscopic images of real cells



Measurement of VSDs in silico



- VSDs require to compute the volume and surface integrals (areas) of all organelles
 - Computationally intensive process
 - Computation of single model can take up to hours
- In an iterative process, computations of tens of models are performed
 - Models can be computed individually
 - Grid offers suitable environment



Grid requirement summary

- Computation of intensive parametric studies
 - VSDs computation
- Heterogeneous platform support
 - Windows-Linux platform
- Retrieval of existing results
 - Retrieve the required computed VSDs and models for further use
 - Metadata catalog service (MCS)



Grid requirement summary

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Metadata Intro

- Data about data
- Metadata types:
 - Technical (file level, security)
 - Application specific
- Discovery and retrieval of existing data
- Scientific Metadata Generation
 - Manual annotation
 - Automatic generation

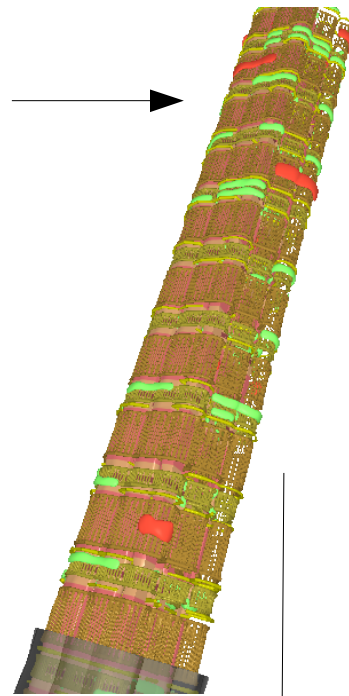


Motivation for metadata utilization

- Representation of a large amount of cell data
 - Many results are generated, which requires a suitable representation model
- Retrieval of existing cell models and VSDs
 - Quick retrieval of demanded data
- Sharing the results
 - In order to utilize the existing cell models by various users, it is required to access the data of interests by each user independently

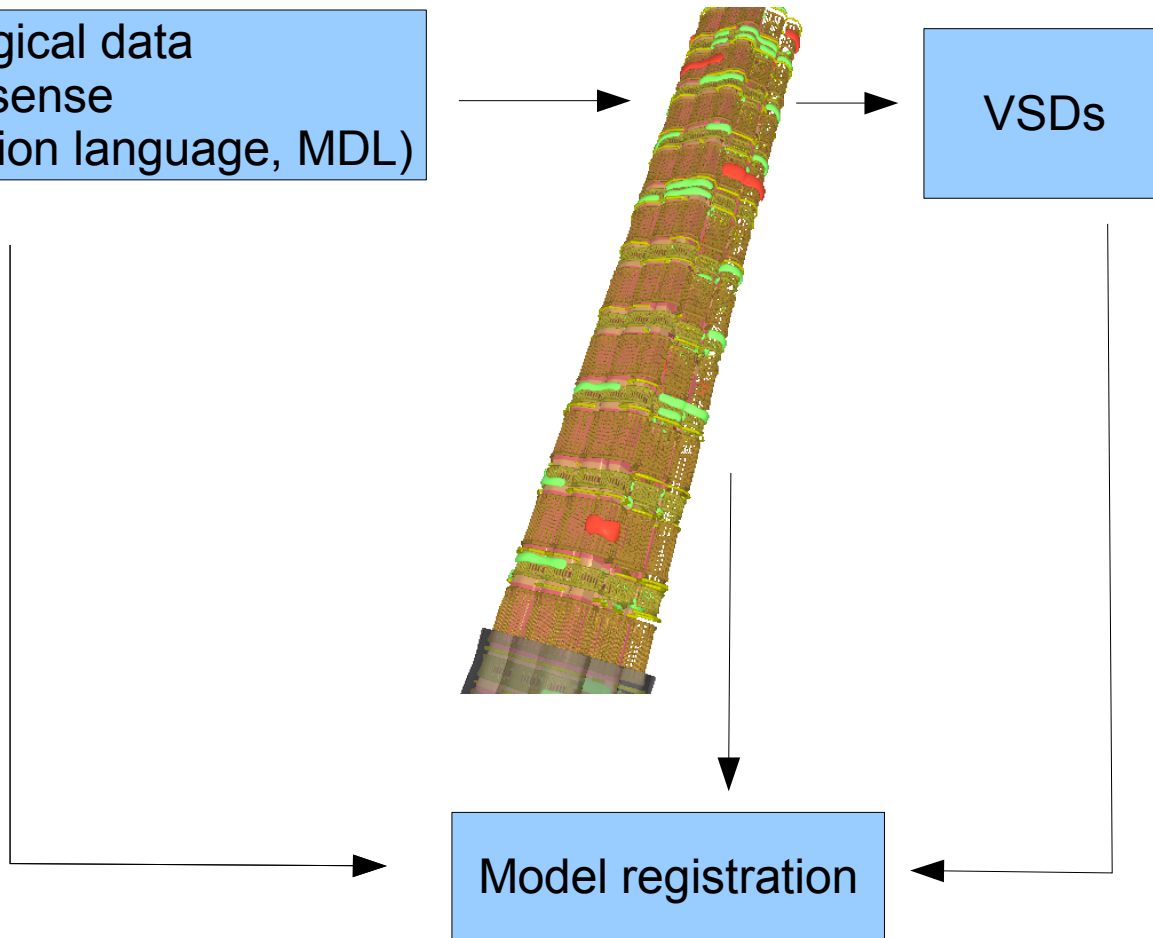
Automatic model registration for further use

Input morphological data
in probabilistic sense
(Model description language, MDL)



VSDs

Model registration





Metadata file example

```
<metadataCatalogue LFN="070905-29728-conf_f9.xml" VDIR="/cell/070905-29728">  
  <attribute name="experiment UID" type="string"/> 070905-29728 </attribute>  
  <attribute name="MyofVD" type="float"/> 0.449557 </attribute>  
  <attribute name="MitchVD" type="float"/> 0.012242 </attribute>  
  <attribute name="TubVD" type="float"/> 0.006543 </attribute>  
  <attribute name="SRVD" type="float"/> 0.037858 </attribute>  
  <attribute name="MyofSD" type="float"/> 0.450307 </attribute>  
  <attribute name="MitchSD" type="float"/> 0.038821 </attribute>  
  <attribute name="TubSD" type="float"/> 0.02182 </attribute>  
  <attribute name="SRSD" type="float"/> 0.110174 </attribute>  
  <attribute name="Length" type="float"/> 2000 </attribute>  
  <attribute name="SarcNum" type="float"/> 3 </attribute>  
  <attribute name="I_Band_Length" type="float"/> 1200 </attribute>  
  <attribute name="A_Band_Length" type="float"/> 700 </attribute>  
</metadataCatalogue>
```



Metadata utilization in grid

Client

Metadata Service

Replica Location
Service

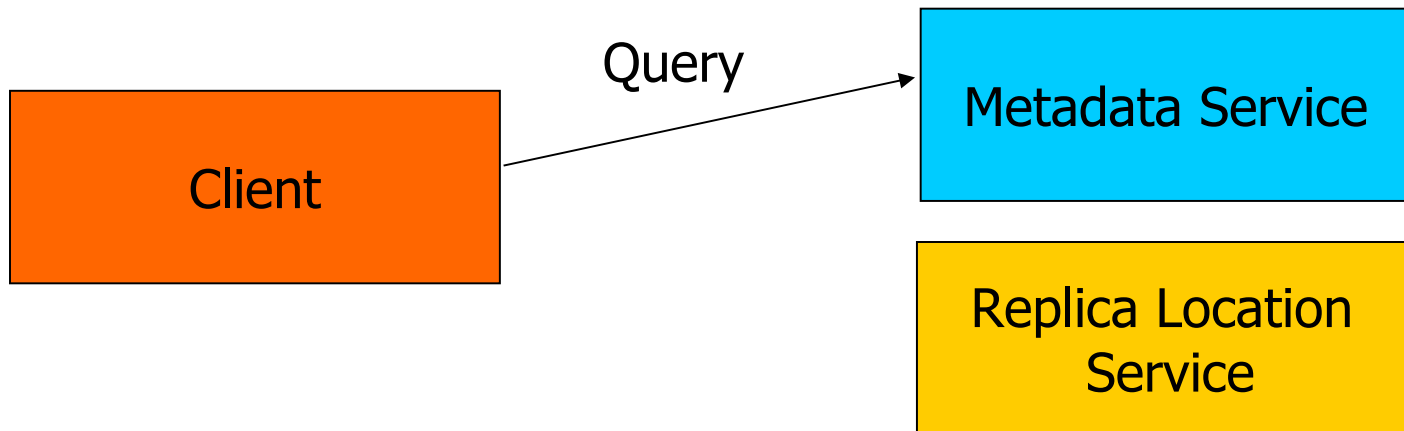
Storage
Resource

Storage
Resource

Storage
Resource



Metadata utilization in grid



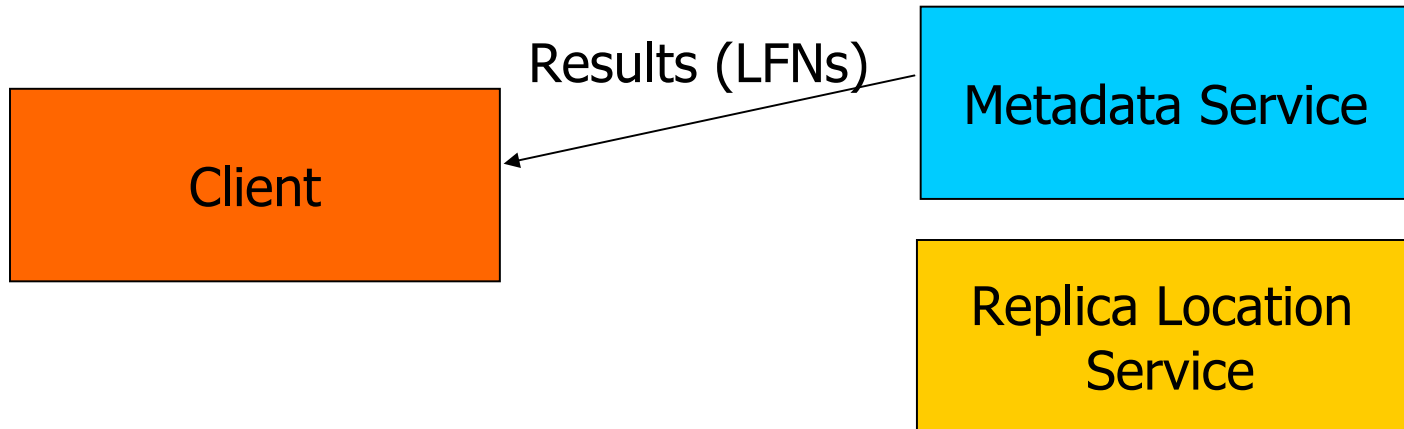
Storage
Resource

Storage
Resource

Storage
Resource



Metadata utilization in grid

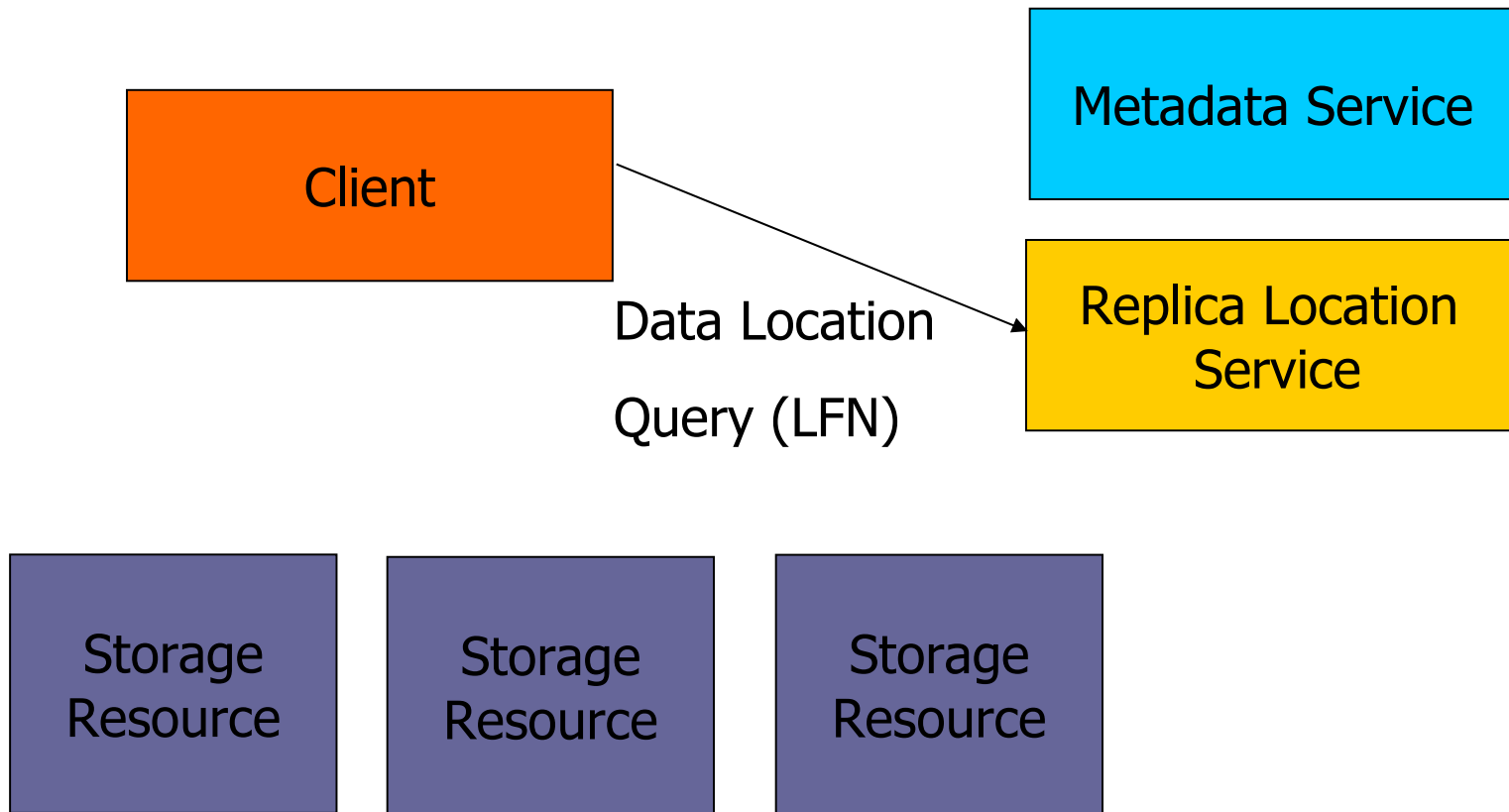


Storage
Resource

Storage
Resource

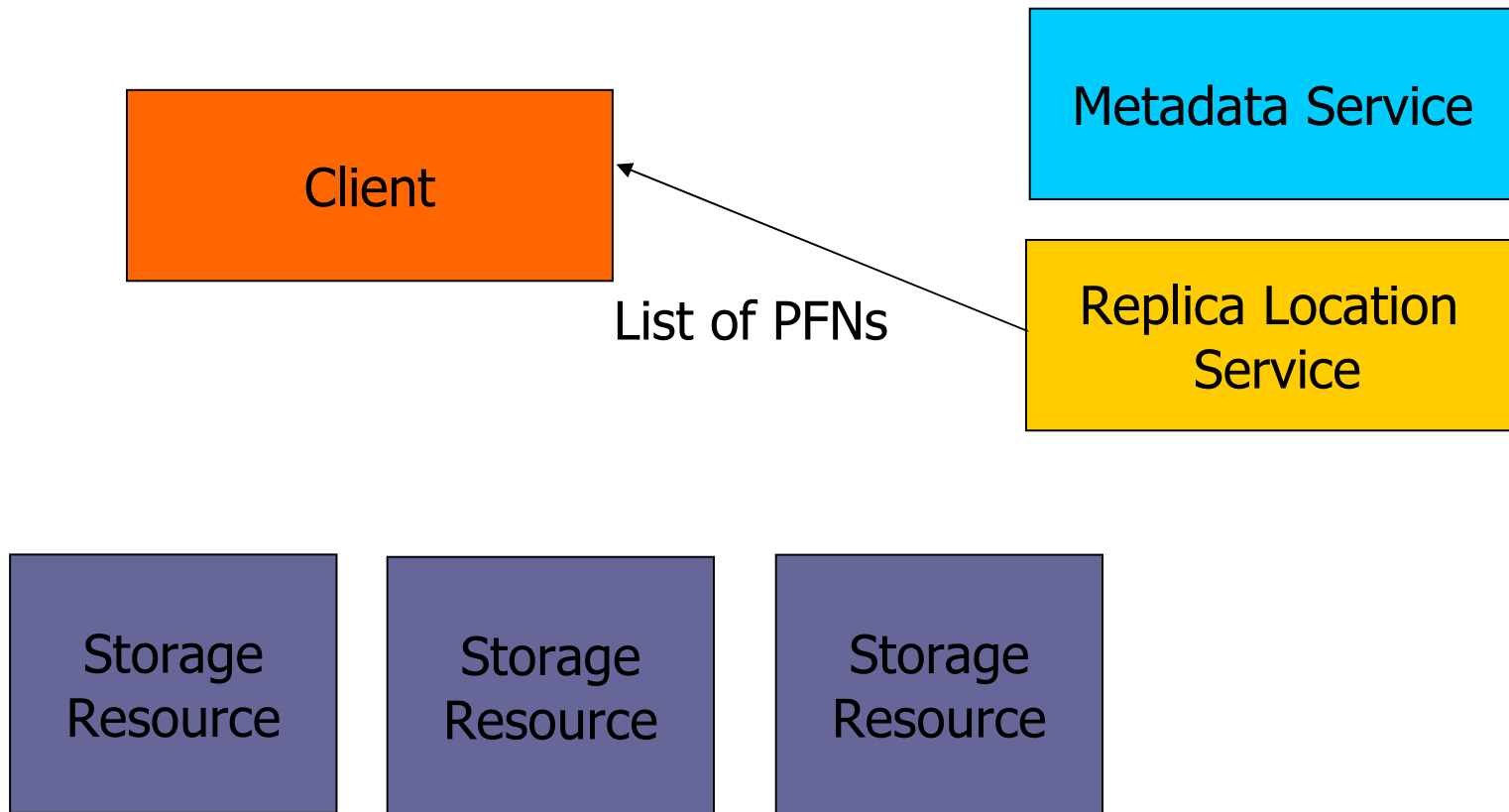
Storage
Resource

Metadata utilization in grid

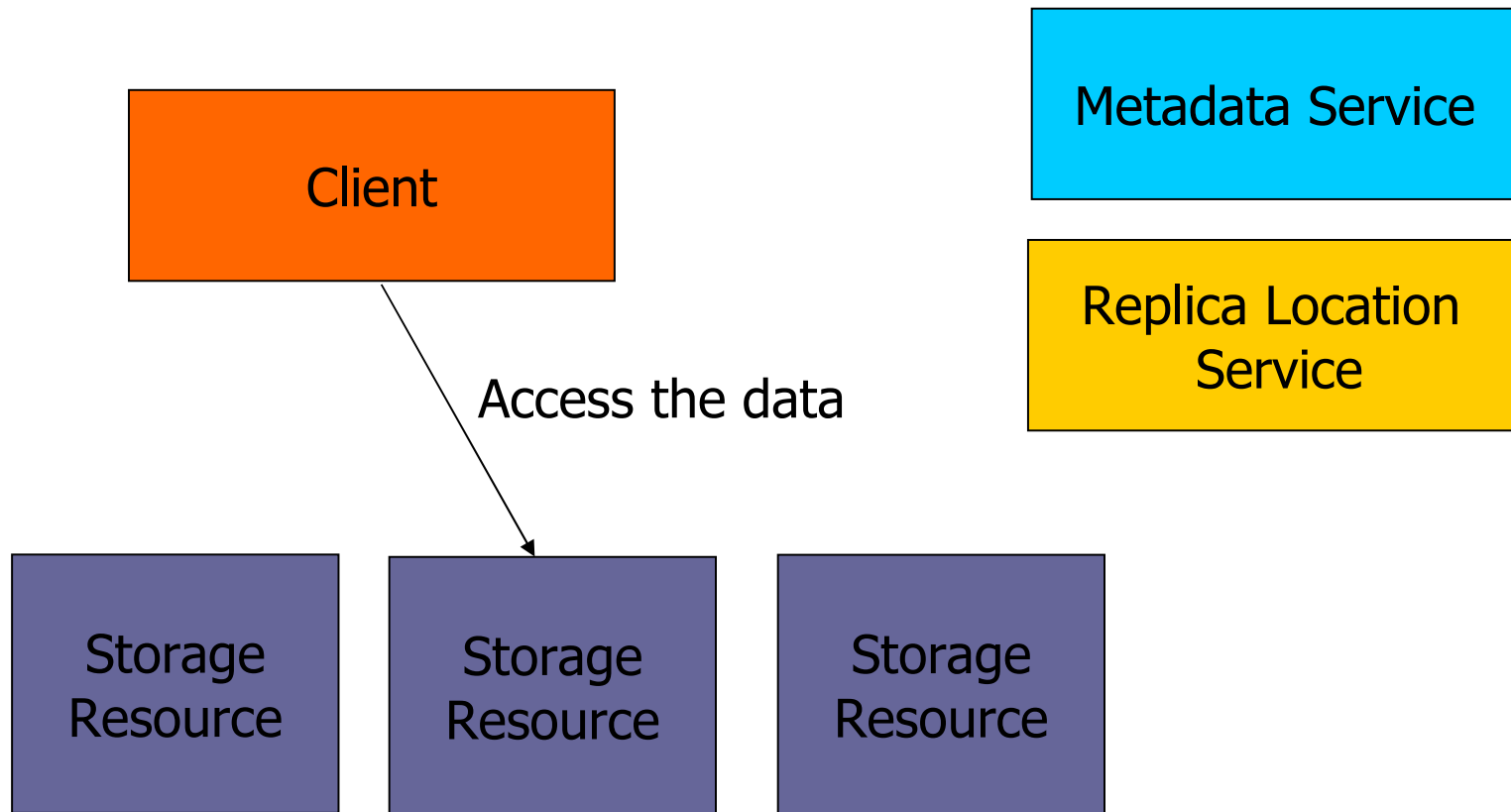




Metadata utilization in grid



Metadata utilization in grid





Metadata management in application portal

- Navigation in Metadata catalog
- View metadata
- Query metadata
- Retrieve files of interest described by metadata

Virtual Filesystem Browser

Virtual Filesystem Browser	
..	..
070830-261	DIR
070904-26316	DIR
070904-14679	DIR
070904-2273	DIR
070904-25992	DIR
070904-27501	DIR
070904-6385	DIR
070905-29728	DIR
070905-29728-jobs	.jcc
070905-29728-conf	.mcc
070905-29728-070905-29728-conf_f.tar	.gz
070905-29728-070905-29728-conf_d.tar	.gz
070905-29728-070905-29728-conf_c.tar	.gz
070905-29728-070905-29728-conf_b.tar	.gz
070905-29728-070905-29728-conf_a.tar	.gz
070905-29728-070905-29728-conf	.mcc
070905-29728-070905-29728-jobs	.jcc
070905-29728-conf_a5_vol	.xml
070905-29728-conf_c4_vol	.xml
070905-29728-conf_d6_vol	.xml
070905-29728-conf_a4_surf	.xml
070905-29728-conf_b2_vol	.xml
070905-29728-conf_c3_surf	.xml
070905-29728-conf_d5_surf	.xml
070905-29728-conf_a4_vol	.xml
070905-29728-conf_c3_vol	.xml
070905-29728-conf_d5_vol	.xml
070905-29728-conf_f0_surf	.xml
070905-29728-conf_a3_surf	.xml
070905-29728-conf_b1_surf	.xml
070905-29728-conf_d4_surf	.xml
070905-29728-conf_c2_surf	.xml
070905-29728-conf_a3_vol	.xml
070905-29728-conf_d4_vol	.xml
070905-29728-conf_a2_surf	.xml
070905-29728-conf_b1_vol	.xml
070905-29728-conf_c2_vol	.xml
070905-29728-conf_a2_vol	.xml

Metadata Attributes

070905-29728-conf_f9.xml

Data_id	871
Logical_name	070905-29728-conf_f9.xml
Version	1
Data_type	.xml
Collection_id	0
Container_service	null
Is_Valid	1
Creator_Dn	
Last_Modifier_Dn	
Create_Time	2007-08-05 13:52:16
Last_Modify_Time	2007-08-05 13:52:16
Master_Copy	null
audit	0
xml	NO
experiment_UID	070905-29728
A_Band_Length	1200
I_Band_Length	700
Length	2000
MitchSD	0.038821
MitchVD	0.012242
MyofSD	0.450307
MyofVD	0.449557
SarcNum	3
SRSD	0.118174
SRVD	0.037858
TubSD	0.02182
TubVD	0.006543

Delete Update

: String :

Add Attribute

Virtual Filesystem Browser

Virtual Filesystem Browser	
..	..
070830-261	DIR
070904-26316	DIR
070904-14679	DIR
070904-2273	DIR
070904-25992	DIR
070904-27501	DIR
070904-6385	DIR
070905-29728	DIR
070905-29728-jobs	.jcc
070905-29728-conf	.mcc
070905-29728-070905-29728-conf_f.tar	.gz
070905-29728-070905-29728-conf_d.tar	.gz
070905-29728-070905-29728-conf_c.tar	.gz
070905-29728-070905-29728-conf_b.tar	.gz
070905-29728-070905-29728-conf_a.tar	.gz
070905-29728-070905-29728-conf	.mcc
070905-29728-070905-29728-jobs	.jcc
070905-29728-conf_a5_vol	.xml
070905-29728-conf_c4_vol	.xml
070905-29728-conf_d6_vol	.xml
070905-29728-conf_a4_surf	.xml
070905-29728-conf_b2_vol	.xml
070905-29728-conf_f0_surf	.xml
070905-29728-conf_a3_surf	.xml
070905-29728-conf_b1_surf	.xml
070905-29728-conf_d4_surf	.xml
070905-29728-conf_c2_surf	.xml
070905-29728-conf_a3_vol	.xml
070905-29728-conf_d4_vol	.xml
070905-29728-conf_a2_surf	.xml
070905-29728-conf_b1_vol	.xml
070905-29728-conf_c2_vol	.xml
070905-29728-conf_a2_vol	.xml

Virtual Directory System (navigation in metadata catalog)

Metadata Attributes

070905-29728-conf_f9.xml

Data_id	871
Logical_name	070905-29728-conf_f9.xml
Version	1
Data_type	.xml
Collection_id	0
Container_service	null
Is_Valid	1
Creator_Dn	
Last_Modifier_Dn	
Create_Time	2007-08-05 13:52:16
Last_Modify_Time	2007-08-05 13:52:16
Master_Copy	null
audit	0
xml	NO
experiment_UID	070905-29728
A_Band_Length	1200
I_Band_Length	700
Length	2000
MitchSD	0.038821
MitchVD	0.012242
MyofSD	0.450307
MyofVD	0.449557
SarcNum	3
SRSD	0.118174
SRVD	0.037858
TubSD	0.02182
TubVD	0.006543

Delete Update

: String :

Add Attribute

Virtual Filesystem Browser

Virtual Filesystem Browser	
..	..
070830-261	DIR 070905-29728-jobs
070904-26316	DIR 070905-29728-conf
070904-14679	DIR 070905-29728-070905-29728-conf_f.tar
070904-2273	DIR 070905-29728-070905-29728-conf_d.tar
070904-25992	DIR 070905-29728-070905-29728-conf_c.tar
070904-27501	DIR 070905-29728-070905-29728-conf_b.tar
070904-6385	DIR 070905-29728-070905-29728-conf_a.tar
070905-29728	DIR 070905-29728-070905-29728-conf
	070905-29728-070905-29728-jobs
	070905-29728-conf_a5_vol
	070905-29728-conf_c4_vol
	070905-29728-conf_d6_vol
	070905-29728-conf_a4_surf
	070905-29728-conf_b2_vol
	070905-29728-conf_f0_surf
	070905-29728-conf_a3_surf
	070905-29728-conf_b1_surf
	070905-29728-conf_d4_surf
	070905-29728-conf_c2_surf
	070905-29728-conf_a3_vol
	070905-29728-conf_d4_vol
	070905-29728-conf_a2_surf
	070905-29728-conf_b1_vol
	070905-29728-conf_c2_vol
	070905-29728-conf_a2_vol

Metadata Attributes

070905-29728-conf_f9.xml	
Data_id	871
Logical_name	070905-29728-conf_f9.xml
Version	1
Last_Modifier_Dn	
Create_Time	2007-08-05 13:52:16
Last_Modify_Time	2007-08-05 13:52:16
Master_Copy	null
audit	0
xml	NO
experiment_UID	070905-29728
A_Band_Length	1200
I_Band_Length	700
Length	2000
MitchSD	0.038821
MitchVD	0.012242
MyofSD	0.450307
MyofVD	0.449557
SarcNum	3
SRSD	0.118174
SRVD	0.037858
TubSD	0.02182
TubVD	0.006543

Delete Update

: String :

Add Attribute

View of Metadata Attributes (Describe cell model file)

Virtual Directory System (navigation in metadata catalog)

Virtual Filesystem Browser

Metadata search

Metadata Attributes

Virtual Filesystem Browser

- 070830-261
- 070904-26316
- 070904-14679
- 070904-2273
- 070904-25992
- 070904-27501
- 070904-6385
- 070905-29728

- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-
- DIR 070905-29728-

- 070905-29728-conf_c4_vol .xml
- 070905-29728-conf_d6_vol .xml
- 070905-29728-conf_a4_surf .xml
- 070905-29728-conf_b2_vol .xml
- 070905-29728-conf_f0_surf .xml
- 070905-29728-conf_a3_surf .xml
- 070905-29728-conf_b1_surf .xml
- 070905-29728-conf_d4_surf .xml
- 070905-29728-conf_c2_surf .xml
- 070905-29728-conf_a3_vol .xml
- 070905-29728-conf_d4_vol .xml
- 070905-29728-conf_a2_surf .xml
- 070905-29728-conf_b1_vol .xml
- 070905-29728-conf_c2_vol .xml
- 070905-29728-conf_a2_vol .xml

Add search condition:
[] : String : = : []
Add Condition
Search
Clear Conditions

Conditions:

Attribute	Type	Condition	Value
length	MCS_FLOAT	<	2500
MitchVD	MCS_FLOAT	>	3.5
MyofVD	MCS_STRING	>	73

Results:

Metadata search

Virtual Directory System
(navigation in metadata catalog)

xml	NO
experiment_UID	070905-29728
A_Band_Length	1200
I_Band_Length	700
Length	2000
MitchSD	0.038821
MitchVD	0.012242
MyofSD	0.450307
MyofVD	0.449557
SarcNum	3
SRSD	0.118174
SRVD	0.037858
TubSD	0.02182
TubVD	0.006543

Delete Update

[] : String : []
Add Attribute

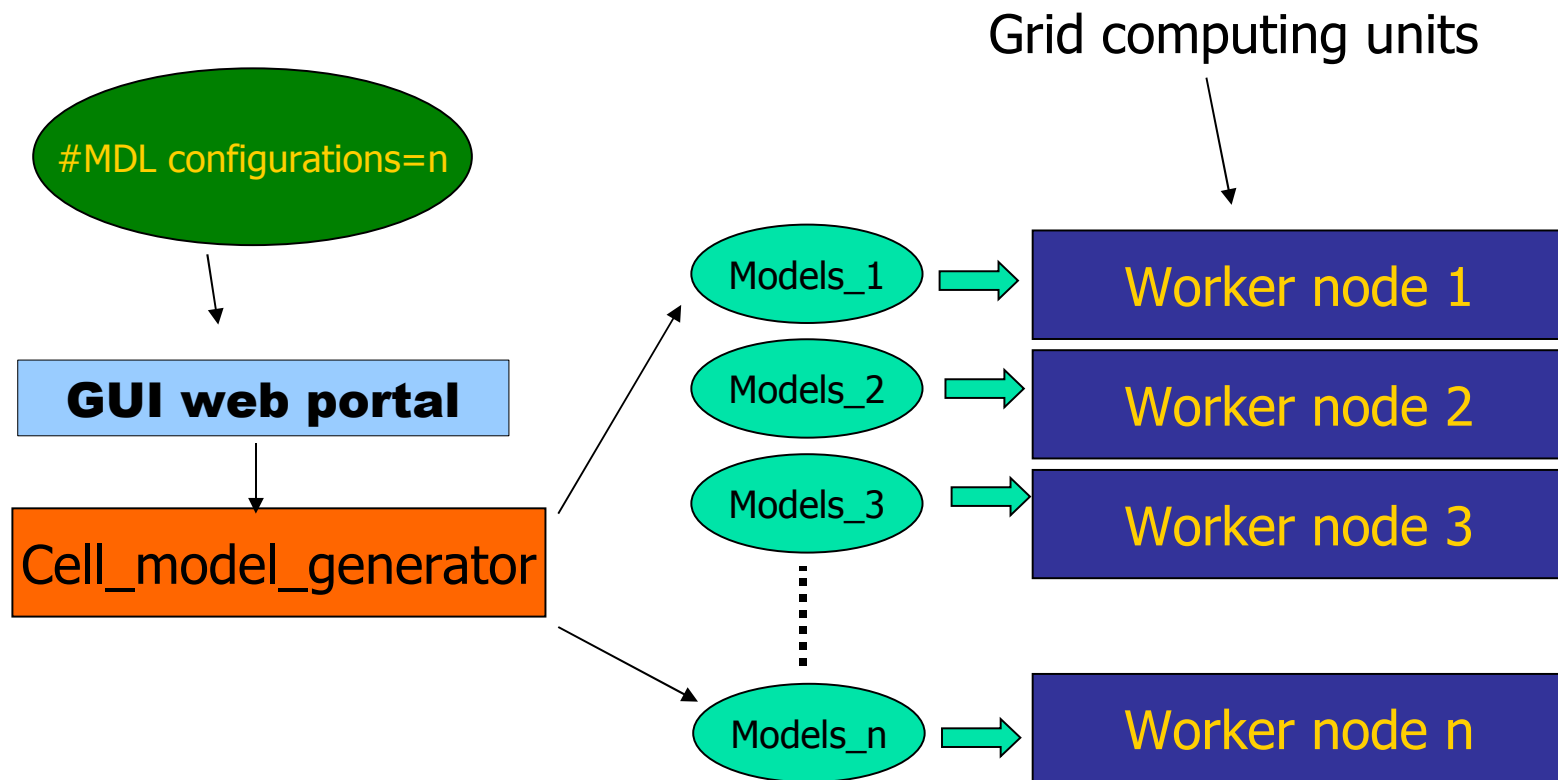
Thank you for your attention

The screenshot displays a web-based interface for job management and data visualization. The interface is divided into several panels:

- Job creation:** A panel with a dropdown menu set to "Cell Model Computation" and a "Select" button.
- User job list:** A panel showing a list of jobs. The first job is highlighted: "Job: Cell Model Computation State: RUNNING Creation date: 2007-06-25 15:08:25.623". Below the job name are buttons for "Run", "Cancel", "Delete", "Outputs", and "View mapset".
- Directory browser:** A panel showing a file tree for the host "All resources #jobs# / 2007-06-25-15-08_2A6E0780-231D-11DC-BE7F-F777AB143692". The file list includes: a0_st_data.txt, job-wrapper.sh, stdout, stderr, runCellComp.sh, edglog.log, jobid, a0_2048_p4.bmp, currentStatus.txt, a0.xml, and a0_i_1.bmp. Each file has "View" and "Attributes" options. An arrow points from "a0.xml" to the "File Content" panel.
- File Content:** A panel displaying a 3D visualization of a biological structure, likely a cell model, with various colored regions (green, yellow, pink, blue) representing different components.
- Table:** A table showing organelle data:

Organelles	V_V [%]	S_V [μm^{-1}]
Mitochondria	5.32	0.46
T tubules	0.57	0.252
Myofibrils	82.26	1.53
Sarcoplasmic reticulum	7.54	1.34

Cell model generation



Automatic metadata generation

process

Metadata file describes the model file

Worker node

