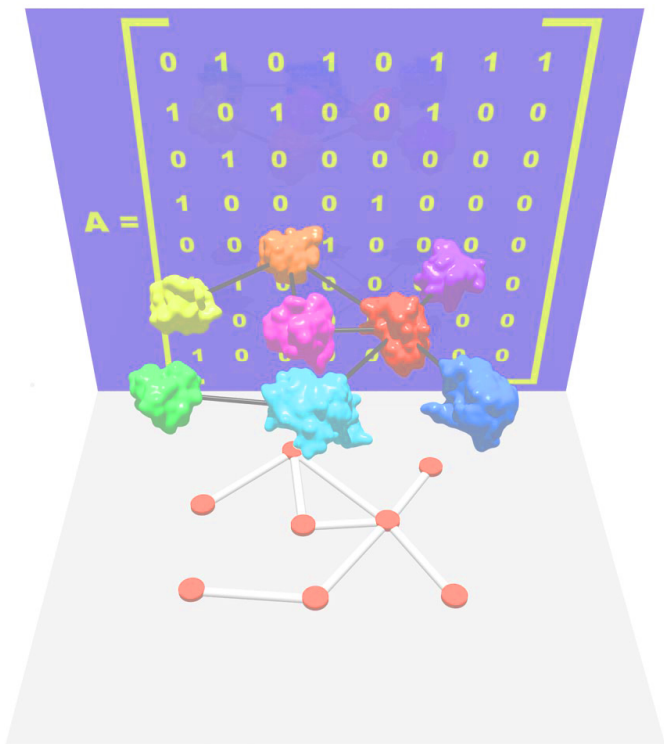
Statistical analysis of network data and evolution on GPUs: High-performance statistical computing



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25/01/2012

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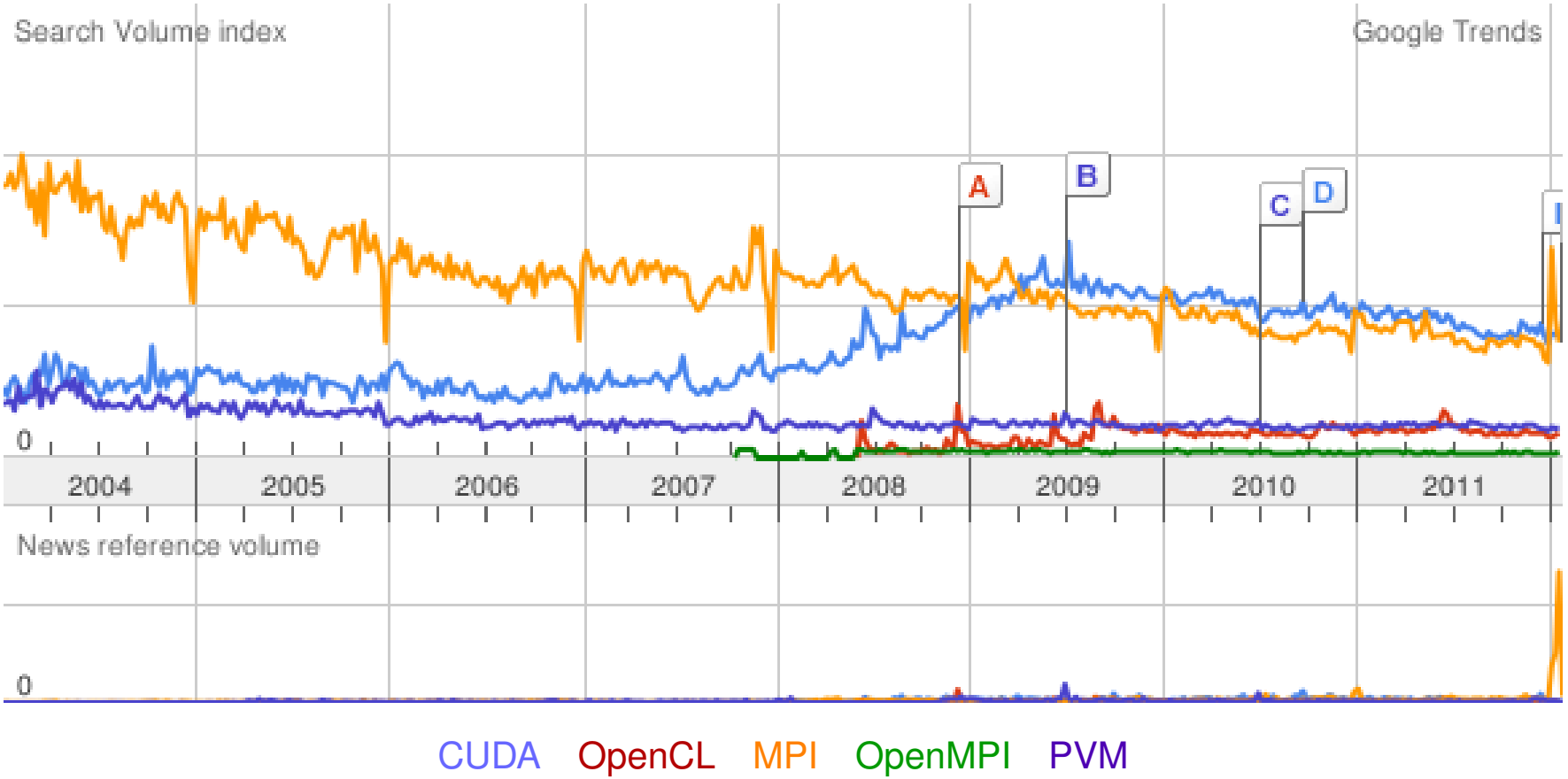
Trends in High-Performance Computing



CUDA OpenCL MPI OpenMPI PVM

(Hidden) Costs of Computing

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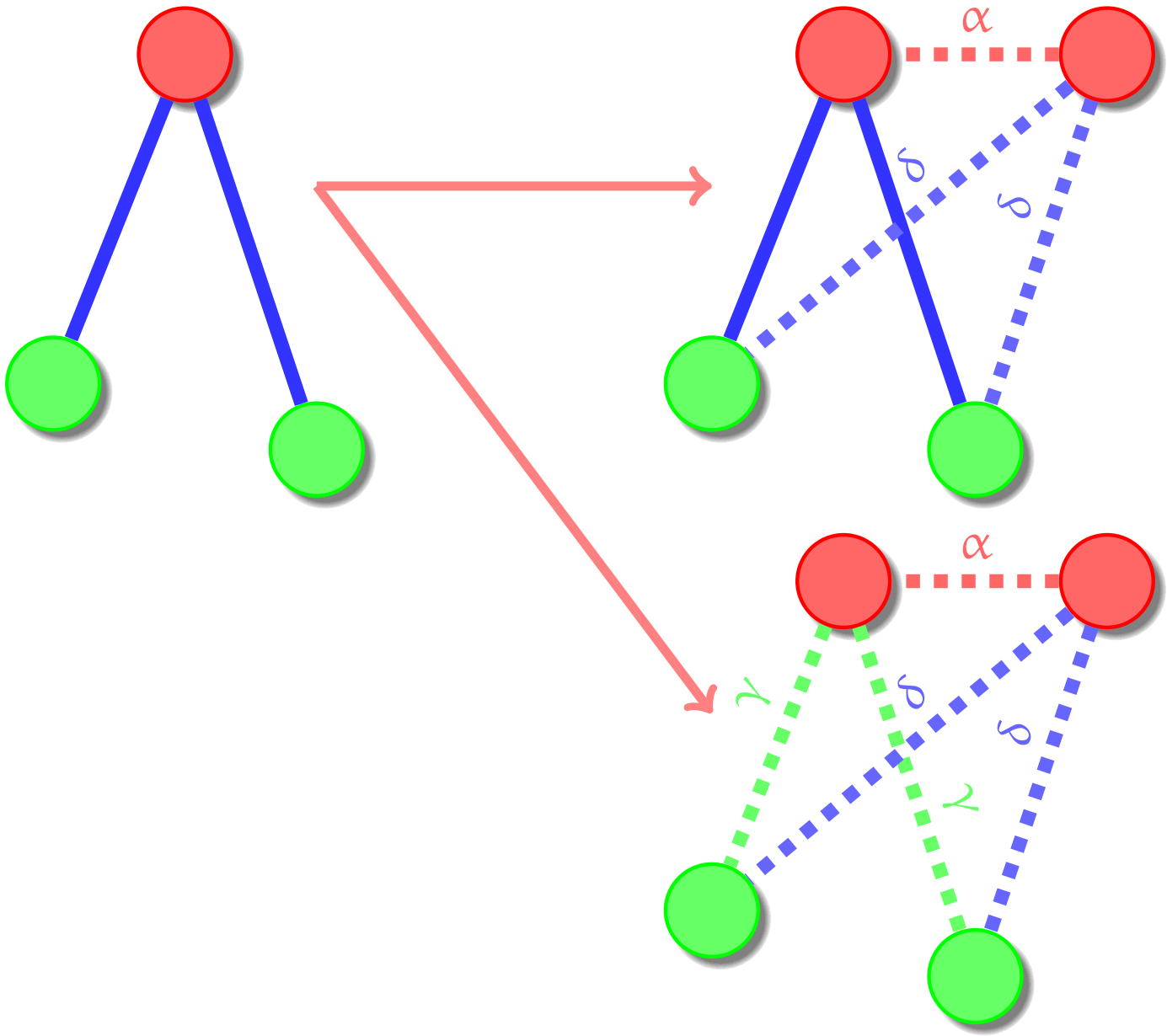
The role of GPUs

- GPUs can be accessed from many different programming languages (e.g. PyCUDA).
- GPUs have a comparatively small footprint and relatively modest energy requirements compared to clusters of CPUs.
- GPUs were designed for consumer electronics: computer gamers have different needs from the HPC community.

Evolving Networks

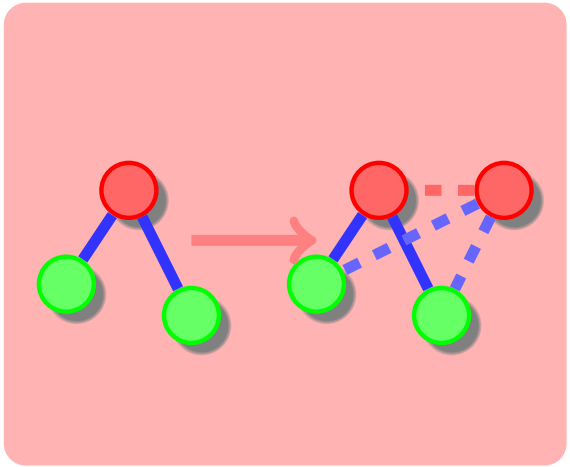


Evolving Networks

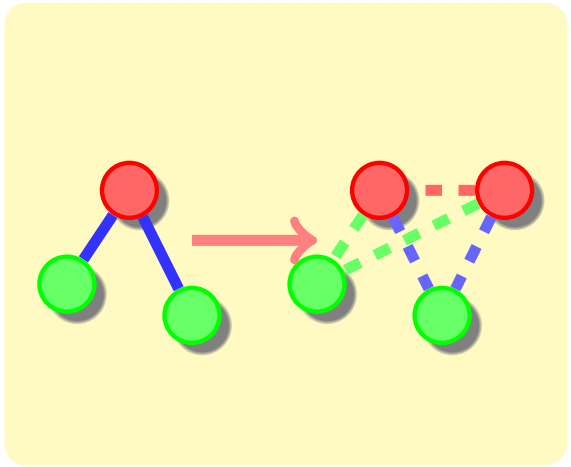
Model-Based Evolutionary Analysis

- For sequence data we use models of nucleotide substitution in order to infer phylogenies in a likelihood or Bayesian framework.
- None of these models — even the general time-reversible model — are particularly realistic; but by allowing for complicating factors e.g. rate variation we capture much of the variability observed across a phylogenetic panel.
- Modes of network evolution will be even more complicated and exhibit high levels of contingency; moreover the structure and function of different parts of the network will be intricately linked.
- Nevertheless we believe that modelling the processes underlying the evolution of networks can provide useful insights; in particular we can study how functionality is distributed across groups of genes.

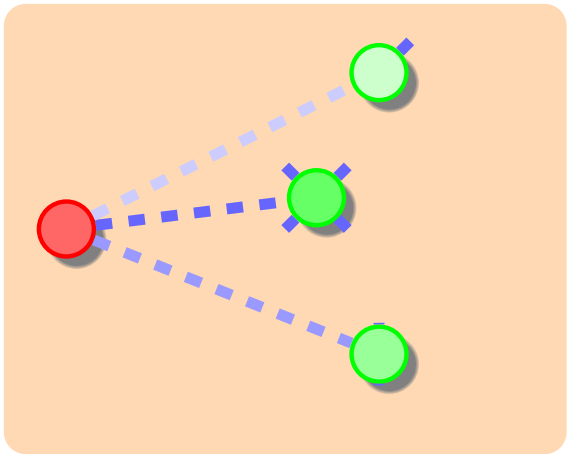
Network Evolution Models



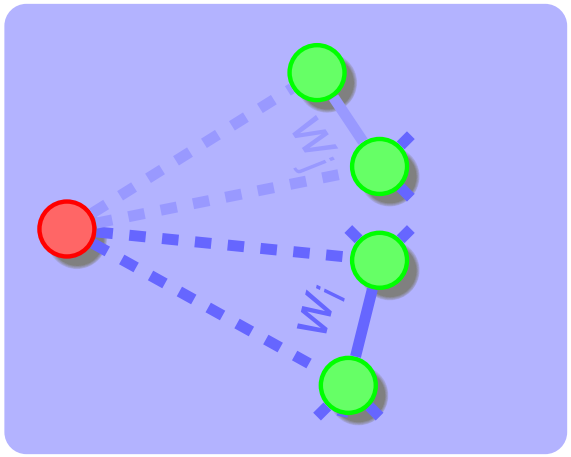
(a) Duplication attachment



(b) Duplication attachment with complimentarity



(c) Linear preferential attachment



(d) General scale-free

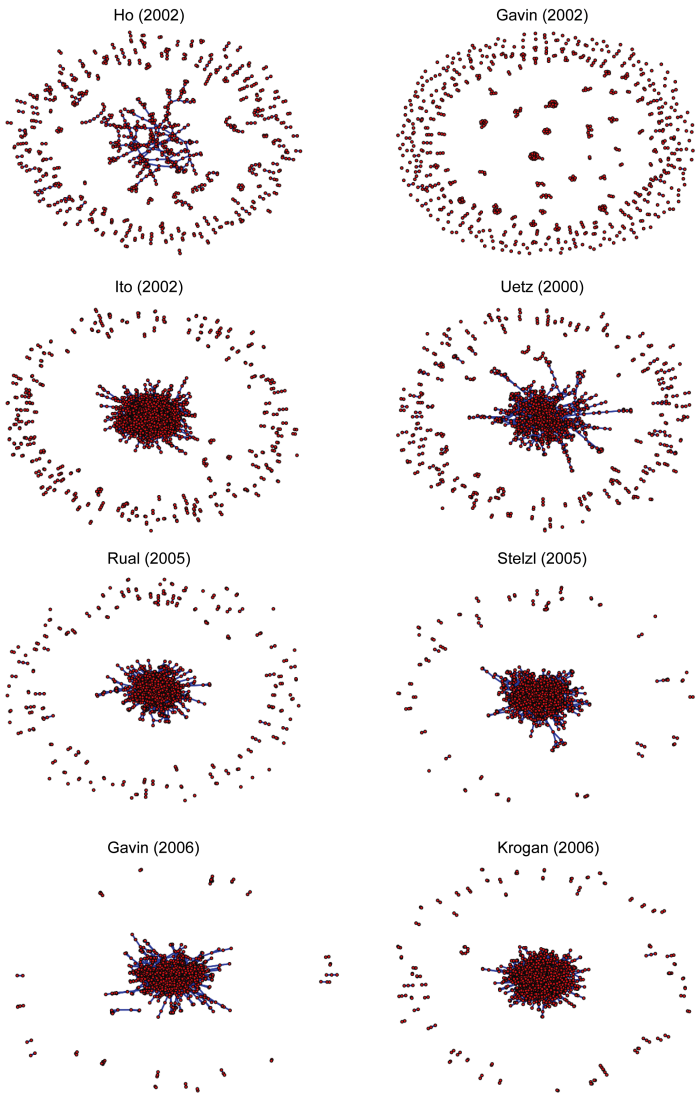
ABC on Networks

Summarizing Networks

- Data are noisy and incomplete.
- We can simulate models of network evolution, but this does not allow us to calculate likelihoods for all but very trivial models.
- There is also no sufficient statistic that would allow us to summarize networks, so ABC approaches require some thought.
- Many possible summary statistics of networks are expensive to calculate.

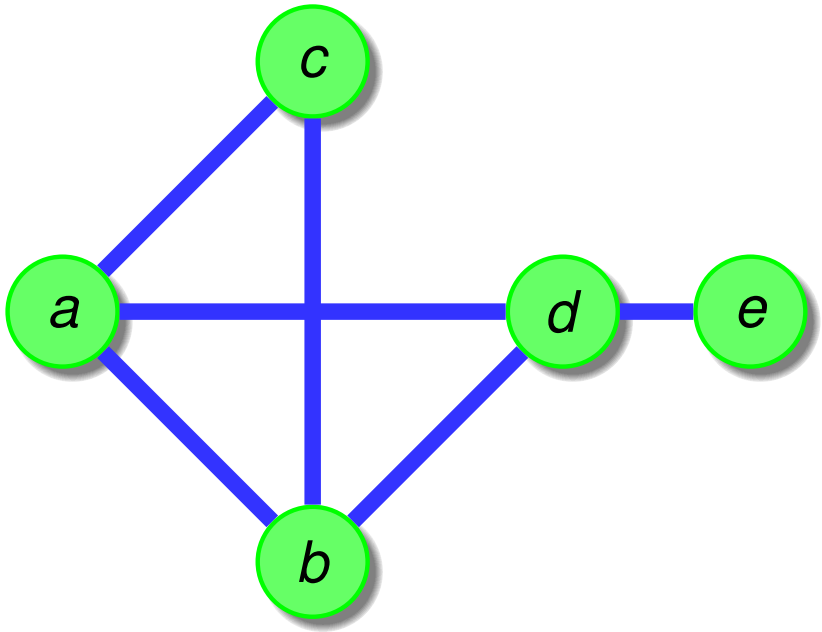
Full likelihood: Wiuf et al., PNAS (2006).

ABC: Ratman et al., PLoS Comp.Biol. (2008).



Stumpf & Wiuf, J. Roy. Soc. Interface (2010).

Graph Spectrum



$$A = \begin{array}{c} \begin{array}{ccccc} a & b & c & d & e \end{array} \\ \begin{pmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \end{array} \begin{array}{c} a \\ b \\ c \\ d \\ e \end{array}$$

Graph Spectra

Given a graph G comprised of a set of nodes N and edges $(i, j) \in E$ with $i, j \in N$, the adjacency matrix, A, of the graph is defined by

$$a_{i,j} = \begin{cases} 1 & \text{if } (i, j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

The eigenvalues, λ, of this matrix provide one way of defining the graph spectrum.

Spectral Distances

A simple distance measure between graphs having adjacency matrices A and B, known as the edit distance, is to count the number of edges that are not shared by both graphs,

$$D(A, B) = \sum_{i,j} (a_{i,j} - b_{i,j})^2.$$

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Given a spectrum (which is relatively cheap to compute) we have

$$D'(A,B) = \sum_{l} \left(\lambda_l^{(\alpha)} - \lambda_l^{(\beta)}\right)^2$$

ABC using Graph Spectra

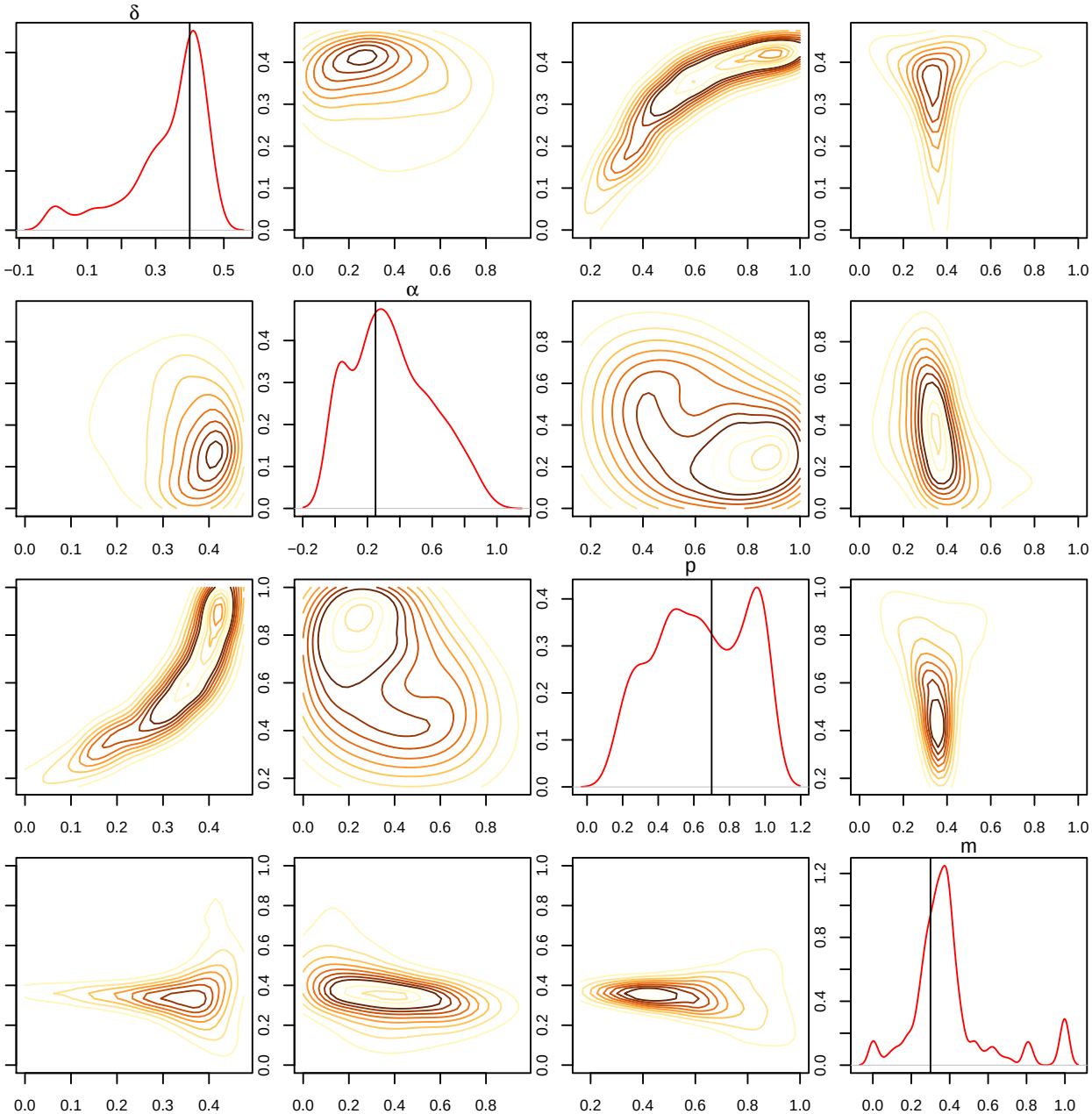
For an observed network, $\mathcal{N}$, and a simulated network, $\mathcal{S}_\theta$, we use the distance between the spectra

$$D'(\mathcal{N}, \mathcal{S}_\theta) = \sum_l \left(\lambda_l^{(\mathcal{N})} - \lambda_l^{(\mathcal{S})}\right)^2,$$

in our ABC SMC procedure. Note that this distance is a close lower bound on the distance between the raw data; we therefore do not have to bother with summary statistics.

Also, calculating graph spectra costs as much as calculating other $O(N^3)$ statistics (such as *all shortest paths*, the *network diameter* or the *within-reach distribution*).

Simulated Data



Protein Interaction Network Data

Species	Proteins	Interactions	Genome size	Sampling fraction
S.cerevisiae	5035	22118	6532	0.77
D. melanogaster	7506	22871	14076	0.53
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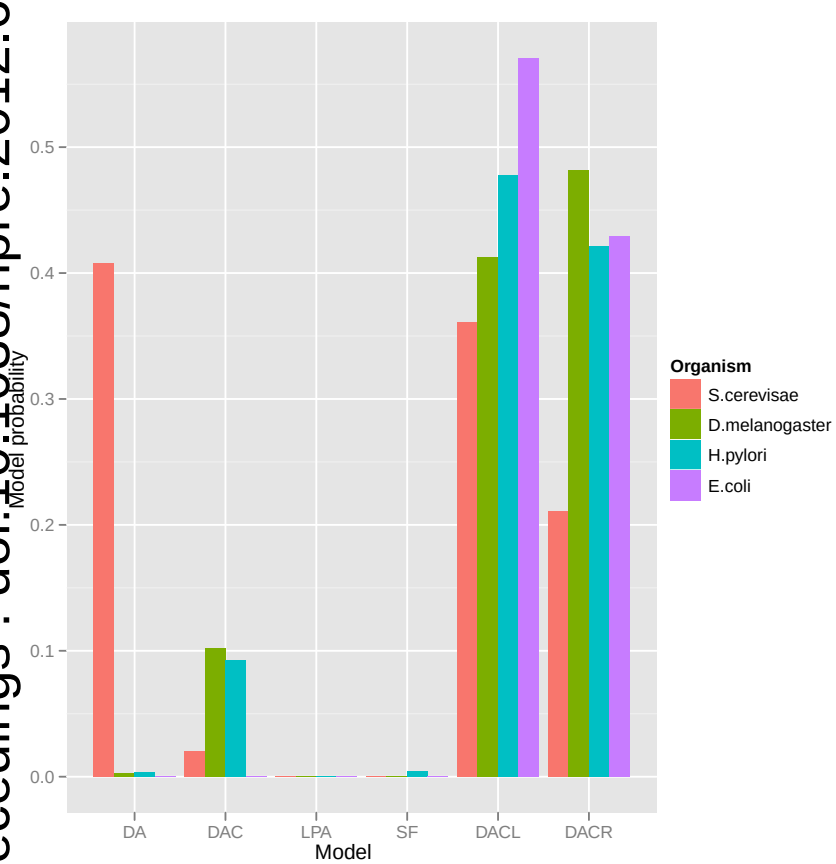

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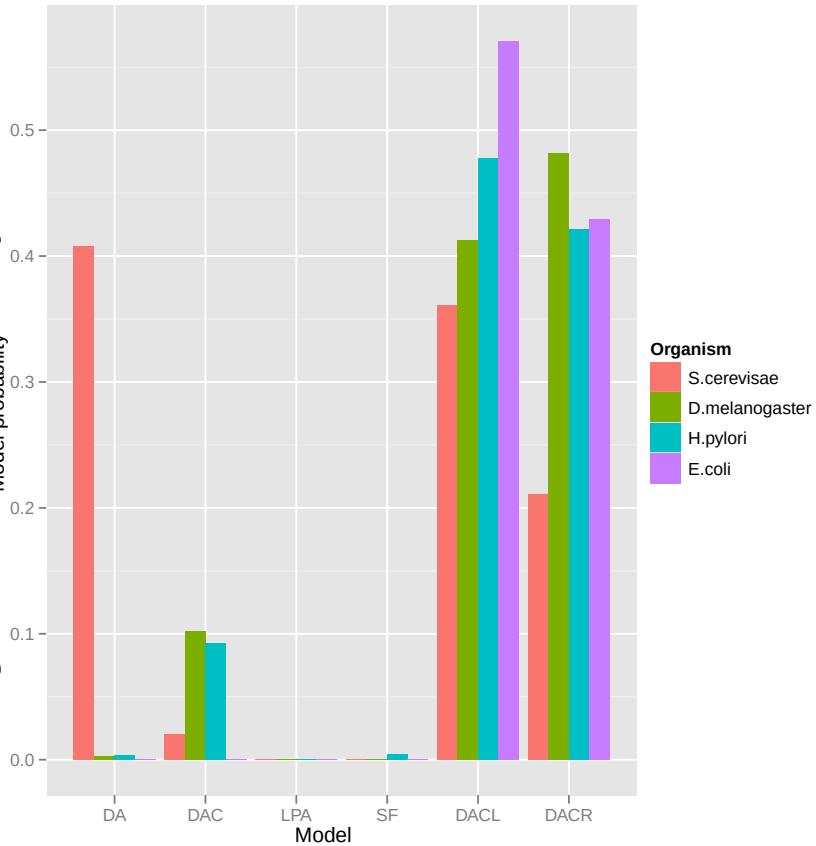

Model Selection

- Inference here was based on all the data, not summary statistics.
- Duplication models receive the strongest support from the data.
- Several models receive support and no model is chosen unambiguously.

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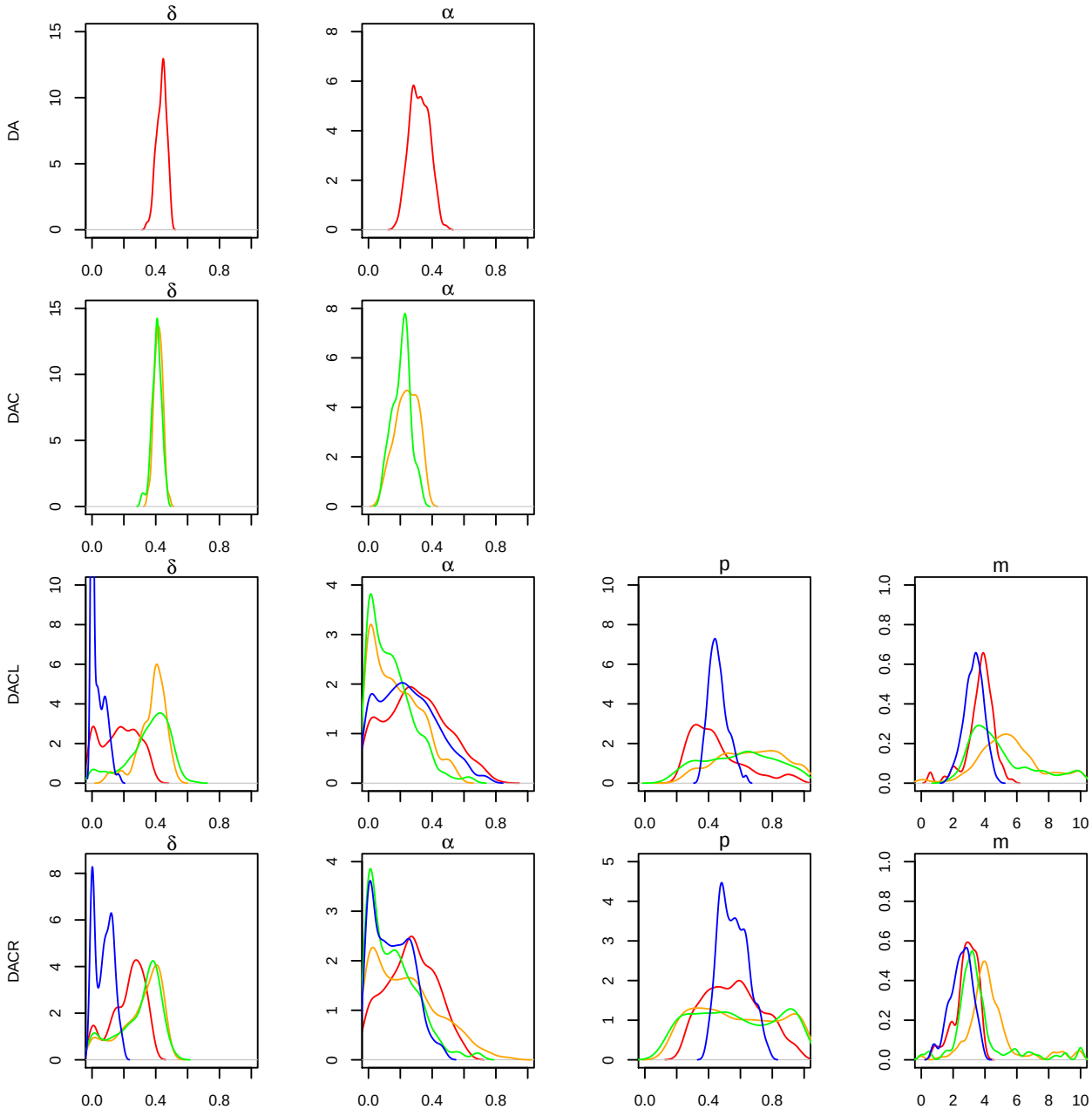

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GPUs in Computational Statistics

Performance

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- GPU hardware was initially conceived for different purposes — computer gamers need fewer random numbers than MCMC or SMC procedures. The address space accessible to single-precision numbers also suffices to kill zombies etc .

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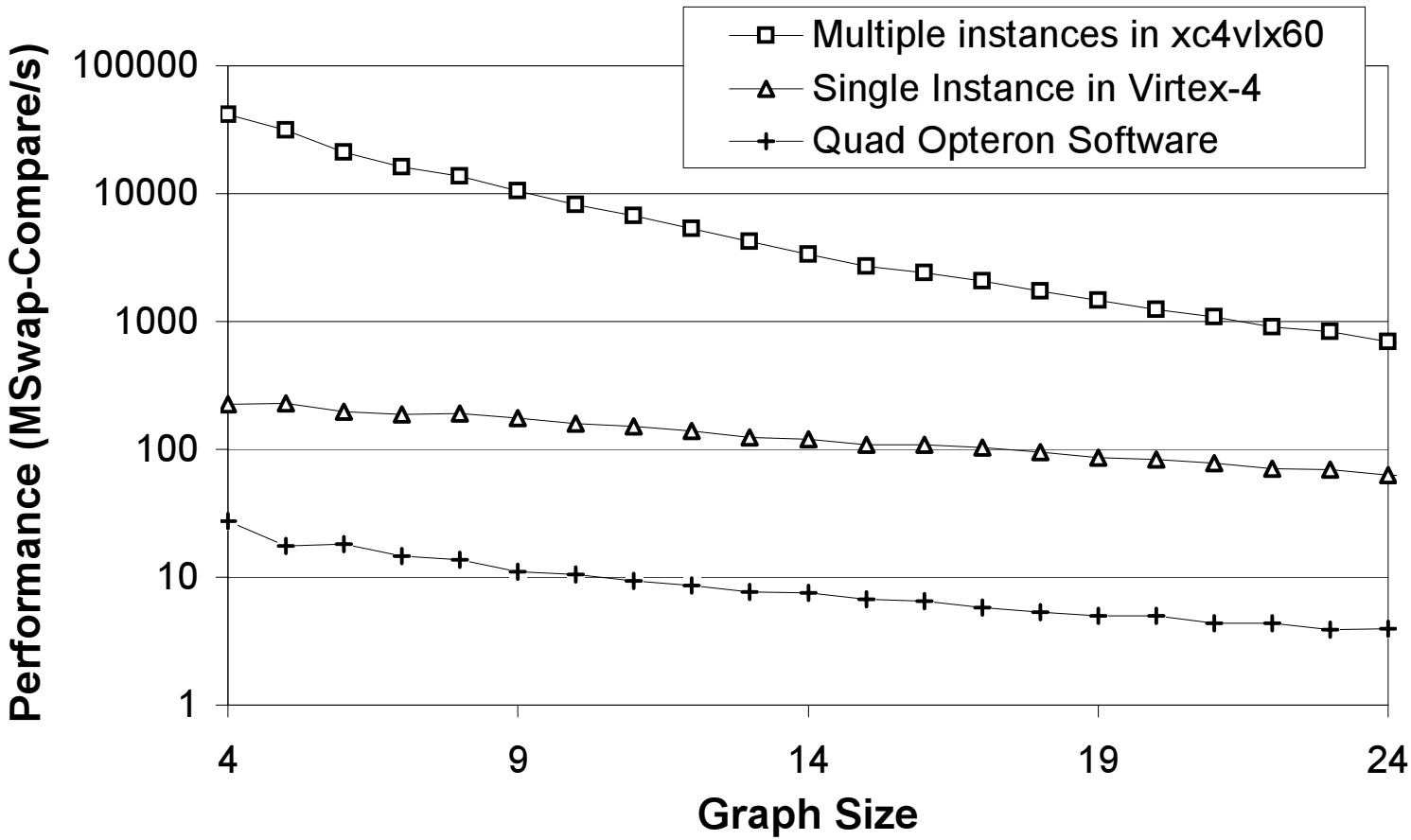
- Combining several GPUs requires additional work, using e.g. MPI.

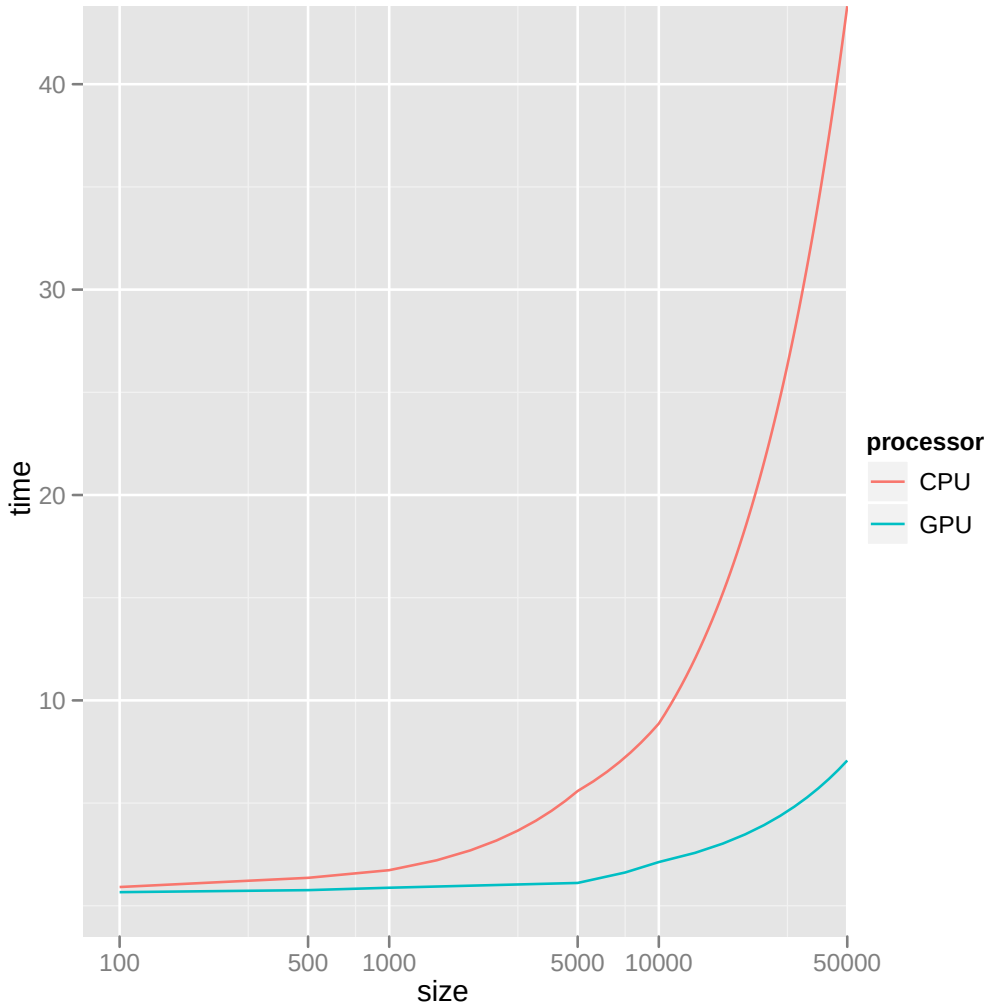
Alternatives to GPUs: FPGAs

Field Programmable Gate Arrays are configurable electronic circuits that are partly (re)configurable. Here the hardware is adapted to the problem at hand and encapsulates the programme in its programmable logic arrays.



Alternatives to GPUs: CPUs (and MPI. . .)

CPUs with multiple cores are flexible, have large address spaces and a wealth of flexible numerical routines. This makes implementation of numerically demanding tasks relatively straightforward. In particular there is less of an incentive to consider how a problem is best implemented in software that takes advantage of hardware features.



6-core Xeon vs M2050 (448 cores) programmed in OpenCL

(Pseudo) Random Numbers

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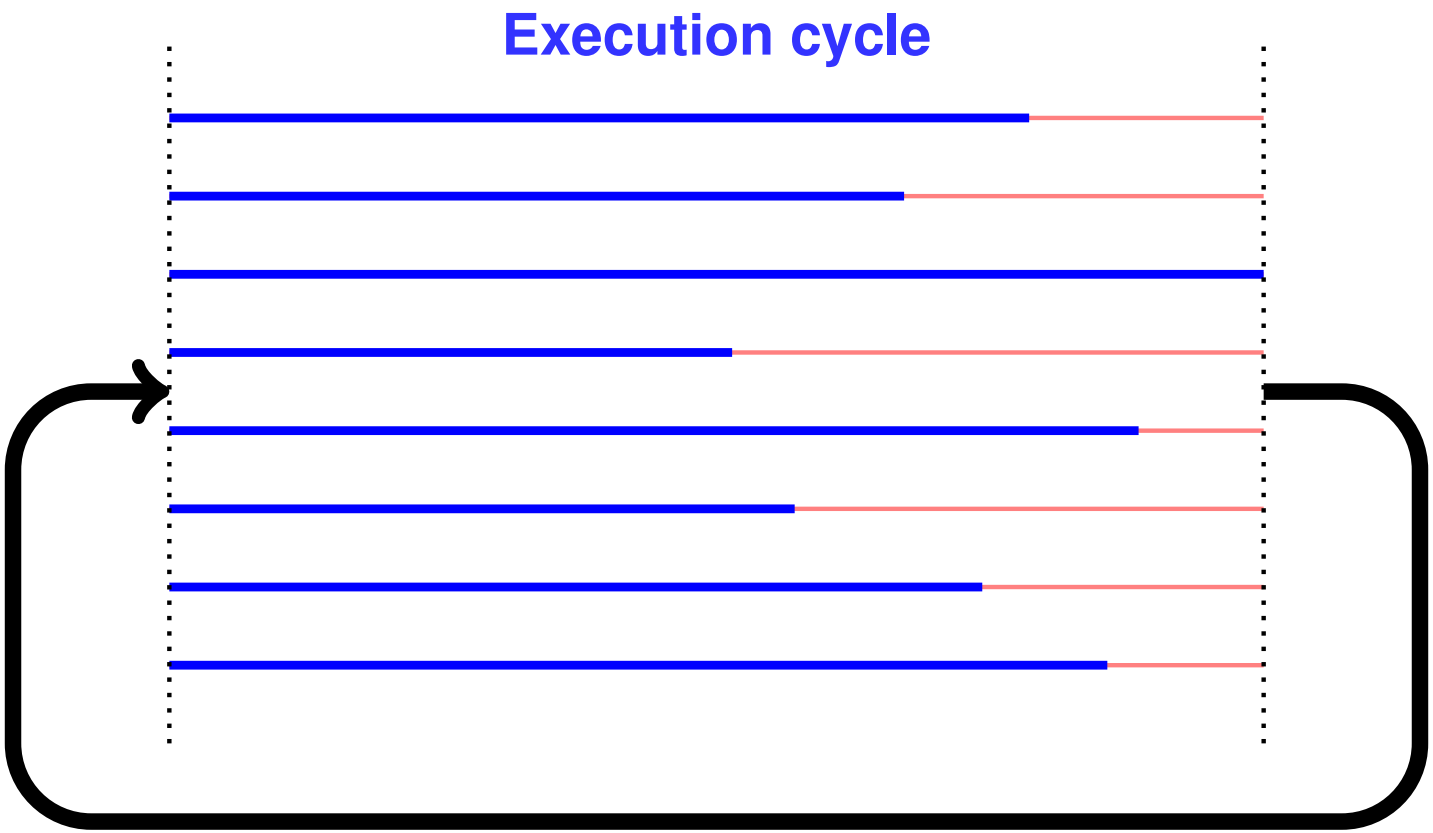
Parallel Random Number Generation

- Running RNGs in parallel does not produce reliable sets of random numbers.
- We need algorithms produce large numbers of parallel streams of "good" random numbers.
- We also need better algorithms for weighted sampling.

What GPUs are Good At

- GPUs are good for linear threads involving mathematical functions.
- We should avoid loops and branches in the code.
- In an optimal world we should aim for all threads to finish at the same time.



Generating RNGs in Parallel

We assume that we have a function $x_{n+1} = f(x_n)$ which generates a stream of (pseudo) random numbers

$$x_0, x_1, x_2, \ldots, x_r, \ldots, x_s, \ldots, x_t, \ldots, x_z$$

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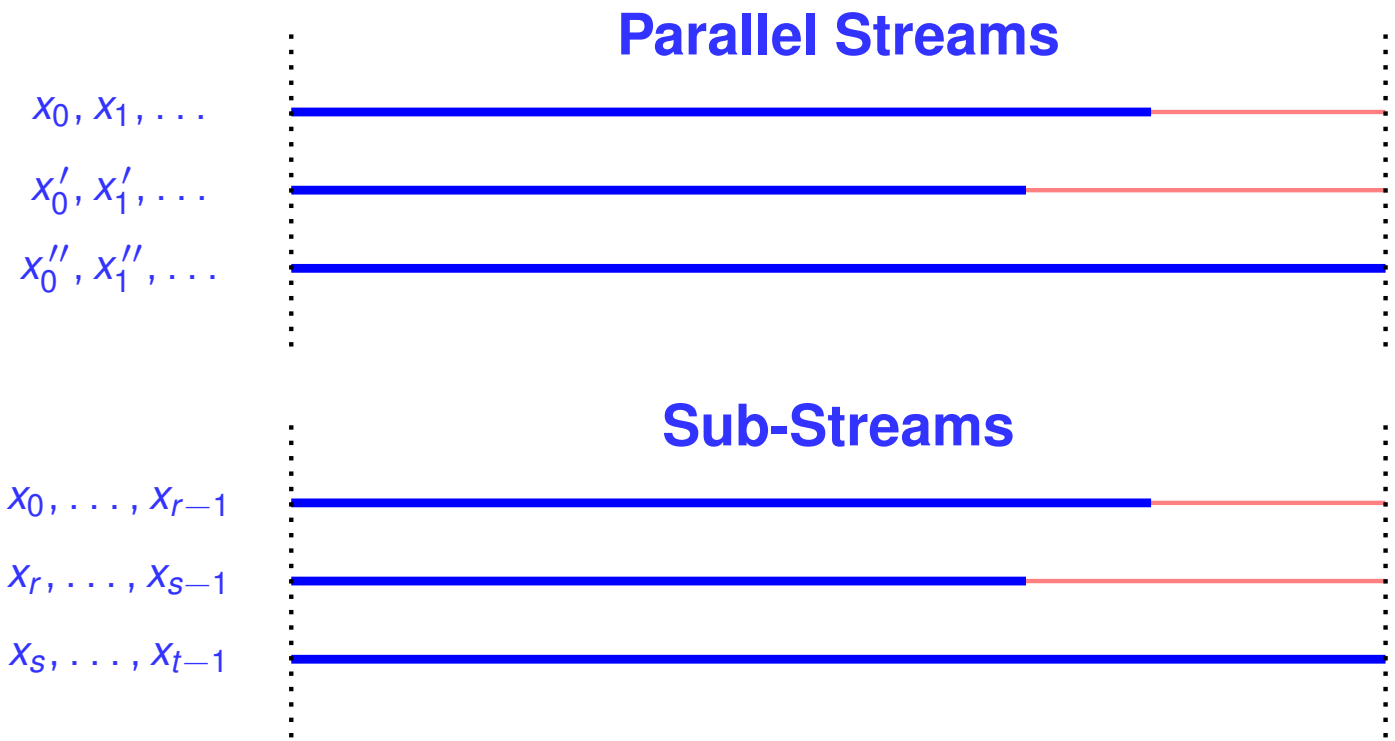

Counter-Based RNGs

We can represent RNGs as state-space processes,

$$y_{n+1} = f(y_n) \quad \text{with} \quad f : Y \longrightarrow Y$$
$$x_{n+1} = g_{k,n \bmod J}(y_{\lfloor n+1/J \rfloor}) \quad \text{with} \quad g : Y \times \mathcal{K} \times \mathbb{Z}_J \longrightarrow X,$$

where x are essentially behaving as $x \sim \mathcal{U}_{[0,1]}$; here $\mathcal{K}$ is the key space, J the number of random numbers generated from the internal state of the RNG.

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For a sufficiently complex bijection b_k we can use simple updates and leave the randomization to b_k. Here cryptographic routines come in useful.

RNG Performance on CPUs and GPUs

Method	Max. input	Min. state	Output size	Intel CPU cpB	Intel CPU GB/s	Nvidia GPU cpB	Nvidia GPU GB/s	AMD GPU cpB	AMD GPU GB/s
Counter-based, Cryptographic									
AES(sw)	(1+0)×16	11×16	1×16	31.2	0.4	–	–	–	–
AES(hw)	(1+0)×16	11×16	1×16	**1.7**	**7.2**	–	–	–	–
Threefish (Threefry-4×64-72)	(4+4)×8	0	4×8	7.3	1.7	51.8	15.3	302.8	4.5
Counter-based, Crush-resistant									
ARS-5(hw)	(1+1)×16	0	1×16	0.7	17.8	–	–	–	–
ARS-7(hw)	(1+1)×16	0	1×16	**1.1**	**11.1**	–	–	–	–
Threefry-2×64-13	(2+2)×8	0	2×8	2.0	6.3	13.6	58.1	25.6	52.5
Threefry-2×64-20	(2+2)×8	0	2×8	2.4	5.1	15.3	51.7	30.4	44.5
Threefry-4×64-12	(4+4)×8	0	4×8	1.1	11.2	9.4	84.1	15.2	90.0
Threefry-4×64-20	(4+4)×8	0	4×8	**1.9**	**6.4**	15.0	52.8	29.2	46.4
Threefry-4×32-12	(4+4)×4	0	4×4	2.2	5.6	9.5	83.0	12.8	106.2
Threefry-4×32-20	(4+4)×4	0	4×4	3.9	3.1	15.7	50.4	25.2	53.8
Philox2×64-6	(2+1)×8	0	2×8	2.1	5.9	8.8	90.0	37.2	36.4
Philox2×64-10	(2+1)×8	0	2×8	4.3	2.8	14.7	53.7	62.8	21.6
Philox4×64-7	(4+2)×8	0	4×8	2.0	6.0	8.6	92.4	36.4	37.2
Philox4×64-10	(4+2)×8	0	4×8	3.2	3.9	12.9	61.5	54.0	25.1
Philox4×32-7	(4+2)×4	0	4×4	2.4	5.0	3.9	201.6	12.0	113.1
Philox4×32-10	(4+2)×4	0	4×4	3.6	3.4	**5.4**	**145.3**	**17.2**	**79.1**
Conventional, Crush-resistant									
MRG32k3a	0	6×4	1000×4	3.8	3.2	–	–	–	–
MRG32k3a	0	6×4	4×4	20.3	0.6	–	–	–	–
MRGk5-93	0	5×4	1×4	7.6	1.6	9.2	85.5	–	–
Conventional, Crushable									
Mersenne Twister	0	312×8	1×8	2.0	6.1	43.3	18.3	–	–
XORWOW	0	6×4	1×4	1.6	7.7	5.8	136.7	16.8	81.1

Taken from Salmon et al.(see References).

Computational Challenges of GPUs

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- There are some differences from conventional ANSI standards for mathematics (e.g. rounding).

References

GPUs and ABC

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- Liepe, Barnes, Cule, Erguler, Kirk, Toni, Stumpf (2010) *ABC-SysBioapproximate Bayesian computation in Python with GPU support.* Bioinformatics **26**:1797-1799.

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bbsrc biotechnology and biological sciences research council
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EPSRC Engineering and Physical Sciences Research Council
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The Leverhulme Trust
EMBO
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