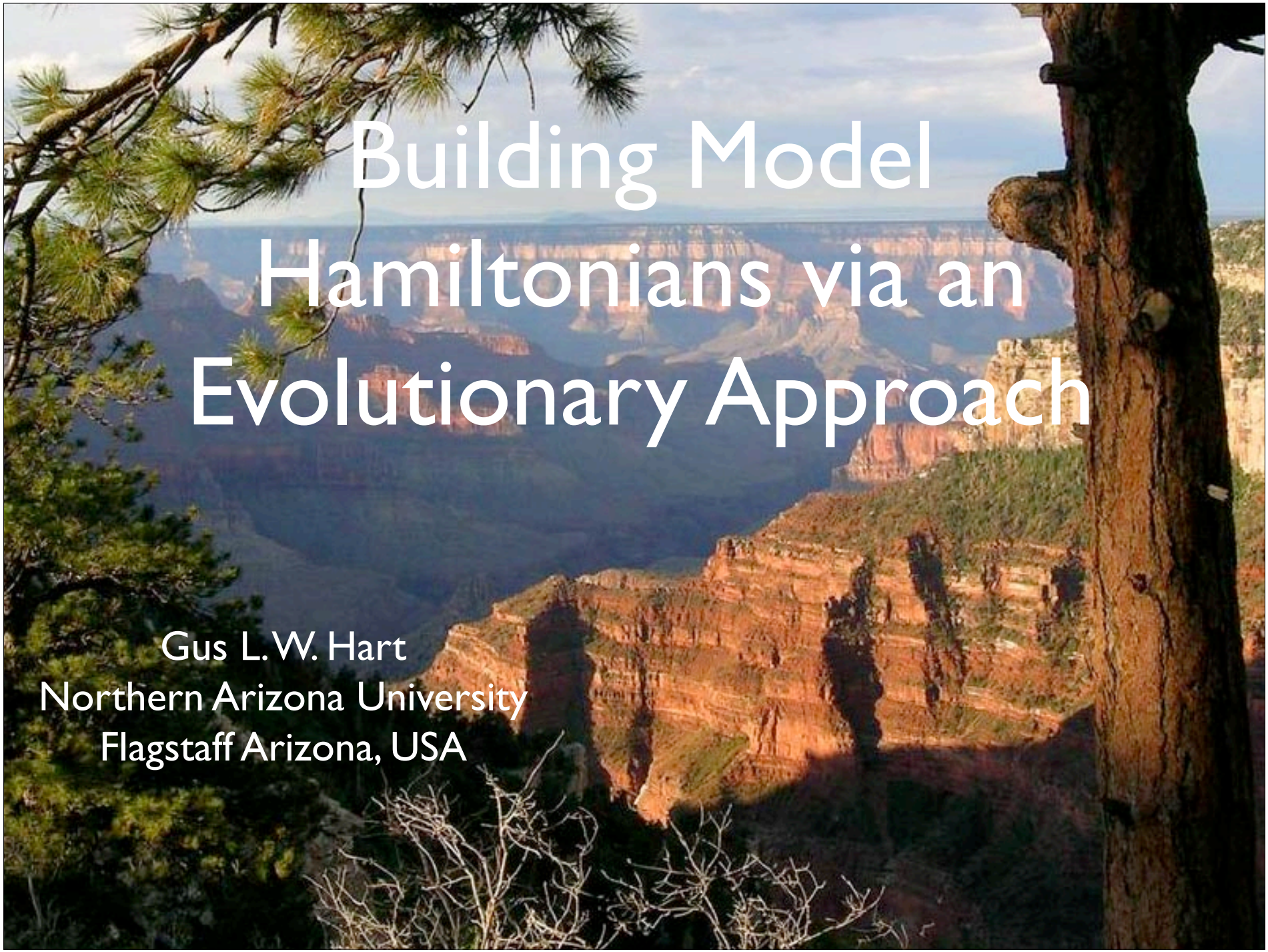
Building Model Hamiltonians via an Evolutionary Approach
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Flagstaff Arizona, USA

PLEASE!

Interrupt me
Ask questions
Make comments
Respond to questions

Shameless self-promotion

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LETTERS

NEWS & VIEWS

Evolutionary approach for determining first-principles hamiltonians

ABINITIOMODELLING

Genesis of crystal structures

GER[2]

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Genetic algorithms prove useful to distil a complex quantum mechanical calculation of interatomic interactions down to its simplest mathematical expression. This makes it possible to predict the structure of new compounds from first principles.

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Modern condensed-matter theory from first principles is highly successful when applied to materials of given structure-type or restricted unit cell size. But this approach is limited ... over the past two decades, quantum mechanical ... large cells or searches over ... cluster expansion ... of the configurational energy $E(\sigma)$ in terms of effective ... atom–atom interactions ...

... methods. However, as the nature of the interactions in a given system are not known a priori, the limiting step in the construction of a cluster expansion is the question of which interactions play an important role and which can be safely neglected. Indeed, given that the number of ways to choose a set of clusters ... (1)

The argument for "fancy"

Goal: A fast, but *quantitatively* accurate, Hamiltonian

- Such models are complex, almost by definition—generally not even the "shape" of the model is simple
- That is, the *value* of parameters is not the issue, which parameters to use in the model (or even how many!) is essentially *unguessable*

Fancy or not, we need an approach that "works"

An Illustration: Cluster expansion (Ising)

$$Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots$$

where:

Z is any configurational-dependent quantity

$\{J\}$ are "interaction parameters" (to be fitted)

$\{S\}$ are the site variables ($S = \pm 1$)

Formally exact but useless unless sums can be truncated

An Illustration: Cluster expansion (Ising)

$$Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots$$

Approach:

Determine Z for a "few" structures via DFT

Use fitting to find values for { *J* }

Predict Z for new structures, check against DFT

Add new structures to your computed set of Z's

Iterate until we have a *universal* set of *J*'s

→ Result: a robust, *extremely fast*, model Hamiltonian

(millions of atoms, millions of configurations)

How do we truncate? Determine the model's "shape?"

$$Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j + \sum J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \dots$$

Can be handled efficiently
by a constrained, k-space fit

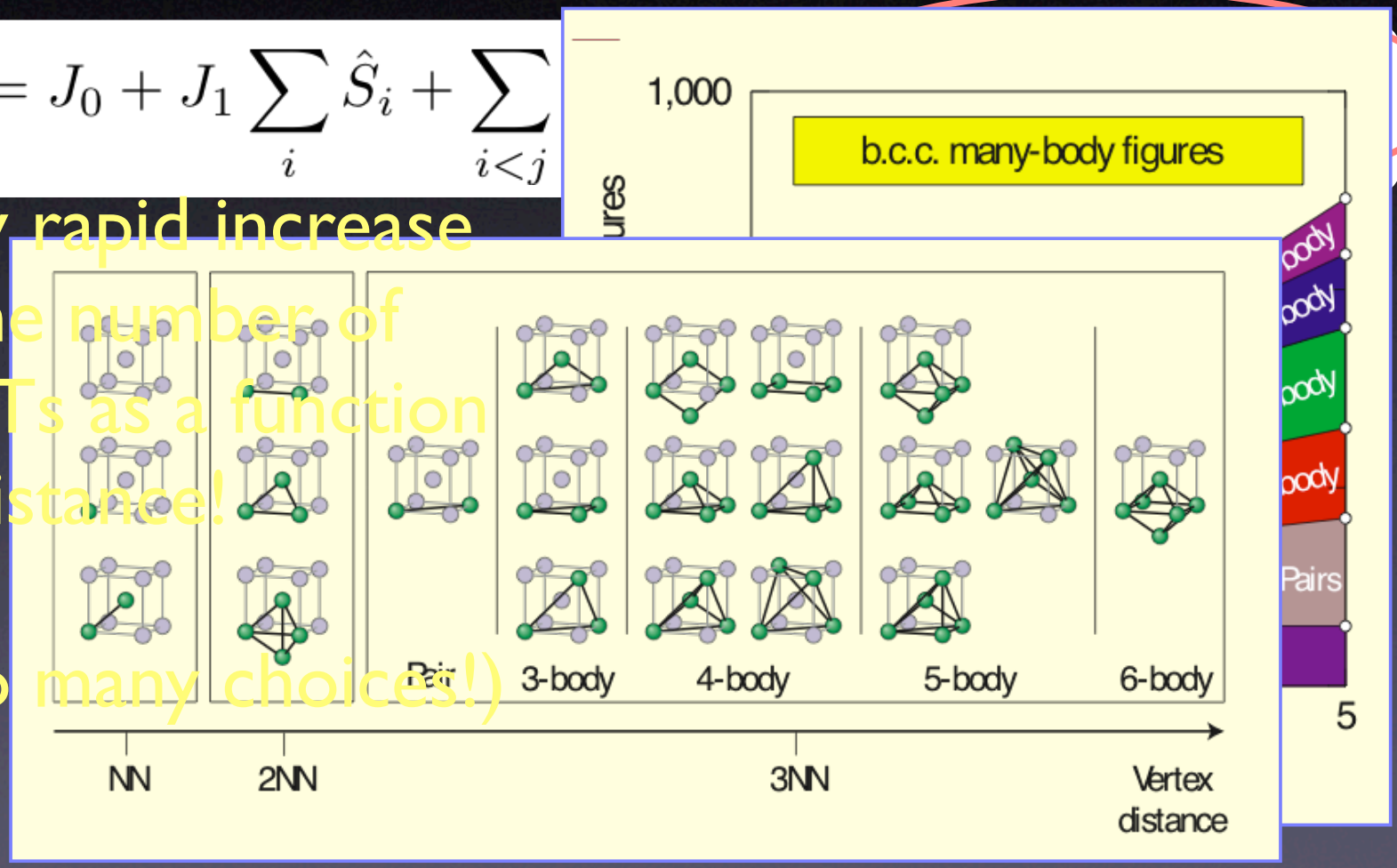
But truncating the multi-body interaction types (MBITs) is hard (Why?)

Selecting the multi-body interaction types (MBITs)

$$Z = J_0 + J_1 \sum_i \hat{S}_i + \sum_{i<j}$$

Very rapid increase in the number of MBITs as a function of distance!

(Too many choices!)



Selecting the multi-body interaction types (MBITs)

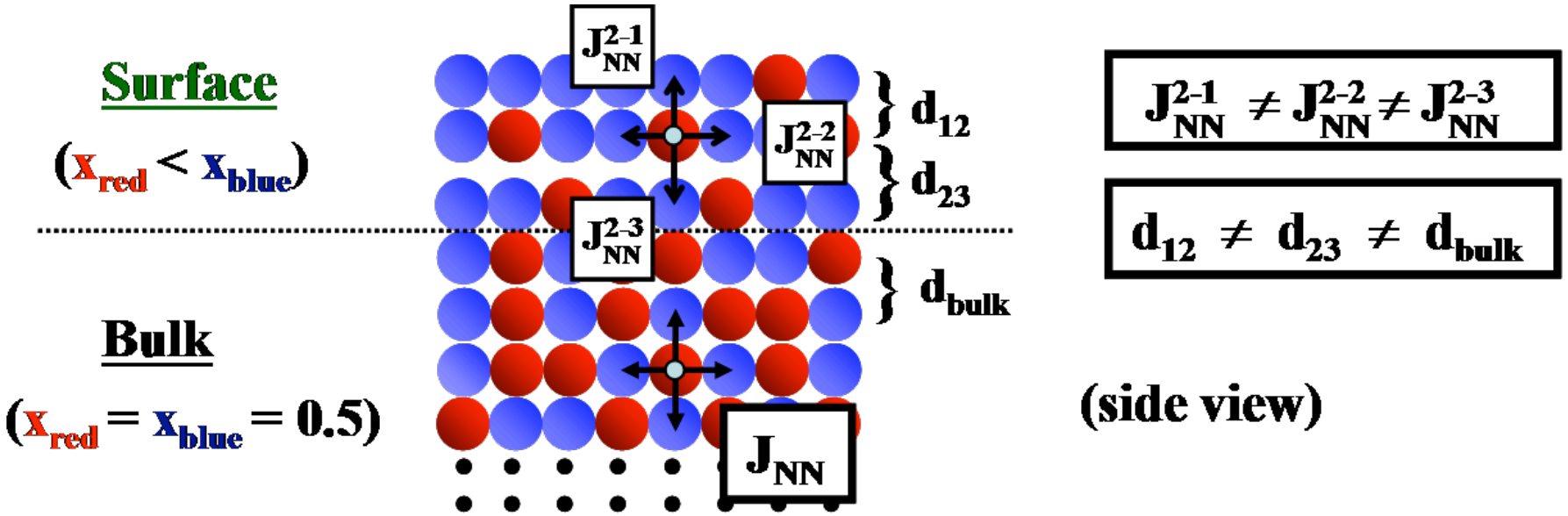
- Optimization (search) problem:

Out of $\binom{50\text{–}100}{5\text{–}10}$ possibilities...

$(\sim 10^6\text{—}10^{13})$

...find (one of) the best model

(Actually, the problem is *even worse* for surfaces...)

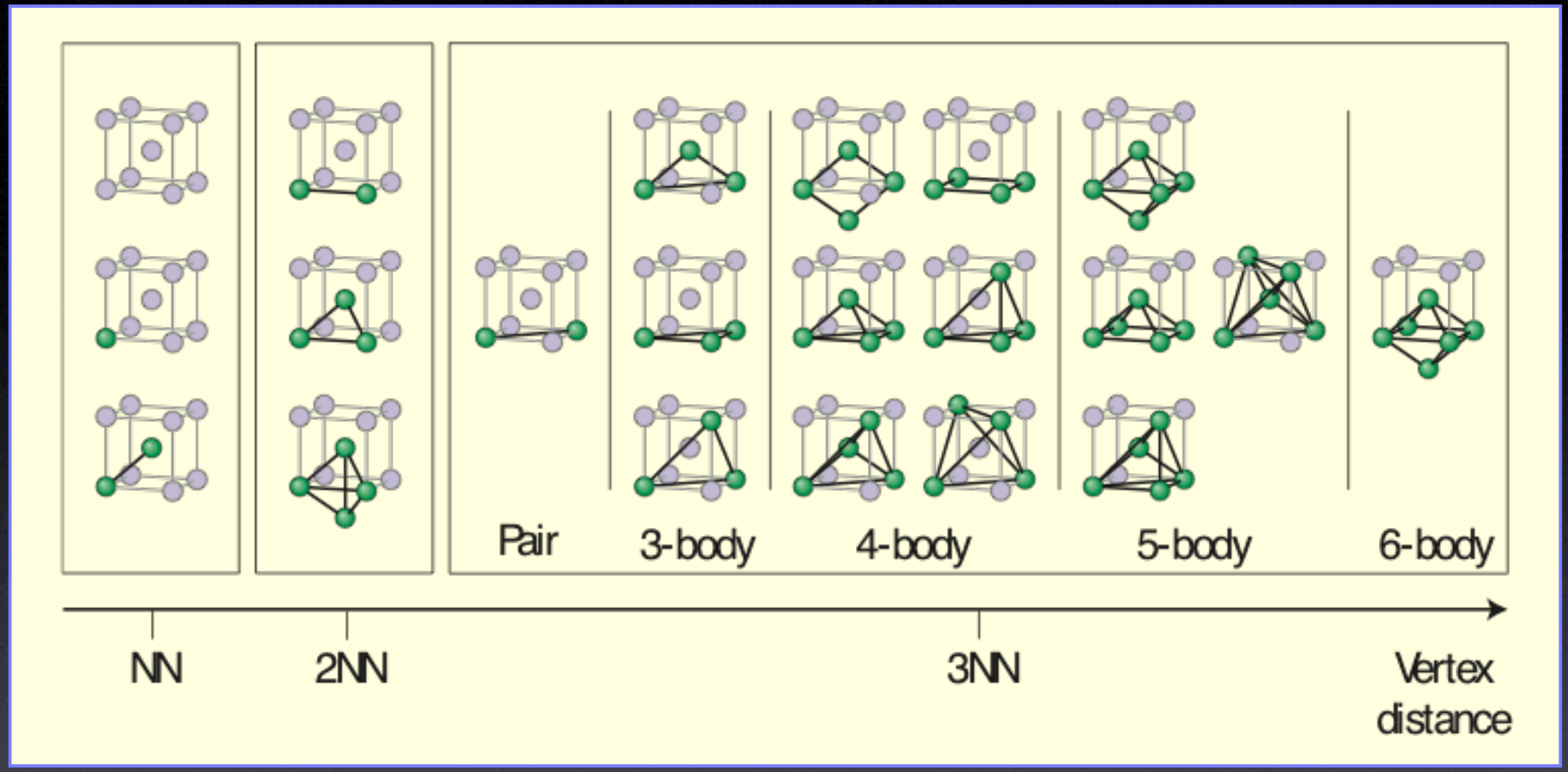


~400 interactions to choose from!

$$\binom{400}{20} \approx 10^{33}$$

How to pick the terms

- By physics "intuition"—dangerous
  (and physics shouldn't be an "art")
- Formal hierarchy
  (converges way too slow to be practical)
- Simulated annealing
  (didn't work—highly correlated problem)
- Systematic "guessing"—hierarchal approach
- Something "fancier" (anything that works!)



“Physical” choices aren’t obvious

How to pick the terms

- By "physics" intuition—dangerous (and physics shouldn't be an "art")
- Formal hierarchy (converges way too slow to be practical)
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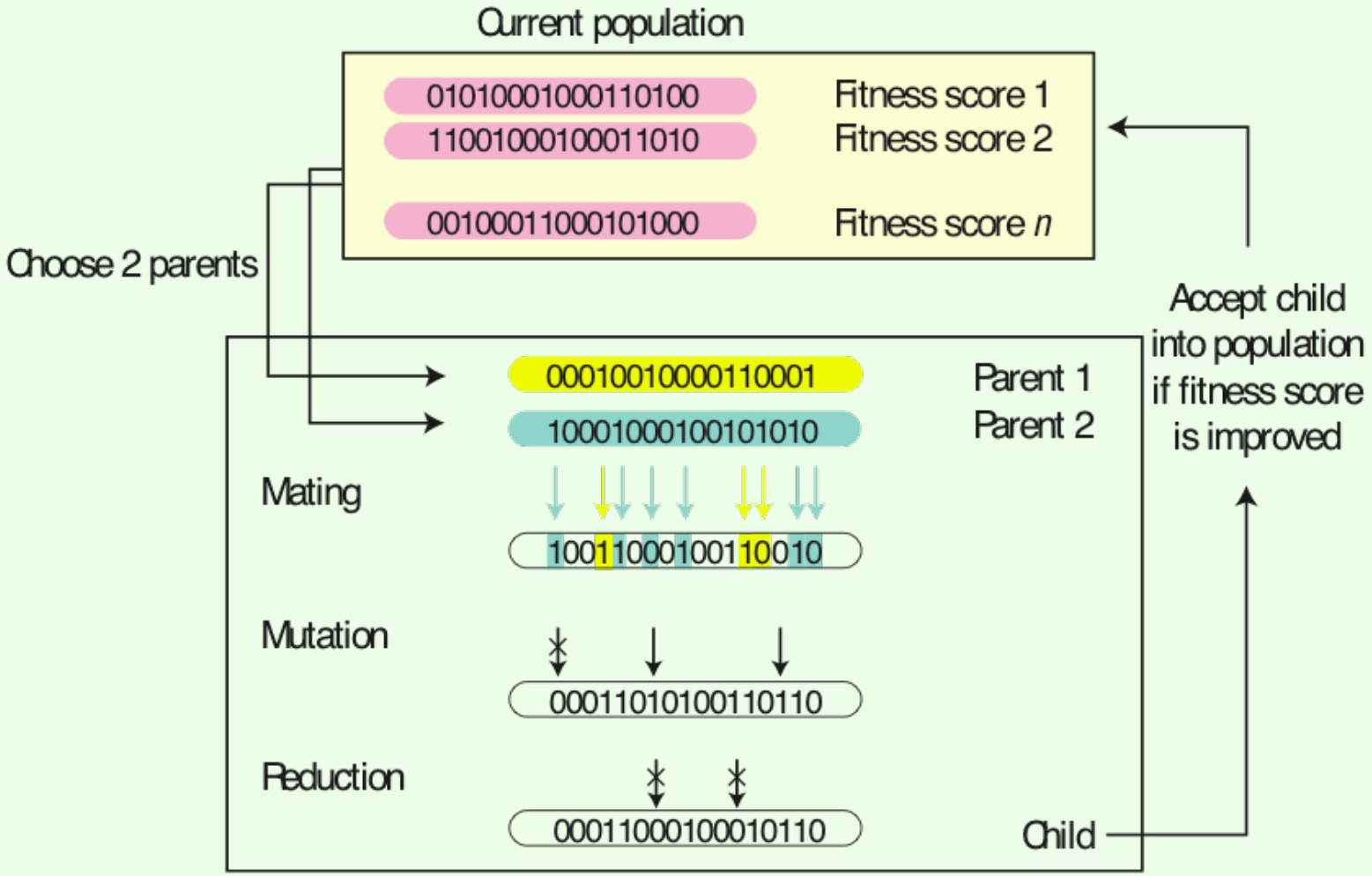
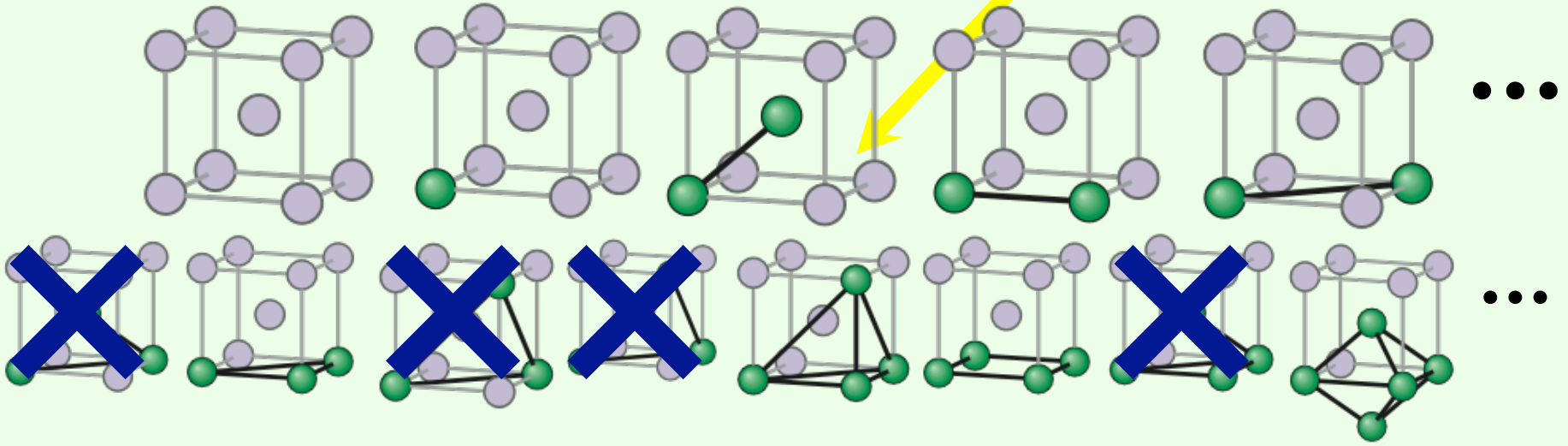
Evolutionary optimization

- Good approach for some highly correlated problems
- Not "too fancy" if it's the simplest thing that works

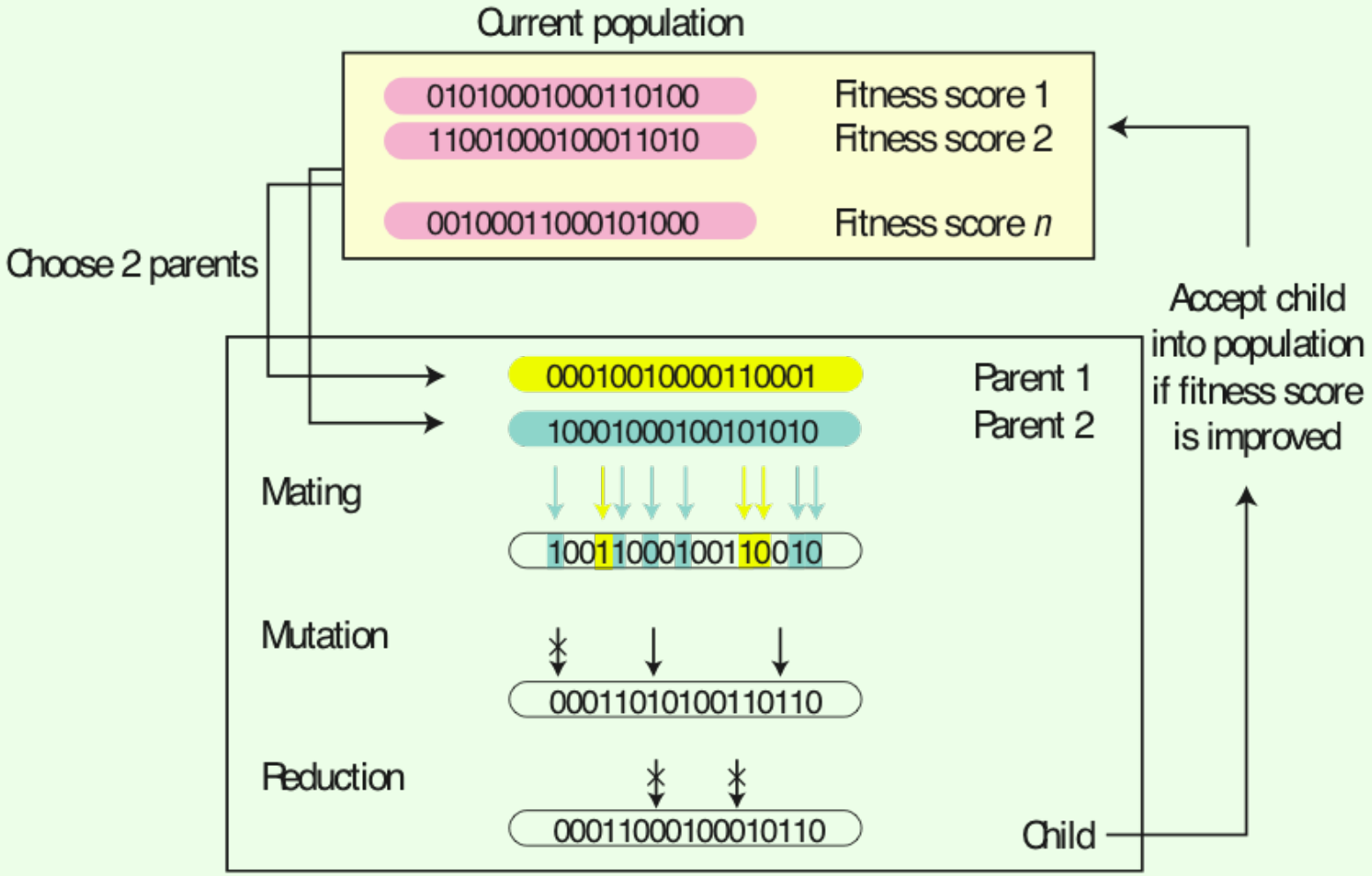


Flowchart of a genetic algorithm for choosing the terms to retain in a model hamiltonian. Each candidate model is represented by a series of zeros and ones, a one indicating that the corresponding term is included.

$$Z = J_0 + J_1 \underbrace{\sum_i \hat{S}_i} + \underbrace{\sum_{i<j} J_{ij} \hat{S}_i \hat{S}_j} + \underbrace{\sum J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k} + \ldots$$



0 1 0 0 1 1 0 1



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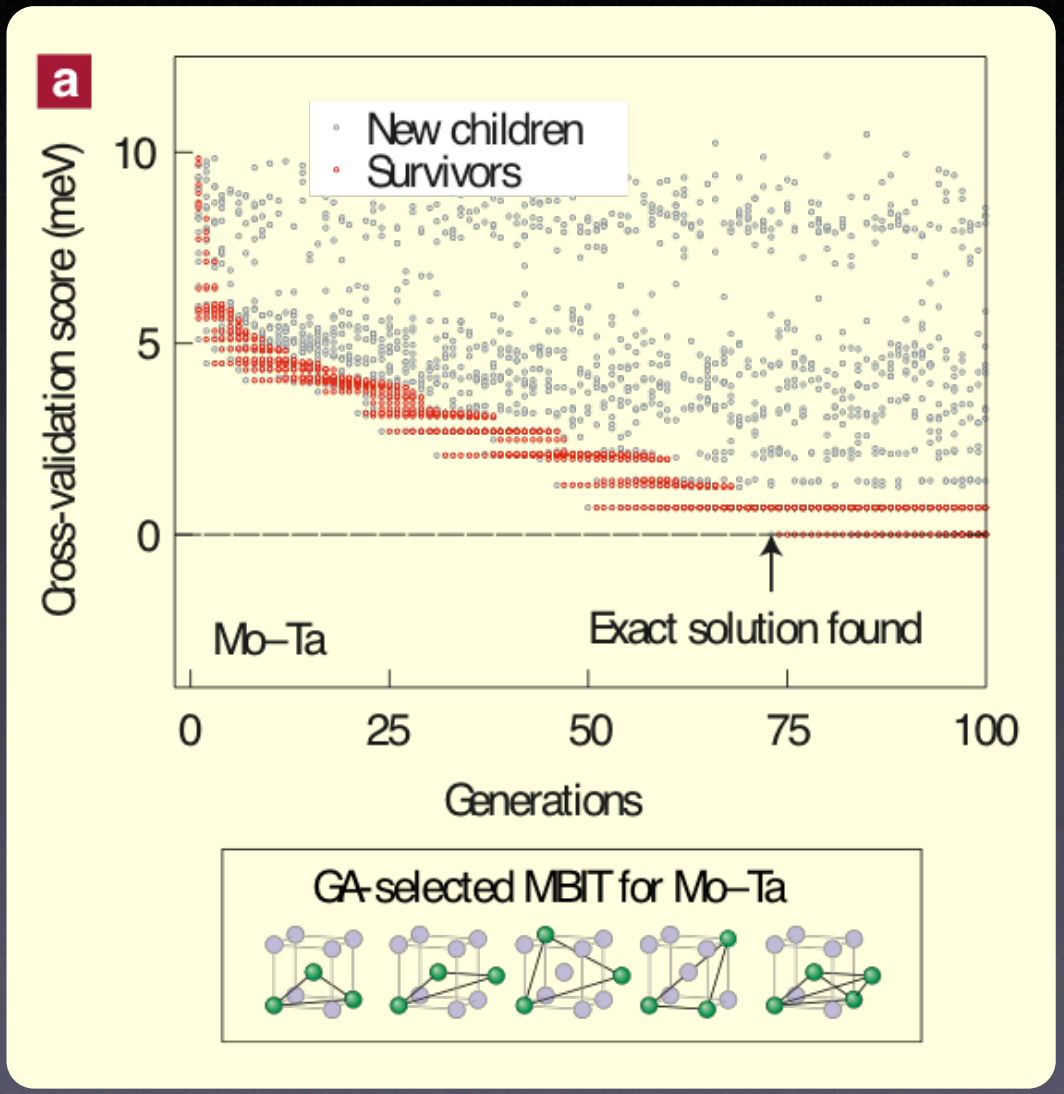
But does it work?

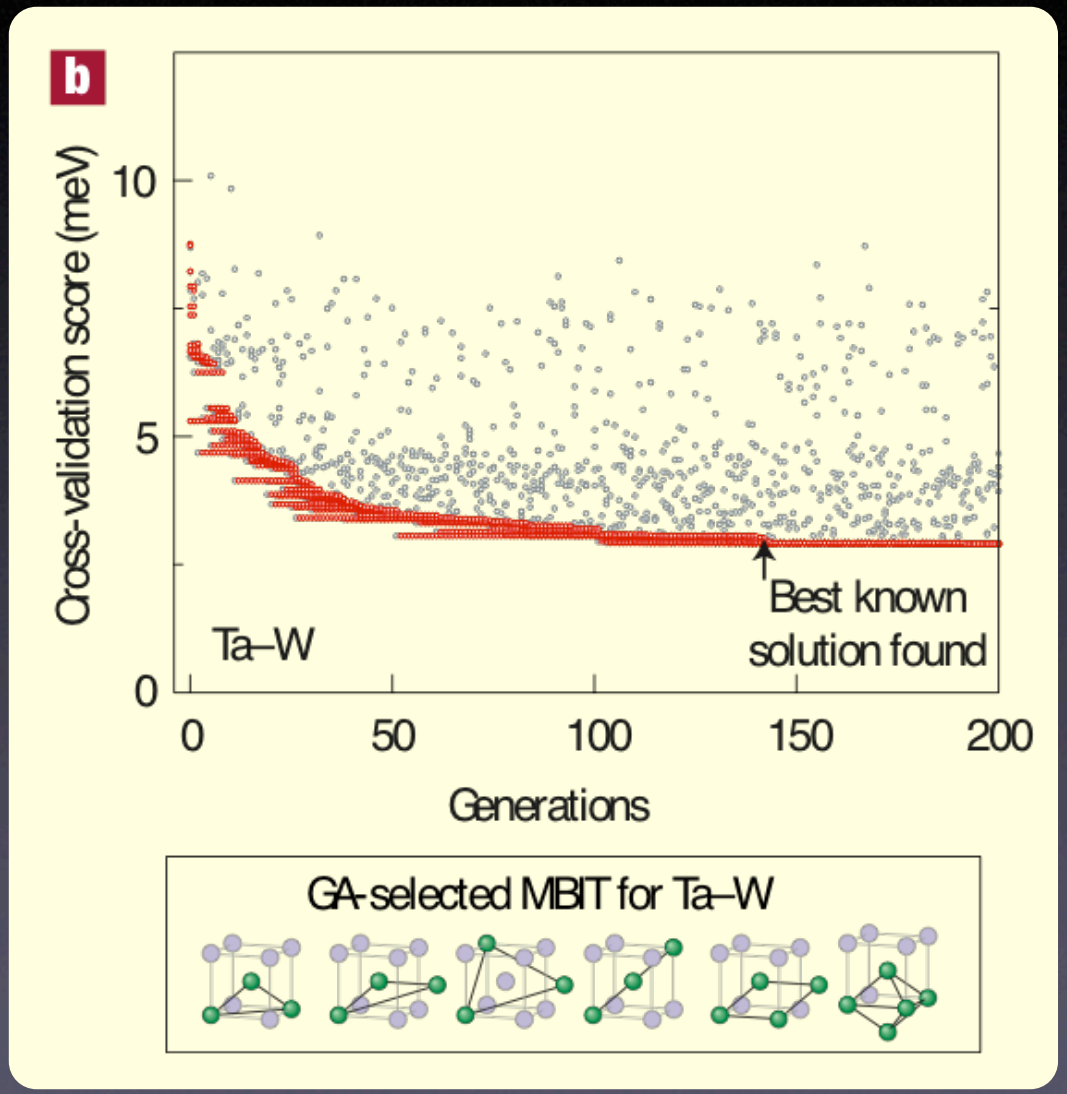


Exact case:

$$\binom{45}{5} = 1.22 \times 10^6$$

Total solutions explored: 975 (< 0.1%)

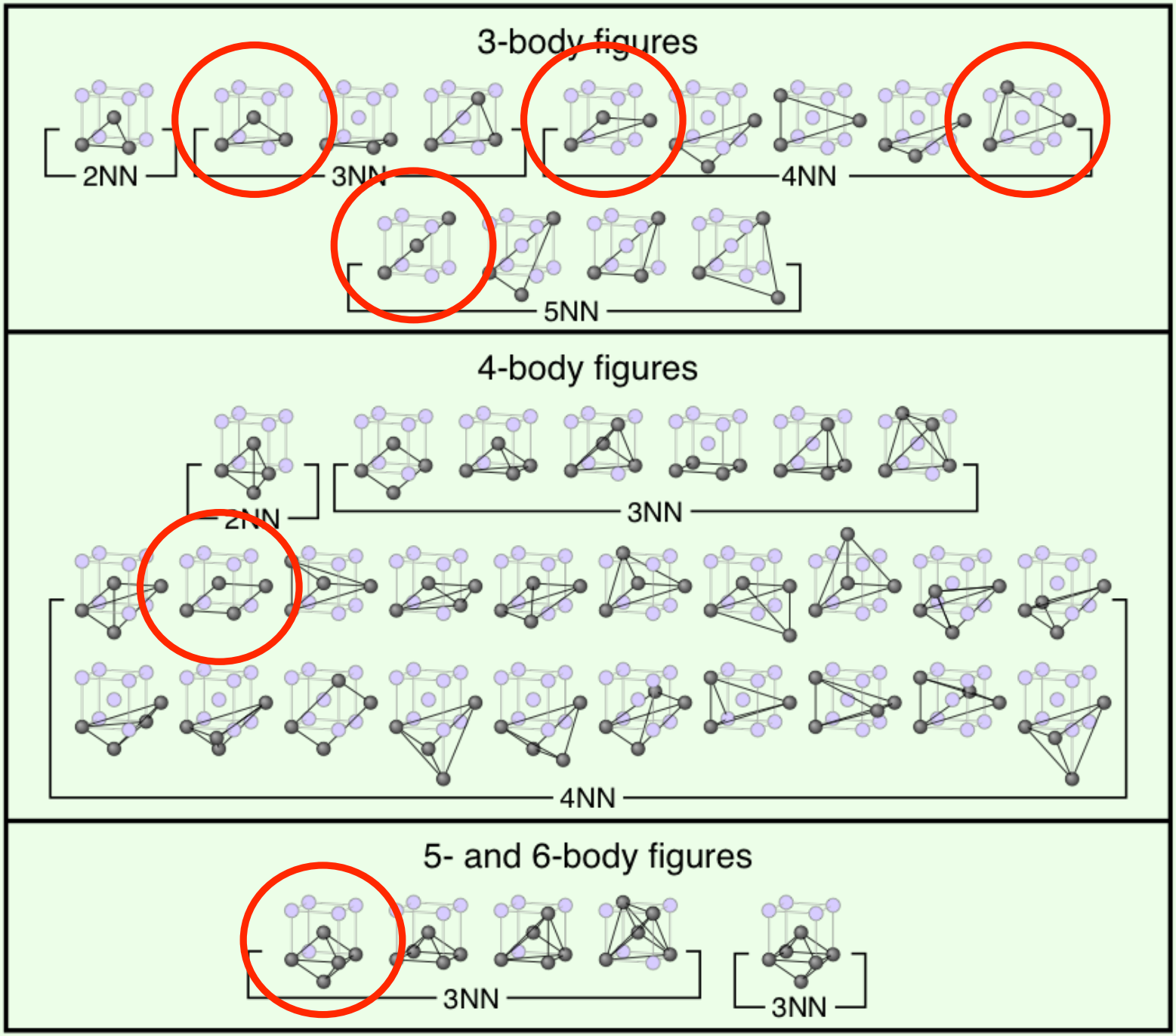
But does it work?



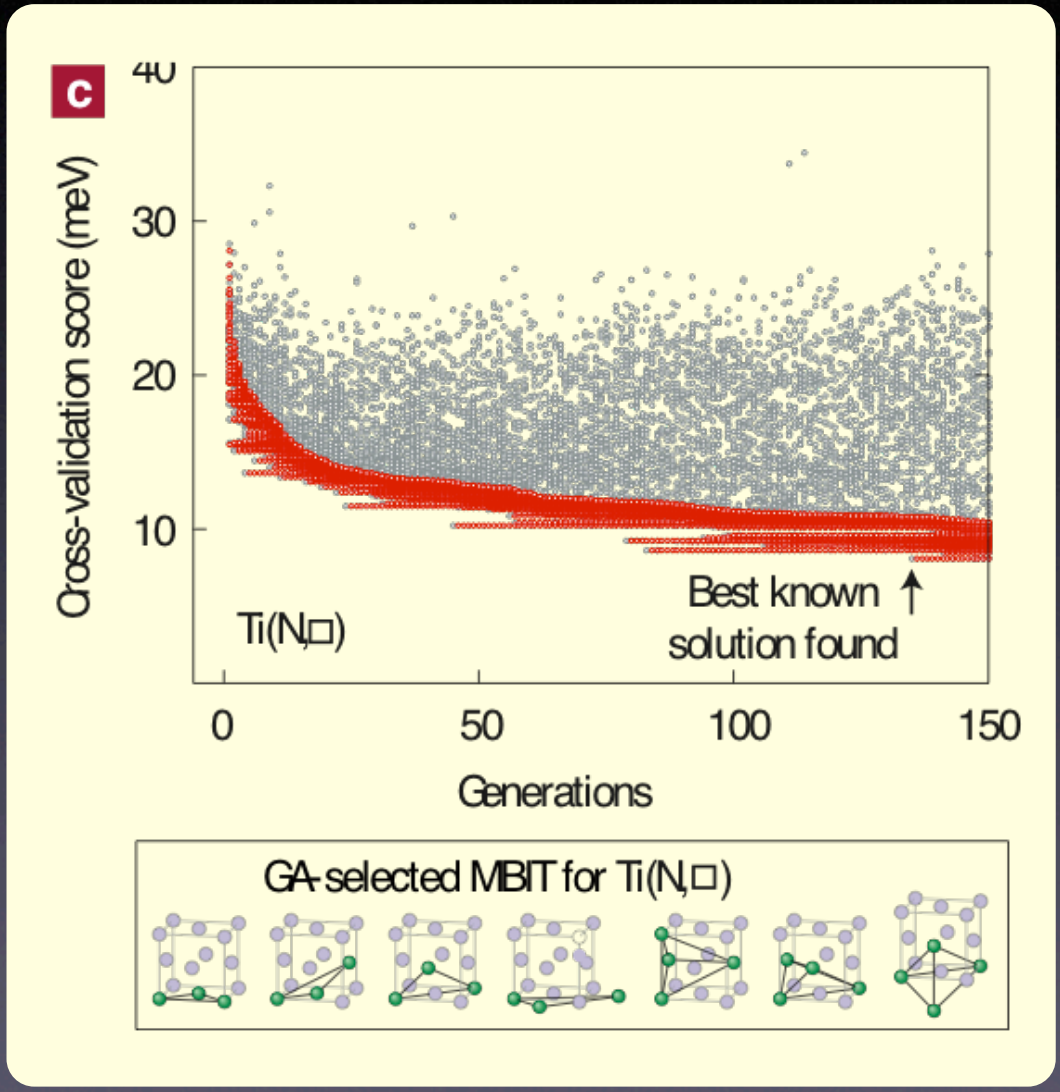
$$\binom{45}{6} = 8.1 \times 10^6$$

Only 0.02% of the solution space is explored by the GA

Best set of MBITs doesn't follow a systematic scheme


3-body figures
2NN
3NN
4NN
5NN
4-body figures
2NN
3NN
4NN
5- and 6-body figures
3NN
3NN

But does it work?

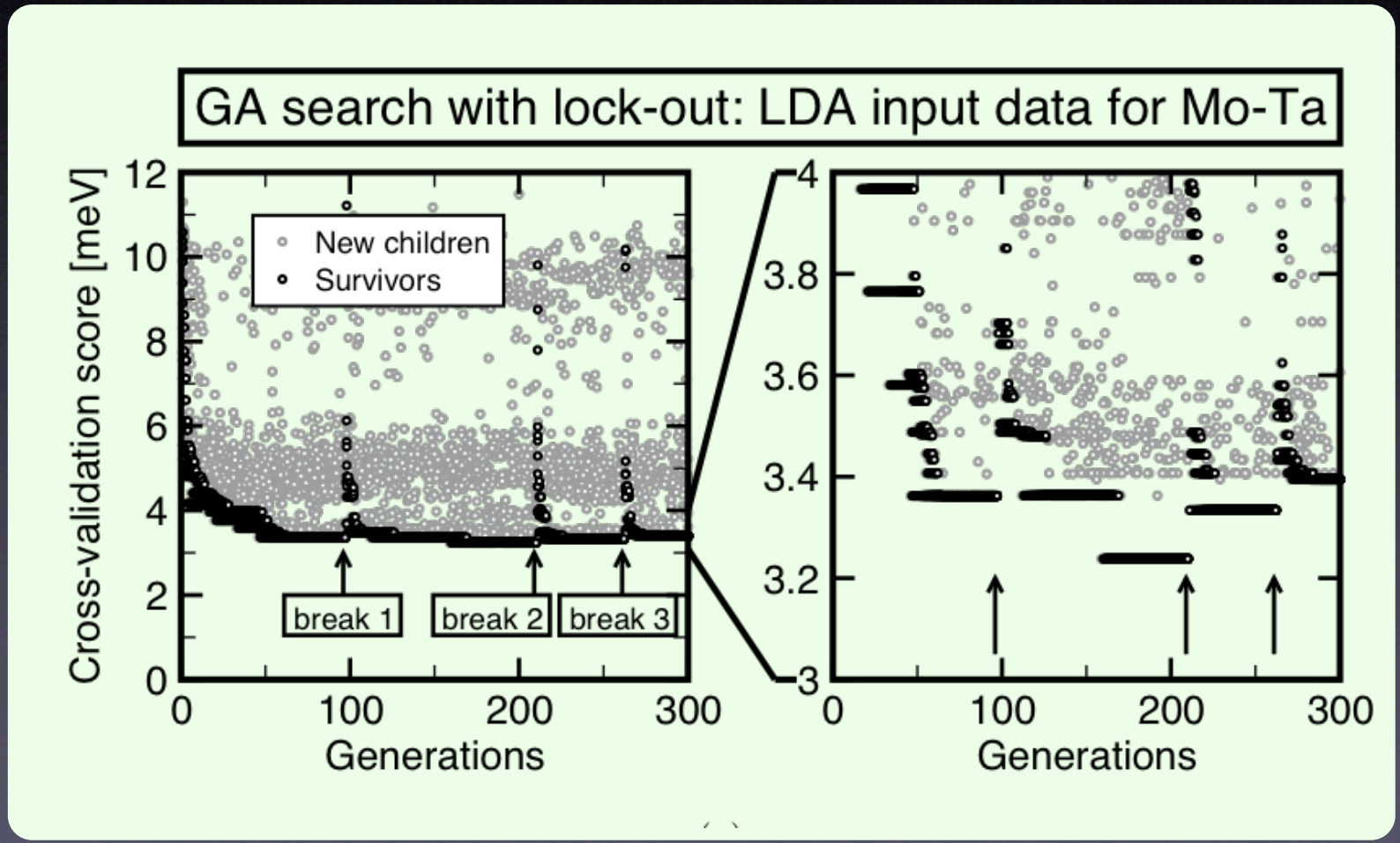


$$\binom{58}{7} \approx 3 \times 10^8$$

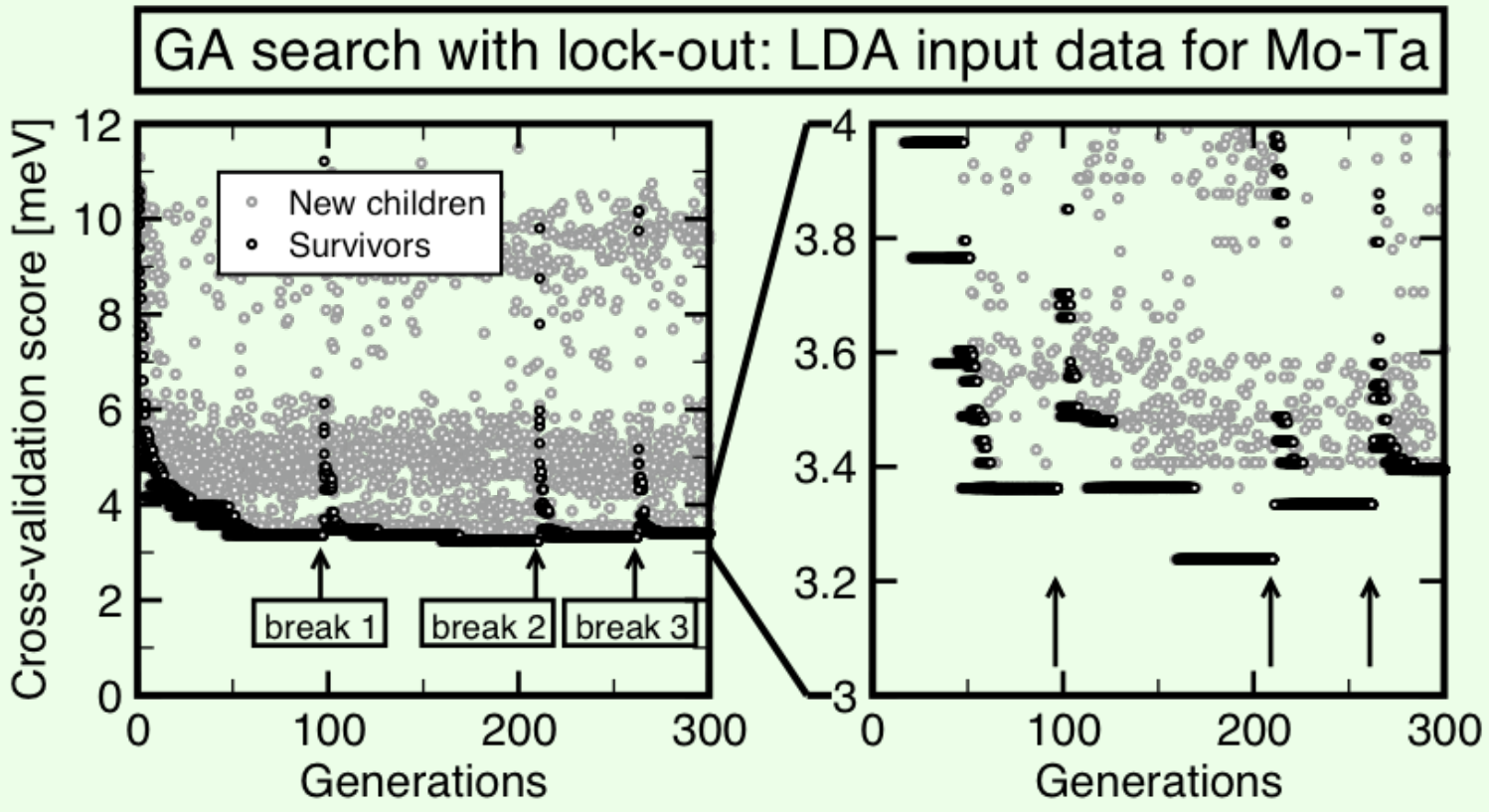
Only 1/30 000 of the solution space is explored by the GA

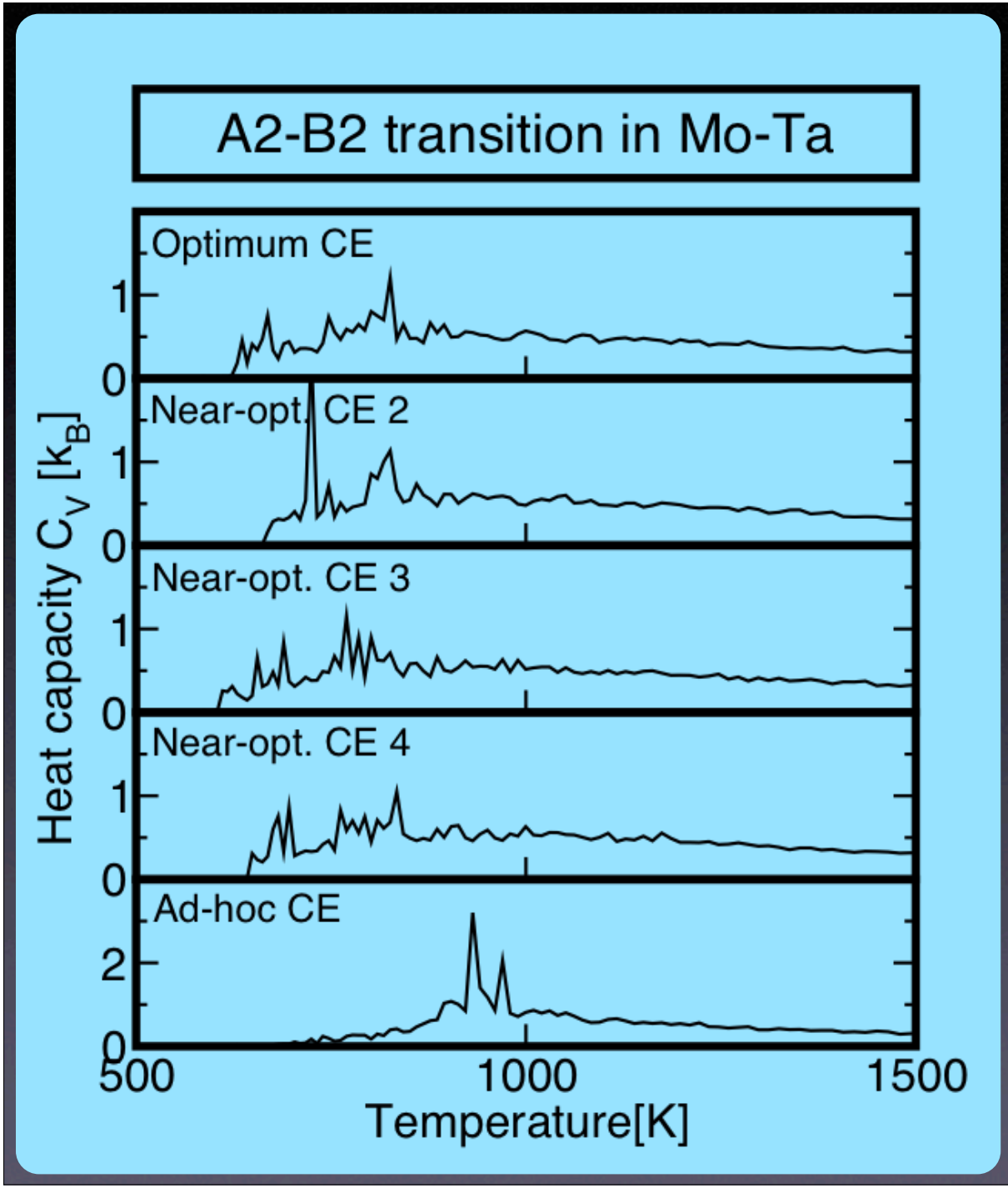
Different lattice (fcc)
Different chemistry

Still have problems with local minima...



“Lock-out” makes the approach completely robust



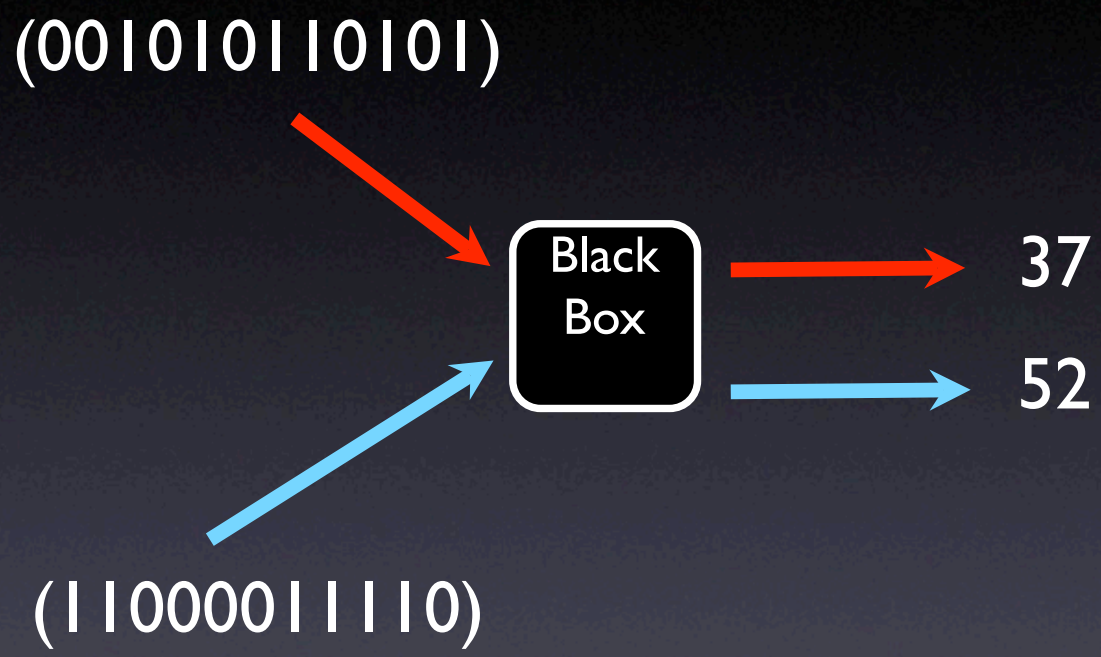


Do we *really* need all this accuracy in the fitting/ construction ?

Does it really make a difference?!

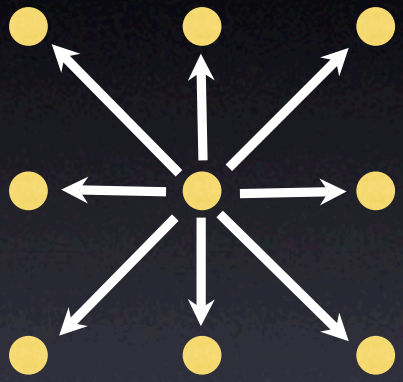
Now for the fun part...
(Today's lab)

A simple view of the problem



What string of zeroes and ones will minimize the output?

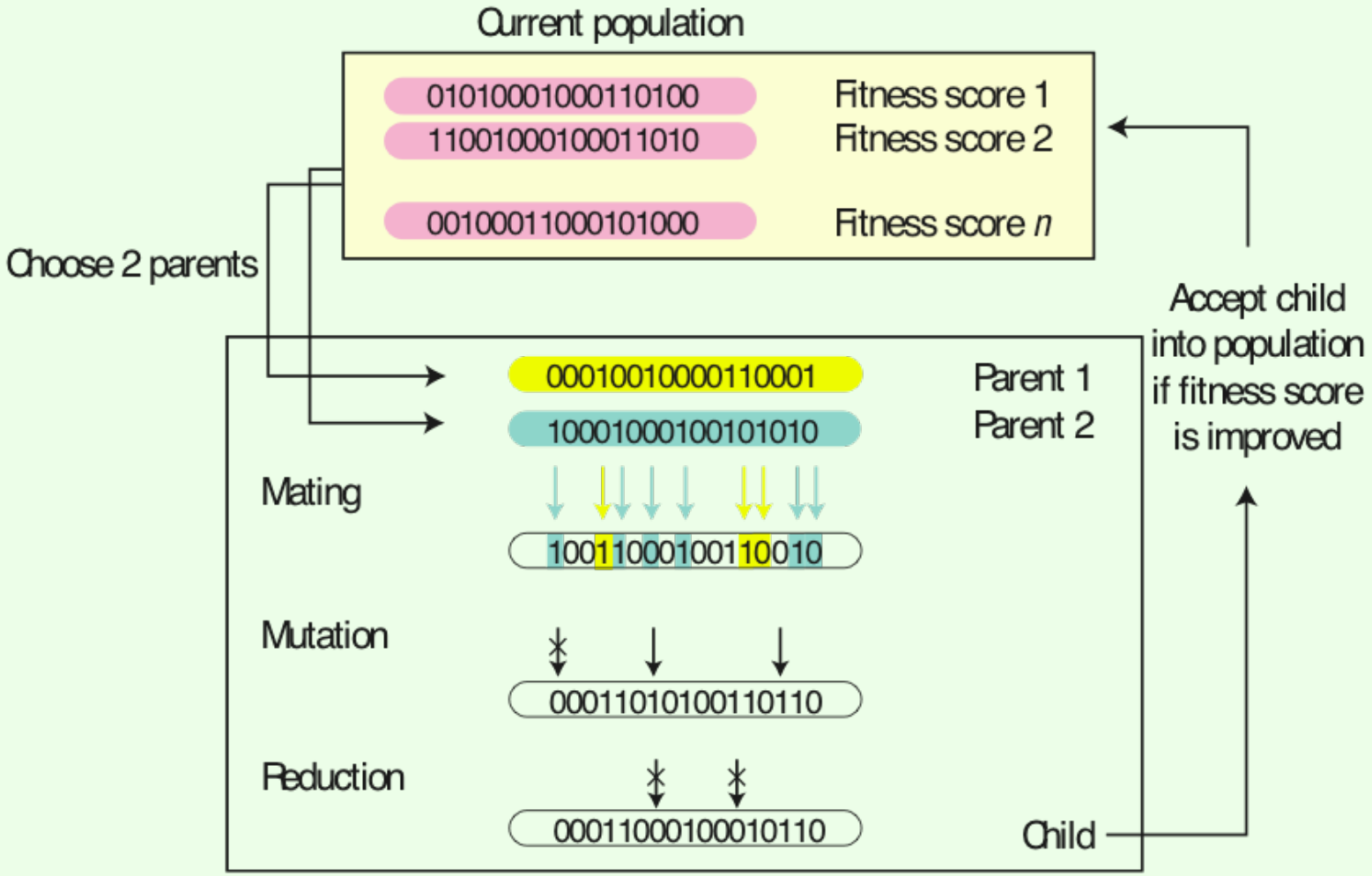
The specific problem for today



3x3 Lattice
Every site is connected
(9x9-9)/2 connections
Each interaction is different
Compute the energy by summing over occupied “pairs”

Computing the energy

$$E(\vec{\xi}) = (\xi_1, \xi_2, \cdots, \xi_N) \begin{pmatrix} J_{1,1} & J_{1,2} & \cdots & J_{1,N} \\ J_{2,1} & J_{2,2} & \cdots & J_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ J_{N,1} & J_{N,2} & \cdots & J_{N,N} \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_N \end{pmatrix}$$



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