

# Metadata in Problem Solving Environment for Stereology Based Modeling

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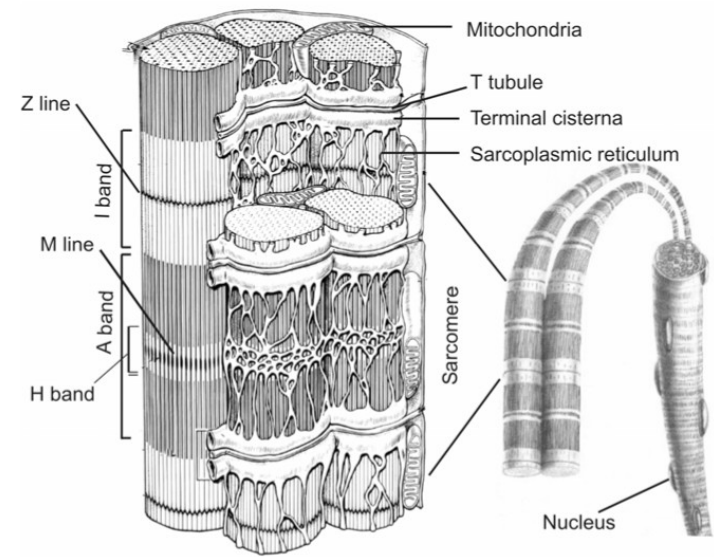
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(3) Institute of Molecular Physiology and Genetics, Slovak Academy of Sciences, Slovakia

(4) Austrian Academy of Sciences, Austria

# Main goal

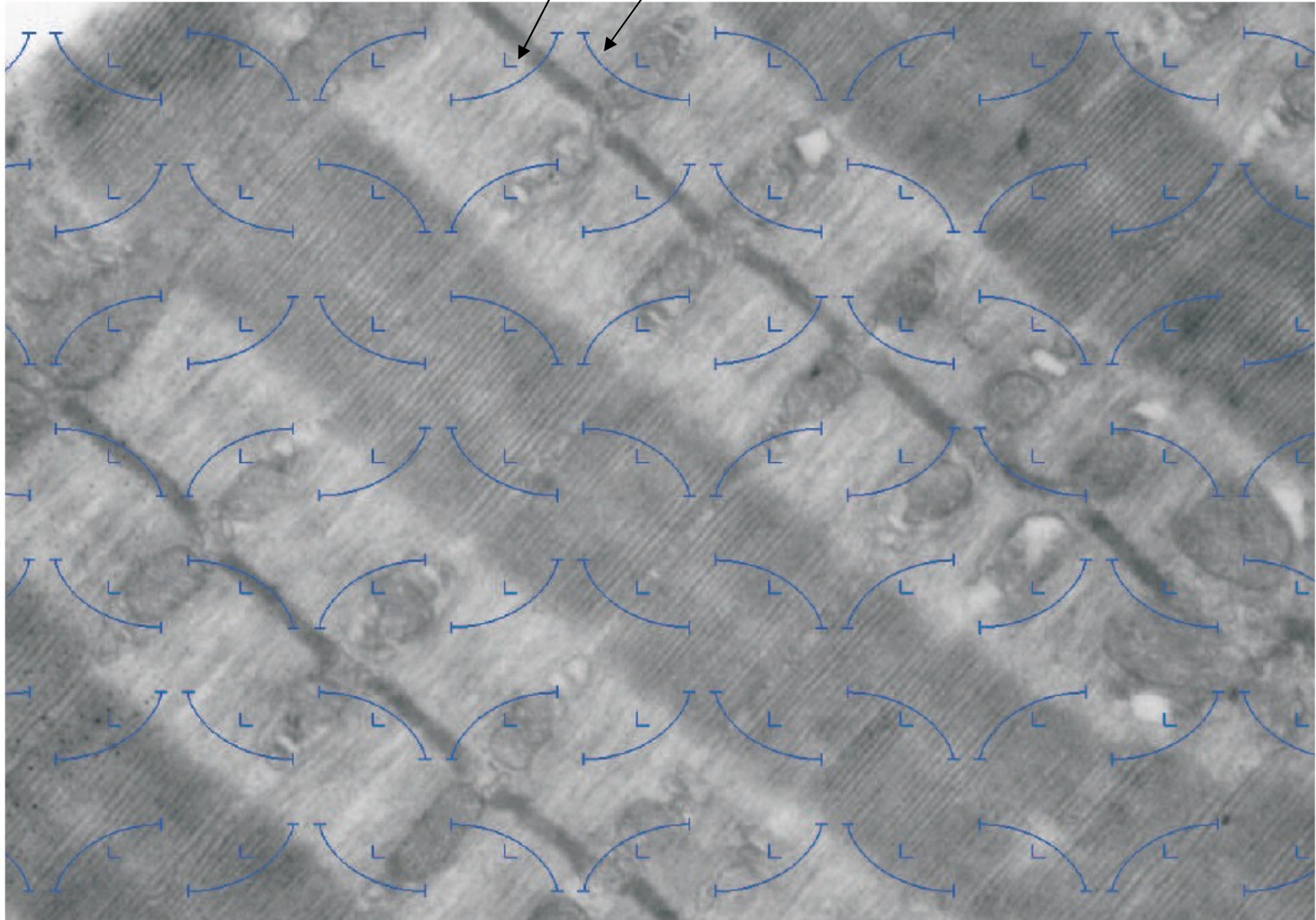
- To create environment that would enable users to
  - **Create** muscle cell models by means of a specialized model description language
  - **Verify** these models according to volume and surface densities (VSDs) of basic cell components - organelles
  - **Visualize** these models



# Measurement of VSDs

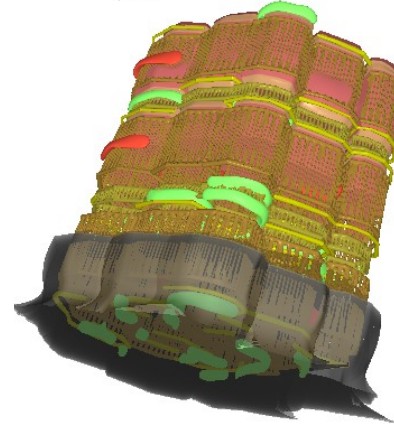
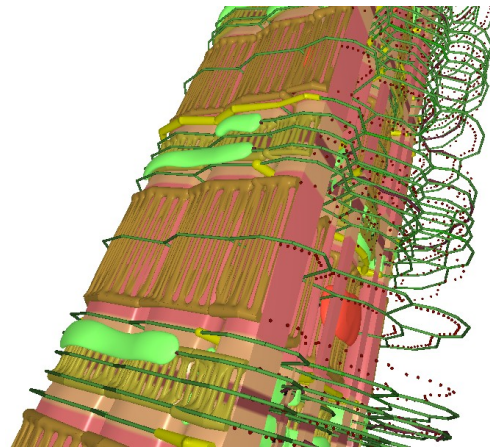
on real cells

L-type points – Volume density  
Cycliodes – 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
- Interactivity support
  - Cancel/restart computations
  - Inspection of intermediate results
- Retrieval of existing results
  - Retrieve the required data
  - Metadata utilization

# Grid requirement summary

- Computation of intensive parametric studies
  - VSDs computation
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- Retrieval of existing results
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  - Metadata utilization

# Metadata Intro

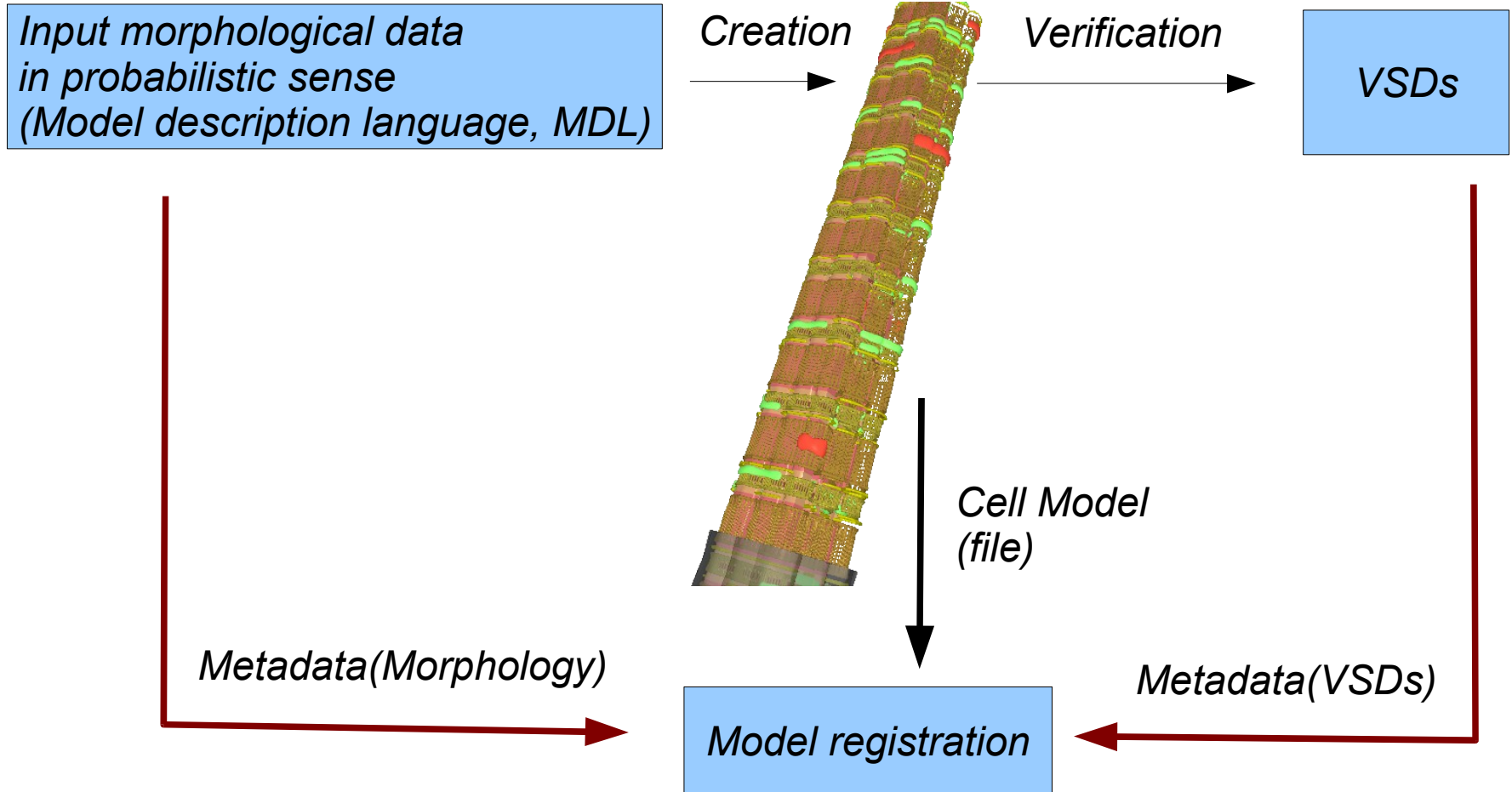
- Data about data
- Metadata types:
  - Technical (file and security levels, etc.)
  - Application specific
- Application metadata generation
  - Manual annotation
  - Automatic generation
- Discovery and retrieval of existing data



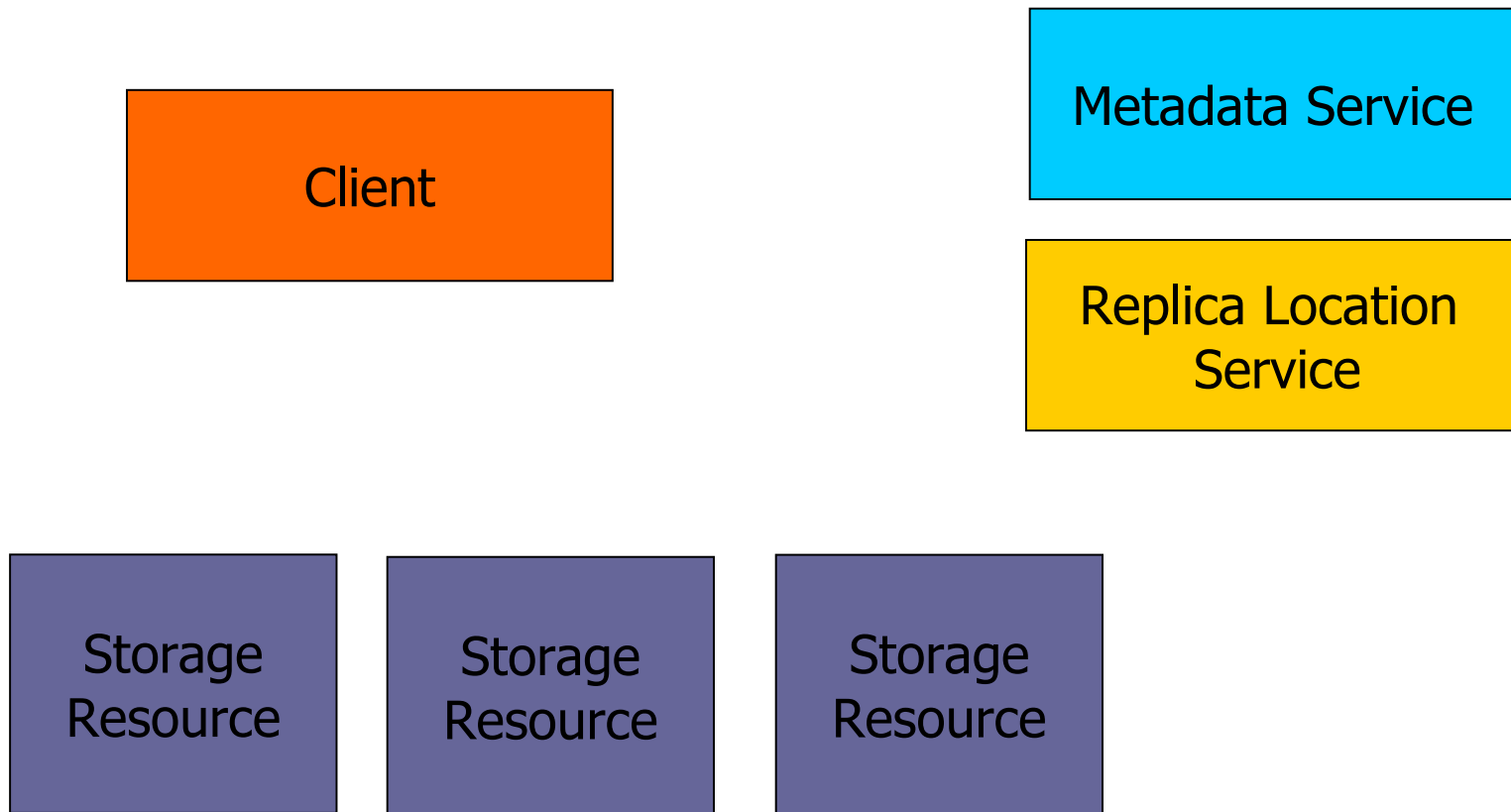
# Motivation for metadata utilization

- Representation of a large amount of cell data
  - Many results are generated, which require 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

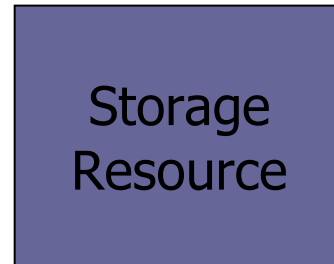
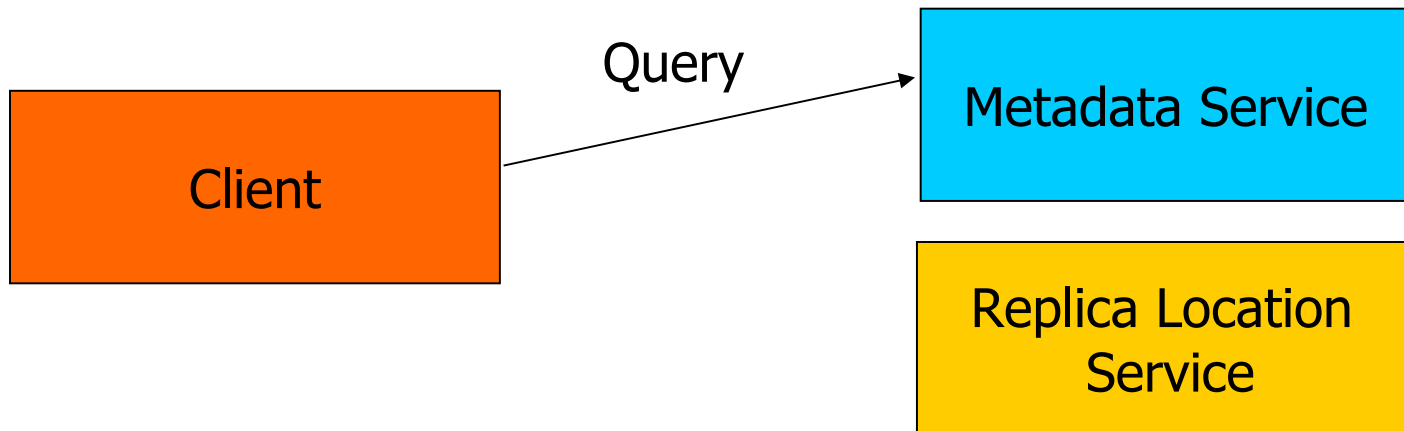
# Cell model registration for further use



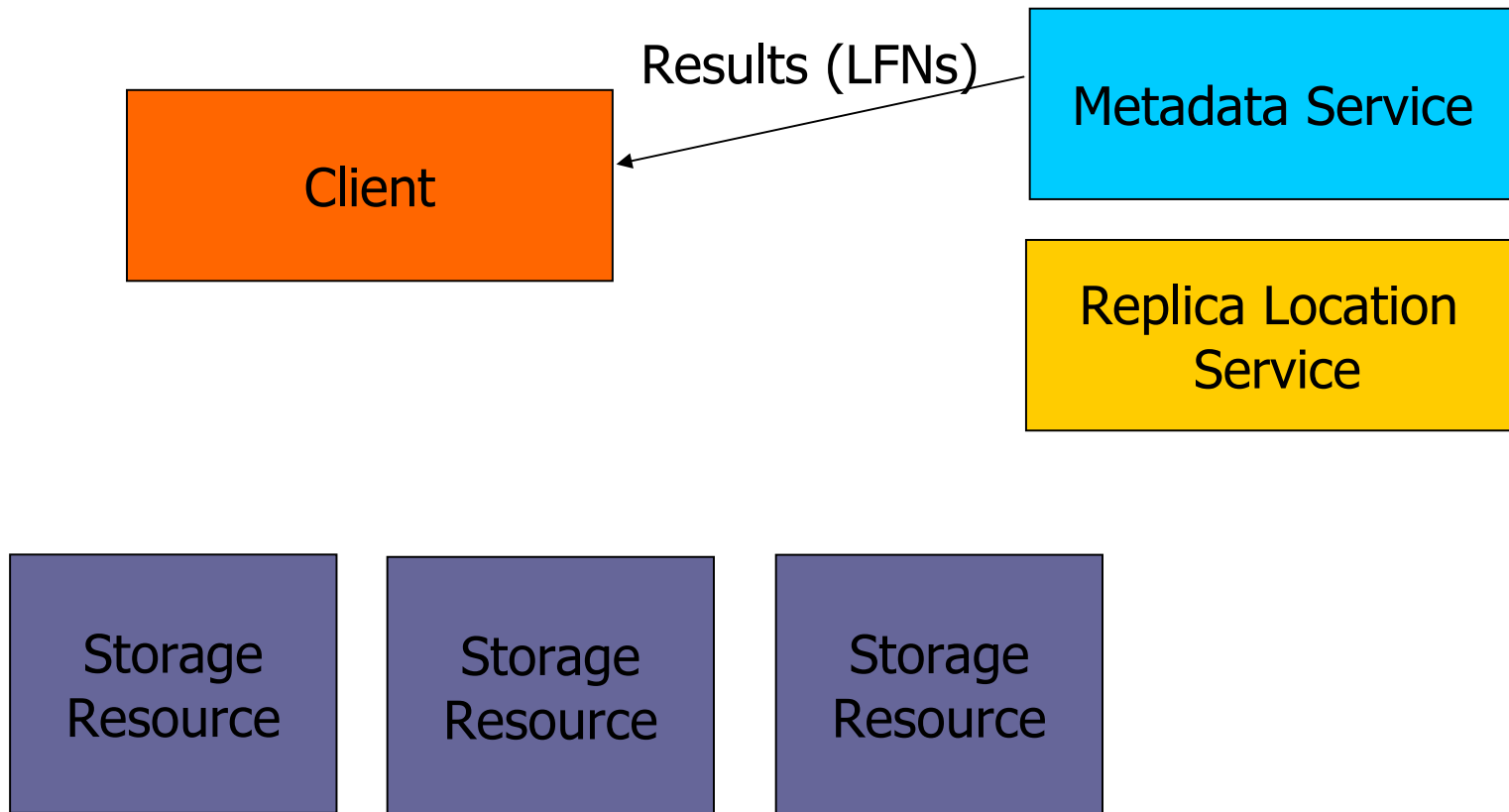
# Metadata utilization in grid



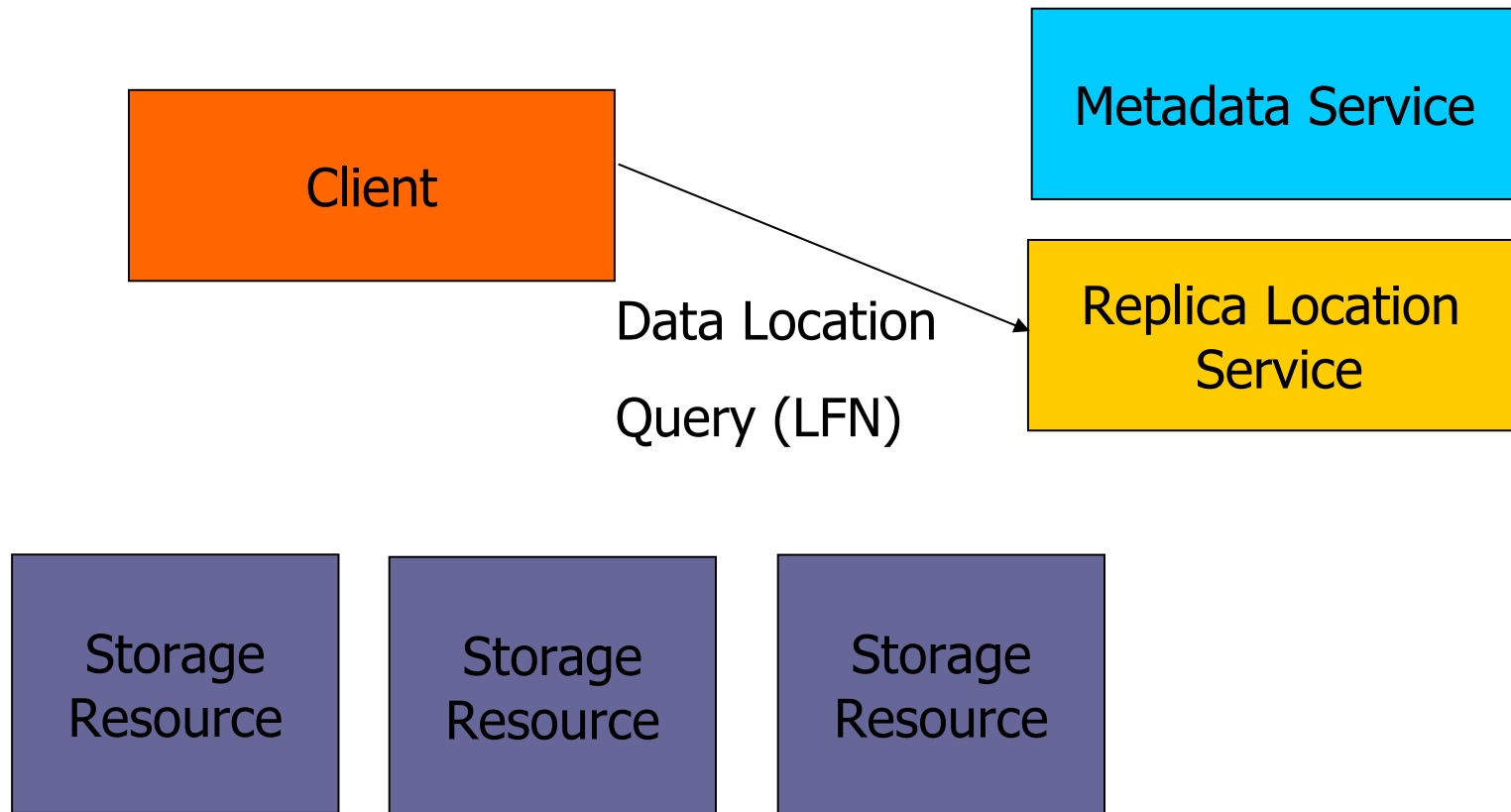
# Metadata utilization in grid



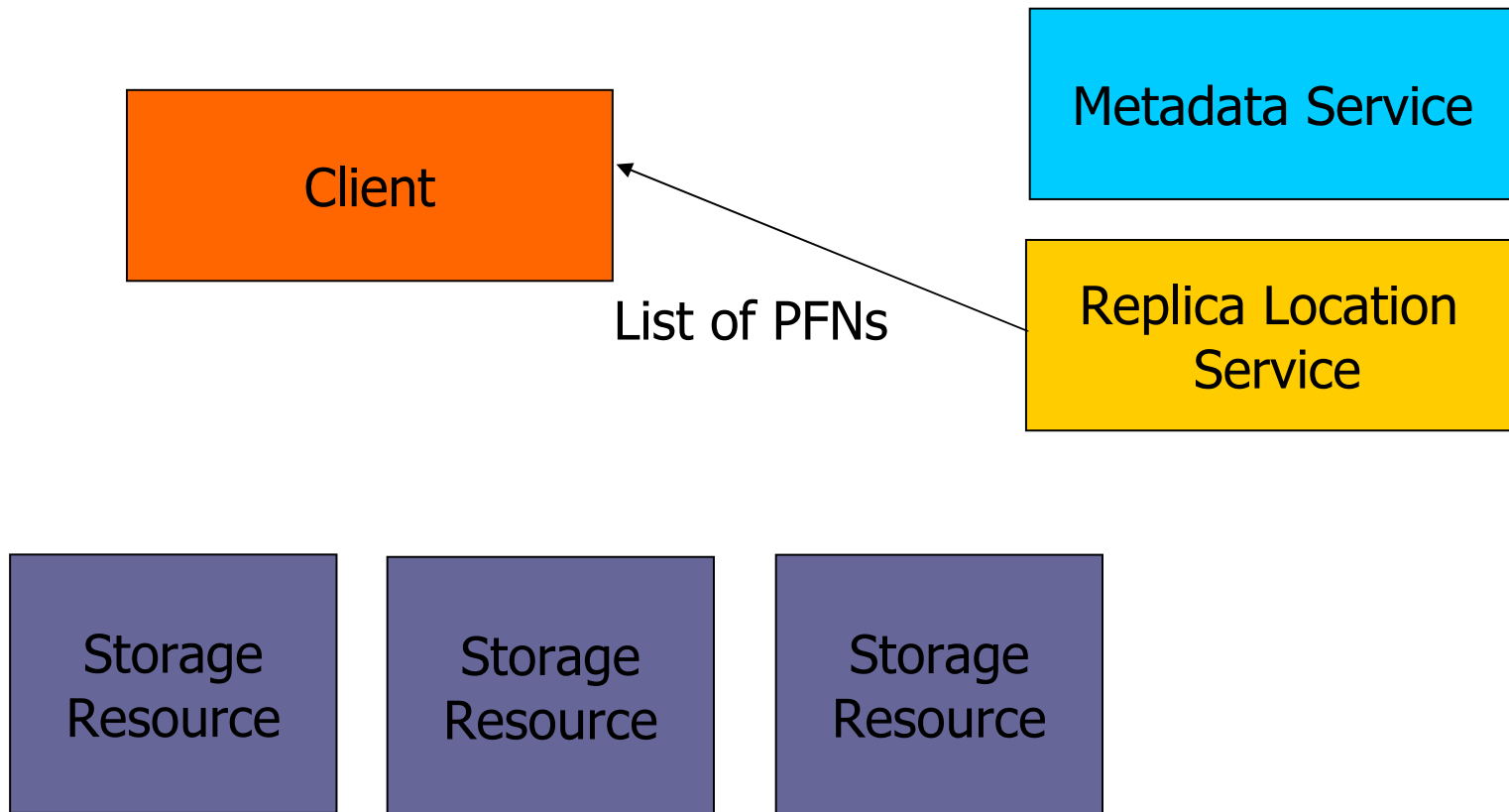
# Metadata utilization in grid



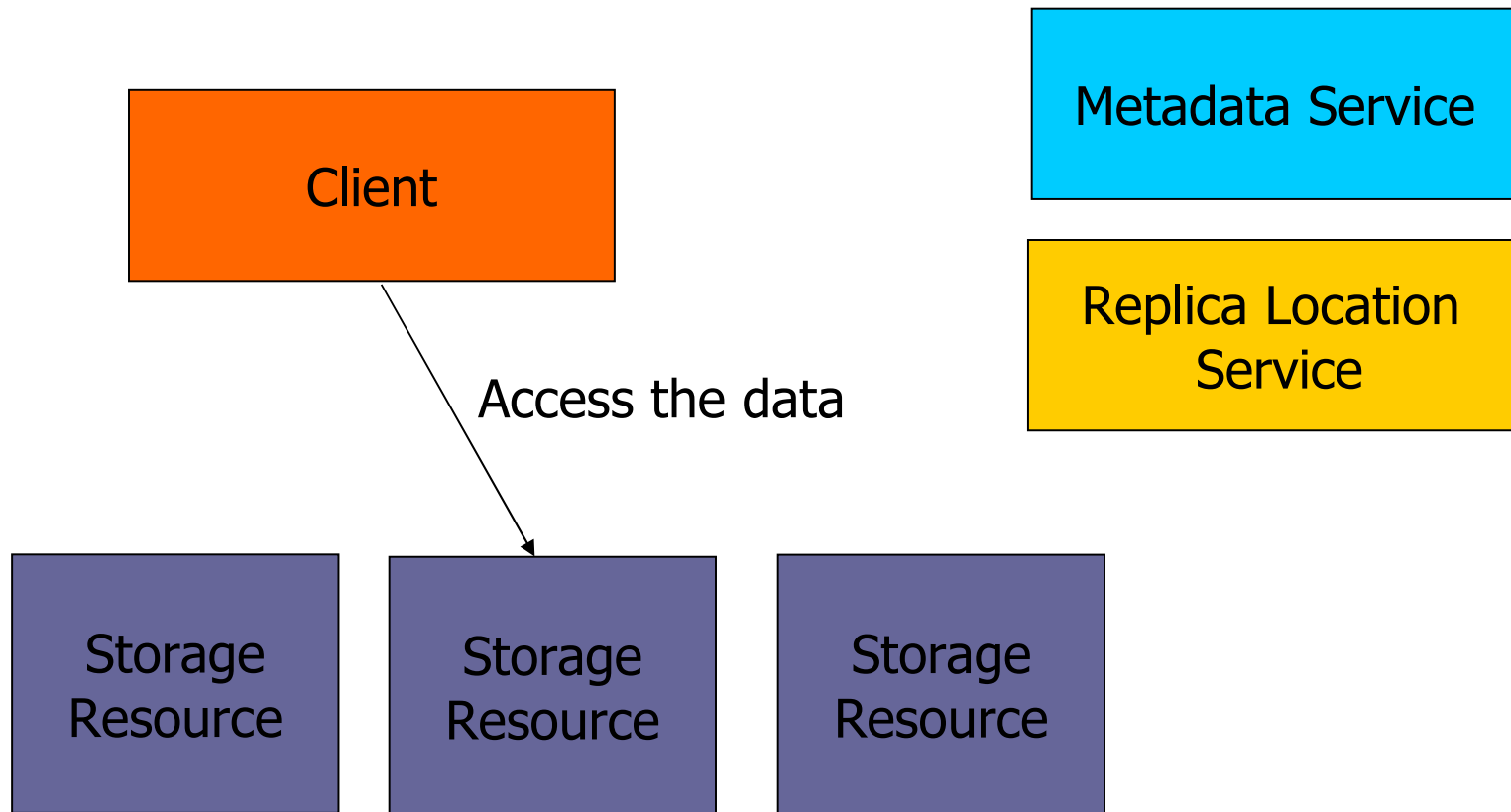
# Metadata utilization in grid



# Metadata utilization in grid

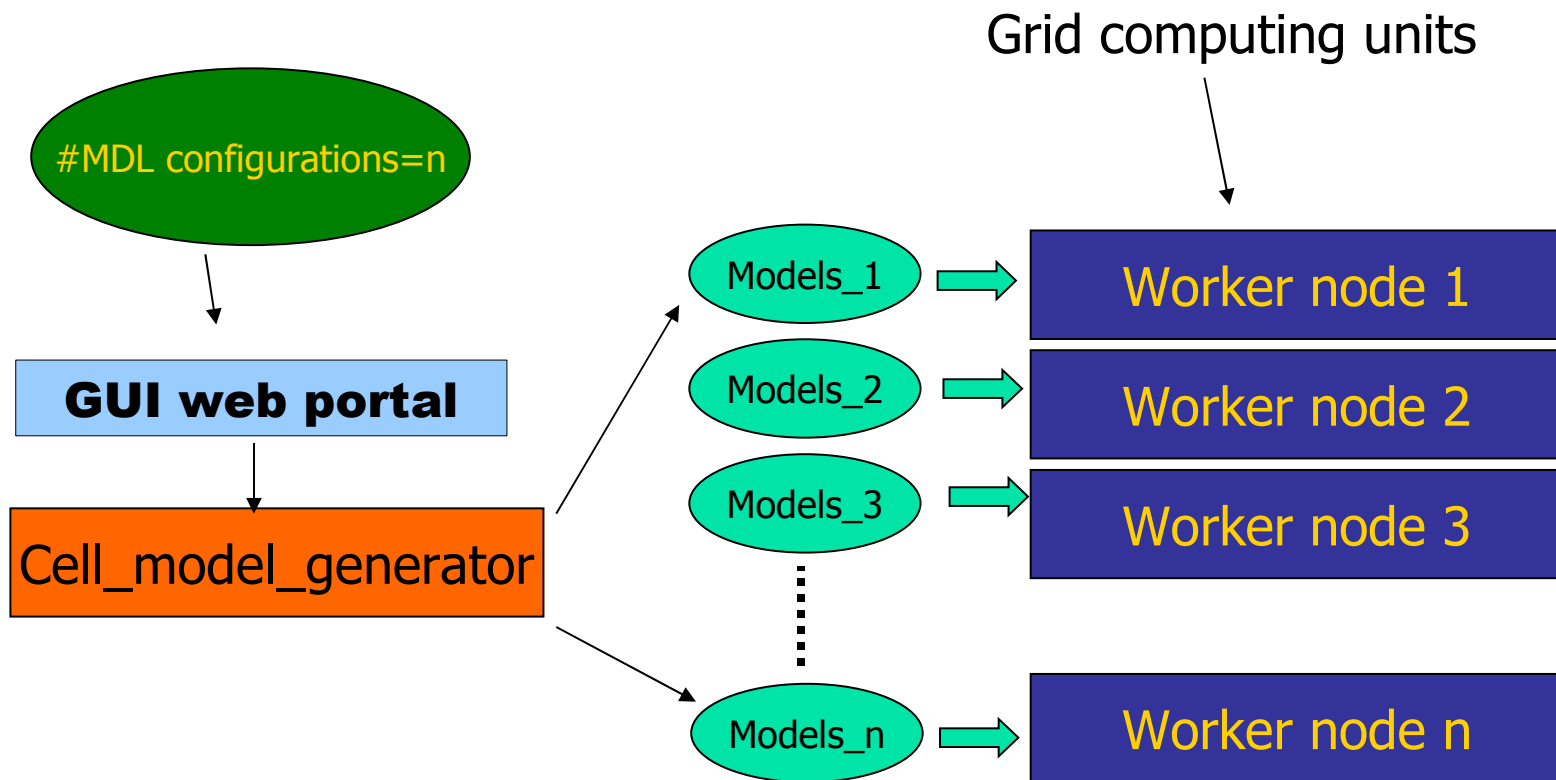


# Metadata utilization in grid





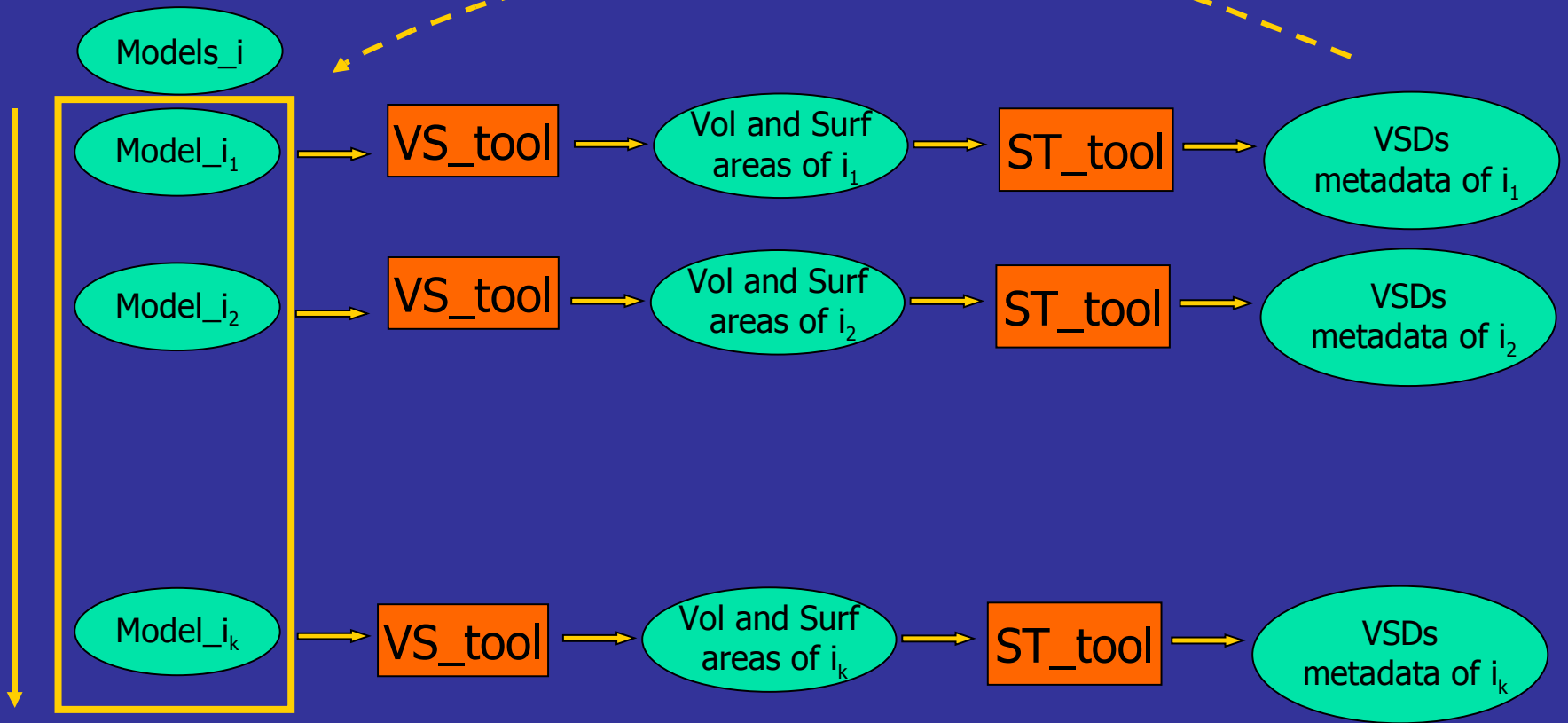
# Cell model generation



# Automatic metadata generation process

Metadata file describes the model file

Worker node



# 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 management in application portal

- Navigation in Metadata catalog
- View/Edit 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

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..	..
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
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MitchSD	0.038821
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Delete Update

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Add Attribute

Virtual Filesystem Browser

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..	..
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

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070905-29728-conf_f9.xml	
Data_id	871
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Version	1
Last_Modifier_Dn	
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Delete Update

: String :

Add Attribute

View of Metadata Attributes (Describe cell model file)

Virtual Directory System (navigation in metadata catalog)





# Thank you for your attention

The screenshot displays a web-based interface for job management and 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 job entry: "Job: Cell Model Computation State: RUNNING Creation date: 2007-06-25 15:08:25.623". Below the entry are buttons for "Run", "Cancel", "Delete", "Outputs", and "View mapset".
- Directory browser:** A panel showing the contents of a directory. The files listed are: 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 a "View" button and an "Attributes" button. An arrow points from the "a0.xml" file to the table below.
- File Content:** A panel displaying a 3D visualization of a cell model. The model is a cylindrical structure with various internal components highlighted in different colors (green, yellow, pink, blue). An arrow points from the "a0.xml" file in the directory browser to this visualization.
- Table:** A table with the following data:

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