Hasso Plattner Institut
IT Systems Engineering | Universität Potsdam

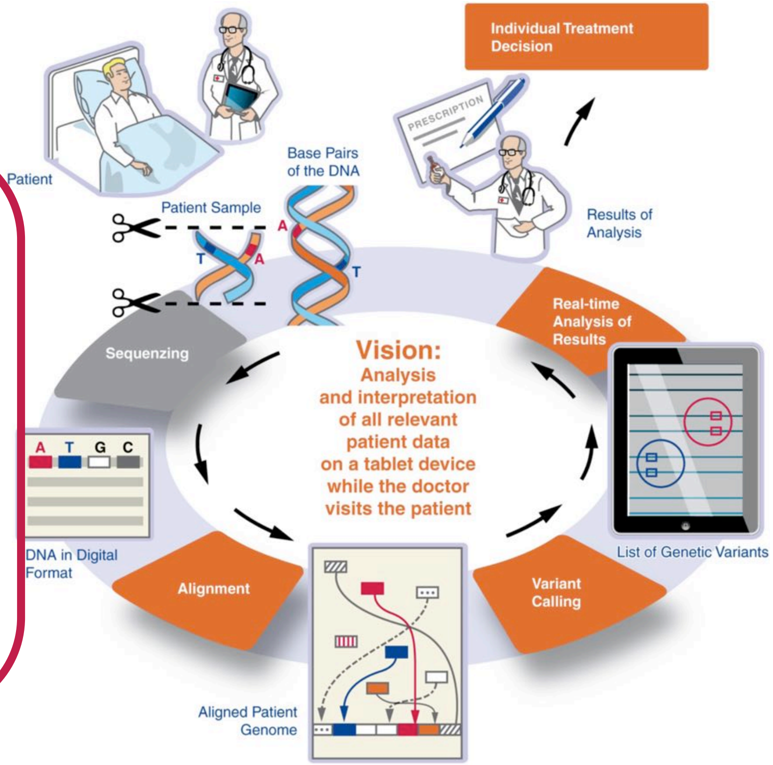
Use Case Oncology Data Management

Dr. Matthieu-P. Schapranow

Data Management for Digital Health
Summer 2017

From Raw Genome Data to Analysis

- **Sequencing**: Acquire digital DNA data
- Alignment: Reconstruction of complete genome with snippets
- Variant Calling: Identification of genetic variants
- Data Annotation: Linking genetic variants with research findings



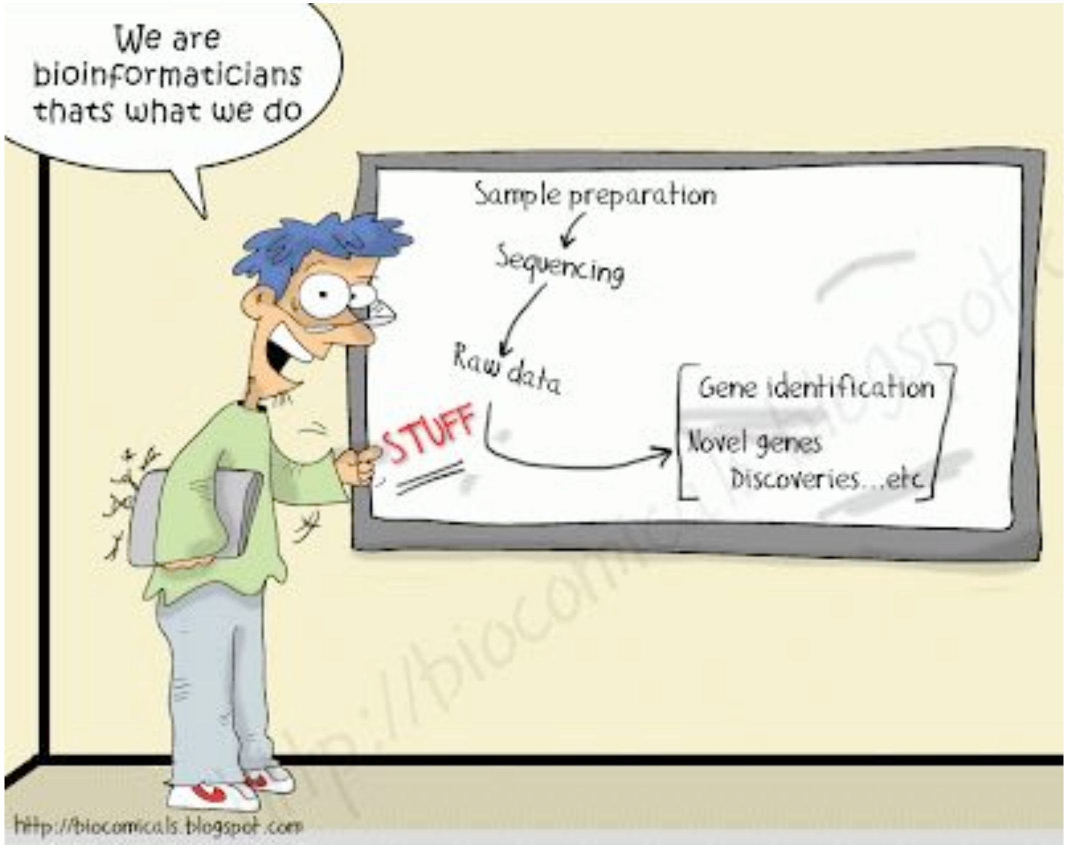
Genome Data Processing Pipelines
Motivation

- Currently Genome Data Processing Pipelines (GDPPs) consist of individually combined command line scripts

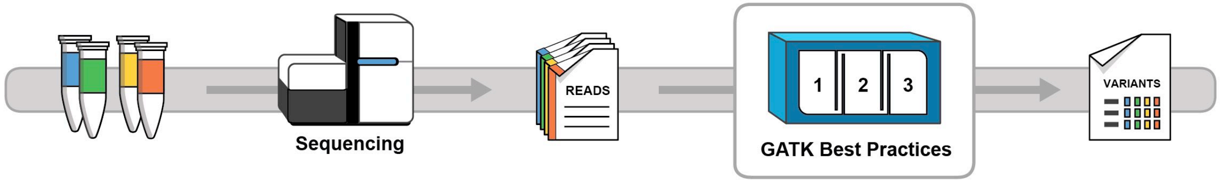
- Complex to
  - Understand,
  - Maintain and update, and
  - Reproduce

- Objective: Model GDPPs in a…
  - Graphical and machine-readable representation
  - Reproducible and exchangeable format

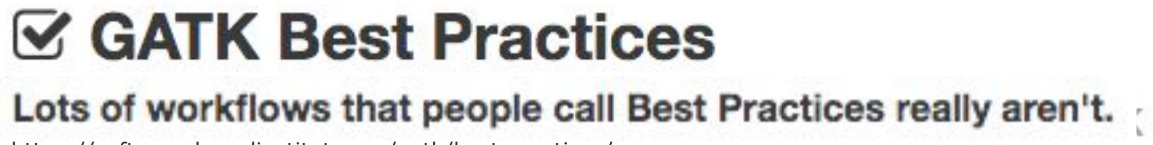
How to Find a Solution?
Call a Bioinformatician



BROAD INSTITUTE



- The BROAD is a joint institute of MIT and Harvard established 2004 in Cambridge, MA
- Genome Analysis Toolkit (GATK) focuses on variant detection
- Open-source tools and shared best-practices



☑ GATK Best Practices

Lots of workflows that people call Best Practices really aren't.

https://software.broadinstitute.org/gatk/best-practices/

Genome Data Processing Pipelines
State of the Art

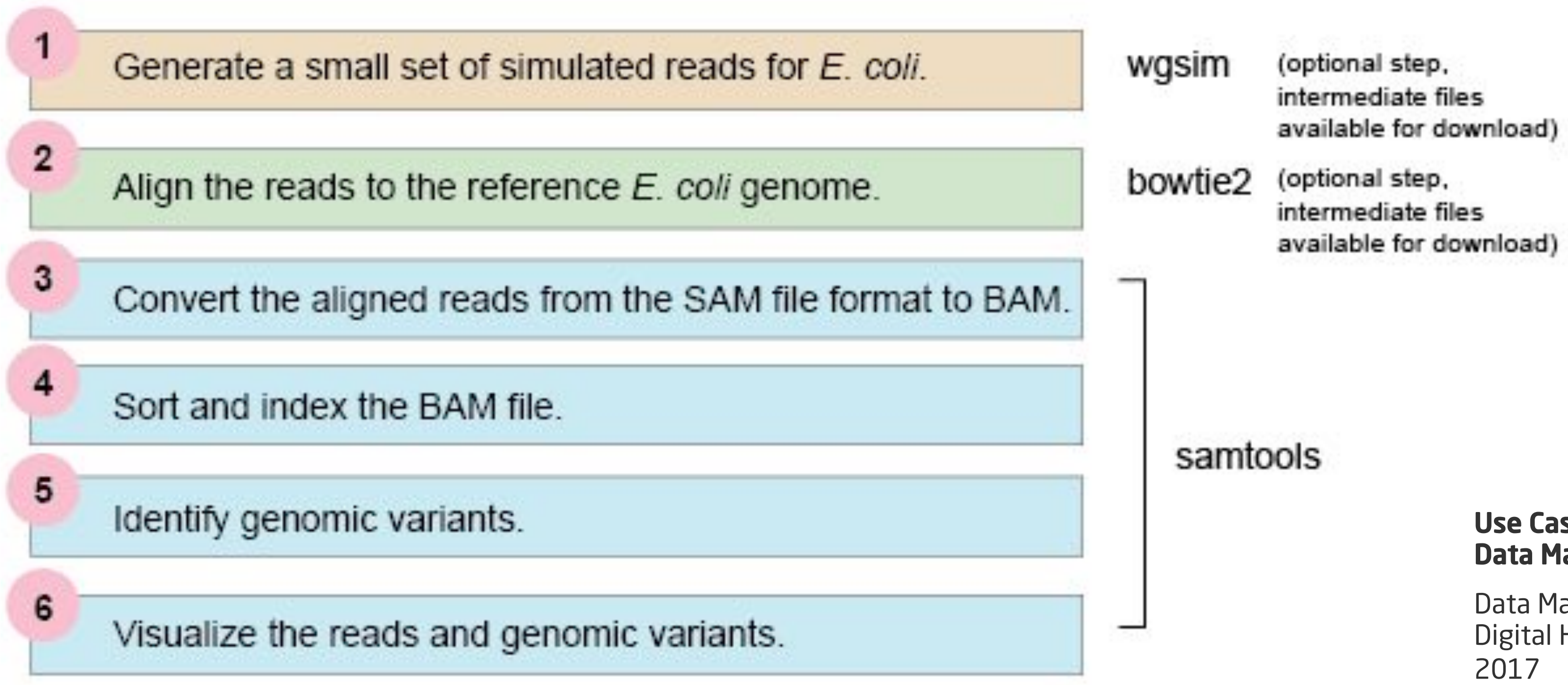
```
bwa aln hg19.fa sample.fastq | bwa samse hg19.fa – sample.fastq | samtools view -Su - | samtools sort …
```

- Concatenation of command line tools reading/writing files
- Lack of standardization and exchangeability

- Requires dedicated expertise for
  - □ Setup and configuration,
  - □ Error handling, and
  - □ Scalable processing

- Objective: Enable modeling, configuration, and execution of reproducible pipelines without involving IT experts

Let us Make it a Workflow!



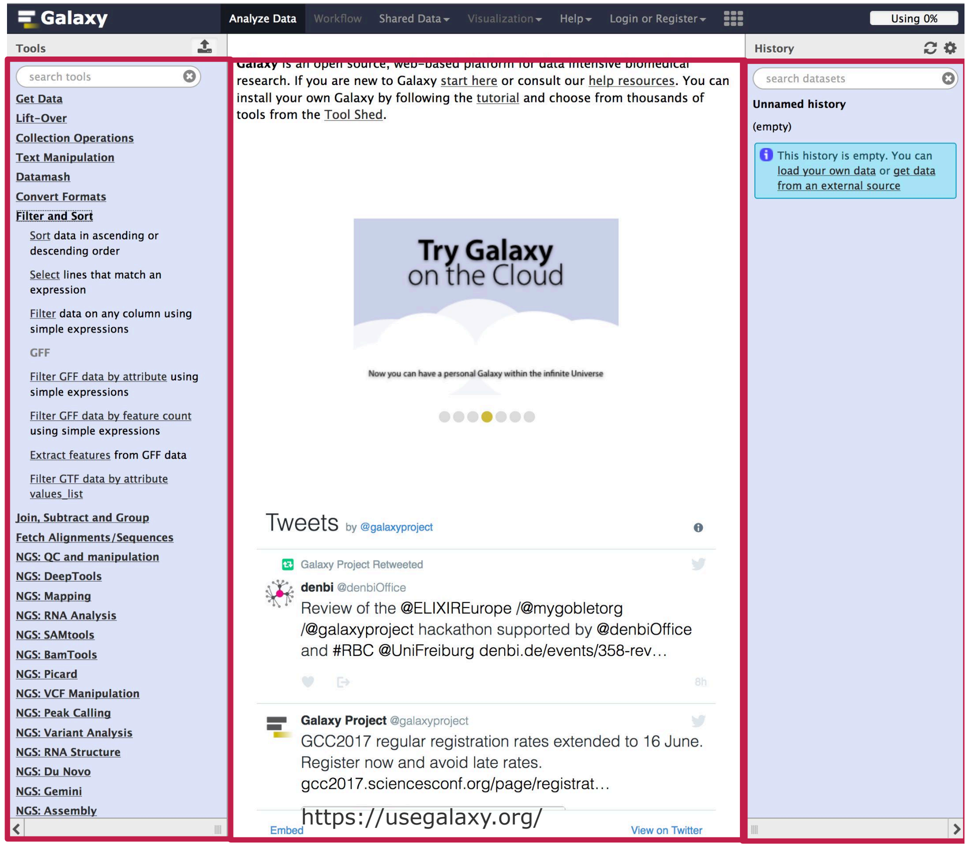
1. Generate a small set of simulated reads for *E. coli*.
2. Align the reads to the reference *E. coli* genome.
3. Convert the aligned reads from the SAM file format to BAM.
4. Sort and index the BAM file.
5. Identify genomic variants.
6. Visualize the reads and genomic variants.

wgsim
(optional step, intermediate files available for download)
bowtie2
(optional step, intermediate files available for download)
samtools

http://biobits.org/samtools_primer.html

Galaxy Workbench

- Open-source, web-based platform
- Supports data-intensive research
- Focuses on process automation and high-throughput sequencing



Get Data
Lift-Over
Collection Operations
Text Manipulation
Datamash
Convert Formats
Filter and Sort

- Sort data in ascending or descending order
- Select lines that match an expression
- Filter data on any column using simple expressions
- GFF
- Filter GFF data by attribute using simple expressions
- Filter GFF data by feature count using simple expressions
- Extract features from GFF data
- Filter GTF data by attribute values_list

Join, Subtract and Group
Fetch Alignments/Sequences
NGS: QC and manipulation
NGS: DeepTools
NGS: Mapping
NGS: RNA Analysis
NGS: SAMtools
NGS: BamTools
NGS: Picard
NGS: VCF Manipulation
NGS: Peak Calling
NGS: Variant Analysis
NGS: RNA Structure
NGS: Du Novo
NGS: Gemini
NGS: Assembly

Galaxy is an open source, web-based platform for data intensive biomedical research. If you are new to Galaxy start here or consult our help resources. You can install your own Galaxy by following the tutorial and choose from thousands of tools from the Tool Shed.

Try Galaxy on the Cloud

Now you can have a personal Galaxy within the infinite Universe

Tweets by @galaxyproject

Galaxy Project Retweeted

denbi @denbiOffice
Review of the @ELIXIREurope /@mygobletorg /@galaxyproject hackathon supported by @denbiOffice and #RBC @UniFreiburg denbi.de/events/358-rev…
8h

Galaxy Project @galaxyproject
GCC2017 regular registration rates extended to 16 June. Register now and avoid late rates. gcc2017.sciencesconf.org/page/registrat…

Embed
View on Twitter

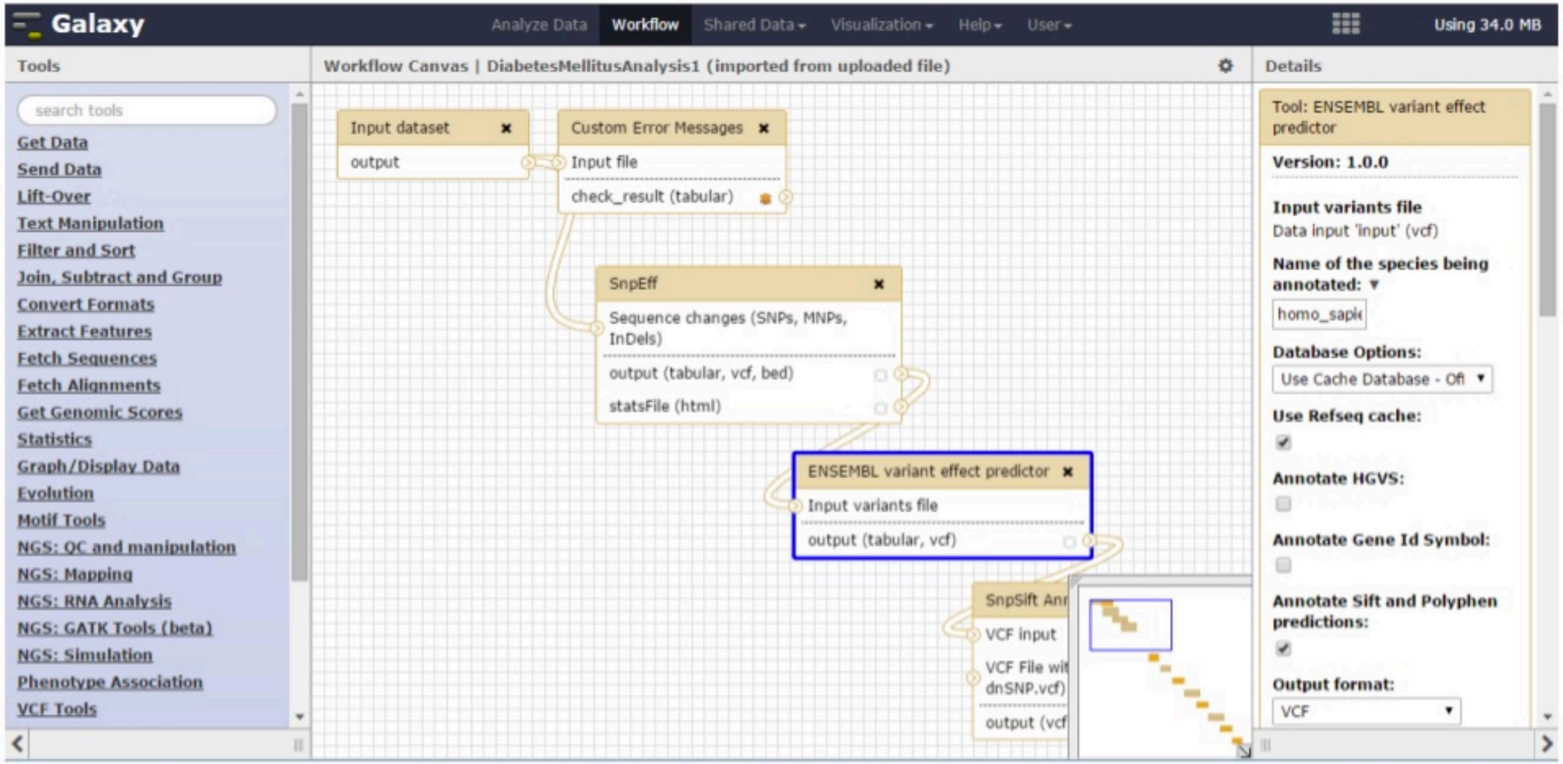
Unnamed history

(empty)

This history is empty. You can load your own data or get data from an external source

https://usegalaxy.org/

Galaxy
Workflow Modeling



Tool: ENSEMBL variant effect predictor

Version: 1.0.0

Input variants file
Data input 'input' (vcf)

Name of the species being annotated: ▾
homo_sapi

Database Options:
Use Cache Database - Off ▾

Use Refseq cache:
☑

Annotate HGVS:
□

Annotate Gene Id Symbol:
□

Annotate Sift and Polyphen predictions:
☑

Output format:
VCF ▾

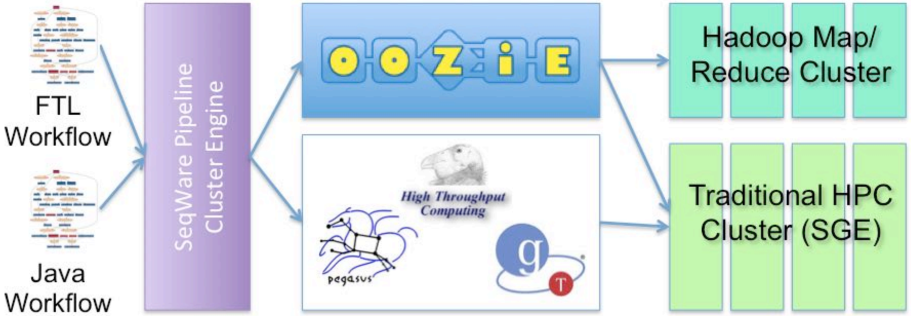
https://usegalaxy.org/

Use Case Oncology Data Management

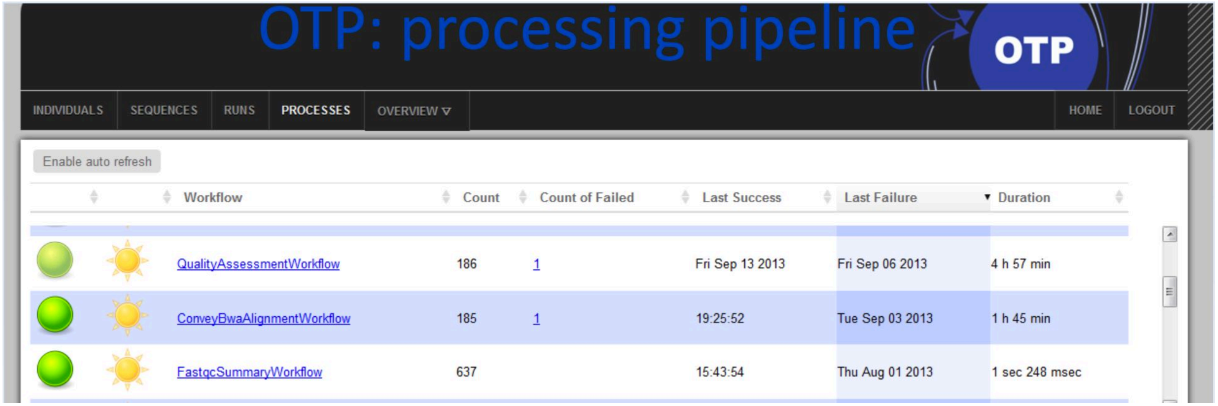
Data Management for Digital Health, Summer 2017

DKFZ One Touch Platform

- IT process automation at DKFZ, HD
- Builds upon OpenStack and Vagrant to reduce setup time
- Workflow managed by SeqWare Pipeline Manager
- Special-purpose developed for DKFZ requirements


FTL Workflow
Java Workflow
SeqWare Pipeline Cluster Engine
OOZIE
High Throughput Computing
pegasus
Hadoop Map/ Reduce Cluster
Traditional HPC Cluster (SGE)

https://seqware.github.io/docs/6-pipeline/

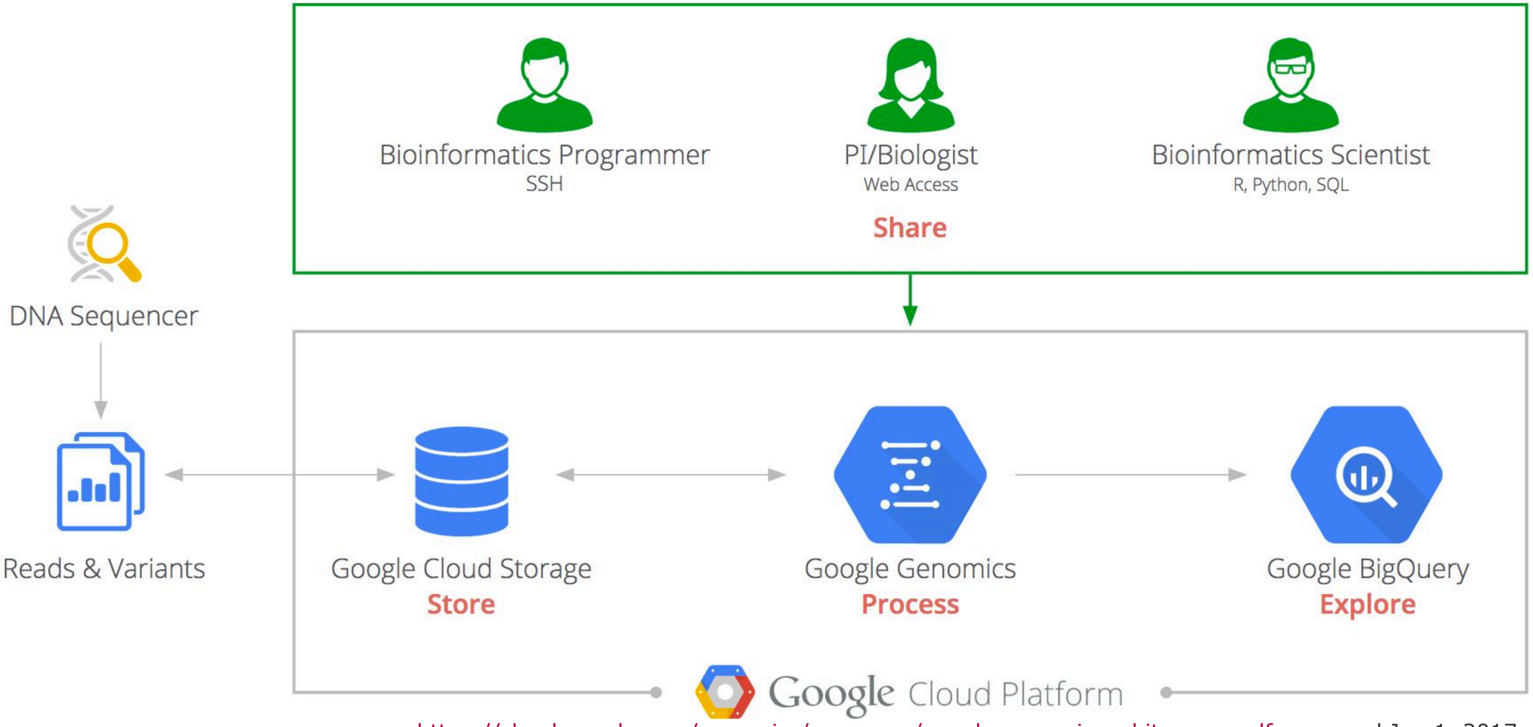


		Workflow	Count	Count of Failed	Last Success	Last Failure	Duration
●	☀	QualityAssessmentWorkflow	186	1	Fri Sep 13 2013	Fri Sep 06 2013	4 h 57 min
●	☀	ConveyBwaAlignmentWorkflow	185	1	19:25:52	Tue Sep 03 2013	1 h 45 min
●	☀	FastqcSummaryWorkflow	637		15:43:54	Thu Aug 01 2013	1 sec 248 msec

Use Case Oncology Data Management

Google Genomics

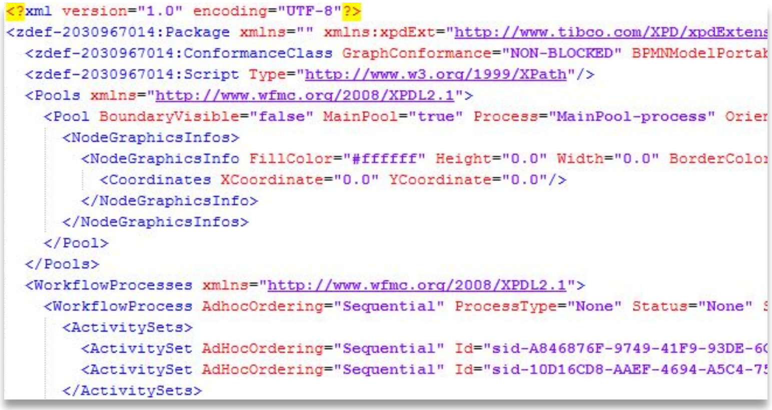
- Integration of existing Google services to genome data processing



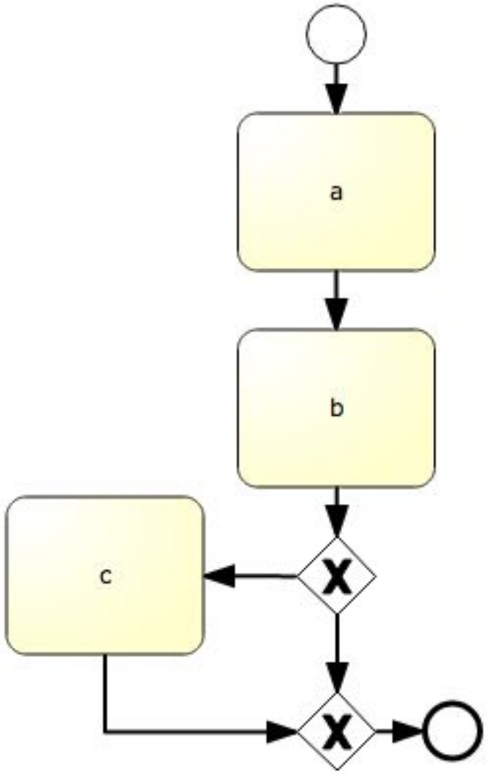
https://cloud.google.com/genomics/resources/google-genomics-whitepaper.pdf, accessed Jun 1, 2017

Business Process Modeling and Notation (BPMN) 2.0

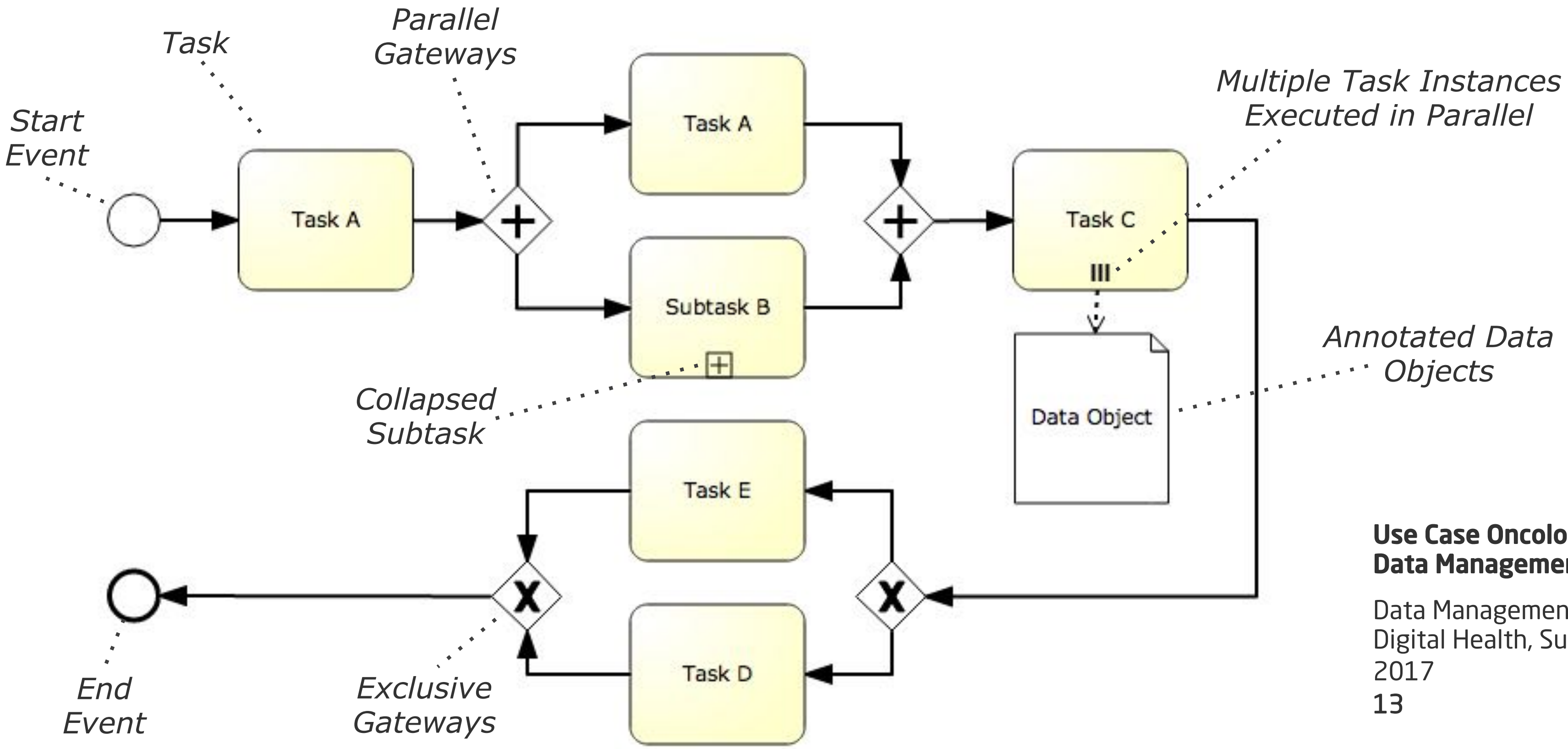
- Used for functional modeling of business processes and workflows
- Graphical notation addresses business and technical users → intuitive modeling and understanding
- Can be serialized and exchanged using XML Process Definition Language (XPDL)



```
<?xml version="1.0" encoding="UTF-8"?>
<zdef-2030967014:Package xmlns="" xmlns:xpdExt="http://www.tibco.com/XPD/xpdExtens
  <zdef-2030967014:ConformanceClass GraphConformance="NON-BLOCKED" BPMNModelPorta
  <zdef-2030967014:Script Type="http://www.w3.org/1999/XPath"/>
  <Pools xmlns="http://www.wfmc.org/2008/XPDL2.1">
    <Pool BoundaryVisible="false" MainPool="true" Process="MainPool-process" Orie
      <NodeGraphicsInfos>
        <NodeGraphicsInfo FillColor="#ffffff" Height="0.0" Width="0.0" BorderColo
          <Coordinates XCoordinate="0.0" YCoordinate="0.0"/>
        </NodeGraphicsInfo>
      </NodeGraphicsInfos>
    </Pool>
  </Pools>
  <WorkflowProcesses xmlns="http://www.wfmc.org/2008/XPDL2.1">
    <WorkflowProcess AdhocOrdering="Sequential" ProcessType="None" Status="None"
      <ActivitySets>
        <ActivitySet AdHocOrdering="Sequential" Id="sid-A846876F-9749-41F9-93DE-6
        <ActivitySet AdHocOrdering="Sequential" Id="sid-10D16CD8-AAEF-4694-A5C4-7
      </ActivitySets>
```



BPMN 2.0: Basic Notation Overview

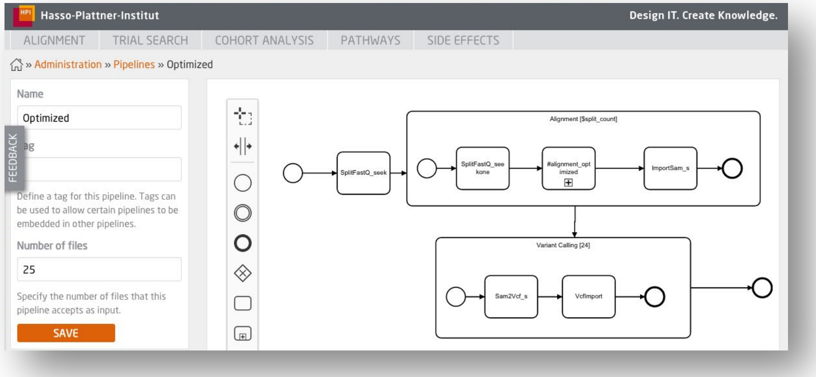


Reproducibility
Modeling of Data Analysis Pipelines

1. Design time (researcher, process expert)
   - □ Definition of parameterized process model
   - □ Uses graphical editor and jobs from repository

2. Configuration time (researcher, lab assistant)
   - □ Select model and specify parameters, e.g. aln opts
   - □ Results in model instance stored in repository

3. Execution time (researcher)
   - □ Select model instance
   - □ Specify execution parameters, e.g. input files



» Administration » Pipelines » Optimized

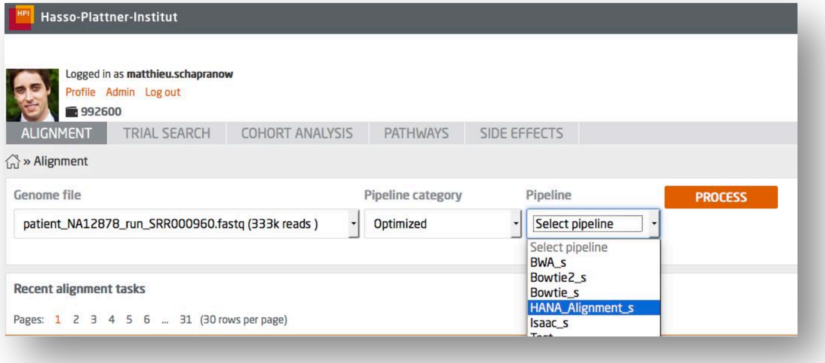
Name: Optimized

Tag:

Define a tag for this pipeline. Tags can be used to allow certain pipelines to be embedded in other pipelines.

Number of files: 25

Specify the number of files that this pipeline accepts as input.



Logged in as **matthieu.schapranow**

992600

» Alignment

Genome file: patient_NA12878_run_SRR000960.fastq (333k reads)

Pipeline category: Optimized

Pipeline: Select pipeline

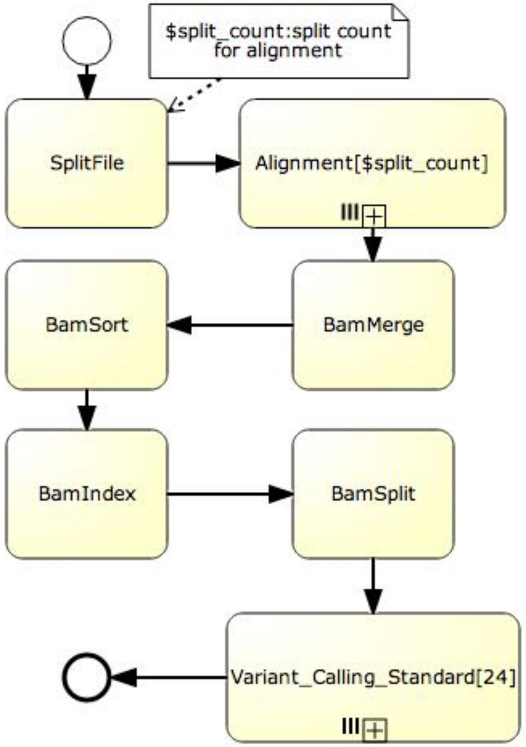
Recent alignment tasks

Pages: 1 2 3 4 5 6 ... 31 (30 rows per page)

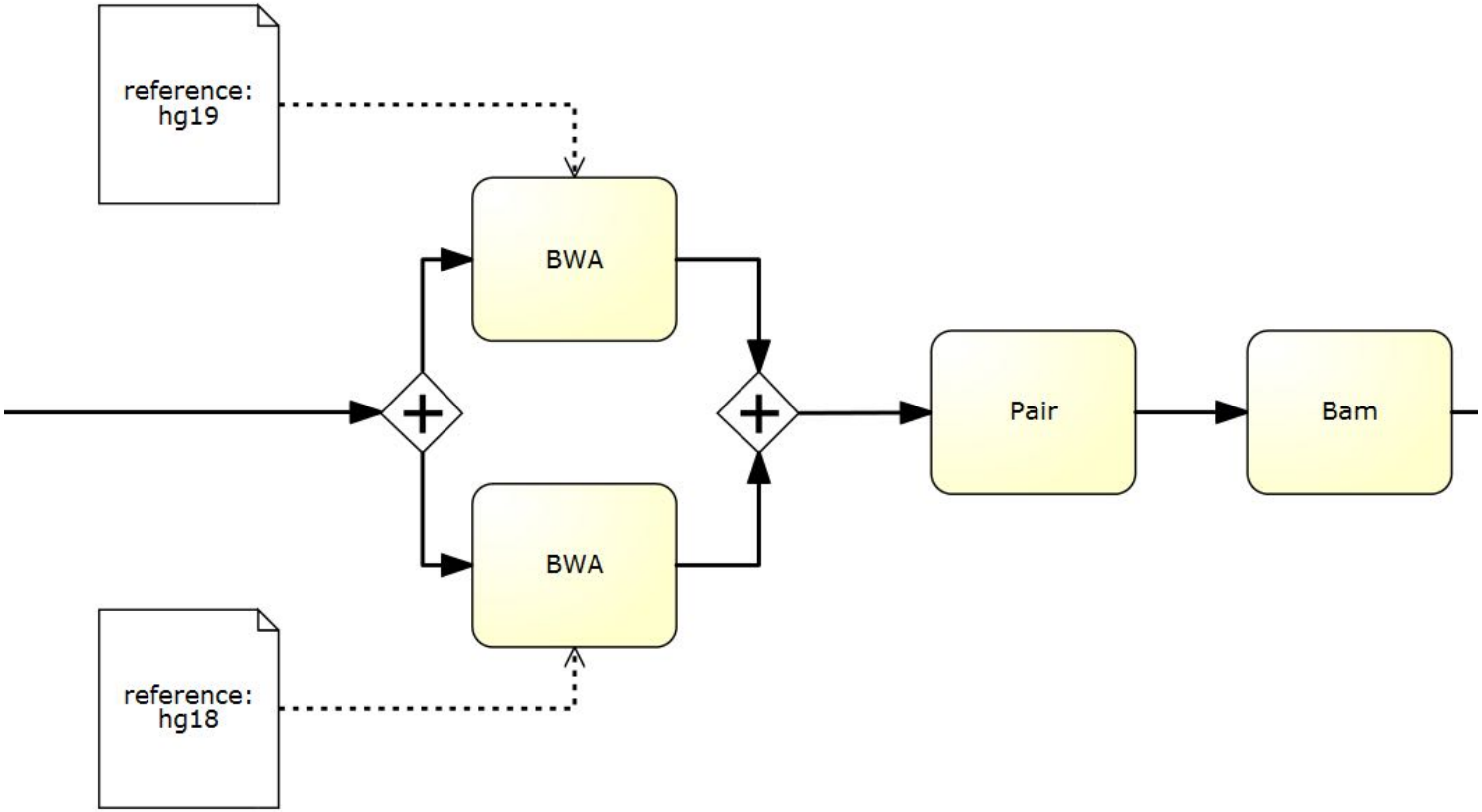
Standardized Graphical Modeling

- Graphical modeling notation compliant with Business Process Modeling and Notation 2.0 extended by
  - □ Modular structure
  - □ Parallelization annotations
  - □ Parameters and variables

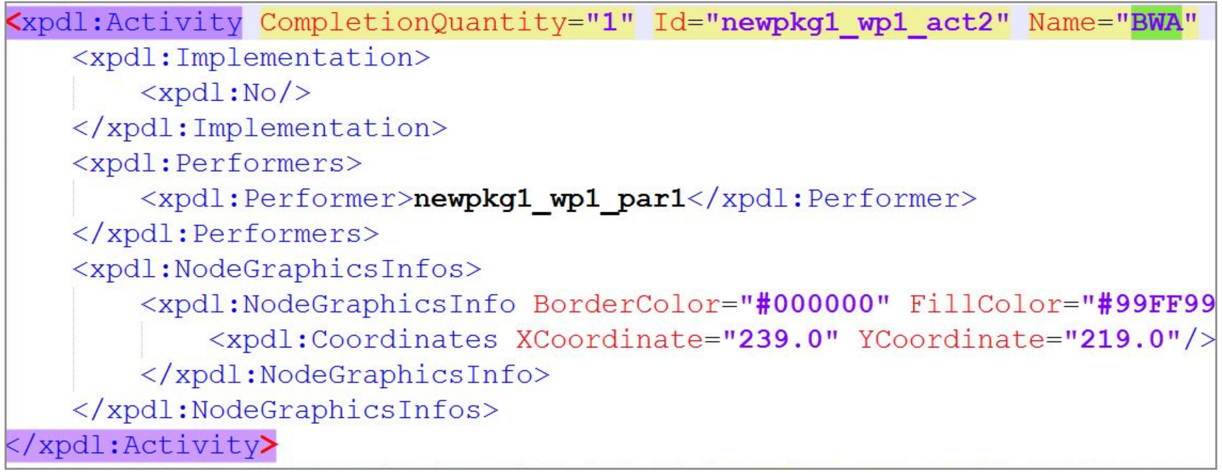
- Model descriptions are stored within IMDB
- Model instances are transformed into graph structure for execution by dedicated runtime environment


$split_count:split count for alignment
SplitFile
Alignment[$split_count]
BamSort
BamMerge
BamIndex
BamSplit
Variant_Calling_Standard[24]

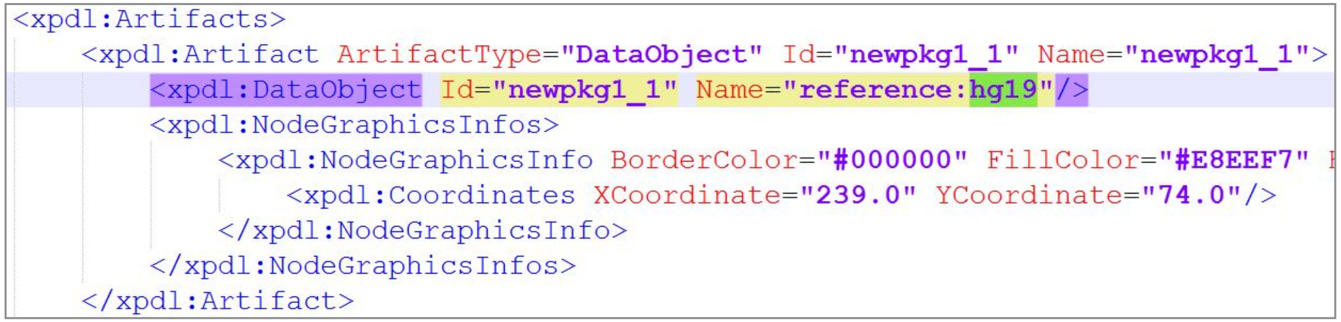
BPMN Example



Persisting Pipelines
XML Process Definition Language



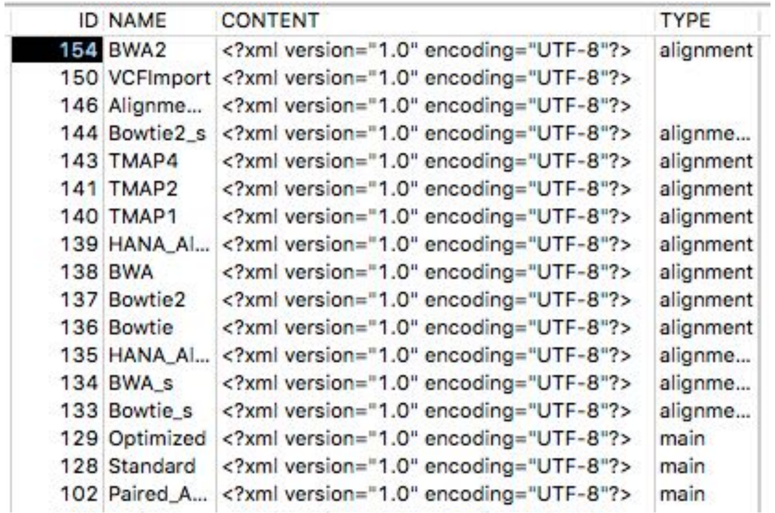
```
<xpdl:Activity CompletionQuantity="1" Id="newpkg1_wp1_act2" Name="BWA"
    <xpdl:Implementation>
        <xpdl:No/>
    </xpdl:Implementation>
    <xpdl:Performers>
        <xpdl:Performer>newpkg1_wp1_par1</xpdl:Performer>
    </xpdl:Performers>
    <xpdl:NodeGraphicsInfos>
        <xpdl:NodeGraphicsInfo BorderColor="#000000" FillColor="#99FF99
            <xpdl:Coordinates XCoordinate="239.0" YCoordinate="219.0"/>
        </xpdl:NodeGraphicsInfo>
    </xpdl:NodeGraphicsInfos>
</xpdl:Activity>
```



```
<xpdl:Artifacts>
    <xpdl:Artifact ArtifactType="DataObject" Id="newpkg1_1" Name="newpkg1_1">
        <xpdl:DataObject Id="newpkg1_1" Name="reference:hg19"/>
        <xpdl:NodeGraphicsInfos>
            <xpdl:NodeGraphicsInfo BorderColor="#000000" FillColor="#E8EEF7"
                <xpdl:Coordinates XCoordinate="239.0" YCoordinate="74.0"/>
            </xpdl:NodeGraphicsInfo>
        </xpdl:NodeGraphicsInfos>
    </xpdl:Artifact>
```

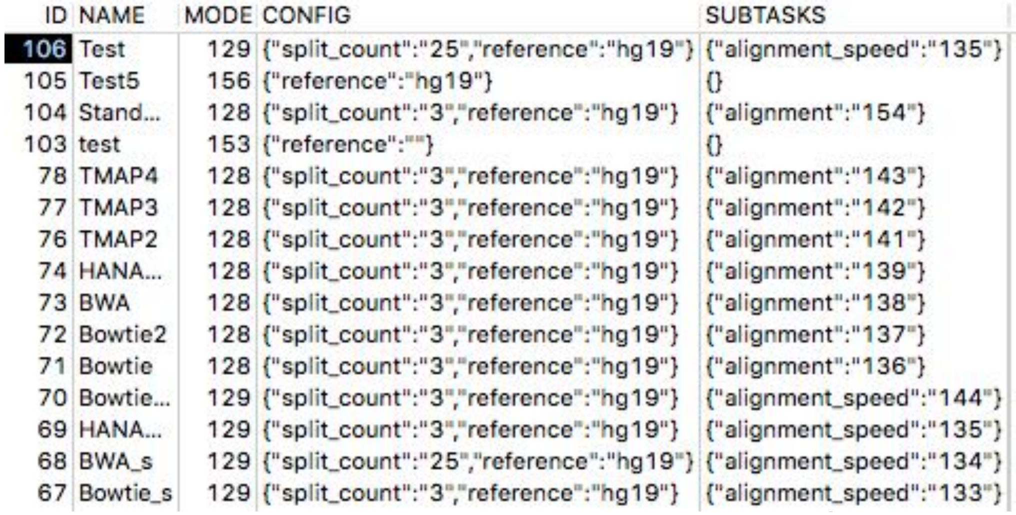
Database Structure

PIPELINES.MODELS



ID	NAME	CONTENT	TYPE
154	BWA2	<?xml version="1.0" encoding="UTF-8"?>	alignment
150	VCFImport	<?xml version="1.0" encoding="UTF-8"?>	
146	Alignme...	<?xml version="1.0" encoding="UTF-8"?>	
144	Bowtie2_s	<?xml version="1.0" encoding="UTF-8"?>	alignme...
143	TMAP4	<?xml version="1.0" encoding="UTF-8"?>	alignment
141	TMAP2	<?xml version="1.0" encoding="UTF-8"?>	alignment
140	TMAP1	<?xml version="1.0" encoding="UTF-8"?>	alignment
139	HANA_Al...	<?xml version="1.0" encoding="UTF-8"?>	alignment
138	BWA	<?xml version="1.0" encoding="UTF-8"?>	alignment
137	Bowtie2	<?xml version="1.0" encoding="UTF-8"?>	alignment
136	Bowtie	<?xml version="1.0" encoding="UTF-8"?>	alignment
135	HANA_Al...	<?xml version="1.0" encoding="UTF-8"?>	alignme...
134	BWA_s	<?xml version="1.0" encoding="UTF-8"?>	alignme...
133	Bowtie_s	<?xml version="1.0" encoding="UTF-8"?>	alignme...
129	Optimized	<?xml version="1.0" encoding="UTF-8"?>	main
128	Standard	<?xml version="1.0" encoding="UTF-8"?>	main
102	Paired_A...	<?xml version="1.0" encoding="UTF-8"?>	main

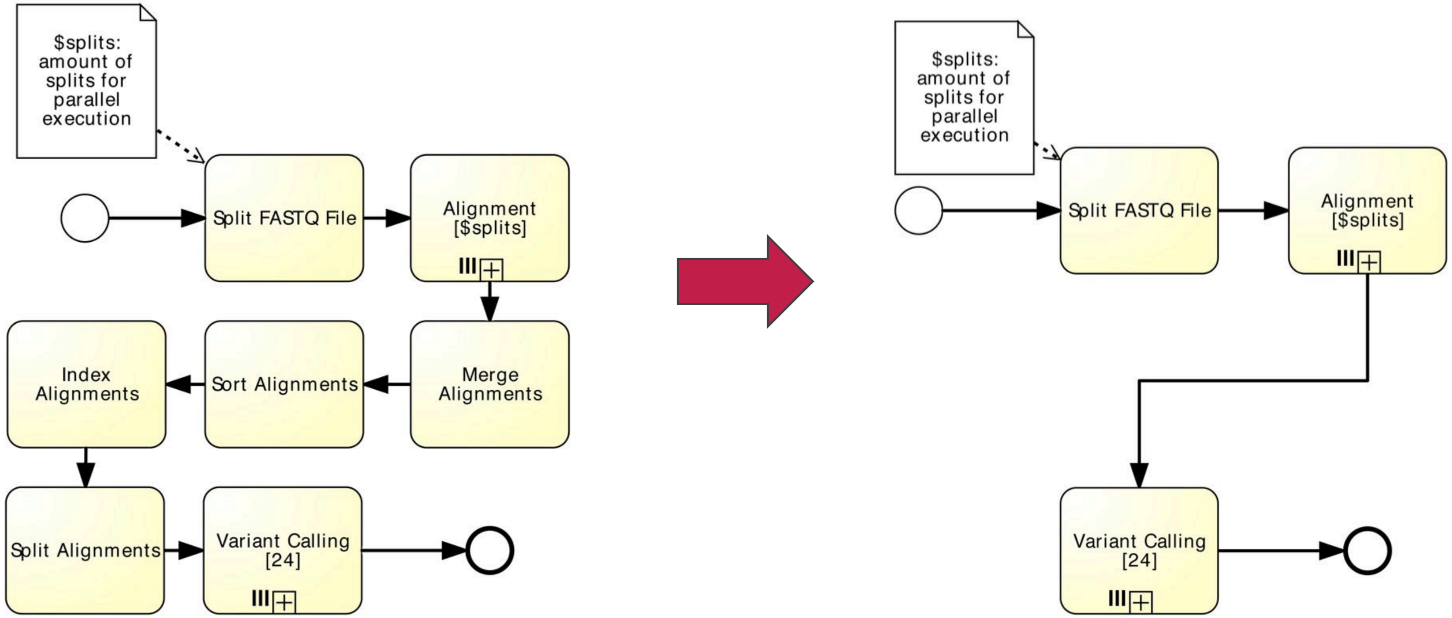
PIPELINES.PIPELINES



ID	NAME	MODE	CONFIG	SUBTASKS
106	Test	129	{"split_count":"25","reference":"hg19"}	{"alignment_speed":"135"}
105	Test5	156	{"reference":"hg19"}	{}
104	Stand...	128	{"split_count":"3","reference":"hg19"}	{"alignment":"154"}
103	test	153	{"reference":""}	{}
78	TMAP4	128	{"split_count":"3","reference":"hg19"}	{"alignment":"143"}
77	TMAP3	128	{"split_count":"3","reference":"hg19"}	{"alignment":"142"}
76	TMAP2	128	{"split_count":"3","reference":"hg19"}	{"alignment":"141"}
74	HANA...	128	{"split_count":"3","reference":"hg19"}	{"alignment":"139"}
73	BWA	128	{"split_count":"3","reference":"hg19"}	{"alignment":"138"}
72	Bowtie2	128	{"split_count":"3","reference":"hg19"}	{"alignment":"137"}
71	Bowtie	128	{"split_count":"3","reference":"hg19"}	{"alignment":"136"}
70	Bowtie...	129	{"split_count":"3","reference":"hg19"}	{"alignment_speed":"144"}
69	HANA...	129	{"split_count":"3","reference":"hg19"}	{"alignment_speed":"135"}
68	BWA_s	129	{"split_count":"25","reference":"hg19"}	{"alignment_speed":"134"}
67	Bowtie_s	129	{"split_count":"3","reference":"hg19"}	{"alignment_speed":"133"}

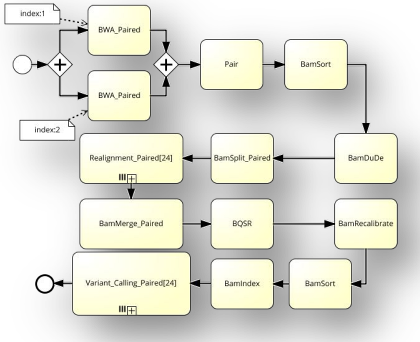
Traditional vs. IMDB Approach

- Processing and results are kept within IMDB
- Optimization reduced execution time by >50%



Available Tools

- Pipeline categories (each traditional and optimized):
  - □ Single read,
  - □ Paired read,
  - □ Amplicon



- Alignment: IMDB-based, TMAP, BWA, Bowtie, Isaac
- Variant Calling: IMDB-based, BcfTools, GATK
- Intermediate steps: SAMtools, Picard, GATK

From Model to Execution

1. Design time (researcher, process expert)
   - □ Definition of parameterized process model
   - □ Uses graphical editor and jobs from repository

2. Configuration time (researcher, lab assistant)
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   - □ Results in model instance stored in repository

3. Execution time (researcher)
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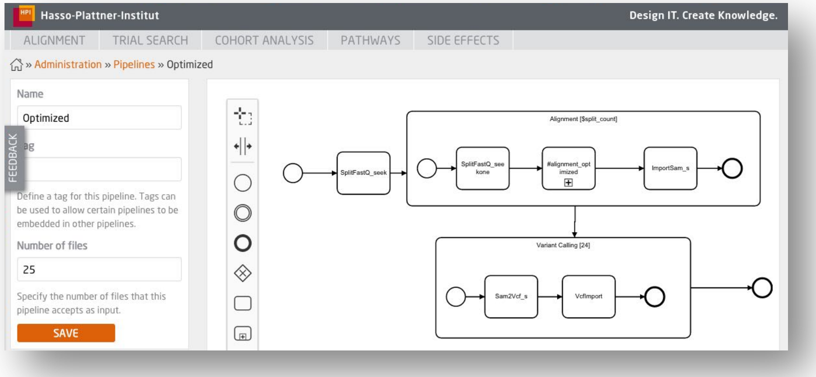
   - □ Specify execution parameters, e.g. input files



» Administration » Pipelines » Optimized

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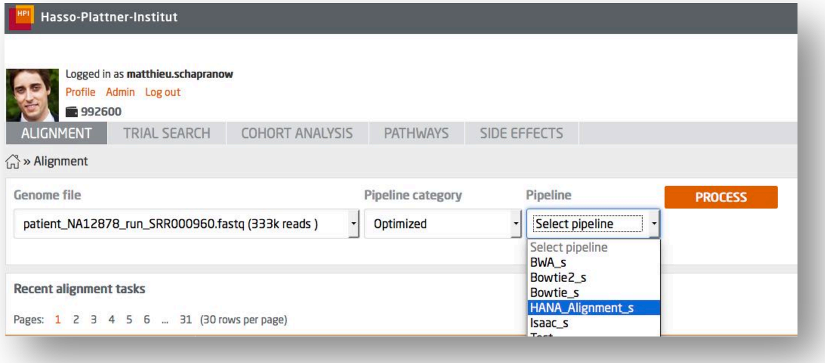


Logged in as **matthieu.schapranow**

992600

» Alignment

Genome file: patient_NA12878_run_SRR000960.fastq (333k reads)

Pipeline category: Optimized

Pipeline: Select pipeline

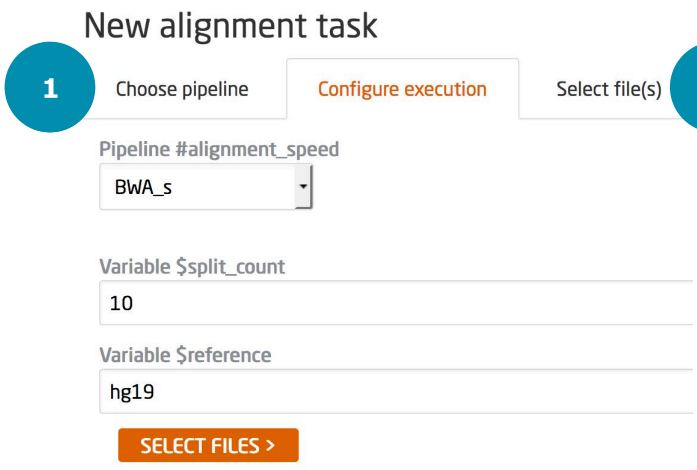
Select pipeline
BWA_s
Bowtie2_s
Bowtie_s
HANA_Alignment_s
Isaac_s

Recent alignment tasks

Pages: 1 2 3 4 5 6 ... 31 (30 rows per page)

Execution of GDPPs

- Uses workflow, which is…
  - □ Predefined by a subject-matter expert
  - □ Preconfigured for a specific run or set of experiments
- Requires only minimal configuration whilst enabling reproducibility



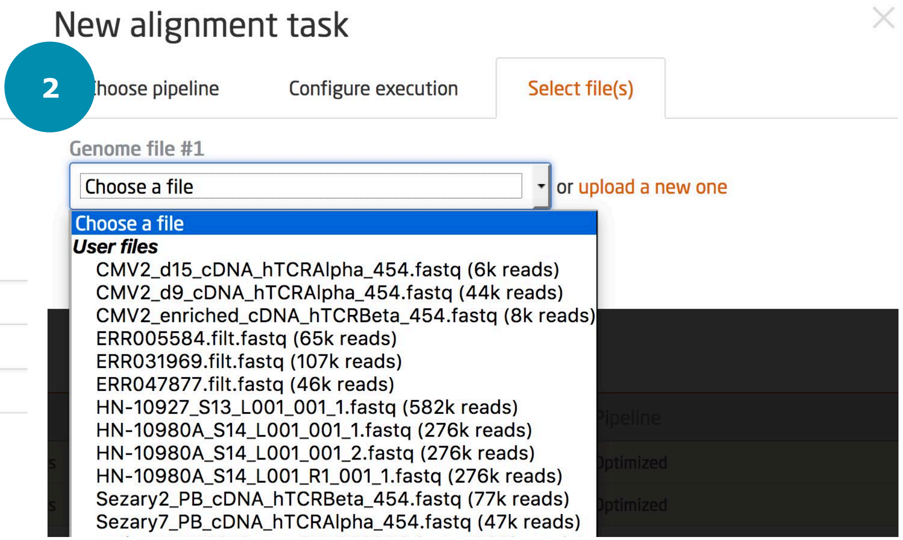
1

New alignment task

Pipeline #alignment_speed: BWA_s

Variable $split_count: 10

Variable $reference: hg19



2

New alignment task

Genome file #1: Choose a file or upload a new one

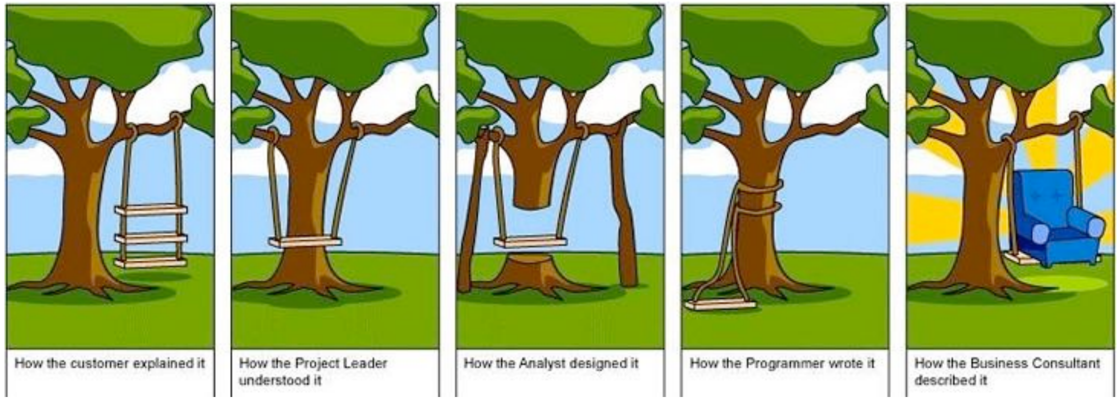
Choose a file

User files

CMV2_d15_cDNA_hTCRAlpha_454.fastq (6k reads)
CMV2_d9_cDNA_hTCRAlpha_454.fastq (44k reads)
CMV2_enriched_cDNA_hTCRBeta_454.fastq (8k reads)
ERR005584.filt.fastq (65k reads)
ERR031969.filt.fastq (107k reads)
ERR047877.filt.fastq (46k reads)
HN-10927_S13_L001_001_1.fastq (582k reads)
HN-10980A_S14_L001_001_1.fastq (276k reads)
HN-10980A_S14_L001_001_2.fastq (276k reads)
HN-10980A_S14_L001_R1_001_1.fastq (276k reads)
Sezary2_PB_cDNA_hTCRBeta_454.fastq (77k reads)
Sezary7_PB_cDNA_hTCRAlpha_454.fastq (47k reads)

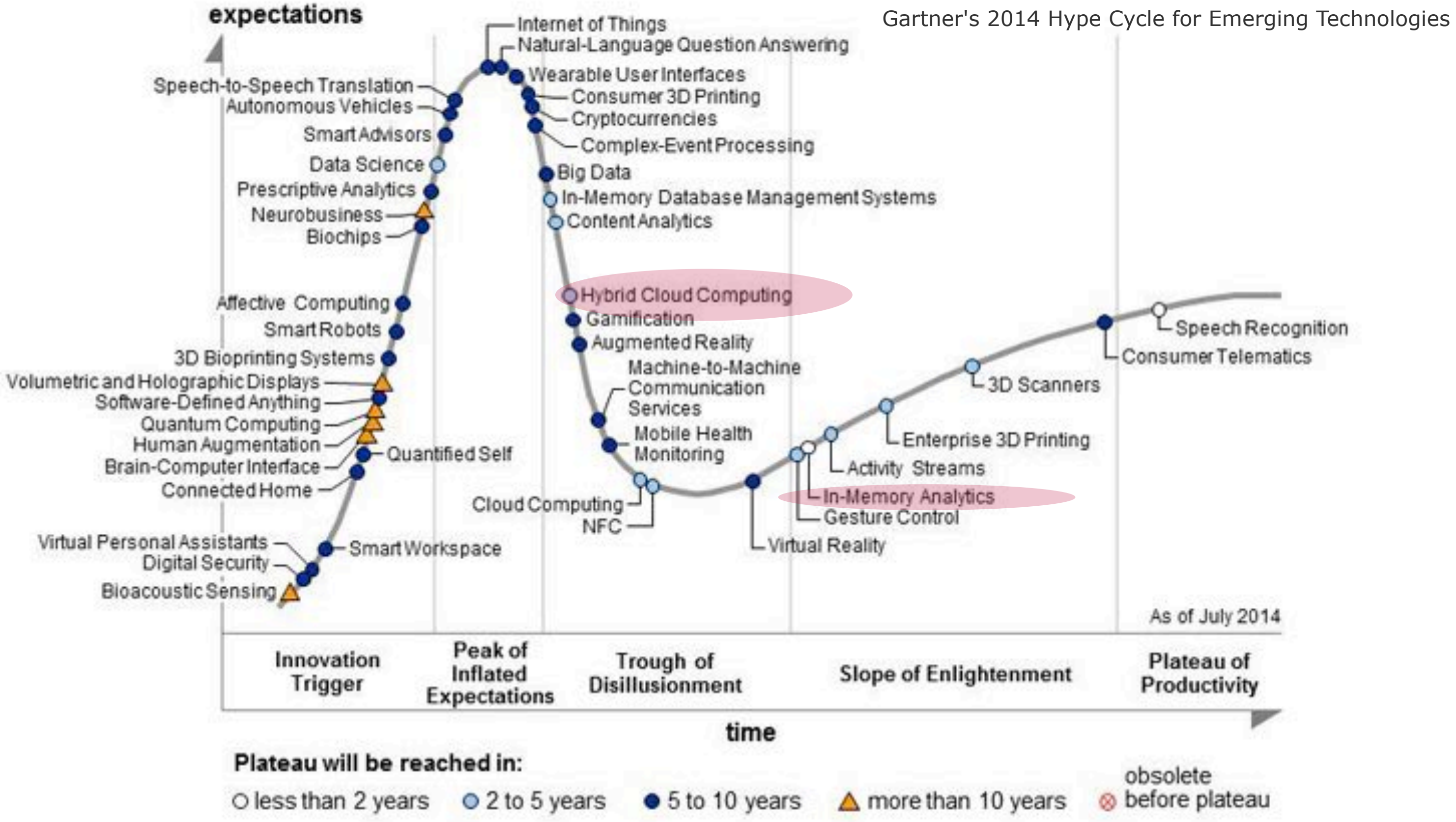
Execution Environment for GDPPs
Software Requirements in Life Sciences

- Requirements
  - □ Managed services
  - □ Reproducibility
  - □ Real-time data analysis of big data
- Restrictions
  - □ Data privacy
  - □ Data locality
  - □ Volume of big medical data
- Solution?
  - □ Federated In-Memory Database System vs. Cloud Computing


How the customer explained it
How the Project Leader understood it
How the Analyst designed it
How the Programmer wrote it
How the Business Consultant described it

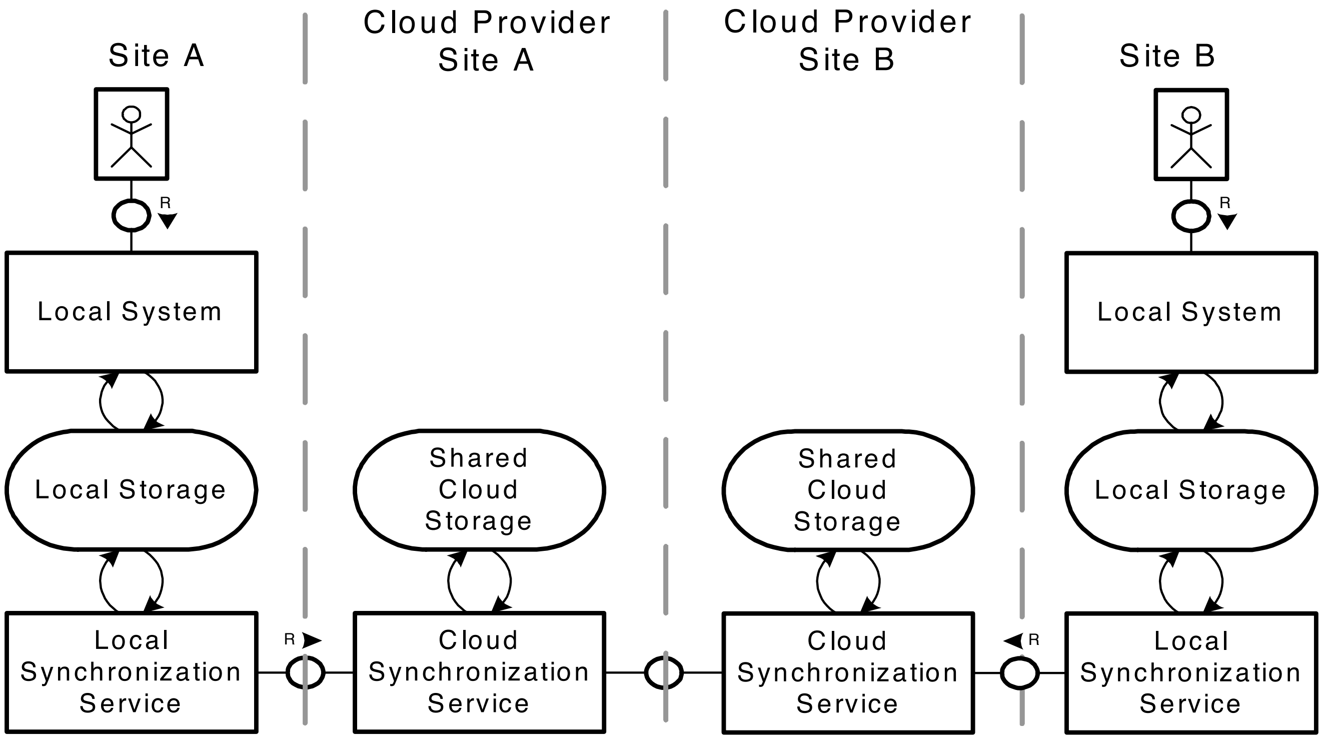
http://stevedempsen.blogspot.de/2013/08/agile-software-requirements-comic.html

Execution Environment for GDPPs Cloud vs. On-Premise?



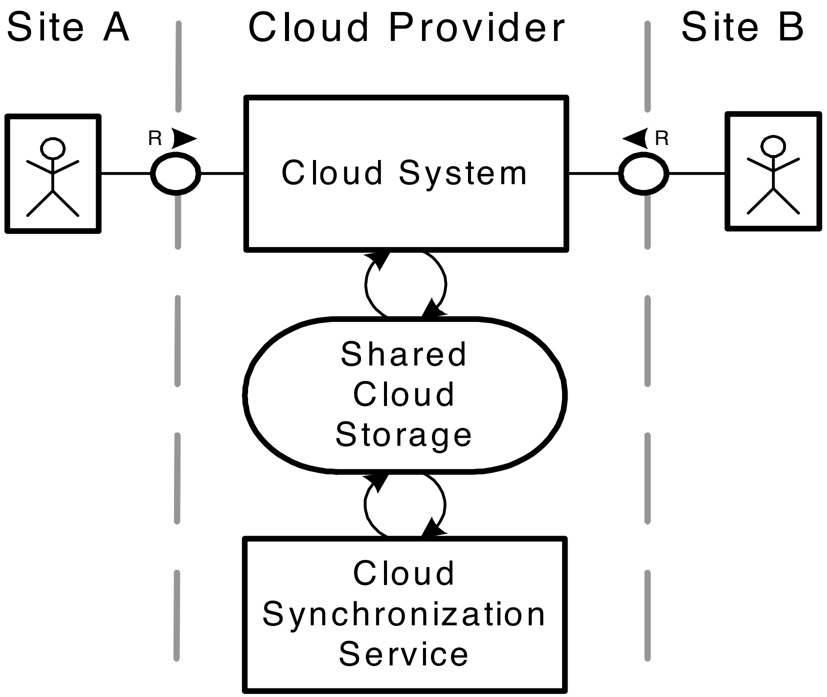
Gartner's 2014 Hype Cycle for Emerging Technologies

Multiple Cloud Service Providers

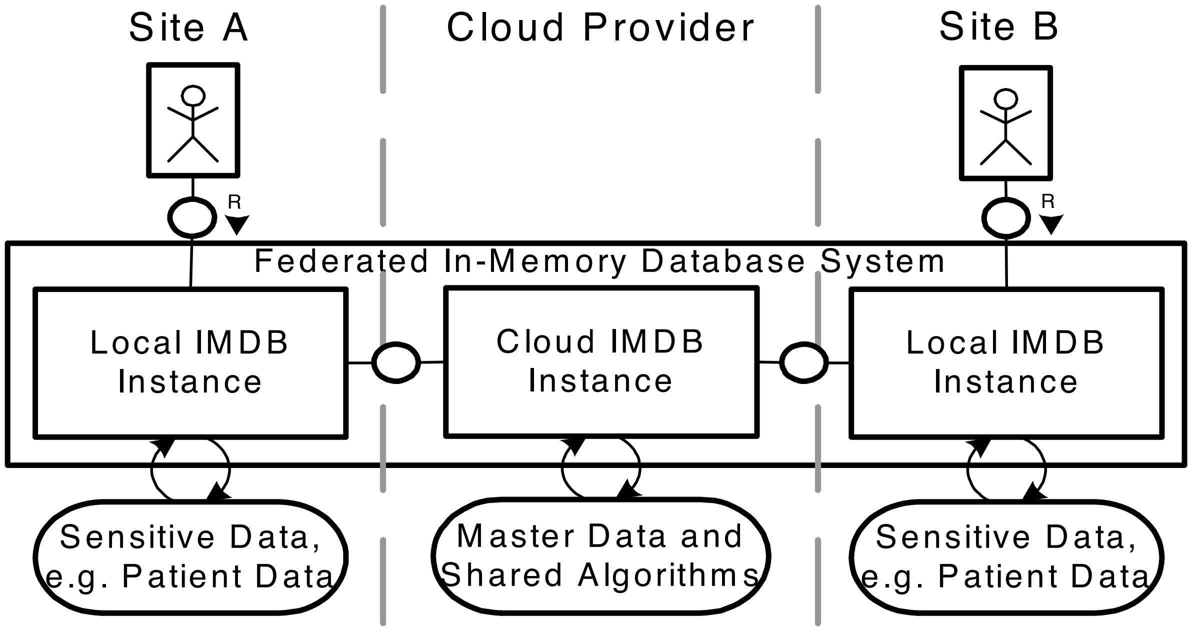


Use Case Oncology Data Management

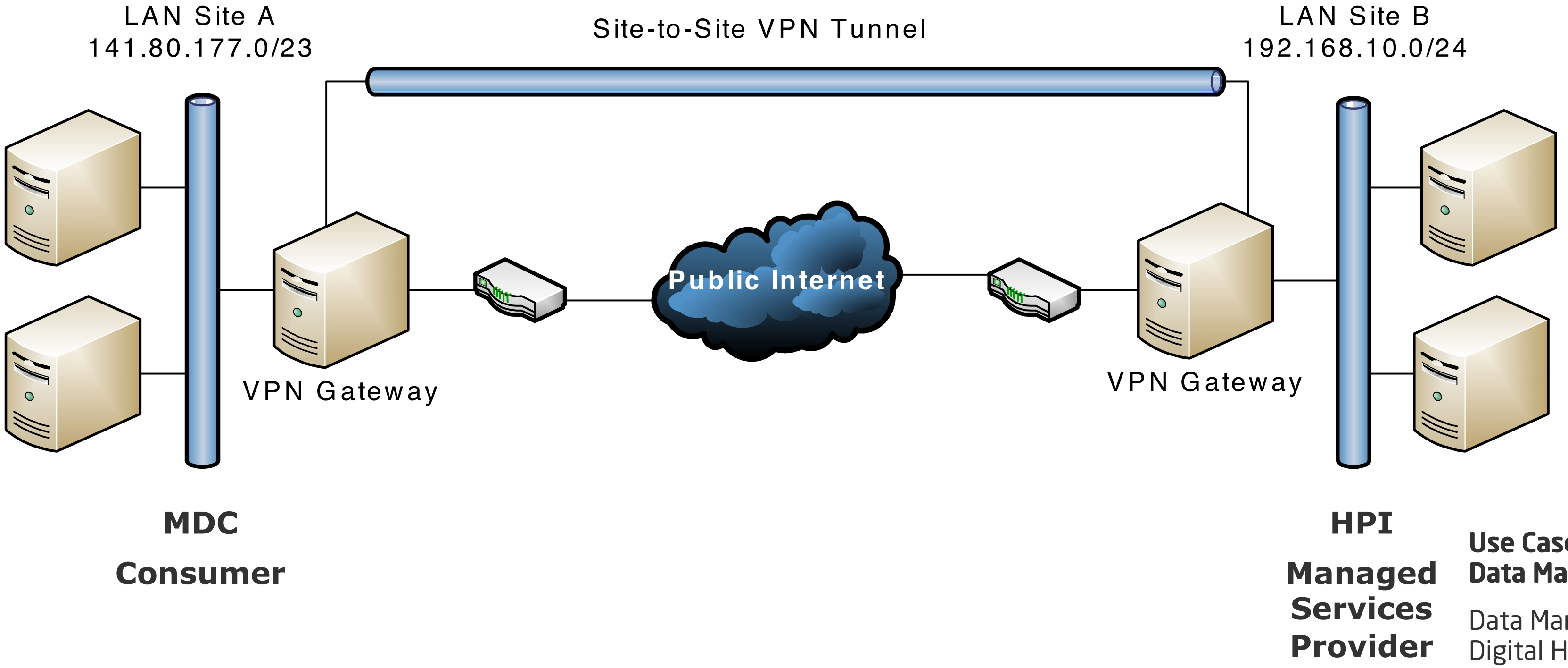
A Single Service Provider



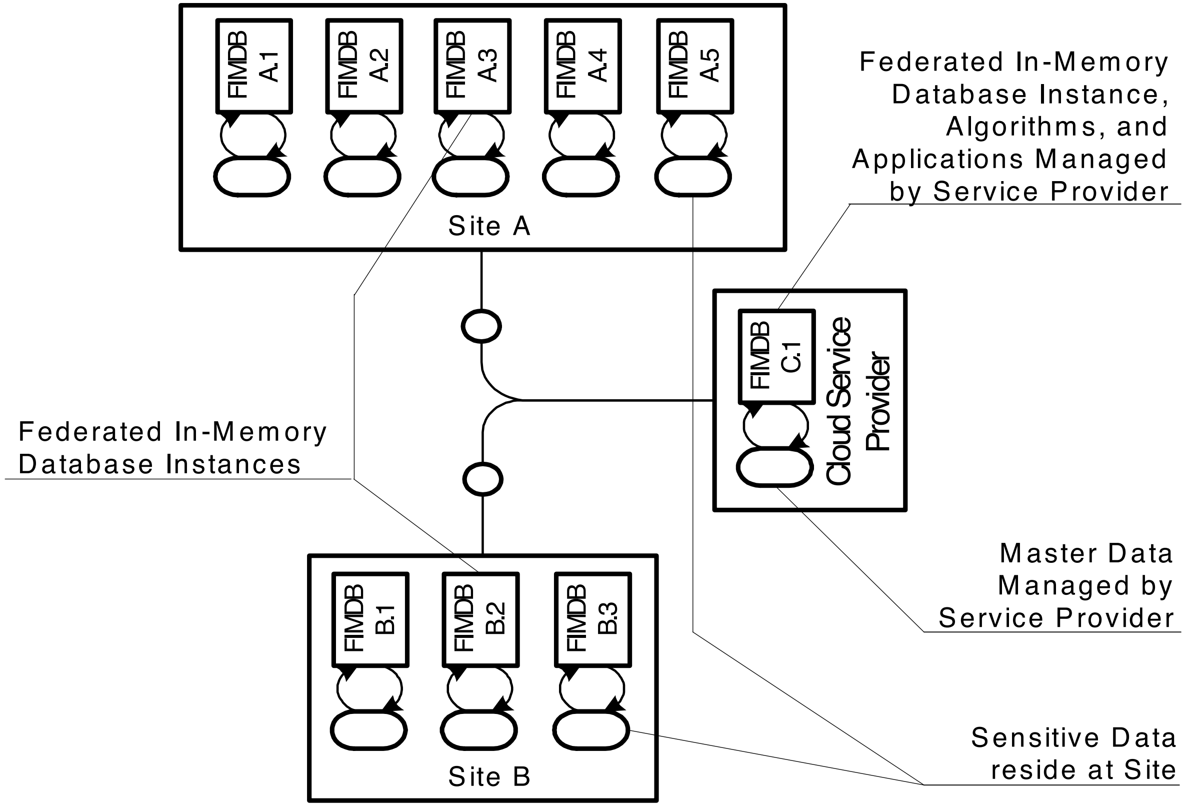
Multiple Sites Forming the Federated In-Memory Database System


Site A
Cloud Provider
Site B
R
R
Federated In-Memory Database System
Local IMDB Instance
Cloud IMDB Instance
Local IMDB Instance
Sensitive Data, e.g. Patient Data
Master Data and Shared Algorithms
Sensitive Data, e.g. Patient Data

Network Setup
Site-to-Site VPN



Federated In-Memory Database (FIMDB) Incorporating Local Compute Resources

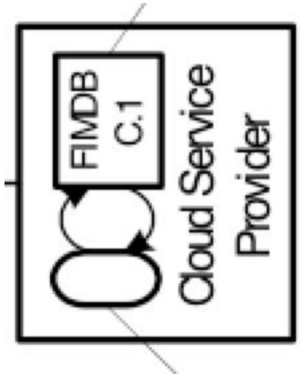


FIMDB A.1
FIMDB A.2
FIMDB A.3
FIMDB A.4
FIMDB A.5
Site A
Federated In-Memory Database Instance, Algorithms, and Applications Managed by Service Provider
FIMDB C.1
Cloud Service Provider
Federated In-Memory Database Instances
Master Data Managed by Service Provider
FIMDB B.1
FIMDB B.2
FIMDB B.3
Site B
Sensitive Data reside at Site

Use Case Oncology Data Management

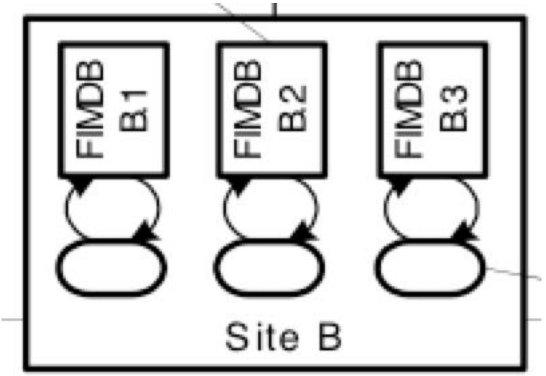
Provided by the Cloud Service Provider

- File System
  - □ Managed services directory
  - □ OS binaries statically compiled for individual platforms
- Database
  - □ In-memory database landscape
  - □ Stored procedures and database algorithms
  - □ Master application data



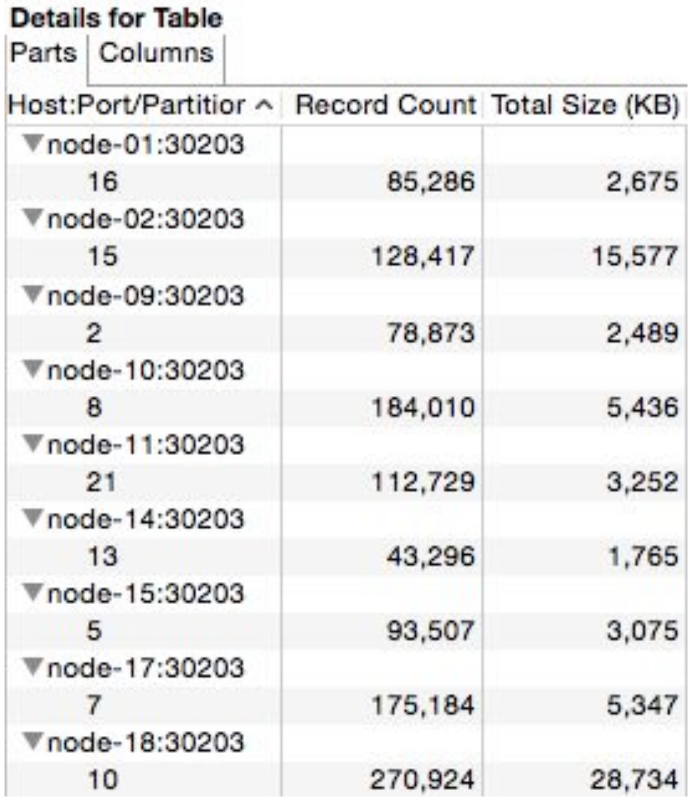
Setup of a New Client

1. Establish site-to-site VPN connection b/w site and cloud service provider
2. Mount remote services directory
3. Install and configure local IMDB instance from services directory
4. Subscribe to and configure selected managed service



Data Partitioning

- Supports parallel query execution
- Protects sensitive data
- Brings algorithms to data



Details for Table

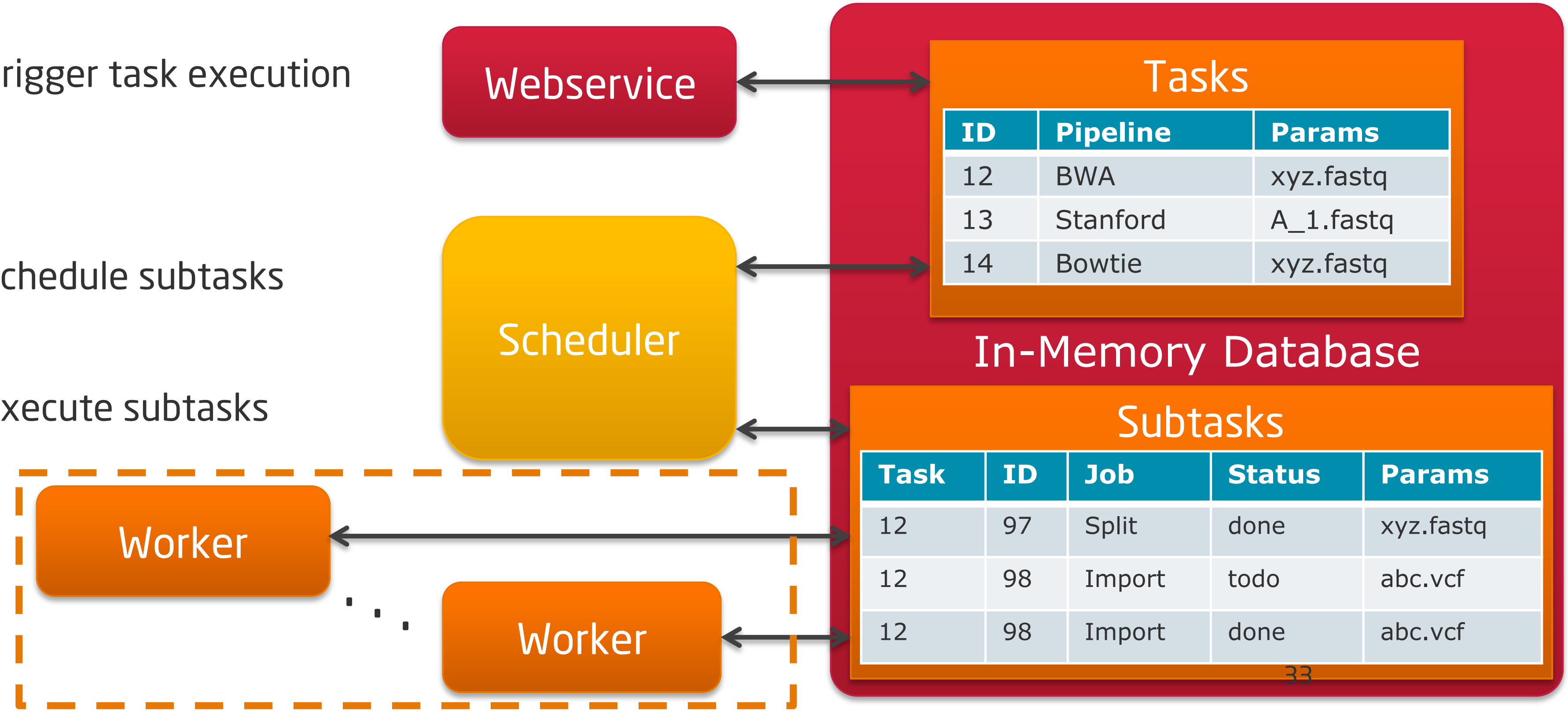
Host:Port/Partitior ^	Record Count	Total Size (KB)
▼node-01:30203		
16	85,286	2,675
▼node-02:30203		
15	128,417	15,577
▼node-09:30203		
2	78,873	2,489
▼node-10:30203		
8	184,010	5,436
▼node-11:30203		
21	112,729	3,252
▼node-14:30203		
13	43,296	1,765
▼node-15:30203		
5	93,507	3,075
▼node-17:30203		
7	175,184	5,347
▼node-18:30203		
10	270,924	28,734

Scheduling and Execution of GDPPs

1. Trigger task execution

2. Schedule subtasks

3. Execute subtasks



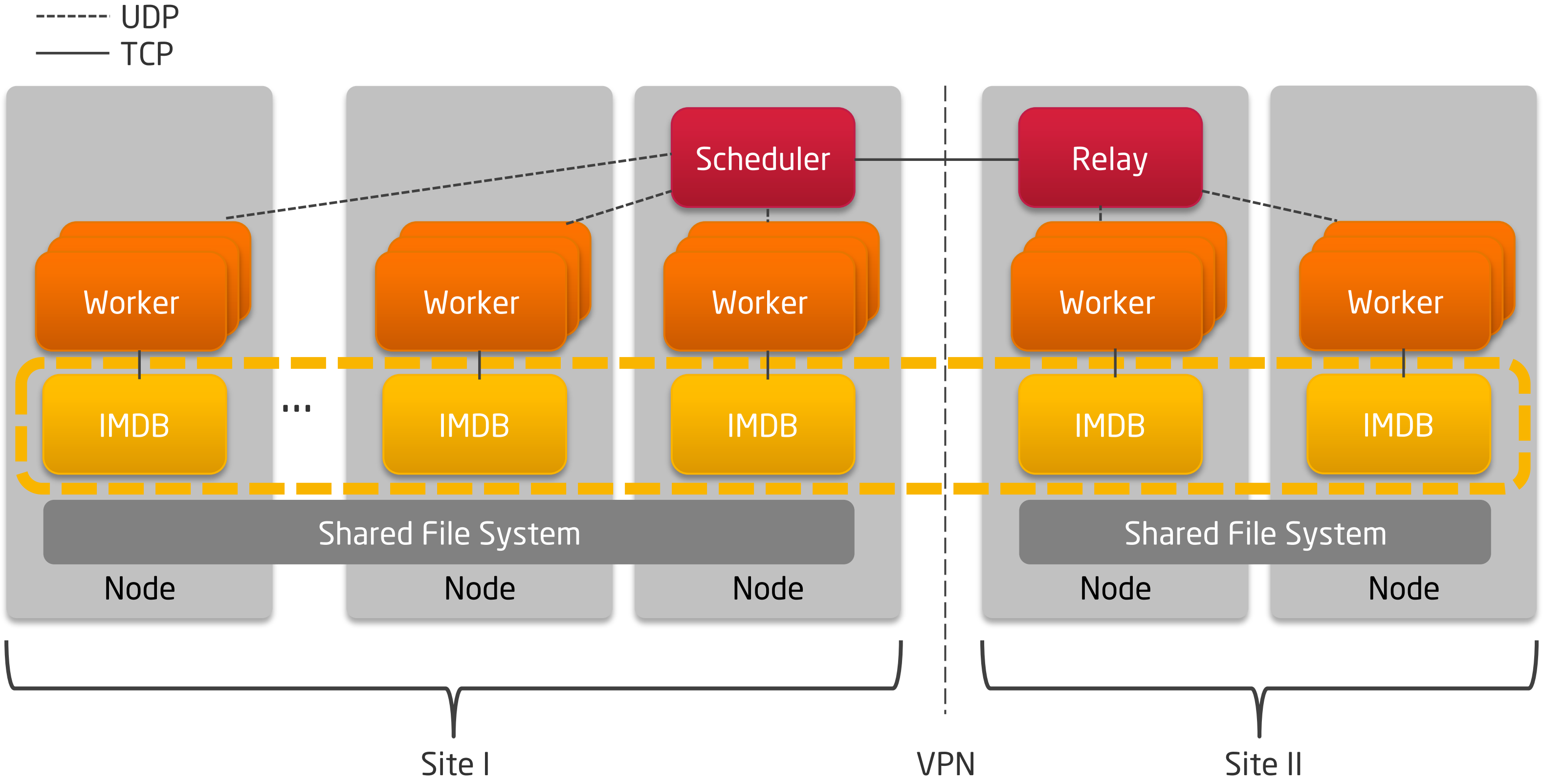
Tasks

ID	Pipeline	Params
12	BWA	xyz.fastq
13	Stanford	A_1.fastq
14	Bowtie	xyz.fastq

Subtasks

Task	ID	Job	Status	Params
12	97	Split	done	xyz.fastq
12	98	Import	todo	abc.vcf
12	98	Import	done	abc.vcf

Software Components and Communication



IMDB Structure
TASKS

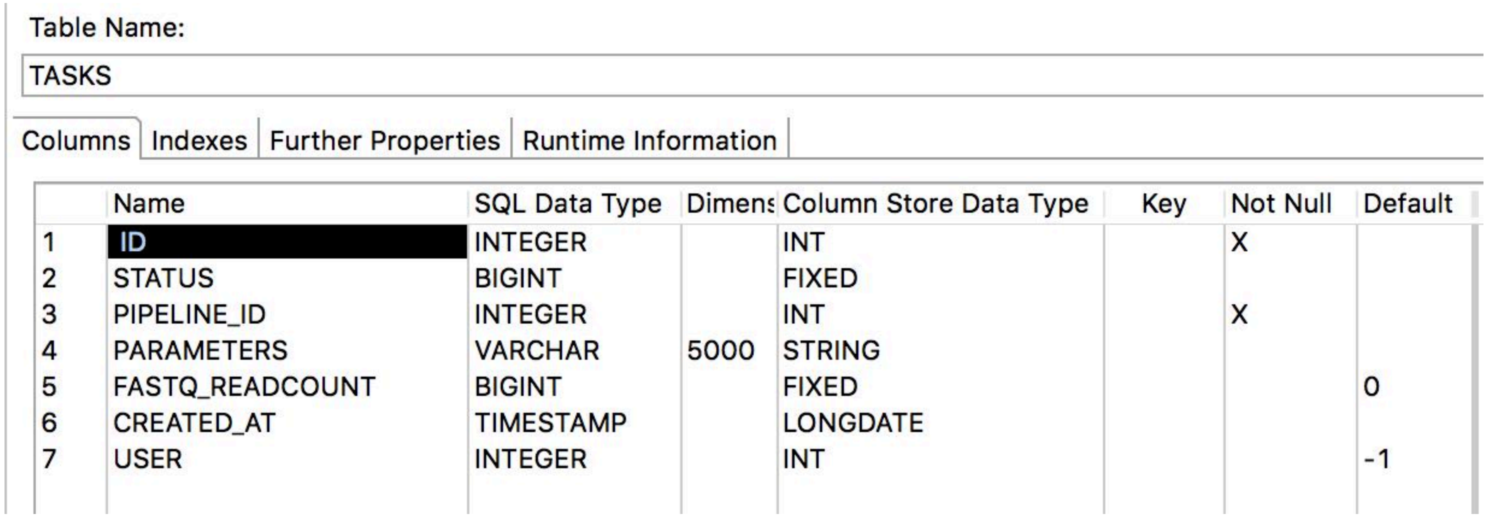
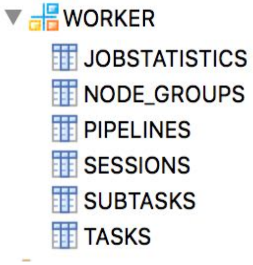


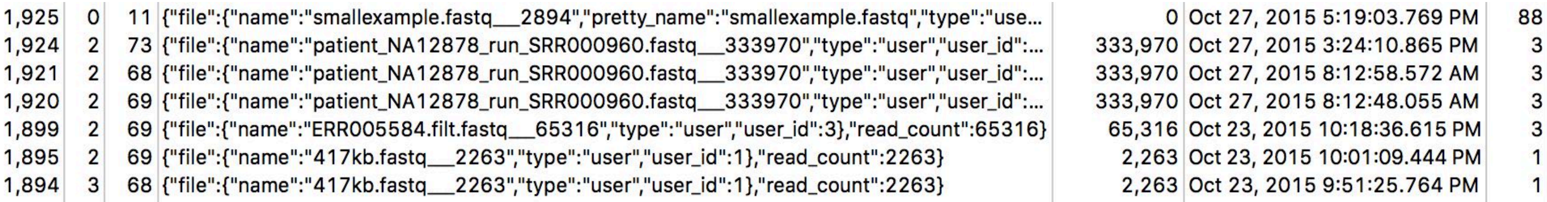
Table Name:

TASKS

	Name	SQL Data Type	Dimens	Column Store Data Type	Key	Not Null	Default
1	ID	INTEGER		INT		X	
2	STATUS	BIGINT		FIXED			
3	PIPELINE_ID	INTEGER		INT		X	
4	PARAMETERS	VARCHAR	5000	STRING			
5	FASTQ_READCOUNT	BIGINT		FIXED			0
6	CREATED_AT	TIMESTAMP		LONGDATE			
7	USER	INTEGER		INT			-1



- WORKER
  - JOBSTATISTICS
  - NODE_GROUPS
  - PIPELINES
  - SESSIONS
  - SUBTASKS
  - TASKS



1,925	0	11	{"file":{"name":"smallexample.fastq___2894","pretty_name":"smallexample.fastq","type":"use...	0	Oct 27, 2015 5:19:03.769 PM	88
1,924	2	73	{"file":{"name":"patient_NA12878_run_SRR000960.fastq___333970","type":"user","user_id":...	333,970	Oct 27, 2015 3:24:10.865 PM	3
1,921	2	68	{"file":{"name":"patient_NA12878_run_SRR000960.fastq___333970","type":"user","user_id":...	333,970	Oct 27, 2015 8:12:58.572 AM	3
1,920	2	69	{"file":{"name":"patient_NA12878_run_SRR000960.fastq___333970","type":"user","user_id":...	333,970	Oct 27, 2015 8:12:48.055 AM	3
1,899	2	69	{"file":{"name":"ERR005584.filt.fastq___65316","type":"user","user_id":3},"read_count":65316}	65,316	Oct 23, 2015 10:18:36.615 PM	3
1,895	2	69	{"file":{"name":"417kb.fastq___2263","type":"user","user_id":1},"read_count":2263}	2,263	Oct 23, 2015 10:01:09.444 PM	1
1,894	3	68	{"file":{"name":"417kb.fastq___2263","type":"user","user_id":1},"read_count":2263}	2,263	Oct 23, 2015 9:51:25.764 PM	1

IMDB Structure
SUBTASKS

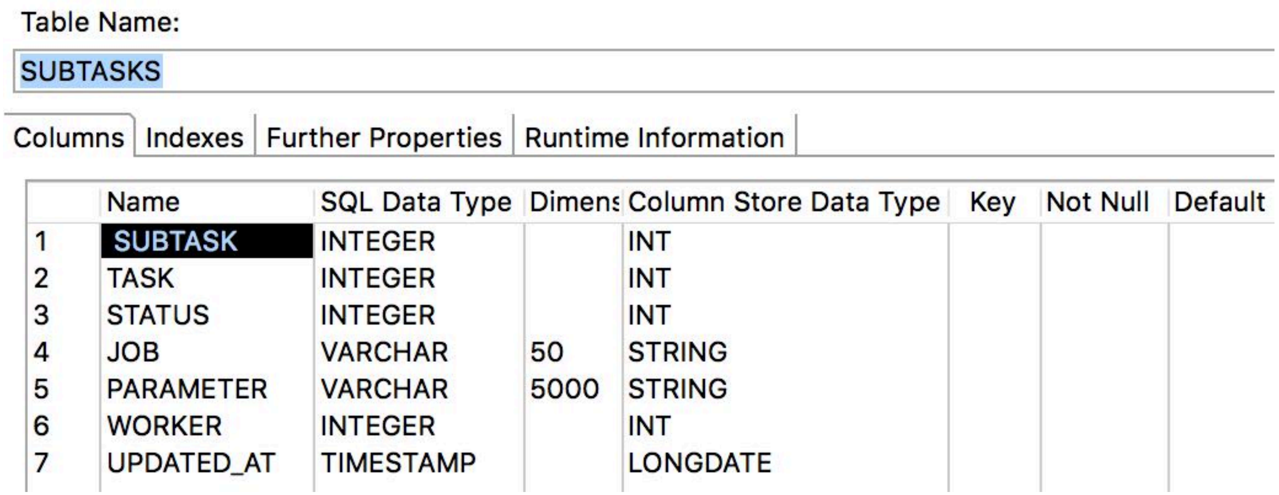
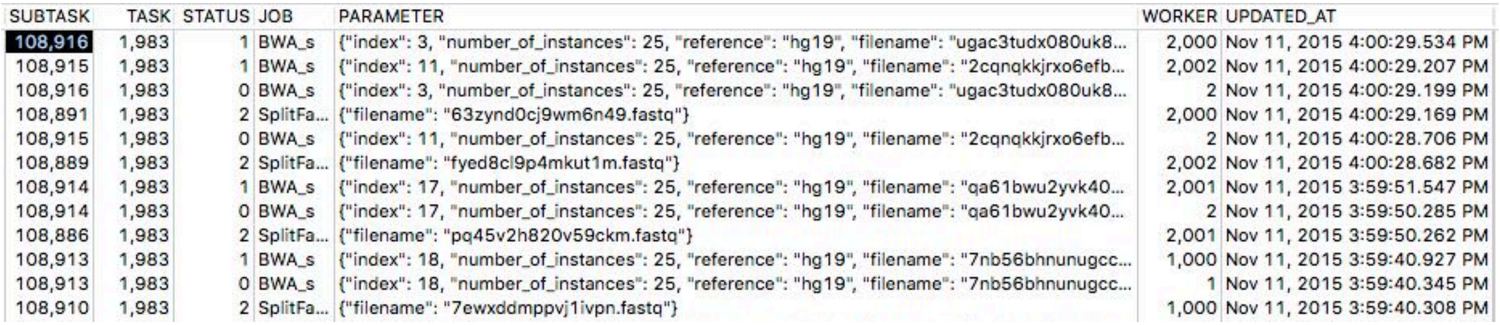


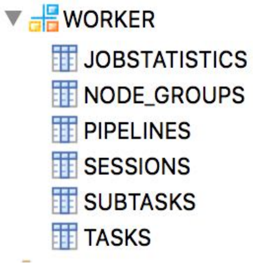
Table Name:

SUBTASKS

	Name	SQL Data Type	Dimens	Column Store Data Type	Key	Not Null	Default
1	SUBTASK	INTEGER		INT			
2	TASK	INTEGER		INT			
3	STATUS	INTEGER		INT			
4	JOB	VARCHAR	50	STRING			
5	PARAMETER	VARCHAR	5000	STRING			
6	WORKER	INTEGER		INT			
7	UPDATED_AT	TIMESTAMP		LONGDATE			



SUBTASK	TASK	STATUS	JOB	PARAMETER	WORKER	UPDATED_AT
108,916	1,983	1	BWA_s	{"index": 3, "number_of_instances": 25, "reference": "hg19", "filename": "ugac3tudx080uk8...	2,000	Nov 11, 2015 4:00:29.534 PM
108,915	1,983	1	BWA_s	{"index": 11, "number_of_instances": 25, "reference": "hg19", "filename": "2cqnqkkjrxo6efb...	2,002	Nov 11, 2015 4:00:29.207 PM
108,916	1,983	0	BWA_s	{"index": 3, "number_of_instances": 25, "reference": "hg19", "filename": "ugac3tudx080uk8...	2	Nov 11, 2015 4:00:29.199 PM
108,891	1,983	2	SplitFa...	{"filename": "63zynd0cj9wm6n49.fastq"}	2,000	Nov 11, 2015 4:00:29.169 PM
108,915	1,983	0	BWA_s	{"index": 11, "number_of_instances": 25, "reference": "hg19", "filename": "2cqnqkkjrxo6efb...	2	Nov 11, 2015 4:00:28.706 PM
108,889	1,983	2	SplitFa...	{"filename": "fyed8cl9p4mkut1m.fastq"}	2,002	Nov 11, 2015 4:00:28.682 PM
108,914	1,983	1	BWA_s	{"index": 17, "number_of_instances": 25, "reference": "hg19", "filename": "qa61bwu2yvk40...	2,001	Nov 11, 2015 3:59:51.547 PM
108,914	1,983	0	BWA_s	{"index": 17, "number_of_instances": 25, "reference": "hg19", "filename": "qa61bwu2yvk40...	2	Nov 11, 2015 3:59:50.285 PM
108,886	1,983	2	SplitFa...	{"filename": "pq45v2h820v59ckm.fastq"}	2,001	Nov 11, 2015 3:59:50.262 PM
108,913	1,983	1	BWA_s	{"index": 18, "number_of_instances": 25, "reference": "hg19", "filename": "7nb56bhnunugcc...	1,000	Nov 11, 2015 3:59:40.927 PM
108,913	1,983	0	BWA_s	{"index": 18, "number_of_instances": 25, "reference": "hg19", "filename": "7nb56bhnunugcc...	1	Nov 11, 2015 3:59:40.345 PM
108,910	1,983	2	SplitFa...	{"filename": "7ewxddmppvj1ivpn.fastq"}	1,000	Nov 11, 2015 3:59:40.308 PM

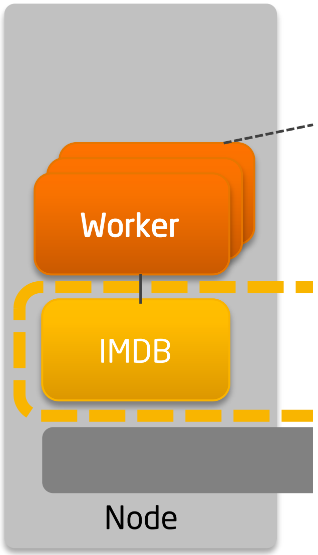


- WORKER
  - JOBSTATISTICS
  - NODE_GROUPS
  - PIPELINES
  - SESSIONS
  - SUBTASKS
  - TASKS

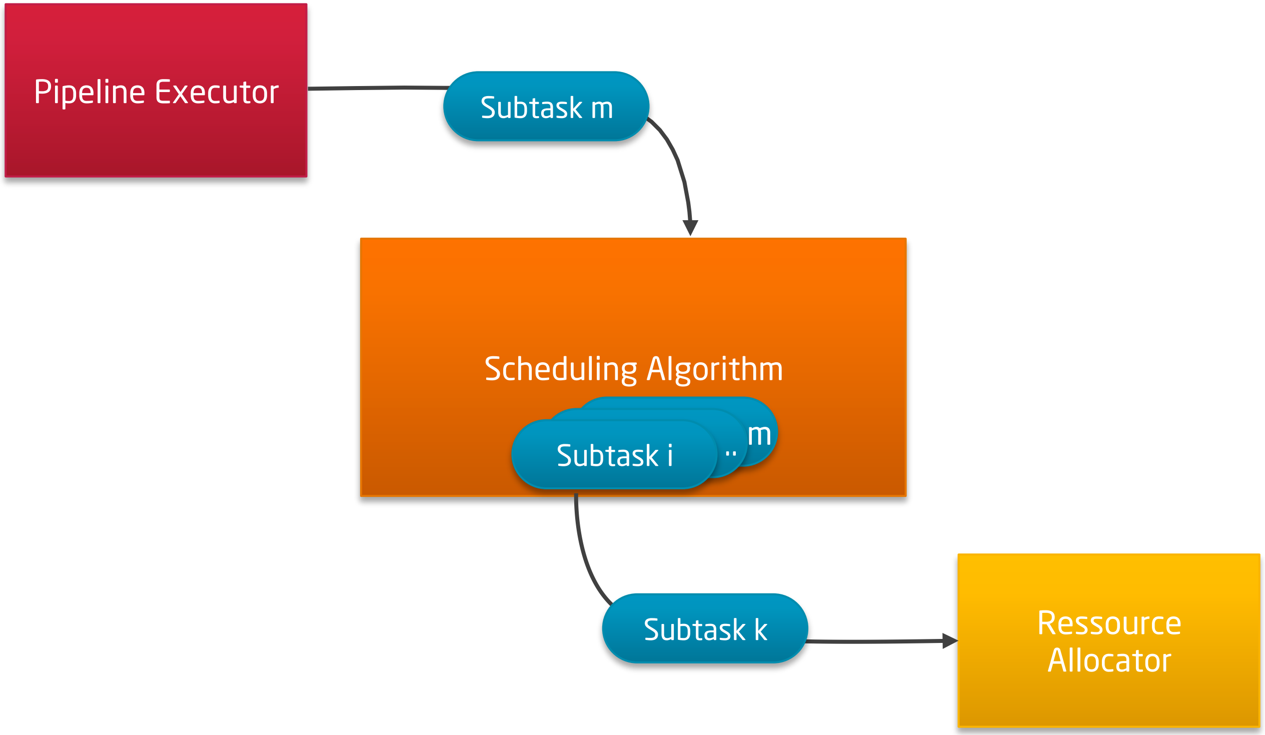
Runtime Layer
Worker

- Workers execute jobs one by one
- Subtask execution status in IMDB:
  - Ready (0),
  - In Progress (1),
  - Done (2), or
  - Erroneous (3).

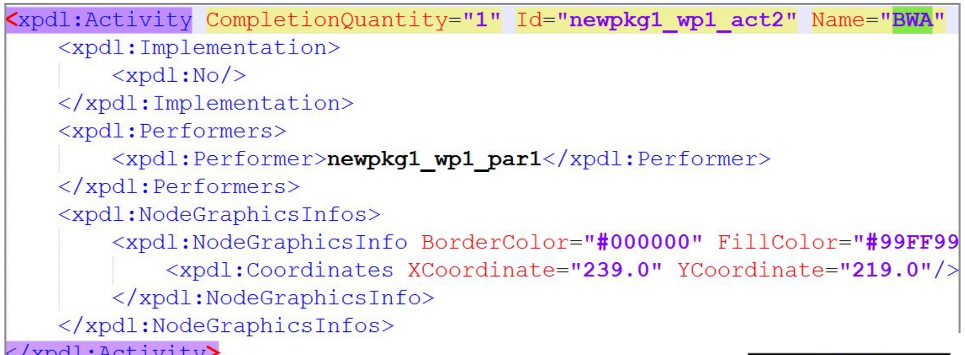
- Jobs implemented as Python modules/classes
  - Can contain arbitrary code
  - Have access to IMDB
  - Can read/write to shared working directory



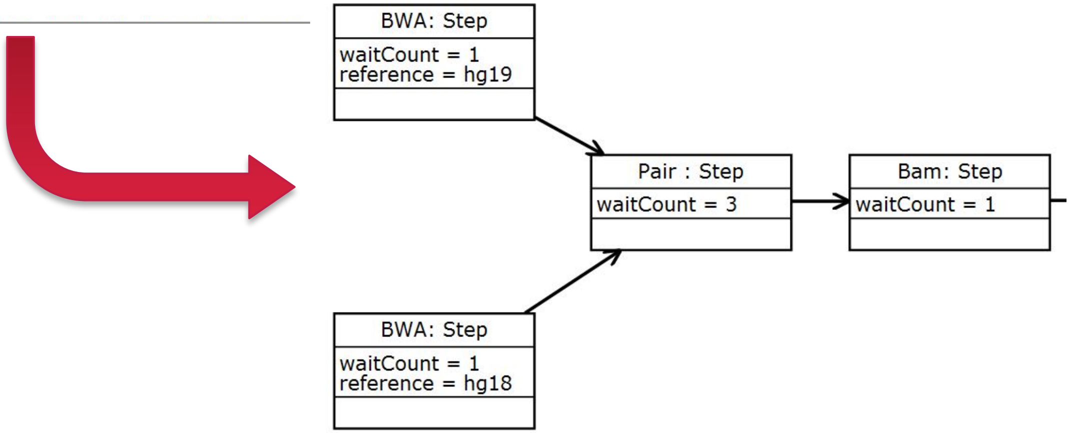
Coordination Layer
Scheduler



Scheduling
Pipeline Executer

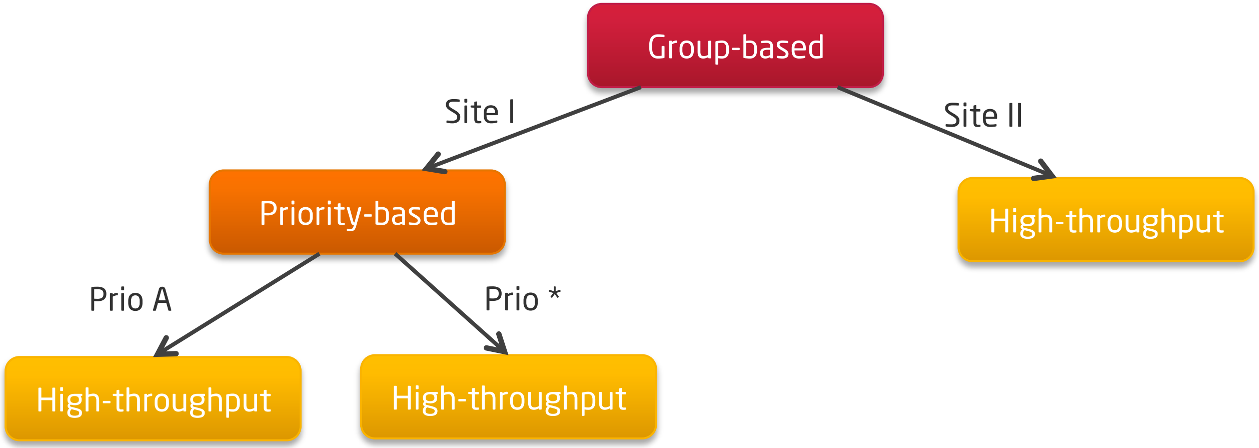


```
<xpdl:Activity CompletionQuantity="1" Id="newpkg1_wp1_act2" Name="BWA"
    <xpdl:Implementation>
        <xpdl:No/>
    </xpdl:Implementation>
    <xpdl:Performers>
        <xpdl:Performer>newpkg1_wp1_par1</xpdl:Performer>
    </xpdl:Performers>
    <xpdl:NodeGraphicsInfos>
        <xpdl:NodeGraphicsInfo BorderColor="#000000" FillColor="#99FF99
            <xpdl:Coordinates XCoordinate="239.0" YCoordinate="219.0"/>
        </xpdl:NodeGraphicsInfo>
    </xpdl:NodeGraphicsInfos>
</xpdl:Activity>
```



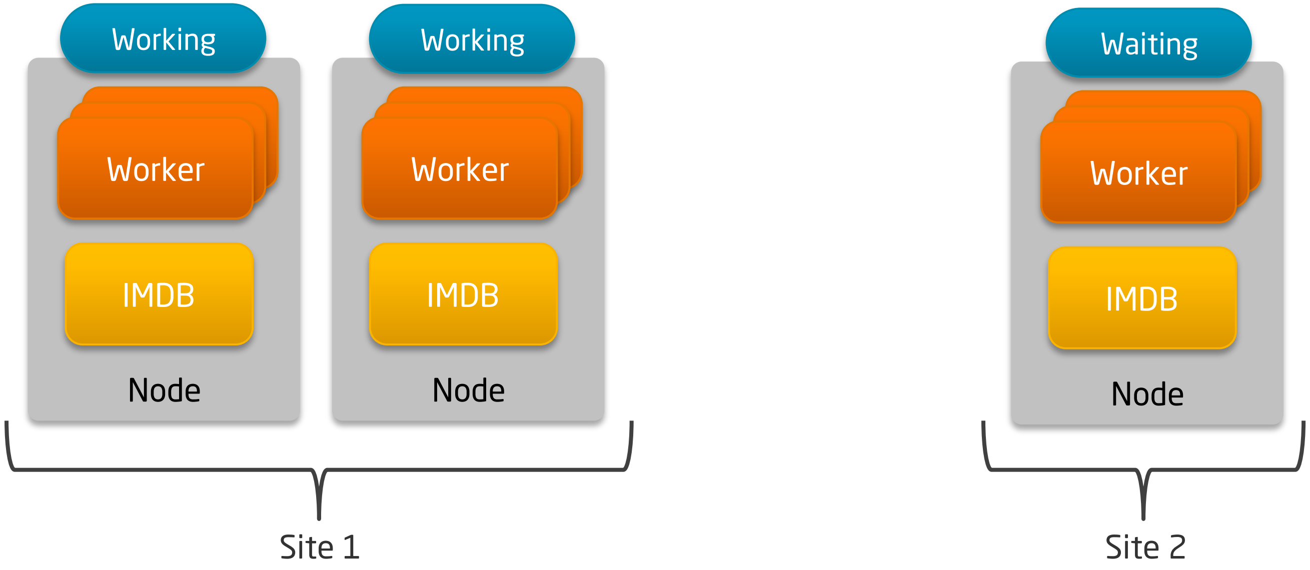
Scheduling Algorithms

- Scheduling algorithms are plug-in software modules
  - □ "User-/Group-based" to let users execute their tasks on their local site only
  - □ "Priority First" to prefer important users
  - □ "High Throughput", i.e. "shortest task first" to deal with high load
- Scheduling algorithms can also be composed hierarchically



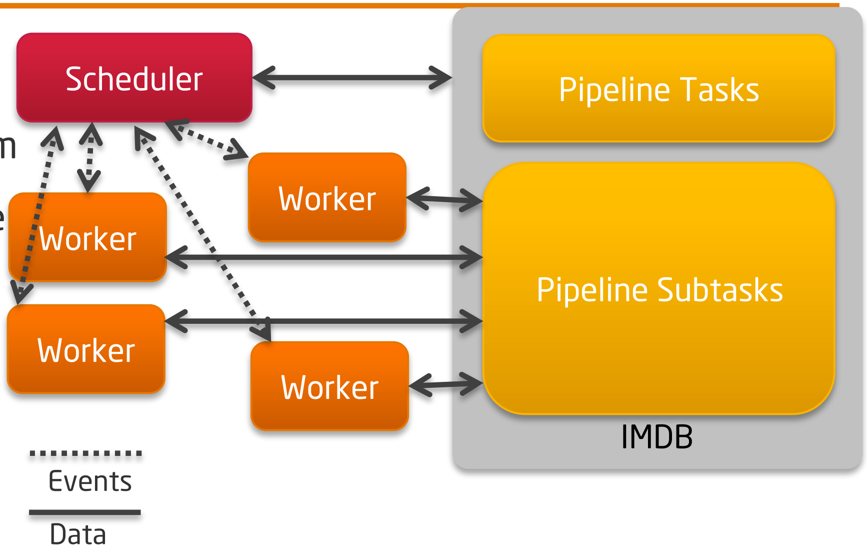
Scheduling
Resource Allocator

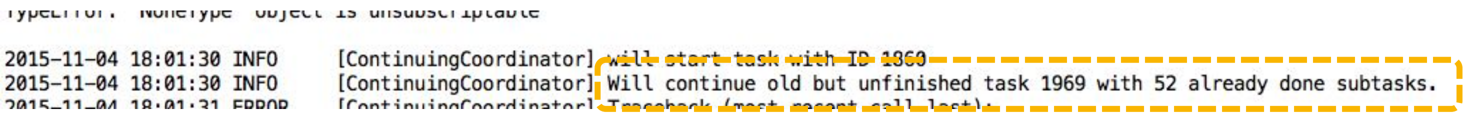
- Maintains lists of running and idle nodes
- Idle worker requests new sub task for its assigned groups
- If there is no matching sub task, it sleeps until a new sub task gets ready



Recoverability

- All execution data is stored in IMDB
- Temporary files on a shared file system
- In case of any failure, the system-wide state can be restored





```
TypeError: 'NoneType' object is unsubscriptable

2015-11-04 18:01:30 INFO      [ContinuingCoordinator] will start task with ID 1969
2015-11-04 18:01:30 INFO      [ContinuingCoordinator] Will continue old but unfinished task 1969 with 52 already done subtasks.
2015-11-04 18:01:31 ERROR     [ContinuingCoordinator] Traceback (most recent call last):
```

FIMDB Comparison

- FIMDB provides (smaller) algorithms to (larger) data
- Forms a single virtual database across sites and locations
- Master data managed by service provider whilst sensitive data resides locally

Pros	Cons
Single database license	Complex operation
Easy to consume services	Single setup required
Query propagation by IMDB	