Université Claude Bernard Lyon 1

INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

LIRIS

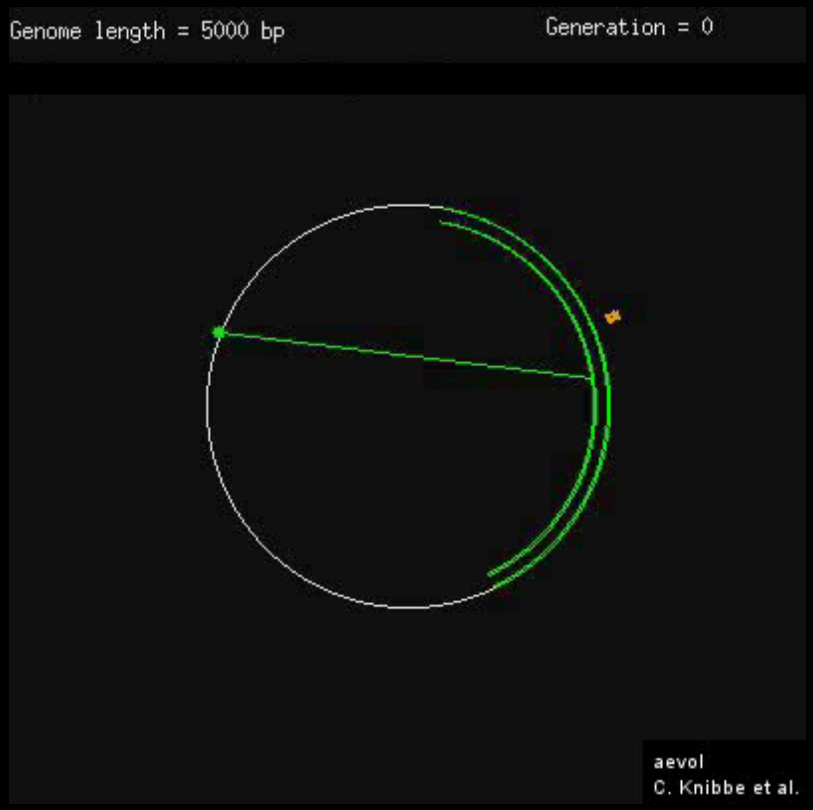
EuroHack 2018
Lugano – October 2018

GPU-Aevol

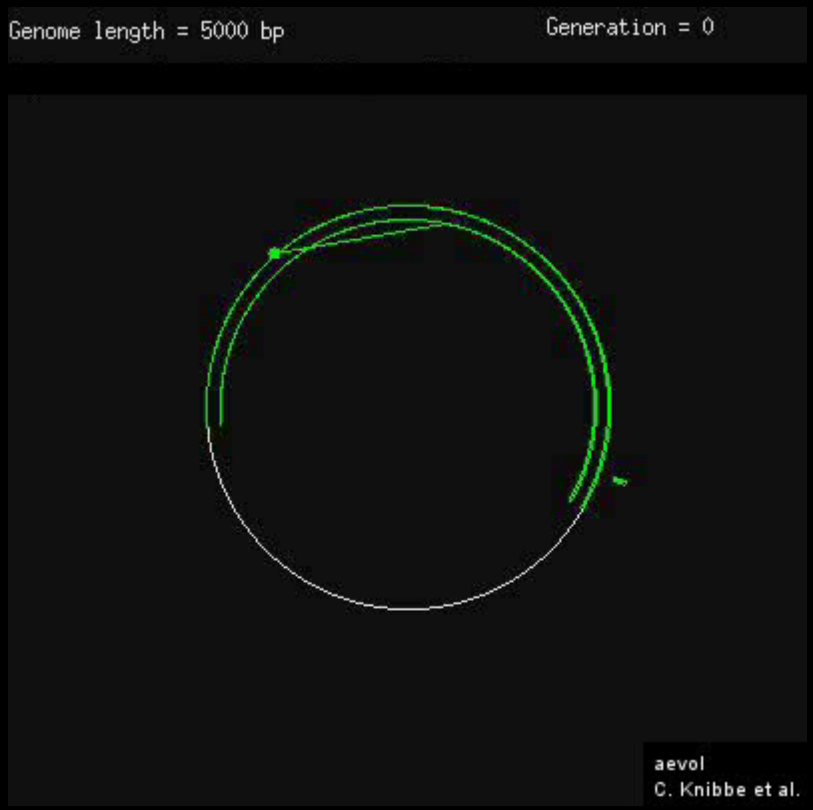
Guillaume Beslon – Computational Biology
David P. Parsons – Software engineering
Jonathan Rouzaud-Cornabas – High Performance Computing
Mentors: Vasileios Karakasis (ETH Zurich), Jeffrey Kelling (HZDR, Dresden)

Inria
INVENTEURS DU MONDE NUMÉRIQUE

Aevol: Evolution in action... *in silico*...



High mutation rate : 2.10^{-4} mut.bp^{-1}.gen^{-1}
for all kind of mutations



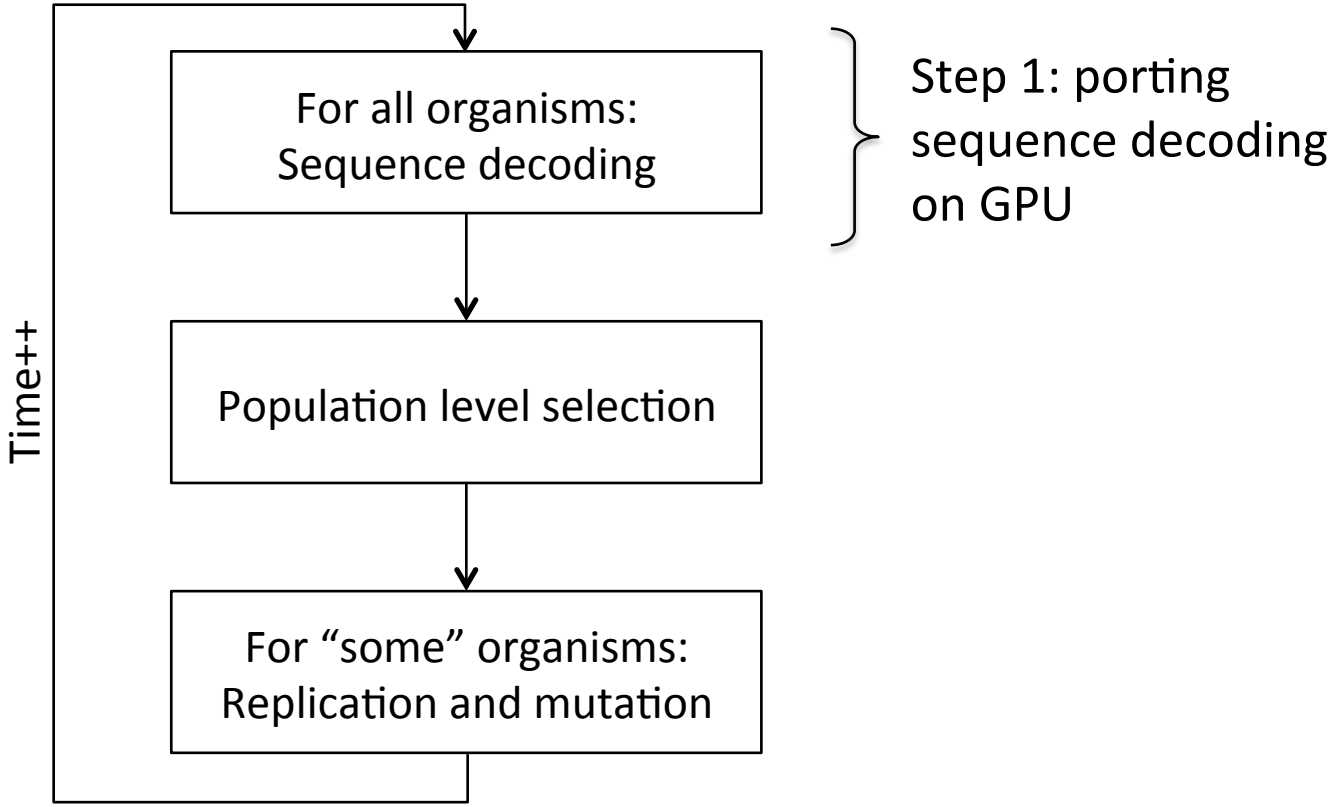
Low mutation rate : 5.10^{-6} mut.bp^{-1}.gen^{-1}
for all kind of mutations

[Knibbe et al., Mol. Biol. Evol. 2007]

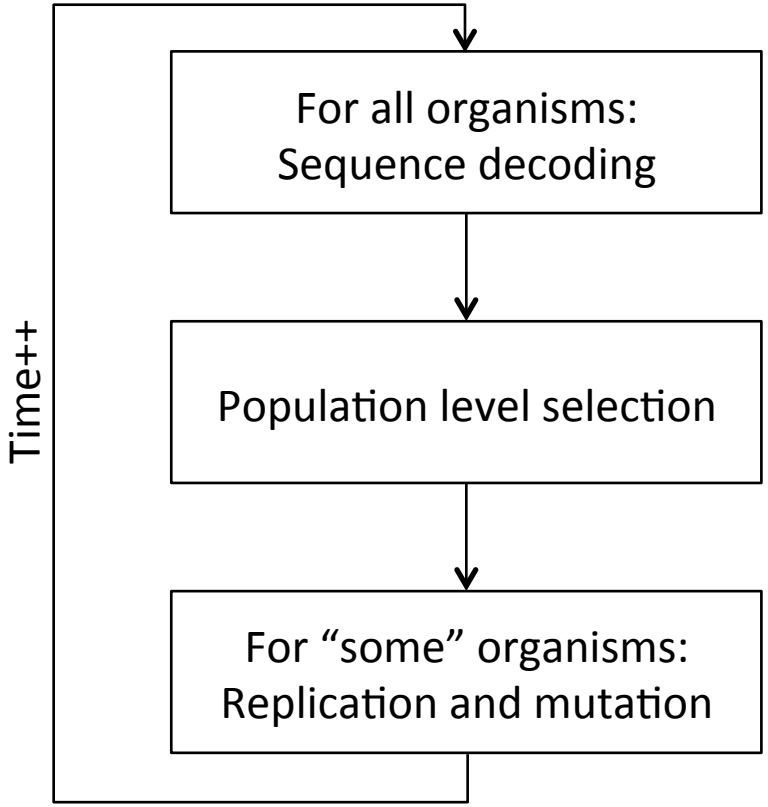
GPU-Aevol − Starting point
(Monday morning)

- Aevol had never been ported on GPU
- Mini-Aevol
  - Aevol simplified and not optimized
  - ~2,000 C++ lines (vs. ~67,000 C++ lines for aevol)
  - One evident parallel scheme: the individual level (but very high heterogeneity)
  - No clear idea on how to efficiently run Aevol on GPU
- Preparation step
  - Optimize Mini-Aevol to enable fair comparisons
  - Replace random-generator by a GPU compatible one

GPU integration in 4 steps



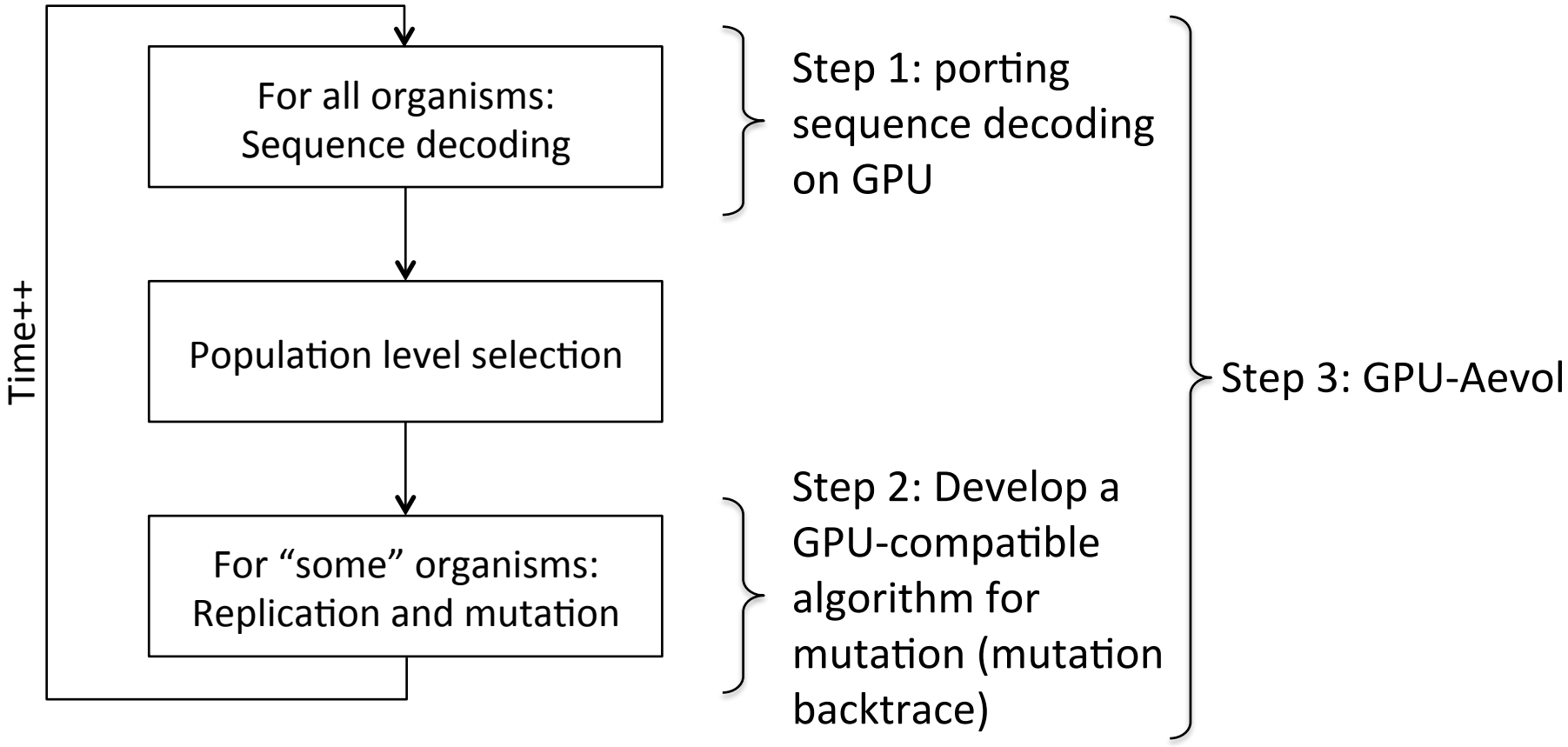
GPU integration in 4 steps



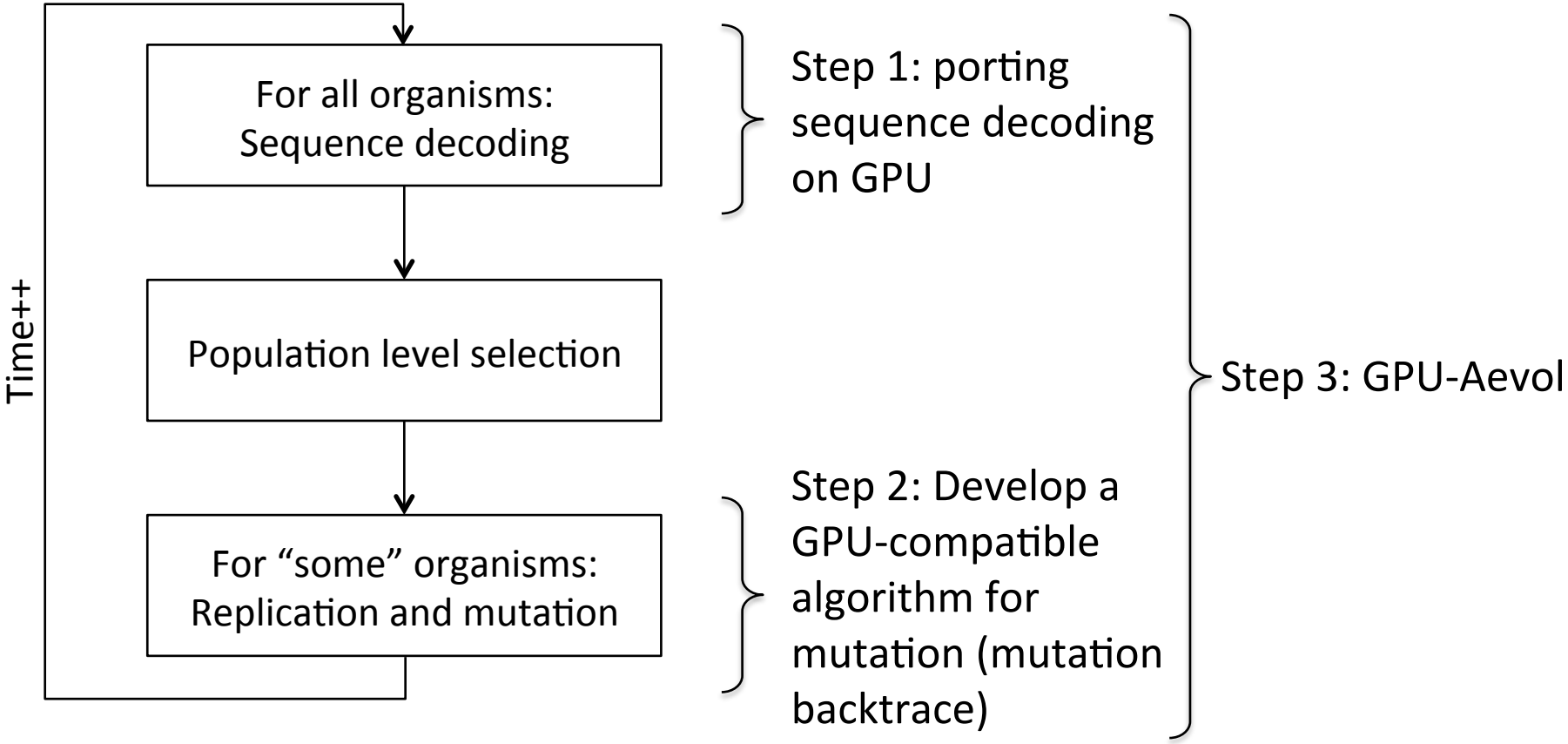
Step 1: porting sequence decoding on GPU

Step 2: Develop a GPU-compatible algorithm for mutation (mutation backtrace)

GPU integration in 4 steps



GPU integration in 4 steps



Step 4: Debugging Optimizing Debugging Optimizing Debugging Optimizing Debugging Optimizing Debugging Optimizing Debugging Optimizing Debugging Debugging Debug Debug Debug Debug

Where we are today

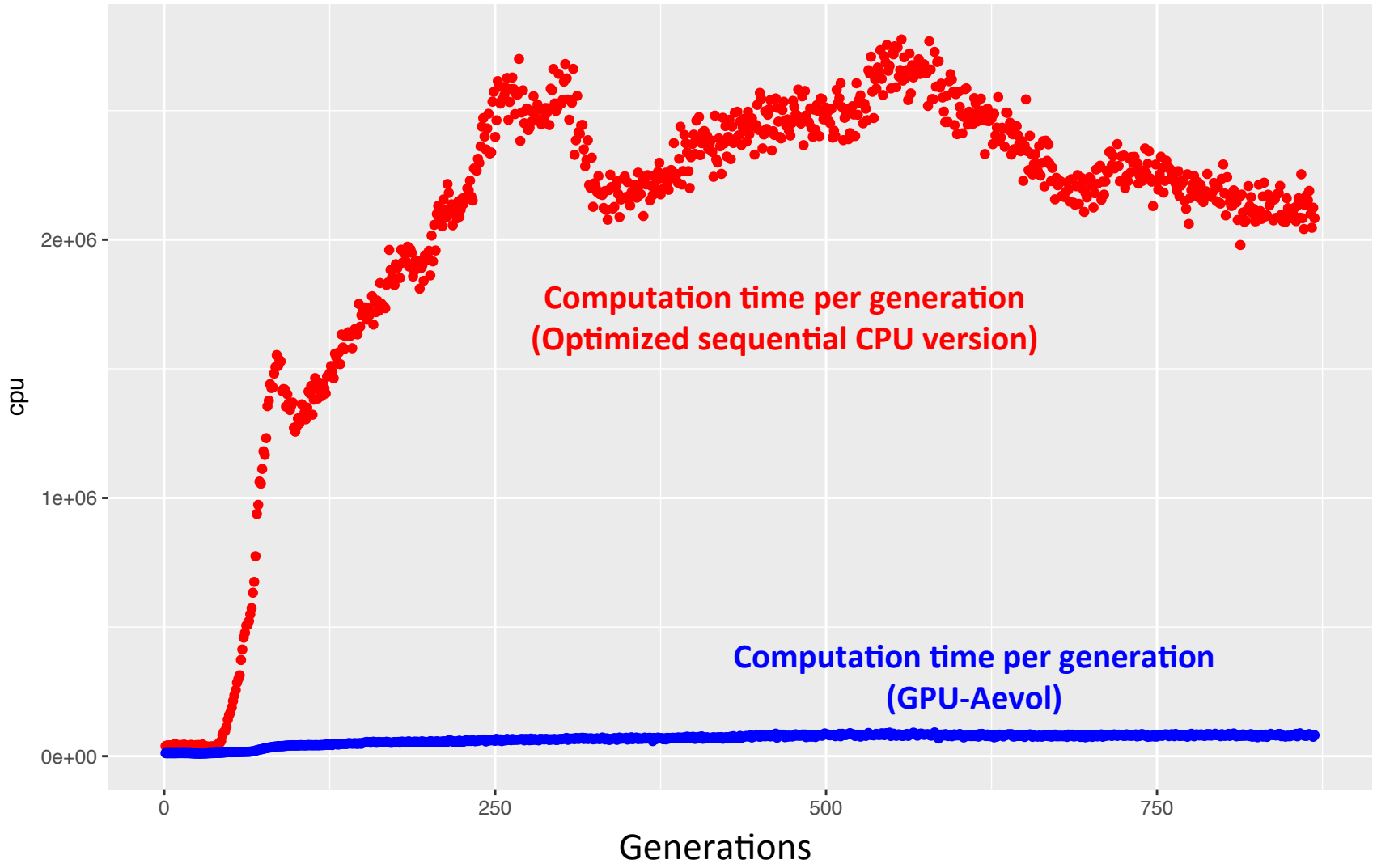
- Full-GPU implem
  - we didn't expect that!
- Speed-up ~X25 **on classical pop sizes**
  - Not much better than CPU openmp speed-up ☹

But

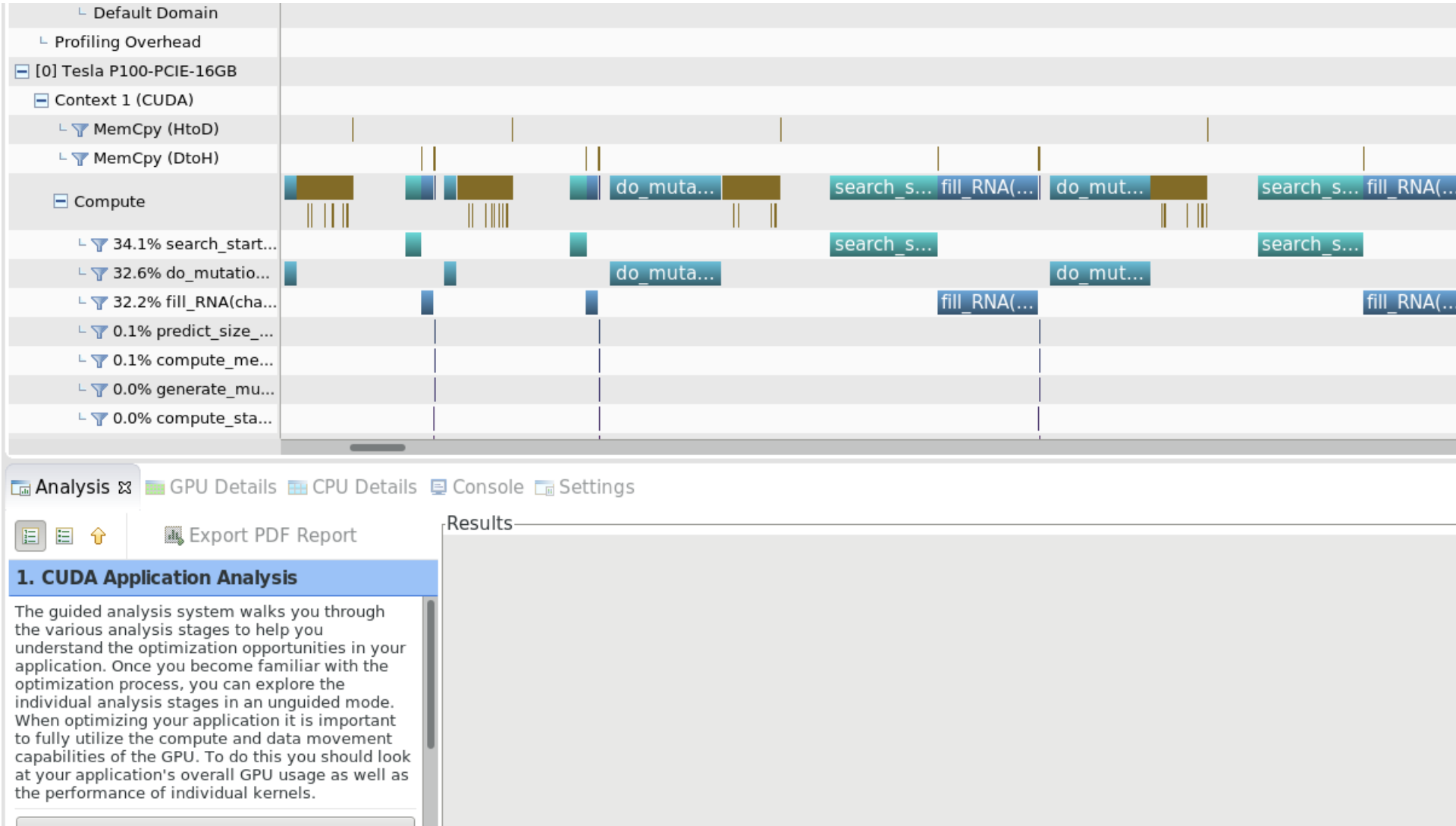
- Large populations run ~as fast as classical ones
  - Far better than CPU openmp speed-up ☺

  → Parallelization scheme seems "reasonable"

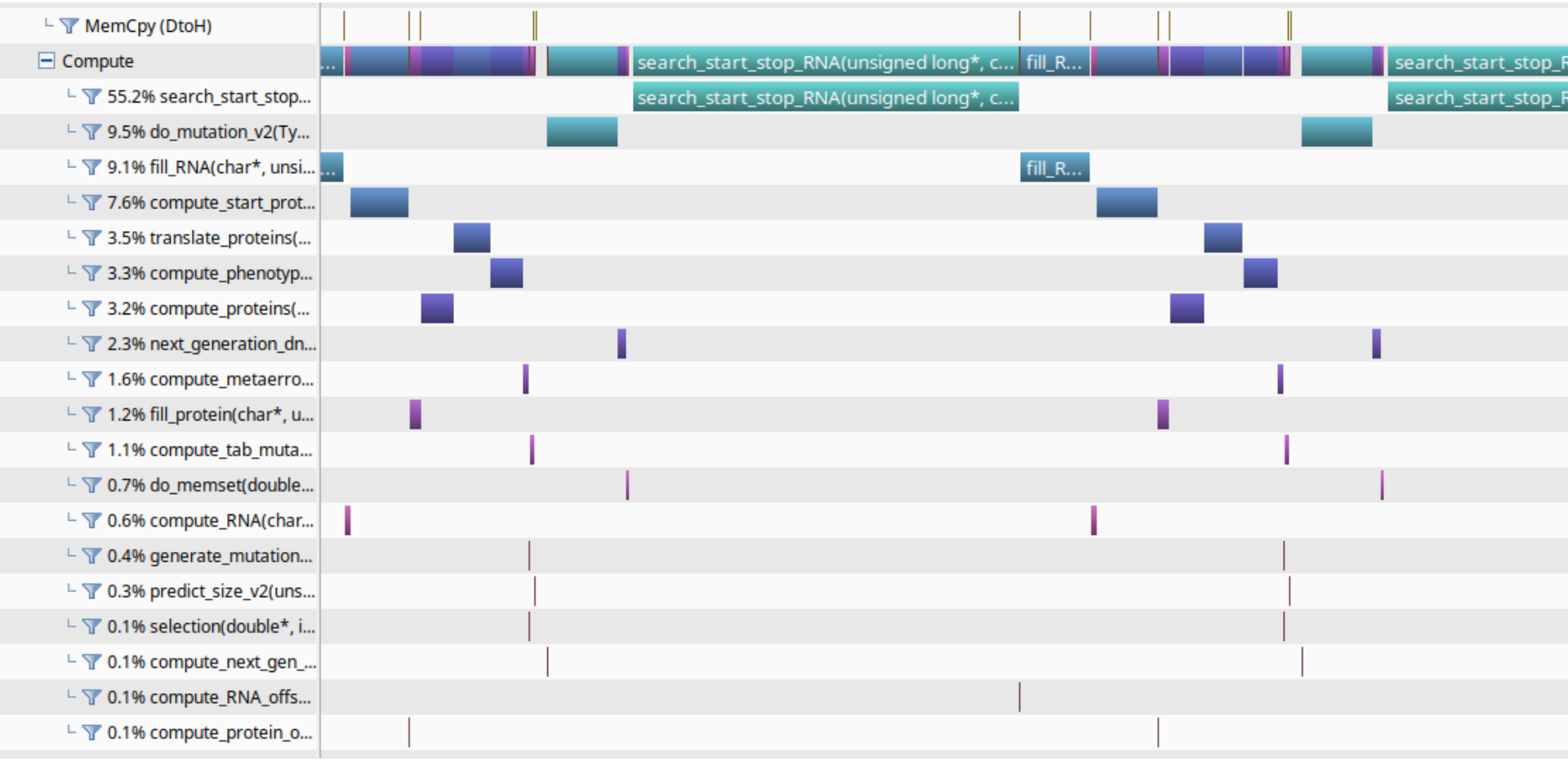
Speedup compared to GPU-optimized Mini-Aevol



Ongoing: profiling of GPU-Aevol (Thursday)



Ongoing: profiling of GPU-Aevol (Friday)



Still many optimization possibilities

- Optimization ideas:
  - Assemble all genomes into a metagenome (suppress heterogeneity)
    - →Done on DNA (estimated gain: >50% in the decoding kernels)
    - →To be done on RNAs
  - Merge decoding and mutation kernels → Easy; To be done
  - Compress genome and metadata
  - Track metadata to avoid "recomputation" (i.e. +/- same optimization idea as on CPU)
    - →Thought to be incompatible with GPU mutation algo.
    - →GPU-compatible algorithm proposed; to be implemented and tested
  - …

Candid feedback on GPU

- Among the three of us…
  - Guillaume had no (recent) experience in programming
    - And was actually wondering what he was doing here!
  - David had no experience in GPU
    - But was eager to learn
  - Jonathan had limited experience on GPU
    - But had a theoretical understanding of the concepts
- Conclusion
  - CUDA is surprisingly easy to dive into but…
  - As GPU noobs, we had to change our vision of prog & algorithmics
  - Debugging is a nightmare… Only for dummies ?
  - Also, in depth knowledge on biology and evolution has revealed essential all along the week to find efficient parallel algorithms

Candid feedback on EuroHack

It’s really been great!

Thanks to the organizers and to our mentors

However…

Candid feedback on EuroHack

Speedup compared to GPU-optimized Mini-Aevol