e-Science: Experience with utilization of the grid computational model based on using of the ARC middleware

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workshop "***Grid Computing for Complex Problems***"
UI SAV Bratislava 30.11.2005

Outline

- ***NorduGrid***

  -characterization
  -in LHC physics
  -technical details

- ***Job submission***

  -parametric task
  -workflow

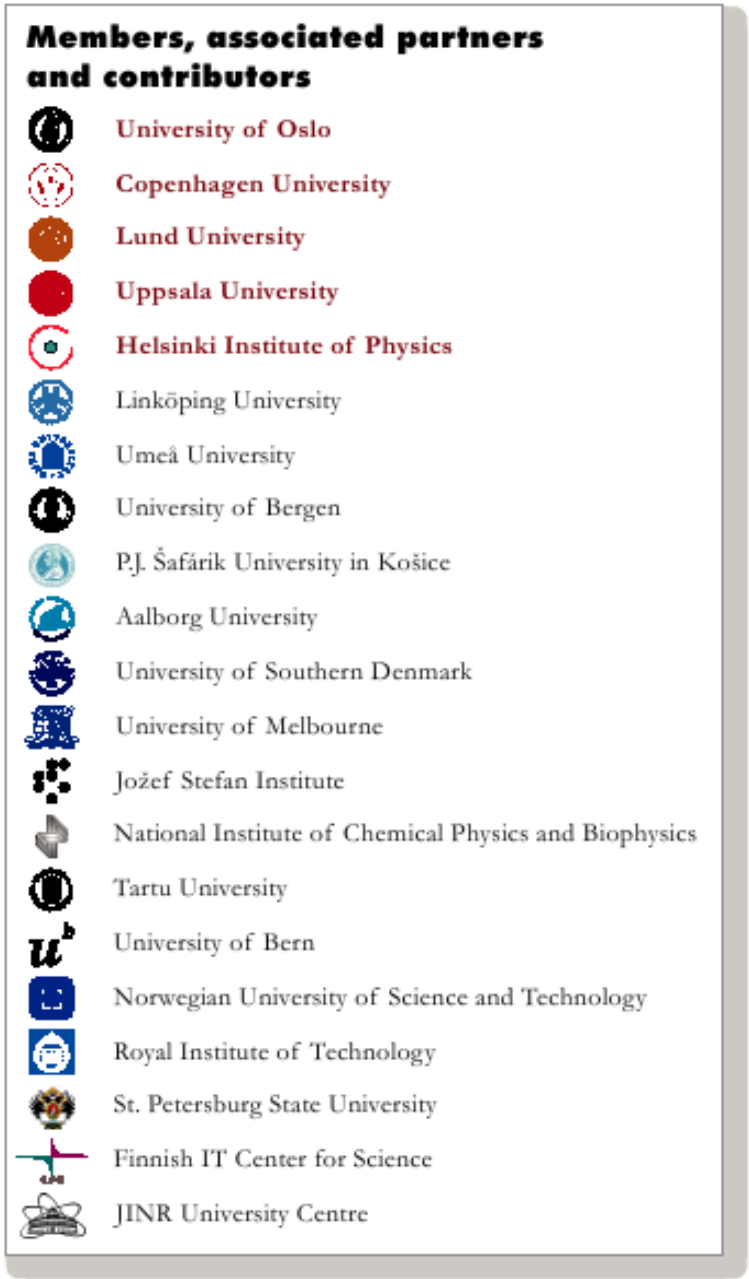
- ***Applications at UPJS***

  -complex systems
  -image processing

- ***Executed jobs -analysis***

- ***Future plan***

Project characterization [2]



- ***Basic***
  Sites ~ 60
  Processors ~ 6000
  Storage ~60TB
  Users ~ 1600

- ***NorduGrid*** is collaboration established by five Nordic academic institutes.

- ***Features***-NorduGrid is fault-tolerant, scalable, portable, light-weighted suitable for global grid computing. The open ARC middleware and sets of tools for different Linux OS were developed in this project. ***Long term experiences with the production quality ARC middleware.***

User oriented programs-Example of Runtime environment

Runtime environment	TEST-MPICH-1.2.5.2
	BIO-GEIJER-0.0.2
	TEST-MPIRUN-MPICH-1.2.5.2
	POVRAY-3.5
	ATLAS-7.0.3
	LOCALDISK
	ATLAS-8.0.1
	GAUSSIAN-03.B05
	PYTHON-1.5.2
	TEST-GAUSSIAN-SINGLE-03.B05
	ATLAS-8.0.3
	TEST-MATLAB-6.5.1
	ATLAS-8.0.4
	TEST-DALTON-PARALLEL-1.2
	ATLAS-8.0.5
	P1SITE
	ATLAS-8.0.7
	MOLCAS-6.0.553
	ATLAS-8.0.8
	TEST/MPICH/1.2.5/GNU
	MOLCAS-6.0.575
	ROOT-4.00.08
	TEST-ATLAS-9.0.3
	PYTHON-2.3.5

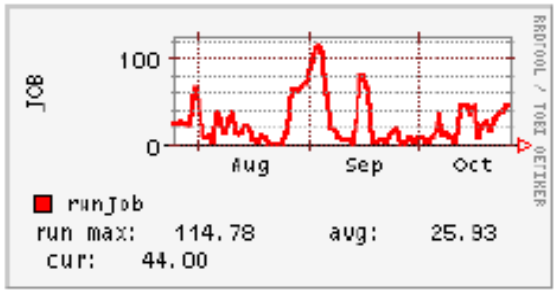
The sites can provide a ***wealth collection of programs from different research areas*** (see example on the left side)

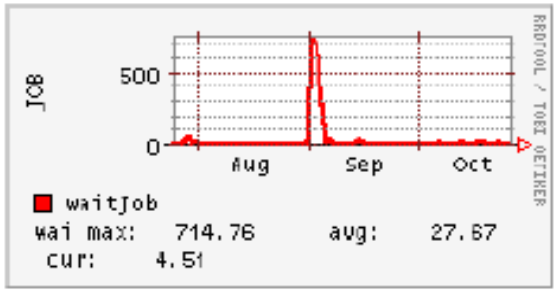
Information about actually installed programs are available on-line via User Information system

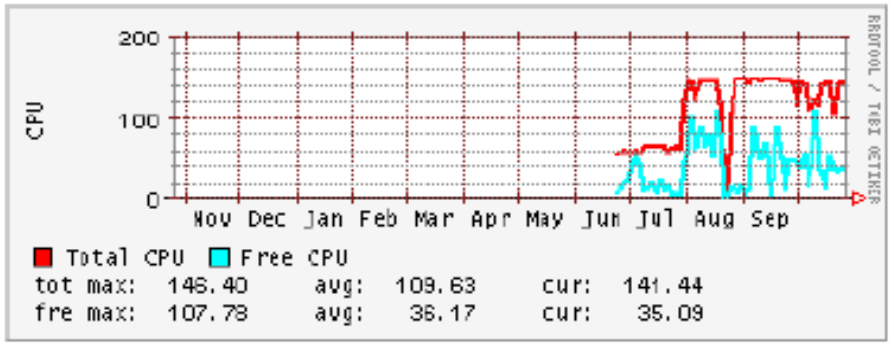
Participation of the grid projects (LCG, Grid3, NorduGrid) on DC2 ATLAS Experiment

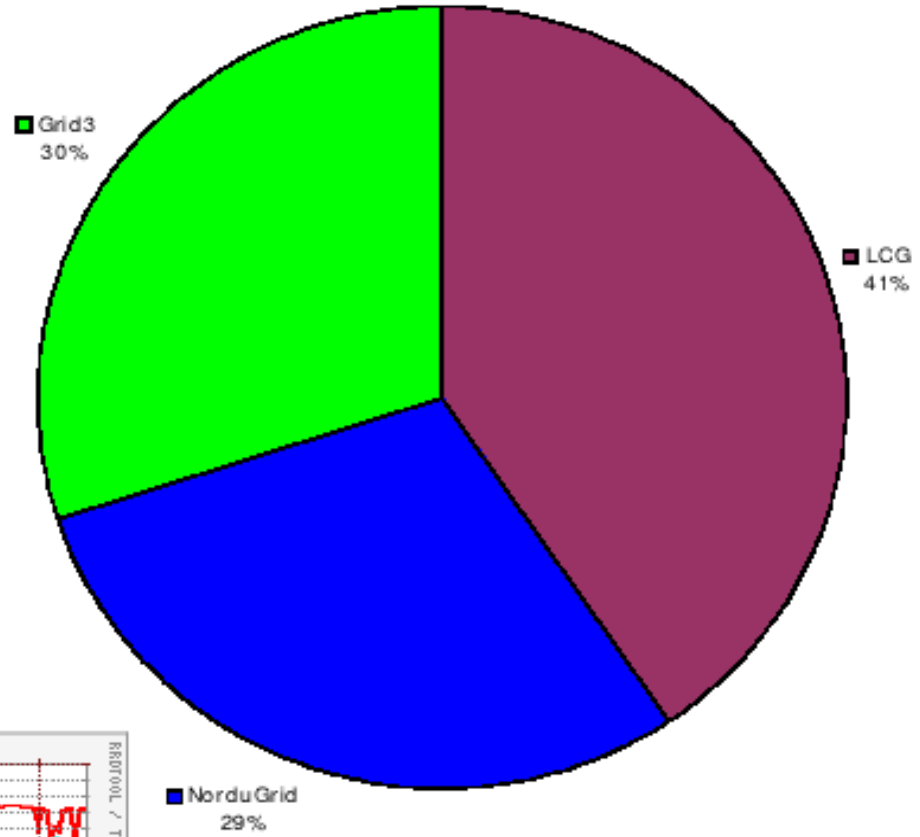
(source: CESNET EGEE, Czech republic)

farma GOLIAS

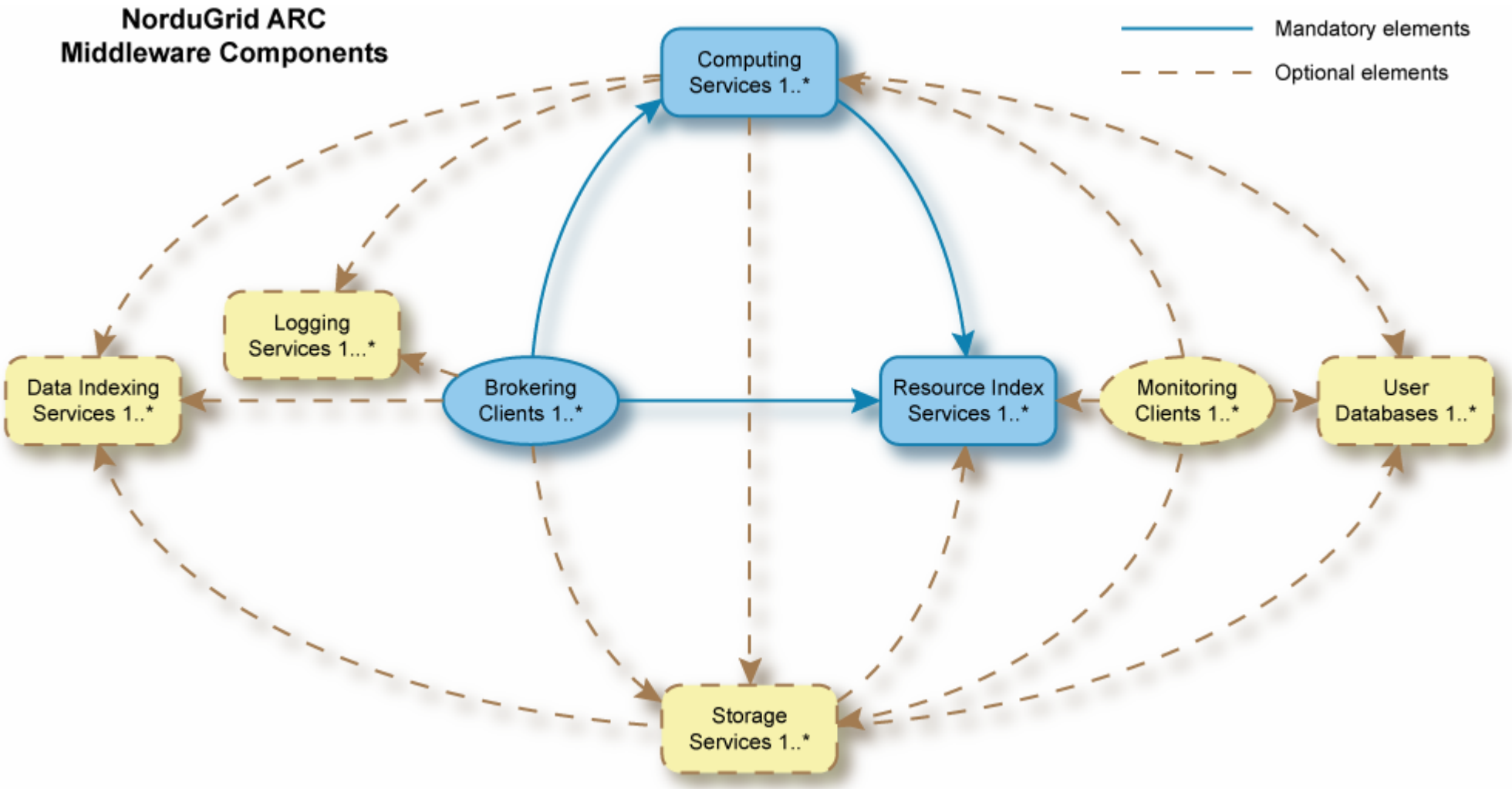








NorduGrid-Technical details



-Computing service

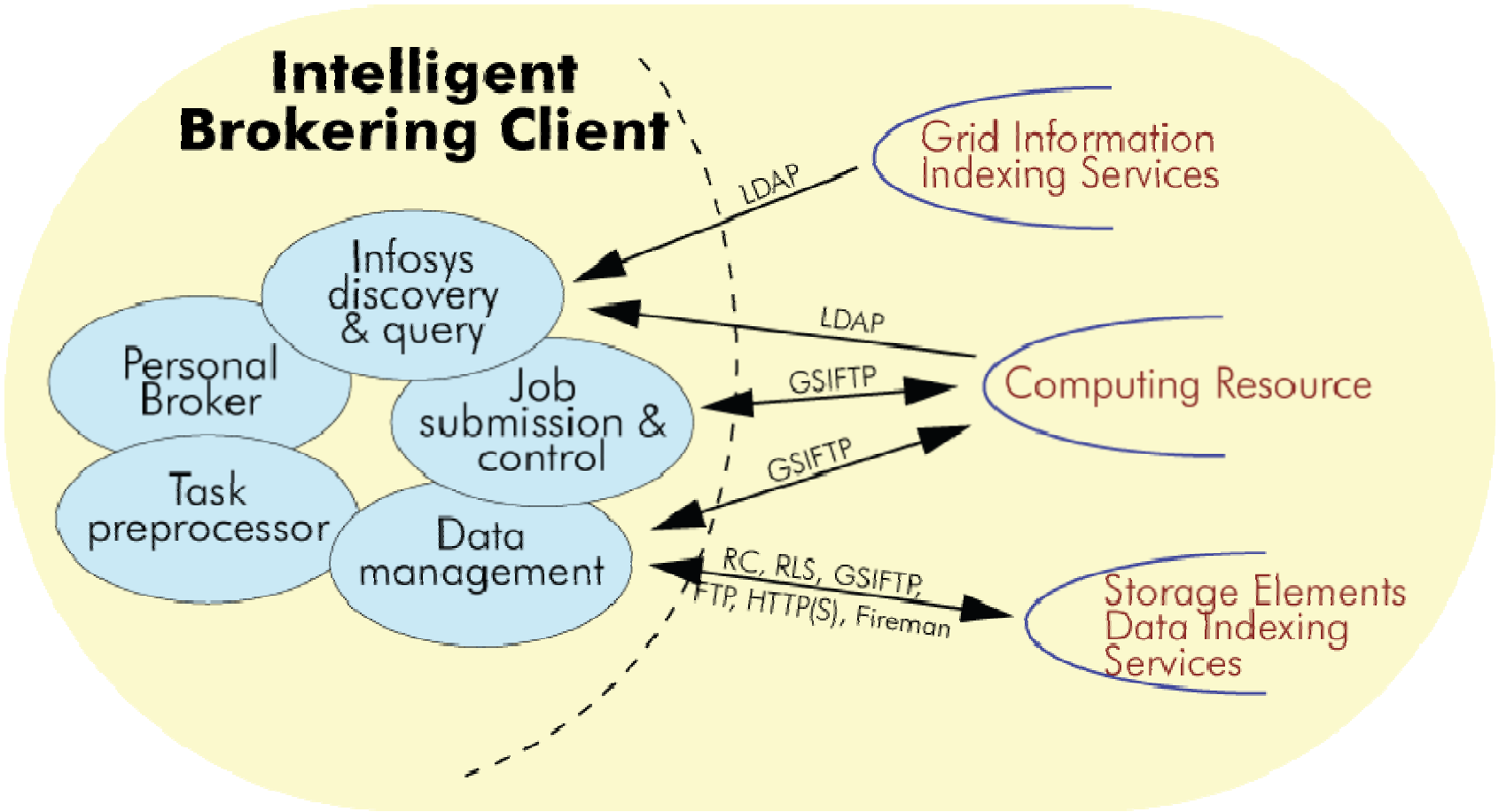
-Intelligent Brokering Client

-Information services

-Conventional storage

-Smart storage

Any user has an own broker - an advantage solution



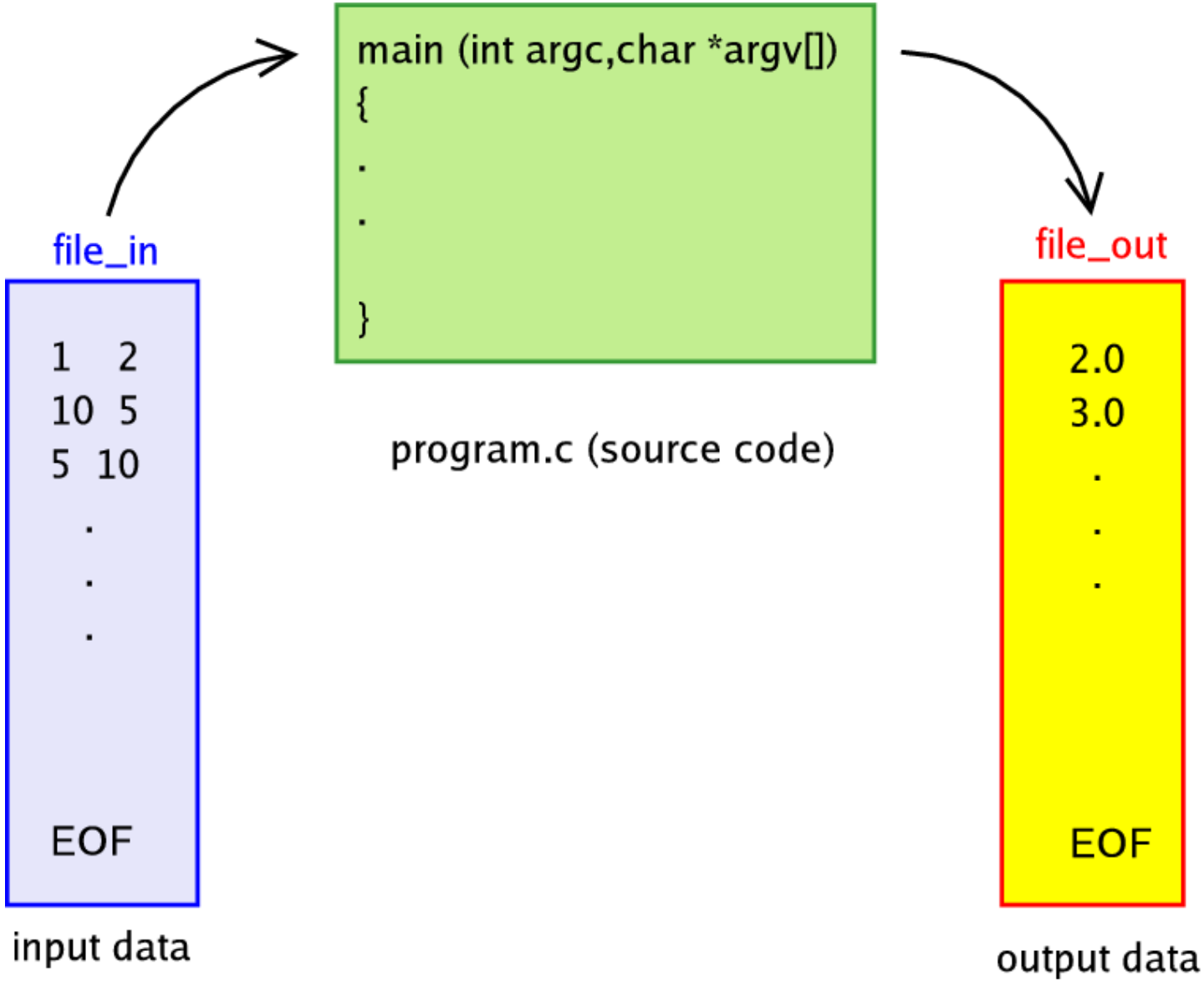
s

- Built on the libraries of the Globus Toolkit 2.x. (solution with the Globus Toolkit 4.x is under development)
- From the Globus Toolkit applied MDS, gsiftp (***GRAM is not used***-own technical solution)
- Advanced Resource Connector Nordugrid (the- original solution ***without central Resource Broker***)
- ***Any user has an own broker***
- Local Job Managers: **PBS**, Condor, SUN Grid Engine - fork (UNIX)
- Clear Information System – many of users data are available online -user name, number jobs and their names, etc.

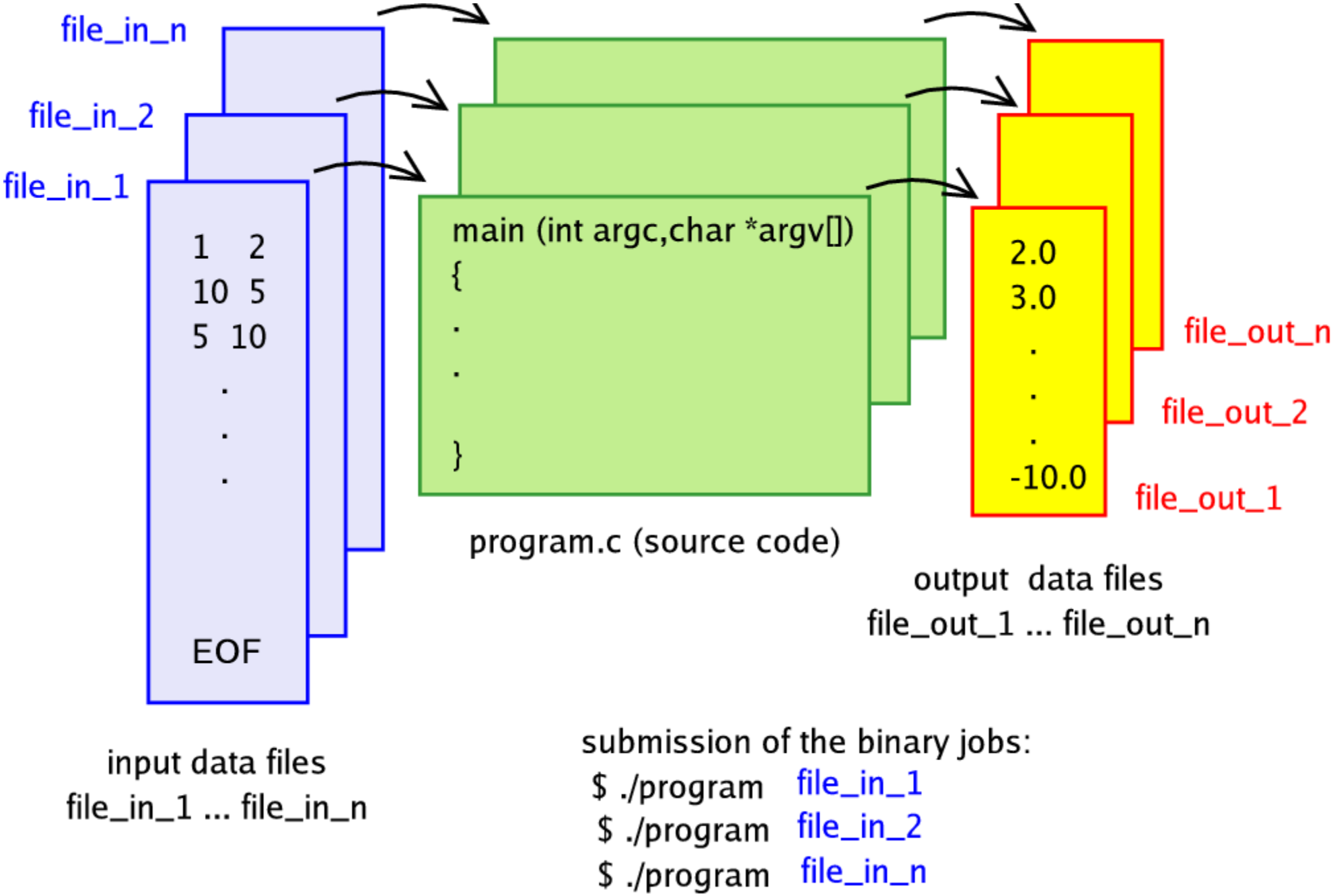
How to prepare my first grid job?

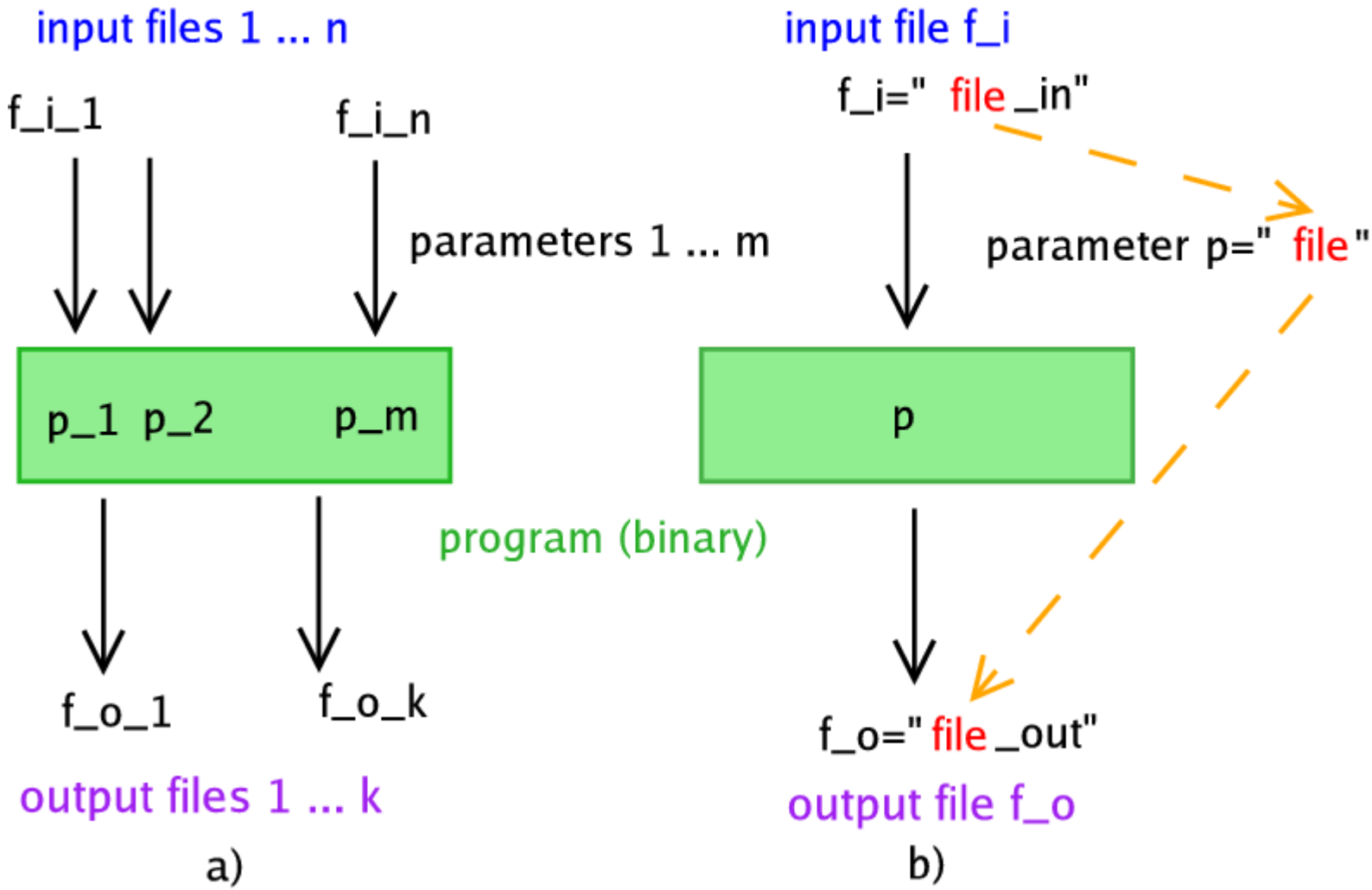
- ***expected skills:***
  -programming language (C, C++.)
  - OS Linux
  - script languages (bash, Perl, Python)
- Personal grid certificate issued by Certification Authority at the Institute of Informatics SAV Bratislava [1]
- The access to the grid server or installed a grid client (NorduGrid).
- Do we need WWW portal to submit jobs?
  No, for the first experiments.

Parametric task [3]



starting of the binary program: $ ./program file_in


file_in_n
file_in_2
file_in_1
1 2
10 5
5 10
.
.
.
EOF
main (int argc,char *argv[])
{
.
.
}
2.0
3.0
.
.
.
-10.0
file_out_n
file_out_2
file_out_1
program.c (source code)
output data files
file_out_1 ... file_out_n
input data files
file_in_1 ... file_in_n
submission of the binary jobs:
$ ./program file_in_1
$ ./program file_in_2
$ ./program file_in_n


input files 1 ... n
f_i_1
f_i_n
parameters 1 ... m
p_1 p_2
p_m
program (binary)
f_o_1
f_o_k
output files 1 ... k
a)
input file f_i
f_i=" file _in"
parameter p=" file "
p
f_o=" file _out"
output file f_o
b)

1) Login into the Grid (standard), for details see [1]

```
[cernak@vls cernak]$ grid-proxy-init
Your identity: /C=SK/O=SlovakGrid/O=UPJS/CN=Jozef Cernak
Enter GRID pass phrase for this identity:
Creating proxy ..................................... Done
Your proxy is valid until: Sun Nov 21 06:10:57 2004
[cernak@vls cernak]$
```

2) Job submission using the script: ***ex1.sh***

```
[cernak@vls data]$ ./ex1.sh
program->program     1 s:        0.0 kB       0.0 kB/s
.
program->program     1 s:        5.5 kB       5.5 kB/s
.
file->file     1 s:        0.0 kB       0.0 kB/s       0.0 kB
file->file     1 s:        0.0 kB       0.0 kB/s       0.0 kB
Job submitted with jobid

gsiftp://vls.science.upjs.sk:2811/jobs/259251100973253%0914
[cernak@vls data]$
```

The shell script ***ex1.sh*** using xRSL in more details [3]

ex1.sh

```
#!/bin/sh
# Example 1: program
ngsub -c vls.science.upjs.sk '&(executable=program)
       (arguments="file")
       (inputfiles=
         ("file" "file")
       )
       (outputfiles=
         ("file_out" "file_out")
       )
       (stdout="out.txt")
       (stderr="err.txt")
       (jobName="program")'
```

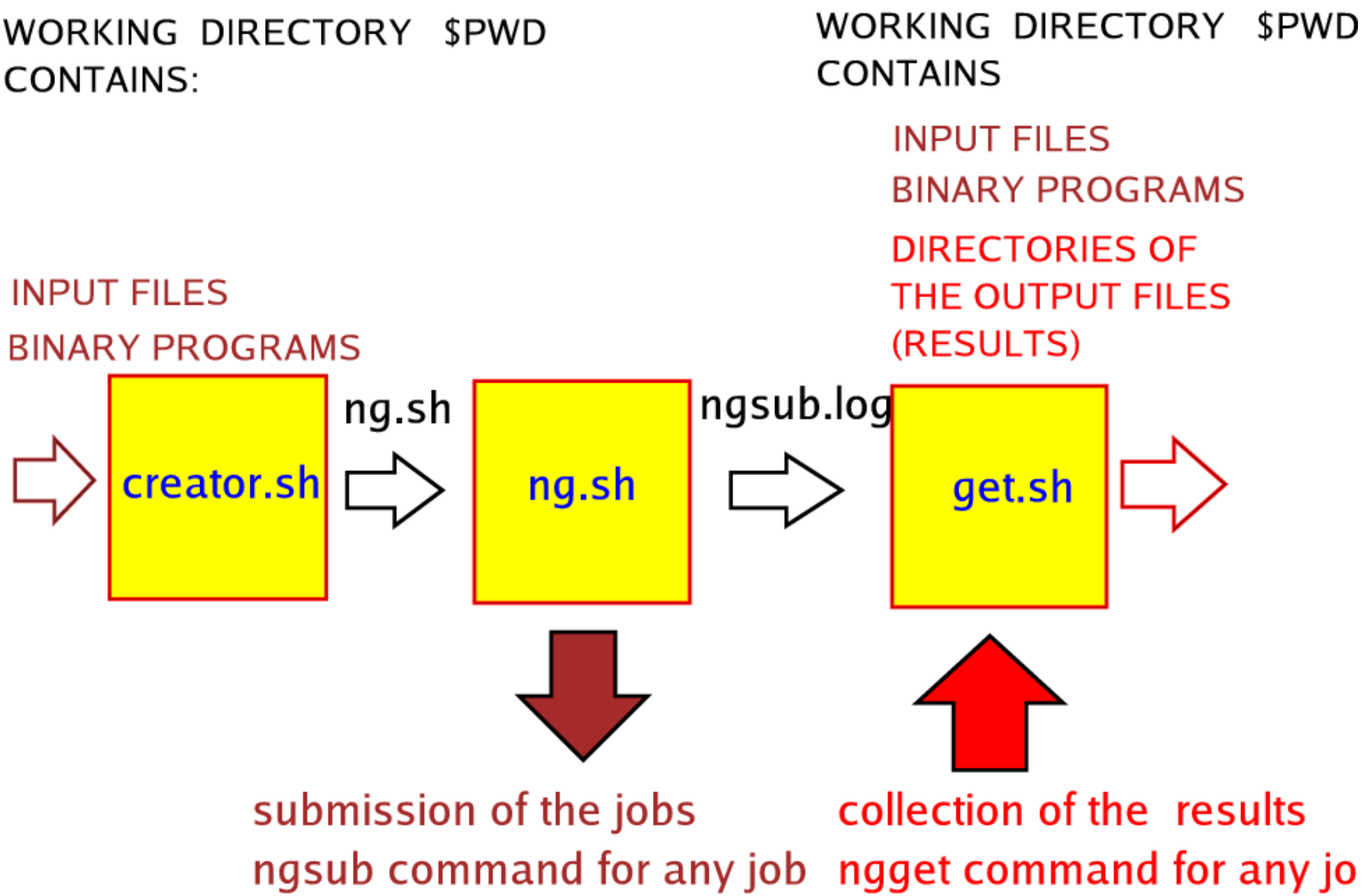
3) Results collection using the ***ngget*** command

```
[cernak@vls data]$ ngget -a
ngget: downloading files to /home/cernak/grid/data/259251100973253968091
ngget: download successful - deleting job from gatekeeper.
[cernak@vls data]$
```

Grid Monitor-online information about tasks and resources

	UiO Grid	33	0+32	0+37
Russia	The SPbSU First Clust>	1	0+0	0+0
Slovakia	UPJS ALICE Grid	1	0+0	0+0
	UPJS AMOS Grid	9	8+0	0+0
	UPJS Grid	1	0+0	0+0
Slovenia	SiGNET	100	0+0	0+0
Sweden	Bluesmoke (Swegrid,NS>	99	95+1	1725+0
	Dayhoff	32	0+26	0+0
	Hagrid (SweGrid, Uppm>	100	58+34	7+0
	Hive (Swegrid, UNICC)	0		0+0
	Ingrid (SweGrid,HPC2N)	95	1+43	0+0
	ISV	4	0+0	0+0

Workflow-during a submission of the jobs



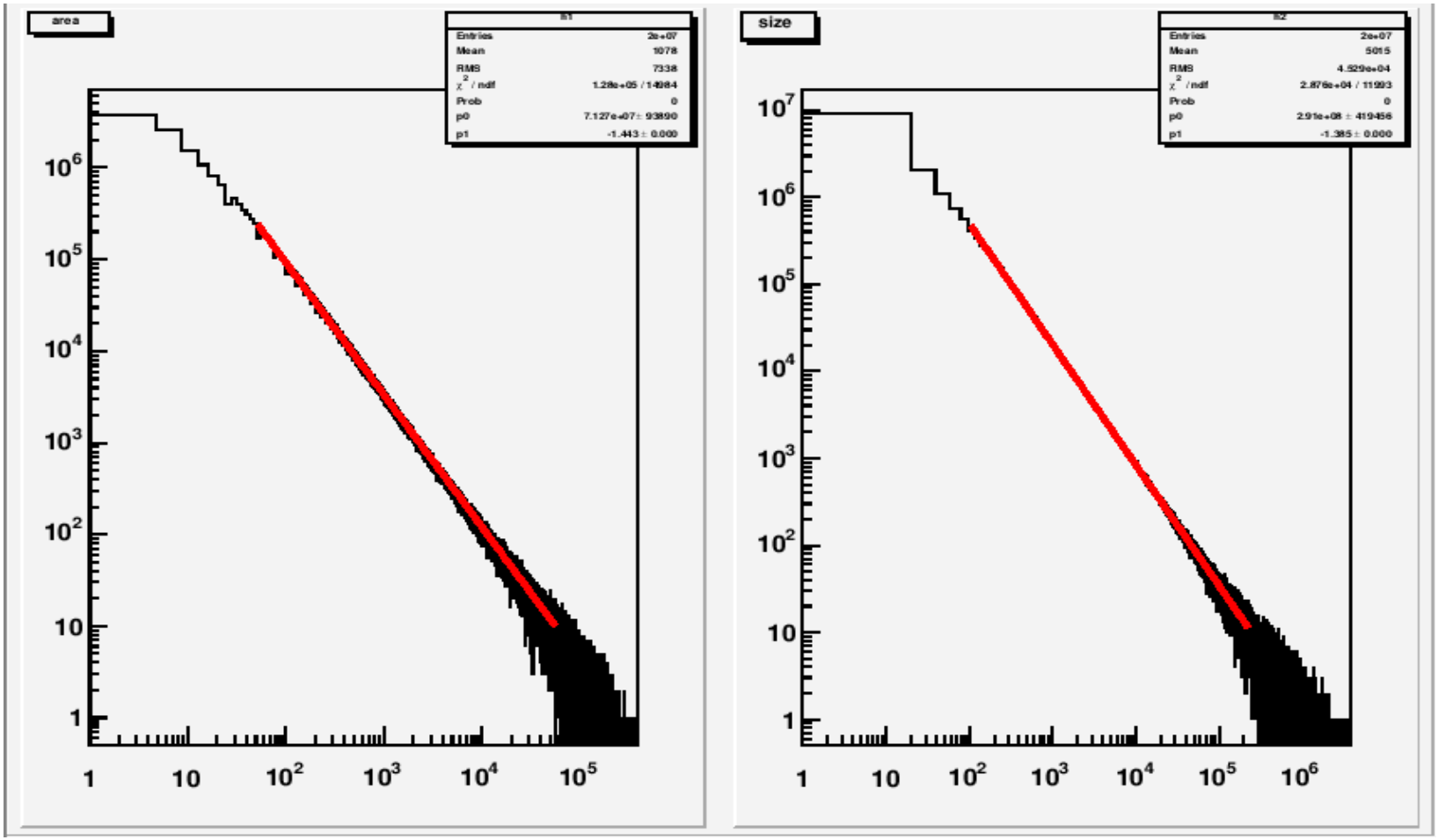
Applications solved in NorduGrid (UPJS group)

- ***Statistical physics (complex systems)*** - avalanche dynamics. This task could be suitable for NEES Grid (USA national project) www: ***it.nees.org***
- ***Image processing*** -generally very useful tasks in medical research and hospital diagnostic [4]
  -our application is from ***"soft condensed matter"*** we study aggregation and diffusion in colloidal systems. Video sequences are taken by CCD.
- ***Future applications:***
  - biochemistry, bioinformatics
  - particle physics
  - nano-technology

Computer simulations of avalanches (SOC approach)

Self organized criticality (SOC) P.Bak, Phys. Rev. Lett. **59** 381 (1987)

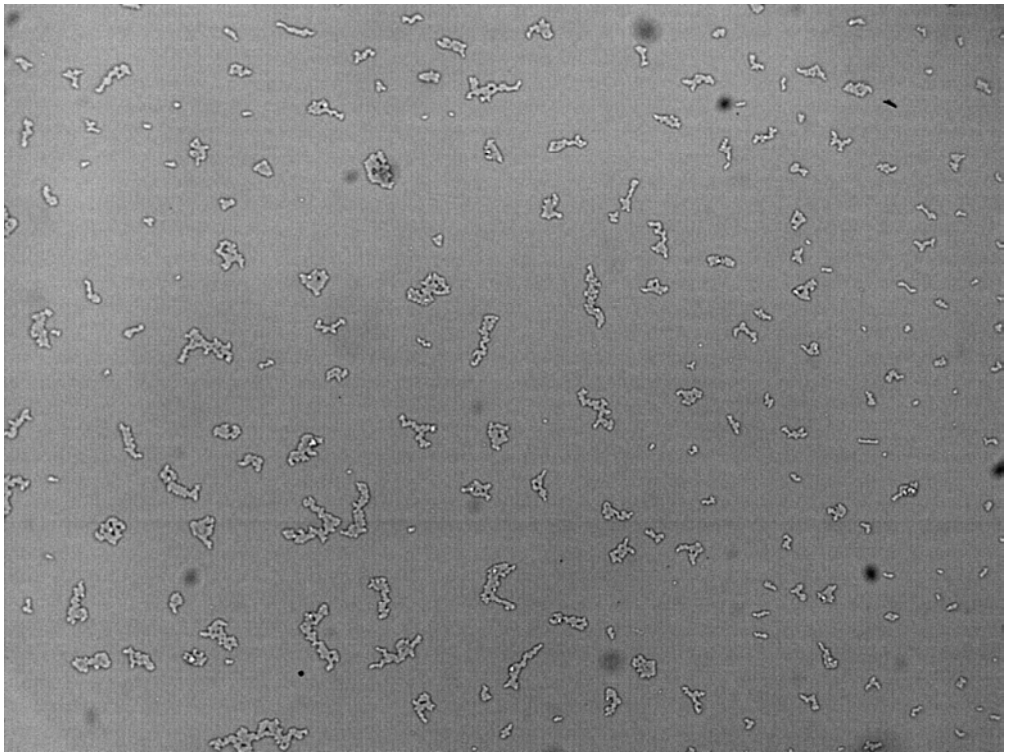
- avalanche dynamics, application at earthquakes,....

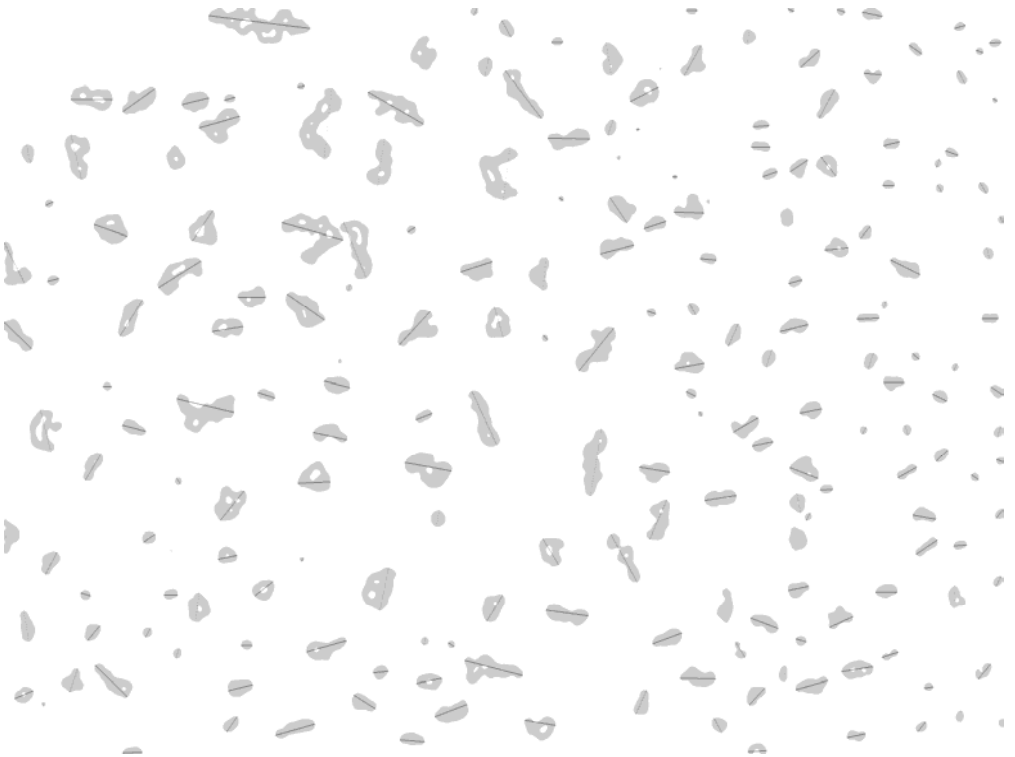


More than 600 jobs, created data 8GB, 1 CPU time (P4@2.4GHz) ~1 year,

in **NorduGrid**…… 30-100 CPUs ~2 weeks

Image processing





Any image can serve as an input file of the parametric task.

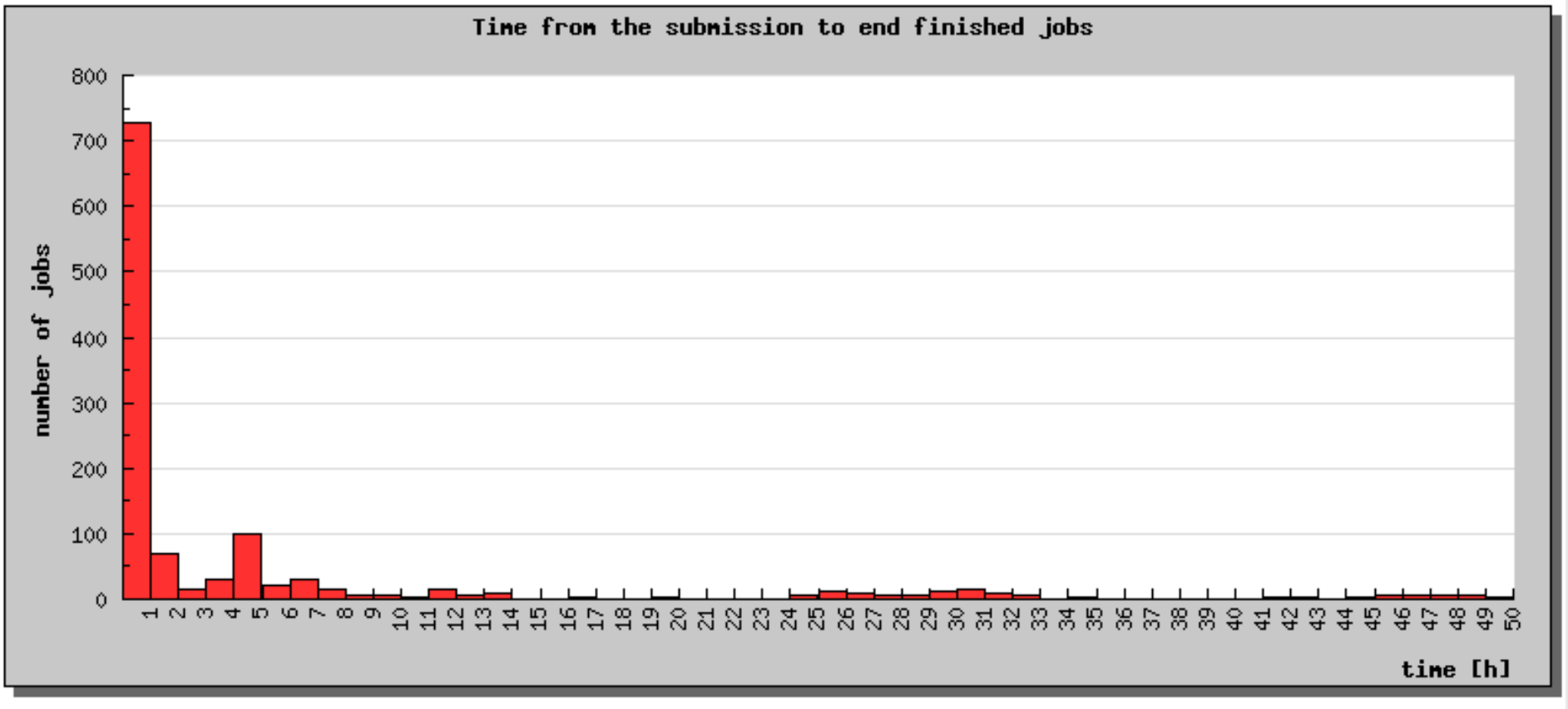
Typical experiment: 4 video sequences of 200-300 frames, 1 frame~5MB

Example: Duration of one frame analysis..... 1min

total time (1CPU) 1200 = 20h

Time distribution of finished “good” jobs (Logger)

More than 2500 good jobs in 2005 (not all are recorded in Logger)



Future plans:

- Security
- Interoperability
- Grid performance analysis
- international collaboration (NorduGrid, Complex, http://www.complexphysics.org/)
- National collaborations (ZU, TU, ...)
- New applications from bio-science
- Support of the new grid users
- ***Contribution to preparation of the national grid project***

References:

[1] M. Dobrucký, Úvod do gridového počítania, 9. marec 2005 VRVS, http://vk.upjs.sk/kalendar
[2] http://www.nordugrid.org
[3] J. Černák, http://bioflab.upjs.sk/~cernak/sys_prog/sys_program.html
[4] http://lyon2003.healthgrid.org/documents/slides_PDF/25_Henning_Muller.pdf