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R, paralelización, datos masivos y aplicaciones web: ejemplos del uso de R en bioinformática

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III Jornadas de Usuarios de R
17-Noviembre-2011

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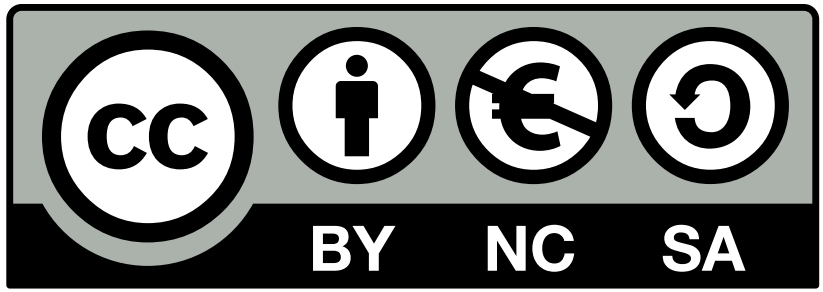

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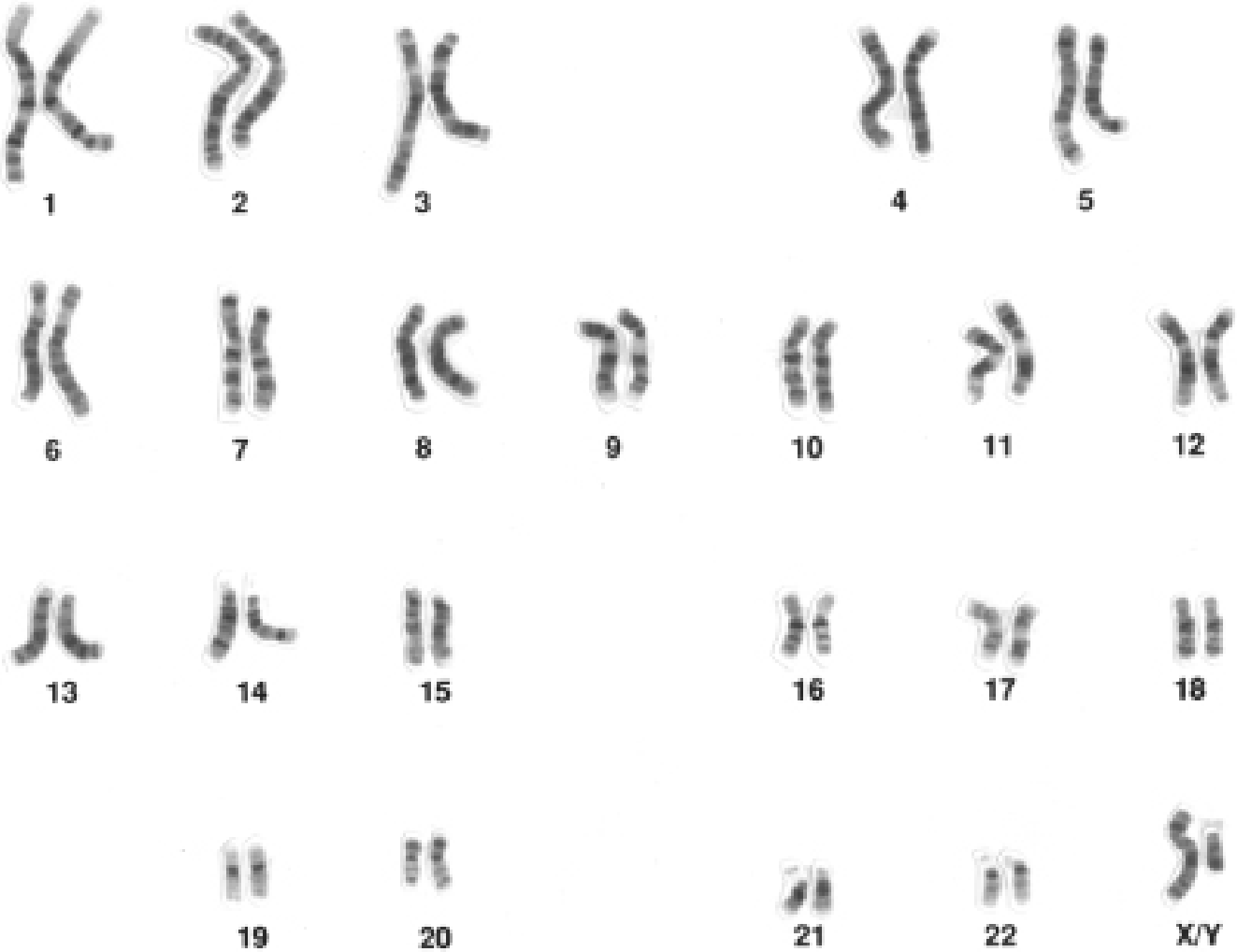
Chromosomes



From the Wikipedia; original source

`http://www.genome.gov/Pages/Hyperion//DIR/VIP/Glossary/Illustration/karyotype.shtml`

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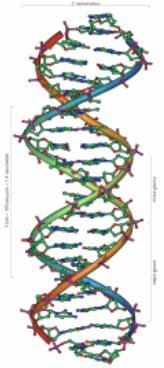
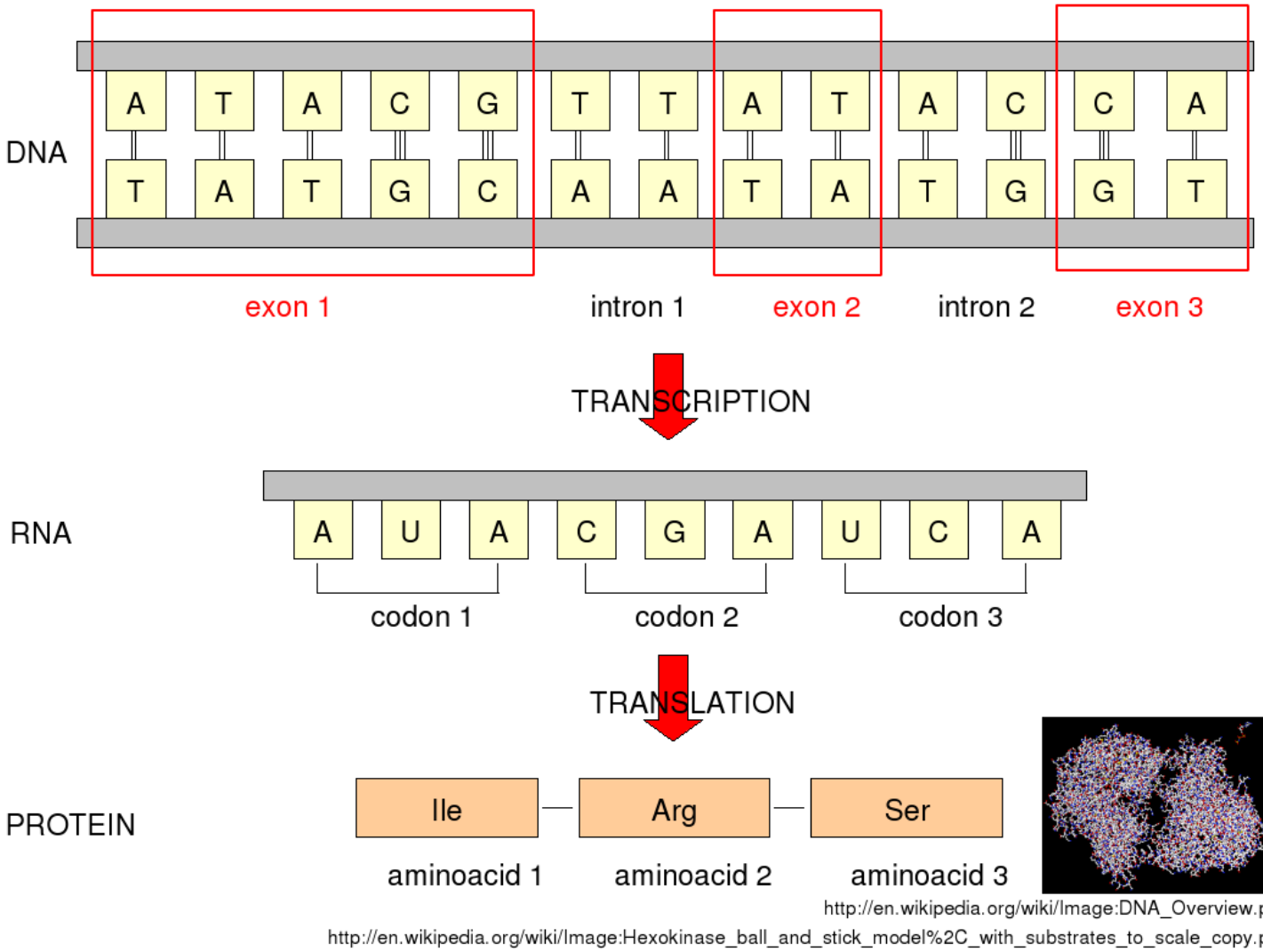
DNA → protein





http://en.wikipedia.org/wiki/Image:DNA_Overview.png
http://en.wikipedia.org/wiki/Image:Hexokinase_ball_and_stick_model%2C_with_substrates_to_scale_copy.png

(From O. Rueda's PhD Thesis)

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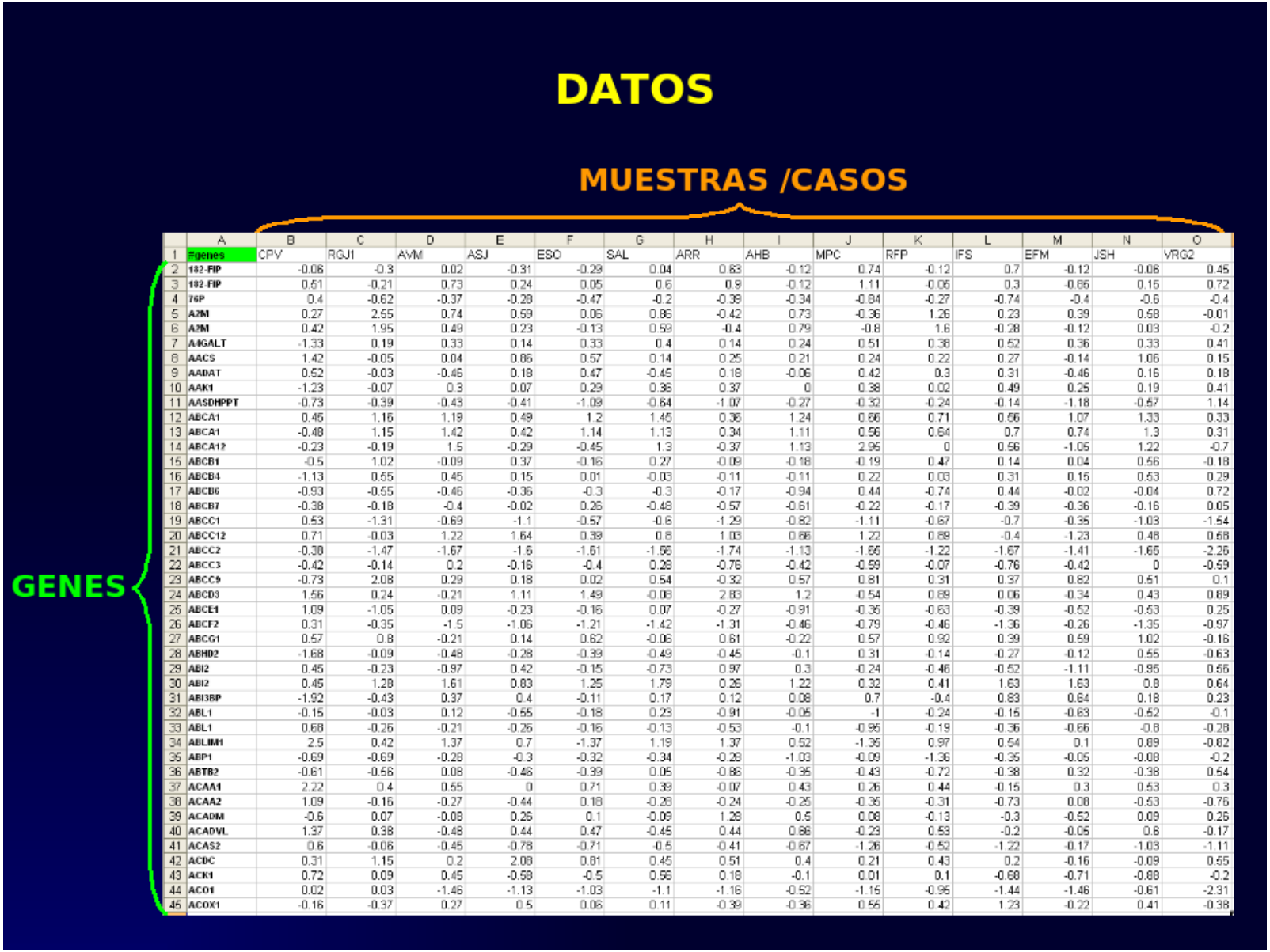
Data from a microarray experiment



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	#genes	CPV	RGJ1	AVM	ASJ	ESO	SAL	ARR	AHB	MPC	RFP	IFS	EFM	JSH	VRG2
2	182-FIP	-0.06	-0.3	0.02	-0.31	-0.29	0.04	0.63	-0.12	0.74	-0.12	0.7	-0.12	-0.06	0.45
3	182-FIP	0.51	-0.21	0.73	0.24	0.05	0.6	0.9	-0.12	1.11	-0.05	0.3	-0.65	0.15	0.72
4	76P	0.4	-0.62	-0.37	-0.28	-0.47	-0.2	-0.39	-0.34	-0.84	-0.27	-0.74	-0.4	-0.6	-0.4
5	A2M	0.27	2.55	0.74	0.59	0.06	0.86	-0.42	0.73	-0.36	1.26	0.23	0.39	0.58	-0.01
6	A2M	0.42	1.95	0.49	0.23	-0.13	0.59	-0.4	0.79	-0.8	1.6	-0.28	-0.12	0.03	-0.2
7	A4GALT	-1.33	0.19	0.33	0.14	0.33	0.4	0.14	0.24	0.51	0.38	0.52	0.36	0.33	0.41
8	AACS	1.42	-0.05	0.04	0.86	0.57	0.14	0.25	0.21	0.24	0.22	0.27	-0.14	1.06	0.15
9	AADAT	0.52	-0.03	-0.46	0.18	0.47	-0.45	0.18	-0.06	0.42	0.3	0.31	-0.46	0.16	0.18
10	AAK1	-1.23	-0.07	0.3	0.07	0.29	0.36	0.37	0	0.38	0.02	0.49	0.25	0.19	0.41
11	AASDHPPT	-0.73	-0.39	-0.43	-0.41	-1.09	-0.64	-1.07	-0.27	-0.32	-0.24	-0.14	-1.18	-0.57	1.14
12	ABCA1	0.45	1.15	1.19	0.49	1.2	1.45	0.36	1.24	0.66	0.71	0.56	1.07	1.33	0.33
13	ABCA1	-0.48	1.15	1.42	0.42	1.14	1.13	0.34	1.11	0.56	0.64	0.7	0.74	1.3	0.31
14	ABCA12	-0.23	-0.19	1.5	-0.29	-0.45	1.3	-0.37	1.13	2.96	0	0.56	-1.05	1.22	-0.7
15	ABCB1	-0.5	1.02	-0.09	0.37	-0.16	0.27	-0.09	-0.18	-0.19	0.47	0.14	0.04	0.56	-0.18
16	ABCB4	-1.13	0.55	0.45	0.15	0.01	-0.03	-0.11	-0.11	0.22	0.03	0.31	0.16	0.53	0.29
17	ABCB6	-0.93	-0.55	-0.46	-0.36	-0.3	-0.3	-0.17	-0.94	0.44	-0.74	0.44	-0.02	-0.04	0.72
18	ABCB7	-0.38	-0.18	-0.4	-0.02	0.26	-0.48	-0.57	-0.61	-0.22	-0.17	-0.39	-0.36	-0.16	0.05
19	ABCC1	0.53	-1.31	-0.69	-1.1	-0.57	-0.6	-1.29	-0.82	-1.11	-0.67	-0.7	-0.35	-1.03	-1.54
20	ABCC12	0.71	-0.03	1.22	1.64	0.39	0.8	1.03	0.86	1.22	0.89	-0.4	-1.23	0.48	0.68
21	ABCC2	-0.38	-1.47	-1.67	-1.6	-1.61	-1.56	-1.74	-1.13	-1.65	-1.22	-1.67	-1.41	-1.65	-2.26
22	ABCC3	-0.42	-0.14	0.2	-0.16	-0.4	0.28	-0.76	-0.42	-0.59	-0.07	-0.76	-0.42	0	-0.59
23	ABCC9	-0.73	2.08	0.29	0.18	0.02	0.54	-0.32	0.57	0.81	0.31	0.37	0.82	0.51	0.1
24	ABCD3	1.56	0.24	-0.21	1.11	1.49	-0.08	2.83	1.2	-0.54	0.89	0.06	-0.34	0.43	0.89
25	ABCE1	1.09	-1.05	0.09	-0.23	-0.16	0.07	-0.27	-0.91	-0.35	-0.63	-0.39	-0.52	-0.53	0.25
26	ABCF2	0.31	-0.35	-1.5	-1.06	-1.21	-1.42	-1.31	-0.46	-0.79	-0.46	-1.36	-0.26	-1.35	-0.97
27	ABCG1	0.57	0.8	-0.21	0.14	0.62	-0.06	0.61	-0.22	0.57	0.92	0.39	0.59	1.02	-0.16
28	ABHD2	-1.68	-0.09	-0.48	-0.28	-0.39	-0.49	-0.45	-0.1	0.31	-0.14	-0.27	-0.12	0.55	-0.63
29	ABI2	0.45	-0.23	-0.97	0.42	-0.15	-0.73	0.97	0.3	-0.24	-0.46	-0.52	-1.11	-0.95	0.56
30	ABI2	0.45	1.28	1.61	0.83	1.25	1.79	0.26	1.22	0.32	0.41	1.63	1.63	0.8	0.64
31	ABI3BP	-1.92	-0.43	0.37	0.4	-0.11	0.17	0.12	0.08	0.7	-0.4	0.83	0.64	0.18	0.23
32	ABL1	-0.15	-0.03	0.12	-0.55	-0.18	0.23	-0.91	-0.05	-1	-0.24	-0.15	-0.63	-0.52	-0.1
33	ABL1	0.68	-0.26	-0.21	-0.26	-0.16	-0.13	-0.53	-0.1	-0.95	-0.19	-0.36	-0.66	-0.8	-0.28
34	ABLIM1	2.5	0.42	1.37	0.7	-1.37	1.19	1.37	0.52	-1.35	0.97	0.54	0.1	0.89	-0.82
35	ABP1	-0.69	-0.69	-0.28	-0.3	-0.32	-0.34	-0.28	-1.03	-0.09	-1.36	-0.35	-0.05	-0.08	-0.2
36	ABTB2	-0.61	-0.56	0.08	-0.46	-0.39	0.05	-0.86	-0.36	-0.43	-0.72	-0.38	0.32	-0.38	0.64
37	ACAA1	2.22	0.4	0.55	0	0.71	0.39	-0.07	0.43	0.26	0.44	-0.15	0.3	0.53	0.3
38	ACAA2	1.09	-0.16	-0.27	-0.44	0.18	-0.26	-0.24	-0.25	-0.36	-0.31	-0.73	0.08	-0.53	-0.76
39	ACADM	-0.6	0.07	-0.08	0.26	0.1	-0.09	1.29	0.5	0.08	-0.13	-0.3	-0.52	0.09	0.26
40	ACADVL	1.37	0.38	-0.48	0.44	0.47	-0.45	0.44	0.86	-0.29	0.53	-0.2	-0.05	0.6	-0.17
41	ACAS2	0.6	-0.06	-0.45	-0.78	-0.71	-0.5	-0.41	-0.67	-1.26	-0.52	-1.22	-0.17	-1.03	-1.11
42	ACDC	0.31	1.15	0.2	2.08	0.81	0.45	0.51	0.4	0.21	0.43	0.2	-0.16	-0.09	0.55
43	ACK1	0.72	0.09	0.45	-0.58	-0.5	0.56	0.18	-0.1	0.01	0.1	-0.68	-0.71	-0.88	-0.2
44	ACO1	0.02	0.03	-1.46	-1.13	-1.03	-1.1	-1.16	-0.52	-1.15	-0.95	-1.44	-1.46	-0.61	-2.31
45	ACOX1	-0.16	-0.37	0.27	0.5	0.06	0.11	-0.39	-0.36	0.56	0.42	1.23	-0.22	0.41	-0.38

Slide from Gema Moreno Bueno, Department of Biochemistry, UAM

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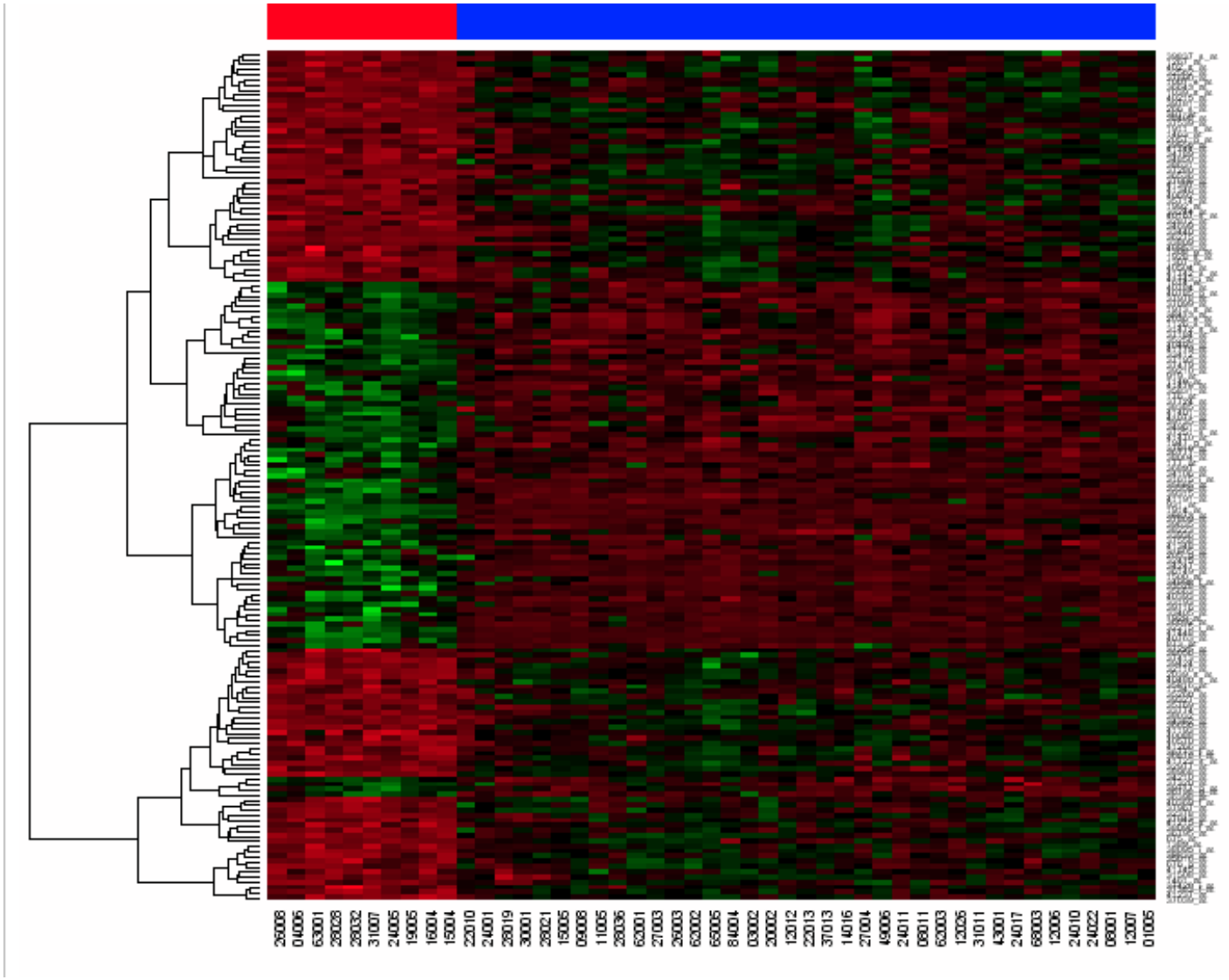
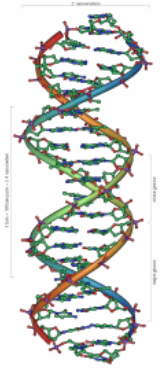
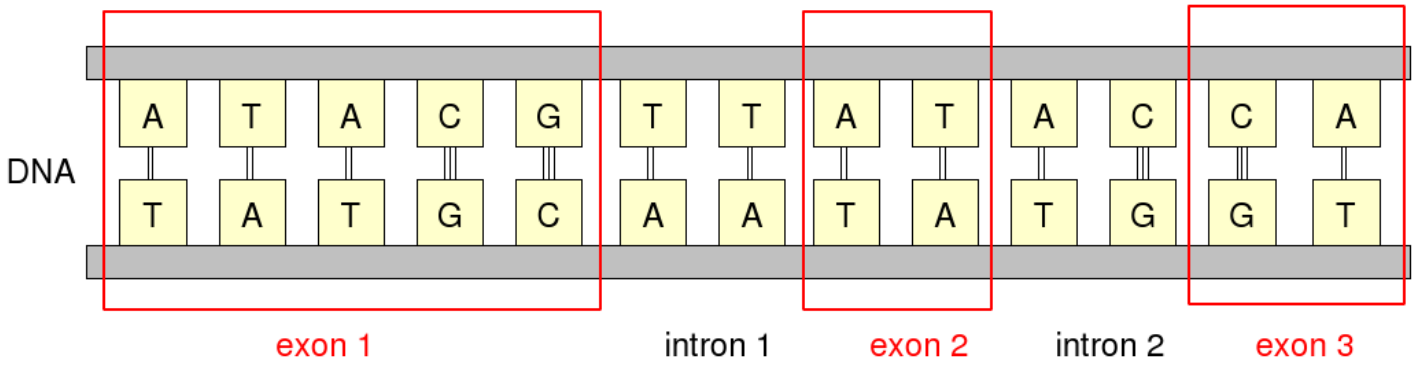
More microarray data

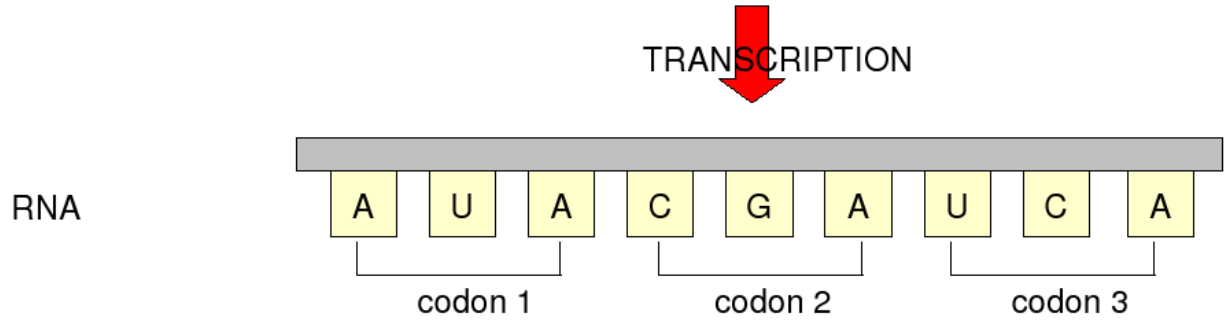


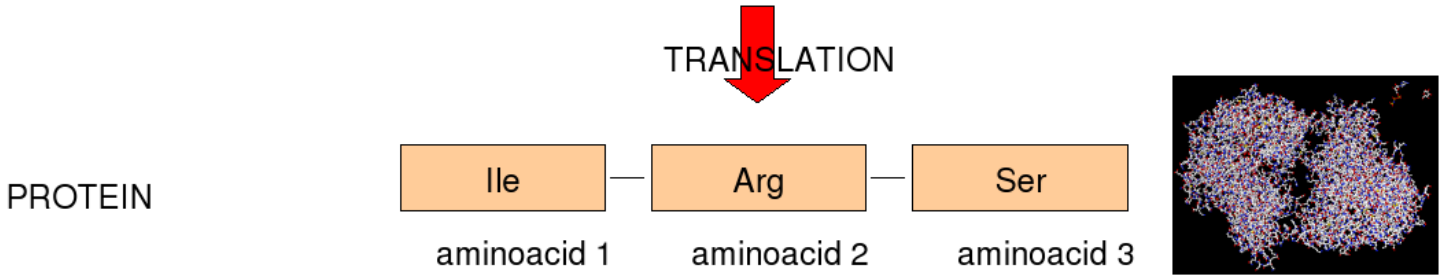
Modified from `http://www2.warwick.ac.uk/fac/sci/moac/students/peter_cock/r/heatmap/scaled_color_key.png`

DNA → protein









http://en.wikipedia.org/wiki/Image:DNA_Overview.png
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(From O. Rueda's PhD Thesis)

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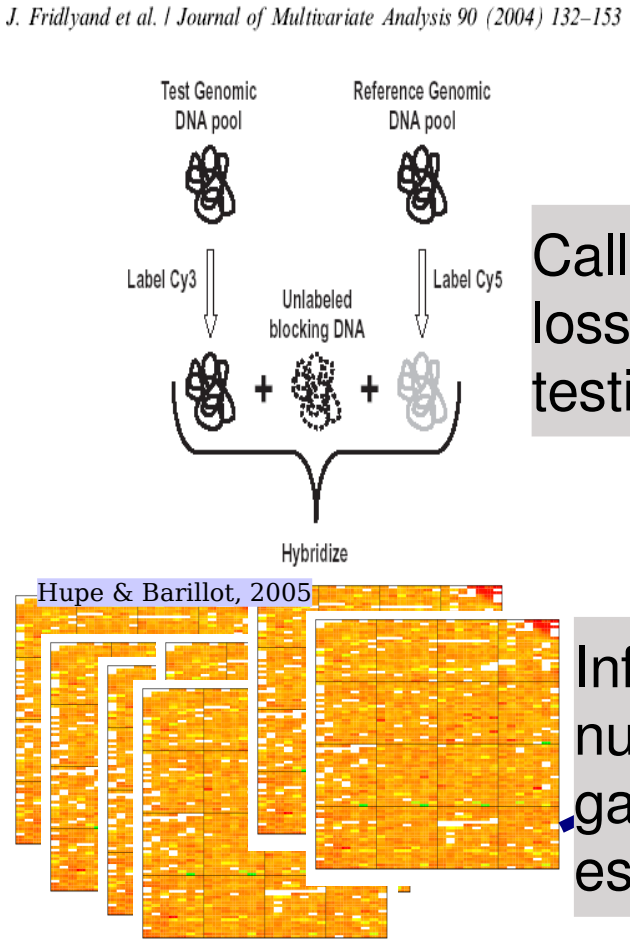
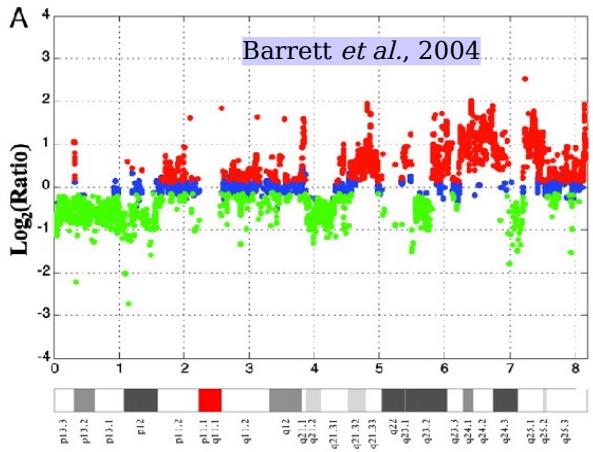
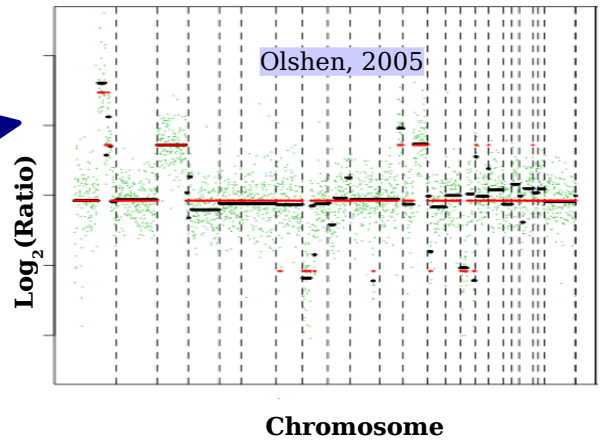
aCGH



Calling gains and losses: hypothesis testing



Inferring number of copy gains/losses: estimation



Arrays: a dot is a DNA fragment. Each array a sample. Each array all chromosomes.

(For analysis, location in chromosome matters)

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Data, data, data (in Gigabytes)

Expression arrays (mRNA) $>$ 40,000 probes

Copy number with aCGH $>$ 400,000 common;
some $>$ 4 x 10^6

... ...

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Multicores and computing clusters

- Increases in CPU speed slowed down (< 20% per year since 2002).
- Increase in the number of “cores”: 2, 4, 8. Next 10 years?
- Inexpensive computing clusters with off-the-shelf components.
- Must design our programs from the start: parallel programming

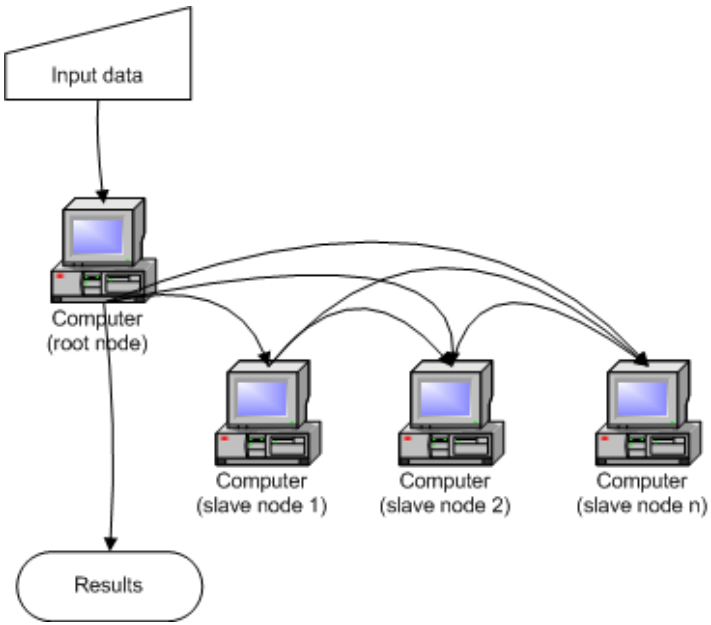

Image from `http://faq.distributed.net/`

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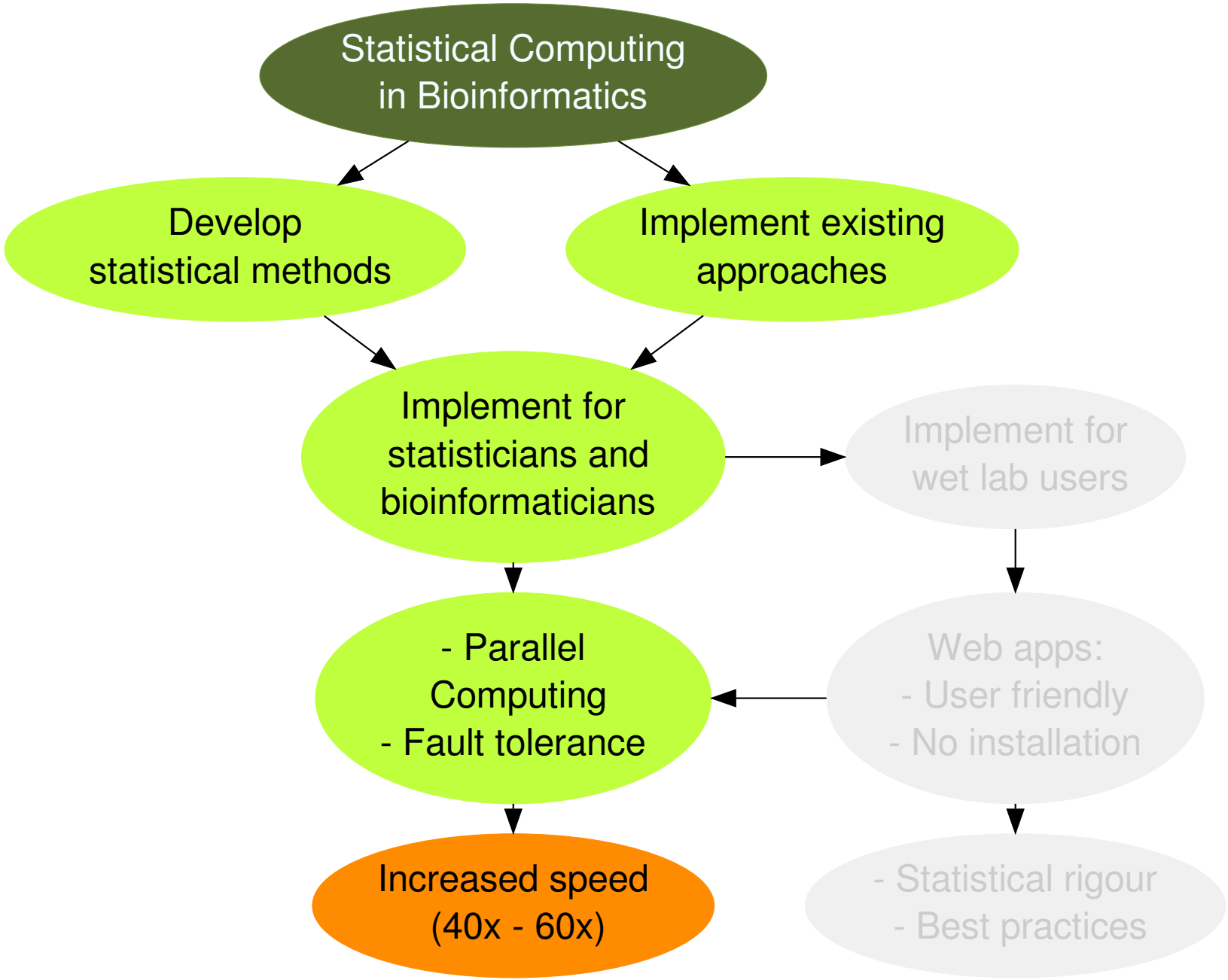
Standalone


Statistical Computing in Bioinformatics
Develop statistical methods
Implement existing approaches
Implement for statisticians and bioinformaticians
Implement for wet lab users
- Parallel Computing
- Fault tolerance
Web apps:
- User friendly
- No installation
Increased speed (40x - 60x)
- Statistical rigour
- Best practices

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R code

- Code available for many procedures (but a few years ago none parallelized!)
- Many computations embarrassingly parallelizable:
  - bootstrapping and cross-validation
  - arrays (or samples)
  - arrays by chromosomes
  - parallel chains in MCMC
- Figure production can be parallelized

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Parallelizing R code

- (Implement missing functionality: R/C)
- MPI: R packages Rmpi, papply, snow, snowfall
- Load balanced
- Wrappers over “mid level” functions in package: ease updating
- Parallelize:
  - Bootstrap samples/Cross-val. runs.
  - arrays
  - arrays by chromosomes
  - (or a combination of both)

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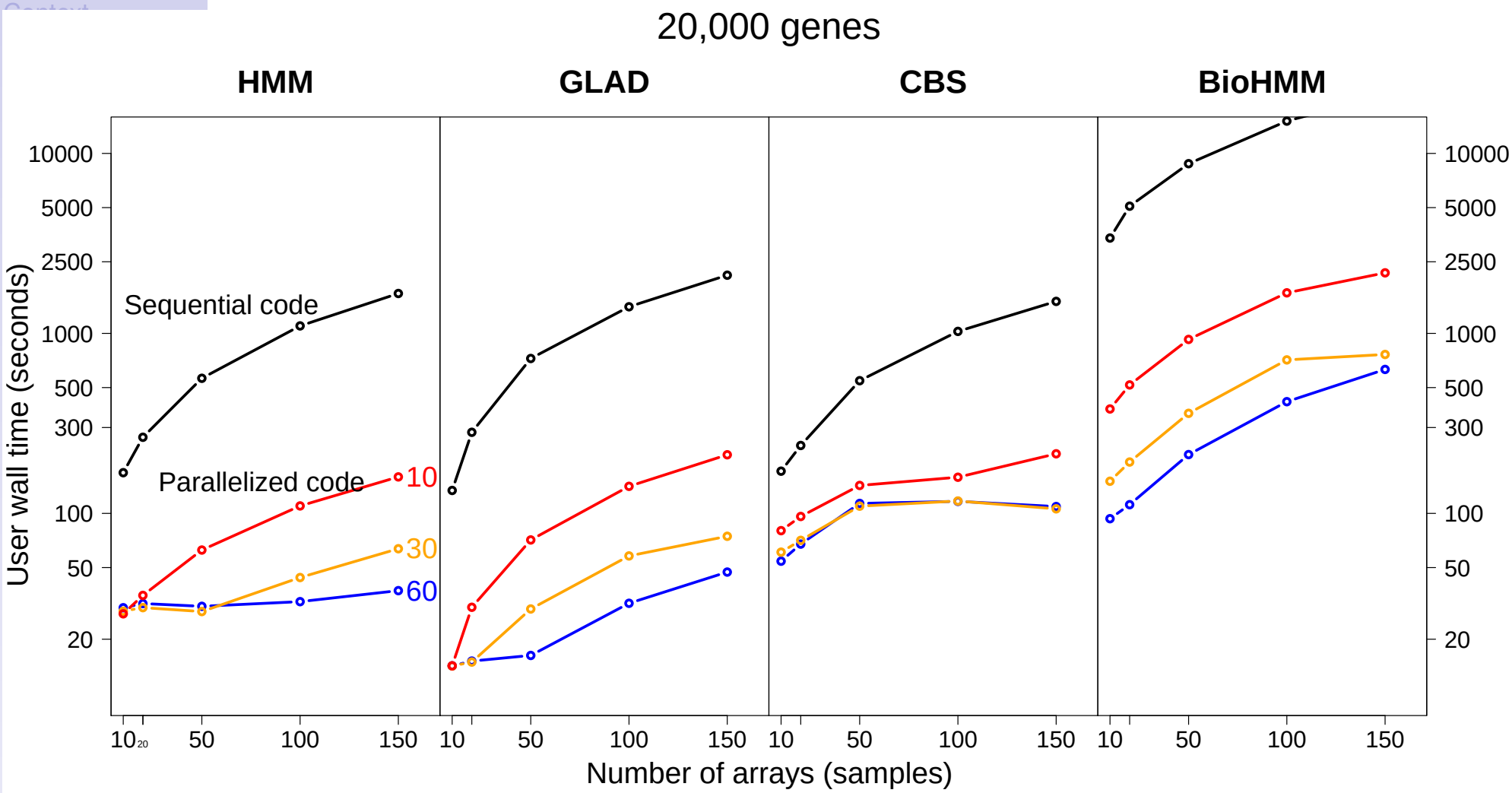
Is it worth it?

- Are speed improvements really worth the effort?
- Over what range of problems do see improvements?
- With what hardware can we see improvements?

What do we gain?



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What do we gain?

Are speed improvements really worth the effort?

Your effort: “R CMD INSTALL ADaCGH2”.

Over what range of problems do see improvements?

10 to 10^3 arrays/samples;
10^4 to 10^6 spots/genes.

With what hardware can we see improvements?

2 cores to 120 cores.

- Smaller clusters: more cost effective
- Single node/multi-core: less communication overhead

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Where is this running?

- *varSelRF* (CRAN)
- *ADaCGH2* (BioConductor)
- *SignS* (launchpad: http://launchpad.net/signs)

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Applications for wet lab researchers

- Analyze data in a reasonably short time.
- User friendly access to methods that are statistically rigorous.

Web-based applications

- User-friendly interface.
- No hardware/software hassles for end users.
- Parallelization is transparent.
- Method selection can be partially transferred (to us).
- Short user wall time: use (hardware/software) resources rarely available to individual biomedical researchers
- Just type in a URL:
  `http://www.some-application`

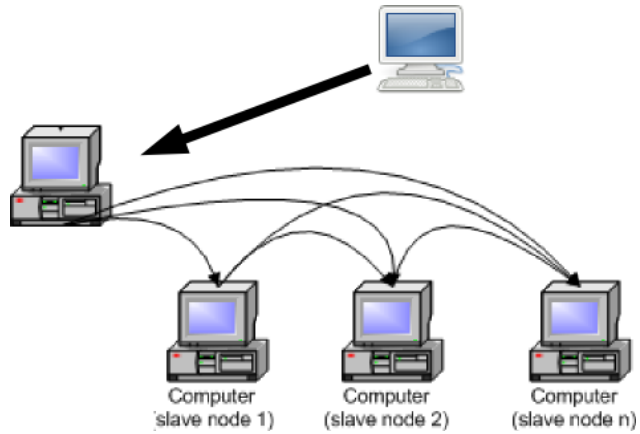

Image modified from `http://faq.distributed.net/`

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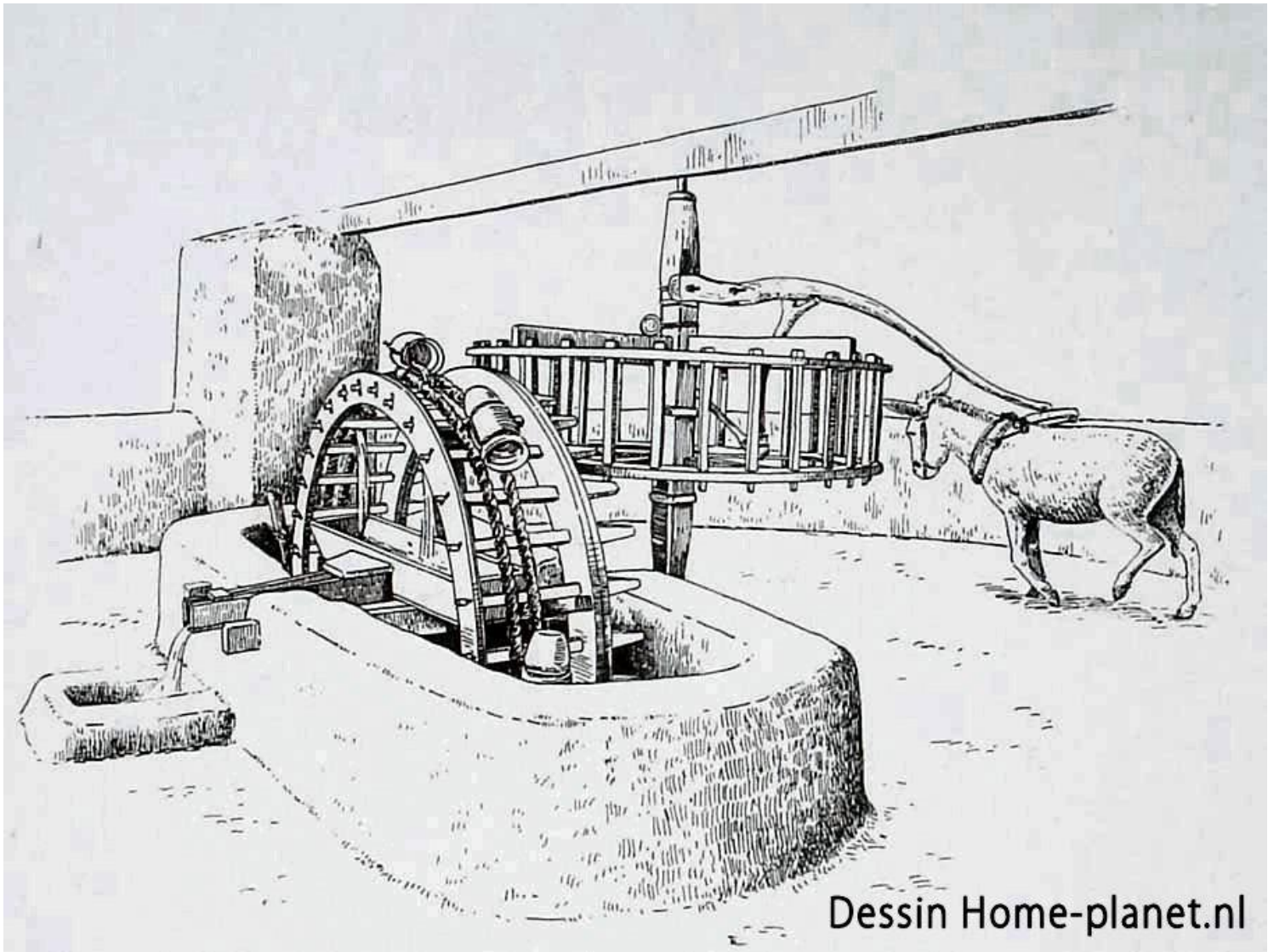
Sometimes collaborations feel like . . .



(From http://www.bitacoradegalileo.com/2010/11/16/giordano-bruno-en-la-cara-oculta-de-la-luna/)

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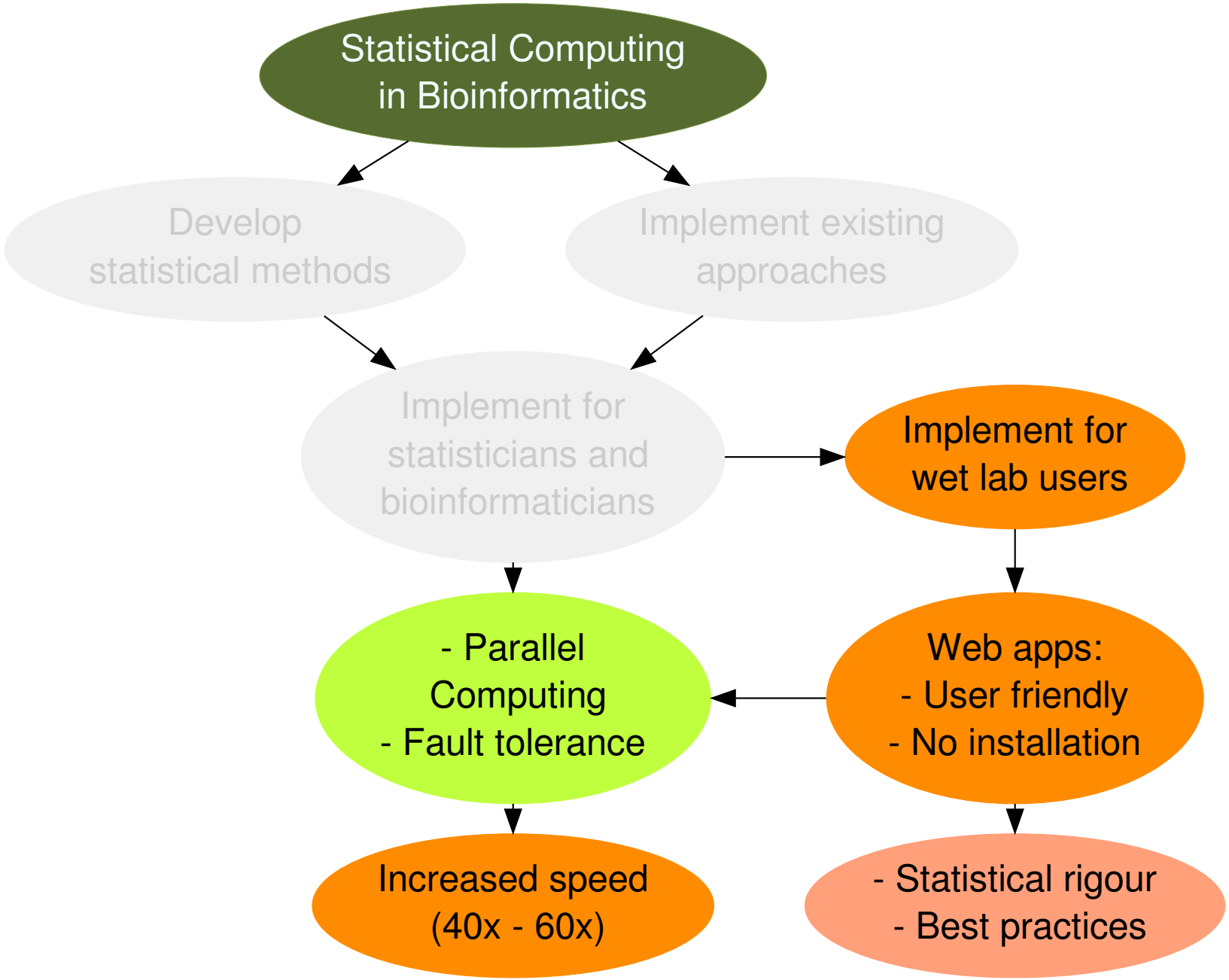
Parallelization in web applications



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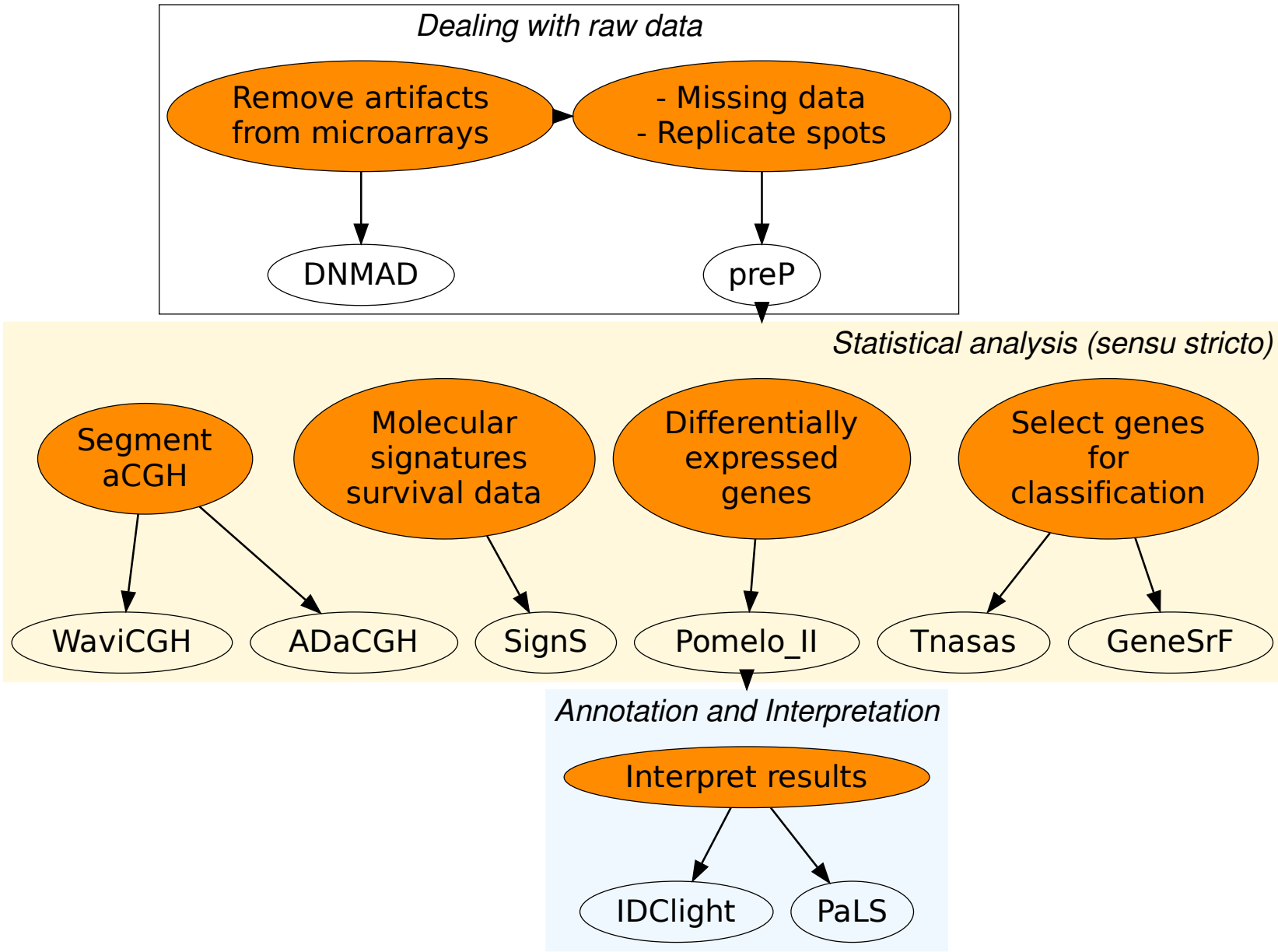
Main web-based applications



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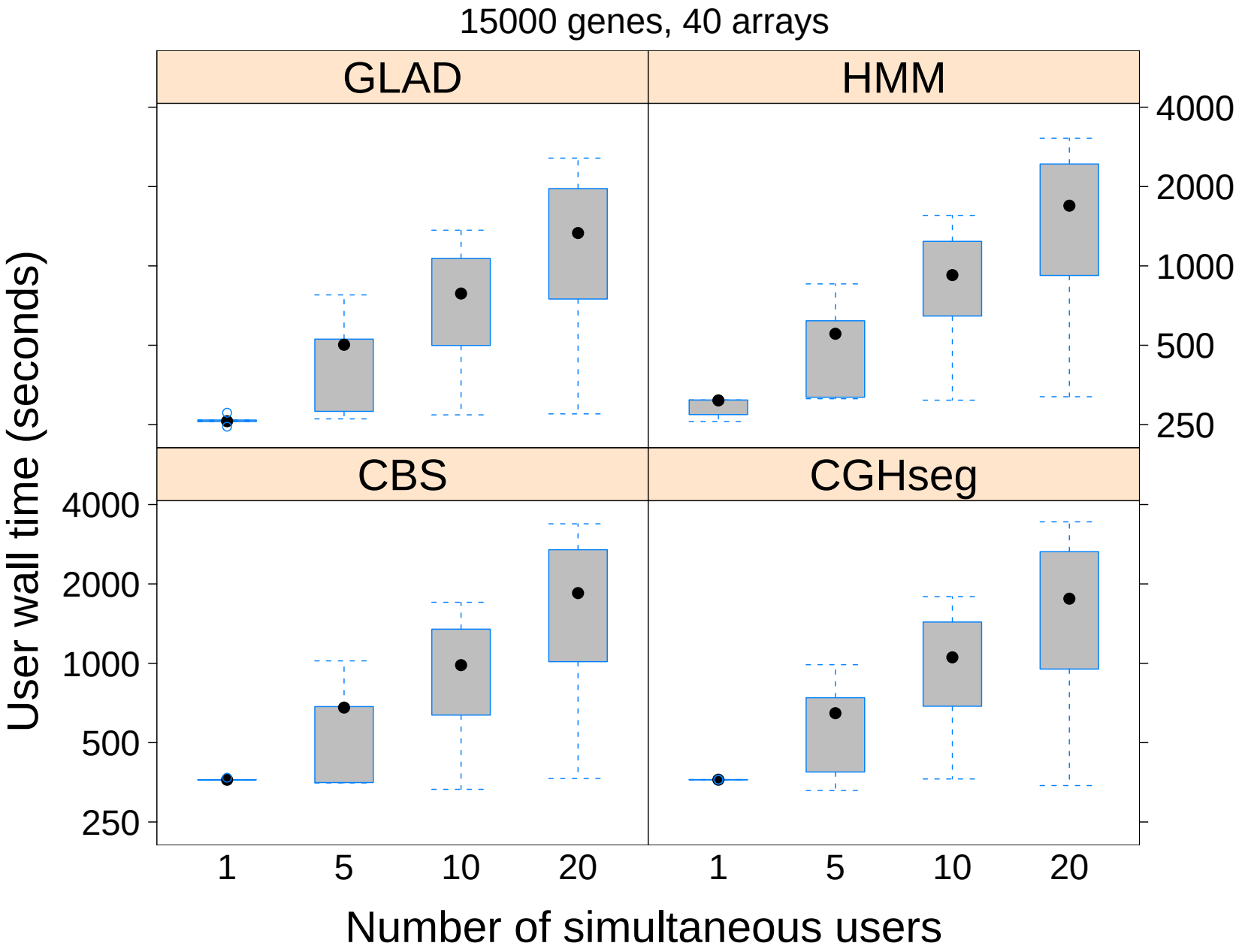
What do we gain?



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How it works: some key ideas

- Each run
  - Parallelization (transparent for users)
  - Fault-tolerance (network problems, machine crashes, bugs)
    - Check-pointing
- Periodic tasks (keep system running 24h, 365 d)
  - Automatic monitorization
  - Automated testing suite

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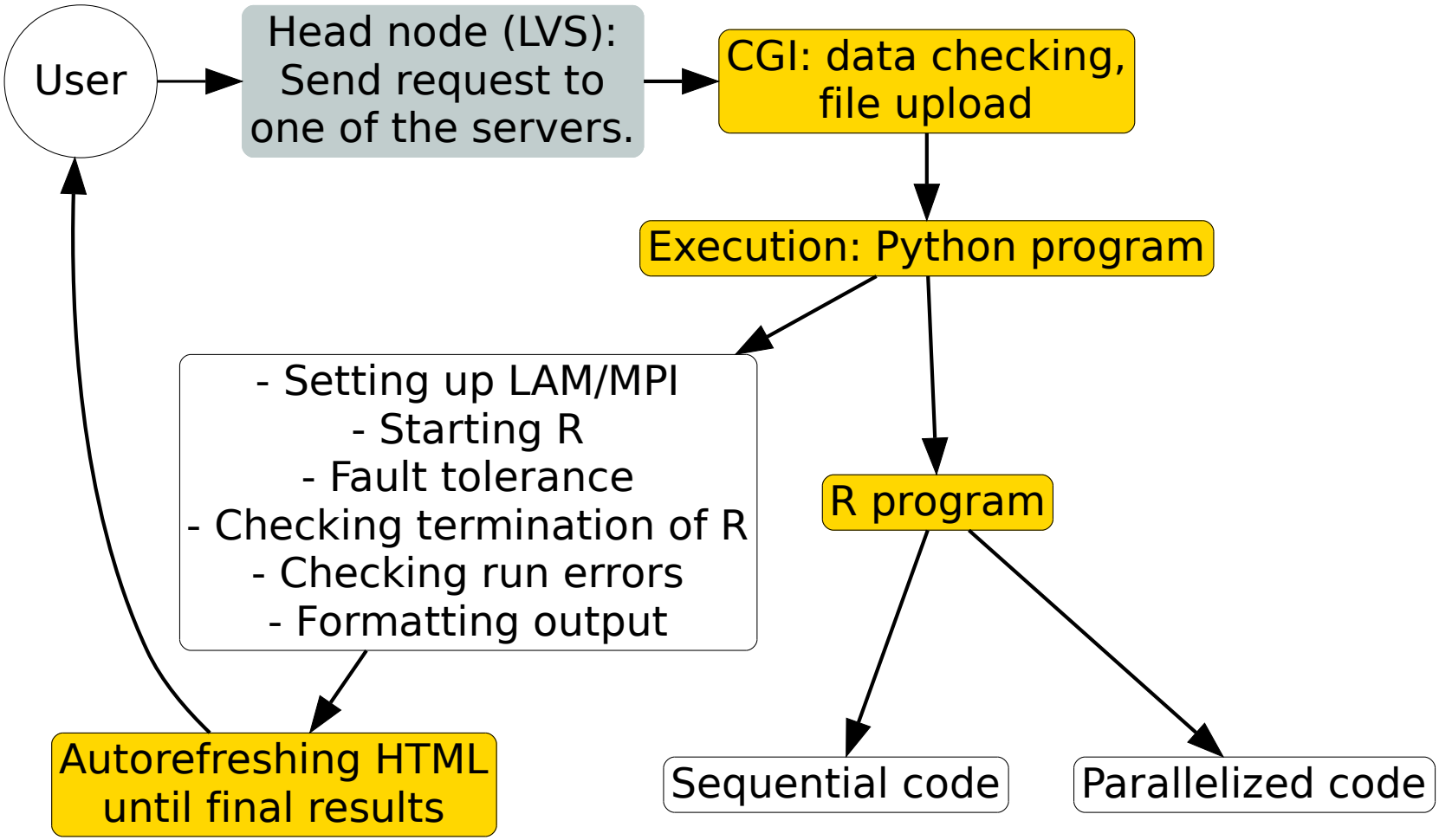
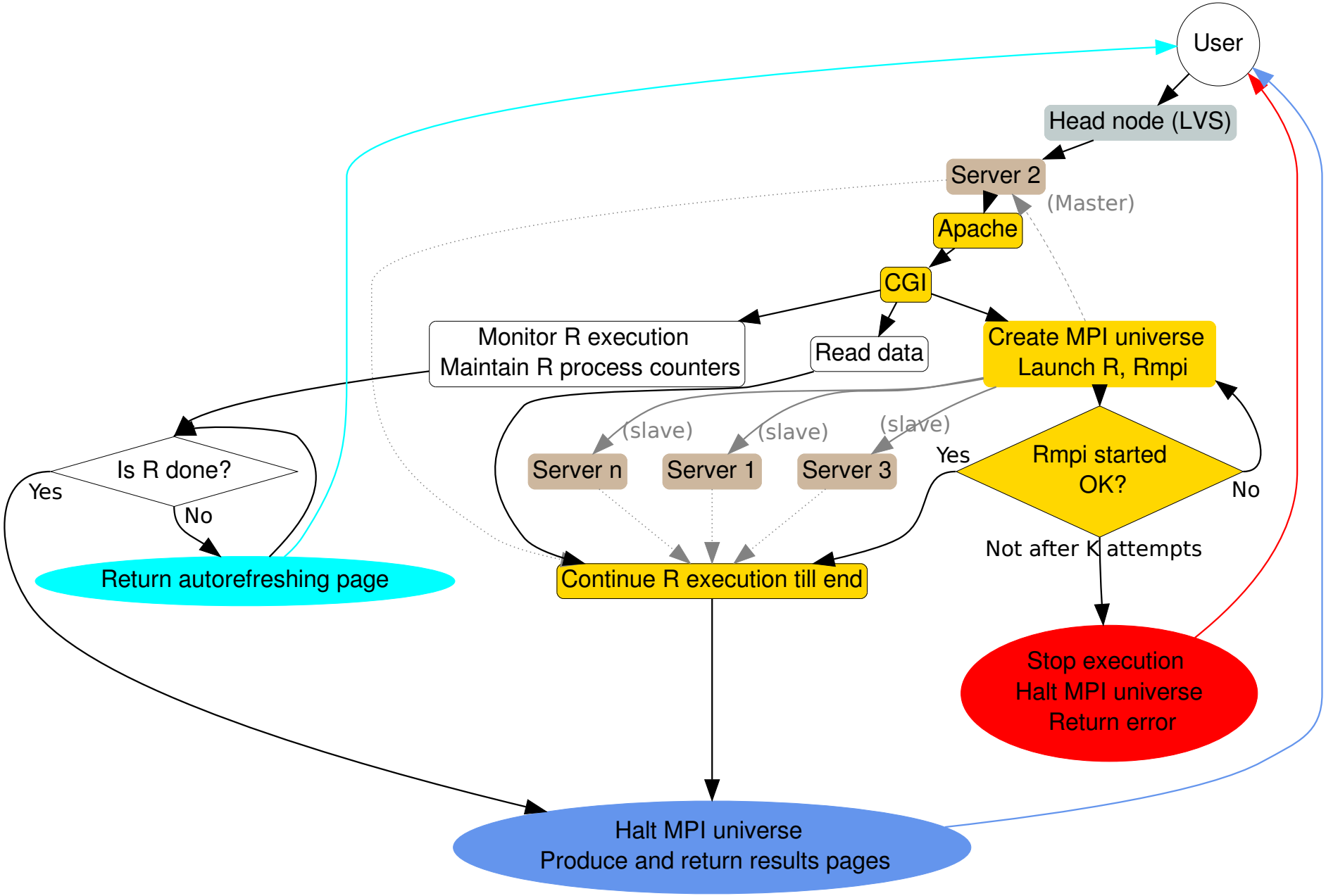
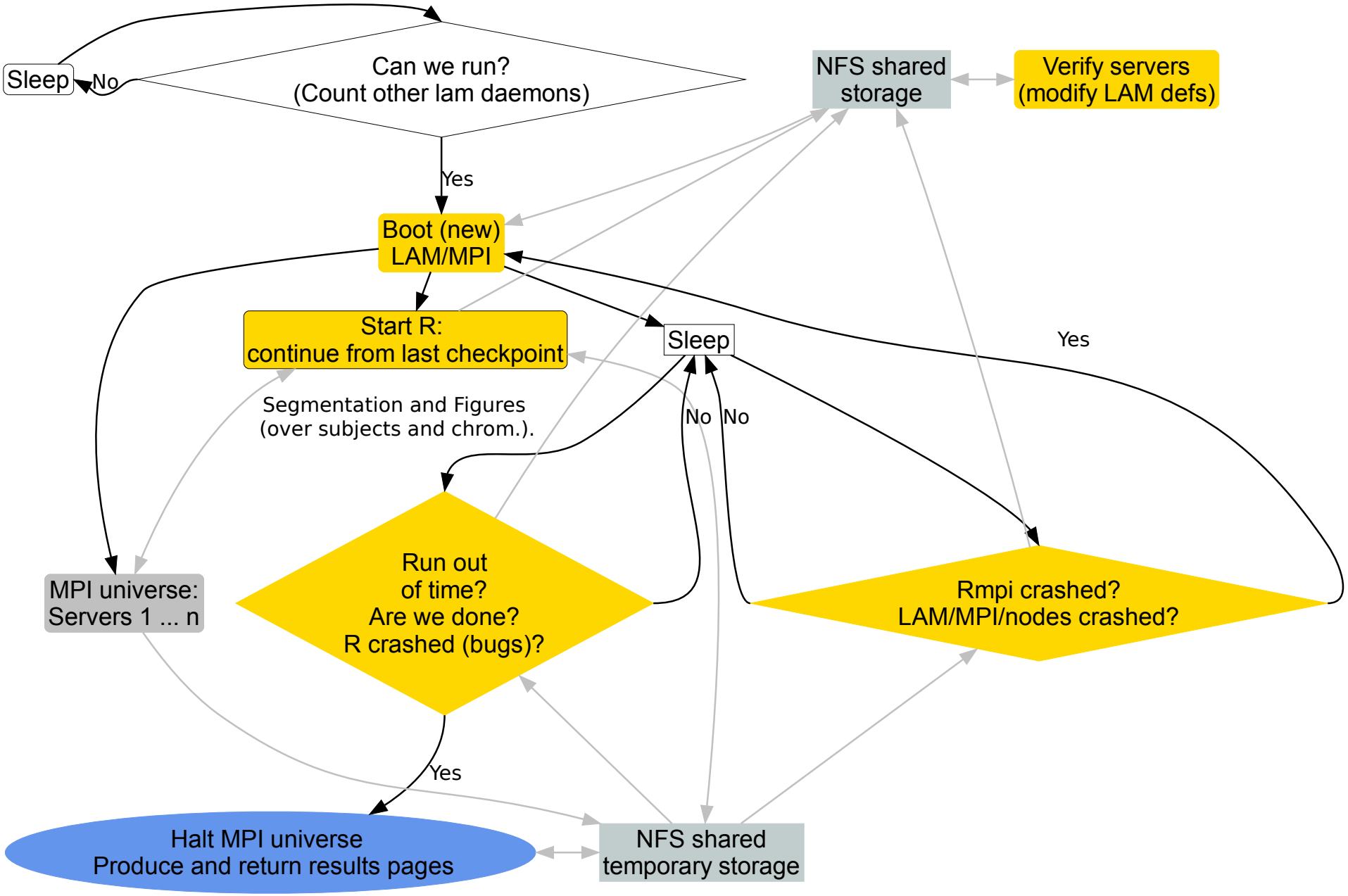
What happens



What happens: details



MPI details


Sleep
No
Can we run?
(Count other lam daemons)
Yes
NFS shared storage
Verify servers (modify LAM defs)
Boot (new) LAM/MPI
Start R: continue from last checkpoint
Sleep
Yes
Segmentation and Figures
(over subjects and chrom.).
No
No
MPI universe: Servers 1 ... n
Run out of time? Are we done? R crashed (bugs)?
Rmpi crashed? LAM/MPI/nodes crashed?
Yes
Halt MPI universe
Produce and return results pages
NFS shared temporary storage

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Where is this running?

- http://signs.bioinfo.cnio.es
- http://wavi.bioinfo.cnio.es
- http://genesrf.bioinfo.cnio.es

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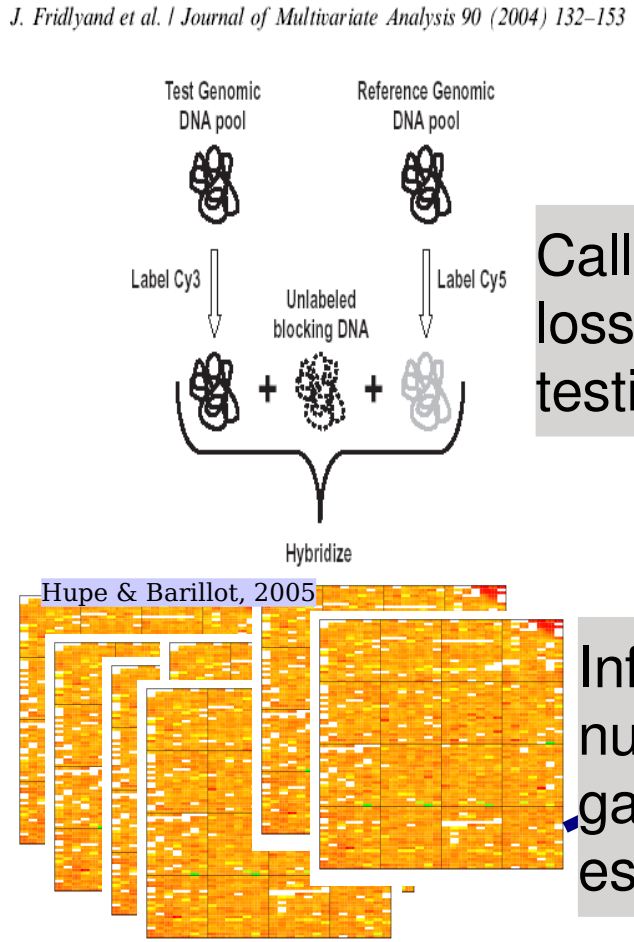
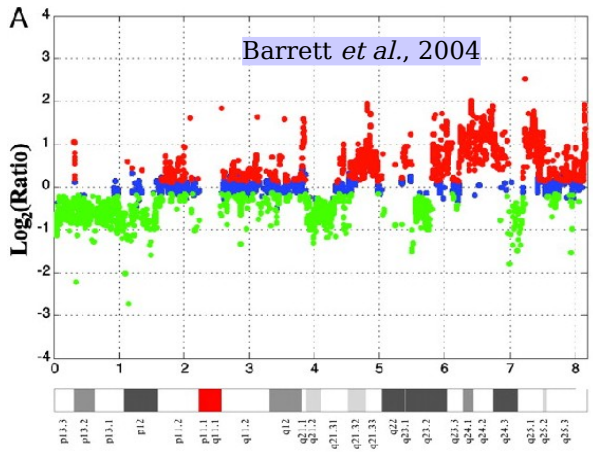
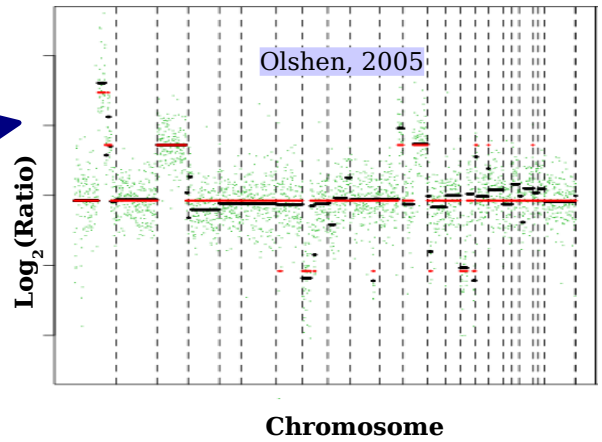


Calling gains and losses: hypothesis testing



Inferring number of copy gains/losses: estimation



Arrays: a dot is a DNA fragment. Each array a sample. Each array all chromosomes.

(For analysis, location in chromosome matters)

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Large data sets

- Millions of spots
- Hundreds or thousands of subjects.
- No need to hold everything in RAM at once.

- Package `ff`: "memory-efficient storage of large data on disk and fast access functions."

- Combined with:
  - parallelization
  - shared storage

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ff and parallelization

- *ff* stores the object on disk.
- Read that object from various R processes.
- Different R processes can write in different *ff* objects

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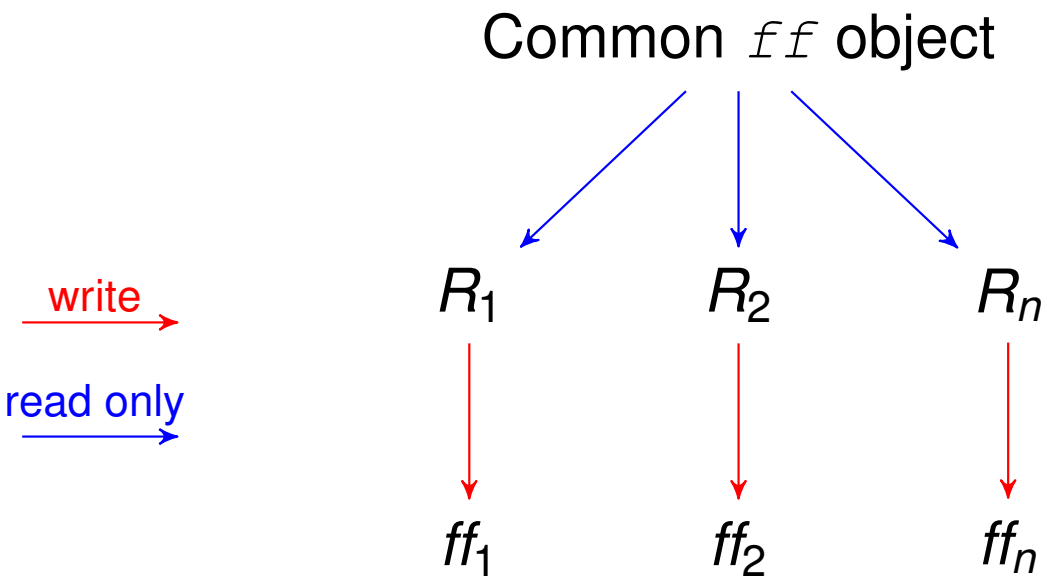
ff and parallelization (I)



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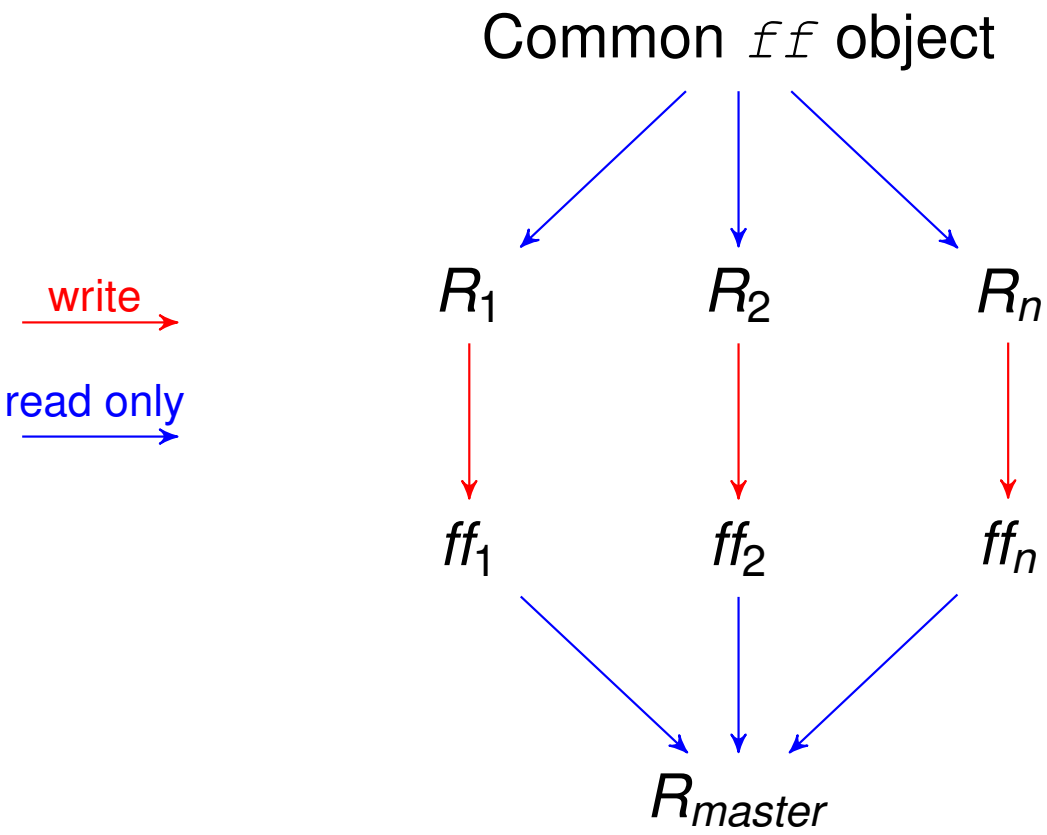
`ff` and parallelization (I)



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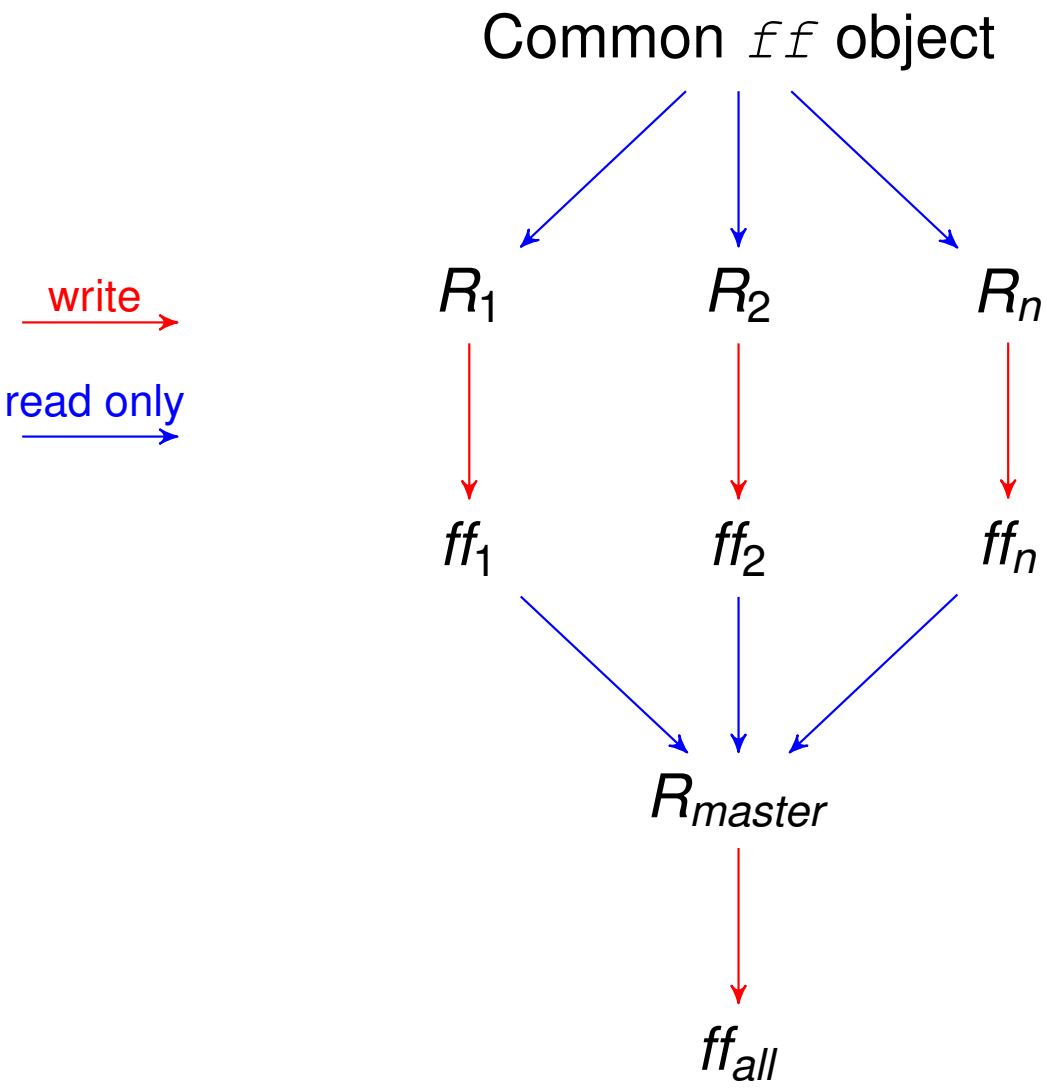

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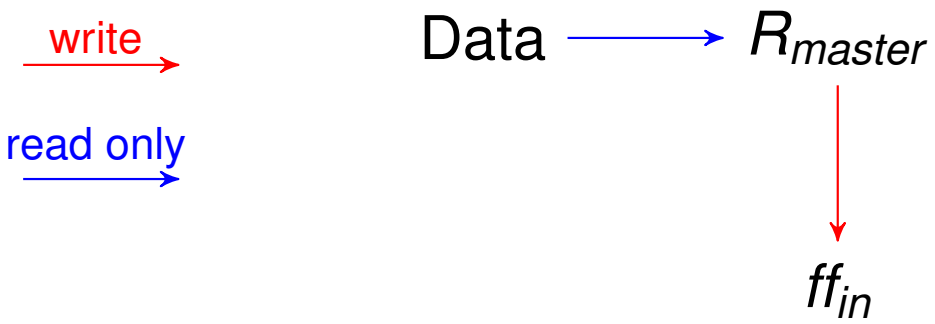
`ff` and parallelization (II)



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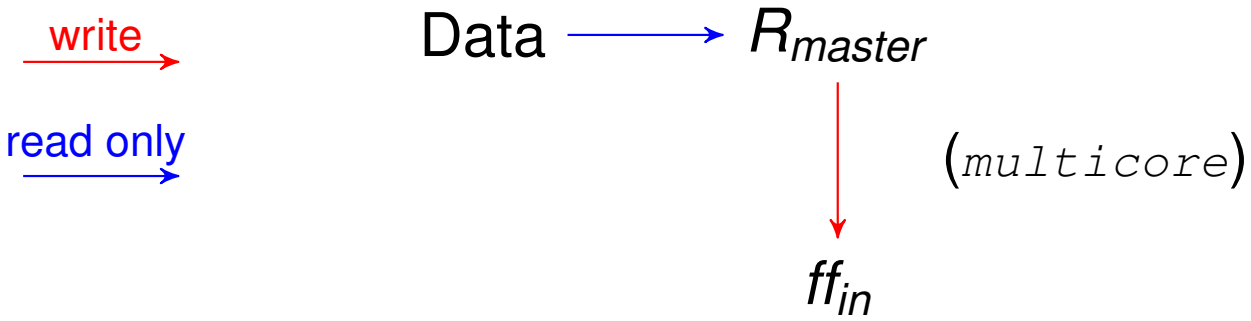

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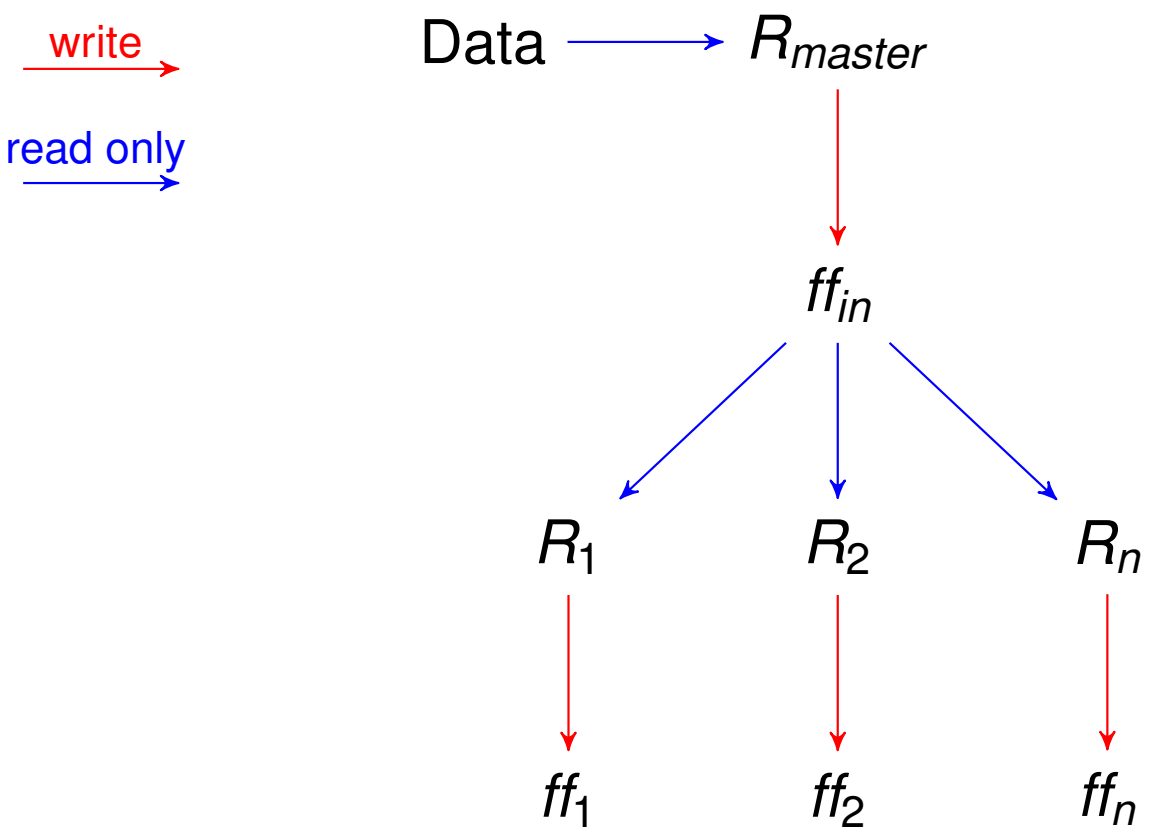

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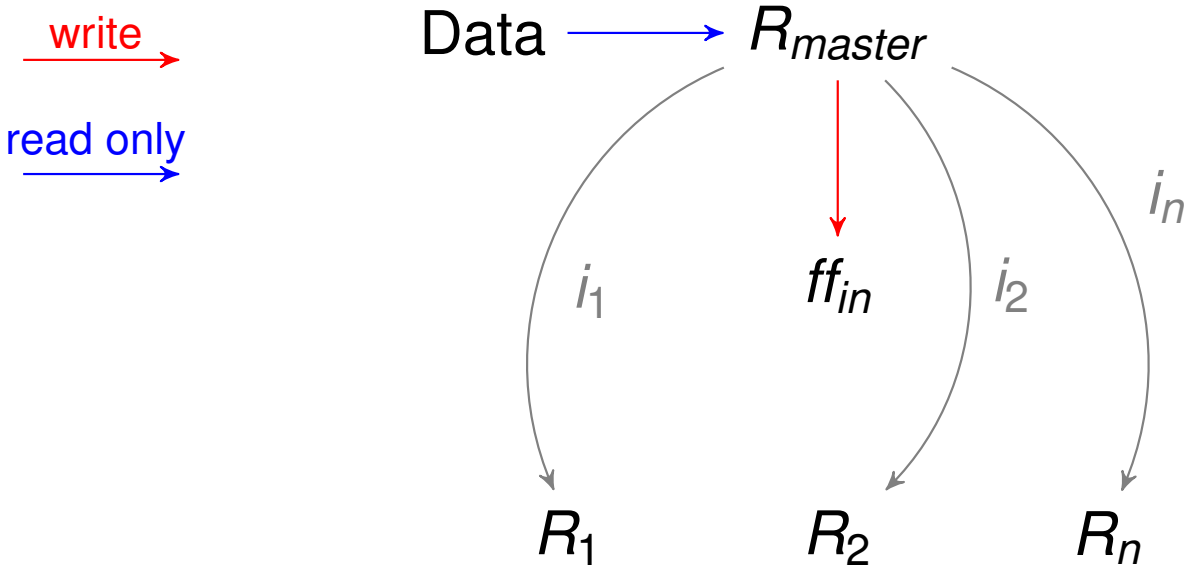

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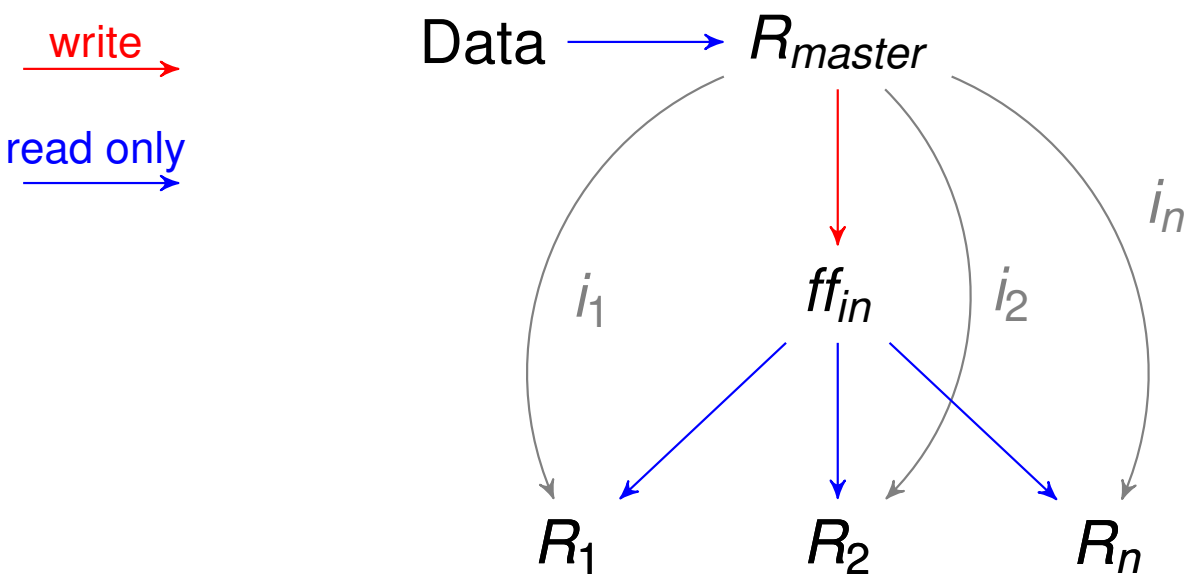

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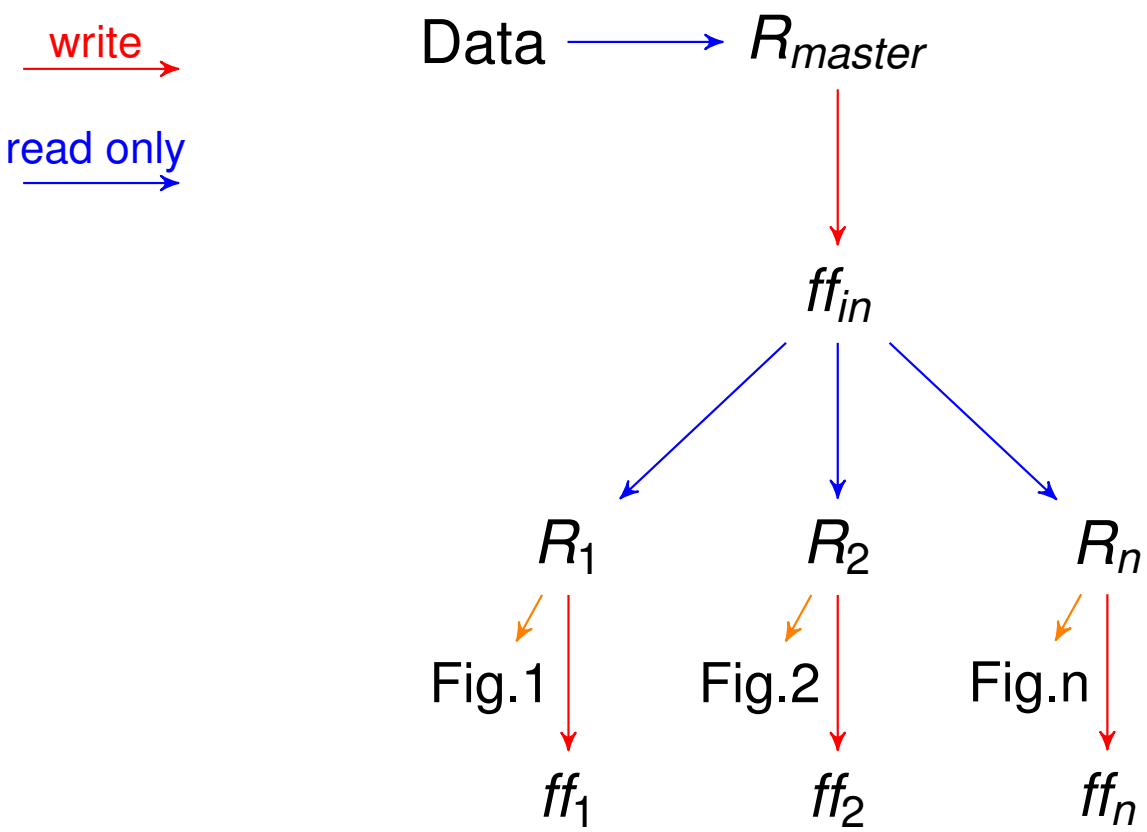

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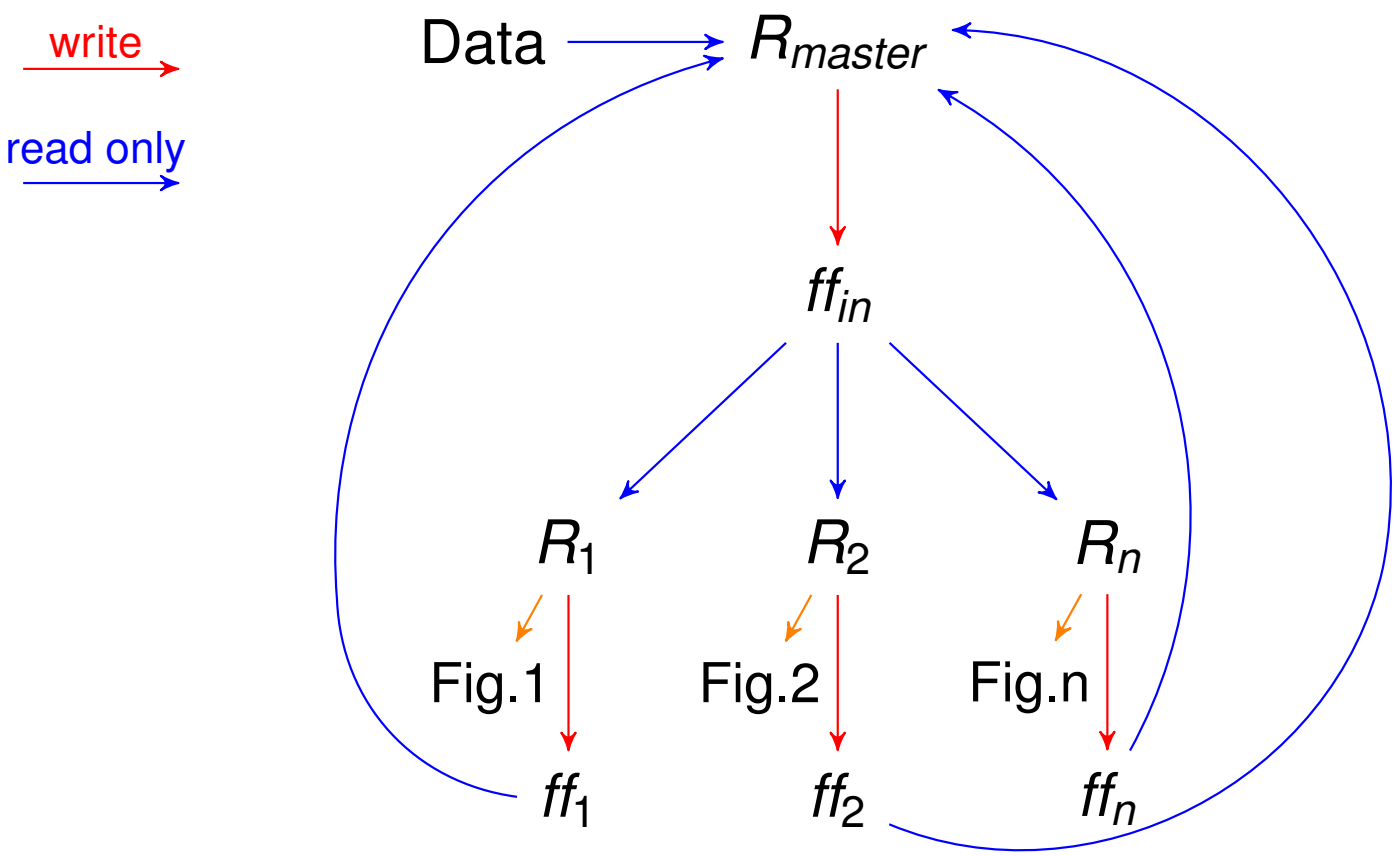

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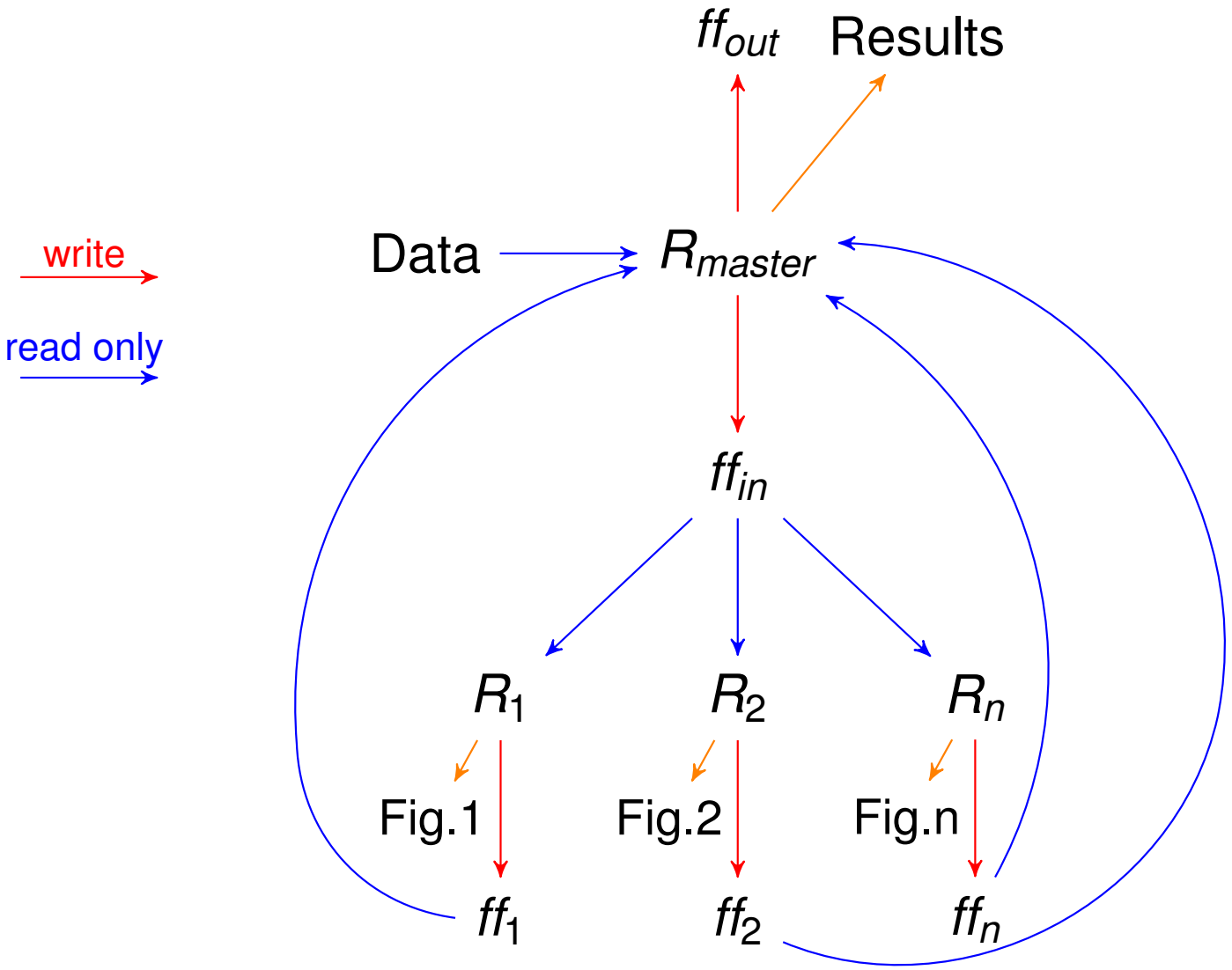

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Where is this running?

- *ADaCGH2* (BioConductor package)
- Web-based application http://wavi.bioinfo.cnio.es.

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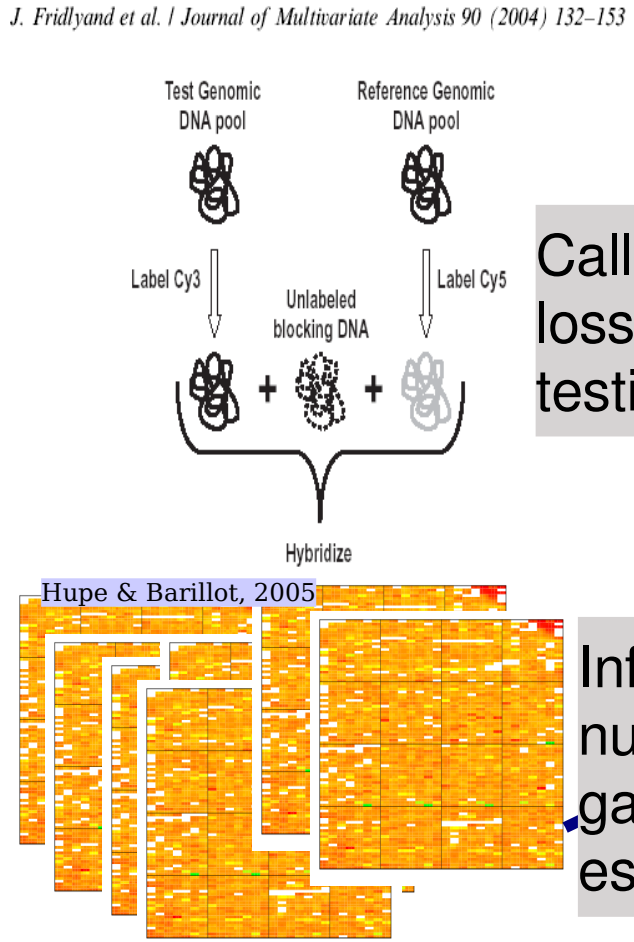

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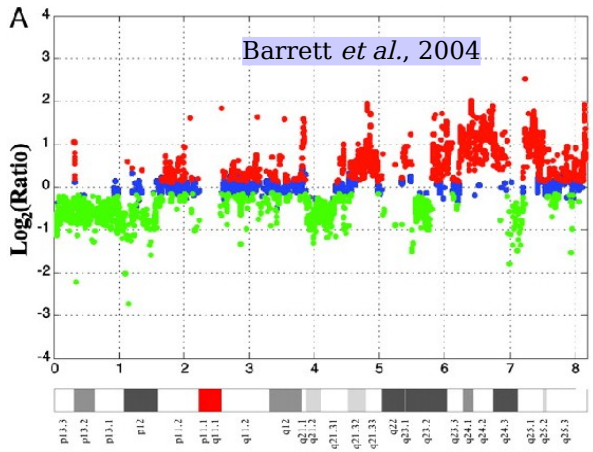

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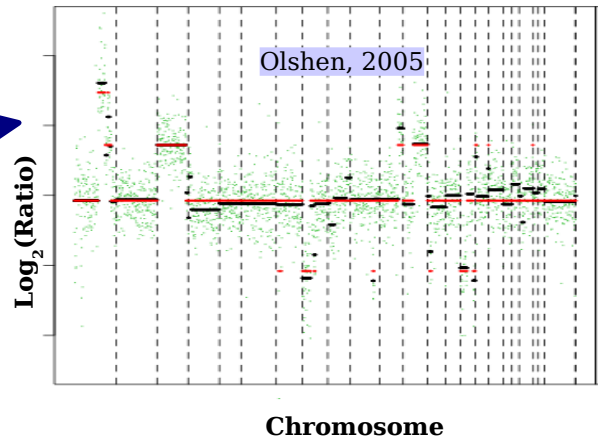

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Store and access (large) pre-computed results

- HMM for aCGH data with Reversible Jump: Viterbi
- Common regions: “count” on the Viterbi paths.

- Fitting HMM/common regions: distinct operations.

- C: number-crunching.
- R: wrapper and figures/tables.
- C: creates large amounts of data.

- In package *RJaCGH* (CRAN).

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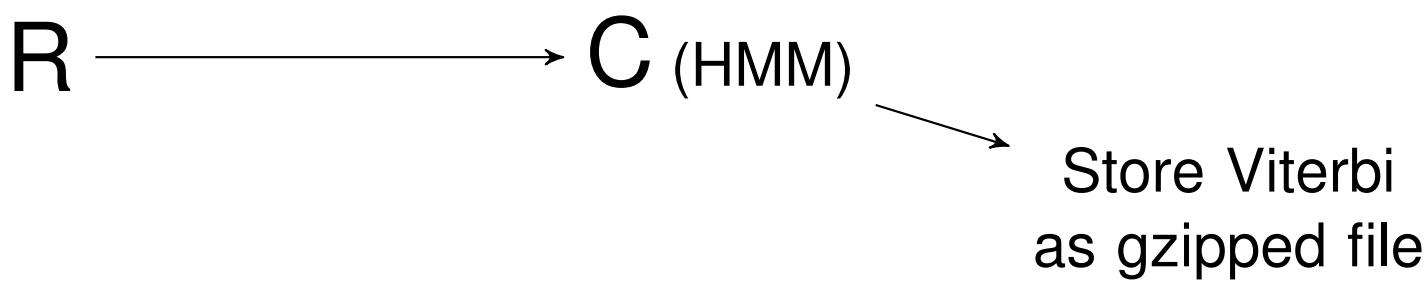
Fit HMM



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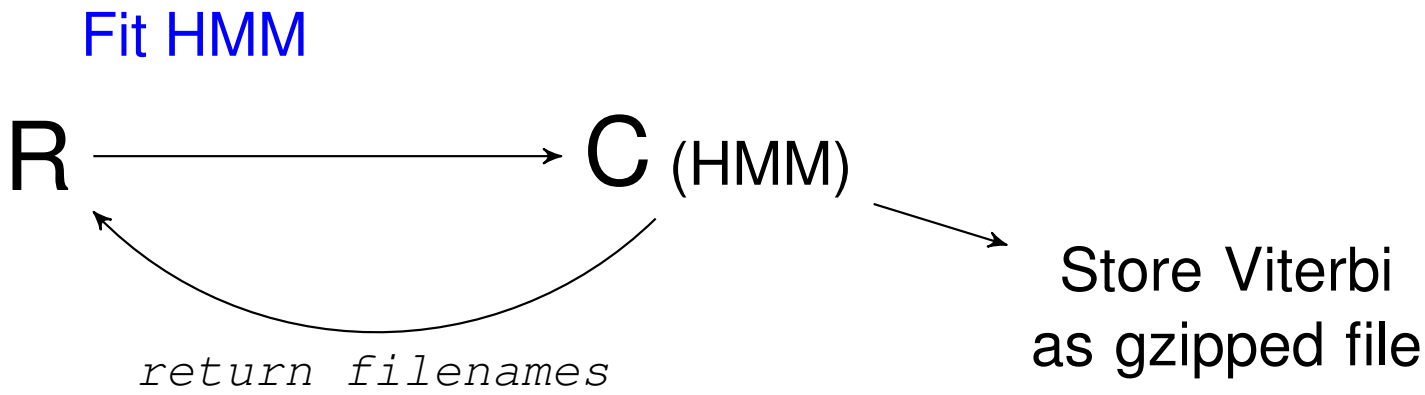

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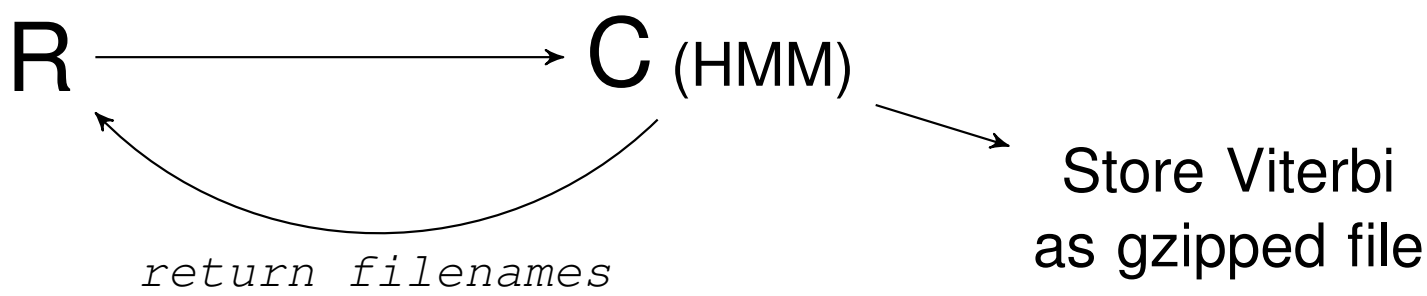
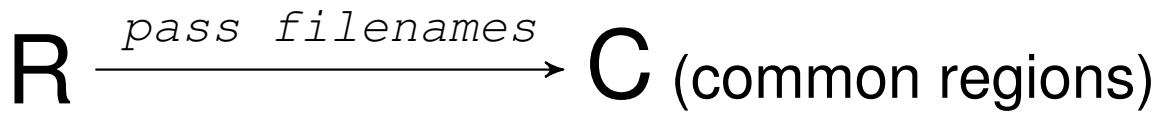


Find common regions



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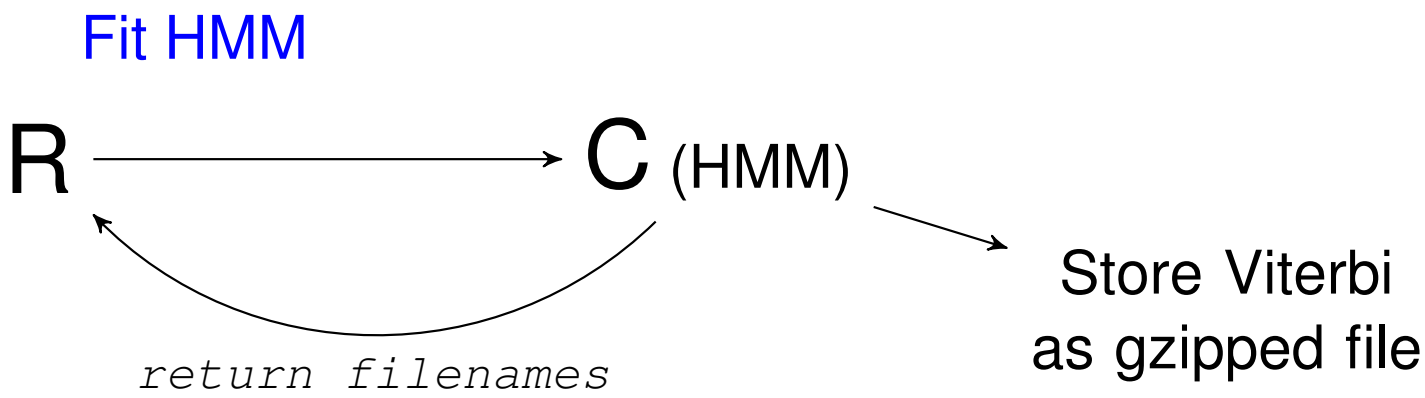

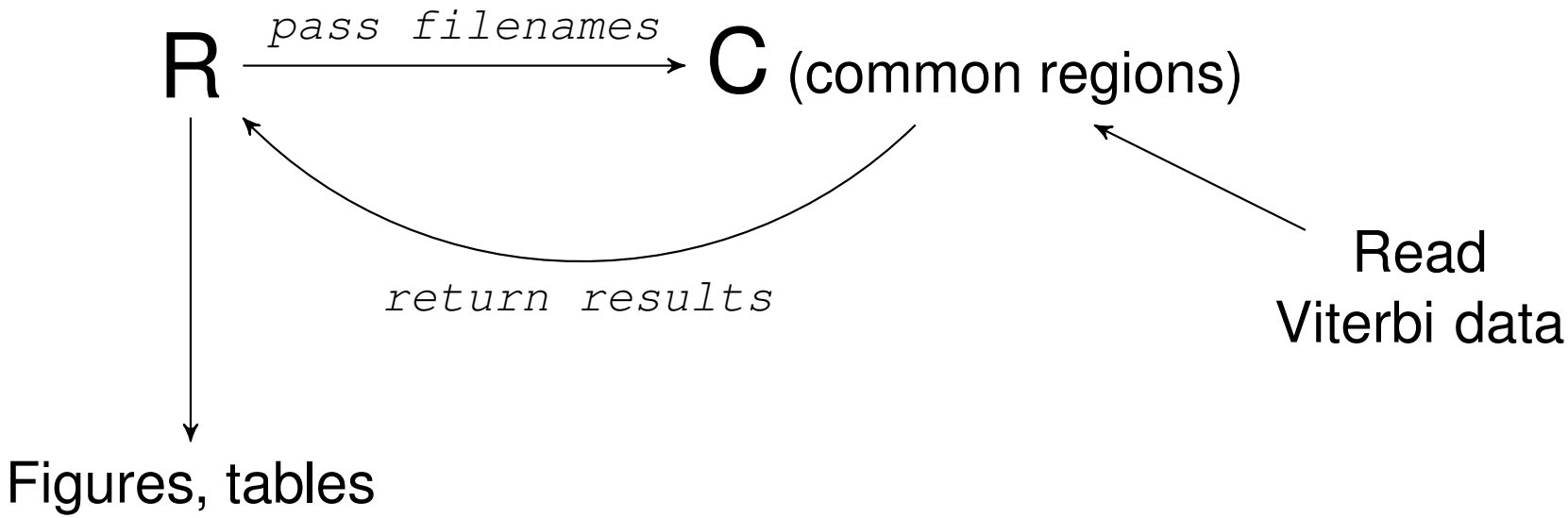

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Web-based: A few things we've learned

- Configuration sucks (if you need to modify $>$ 1 file)
- Too many languages
- Adding test cases to the testing suites: web, R
- Documentation: in the code, web pages, LaTeX ...
- Too much R code to catch errors
- User interfaces: who designs them?

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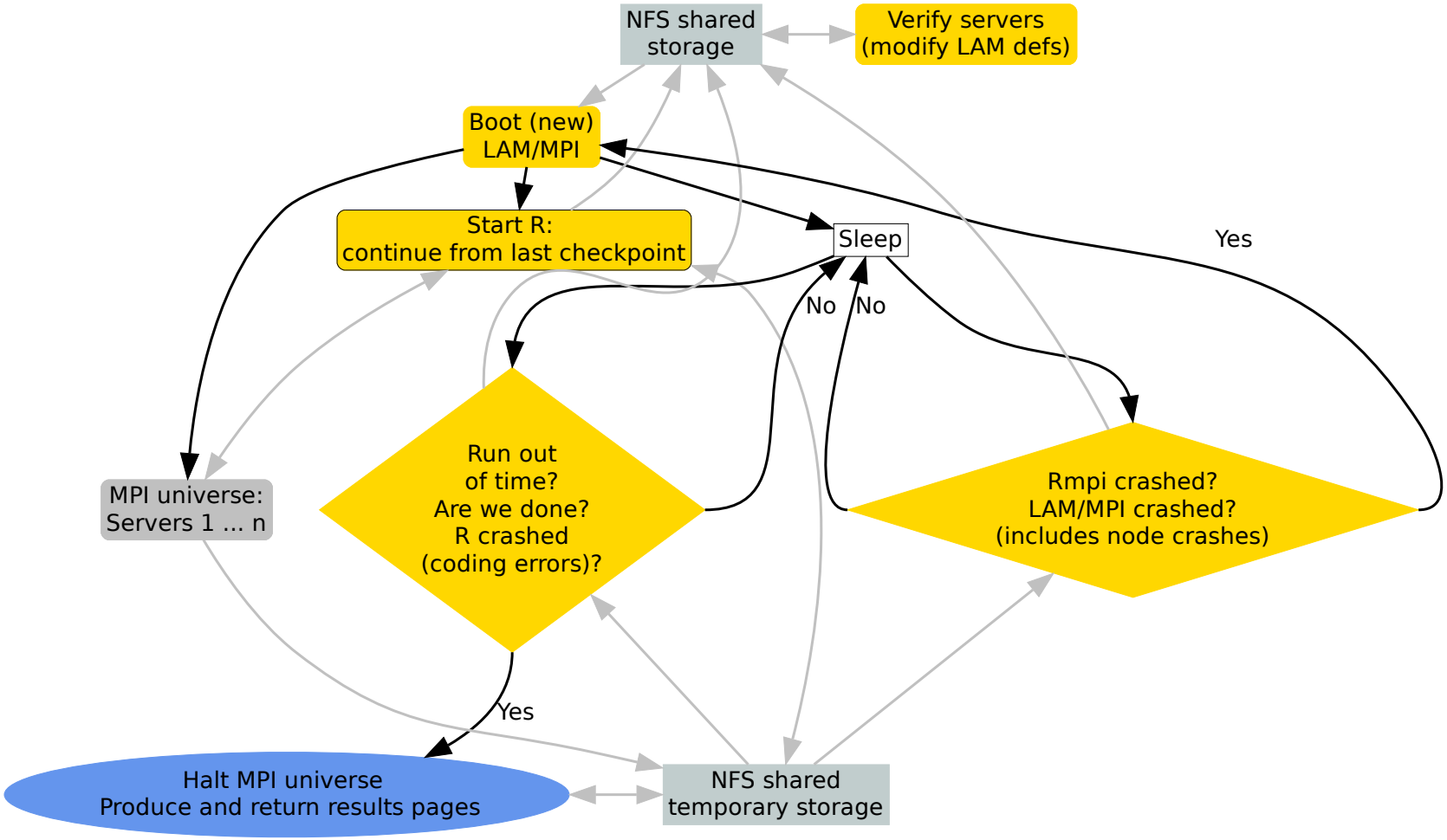
Fault tolerance and communication

- Manual check for errors (R ain't Erlang)
- Too much network traffic



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Solutions?

- Literate programming and org-mode
- Alternatives to MPI and/or use Erlang
- ...
- Keep things as they are (only a few painful events a year)

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Single machine applications

- Run applications in a single, multicore (e.g., 12) machine
- Just verify if the machine is up

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Rethinking web-based applications

- Users can get into trouble.

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Rethinking web-based applications

- Users can get into trouble.

  Sure, but we can do a good job . . .

  - Provide state-of-the art statistical and computational approaches (R ;-)
  - Pedagogical examples and pipelines
  - Minimize the chance of users getting into trouble

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Rethinking web-based applications

- Users can get into trouble.

  Sure, but we can do a good job . . .

  - Provide state-of-the art statistical and computational approaches (R ;-)
  - Pedagogical examples and pipelines
  - Minimize the chance of users getting into trouble

- Web-based applications are here to stay

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. . . so . . .

- Forget about them: just write R (plus C, etc) code
- Go for it
  - R will do its job (which is only part of the job)
  - HPC available
  - No problem with large data sets
  - But other tools and work necessary

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Regardless of web-based applications . . .

- Parallel computing can be used routinely
  - (*library(parallel)* in R $\geq$ 2.14.0)
- Large data sets with *ff* + parallelization.

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Acknowledgements

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- CNIO (Spanish National Cancer Research Center).
- The R users and developers for a vibrant statistical computing community and amazing platform.
- The organizing and scientific committees of the III Jornadas de Usuarios de R.

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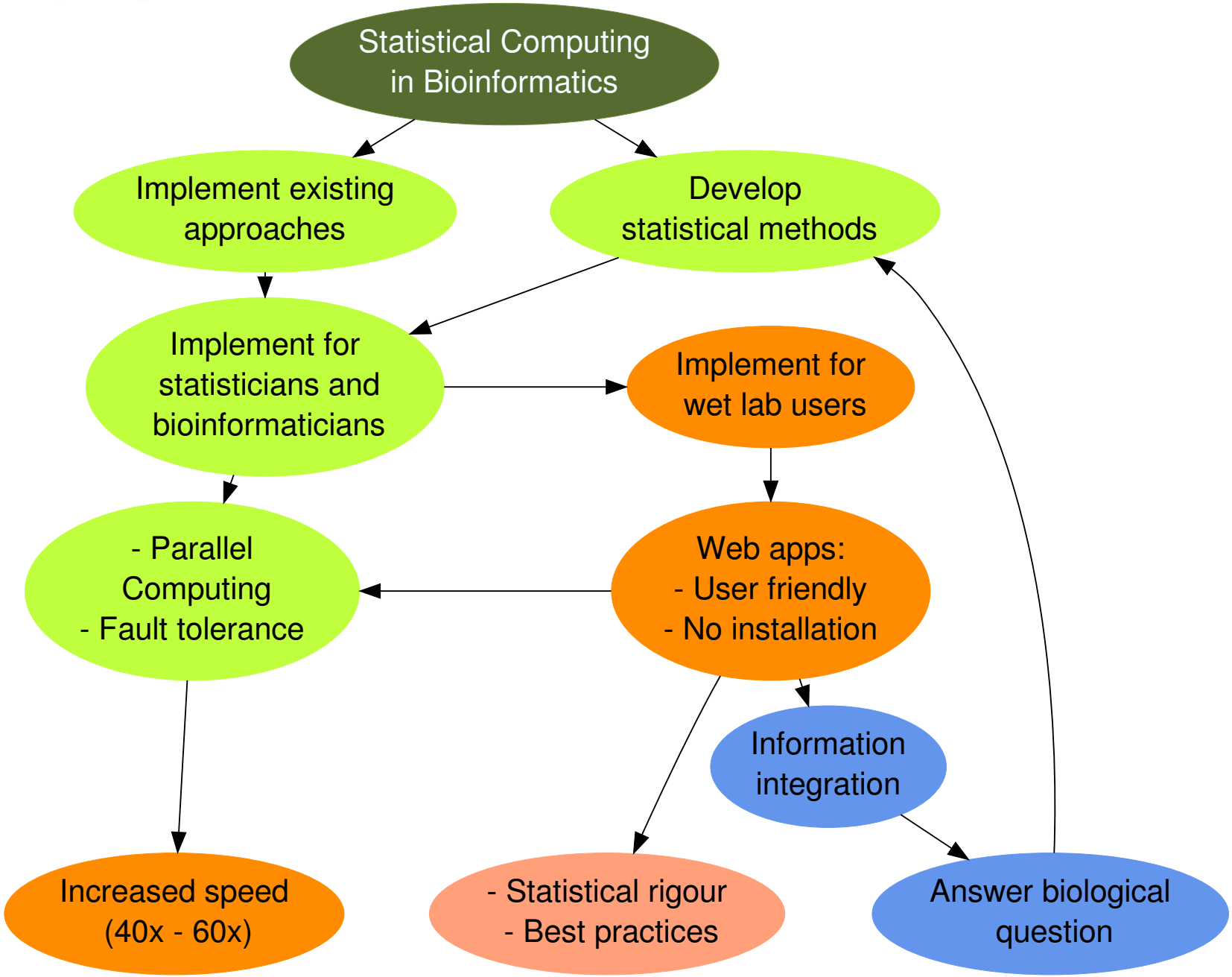
Trying to fit it all



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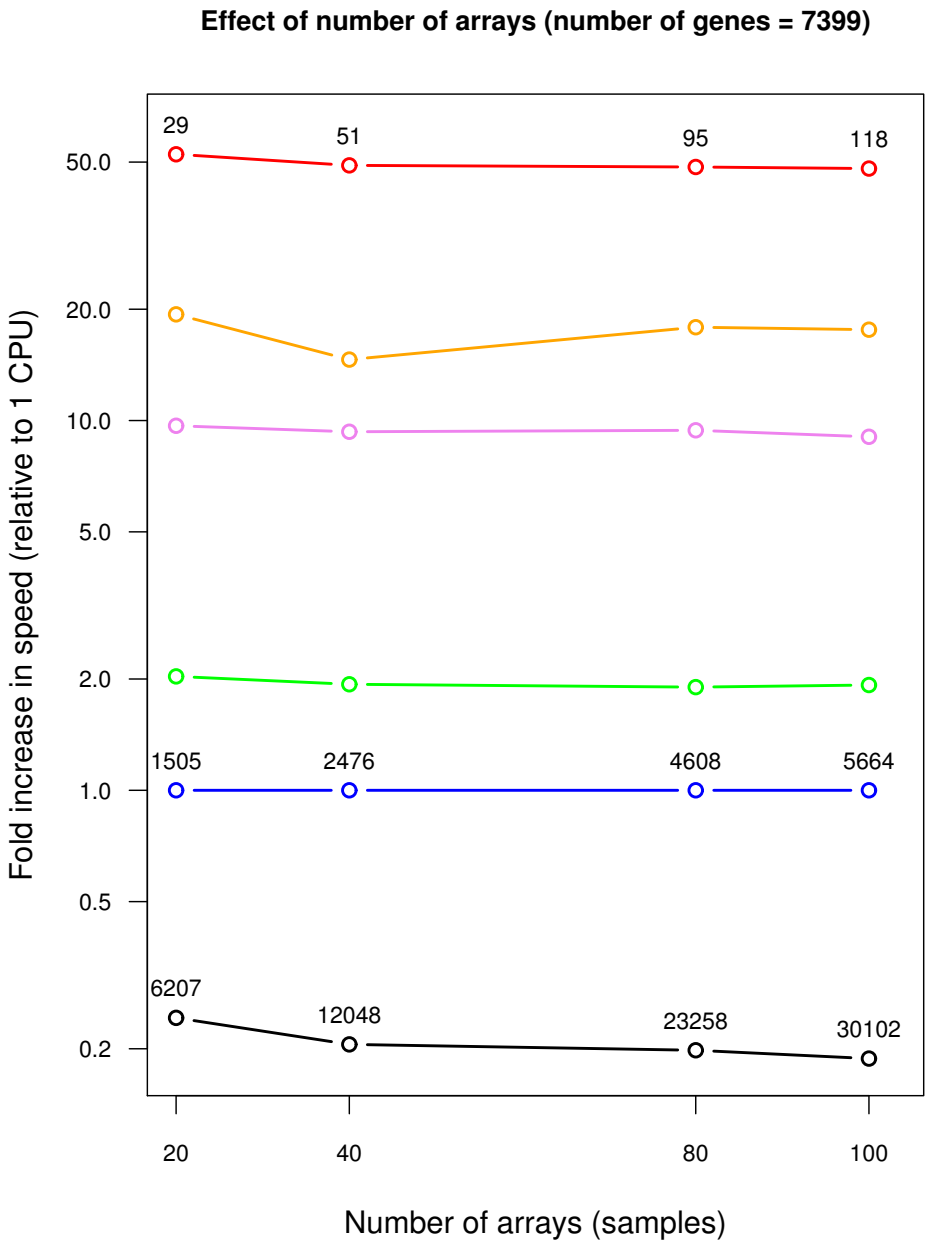

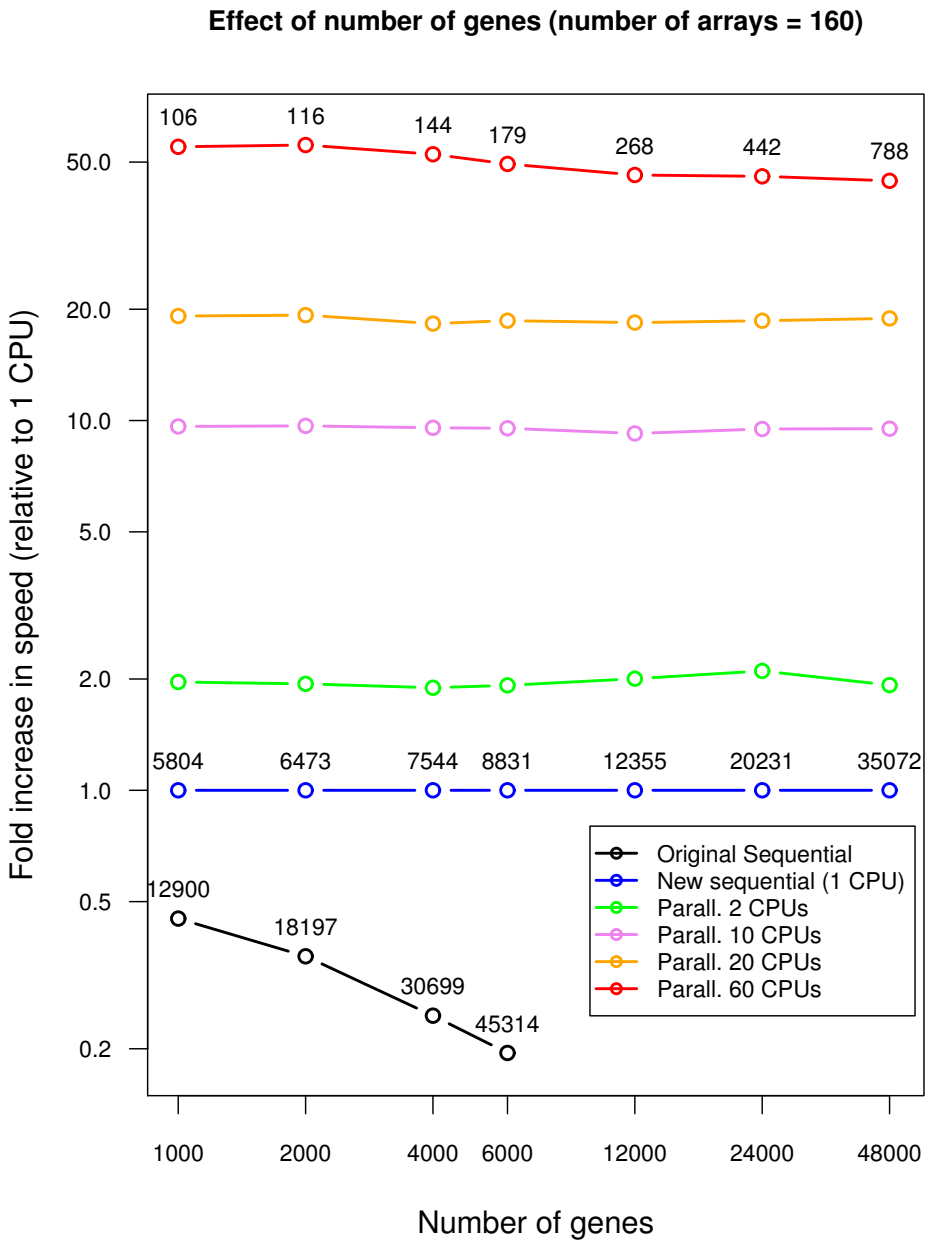

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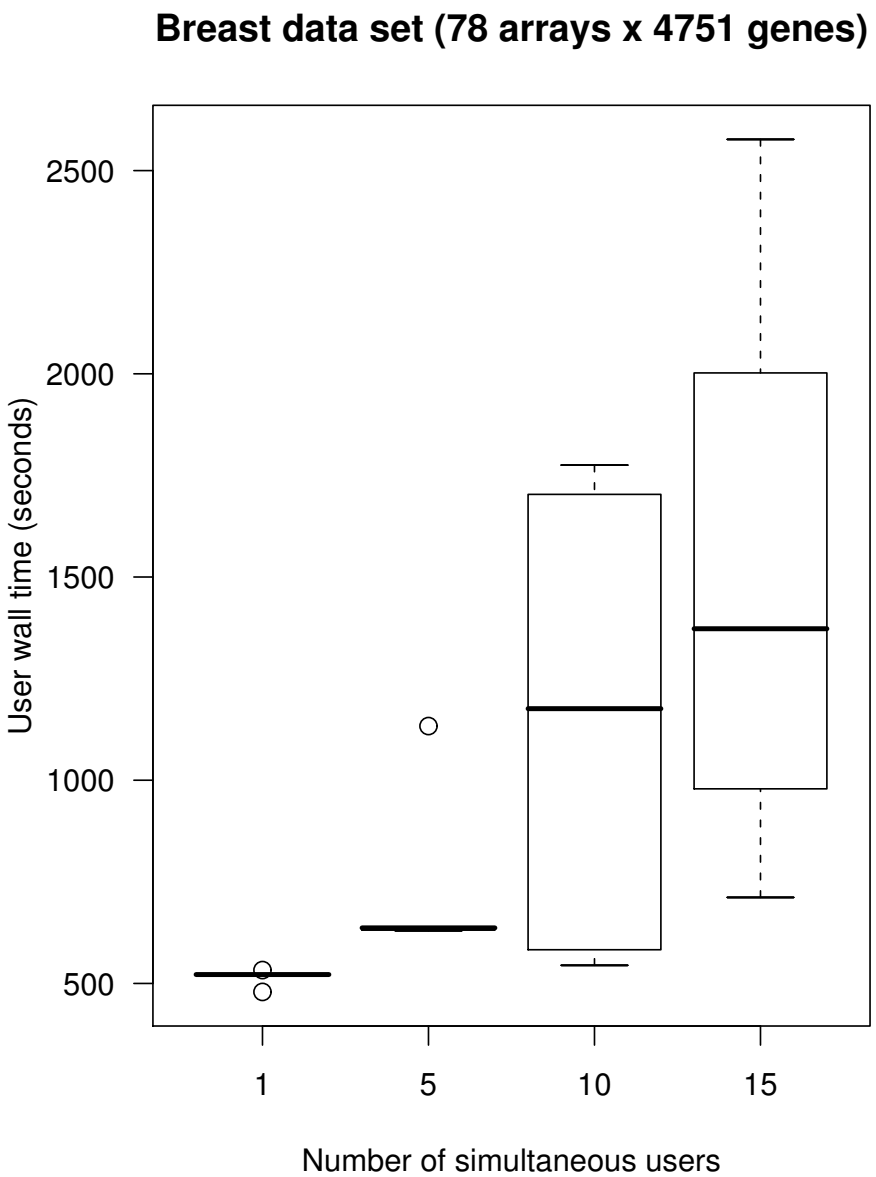

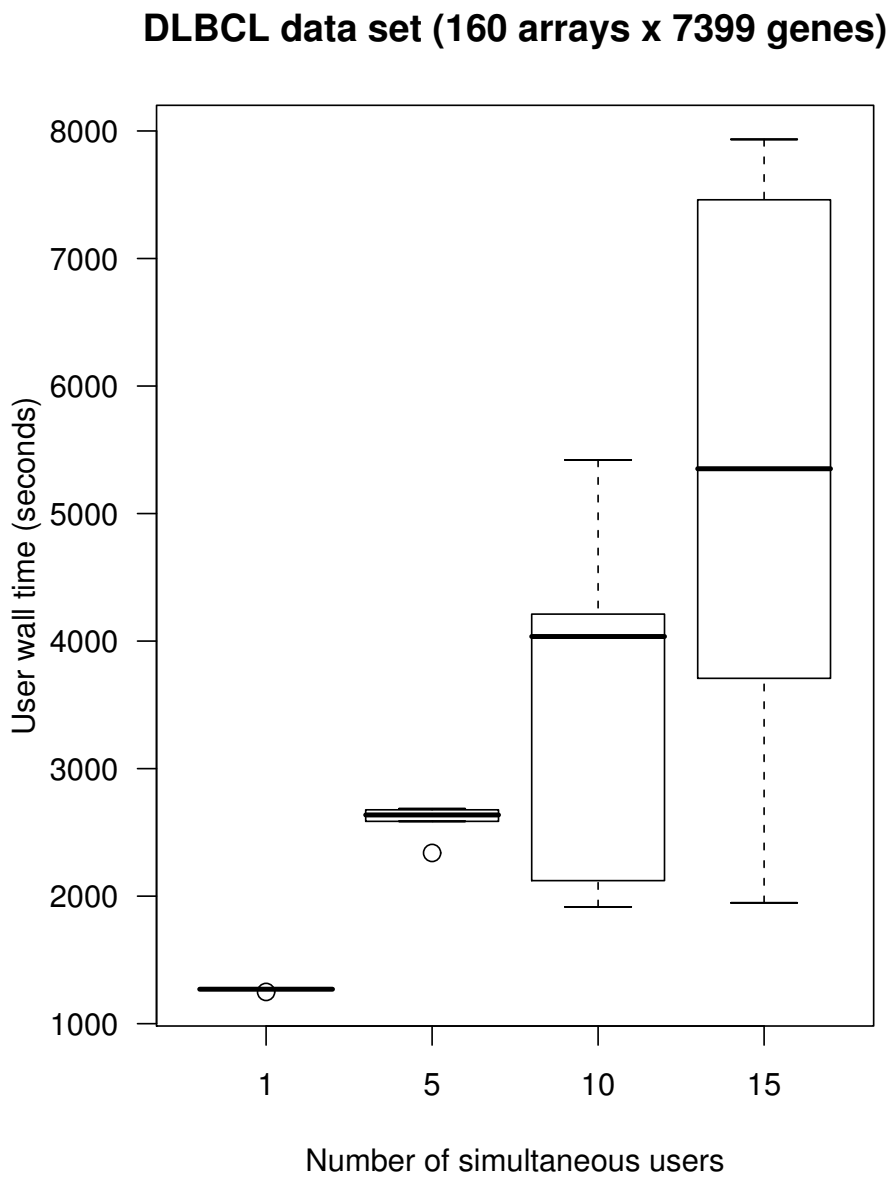

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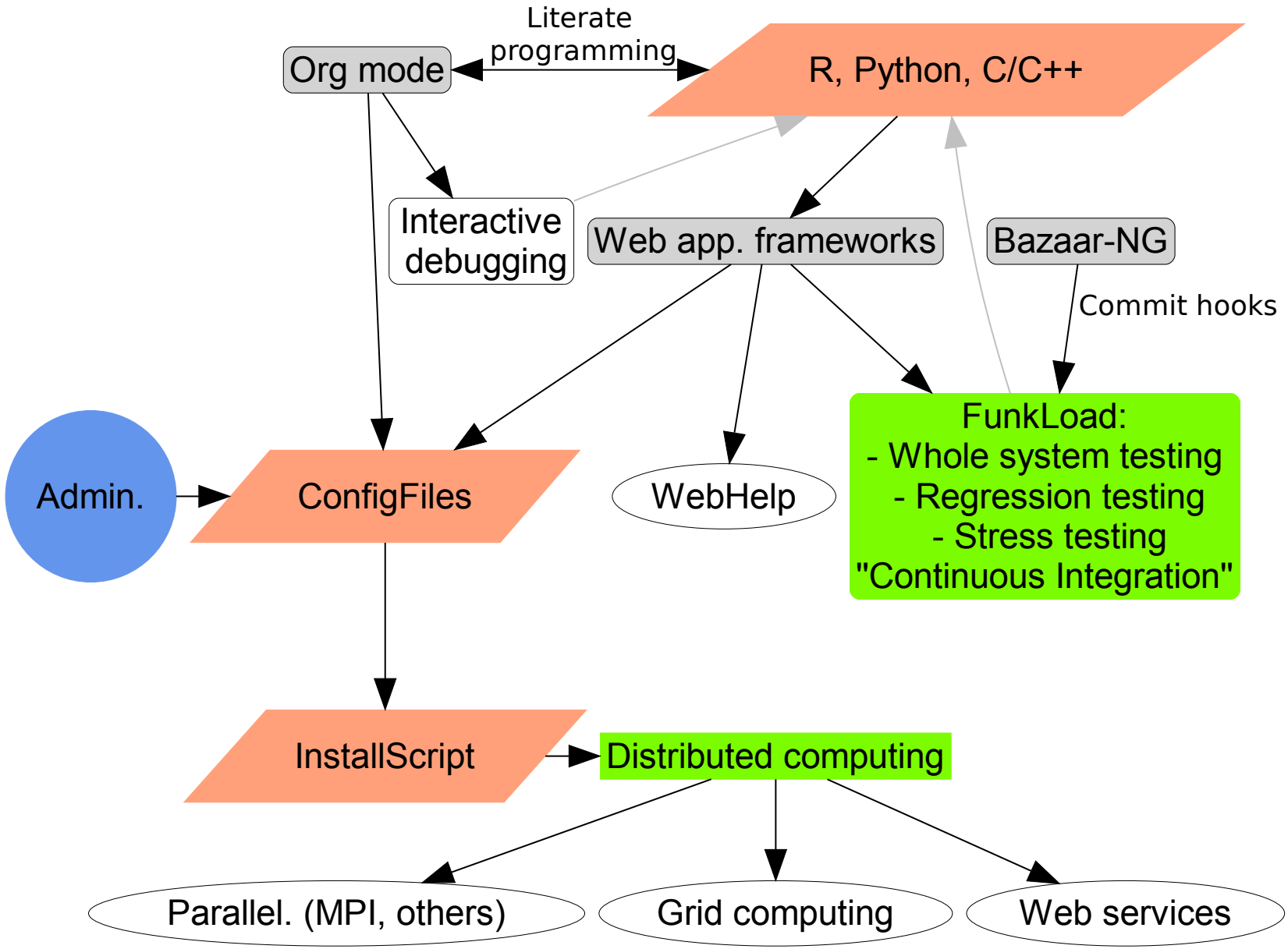
Tools. . .



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Too many languages

Impedance mismatch problem:

"Building Web-based applications requires the mastering of a number of languages/technologies (e.g. HTML, CSS, CGI, ASP, PHP, XML, etc..). Such languages and technologies were created to address different aspects on a by-need evolutionary manner. The result is a plethora of tools that are fitted together in an ad hoc fashion." El-Ansary, Grolaux, Van Roy, Rafea (2005) *"Overcoming the Multiplicity of Languages and Technologies for Web-Based Development Using a Multi-paradigm Approach"*.

- R and C
- HTML and Python: CGI, data entry, display
- Python (and others): control and monitor MPI
- Javascript: AJAX and figures

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Other solutions?

Too many languages Use languages designed to overcome this problem: Hop, Links, QHTML.

Fault tolerance and too much traffic Alternatives to MPI?

- Linda and tuple spaces (also between-language funct.)
- Roll-our-own based on Rserve
- Have Erlang control R processes?