Parallel Genetic Algorithms on the GPU
The Brain Science Version

Amit Aviv, Roy Ben-Shalom and Alon Korngreen

Bar-Ilan University, Israel

My research in one slide...

- I want to understand how the brain works....
  - ...I have to understand single neurons...
    - ...I have to understand how voltage-gated channels modulate neuronal physiology...
      - ...I have to provide experimentally driven models of ion channels!

Ion channel kinetics is best described by Markov chain models.

$$C \underset{k_{2,1}}{\overset{k_{1,2}}{\rightleftharpoons}} C \underset{k_{3,2}}{\overset{k_{2,3}}{\rightleftharpoons}} O$$

$$g_K = \bar{g}_K \cdot O$$

$$k_{i,j} = a_{i,j}\exp(z_{i,j} \cdot v_m)$$

$$k_{j,i} = a_{j,i}\exp(-z_{j,i} \cdot v_m)$$

where $\bar{g}_K$ defined in $pS/\mu m^2$

Things you always wanted to know about Markov kinetic models and didn't bother asking....

$$C \underset{k_{2,1}}{\overset{k_{1,2}}{\rightleftharpoons}} C \underset{k_{3,2}}{\overset{k_{2,3}}{\rightleftharpoons}} O$$

$$\frac{dC_1}{dt} = -k_{12}C_1 + k_{21}C_2$$

$$\frac{dC_2}{dt} = k_{12}C_1 - k_{21}C_2 - k_{23}C_2 + k_{32}O$$

$$\frac{dO}{dt} = k_{23}C_2 - k_{32}O$$

$$\begin{pmatrix} C_1' \\ C_2' \\ O' \end{pmatrix} = \begin{pmatrix} -k_{12} & k_{12} & 0 \\ k_{21} & -k_{21} - k_{23} & k_{23} \\ 0 & k_{32} & -k_{23} \end{pmatrix} \begin{pmatrix} C1 \\ C2 \\ O \end{pmatrix}$$

What we do in the lab?

1. Come in the morning.
2. Kill a rat and take out its brain.
3. Record ionic currents from neurons in the cerebral cortex.
4. Fit Markov models to the data.
5. goto 1

Our first computational challenge

How to automatically fit Markov chain models to ionic currents?

Use stochastic search algorithms to constrain the parameters of such models.

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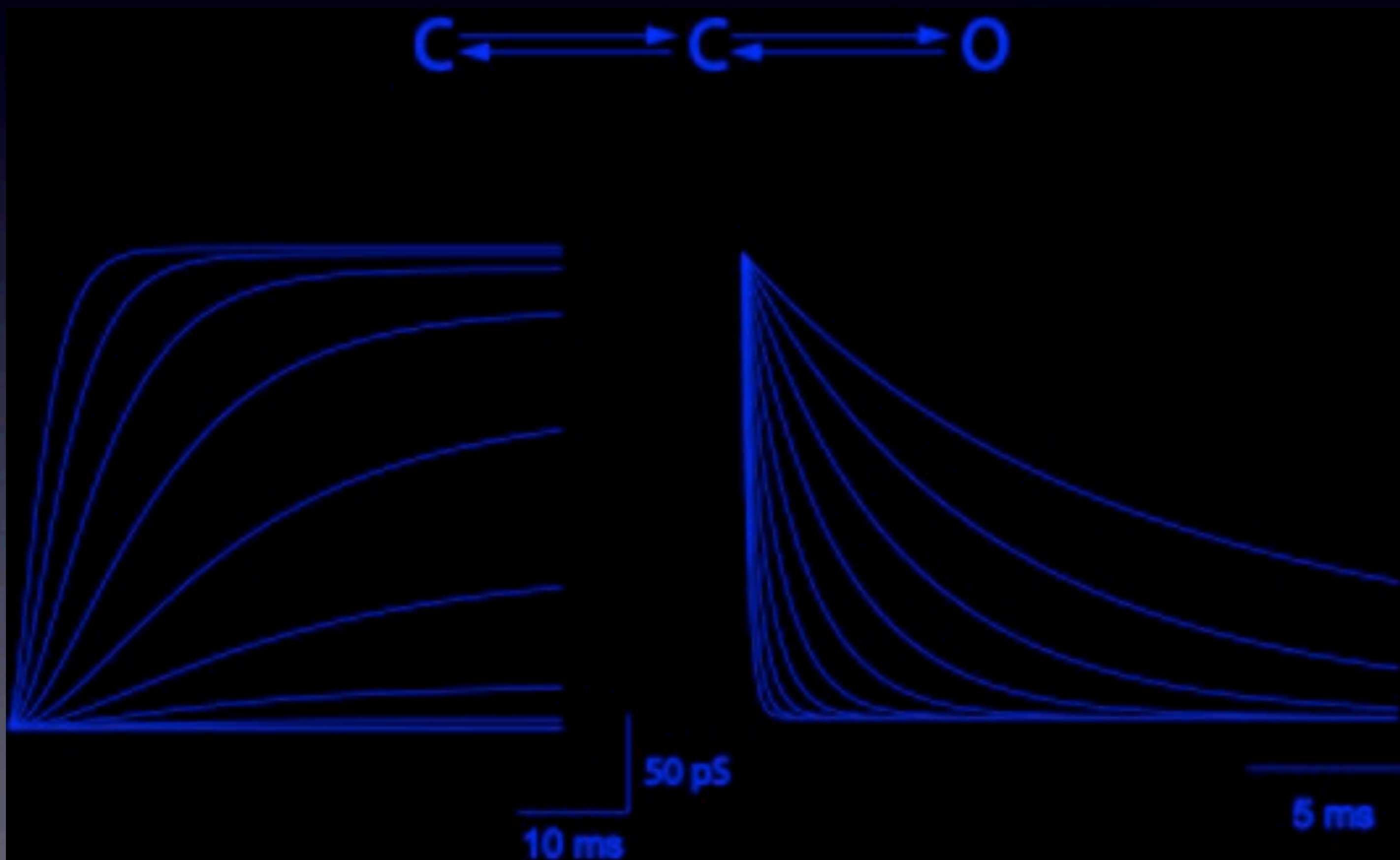
A Numerical Approach to Ion Channel Modelling Using Whole-Cell Voltage-Clamp Recordings and a Genetic Algorithm



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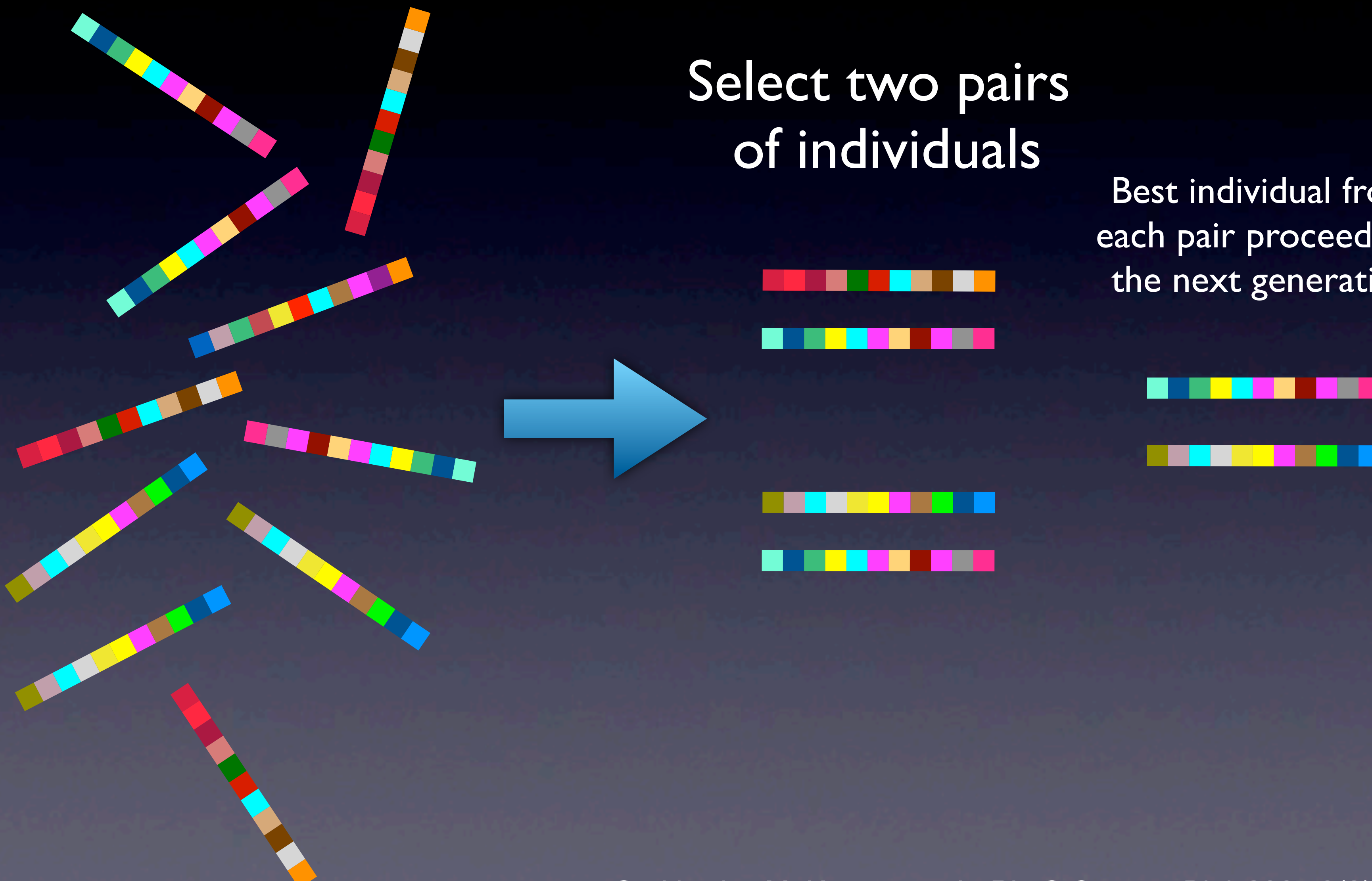
The Genetic Algorithm - Selection

The population



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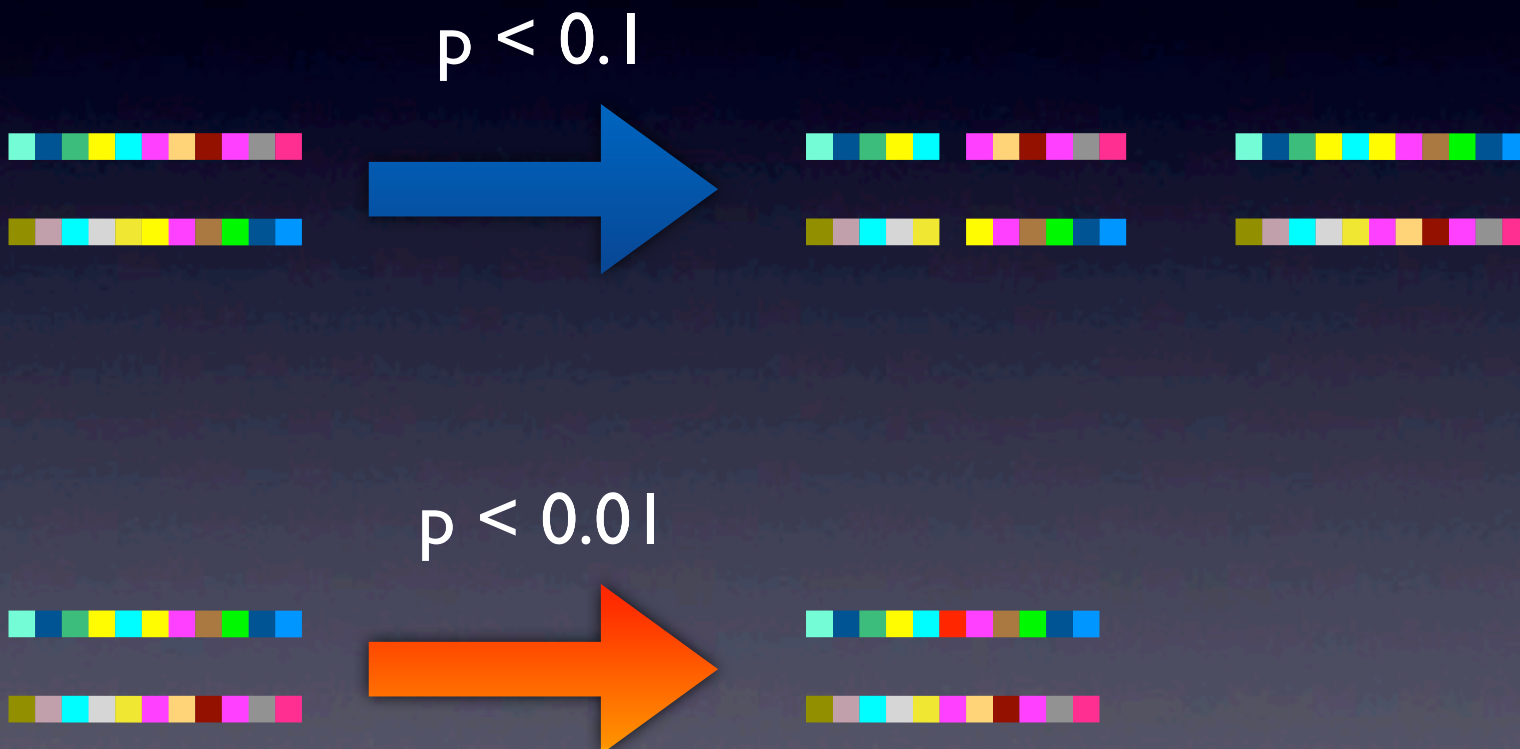
The Genetic Algorithm - Crossover and mutation



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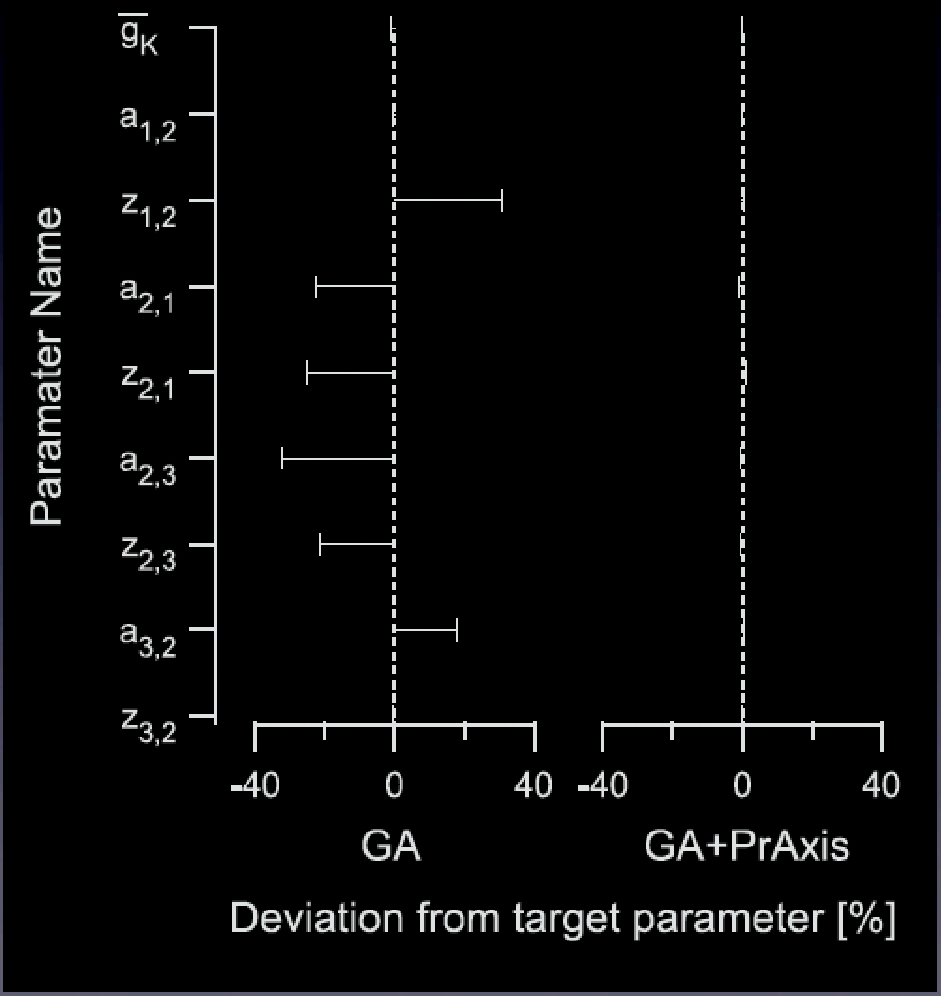
This scheme allowed us to constrain kinetic chain models



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There is no such thing as a free lunch

160 CPU Linux Cluster
OpenSuse Linux 10.3
Torque and Maui for job management
OpenMPI for parallel jobs
The Cluster is used by the entire institute.
Jobs wait in queue for more than a week.
We usually get 80 CPUs.
Jobs can last for several days.
Power hungry.
Needs cooled server room.
No chance of upgrade.

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The second computational challenge

- How to reduce the cost of the computing element?
- How to save on electricity and cooling?
- How to do these things and still compute faster?

↓

GPU

Genetic Algorithm on the GPU

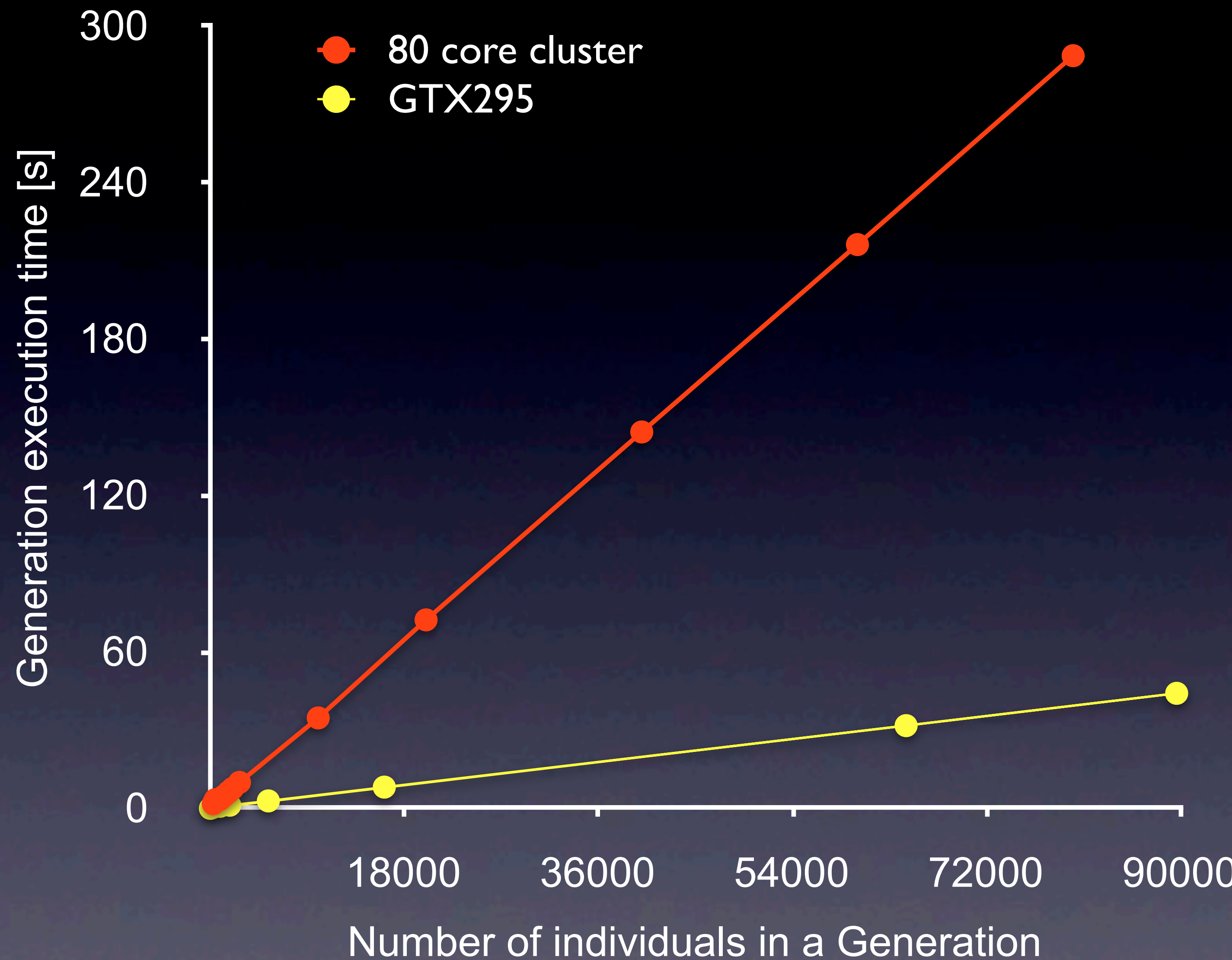
Host
Genetic Algorithm, generates population, reads target data set and kinetic model

GPU
Global Memory
Stores population, kinetic constants and target data.
Collects cost results from threads.

GPU
Lightweight threads (Shared memory)
Solves differential equations for a single individual in the population. Returns score.

The competition

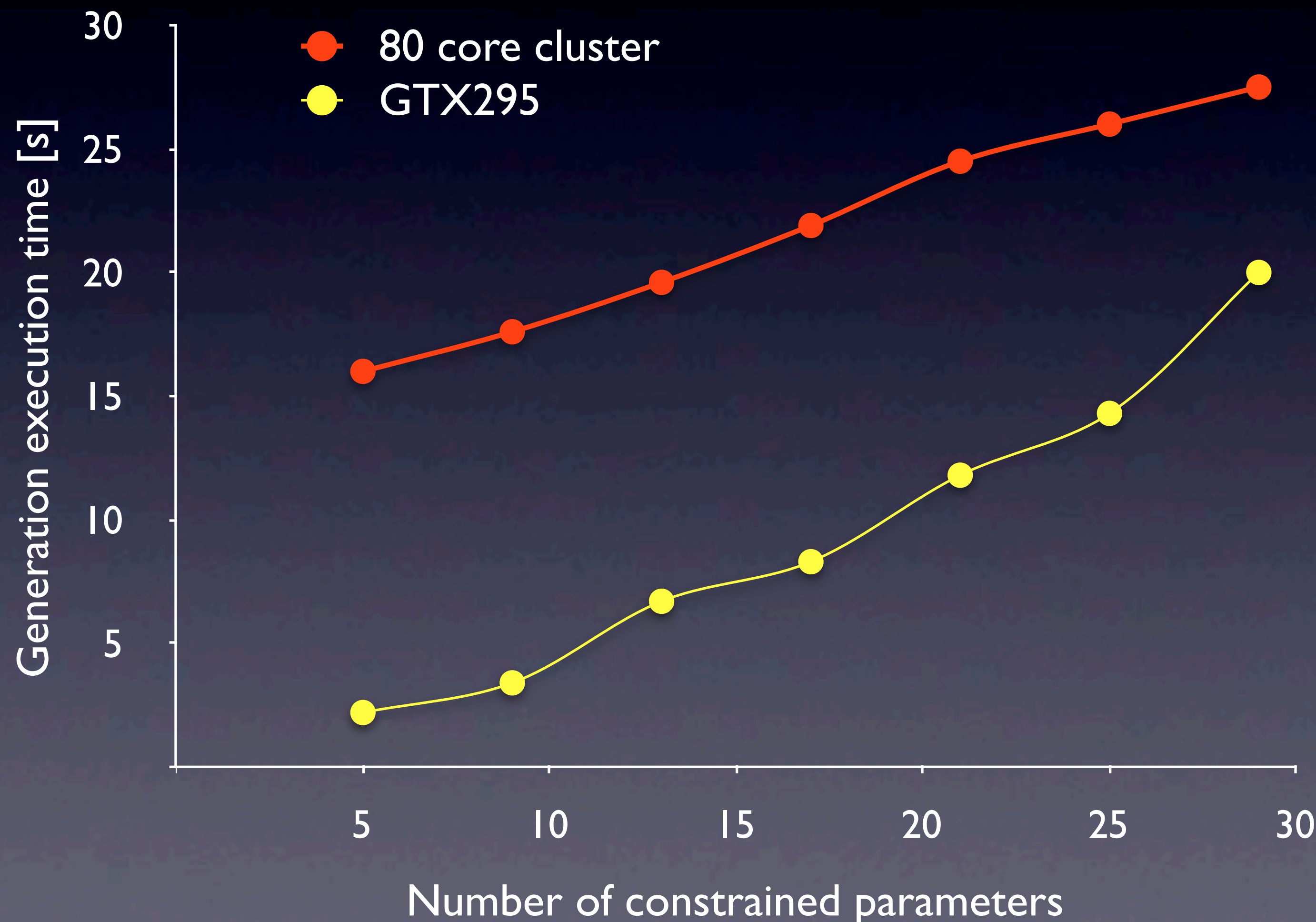
And the winner is!



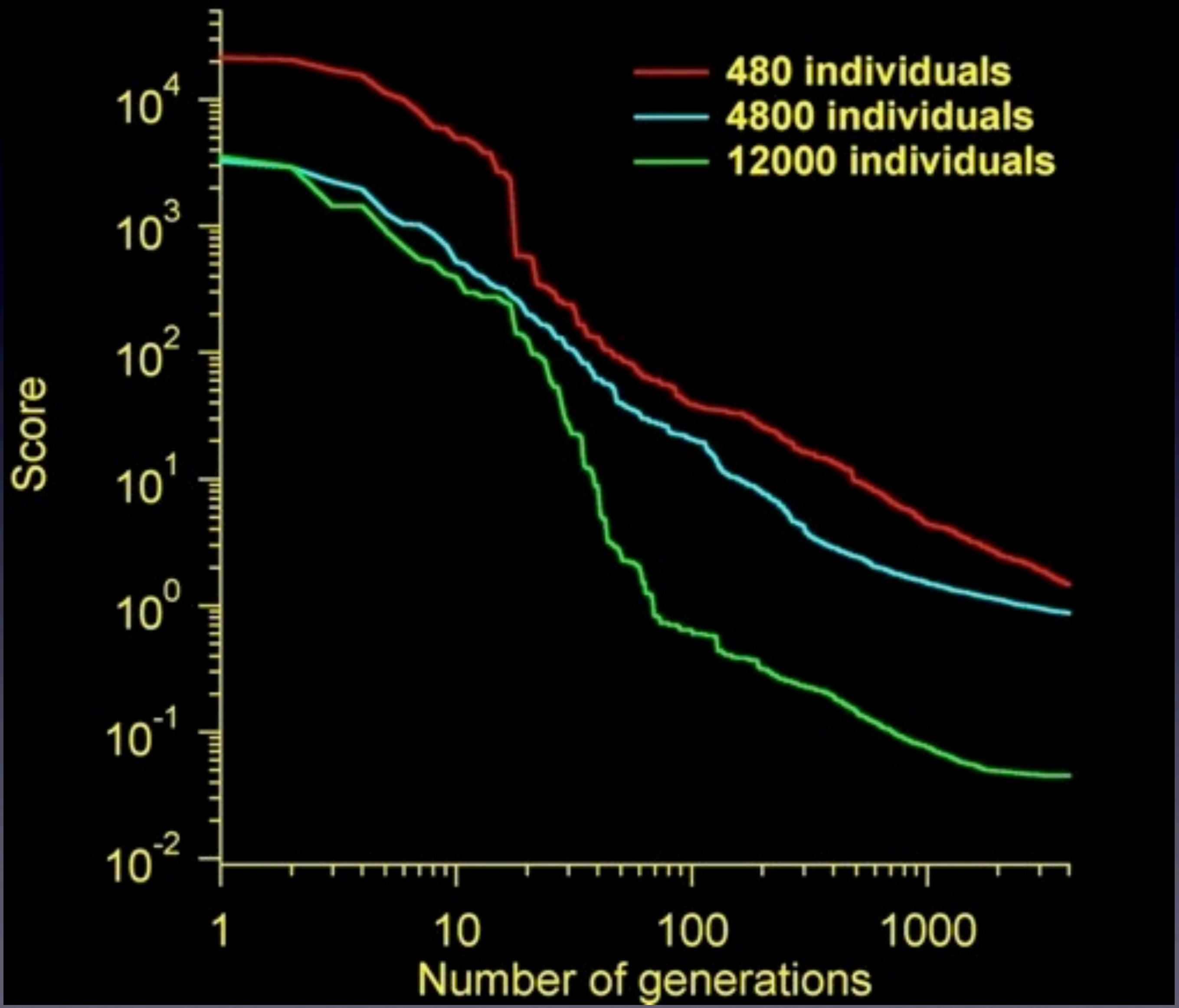
Half a GTX295 is 6 times faster than an 80 CPU cluster.

A speedup of 480 over one CPU!

What happens when we increase the complexity of the model?

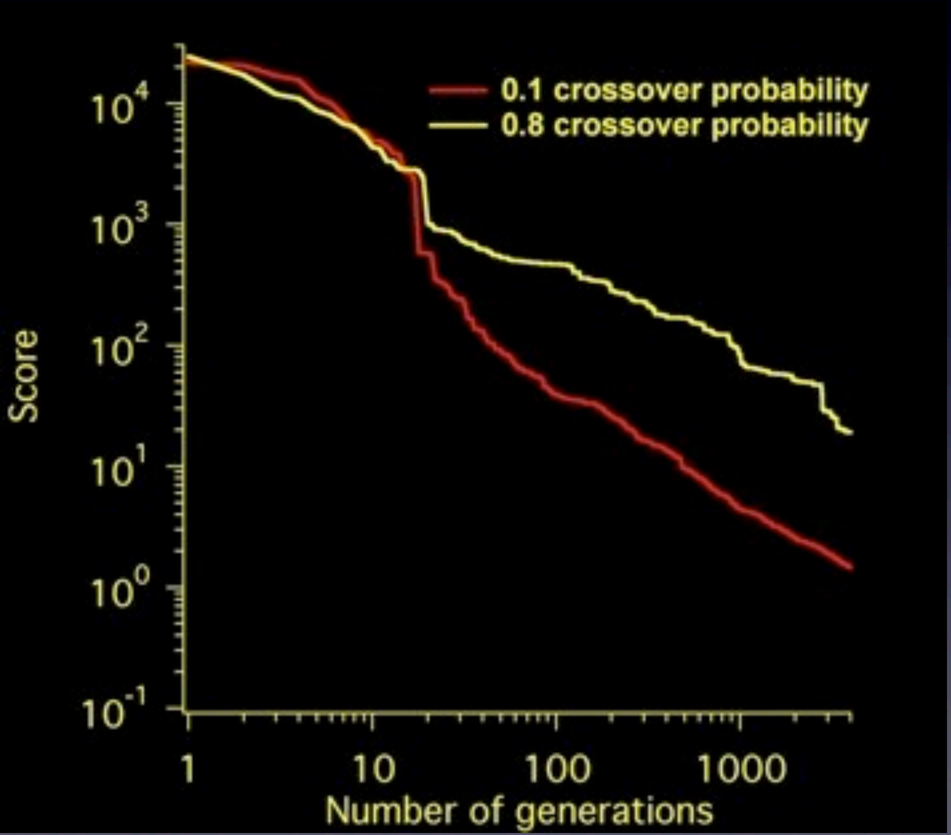


Now we can test MUCH larger generations

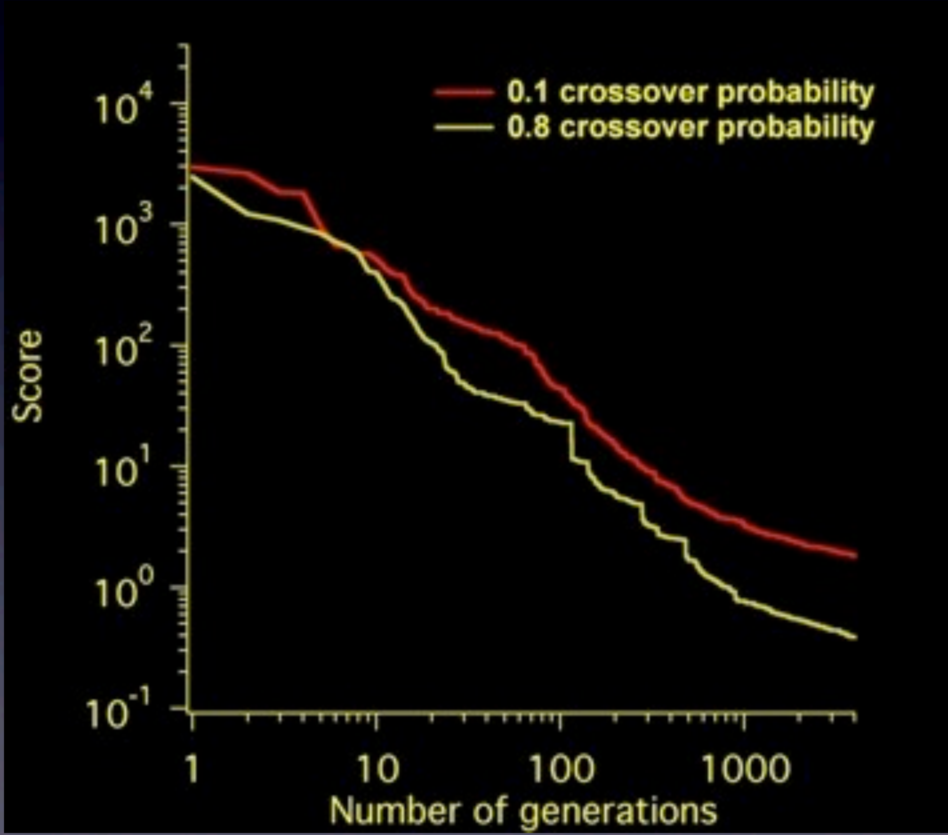


Better performance for larger populations

480 Individuals



4800 Individuals



Summary and outlook

- ☑ Using a genetic search algorithm it is possible to locate the region in parameter space containing the global minimum when fitting simple models of voltage-gated channels.
- ☑ We were able to speedup the process by ~480 fold using CUDA running on a single GTX295.
- ☑ We can now use larger populations!
- ☑ We are currently optimizing the code...
- ☑ We added a user friendly GUI.
- ☑ We plan to speedup the computation further by running the code on several GPU units simultaneously.

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- Roy Ben-Shalom
- Amit Aviv
- All the lab.

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