Crank Web Interface

Remote automated structure solution

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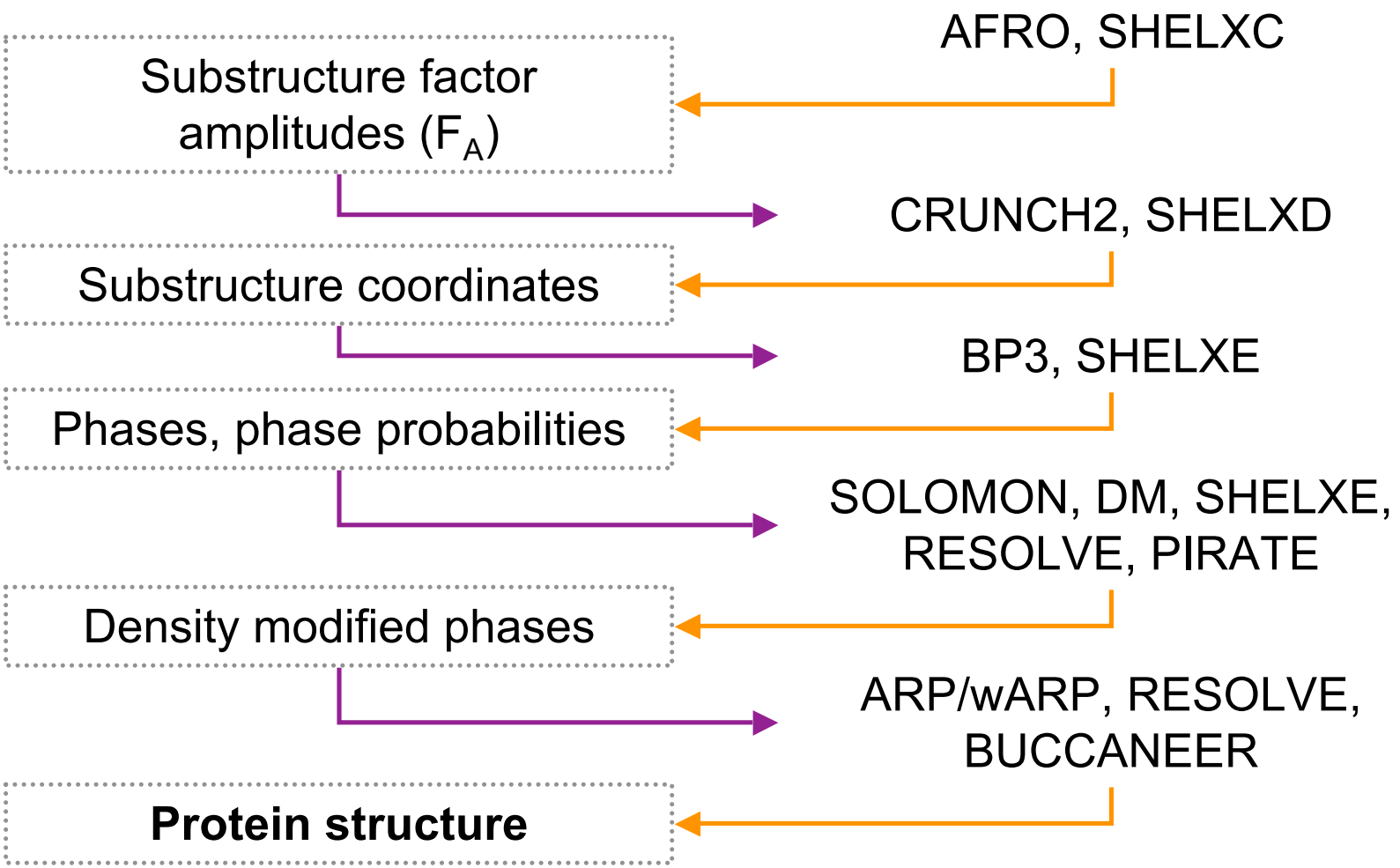
Crank

- Automated macromolecular structure determination for SAD, SIRAS, MAD, and MAD+native experiments

- Interfaces with various crystallographic programs

www.bfsc.leidenuniv.nl/software/crank

Crank : programs



Crank / BP3 : many test cases

- 33 test cases on SAD, MAD, SIRAS data show robustness and speed
  - www.bfsc.leidenuniv.nl/software/crank/tests.html
- Currently testing JCSG-datasets as well
  - www.jcsg.org
- Published results show in 8 out of 10 real SAD cases, BP3 produced better results over SHARP, MLPHARE or SOLVE
  - Ness, de Graaff, Abrahams, Pannu (2004) *Structure*, **12**, 1753-1761

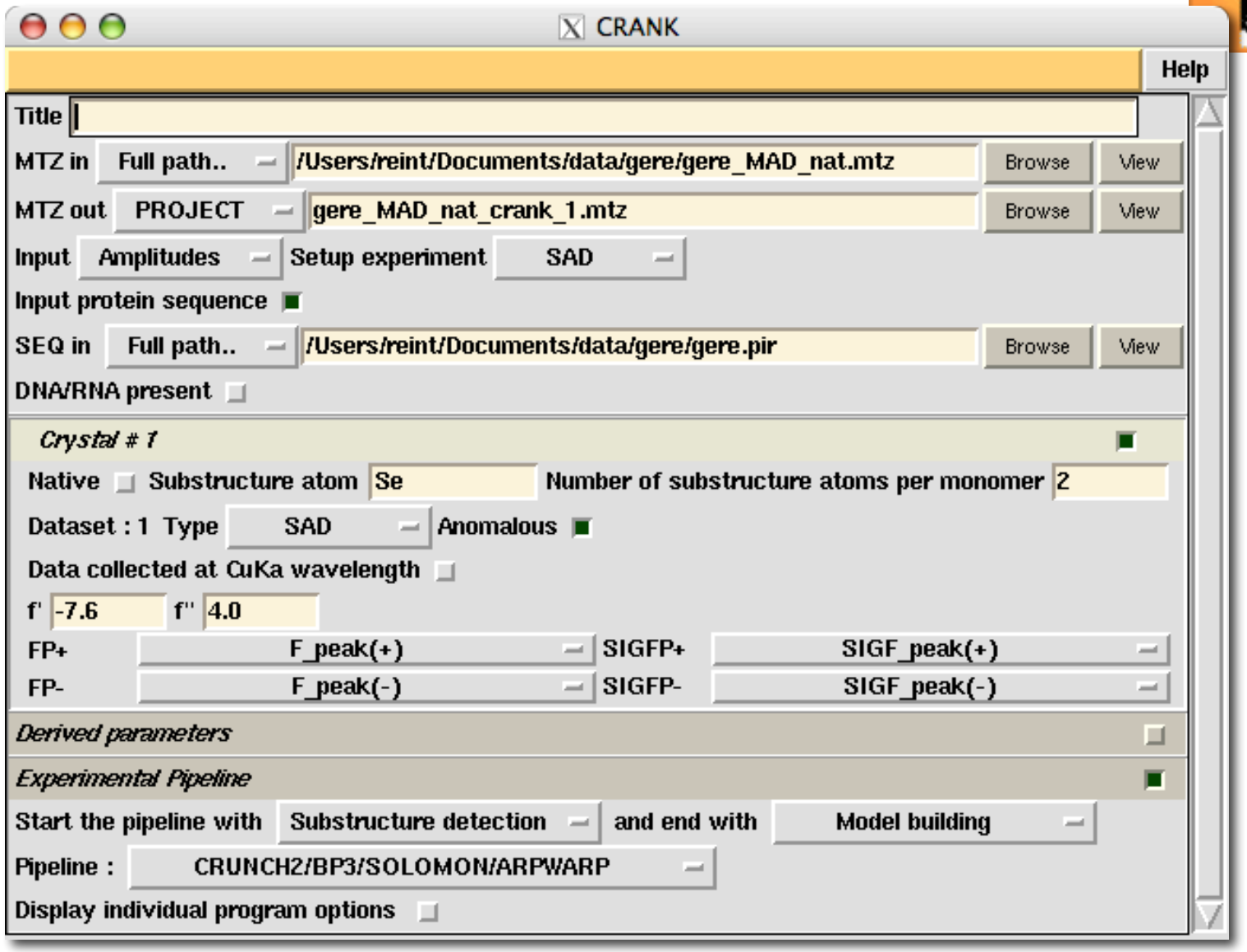
Crank : how to get it

- Download from BFSC or CCP4 (pre-release zone)
  - Suitable for SAD, SIRAS, MAD and MAD+native experiments
  - Supported platforms: Linux, Mac OS X (Intel, PPC)
  - CRUNCH2, BP3 and most of Crank is GPL

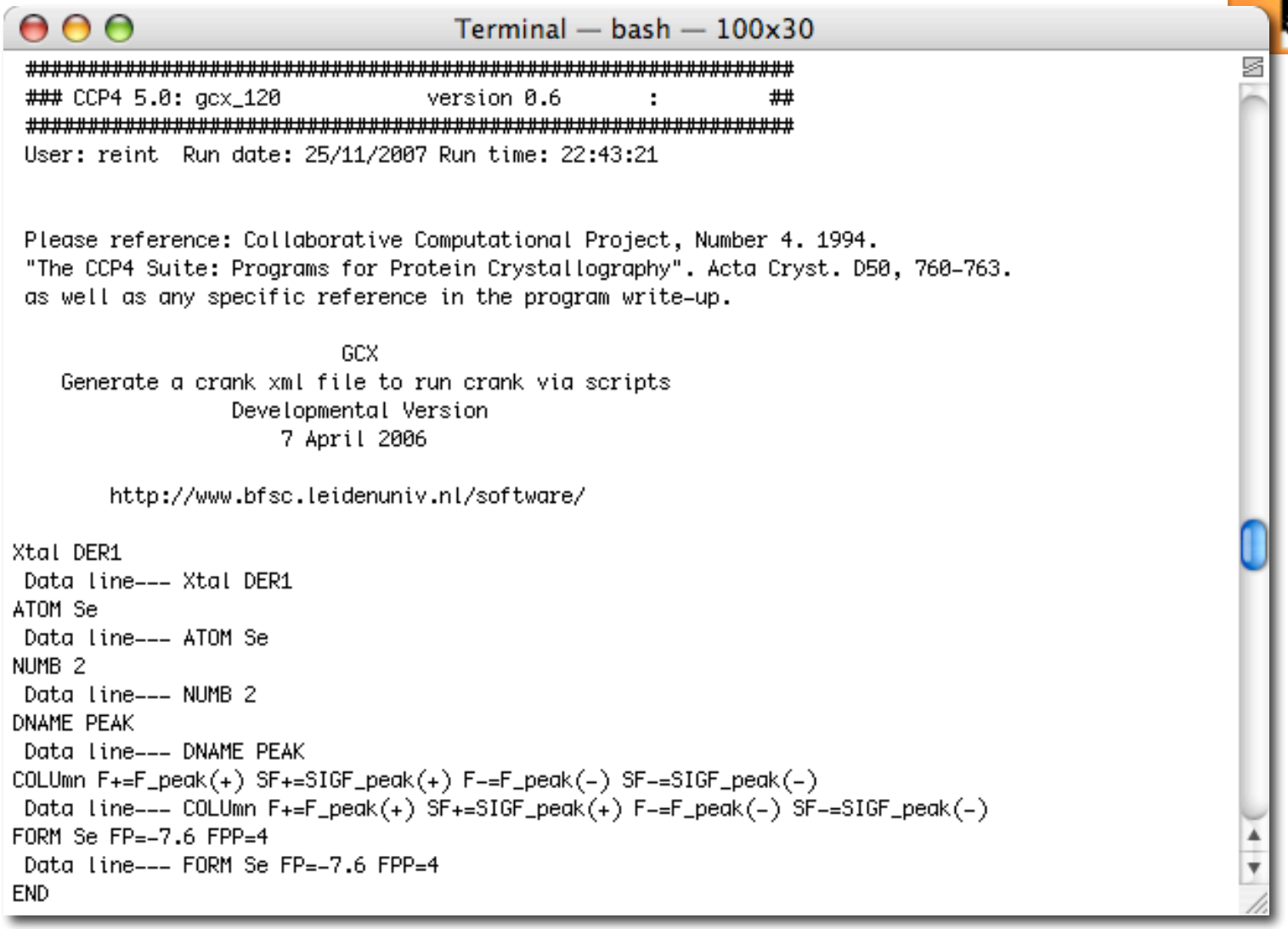
- Version 1.2.0 is available: *much* improved over earlier versions

- Interfaces to BP3 exist in AutoRickshaw (EMBL Hamburg pipeline) and MIFit

Crank : two interfaces



Crank : two interfaces



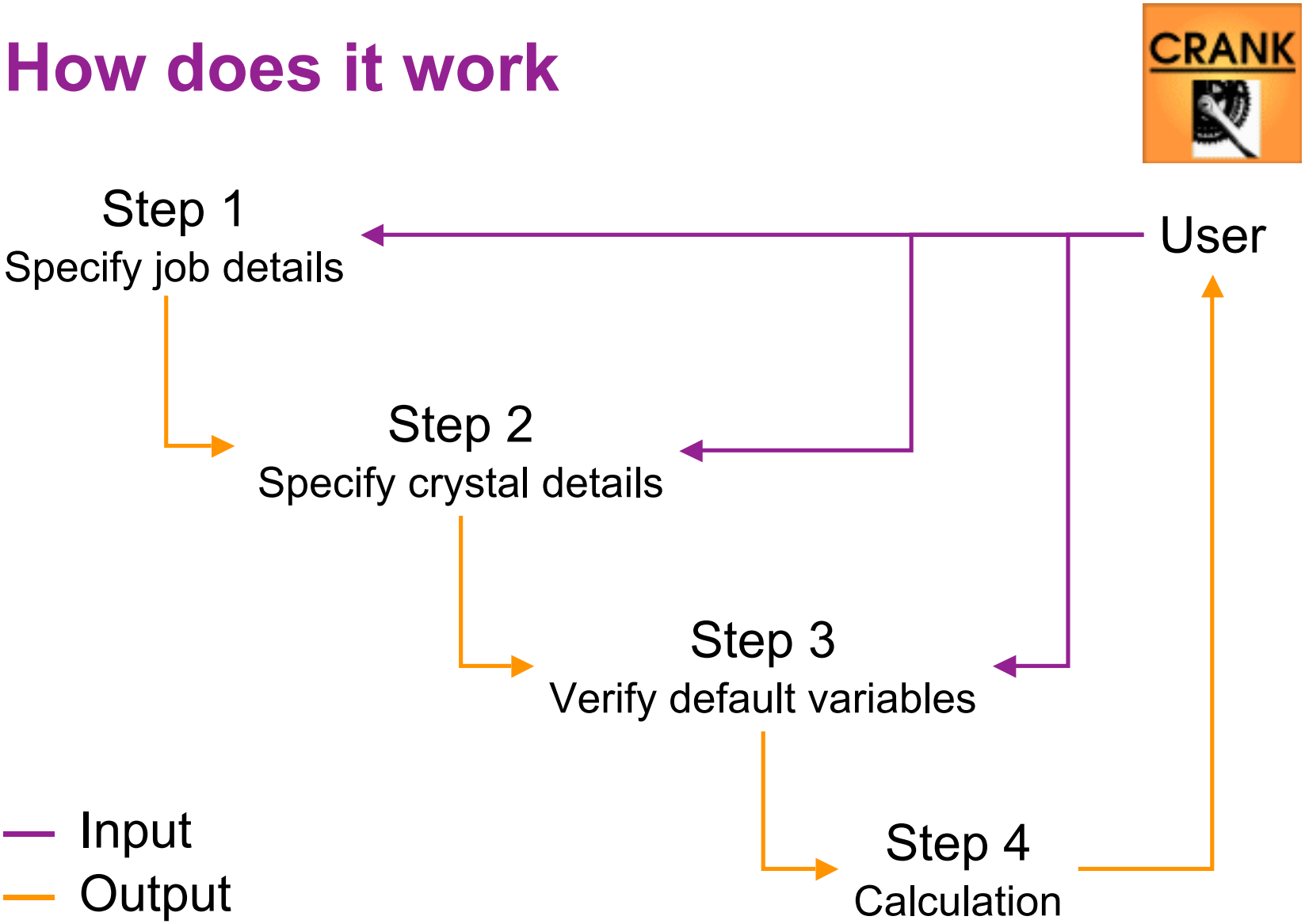
Crank : third interface

- A third interface to Crank has been added
  - Interface Crank to computing cluster for remote job submission
  - Works like CCP4i interface

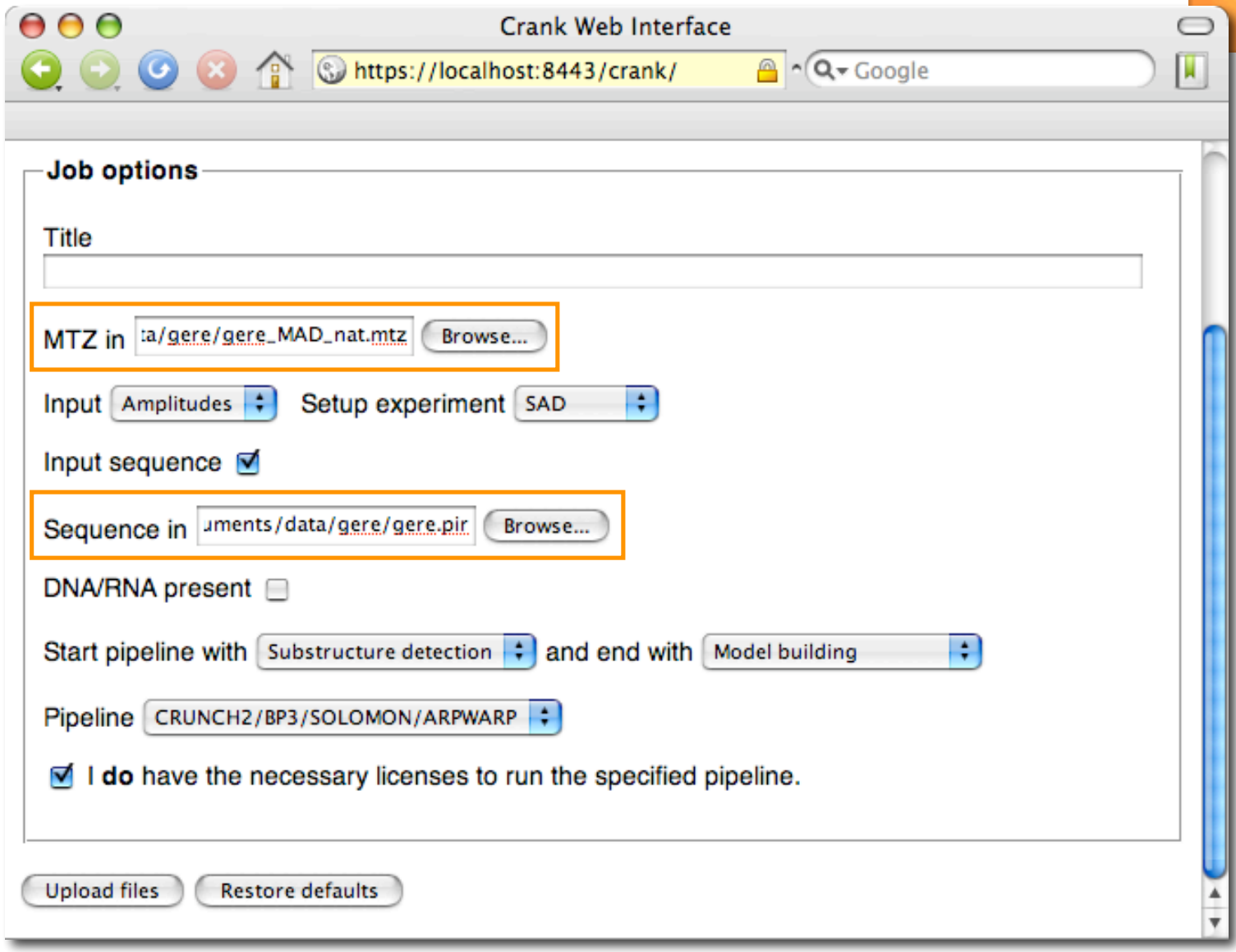
Benefits

- Focus on the science
  - No need to set-up and administer crystallographic software
- Faster computation
- Leiden programs are “free”
  - If user verifies ARP/wARP, CCP4, SHELX license, user can run those suites
- Remote job submission has shown its merits
  - Web-based ARP/wARP / Auto-Rickshaw

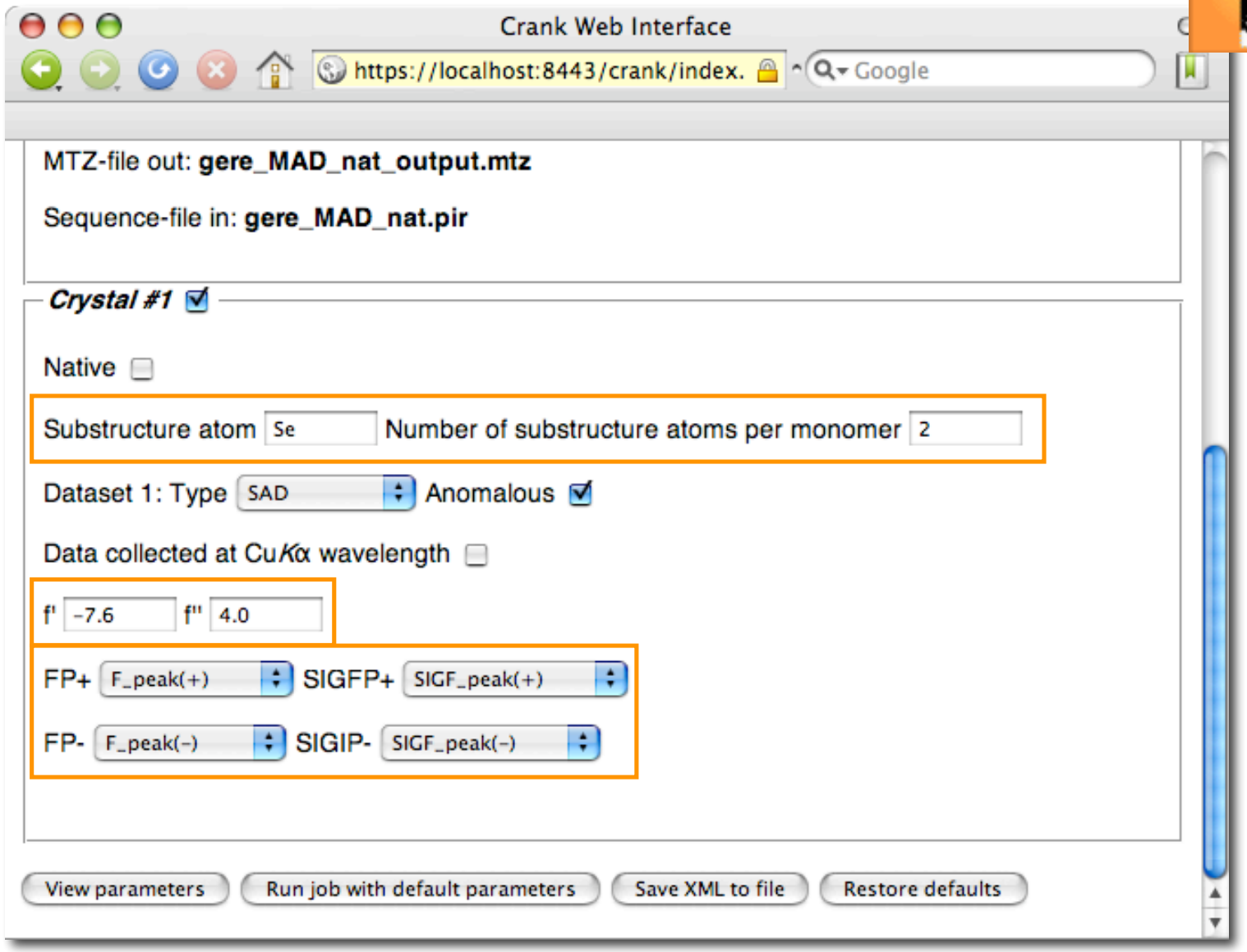
How does it work



How does it work : step 1



How does it work : step 2

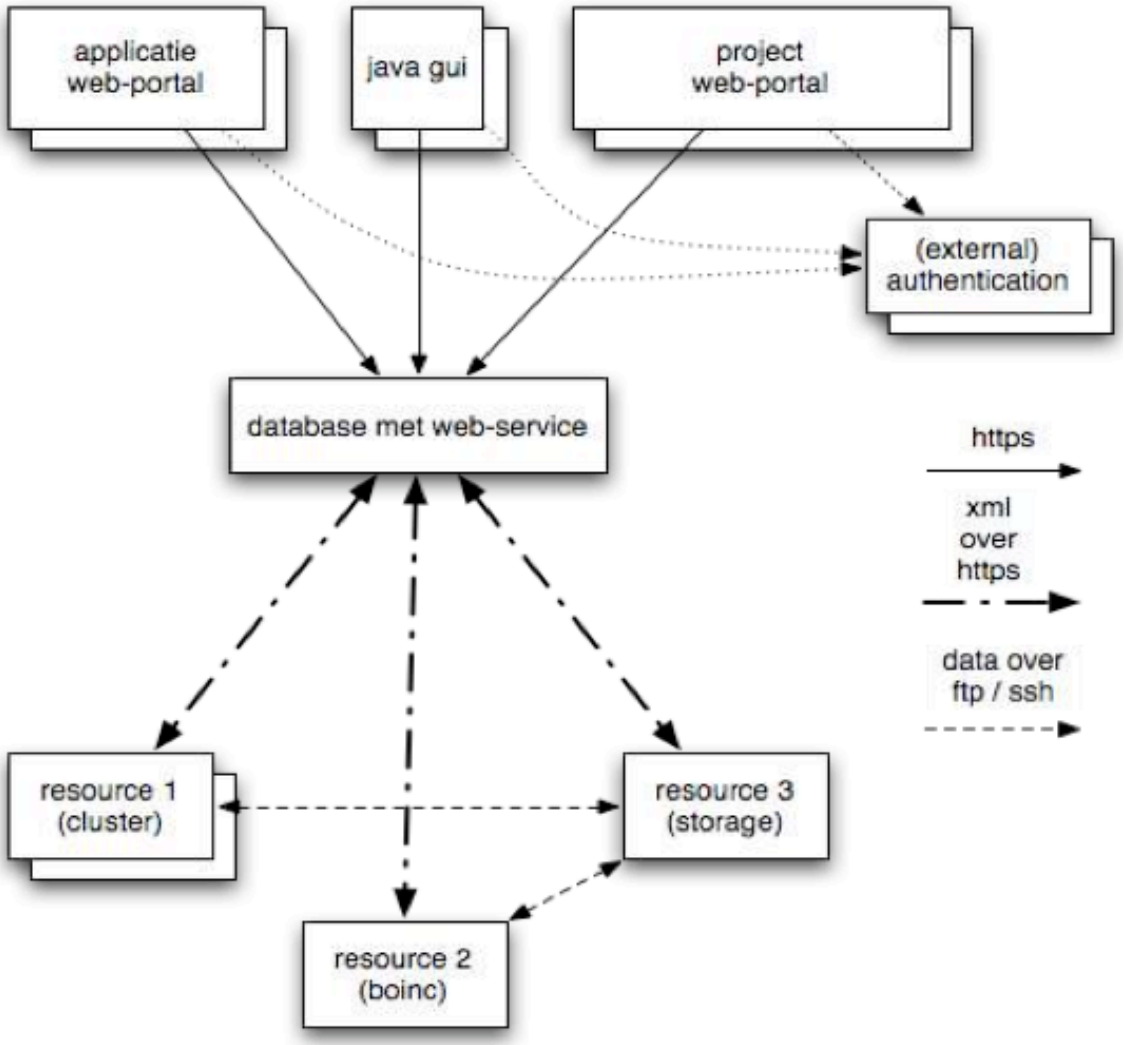


LGI (Leiden Grid Infrastructure)

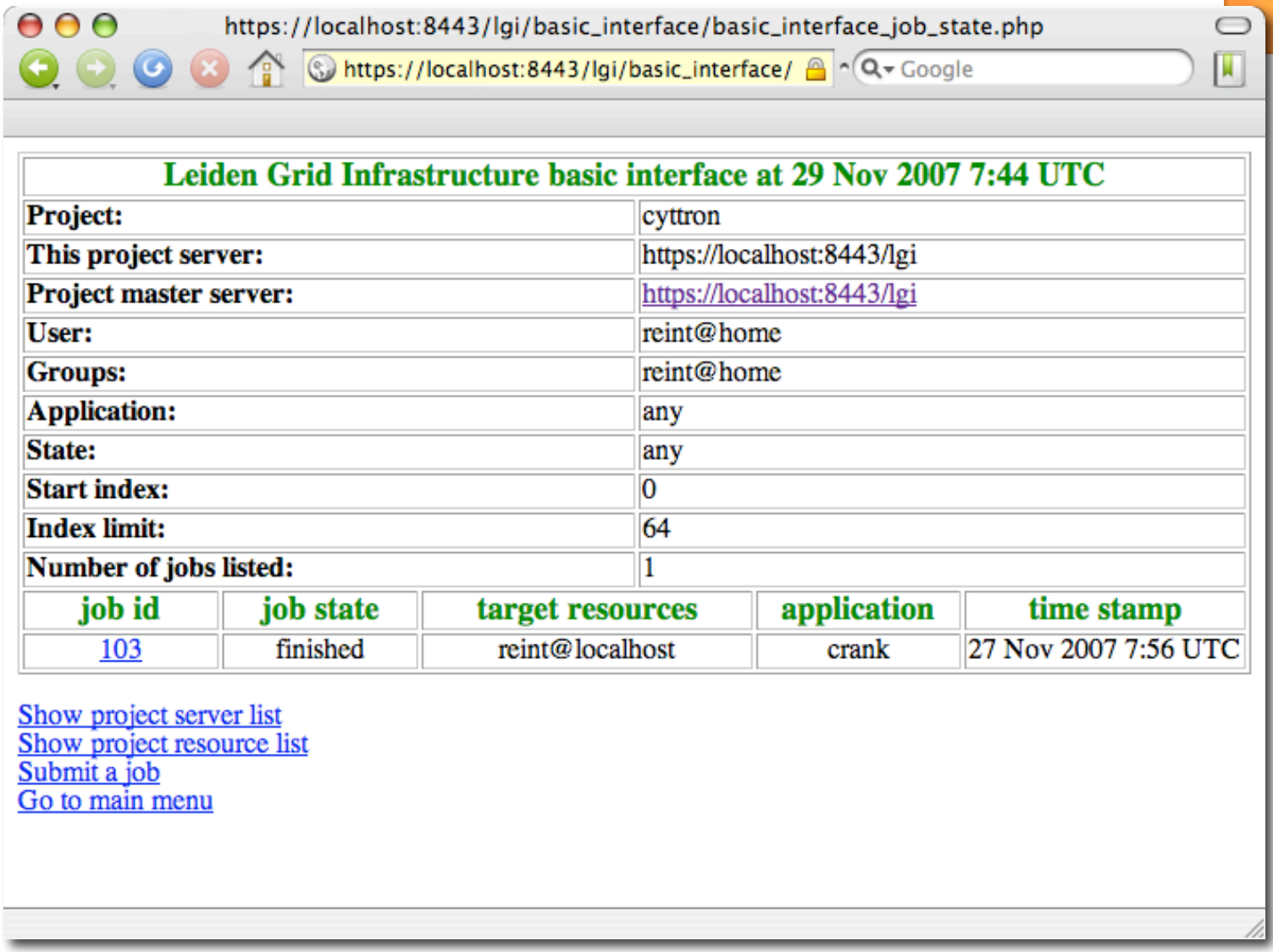
- Lightweight grid middleware
  - Communication between job submission (front-end) and computing grid (backend)
  - Distribution of jobs to various resources
  - Use of standards: HTTPS and XML

- Make programs more intuitive and accessible for most common tasks
- Provide scalability and continuity without interference with the user

LGI (Leiden Grid Infrastructure)



LGI (Leiden Grid Infrastructure)



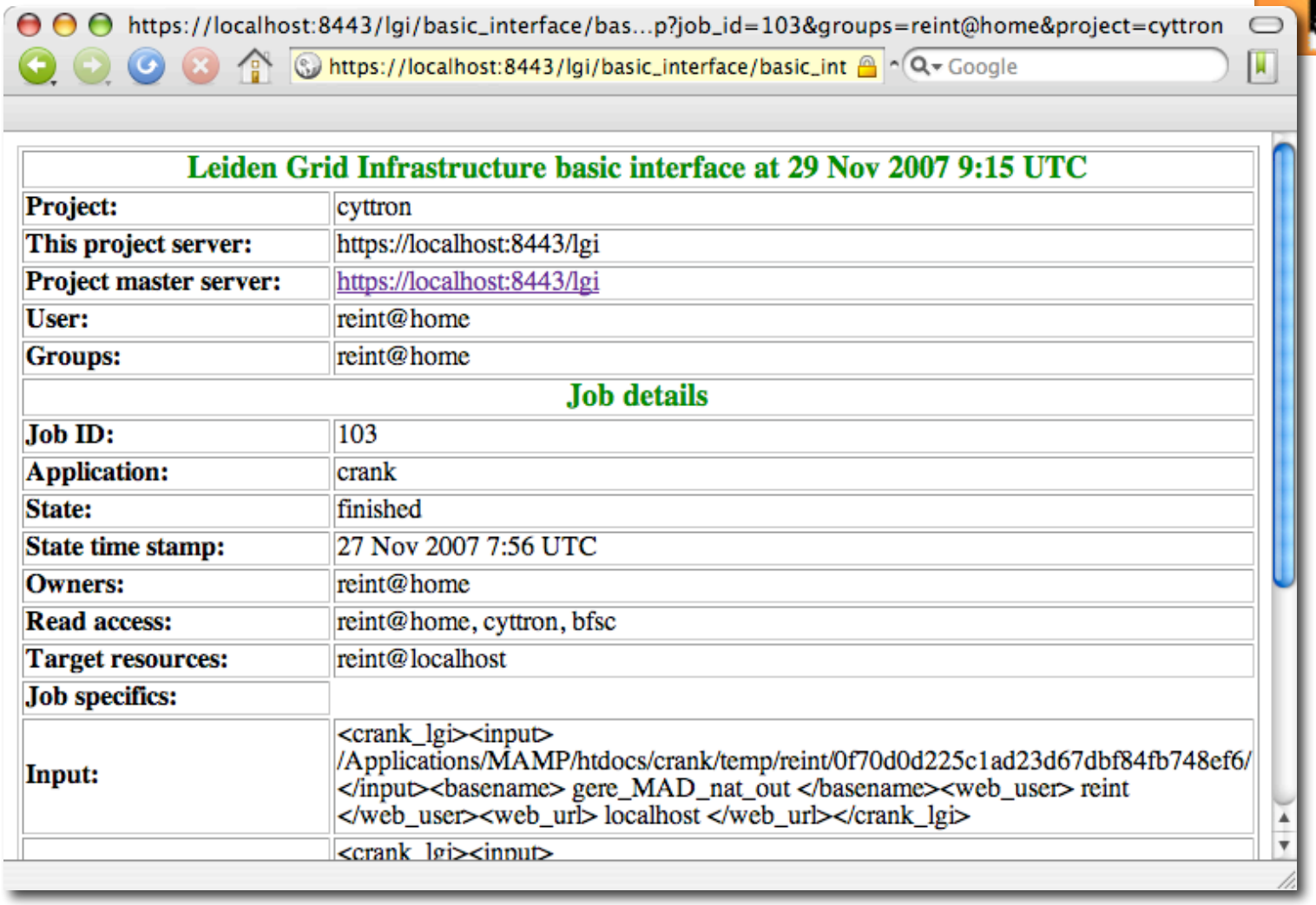
Leiden Grid Infrastructure basic interface at 29 Nov 2007 7:44 UTC

Project:	cyttron
This project server:	https://localhost:8443/lgi
Project master server:	https://localhost:8443/lgi
User:	reint@home
Groups:	reint@home
Application:	any
State:	any
Start index:	0
Index limit:	64
Number of jobs listed:	1

job id	job state	target resources	application	time stamp
103	finished	reint@localhost	crank	27 Nov 2007 7:56 UTC

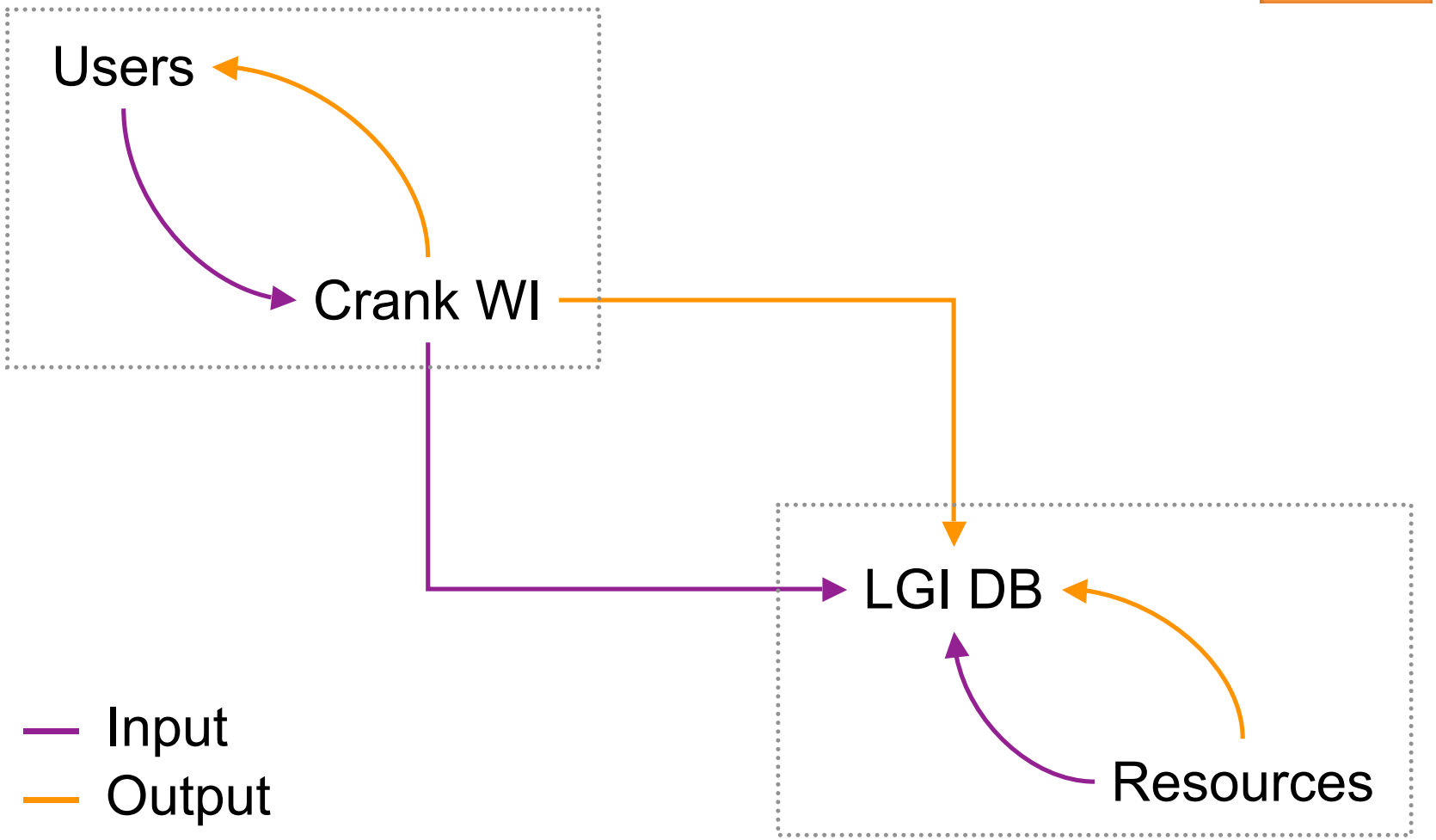
Show project server list
Show project resource list
Submit a job
Go to main menu

LGI (Leiden Grid Infrastructure)



Leiden Grid Infrastructure basic interface at 29 Nov 2007 9:15 UTC	
Project:	cyttron
This project server:	https://localhost:8443/lgi
Project master server:	https://localhost:8443/lgi
User:	reint@home
Groups:	reint@home
Job details	
Job ID:	103
Application:	crank
State:	finished
State time stamp:	27 Nov 2007 7:56 UTC
Owners:	reint@home
Read access:	reint@home, cyttron, bfsc
Target resources:	reint@localhost
Job specifics:	
Input:	<crank_lgi><input> /Applications/MAMP/htdocs/crank/temp/reint/0f70d0d225c1ad23d67dbf84fb748ef6/ </input><basename> gere_MAD_nat_out </basename><web_user> reint </web_user><web_url> localhost </web_url></crank_lgi>
	<crank_lgi><input>

Communication CWI ‹–› LGI



Where are we now

- Simple job submission with default variables
- Calculation on BFSC computing cluster
- Send results back to user

What's next

- Finalise step 3
- User/session management
- Interface with Cyttron Visualisation Platform (CVP)
- A lot of testing …

Acknowledgements

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