Efficient tool deployment to the Galaxy Cloud: An RNA-seq workflow case study

Sebastian J. Schultheiss <sebi@tue.mpg.de>
Machine Learning in Biology, Rätsch Lab, FML of the Max Planck Society
Tübingen, Germany

Friedrich Miescher Laboratory
of the Max Planck Society

MAX-PLANCK-GESELLSCHAFT

oqtans
online
quantitative
transcript
analysis

Web Services Availability

Schultheiss 2011, PLoS CB acc.
Schultheiss et al. 2011, PLoS ONE i.r.

- 927 web services (NAR Web Server Issues)
- Collection of 45 data on every service
- Survey among authors
- Problems:
  - URL change
  - missing example data
  - program on server not functional
  - undocumented changes from updates

Web Servic Availability

chultheiss 2011, PLoS CB acc.
iss et al. 2011, PLoS ONE i.r.

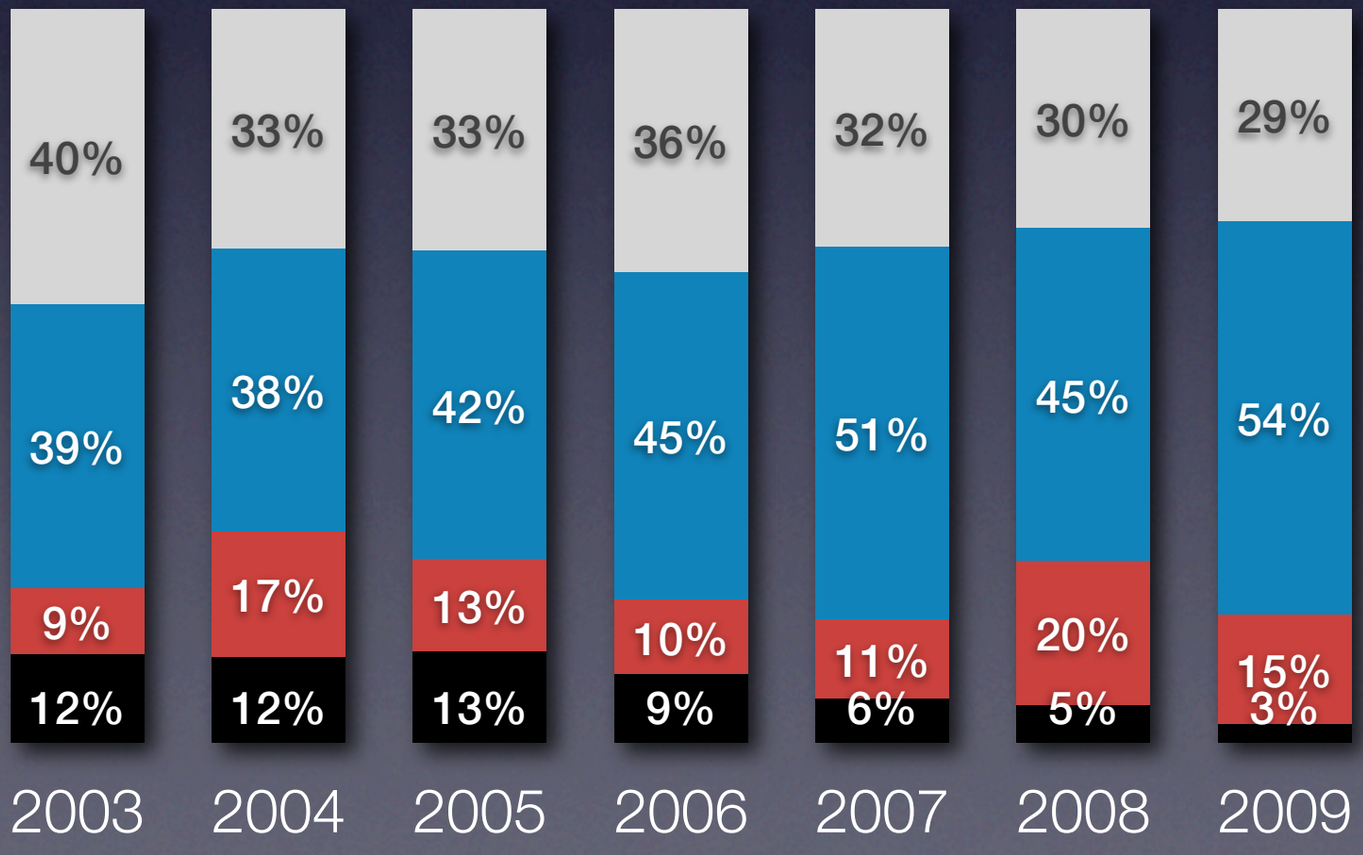
- 927 web servi erver Issues)
- Collection ervice
- Survey a
- Proble
  - URL change

Caution: Published results may not be reproducible

Web Services Availability

- Redirected from URL stated in abstract: 13%
- Unreachable, only via search engine: 7%
- Unreachable and not found: 9%
- Correct URL in abstract: 72%

Schultheiss et al. 2011, PLoS ONE i.r.



Evaluations:
June 2009
August 2010
October 2010

No “fair” testing possibility (33%)
Server is functional (45%)
Server is not functional (13%)
Server is unreachable (9%)

Galaxy Approach

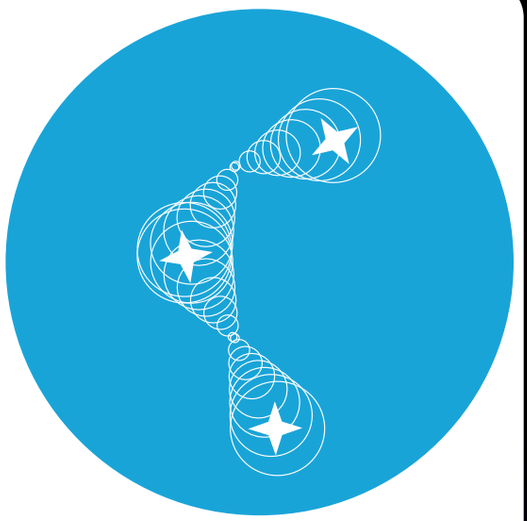
J. Goecks et al. 2010
D. Blankenberg et al. 2010
E. Afgan et al. 2010
S. Koskovsky Pond et al. 2009
W. Miller et al. 2007
J. Taylor et al. 2007
D. Blankenberg et al. 2007
Giardine et al. 2005

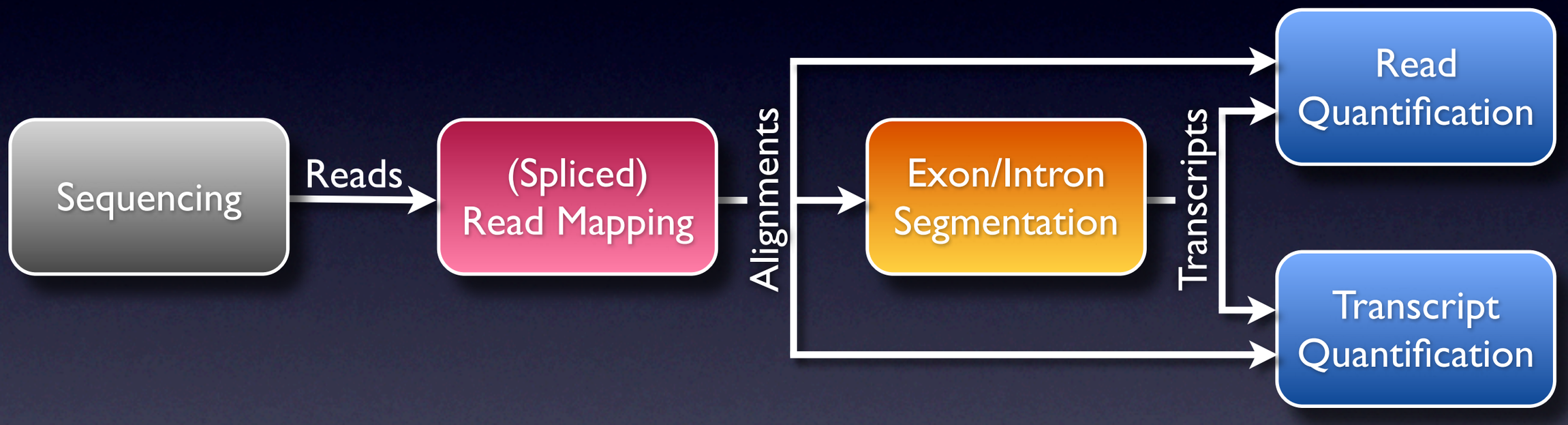
- Persistent, reproducible approach to bioinformatics research
- Integration of tools made simple
- Source code release, VM/AMI, cloud instances, Galaxy pages

Our Galaxy Tools:

oqtans

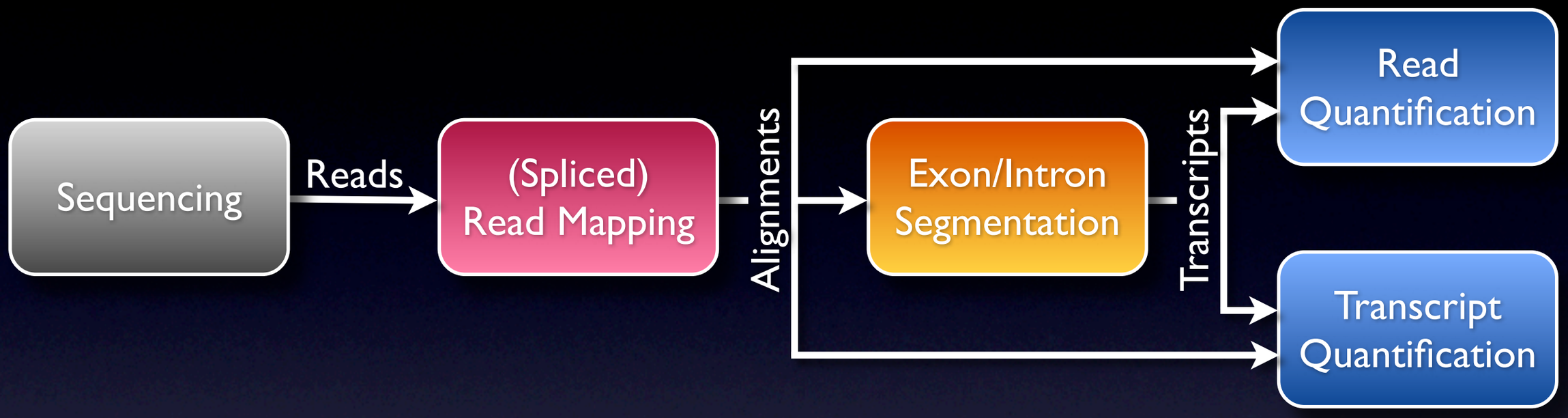
online
quantitative
transcript
analysis





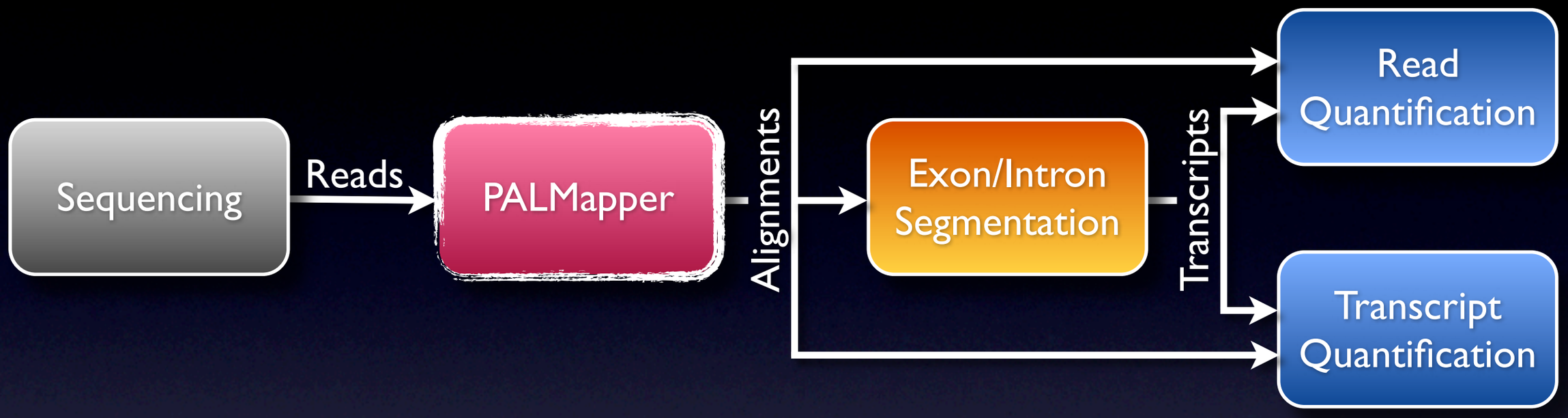
- Machine Learning-powered for quantitative analyses of RNA-seq experiments
- Workflow can be adjusted to your needs

oqtans



- Common experimental setups:
  - Identification of new transcripts
  - Comparison of samples

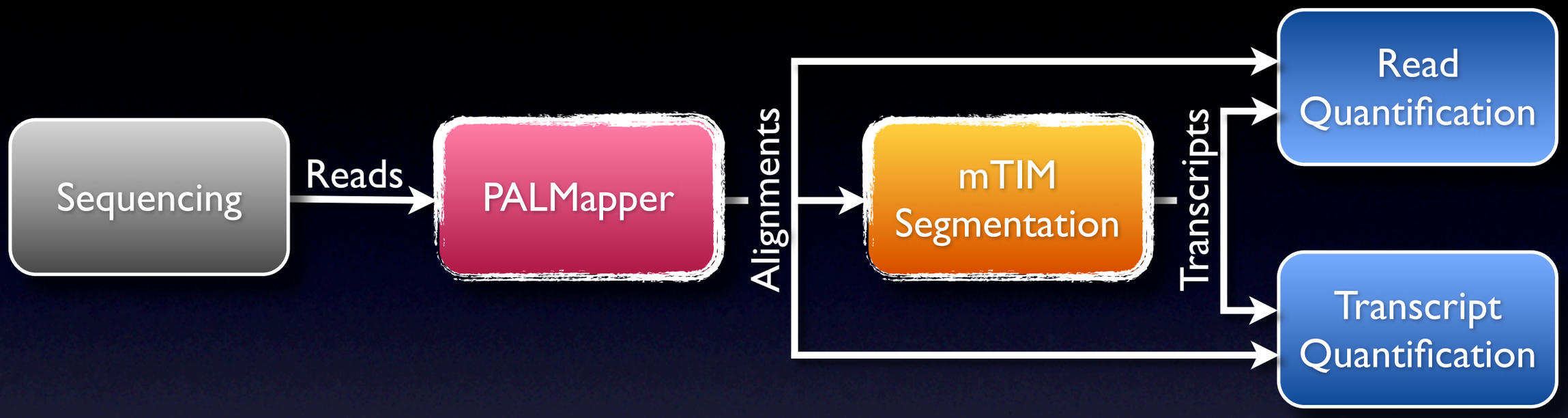
oqtans



- **PALMapper**: highly accurate short-read mapper using base quality and splice site predictions

G. Jean et al. 2010

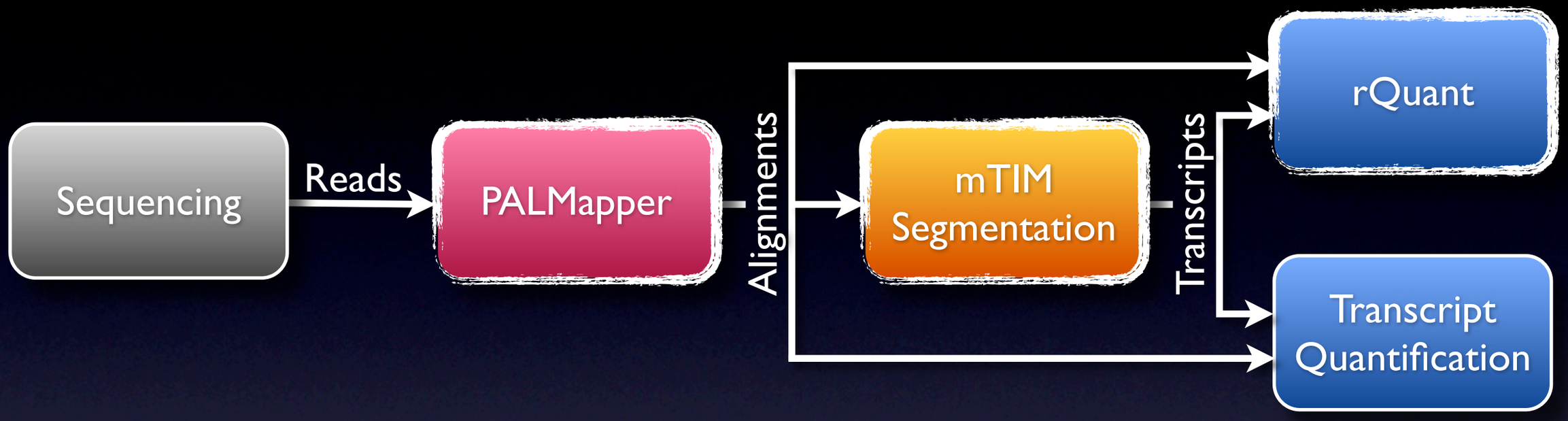
oqtans



- **mTIM**: reconstructs exon-intron structure from alignments and splice site predictions
- **SplAdder**: adds isoforms to known annotation based on splice graph

G. Zeller et al. 2011 i.p.

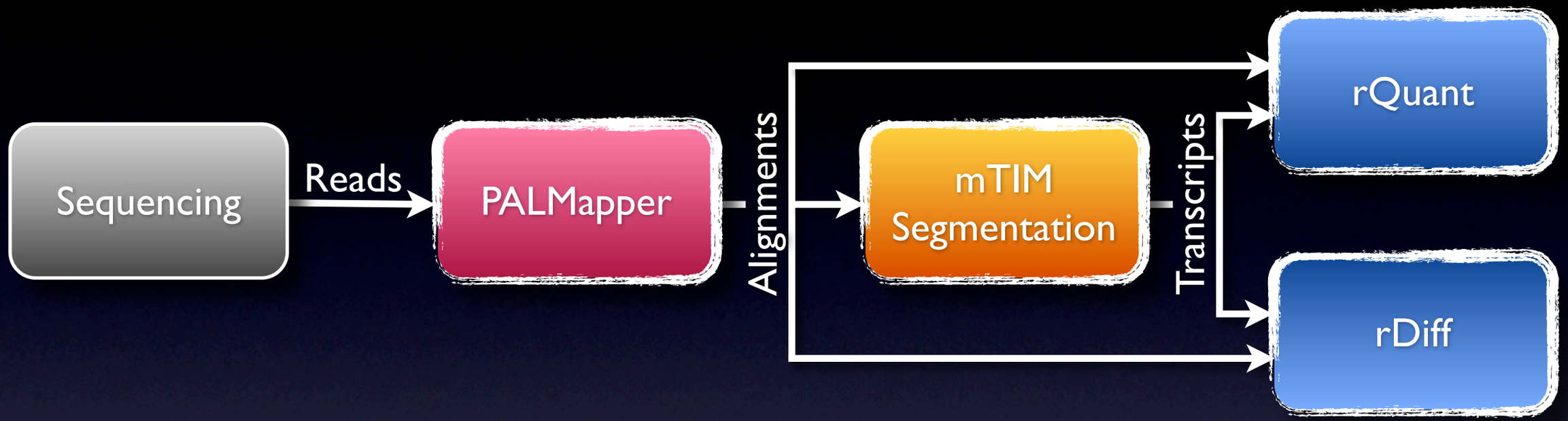
oqtans



- **rQuant**: estimates biases in library prep, sequencing, and read mapping; accurately determines the abundances of transcripts

R. Bohnert et al. 2009

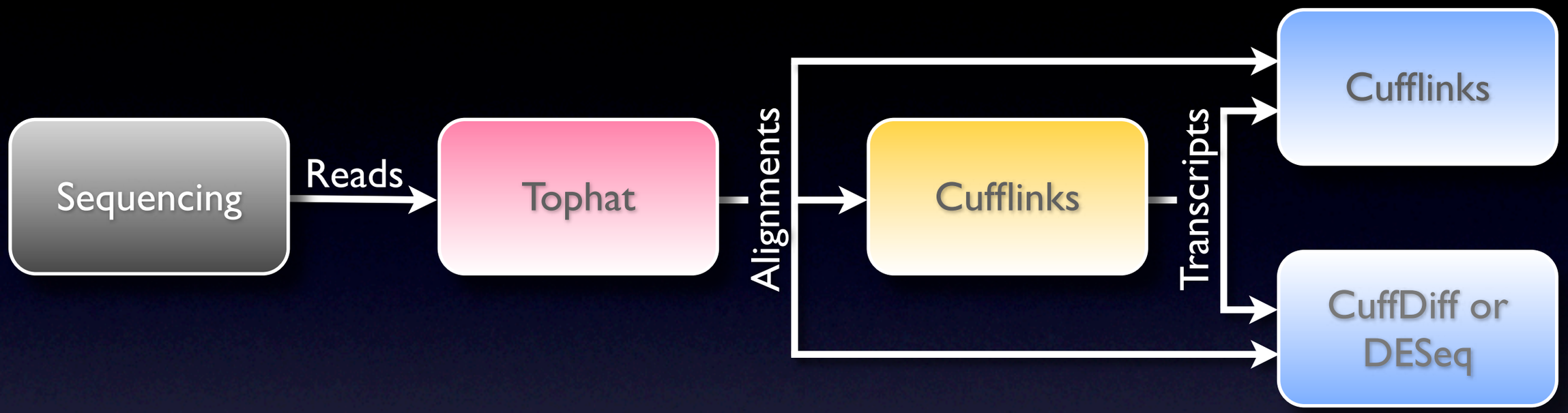
oqtans



- **rDiff**: determines significant differences in transcript expression between experiments using statistical tests

O. Stegle et al. 2010

oqtans



- Performance at or above state-of-the-art
- Tophat, DESeq, Cufflinks, CuffDiff for comparison

A. Roberts et al. 2011
S. Anders and W. Huber 2010
C. Trapnell et al. 2010

Galaxy Tool Installers

Joint work: Enis Afgan & Galaxy Team
James Taylor, Anton Nekrutenko
AG Rätsch

- MLB group tools into any Galaxy installation
- Python Fabric scripts: used to manage automation of a remote server

```
install_cmd("wget %s" % self.tool_env['url'])
install_cmd('chown -R %s %s' % (env.user, install_dir_root))
```

- Available from **Galaxy Tool Shed**
- Adjusted to Ubuntu on Galaxy Cloud Image

Tools with Fabric Scripts

Joint work: Enis Afgan & Galaxy Team
James Taylor, Anton Nekrutenko
AG Rätsch

- Machine Learning Toolbox *Shogun*
- EasySVM tools for easy-to-use SVM classifications
- All oqtans tools
- GFF Toolkit for pre-processing annotations
- KIRMES regulatory modules identification
- WebLogo interface

oqtans Availability

Joint work: Enis Afgan
Galaxy Team
AG Rätsch

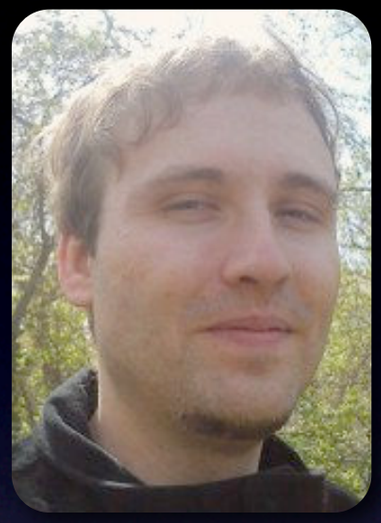
- External cluster (21 nodes, 168 CPUs) handles requests to our Galaxy instance
- Fabrics to install tools from the shed
- AMI instance created
- ‘Instant on’
- Cloudman to launch as many as you need

oqtans Availability

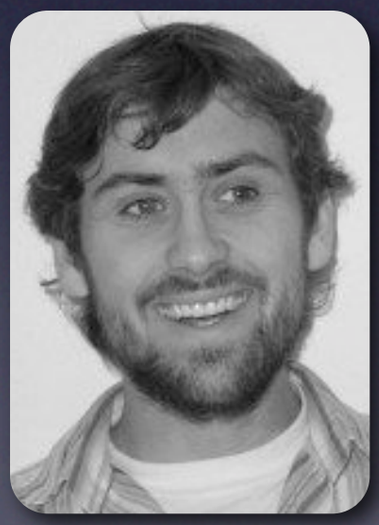
- **MLB Group Galaxy Instance**
  http://galaxy.fml.mpg.de
- EC2 Cloud Instance & AMI
  ami-228a7e4b “Oqtans-Galaxy”
- **Fabric** scripts install Oqtans on your Galaxy
  http://community.g2.bx.psu.edu/
- Source code releases of all tools, email info
  http://fml.mpg.de/oqtans

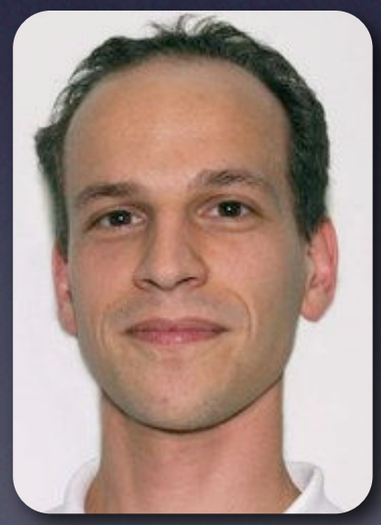
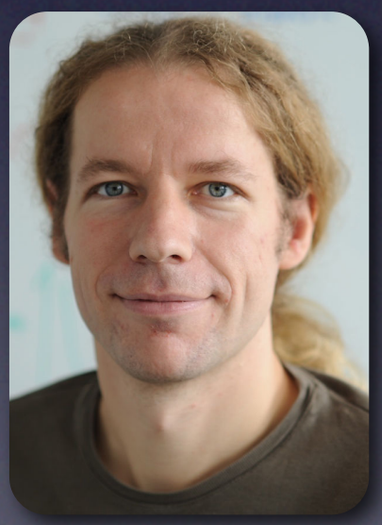
http://fml.mpg.de/oqtans




Jonas Behr, Regina Bohnert, Philipp Drewe, Nico Goernitz, Géraldine Jean



André Kahles, Pramod Mudrakarta, Vipin T. Sreedharan, Georg Zeller, Gunnar Rätsch