

# Data Management and Analysis at the Large Scale Data Facility

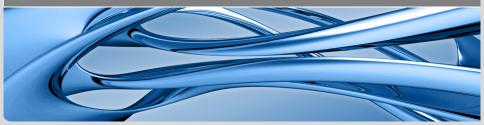
A. García<sup>1</sup>, S. Bourov<sup>1</sup>, A. Hammad<sup>1</sup>, T. Jejkal<sup>2</sup>, J. Otte<sup>3</sup>, S. Pfeiffer<sup>4</sup>, T. Schenker<sup>4</sup>, C. Schmidt<sup>4</sup>, J. van Wezel<sup>1</sup>, B. Neumair<sup>1</sup>, A. Streit<sup>1</sup>

<sup>1</sup> Steinbuch Centre for Computing, KIT

- <sup>2</sup> Institute for Data Processing and Electronics, KIT
- <sup>3</sup> Institute of Toxicology and Genetics, KIT
- <sup>4</sup> Institute for Applied Computer Science, KIT

ICDIM 2011, Melbourne | September 27, 2011





www.kit.edu



- Many experiments have a data-management problem!
- This project aims at improving the situation, with adapted infrastructure and services
- Data Intensive Computing workflows are critical for the value of the data
- We present a concrete data intensive analysis use case at the LSDF

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#### Science produces data!

- Experiments getting exponentially more data
  - $\Rightarrow$  experiments need storage
  - $\Rightarrow$  need sophisticated data analysis workflows

#### Old data is very valuable

- to analyse change in time
- for reprocessing
- for analysis by other scientists, in other contexts
- Invisible (not-found, no-metadata) data is lost data
  - $\Rightarrow$  adequate **meta data** greatly increases data value
  - ⇒ single big scientific DB is more valuable than many small ones
- Data is used by large virtual communities!
  - $\Rightarrow$  access to data is critical

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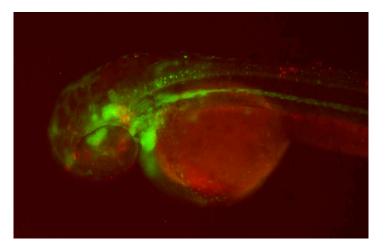
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### Why do experiments produce so much data?





#### Zebrafish embryo, raw picture, 4MB (24 per fish)

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### Why do experiments produce so much data?



- Institute of Toxicology and Genetics @ KIT
  - $\Rightarrow$  Zebra fishes' embryonal development reconstruction
  - $\Rightarrow$  Toxicological studies of drugs
    - High Throughput Microscopy
      - fully automated microscopes
      - robot moves object to microscope
      - can potentially run 24\*7
      - produce high resolution images (4 MB each)
      - over varying parameters (focus point, cell markers, ...)
    - ho
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    - Estimated: 1+ PB/year in 2012, C DB/wear in 2014
      - 6 PB/year in 2014
    - Raw data must be heavily analysed

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### The Large Scale Data Facility Project



#### LSDF started end of 2009 at KIT

- involving several institutes
- in cooperation with BioQuant of Univ. Heidelberg
- to address the needs of Data Intensive Science:
  - providing large scale storage and data processing
  - open protocols and APIs for access to data and metadata
  - added value services for community specific needs (multi-disciplinary)

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### The Large Scale Data Facility Project



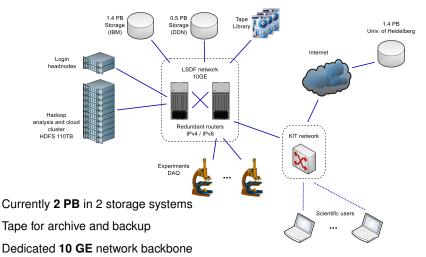
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### What infrastructure are we talking about?



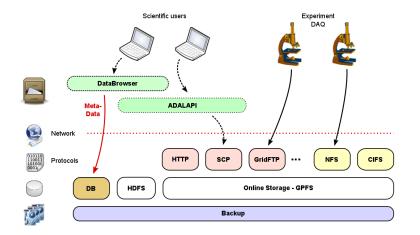


Direct network connection to some institutes

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### The current architecture





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### How to deal with so much data?



#### Metadata is essential

- Needs to be stored and kept up to date with data
- Metadata schema is highly project-dependent
- $\Rightarrow$  use a project metadata DB

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Example:

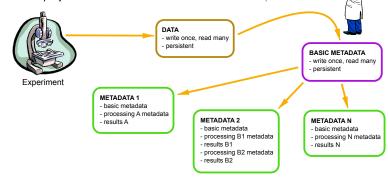
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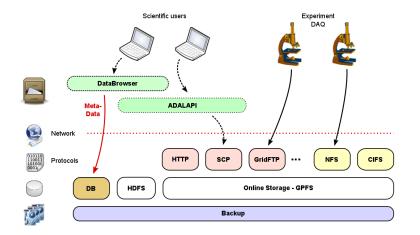


Example:

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### The current architecture





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### Which access APIs and tools?



Different components accessible through different protocols and APIs

- $\Rightarrow$  need a unified access layer
  - Abstract Data Access Layer, low-level interface to LSDF
  - $\Rightarrow$  extensible to support new backends, authentication mechanisms
- For end-users: DataBrowser
  - graphical tool for exploring and managing the LSDF data
  - also library for meta-data access
  - based on ADALAPI
  - connects to the meta-data repository
  - will be available as web GUI

R. Stotzka et. al., Perspective of the Large Scale Data Facility supporting nuclear fusion applications, Proceedings PDP 2011.

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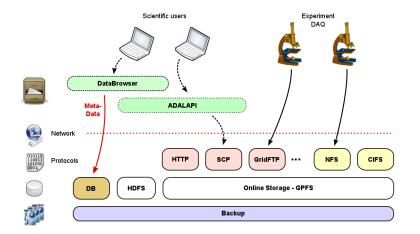


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### The current architecture





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### Can we process the data?



- Data has to be processed!
- Exascale ⇒ bring computing to the data!!

(15 days to transfer 1 PB over ideal 10Gb/s link)

- $\Rightarrow$  dedicated 60 nodes cluster
- Hadoop environment
  - + 110 TB Hadoop filesystem
    - extreme scalability
- Cloud environment OpenNebula
  - users can deploy own dedicated data-processing VMs
  - reliable, highly flexible, and very fast to deploy

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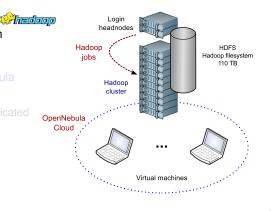
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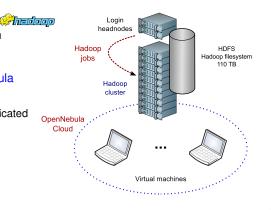
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#### How to deal with data?



With Cloud instances, if customized SW environment is required

- Integrated with the Kepler workflow orquestrator
- user-friendly interface

• With workflows in the Hadoop cluster

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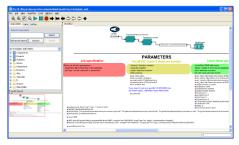
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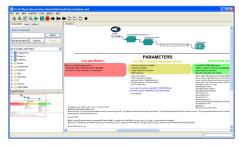
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#### With workflows in the Hadoop cluster

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### Processing data at LSDF



■ Experiments should be able to process data locally ⇒ help the users automate the workflows

- Allow tagging data and triggering execution via DataBrowser
- Data from finished workflows stored and tagged in DB

used for zebrafish microscopy data

T. Jejkal et al., LAMBDA – The LSDF Execution Framework for Data Intensive Applications, Proceedings PDP 2012.

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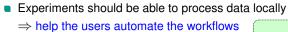
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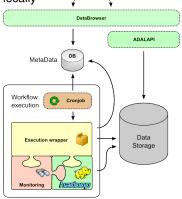




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### Microscopy data analysis

- Zebra-fish data sets
- Data imported with DataBrowser, meta-data added
- ImagingProjectGUI to define image analysis chain
  - based on operators from different libraries (VTK, ITK, Matlab,...)
  - creates sequence-XML, XML description of operators' chain
- User tags data for processing
  - using DataBrowser
  - associating sequence-XML
- Cron job starts execution based on tags
  - projectProcessor
- Executed in Hadoop cluster
  - result-XML stored
- Speedup of 60-120 depending on operators
  - I/O bound analysis

S. Pfeiffer, M. Mai, and J. Calliess, On the Computational Benefit of Tensor Separation for High-Dimensional Discrete Convolutions, Multidimensional Systems and Signal Processing 31, 2010, pp. 1-25.

J.C. Otte, S. Pfeiffer, T. Schenker, and C. Schmidt, Concept of multidimensional image analysis with flexible operators and cluster-computing, 6th European Molecular Imaging Meeting, Leiden, The Netherlands, 2011.

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### What's ahead?



Improved storage, network capacity: 6 PB in 2012

#### Investigate and deploy new technologies

- Data management system iRODS
- Object Storage
- Additional communities being integrated
  - Meteorology and climate research ("archival" quality)
  - Geophysics, seismology data
  - KATRIN experiment, neutrino mass
  - DARIAH, arts and humanities

#### **Project expansion**

to offer more community tailored support

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### **Concluding remarks**



- Infrastructure, 2 PB and storage services up and running
- First software tools available
- Experimental data being stored and processed
- Many scientific communities interested and getting involved

#### Focus on users, added value services

- Can't just "store files"
- Training for new tools, data management workflows
- Same problem at most (all?) research institutions
  - $\Rightarrow$  Open for new partnerships, international collaborations

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# **Questions?**

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