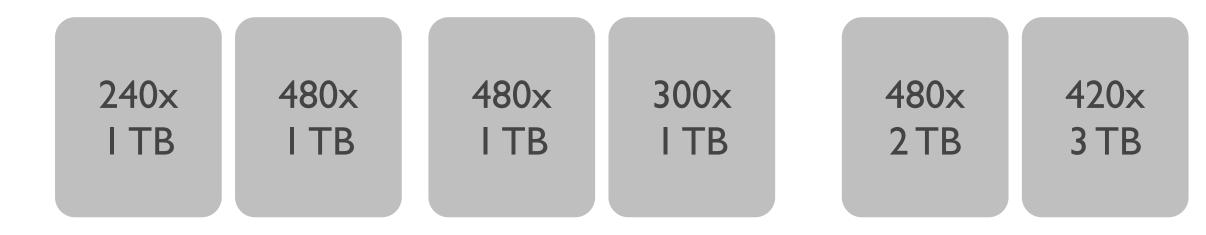
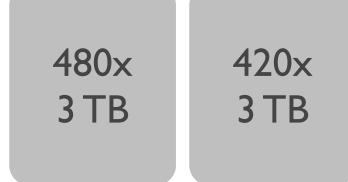
BioQuant's Large Scale Data Facility Usage Patterns, Problems, Solutions

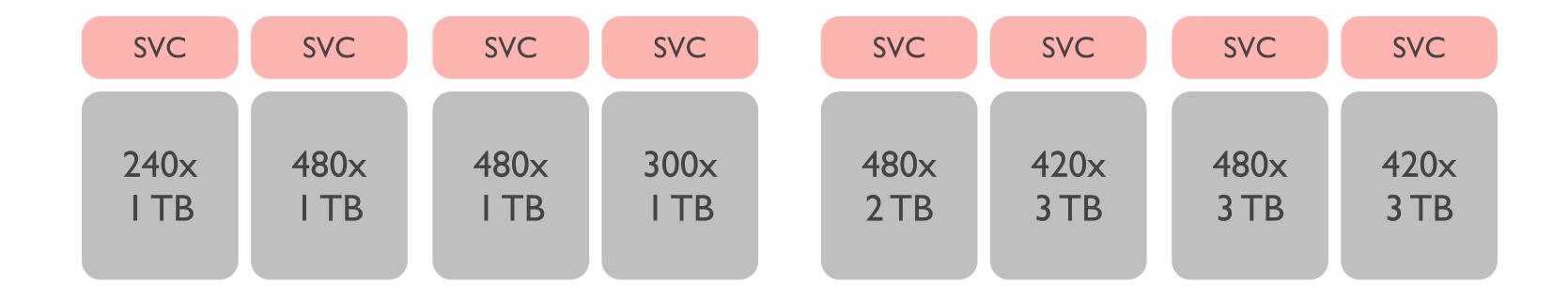
Christian Thiemann Marc Hemberger

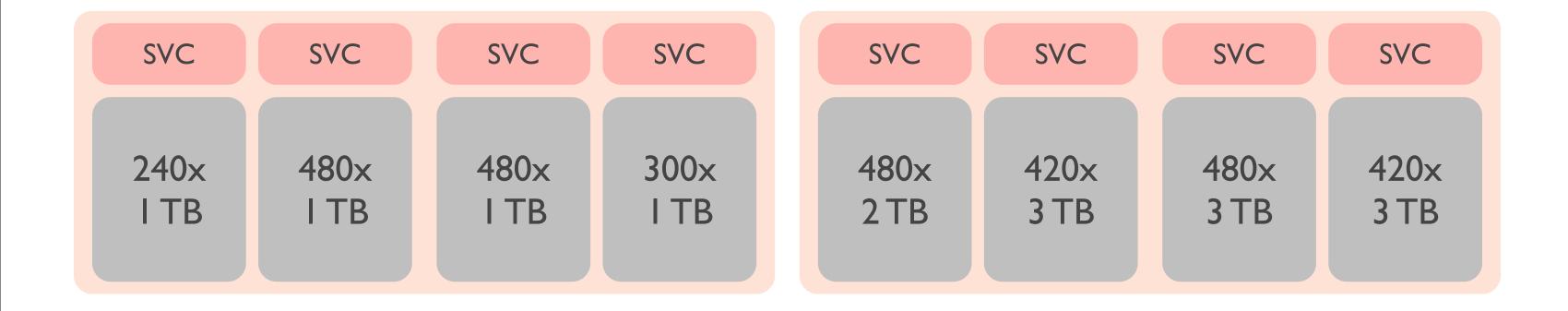
BioQuant IT, Ruprecht-Karls-Universität Heidelberg

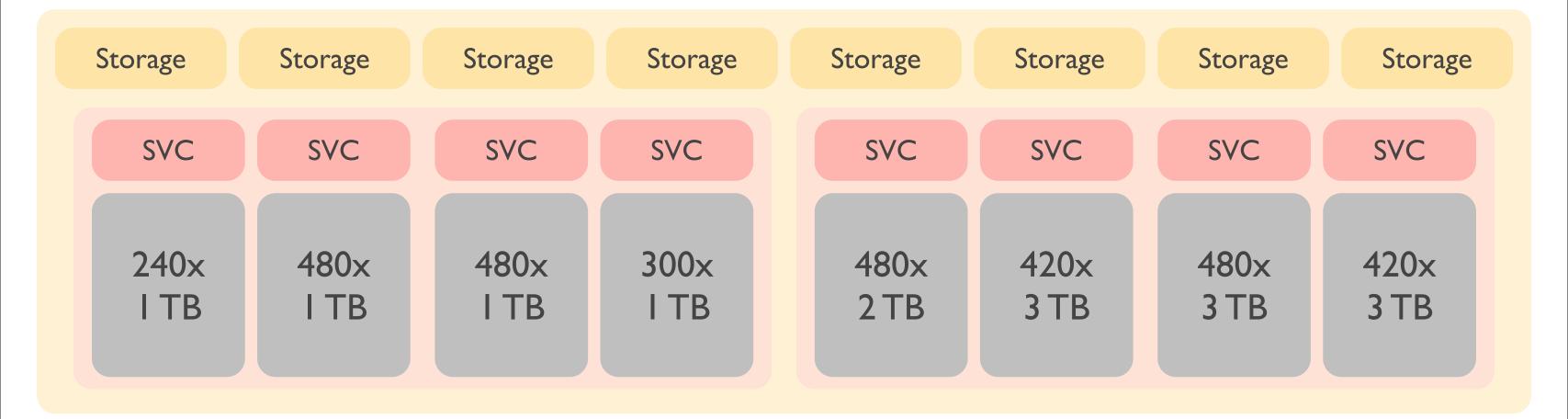
LSDMA 2013 Spring Meeting

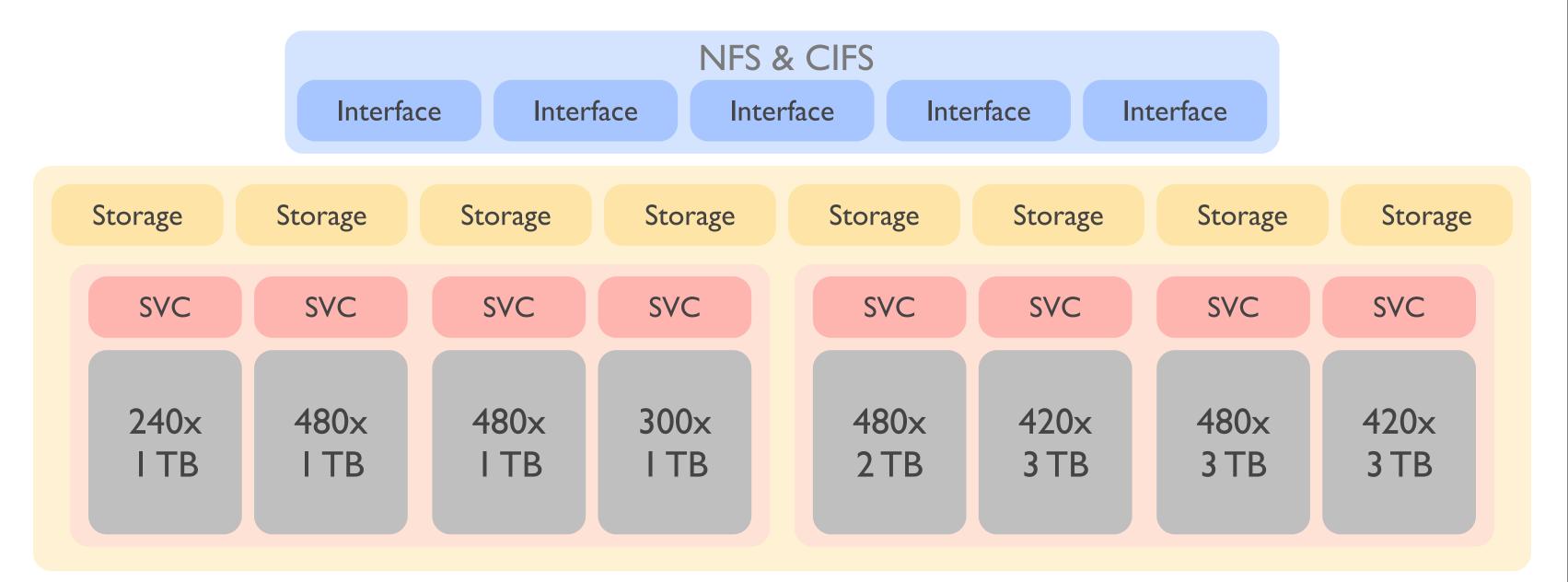


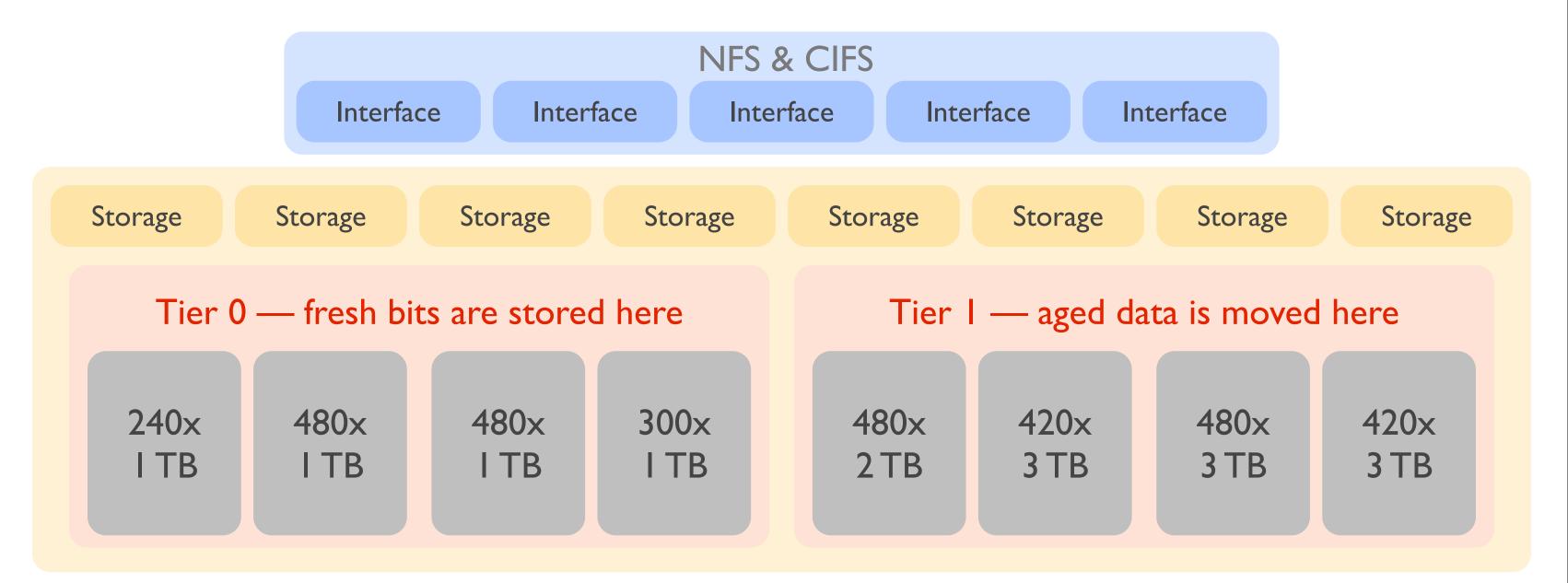


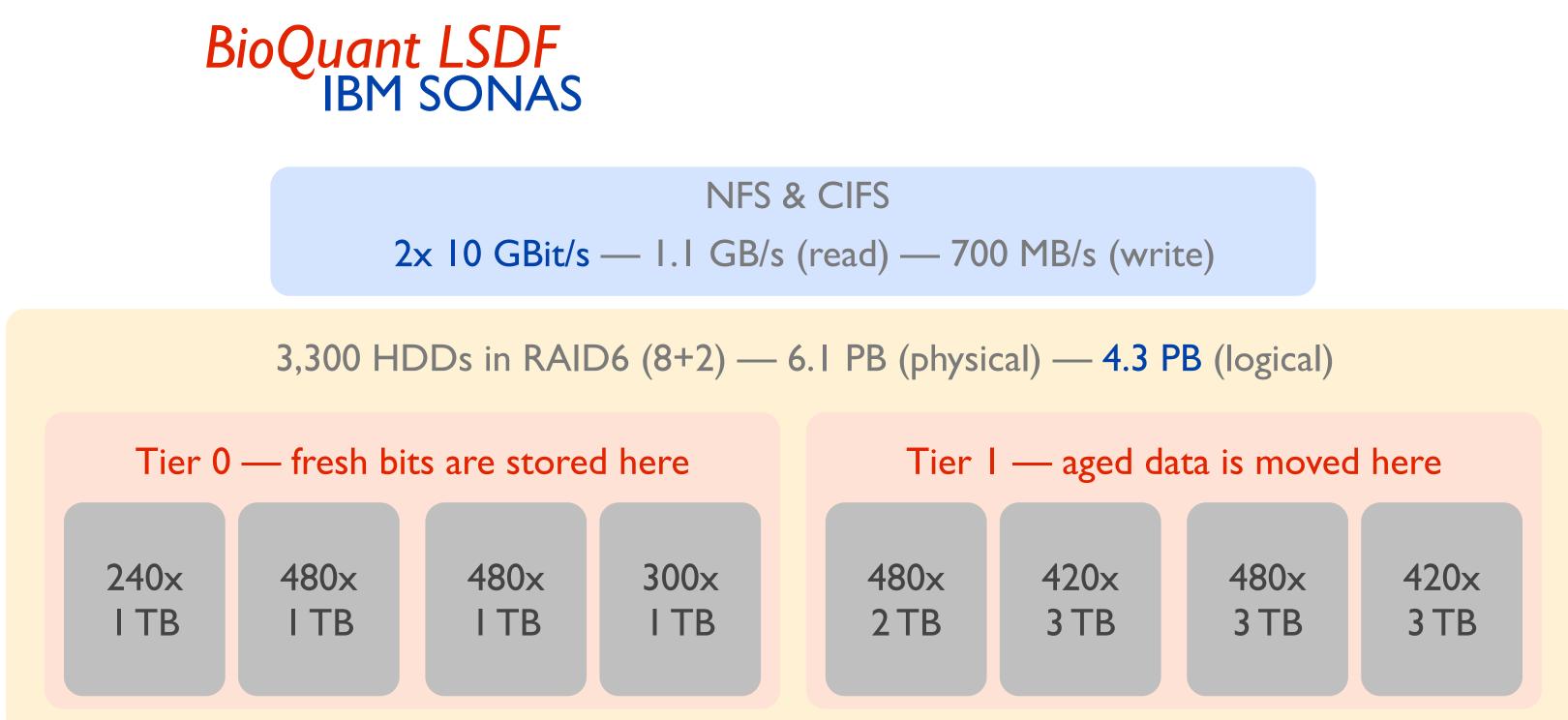






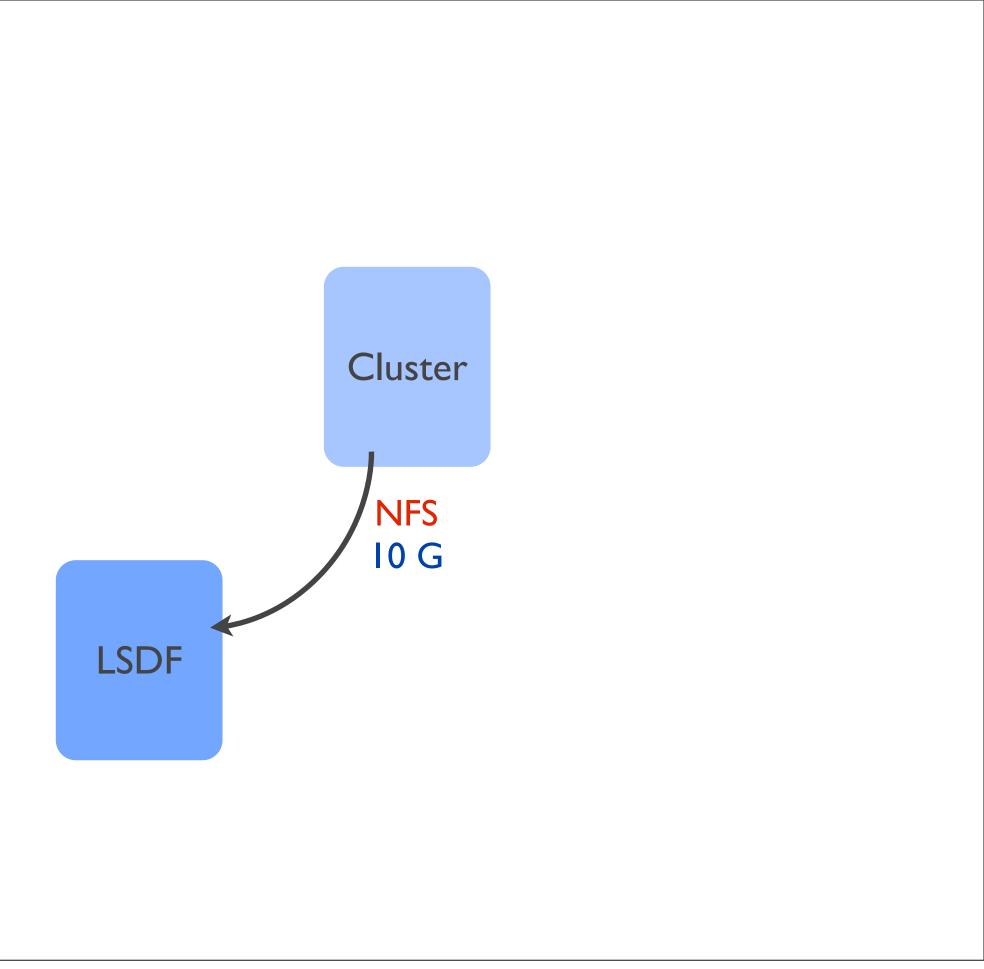


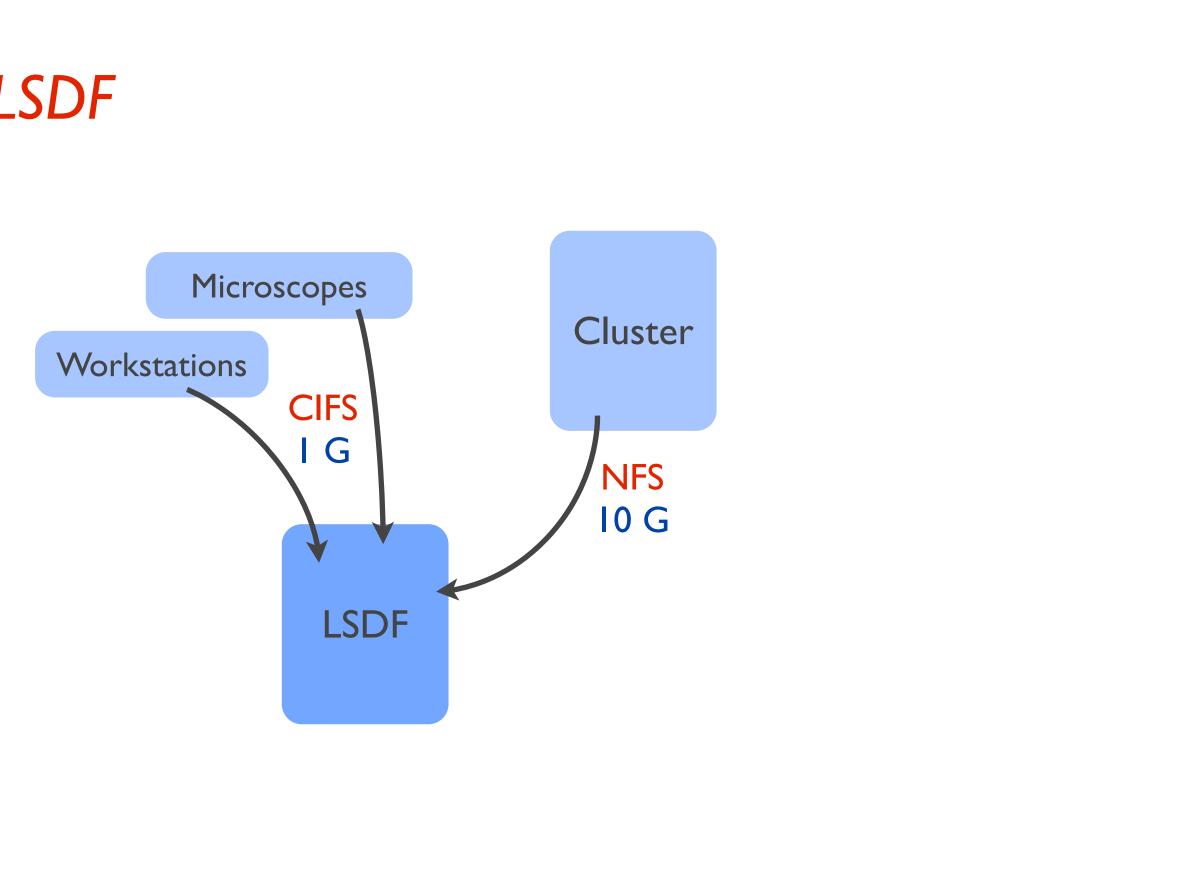


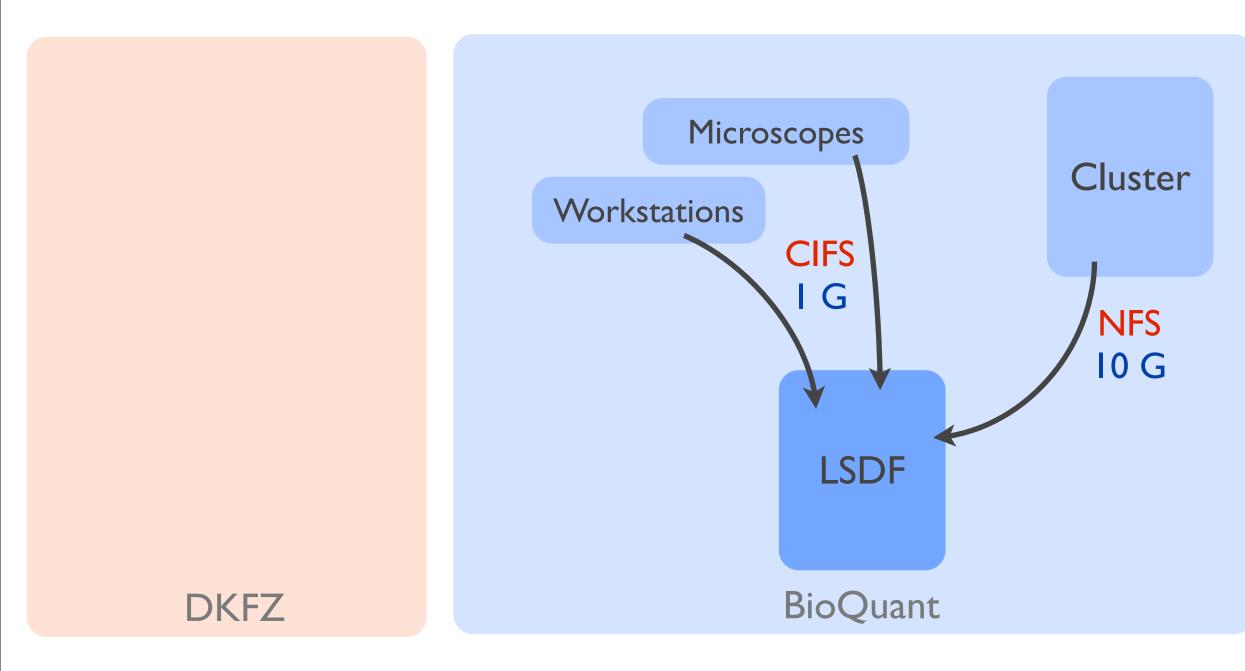


LSDF

Tuesday, March 12, 13

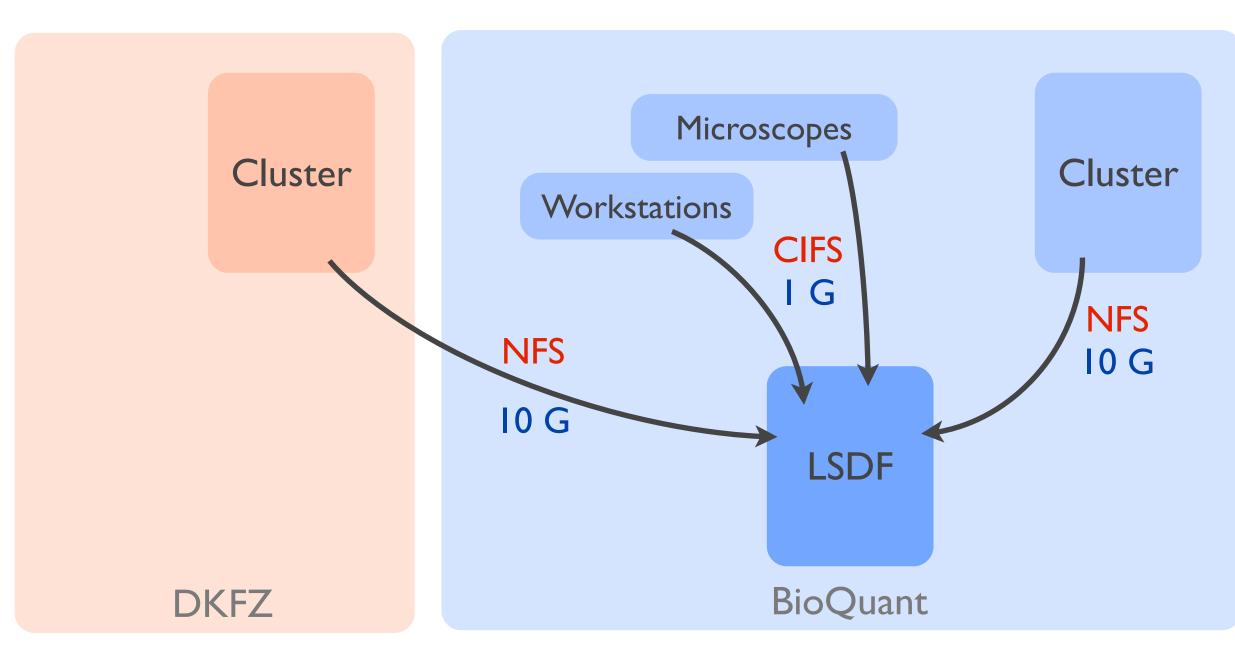






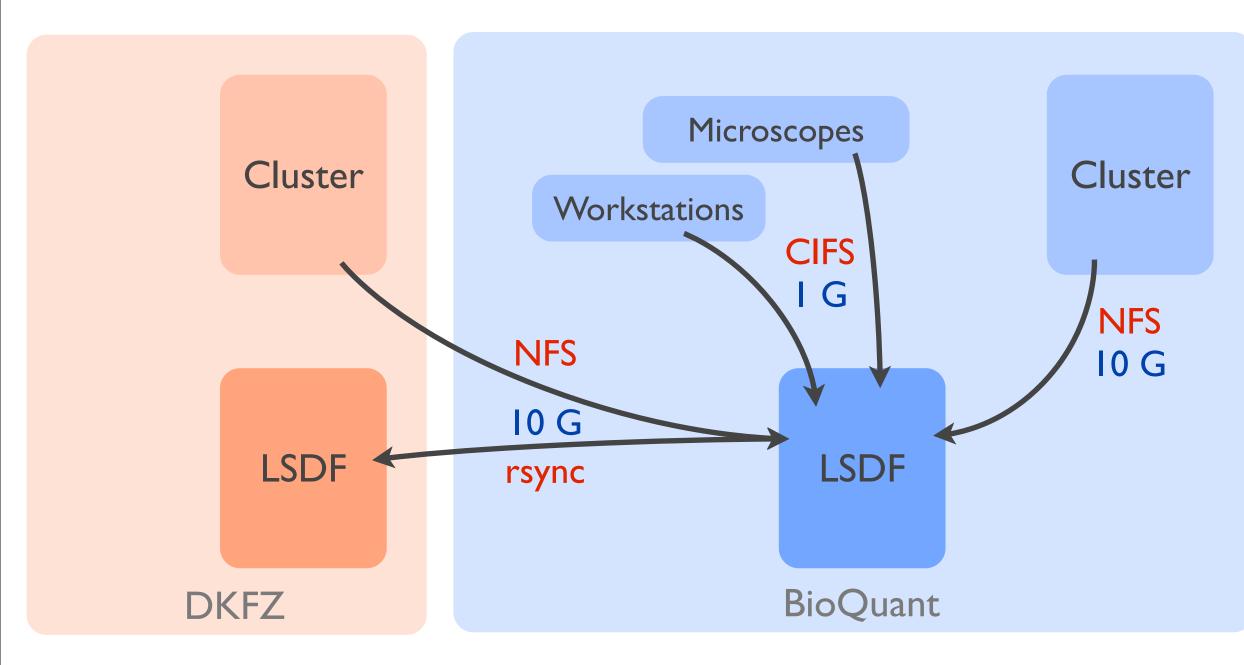
Tuesday, March 12, 13

KIT

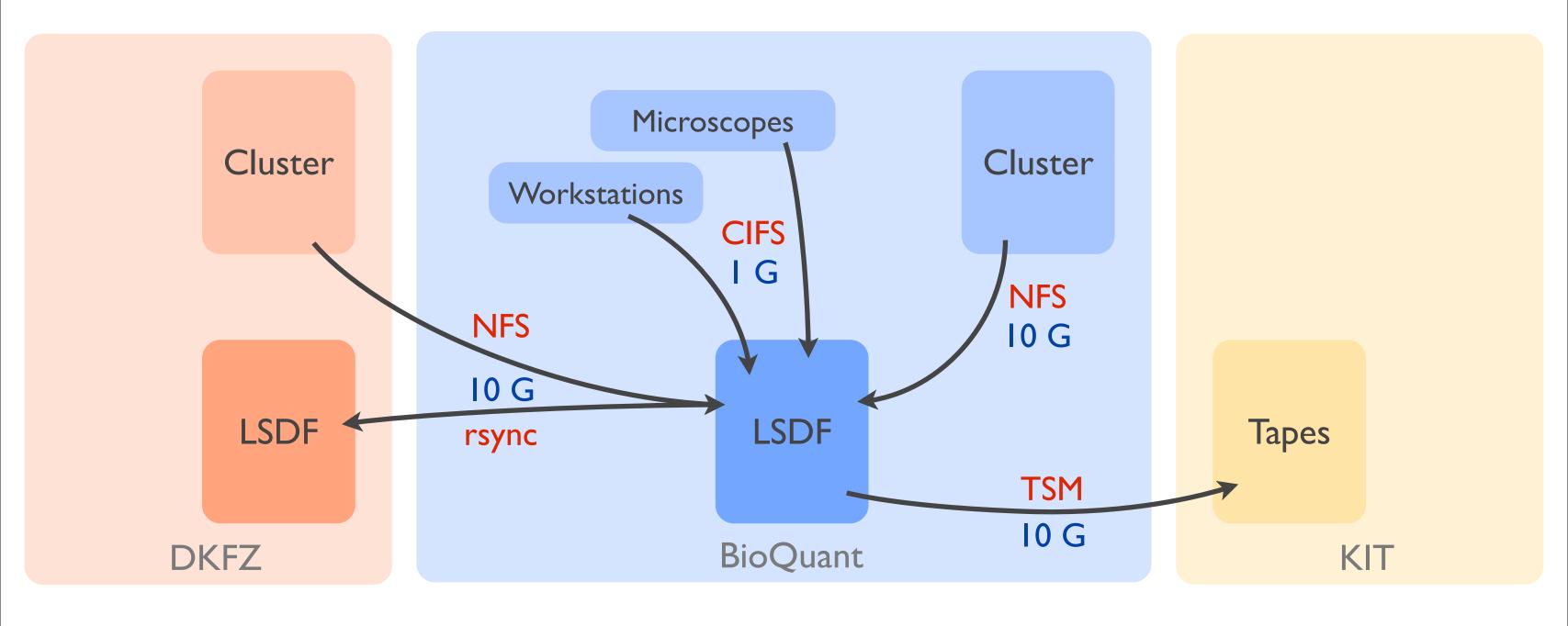


Tuesday, March 12, 13

KIT



KIT



Group Shares

Microscopy

- Group Shares ~ 80 TB
- Microscopy ~ 70 TB
 - Sequencing I.3 PB

- Group Shares ~ 80 TB
- Microscopy ~ 70 TB
 - Sequencing I.3 PB
 - total I.6 PB

Group Shares

Microscopy



Group Shares

RNA interference

Microscopy

Group Shares

RNA interference

Microscopy

image size ~ 2 MB

Microscopy

RNA interference

image size ~ 2 MB

~ 2,000 images per sample / run future runs up to 70,000 images

Tuesday, March 12, 13

Microscopy

RNA interference

image size ~ 2 MB

- ~ 2,000 images per sample / run future runs up to 70,000 images
 - many samples per study / experiment "typical" throughput: 20,000 images per day

peak throughput: 3,000,000 images (3 TB) in three weeks

Microscopy

RNA interference

image size ~ 2 MB

~ 2,000 images per sample / run future runs up to 70,000 images

many samples per study / experiment "typical" throughput: 20,000 images per day

peak throughput: 3,000,000 images (3 TB) in three weeks

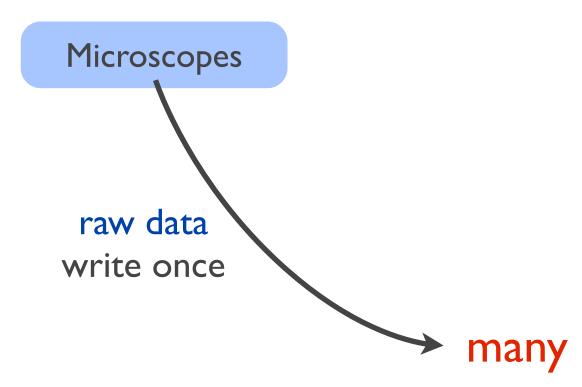
Microscopy

Tuesday, March 12, 13

Group Shares

Microscopy

Sequencing

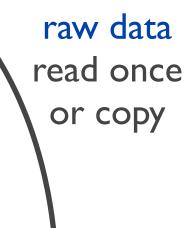


Group Shares

Microscopy

Sequencing

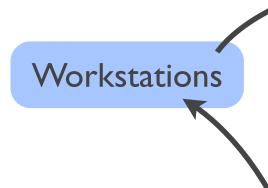


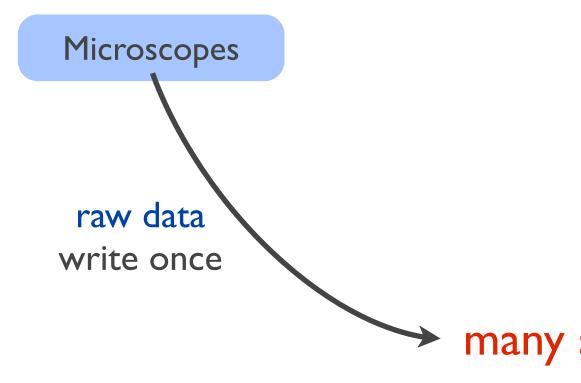


Group Shares

Microscopy

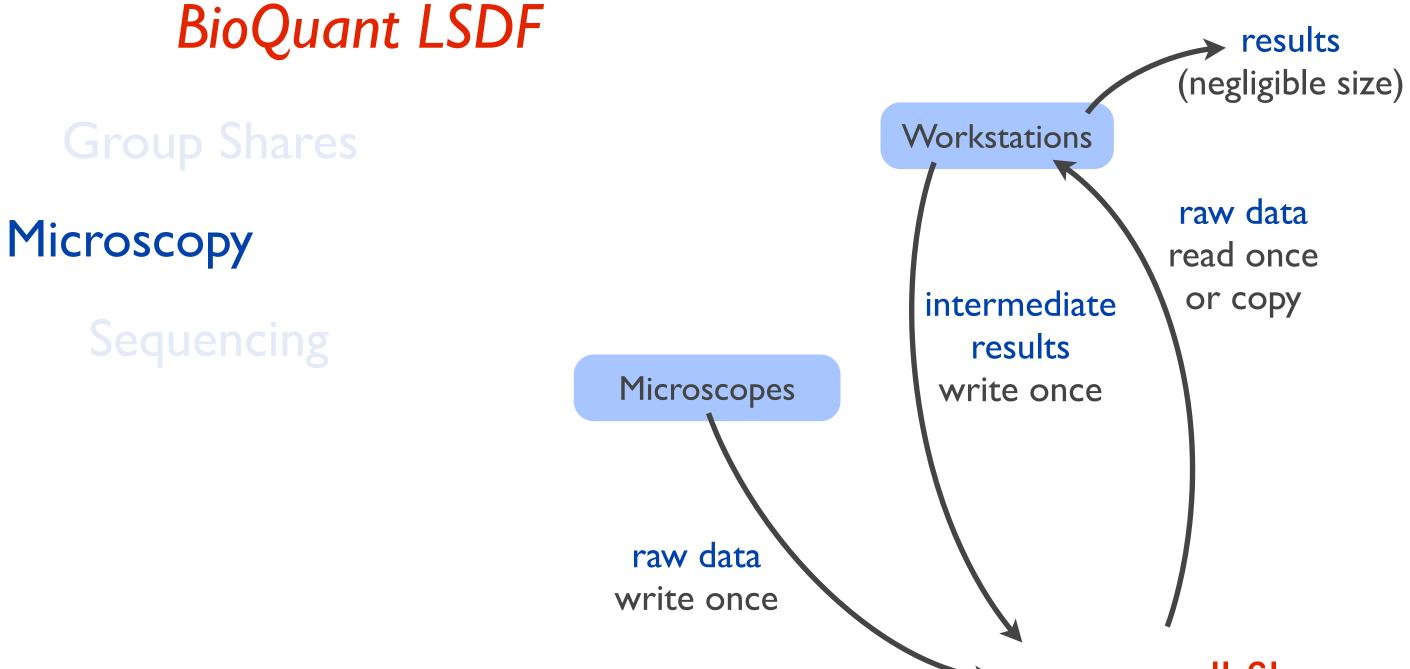
Sequencing





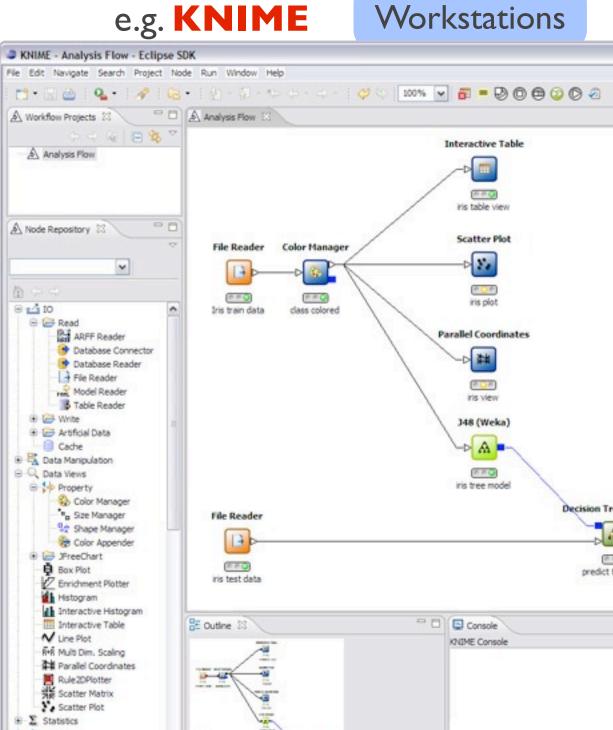


raw data read once or copy



Group Shares

Microscopy





00	A Node Description 2	
	ST wooe perception 12	6
	Scorer	ĺ
	Compares two columns by their attribute value pairs and shows the confusion matrix, i.e. how many rows of which attribute and their classification. Additionally, it is possible to hilight cells of this matrix to determine the data rows that have been predicted wrongly. The dialog allows you to select two columns to compare; the values from the first selected column are represented in the confusion matrix's rows and the values from the second column by the confusion matrix's columns. The output of the node is the confusion matrix.	
	Ports Data Input	
	0 Table containing at least two columns to compare.	
Predictor Scorer	Data Output	
	0 The confusion matrix.	l
t data score prediction	Views	
	Confusion Matrix Displays the confusion matrix	6
	G. 🖬 🖻 🗒 · 📬	C

Group Shares

Microscopy

Group Shares

International Cancer Genome Consortium

Microscopy

International Cancer Genome Consortium

~ 200 GB raw data per genome

Sequencing

International Cancer Genome Consortium

~ 200 GB raw data per genome

~ 2 TB after processing intermediate results are retained



Sequencing

International Cancer Genome Consortium

~ 200 GB raw data per genome

~ 2 TB after processing intermediate results are retained

throughput: 10–20 genomes per week



Sequencing

International Cancer Genome Consortium

~ 200 GB raw data per genome

~ 2 TB after processing intermediate results are retained

throughput: 10–20 genomes per week

total $\sim 2 \text{ PB of data}$ ~ I PB at BioQuant LSDF



Sequencing

International Cancer Genome Consortium

~ 200 GB raw data per genome

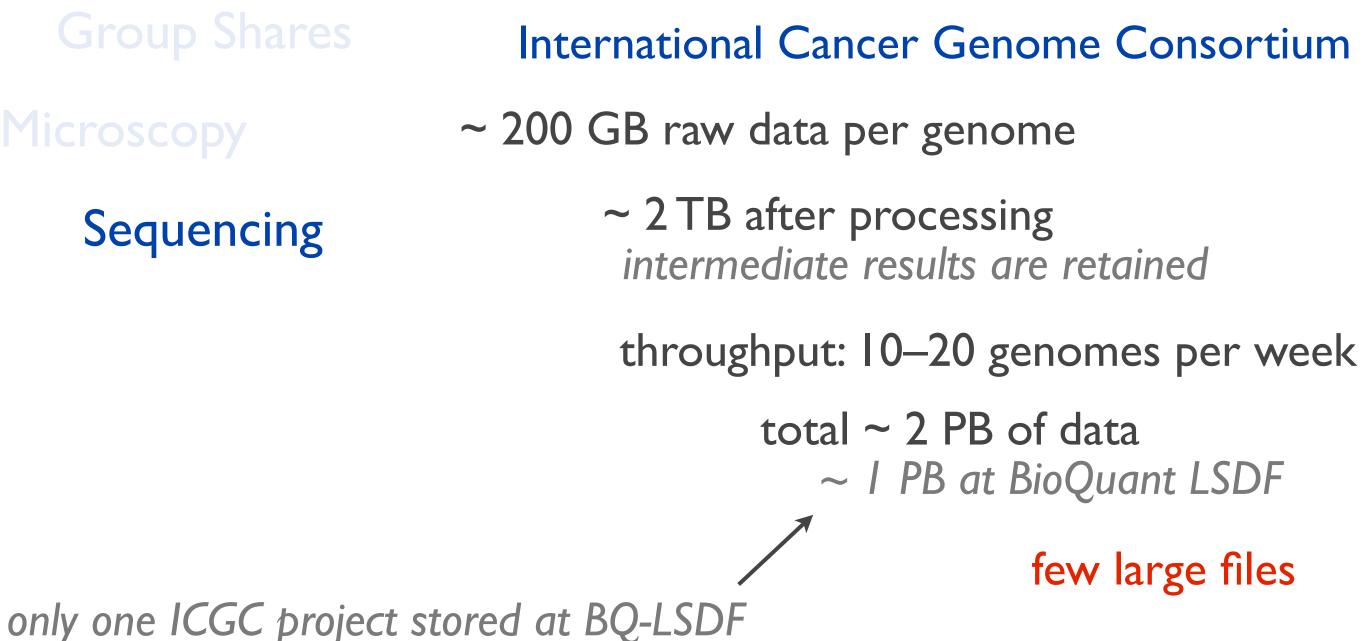
~ 2 TB after processing intermediate results are retained

throughput: 10–20 genomes per week

total $\sim 2 \text{ PB of data}$ ~ I PB at BioQuant LSDF



- few large files



Sequencing

International Cancer Genome Consortium

~ 200 GB raw data per genome

~ 2 TB after processing intermediate results are retained

throughput: 10–20 genomes per week

total $\sim 2 \text{ PB of data}$ ~ 1 PB at BioQuant LSDF

different "views" of same data via symbolic links



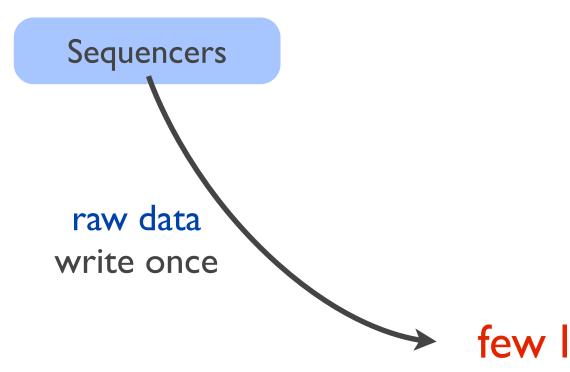
- few large files

Sequencing

Group Shares

Microscopy

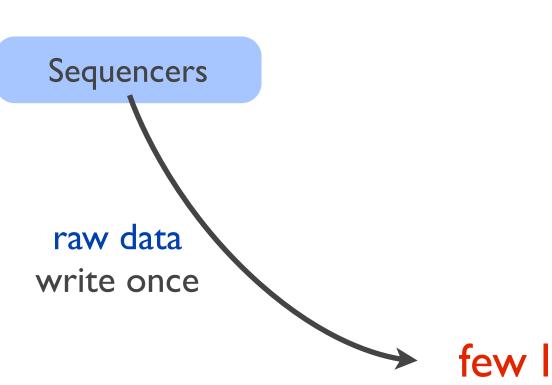
Sequencing



Group Shares

Microscopy

Sequencing



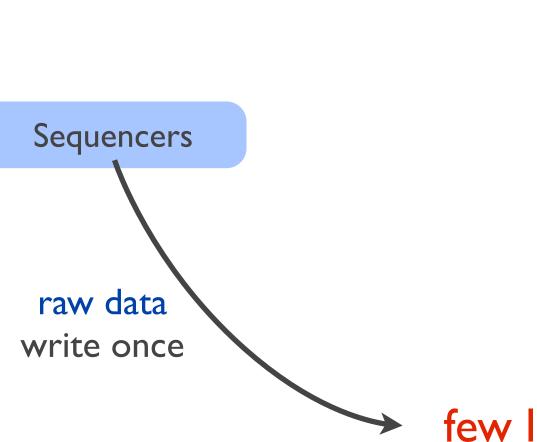
Cluster

raw data & temp data read often

Group Shares

Microscopy

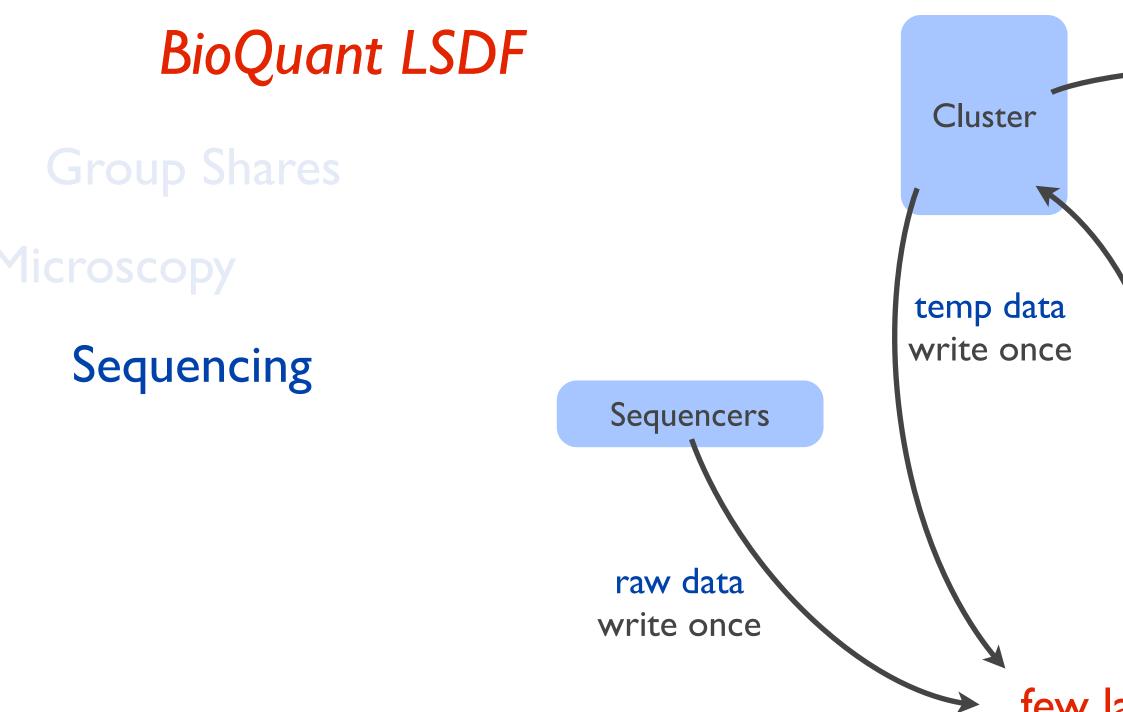
Sequencing



Cluster

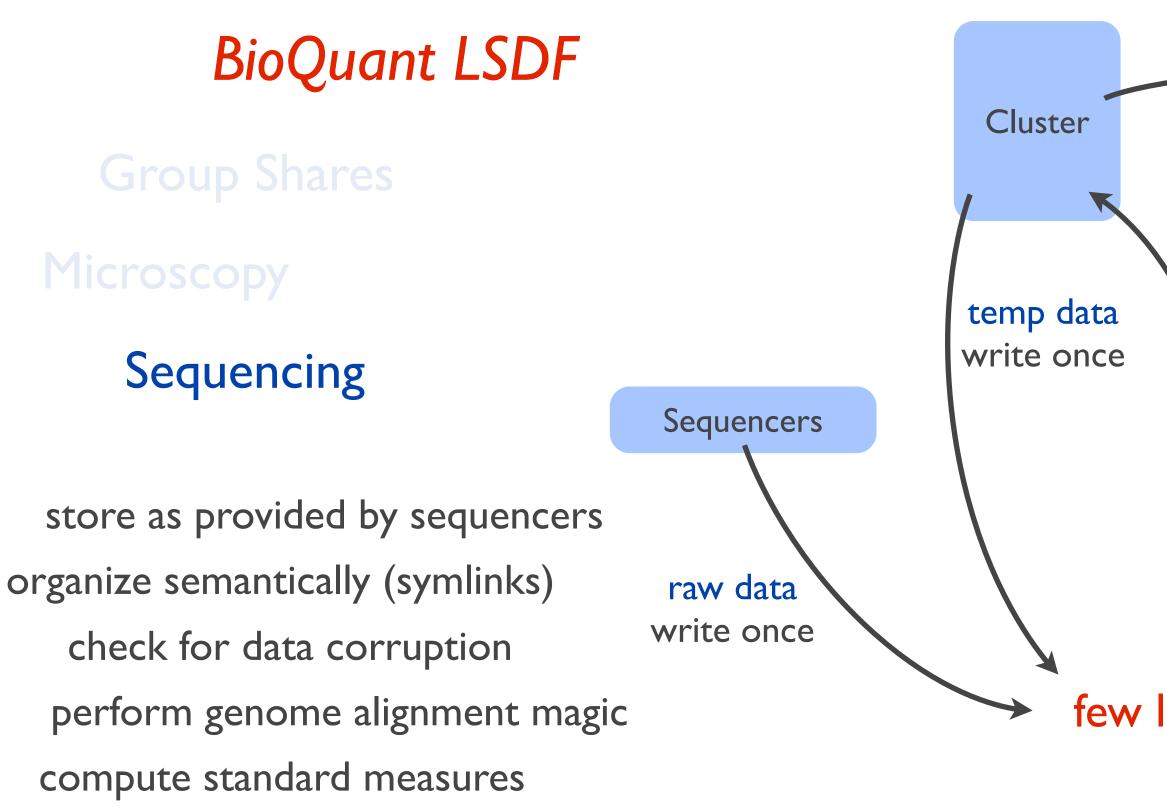
results (negligible size)





results (negligible size)





Tuesday, March 12, 13

results (negligible size)



Cluster

Group Shares

Microscopy

Sequencing One Touch Pipeline

Sylwester Radomski, DKFZ

Home	Overview Individuals Sequen	ces Runs	Progress Processes Ru	n Submit Logout		
	Vorkflows					
Enable auto		0 Count	Count of Failed	Last Success	Last Failure	Duration
	- mergedBamDiscoveryWorkflo	<u>w</u> 0			÷	-
0	FileSystemConsistencyWorkf	<u>low</u> 78		02:51:20 AM		1 h 51 min
0	BwaAlignmentWorkflow	100	<u>52</u>	Sat Dec 22 2012	Sat Dec 22 2012	1 day(s) 13 h
0	FastqcSummaryWorkflow	266		Wed Feb 27 2013	а-	660 msec
0	FastqcWorkflow	2615	<u>153</u>	Wed Feb 27 2013	Tue Feb 05 2013	1 h 31 min
0	runUnpack	2		Thu Oct 18 2012	(e	2 sec 539 msec
0	DataInstallationWorkflow	401	1	Wed Feb 27 2013	Thu Feb 21 2013	19 h 56 min
0	createSeqScan	3898	35	Tue Feb 26 2013	Tue Feb 19 2013	752 msec
0	DataLocationWorkflow	855	<u>44</u>	Fri Oct 12 2012	Fri Oct 12 2012	851 msec
	IoadMetaData	1062	Z	Tue Feb 26 2013	04:42:02 PM	1 min 43 sec

results (negligible size)

Cluster

Shares

Microscopy

Sequencing One Touch Pipeline



ist of Runs								
						Search:		
Name	Center	Storage Realm	Date Created	 Date Executed 	Blacklisted	Multiple Source	Fastqc	\$
130213 SN952 0141 BC1PB8ACXX	dkfz		2013-02-27 04:04:04	1	false	false	NaN	
130212 SN509 0208 BC1R00ACXX	dkfz	dkfz	2013-02-26 01:02:28	2013-02-12	false	false	0.82	
130212 SN509 0207 AD1U4CACXX	dkfz	dkfz	2013-02-26 12:24:40	2013-02-12	false	false	0.80	
130206 SN143 0612 BD1H8EACXX	gatc	bioquant	2013-02-26 10:56:42	2013-02-06	false	false	0.84	
130103 SN509 0201 AC1BVCACXX	dkfz	bioquant	2013-02-25 11:42:06	2013-01-03	false	false	0.83	
NG-6166 Exome Data batch22	gatc	dkfz	2013-02-22 11:48:39		false	false	NaN	
130201 SN486 0373 AC1C15ACXX	gatc	dkfz	2013-02-22 10:04:44	2013-02-01	false	false	NaN	
30205 SN7001397 0049 AC1PLNACXX	dkfz	bioquant	2013-02-21 12:53:22	2013-02-05	false	false	0.86	
30205 SN7001153 0110 BD1RYKACXX	dkfz	bioquant	2013-02-21 12:44:56	2013-02-05	false	false	0.78	
130205 SN 1007 0135 AD 1U 5MACXX	dkfz	bioquant	2013-02-21 11:10:14	2013-02-05	false	false	0.83	
130129 SN486 0372 BD1GWAACXX	gate	bioquant	2013-02-21 10:28:23	2013-01-29	false	false	0.75	
130205 SN 1007 0136 BD 1TBBACXX	dkfz	mixed	2013-02-19 11:51:28	2013-02-05	false	false	0.83	
30130 SN7001103R 0108 BD1N9DACXX	dkfz	bioquant	2013-02-19 11:13:45	2013-01-30	false	false	0.86	
30130 SN7001393 0039 BC1NMCACXX	dkfz	bioquant	2013-02-18 02:10:51	2013-01-30	false	false	0.81	
30130 SN7001103R 0107 AD1T8YACXX	dkfz	bioquant	2013-02-18 12:11:44	2013-01-30	false	false	0.86	
130129 SN7001153 0107 AC1K37ACXX	dkfz	bioquant	2013-02-18 12:07:34	2013-01-29	false	false	0.86	
30131 SN952 0138 AD1J8WACXX	dkfz	mixed	2013-02-18 11:06:32	2013-01-31	false	false	0.64	
30129 SN7001149 0123 BC1PMDACXX	dkfz	bioquant	2013-02-18 10:58:10	2013-01-29	false	false	0.80	
30103 SN952 0135 BD1H60ACXX	dkfz	dkfz	2013-02-15 04:00:00	2013-01-03	false	false	0.81	
30131 SN952 0139 BC1R14ACXX	dkfz	mixed	2013-02-14 10:13:00	2013-01-31	false	false	0.75	
30131 SN7001177 0109 AD1NUKACXX	dkfz	dkfz	2013-02-12 03:23:13	2013-01-31	false	false	0.62	
30129 SN509 0206 BC1K3GACXX	dkfz	dkfz	2013-02-12 03:19:10	2013-01-29	false	false	0.64	
30129 SN509 0205 AD1T51ACXX	dkfz	dkfz	2013-02-12 03:17:51	2013-01-29	false	false	0.61	
130122 SN7001397 0048 BC1DG4ACXX	dkfz	bioquant	2013-02-12 11:09:37	2013-01-22	false	false	0.86	
120122 SN2001207 0047 AD112DACVV	duta	hisauant	2012 02 12 11:02:25	2012.01.22	falso	falsa	0.95	

results (negligible size)

Cluster

Group Shares

Microscopy

Sequencing One Touch Pipeline



Home	e Overview	Individuals	Sequences	Runs	Progress	Processes	Run Submit	Logout
Run d	etails							
Gener	al							
		Name	130206_SN 143	_0612_BD	1H8EACXX			
	Sequenci	ng Center	gatc					
	Sequencing Te	chnology	HiSeq2000					
	Date	Executed	2013-02-06					
	Dat	e Created	2013-02-26 10:5	6:42.65				
	Meta	Data Path	/icgc/lsdf/ftp/ga	tc/				
	Final I	Locations	/icgc/lsdf/projec	t//pedbrair	n/pa/sequenci	ing//whole_gend	me_sequencing/	'gatc/
Proce	ssing							
	DataInstallation	Workflow	Show Details					
	load	MetaData	Show Details					
	FastqcSummary	Workflow	Show Details					
	Data Files							
	130206_SN 143	_0612_BD1	H8EACXX_fasto	ı.tsv				
	8 PABL94 CONTRO WHOLE_GENOME			insert	size: 278			number of b
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	- s <u>s 8 2 s</u> e	equence.txt.	gz	astroc	ytome	🛩 meta-data	🛩 Isdi	🛩 linked
	Files not used:							
	chPipeline Eils Labs		uid: 19h9cc9 (produc	tion/1.9)				

results (negligible size)

				previous run	next run
		2013-02-26		true	
f base	pairs: 37.7 G				
	16.5 GB	2013-02-27	FastQC	(7/4/0)	
	16.8 GB	2013-02-27	FastQC	(8/3/0)	

BioQua



Microscopy

Sequencing Cluster Monitoring

Rolf Kabbe, DKFZ

Rolf Kabbe TBI / eilslabs

02/07/13 | Page 18

Showing details of jobs

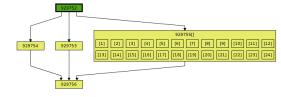
Tbi-cluster

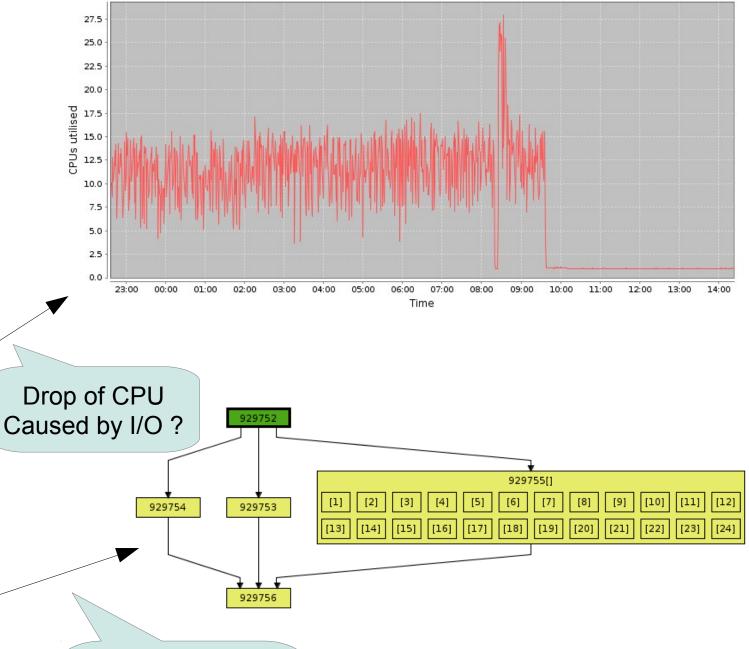
Logged in : Rolf Kabbe | Log out

Active jobs Completed jobs Nodes Job categories Projects Preferences Admin About

Showing details for job : 929752

Use as MinJobId Use as MaxJobId Modify this lob Delete Job Purge Job Extend Walltime Requested and used resources wangq LINA463K_LINA463K_merge_removedup LINACOST_ /LIN463K_IUI12112_INV0/DI33_0095_DI1664CAX_2.ml0qb.bani./rgg/isu/inib/alaiysis/Lin44alaiysis /DKFZLSDF/results_per_pid/LIN463K_temp/alignment /LIN463K_run121127_SN952_0127_AD1HC5ACXX_6.rmdup.bam:/icgc/isdf/mb/analysis/LiN4/analysis /DKFZLSDF/results_per_pid/LIN463K_temp/alignment /LIN463K_run130117_SN7001149_0121_BD1320ACXX_2.rmdup.bam:/icgc/isdf/mb/analysis/LiN4/analysis Submit arguments /LINA463K_run130117_SN7001149_0121_BD1120ACXX_2.rmdup.bam:/lcgc/lsdf/mb/analysis/LiNA/analysis /DKF2LSDF/results_per_jpd/LINA463K_temp/alignment /LINA463K_run130117_SN7001149_0121_BD1120ACXX_3.rmdup.bam:/lcgc/lsdf/mb/analysis/LiNA/analysis /DKF2LSDF/results_per_jpd/LINA463K_temp/alignment /LINA463K_run130117_SN7001149_0121_BD1120ACXX_4.rmdup.bam,OUTPUT_BAM=/lcgc/lsdf/mb/analysis /LINA463K_run130117_SN7001149_0121_BD1120ACXX_4.rmdup.bam,OUTPUT_BAM=/lcgc/lsdf/mb/analysis /LINA463K_Slanes_merged.rmdup.bam,METRICS_FILE=/lcgc/lsdf/mb/analysis/LINA/analysis/DKF2LSDF /results_per_jpd/LINA463K_temp/alignment/LINA463K_Slanes_merged.rmdup.bam.dupmark.rewtrics_txt /home/wangq/SVNrepository/ngs2/branches/pipelines/QCPipeline_BSseq/analysis_tools/MergeBAM_MarkDup.sh verylong Job Type BATCH Status RUNNING Queued Tue Feb 5 22:37:09 2013 Started Tue Feb 5 22:37:09 2013 Ended Exit Code Start count Exec Host tbi-dsx08 50:00:00 Requested wal Elapsed walltime 15:45:47 CPU time 135:19:48 CPU time / core 135:19:48 CPUs avg. utilised 8.59 Cores Memory Requested 5 0 GB Maximum Memory Used 4.4 GB Memory Efficiency 0.89 File Size 250.0 GE Job Categor wangq:LINA463K-LINA463K-merge-removedup:cores=1:mem= 5.0 GB:walltime=5 **CPU** profile ACTIVE BEFOREOK 929753 ACTIVE BEFOREOK 929755[] ACTIVE BEFOREOK 929754 SEVERE More CPU-time used (135:19:48) than expected (15:45:47), ratio : 8.59 SPECIFICATION INFO PBS will prevent that this job can create files larger than 250.0 GB





Dependency-graph Shows progress of workflows



CPU profile

BioQual

iCHIP Web - Image result for gene query - Mozilla Firefox

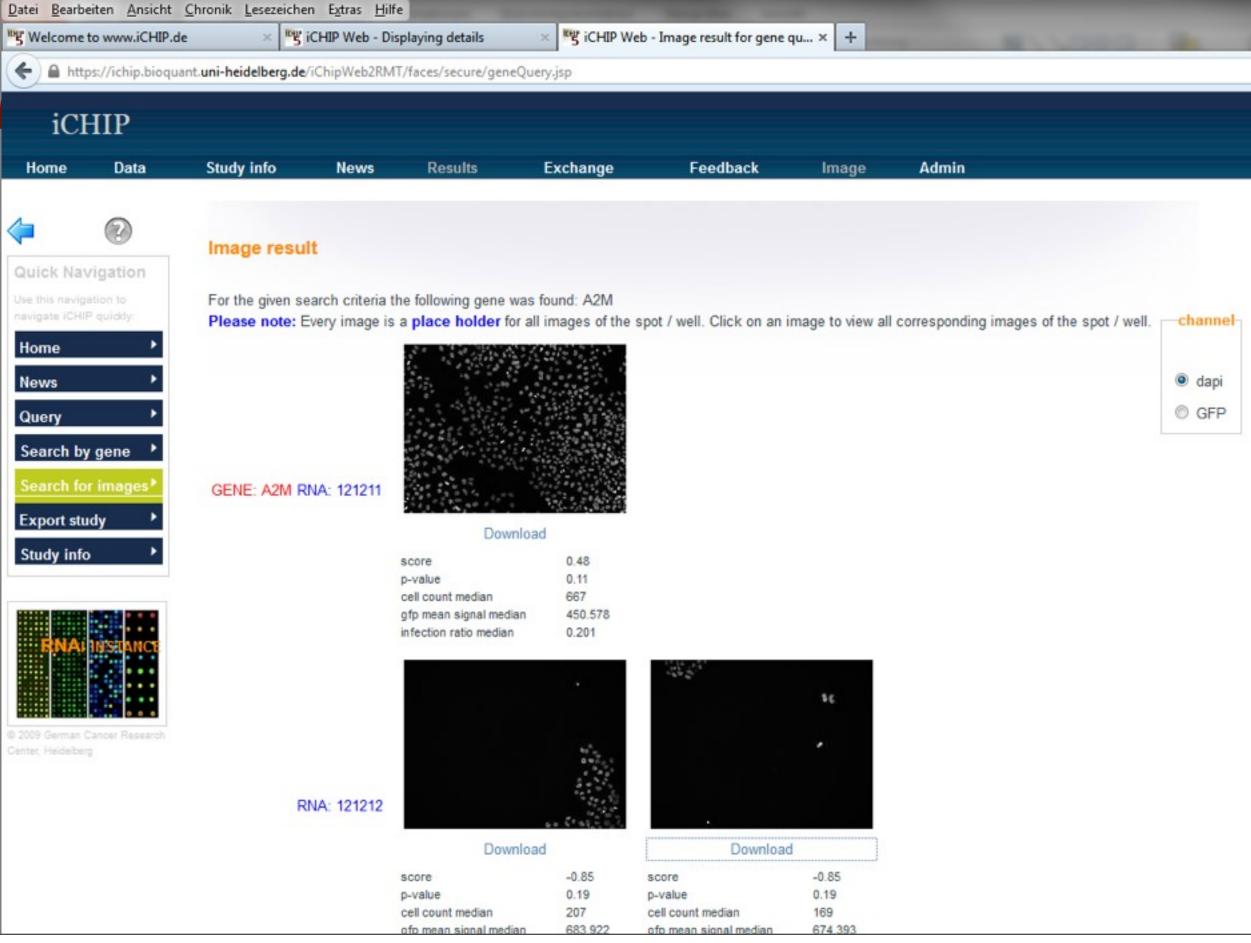
Group Shares

Microscopy

Sequencing

Results Database

Jürgen Eils, DKFZ



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BioQua Group Shares

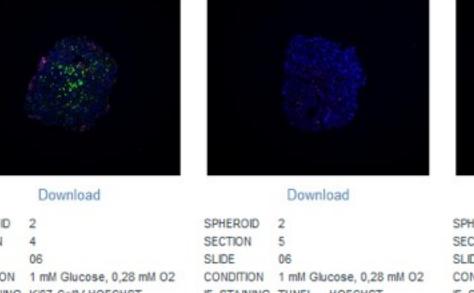
Microscopy

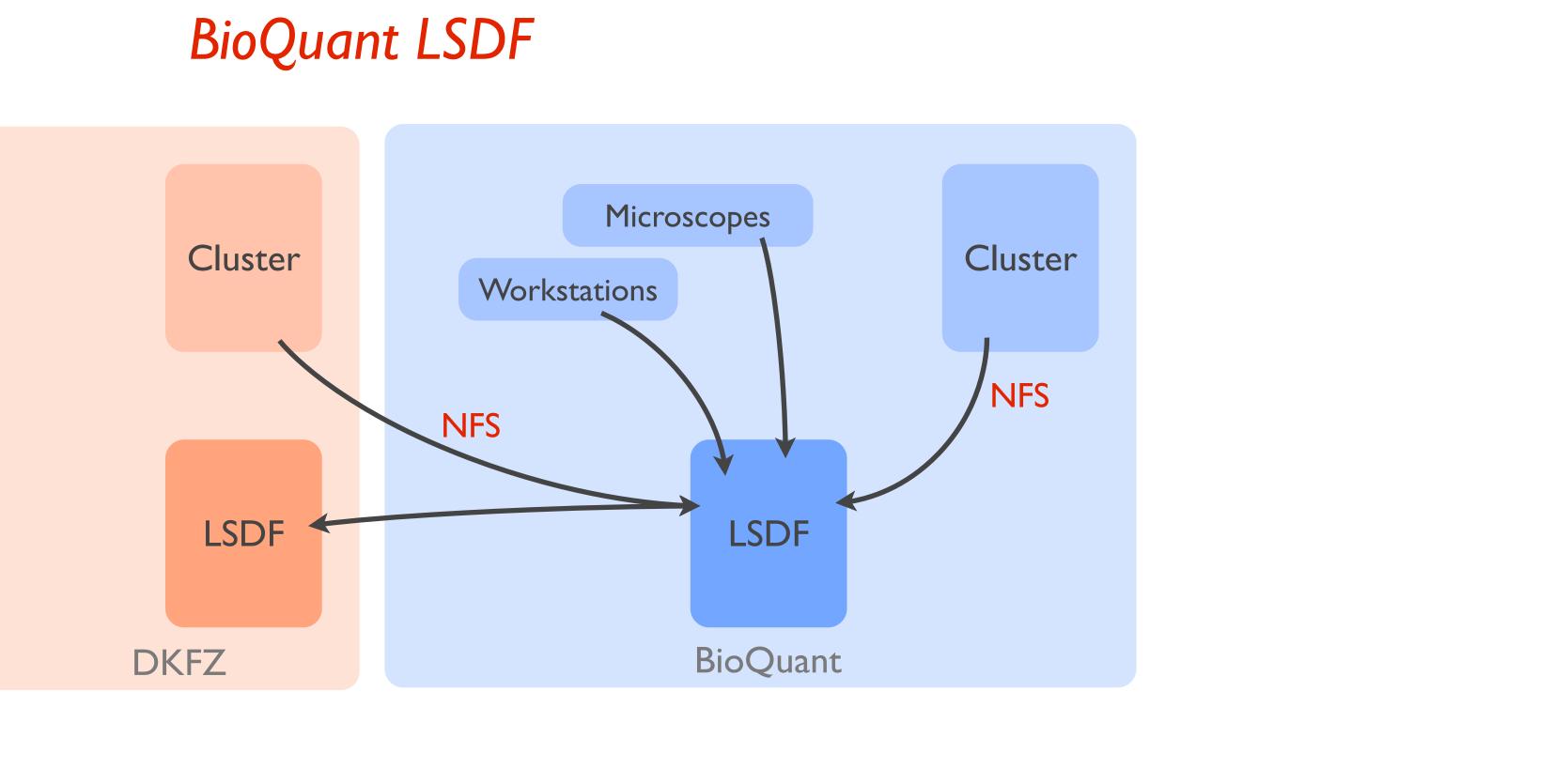
Sequencing

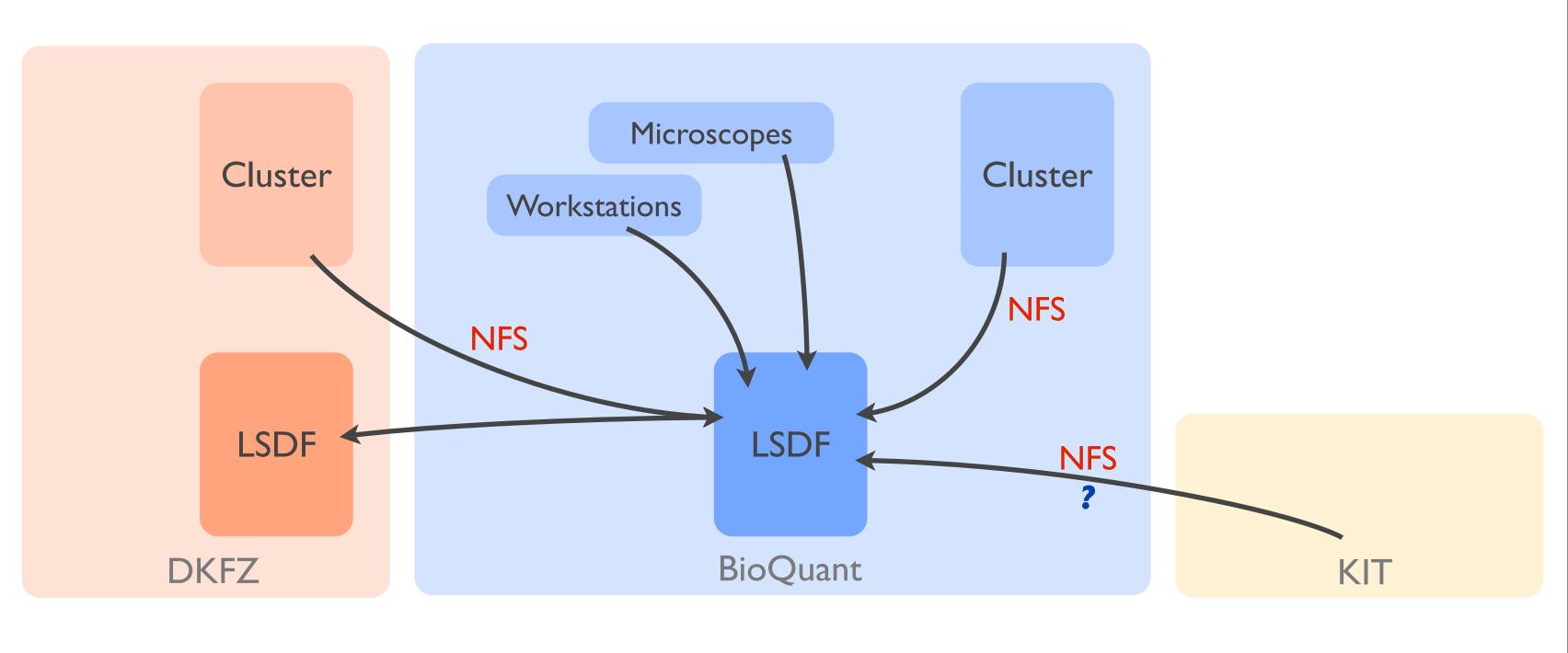
Results Database



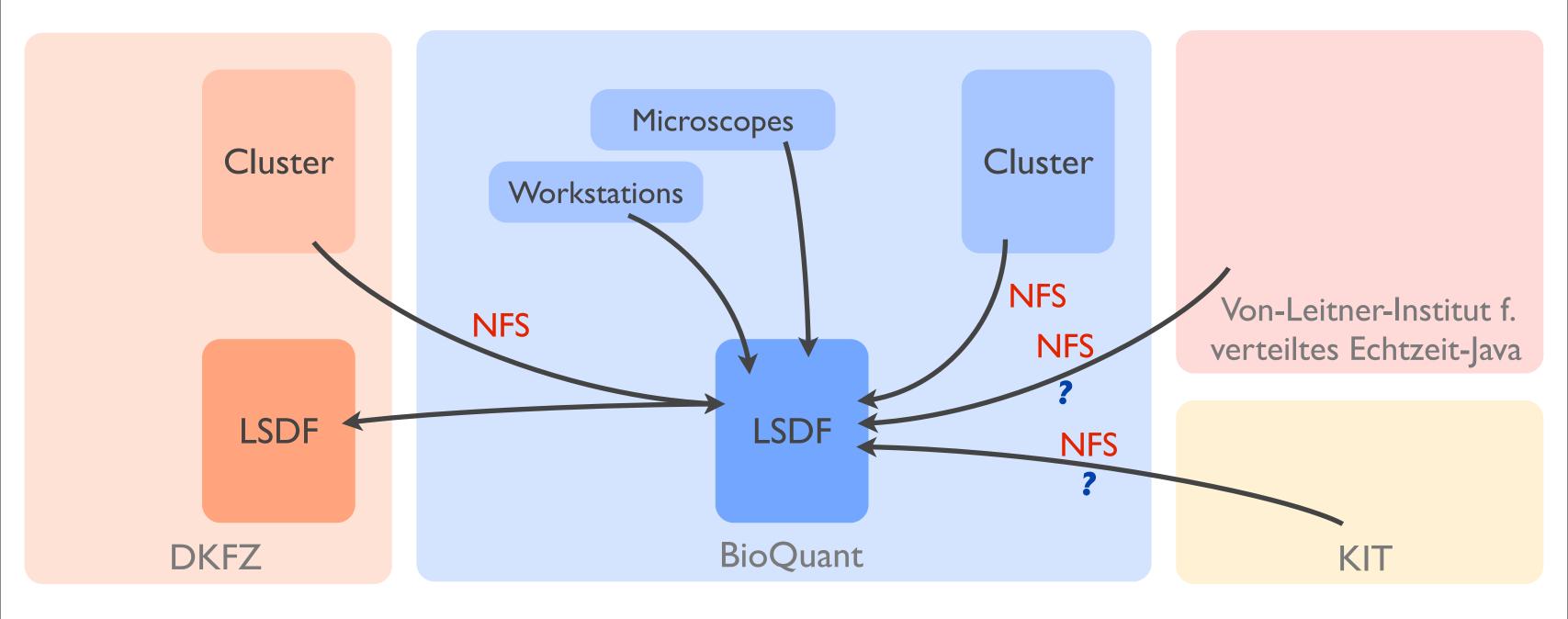
iCHIP Web - Displaying deta	ails - Mozilla Firefox				
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+ https://services.ichip.	.de/web/faces/secure/entityDetail.jsp				
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Study info					
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	SPHEROID 2 SECTION 2	SPHEROID 2 SECTION 3	SPHEROID 2 SECTION 4	SPHEROID 2 SPHER SECTION 5 SECTION	
	SLIDE 06	SLIDE 06	SLIDE 06	SLIDE 06 SLIDE	
	CONDITION 1 mM Glucose, 0,28 mM 02 IF_STAINING Ki67-CollV-HOECHST	CONDITION 1 mM Glucose, 0,28 mM 02 IF_STAINING Ki67-CollV-HOECHST	CONDITION 1 mM Glucose, 0,28 mM 02 IF_STAINING Ki67-CollV-HOECHST	CONDITION 1 mM Glucose, 0,28 mM 02 COND IF_STAINING TUNELHOECHST IF_STA	

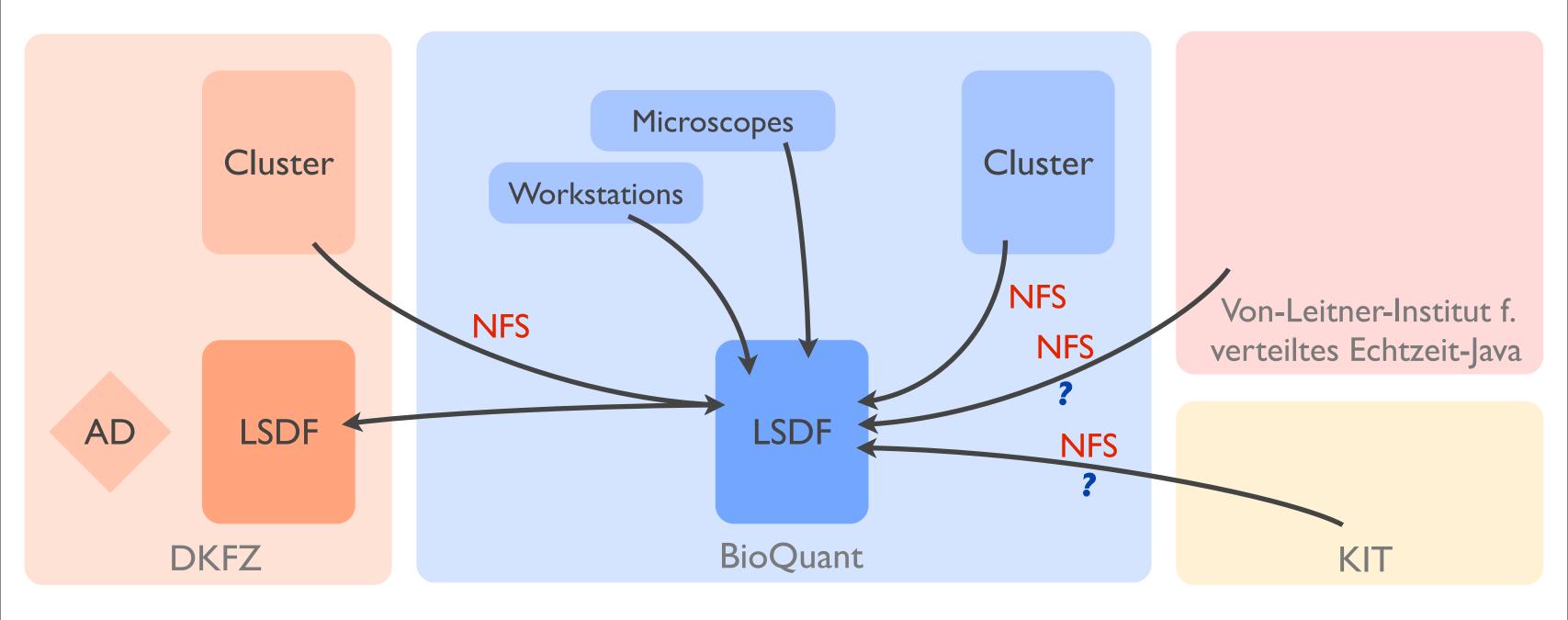


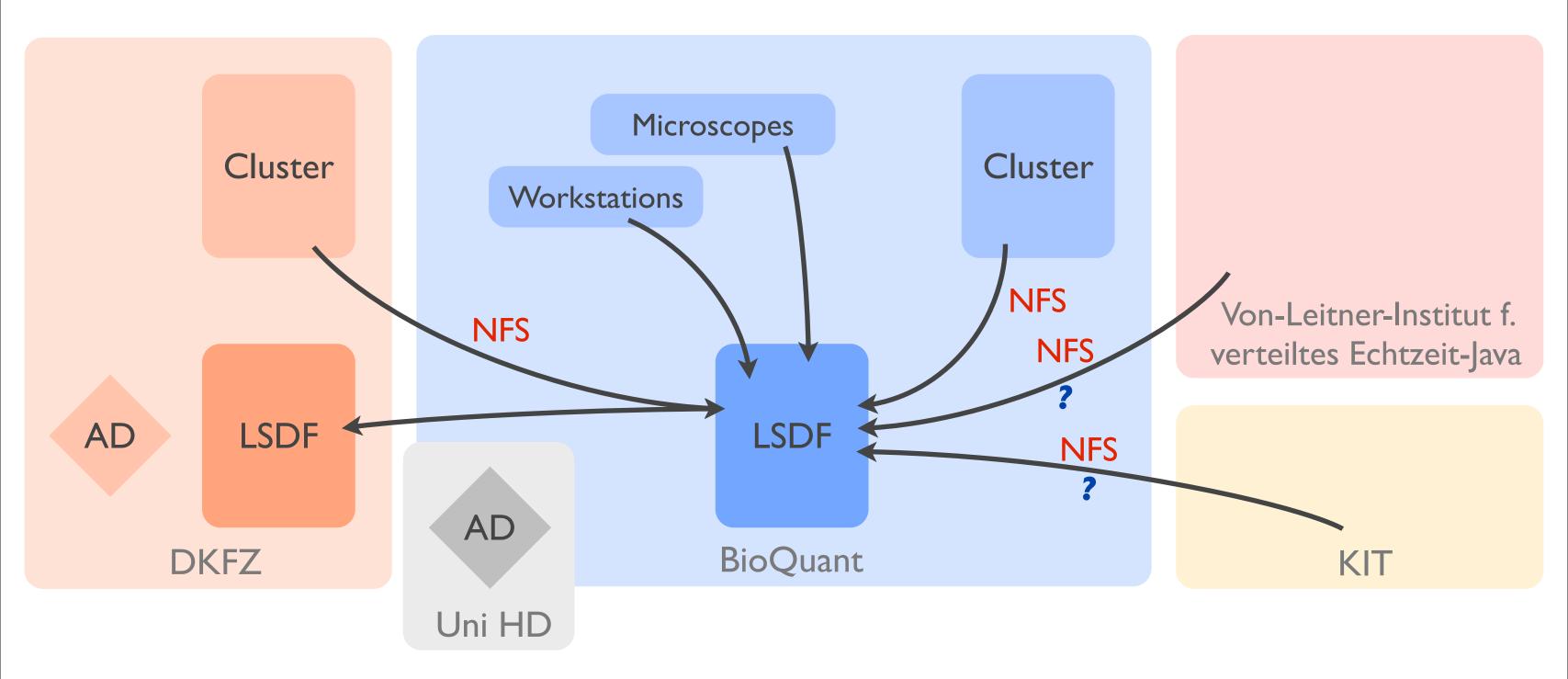


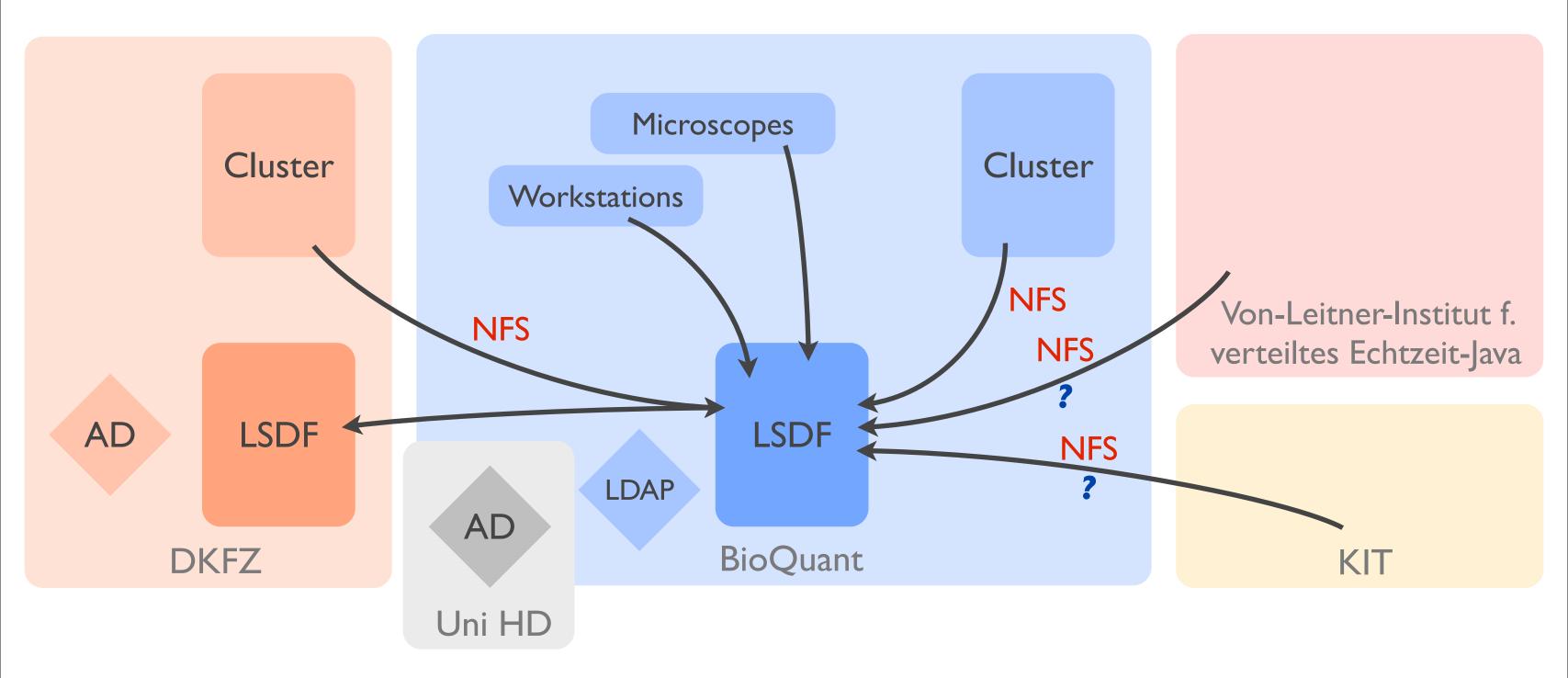


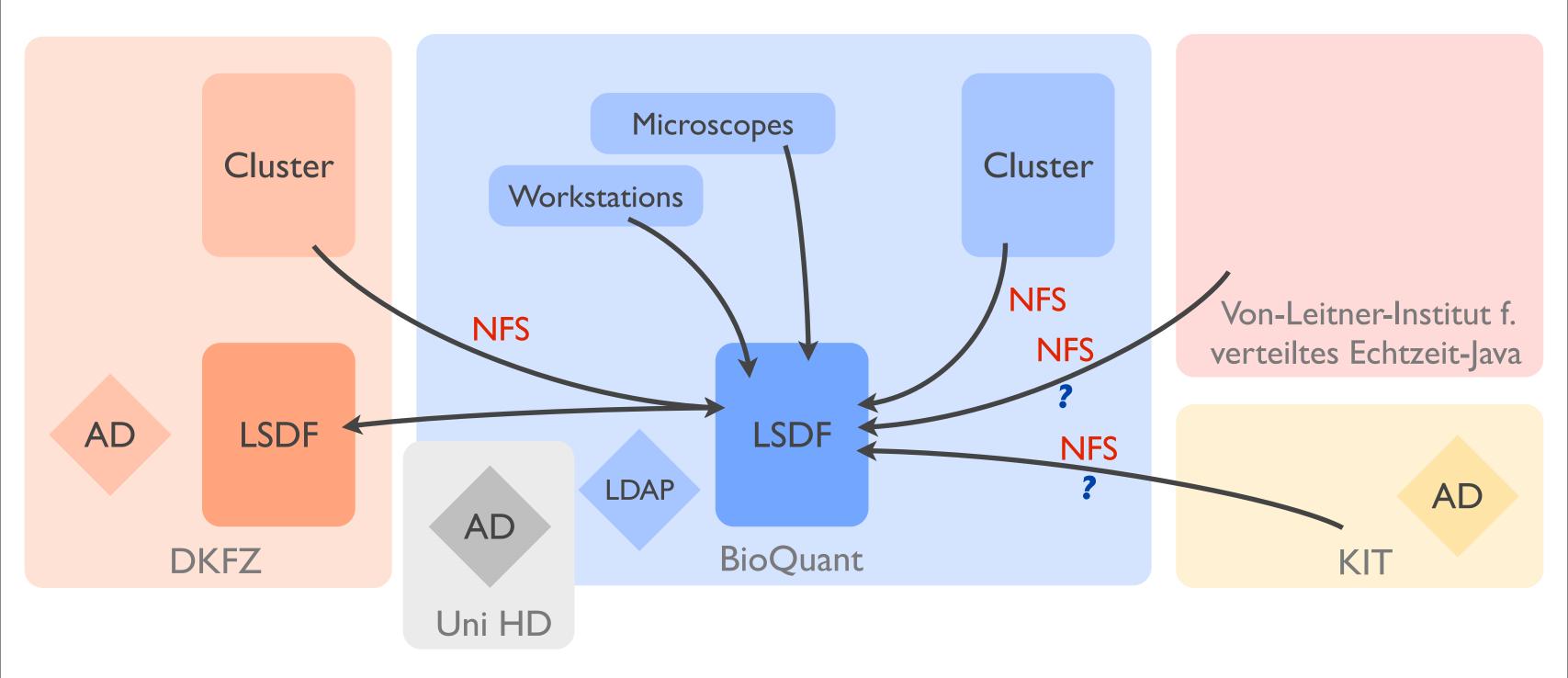
Tuesday, March 12, 13

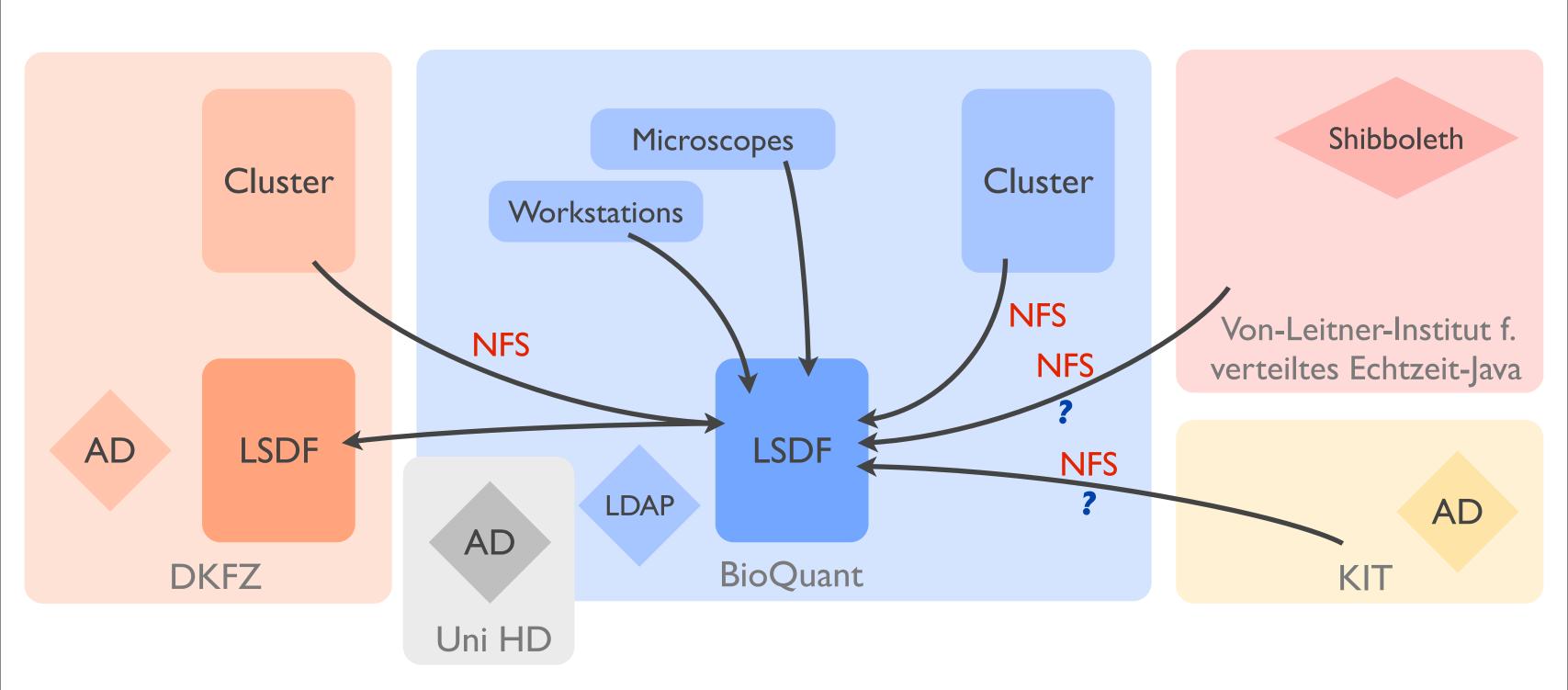








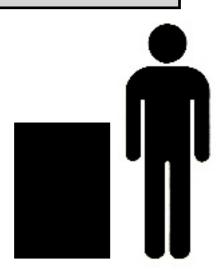




The Problem

COMMUNITY BANK SAFE DEPOSIT BOXES

COMMUNITY BANK SAFE DEPOSIT BOXES



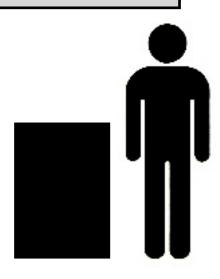






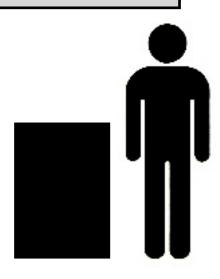


COMMUNITY BANK SAFE DEPOSIT BOXES





COMMUNITY BANK SAFE DEPOSIT BOXES



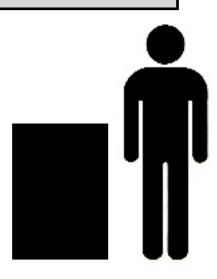






The Solution Authentication NFS via RPCSEC_GSS_KRB5





The Solution Authentication NFS via RPCSEC_GSS_KRB5



The Solution Authentication NFS via RPCSEC_GSS_KRB5



BioQuant: Christian Thiemann is 3224

The Problem Differentiation NFS via RPCSEC_GSS_KRB5 and multiple authorities



The Problem Differentiation NFS via RPCSEC_GSS_KRB5 and multiple authorities



Ok, my records show that you are-Aw crap.

DKFZ: Alice Smith is 3224

The Solution Differentiation NFS via RPCSEC_GSS_KRB5 and multiple authorities and mapped ID spaces



BioQuant: Christian Thiemann Alice Smith is 3224

DKFZ: is 3224

The Solution Differentiation NFS via RPCSEC_GSS_KRB5 and multiple authorities and mapped ID spaces



My records show that you are 103224. Here is your box.

> My records show that you are 203224. Here is your box.

BioQuant: DKFZ: Christian Thiemann Alice Smith is 3224 is 3224

Bank Policy: BioQuant = 10xxxx DKFZ = 20xxxx

The Problem NFSv3 uses numeric UID/GIDs

BioQuant Client LSDF

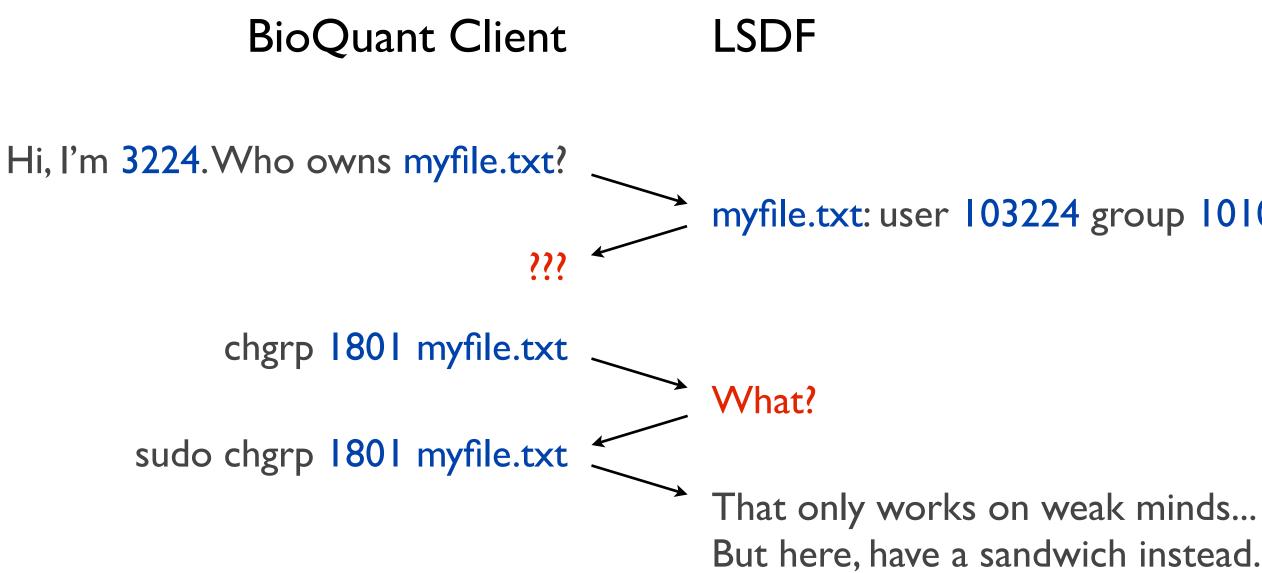
The Problem NFSv3 uses numeric UID/GIDs

BioQuant Client LSDF



myfile.txt: user 103224 group 101000

The Problem NFSv3 uses numeric UID/GIDs



myfile.txt: user 103224 group 101000

BioQuant Client NFS Proxy LSDF

BioQuant Client NFS Proxy

Ok

Hi, I'm 3224. Who owns myfile.txt?

Hi, I'm 103224. Who owns myfile.txt?

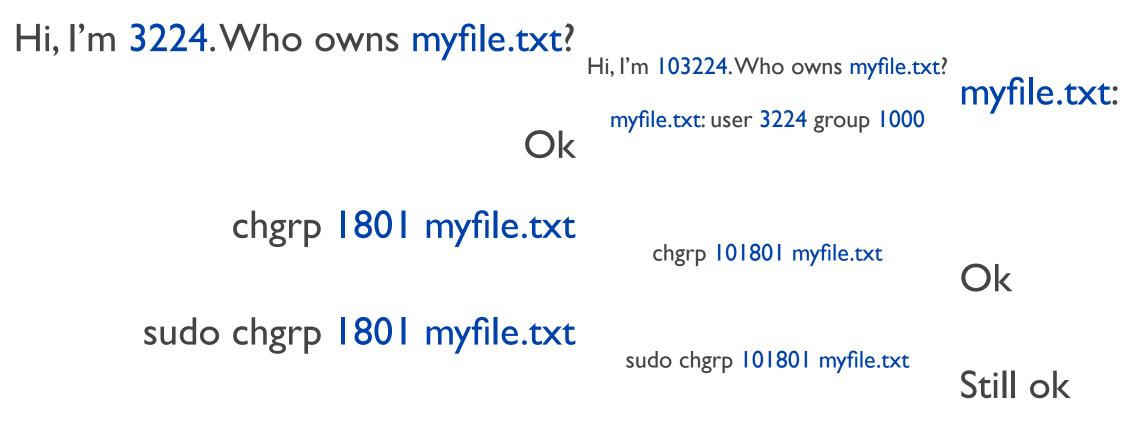
LSDF

myfile.txt: user 3224 group 1000

Tuesday, March 12, 13

myfile.txt: user 103224 group 101000

BioQuant Client NFS Proxy LSDF



myfile.txt: user 103224 group 101000



LSDF



LSDF

Hi, I'm 3224. Who owns myfile.txt?

Hi, I'm bq_cthiemann@bioquant.Who owns myfile.txt?

myfile.txt: user 103224 group 101000

myfile.txt: user bq_cthiemann@BQ group bq_admins@BQ

Ok



LSDF

Hi, I'm 3224. Who owns myfile.txt?

Hi, I'm bq_cthiemann@bioquant.Who owns myfile.txt?

myfile.txt: user 103224 group 101000

myfile.txt: user bq_cthiemann@BQ group bq_admins@BQ

Ok

chgrp 1801 myfile.txt

chgrp rattorturers@BQ myfile.txt

Ok



Hi, I'm 3224. Who was MFSv4 development is slow: "no economical incentive" (IBM / EMC) 103224 group 101000

myfile.txt: user bq_cthiemann@BQ group bq_admins@BQ

Ok

chgrp 1801 myfile.txt

hgrp rattorturers@BQ myfile.txt



Hi, I'm 3224 Who was NFSv4 development is slow: "no economical incentive" (IBM / EMC) 103224 group 101000

myfile.txt: user bq_cthiemann@BQ group bq_admins@BQ

horn 1801 myfile tyt

hgrp rattorturers@BQ myfile.txt

invisible hand



NFSv4 development is slow:

"no economical incentive" (IBM / EMC) 103224 group 101000 IBM SONAS will be NFSv4-capable in 2014

invisible hand

hopefully...

BioQuant Client NFS Proxy LSDF

NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

chgrp 1801 myfile.txt

chgrp 101801 myfile.txt

sudo chgrp 1801 myfile.txt

sudo chgrp 101801 myfile.txt

Still ok

Tuesday, March 12, 13

Hi, I'm 3224. Who owns myfile.tx NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

acts as a trusted client to the LSDF (using AUTH_SYS)

Hi, I'm 3224. Who owns myfile.tx NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

acts as a trusted client to the LSDF (using AUTH SYS) authenticates external clients using RPCSEC GSS KRB5

Hi, I'm 3224. Who owns myfile.tx NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

acts as a trusted client to the LSDF (using AUTH_SYS) authenticates external clients using RPCSEC GSS KRB5 transparently translates UIDs & GIDs between LSDF and external ID spaces

BioQuant Client NFS Proxy LSDF

NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

chgrp 1801 myfile.txt

chgrp 101801 myfile.txt

sudo chgrp 1801 myfile.txt

sudo chgrp 101801 myfile.txt

Still ok

Tuesday, March 12, 13

BioQuant Client NFS Proxy LSDF

NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

user-space daemon intercepting TCP traffic

chgrp 101801 myfile.txt

sudo chgrp 1801 myfile.txt

udo chgrp 101801 myfile.txt

Hi, I'm 3224. Who owns myfile.tx NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

user-space daemon intercepting TCP traffic slows down filesystem operations (directory listings etc.) factor 2–3

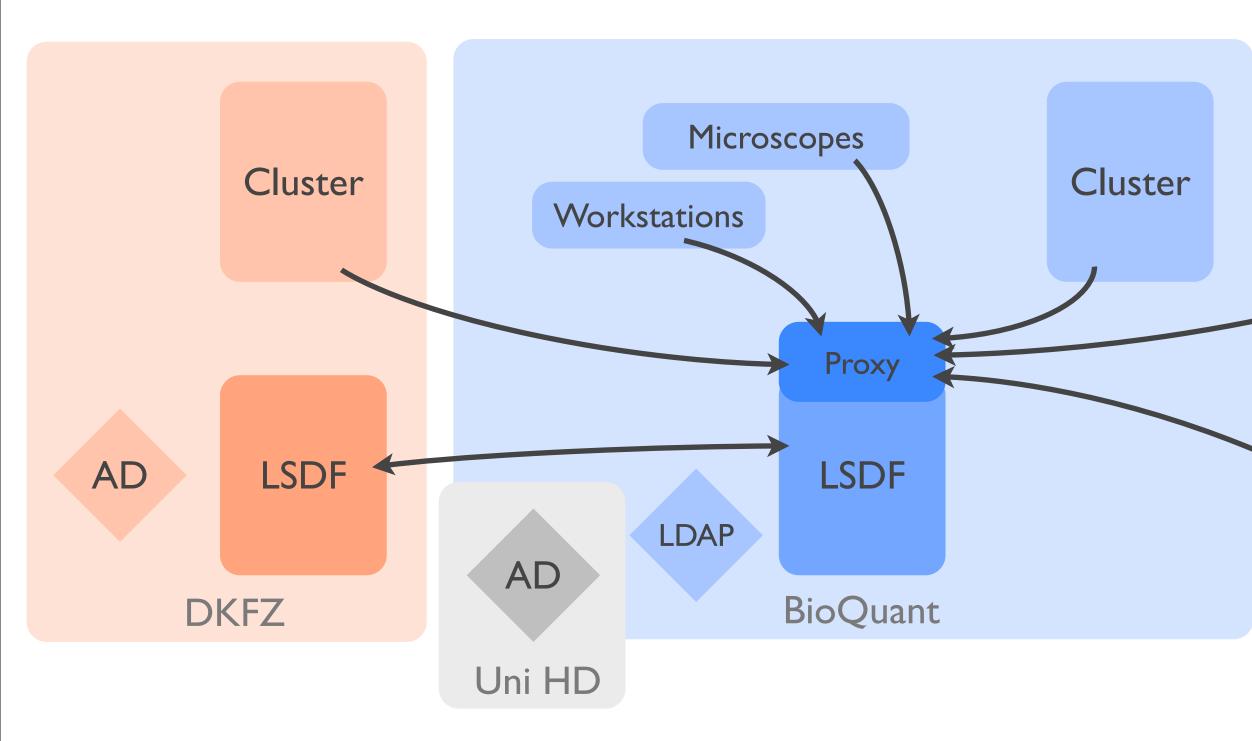
Tuesday, March 12, 13

Hi, I'm 3224. Who owns myfile.tx NFSv3 Ticket Agent: Kerberized Inter-Realm NFS Service

user-space daemon intercepting TCP traffic slows down filesystem operations (directory listings etc.) factor 2–3 sudo charp 1801 myfile of no throughput penalty on read/write operations

10-20 GBit/s

BioQuant LSDF



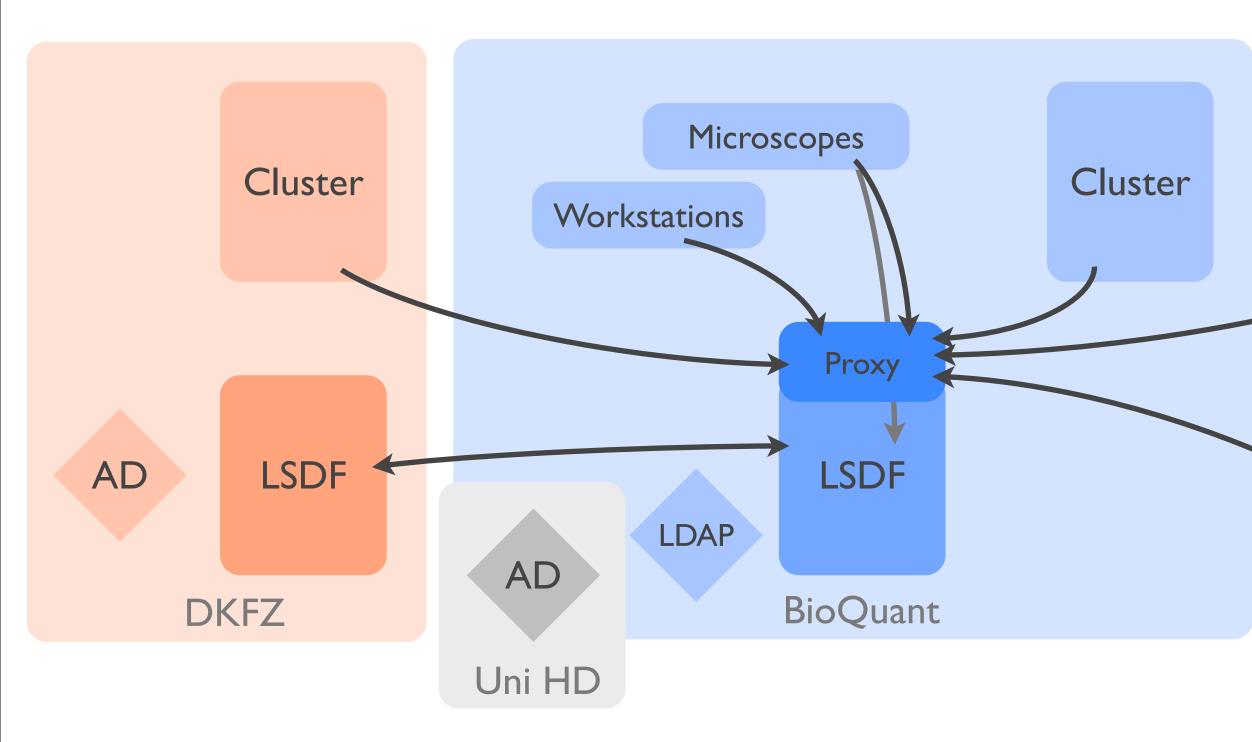
Shibboleth

Von-Leitner-Institut f. verteiltes Echtzeit-Java

KIT

AD

BioQuant LSDF



Shibboleth

Von-Leitner-Institut f. verteiltes Echtzeit-Java

KIT

AD

BioQuant LSDF

