

ANDREW R. MCCLUSKEY ^[a,b], JAMES GRANT ^[a], STEPHEN C. PARKER ^[a] &
KAREN J. EDLER ^[a]

a. Department of Chemistry, University of Bath, Bath

b. Diamond Light Source, Rutherford Appleton Laboratory, Harwell-Oxford



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BATH



diamond

SURFACTANTS AND MOLECULAR DYNAMICS

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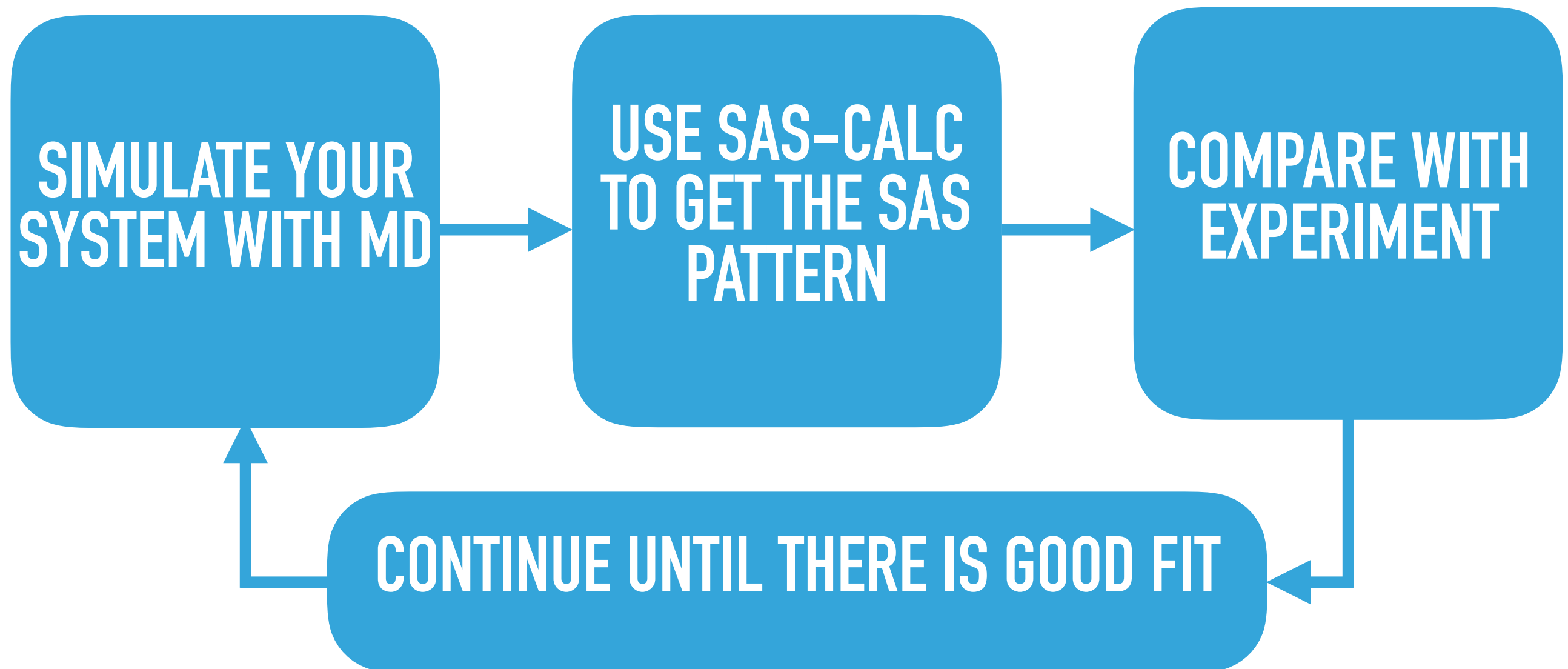


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SURFACTANTS **BUT NOT** MOLECULAR DYNAMICS

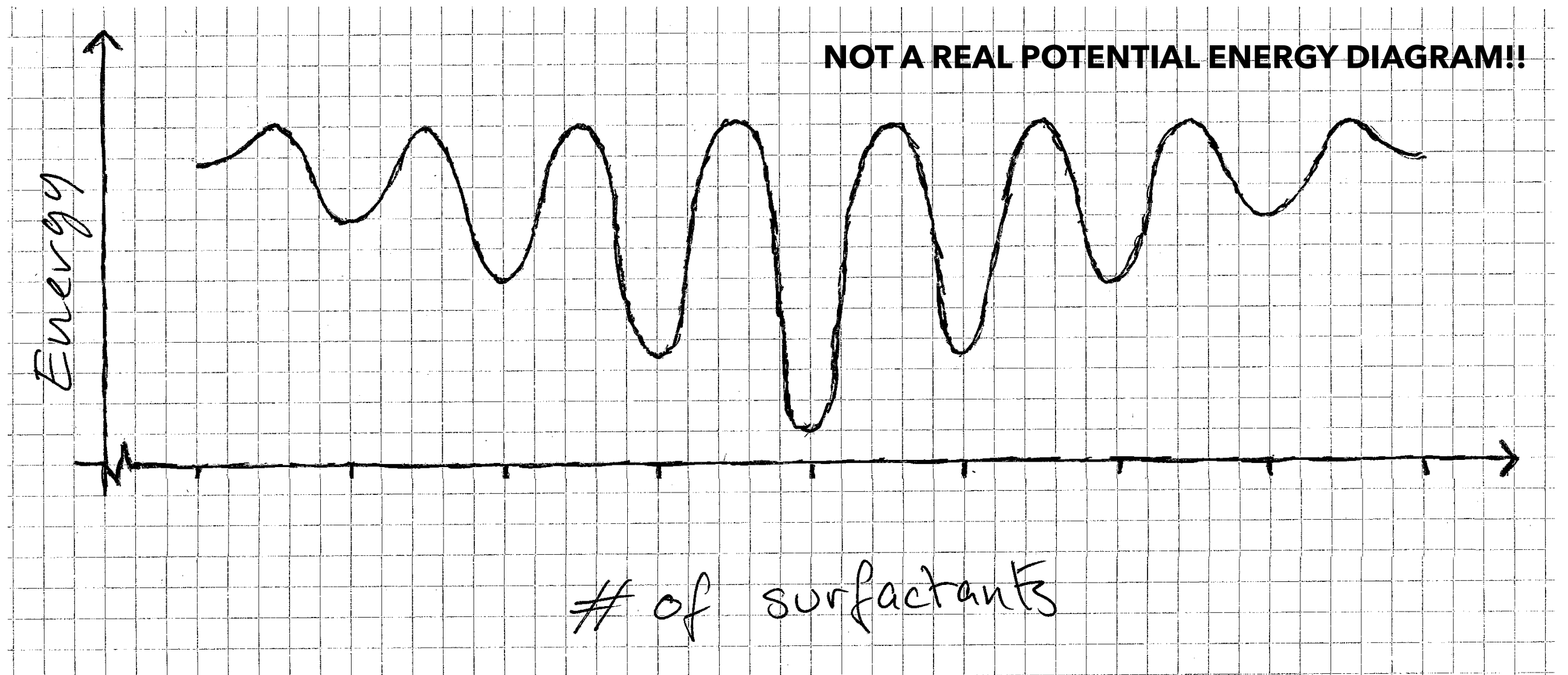


HOW SOFT MATTER PEOPLE USE SASSIE



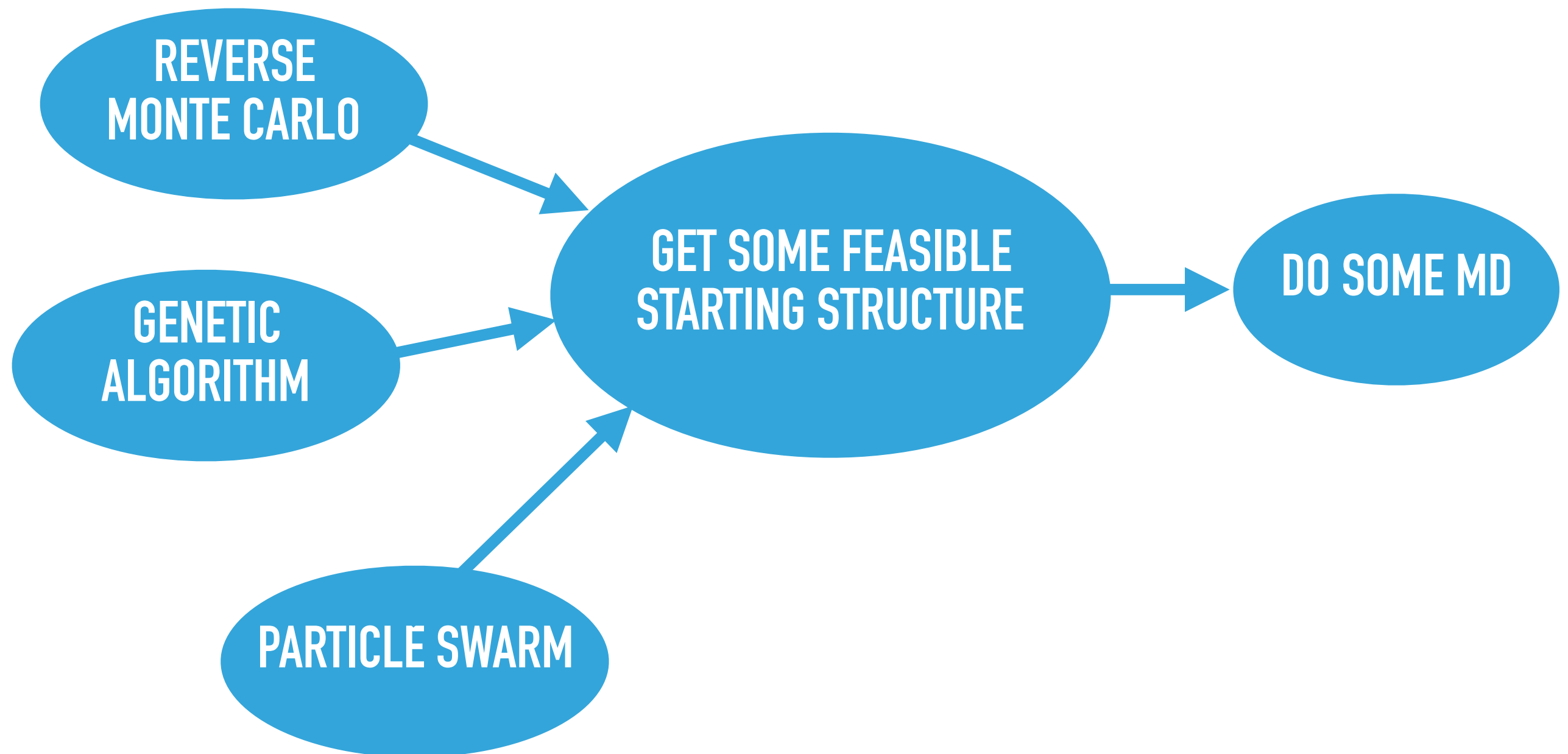


MICELLES ARE TOUGH TO SIMULATE



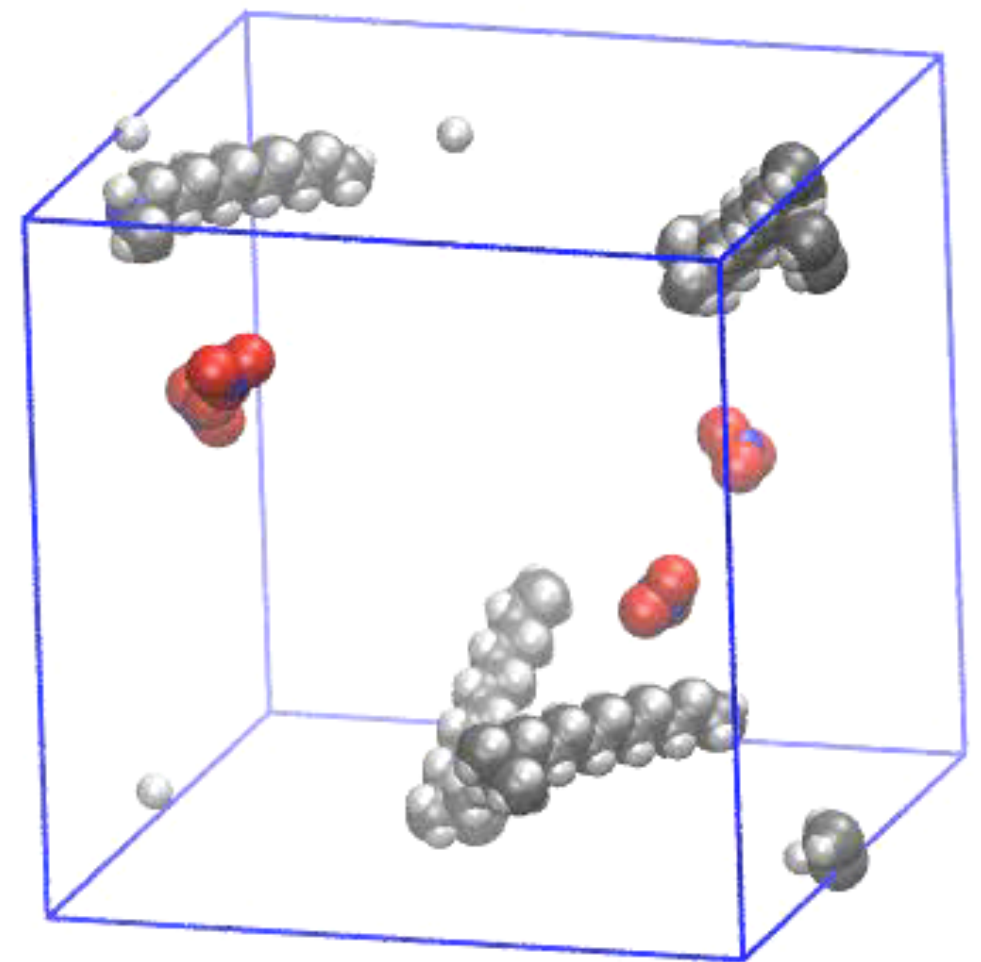
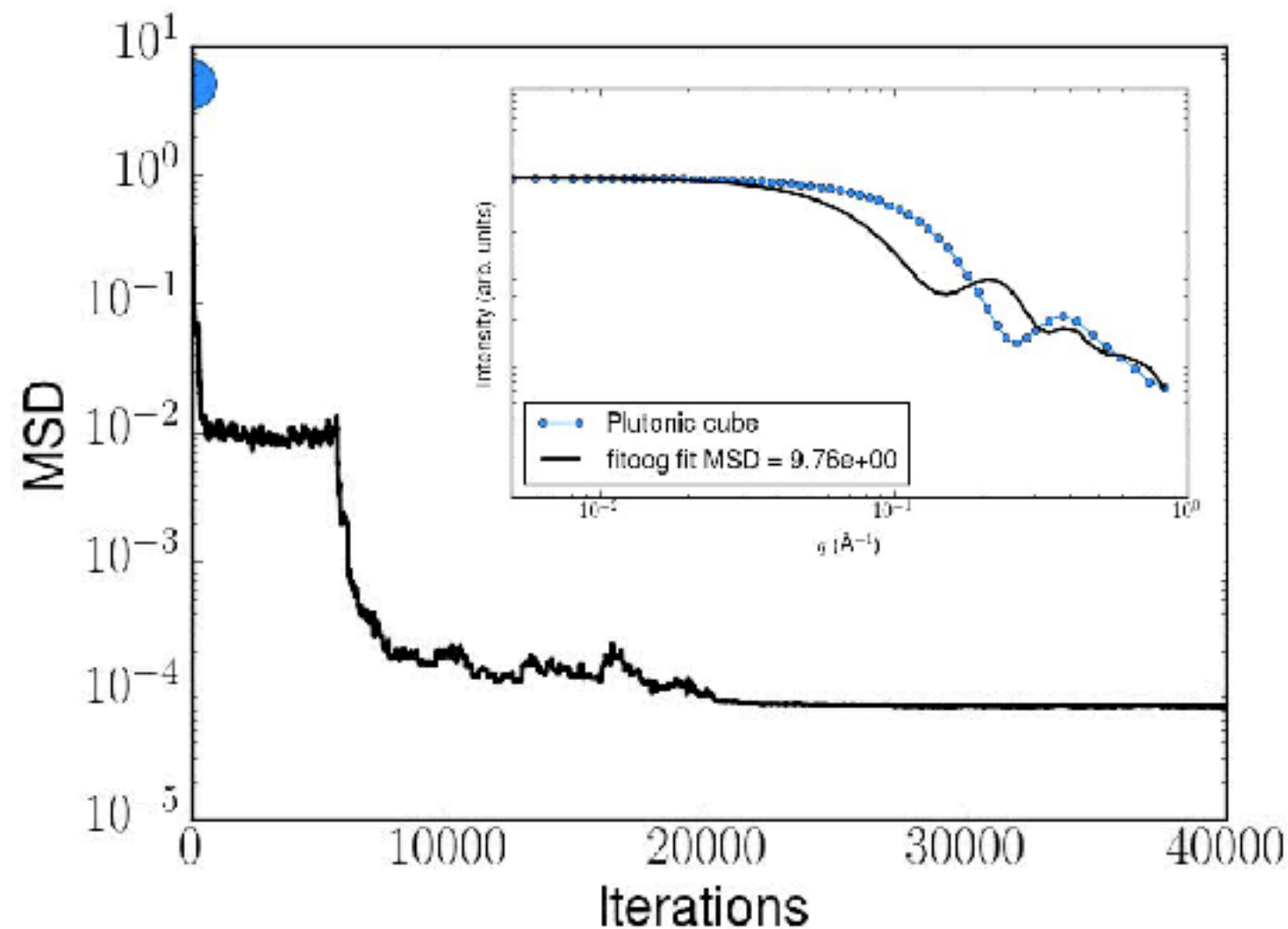


EDUCATE STARTING STRUCTURE WITH EXPERIMENT



FITOOG 1.0

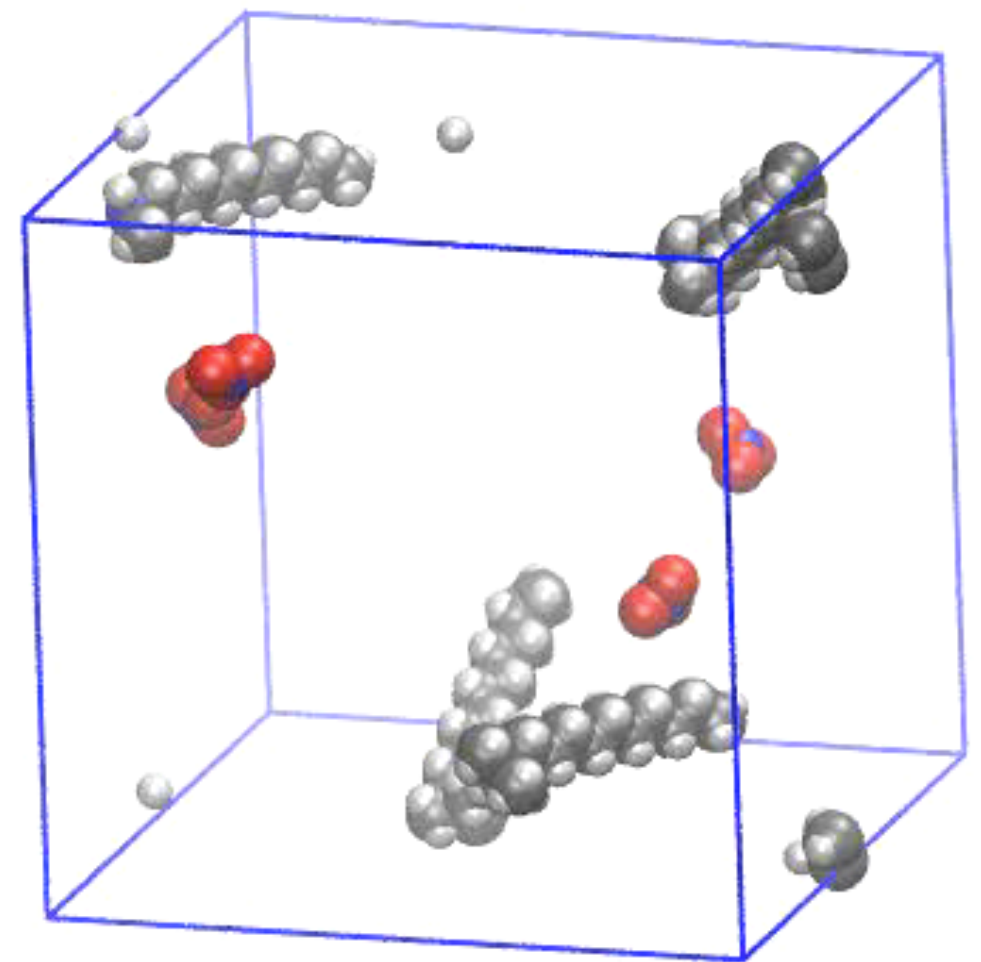
- Fitoog 1.0 was based on reverse Monte-Carlo



FIT00G 1.0

▶ **TOO SLOW**

- Written in python with no parallelisation
- ▶ Single structure
- ▶ The parameter space in a micellisation has hundreds of dimensions
 - Even with the Metropolis condition it is easy to be stuck in local minima



FITOOG 2.0

- ▶ Fitoog 2.0 uses a hybrid particle swarm-genetic algorithm



**INTRODUCING THE NEW
IMPROVED FITOOG 2.0**

PARTICLE SWARM ALGORITHM

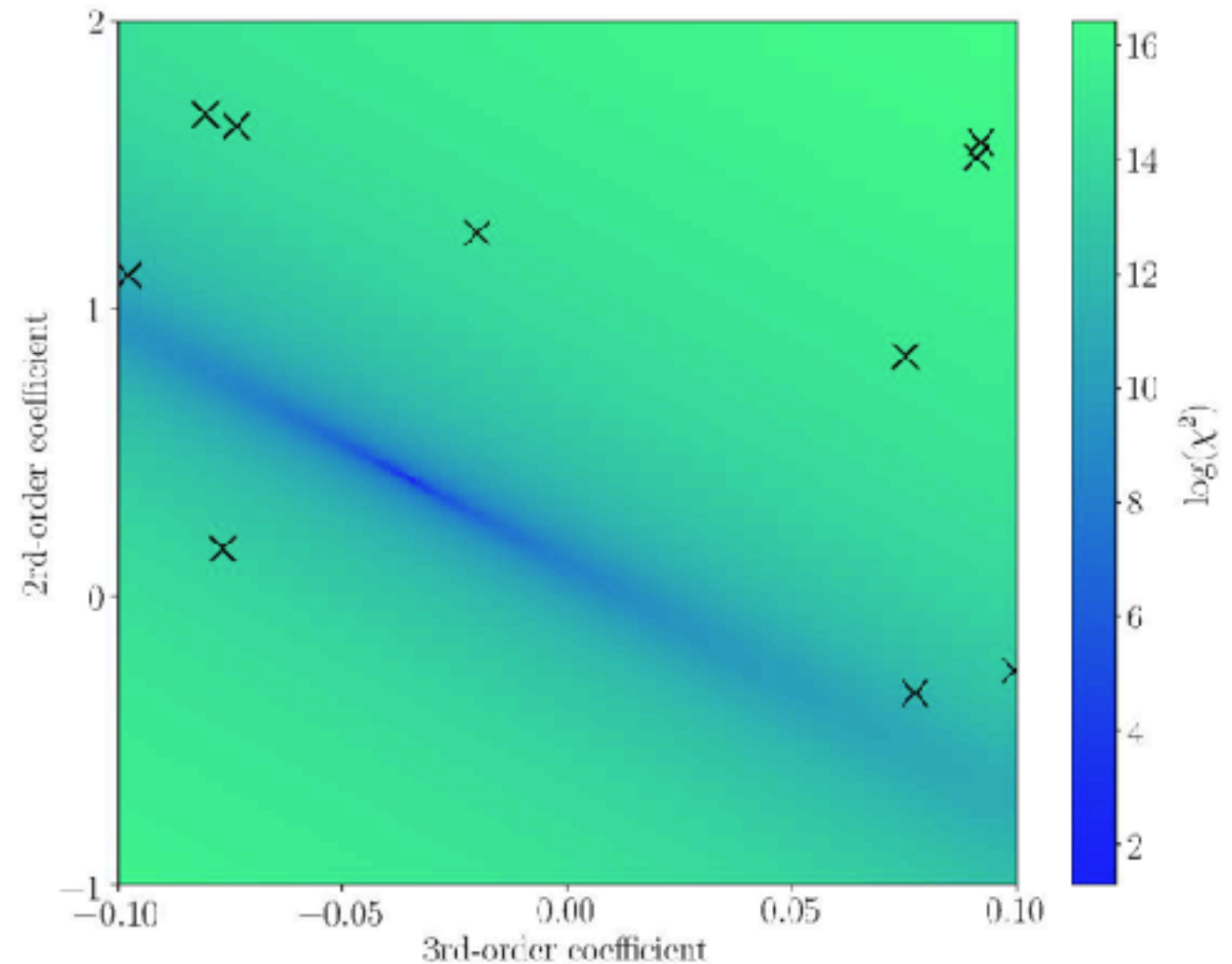
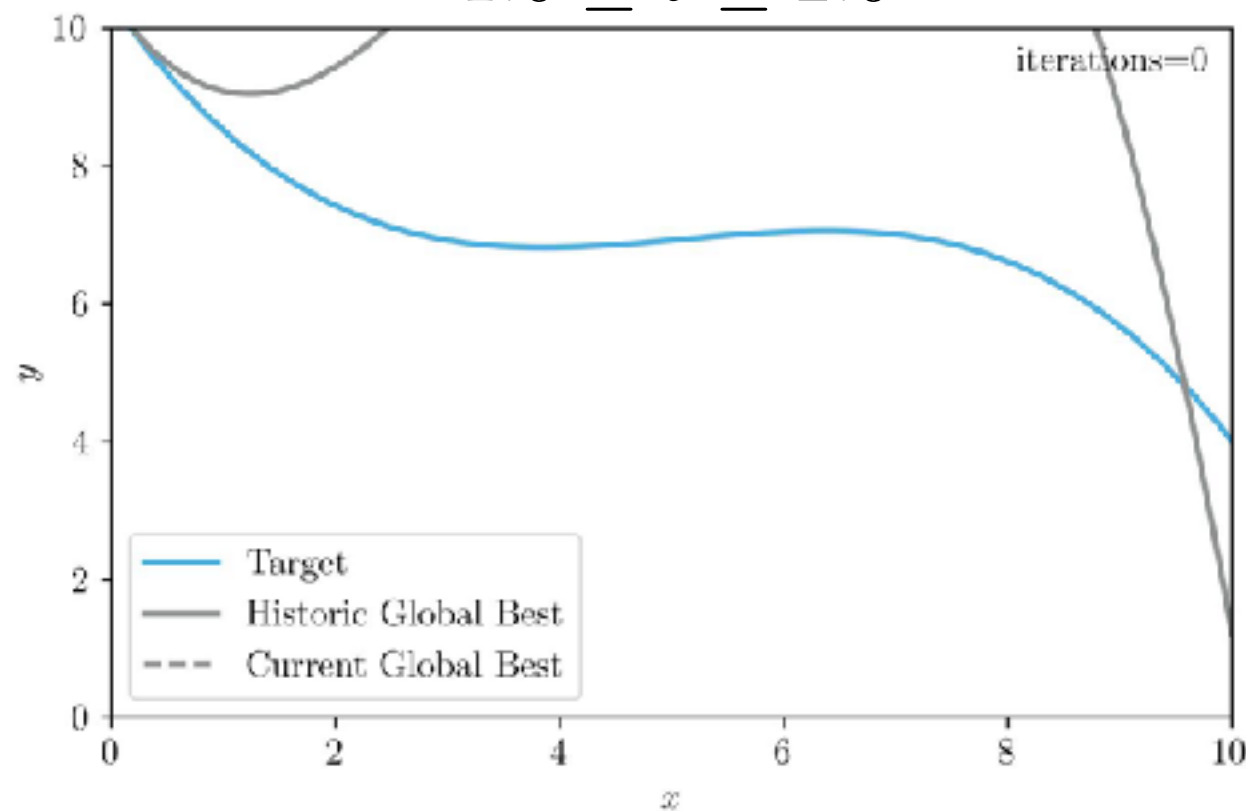
- ▶ Each particle has knowledge of its personal best position and the global best ever position in parameter space
- ▶ Parameters are changed based on a velocity that is determined as follows

$$v_i \leftarrow v_i + U(0, \phi_1) \times (p_i - x_i) + U(0, \phi_2) \times (p_g - x_i)$$

$$x_i \leftarrow x_i + v_i$$

PARTICLE SWARM ALGORITHM

$$y = ax^3 + bx^2 - 2.3188x + 10.386$$
$$-0.1 \leq a \leq 0.1$$
$$-1.0 \leq b \leq 2.0$$



Can get stuck in local minima

GENETIC ALGORITHM

INITIAL POPULATION



GENETIC ALGORITHM

INITIAL POPULATION



SORT



5

6

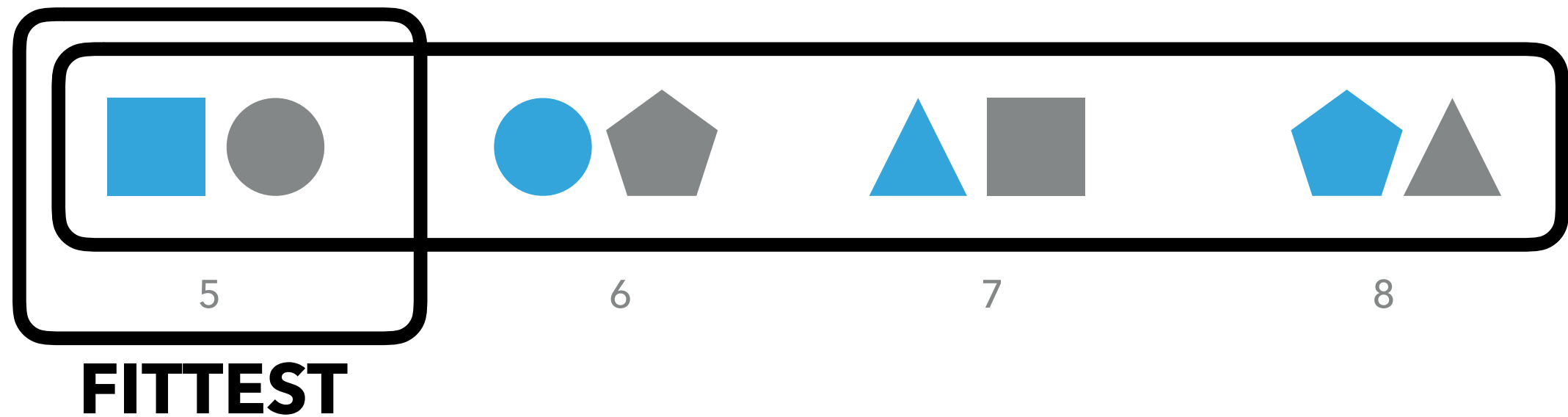
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8

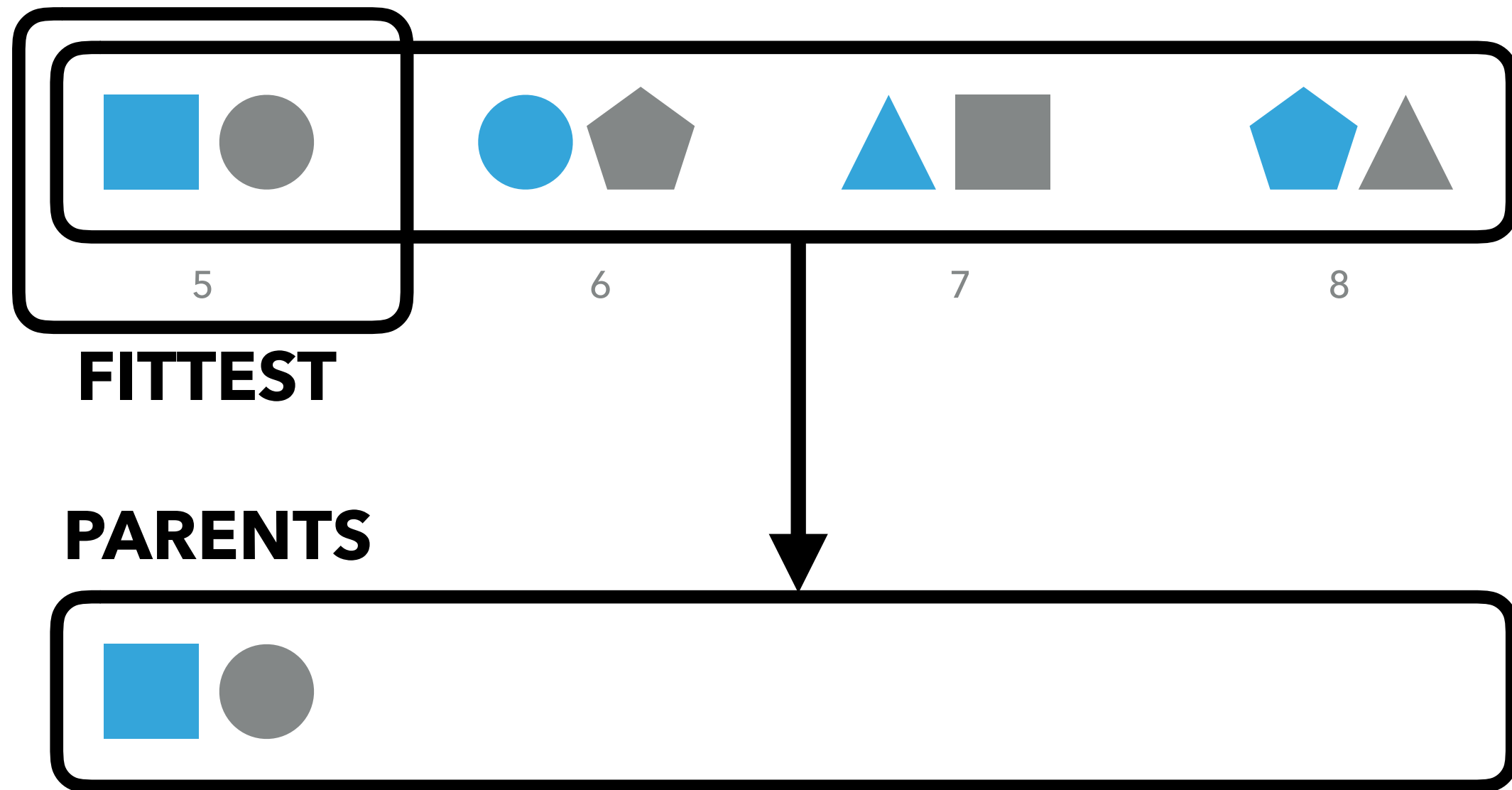
GENETIC ALGORITHM



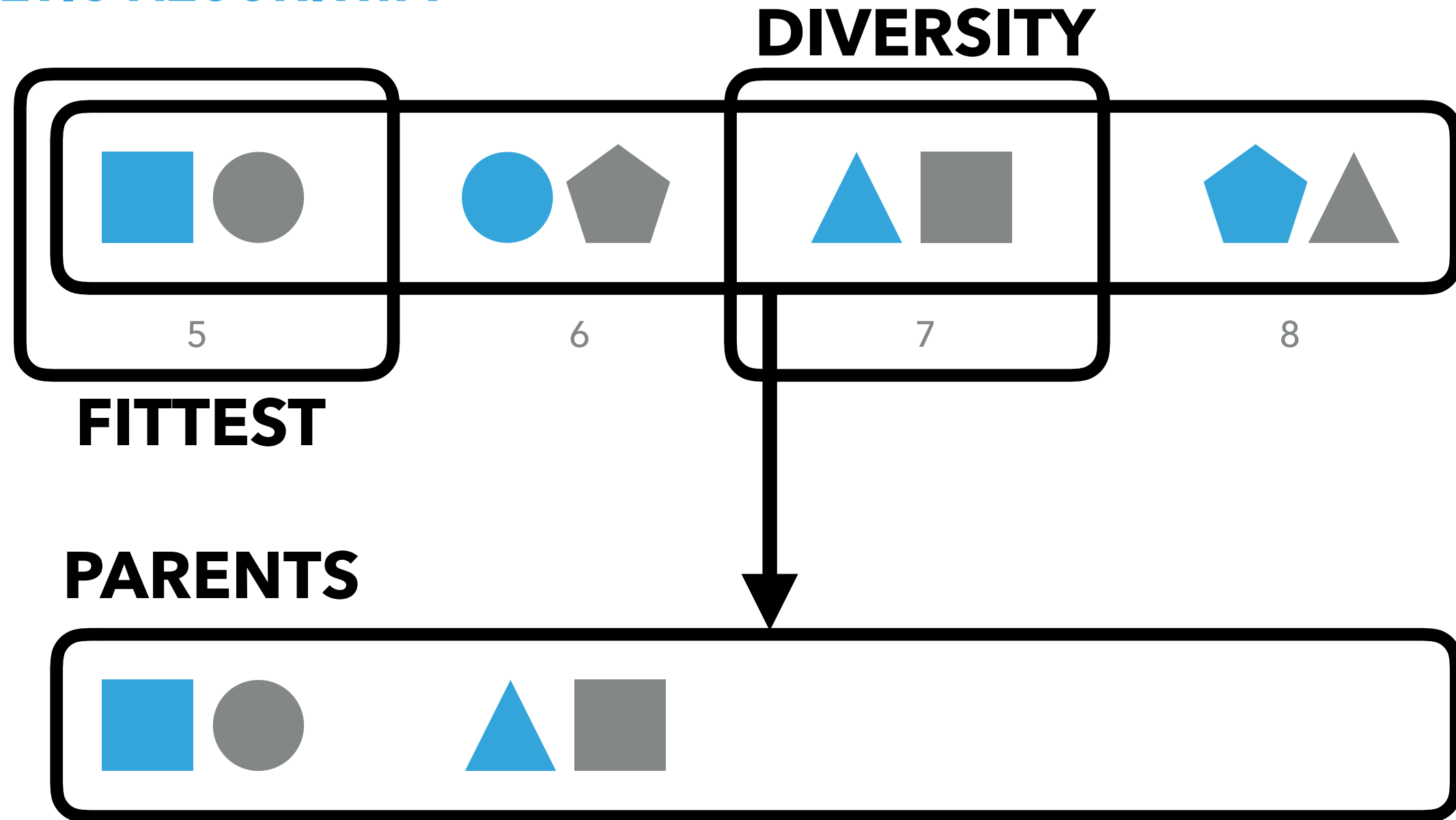
GENETIC ALGORITHM



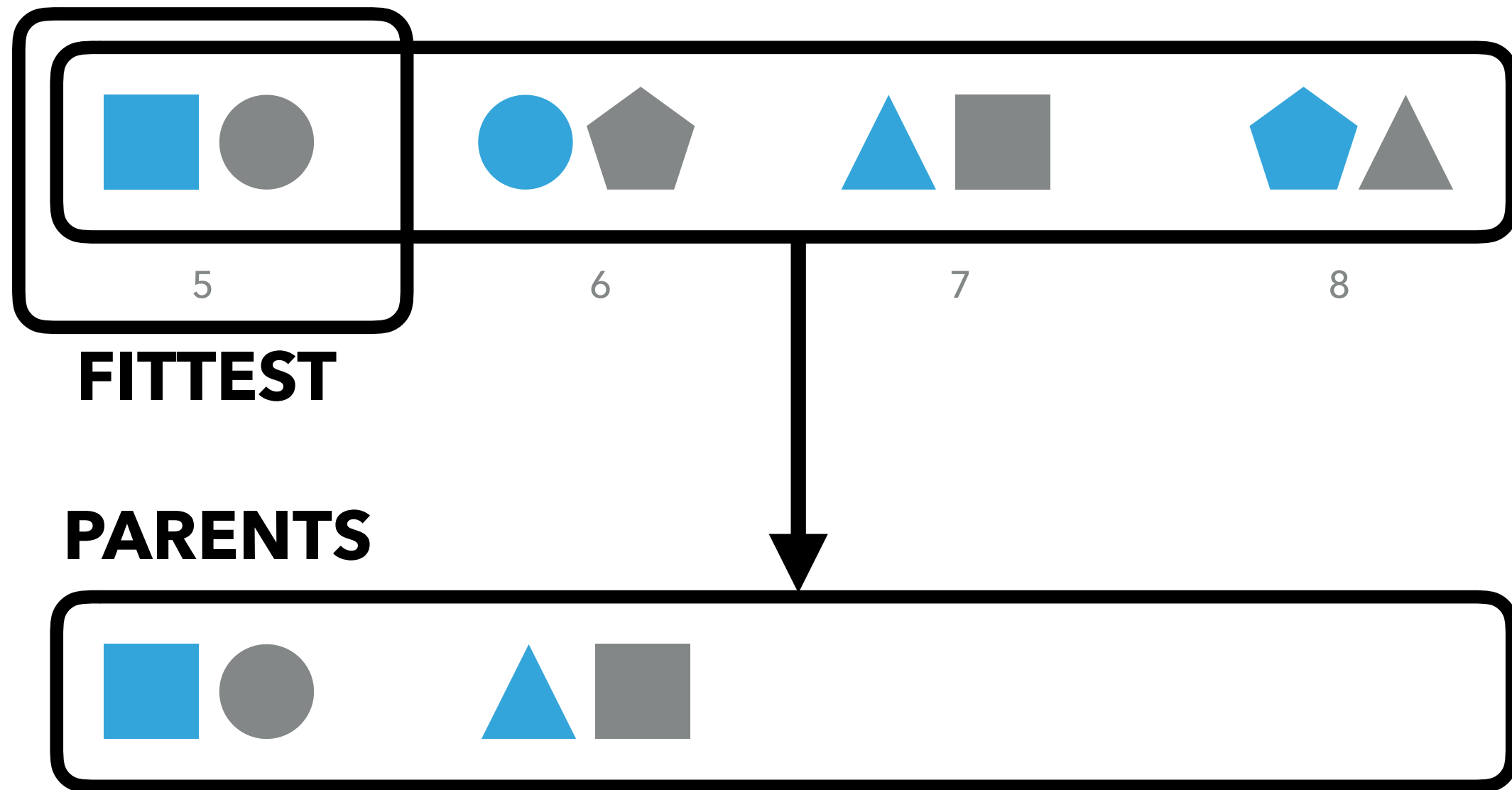
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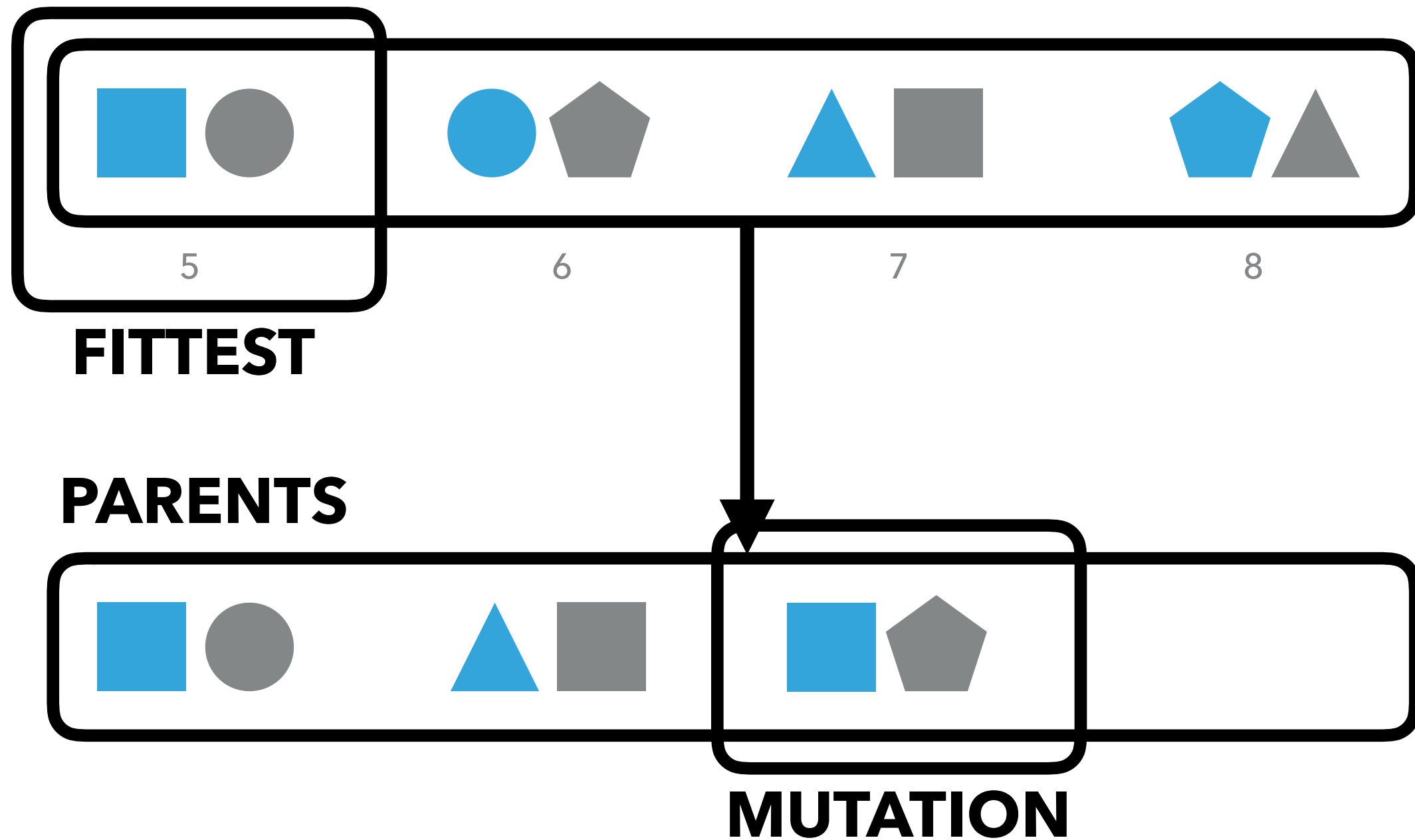
GENETIC ALGORITHM



GENETIC ALGORITHM



GENETIC ALGORITHM



GENETIC ALGORITHM

PARENTS

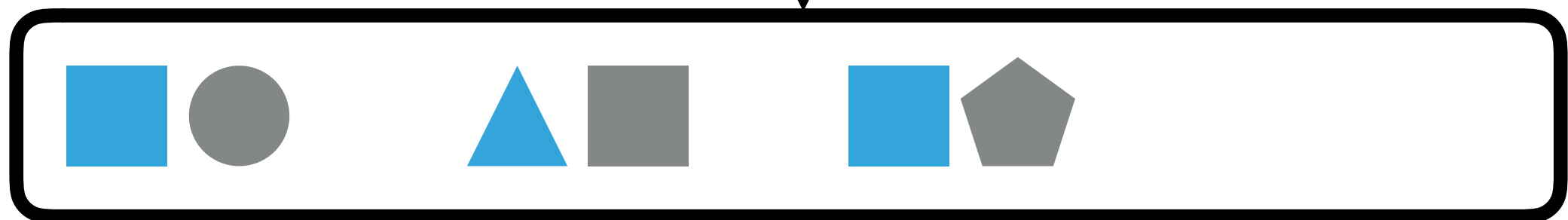


GENETIC ALGORITHM

PARENTS



NEW POPULATION

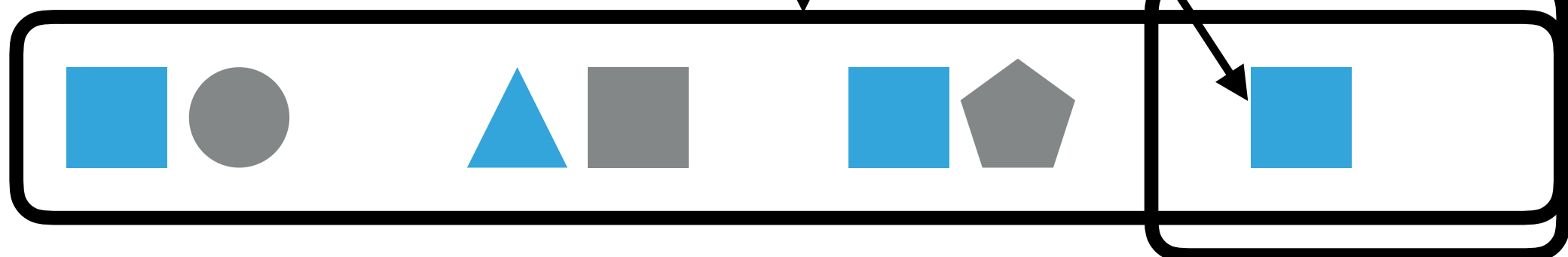


GENETIC ALGORITHM

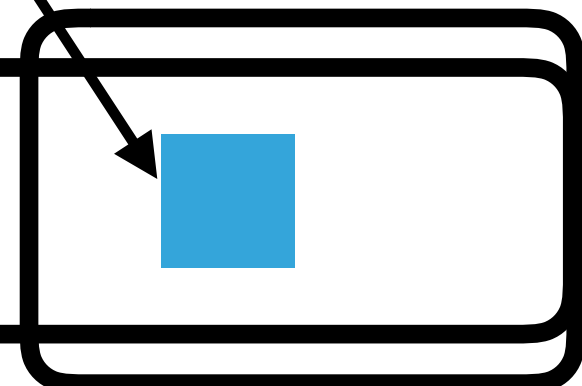
PARENTS



NEW POPULATION



CHILD

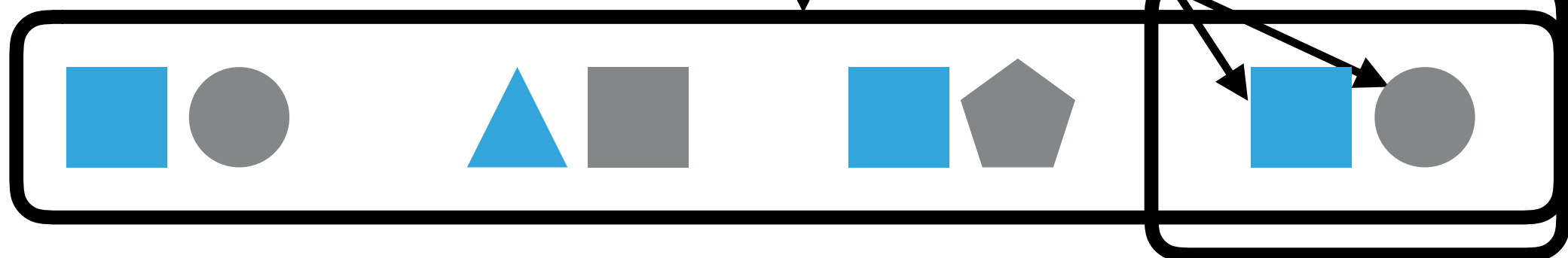


GENETIC ALGORITHM

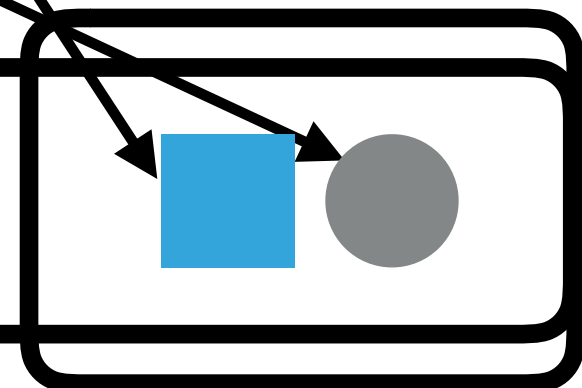
PARENTS



NEW POPULATION

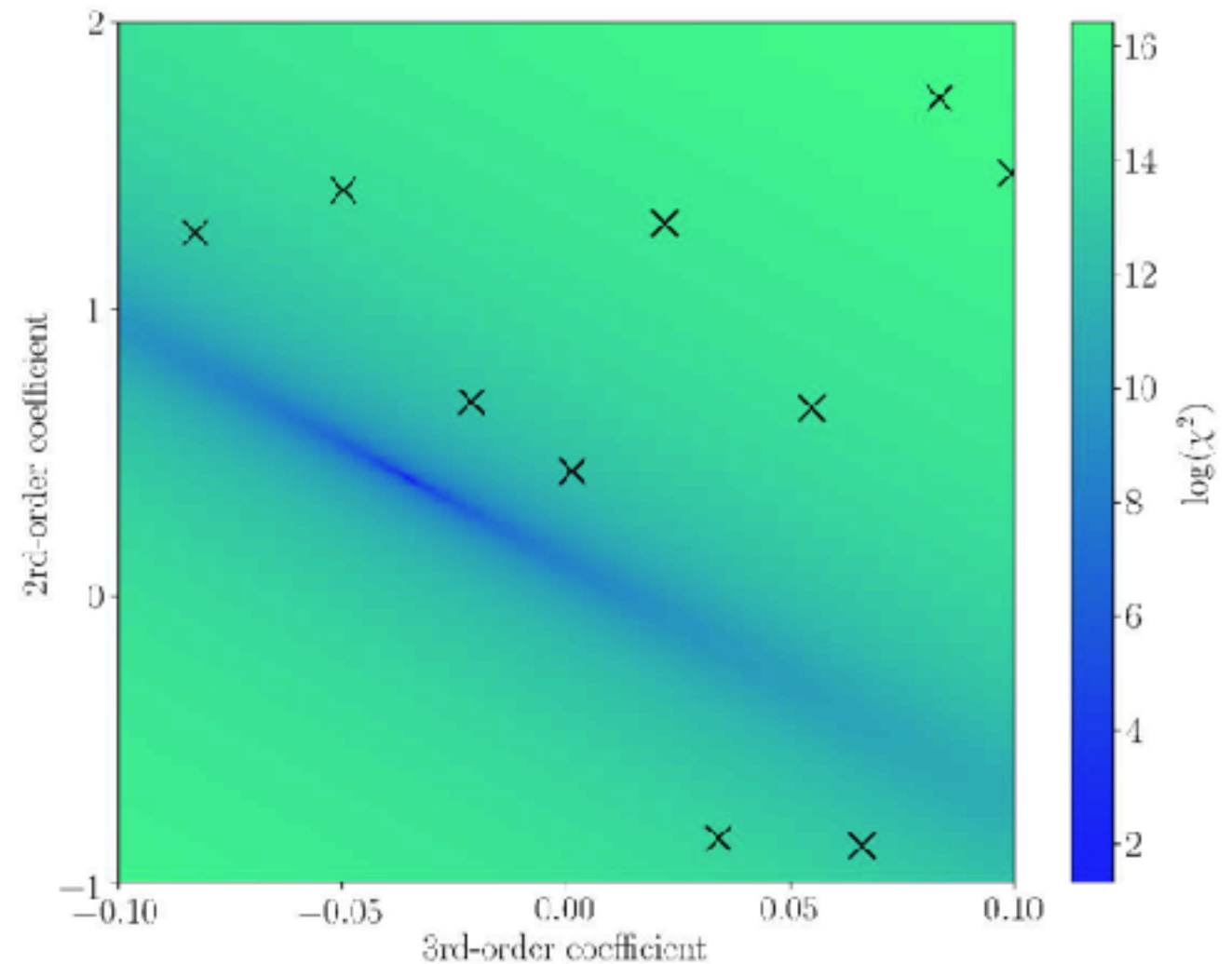
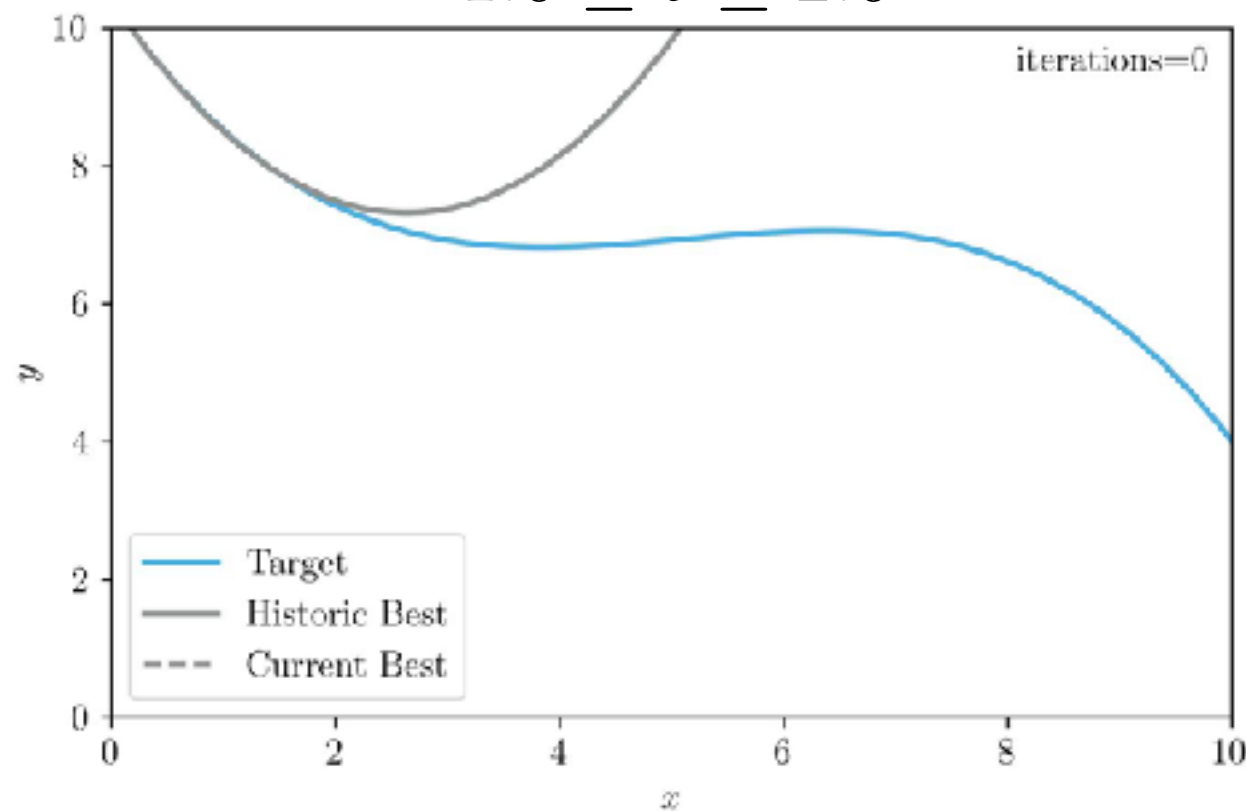


CHILD



GENETIC ALGORITHM

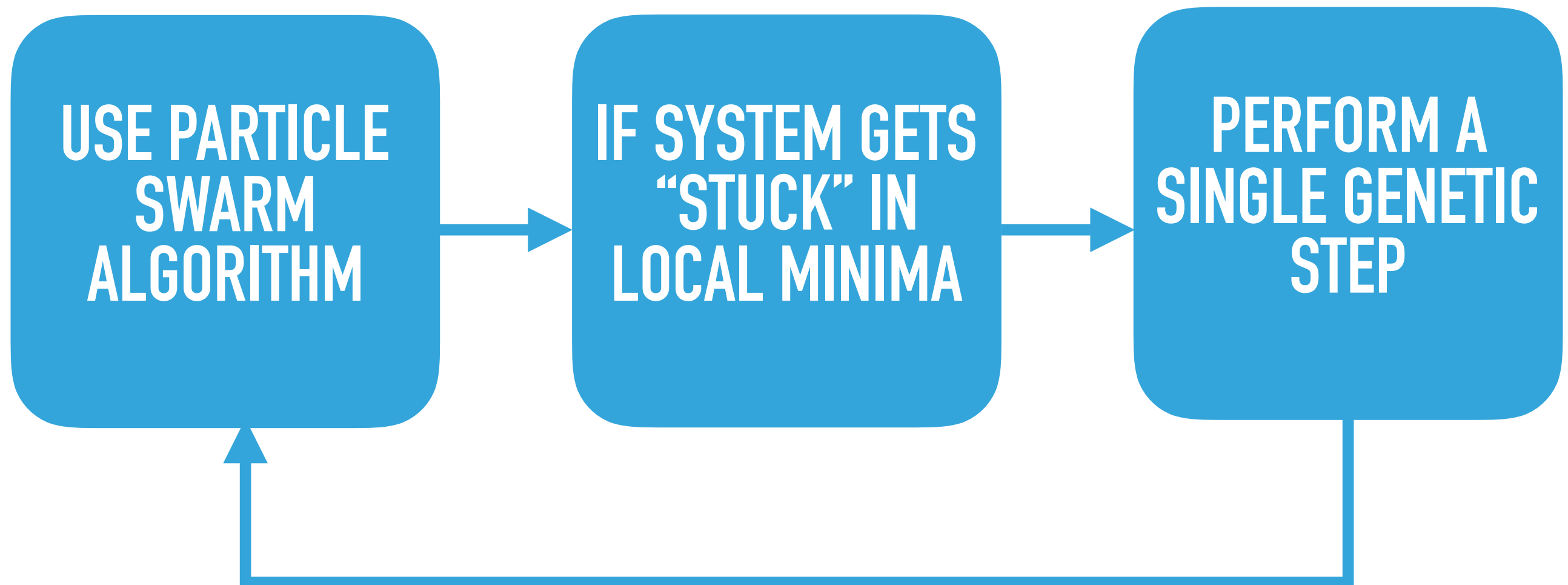
$$y = ax^3 + bx^2 - 2.3188x + 10.386$$
$$-0.1 \leq a \leq 0.1$$
$$-1.0 \leq b \leq 2.0$$



Can struggle to find the bottom of a minimum



BEST OF BOTH WORLDS?

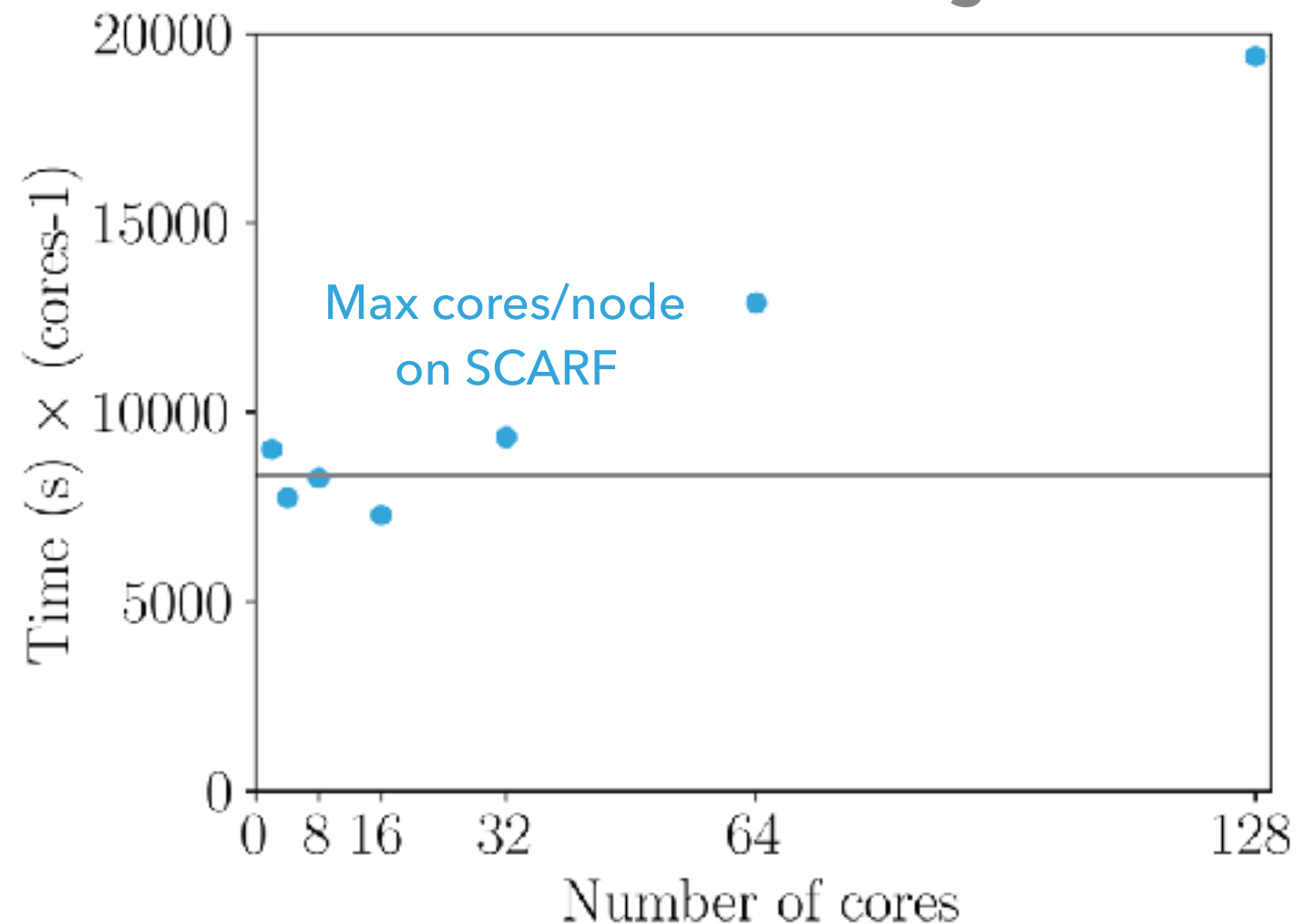




FIT00G 2.0

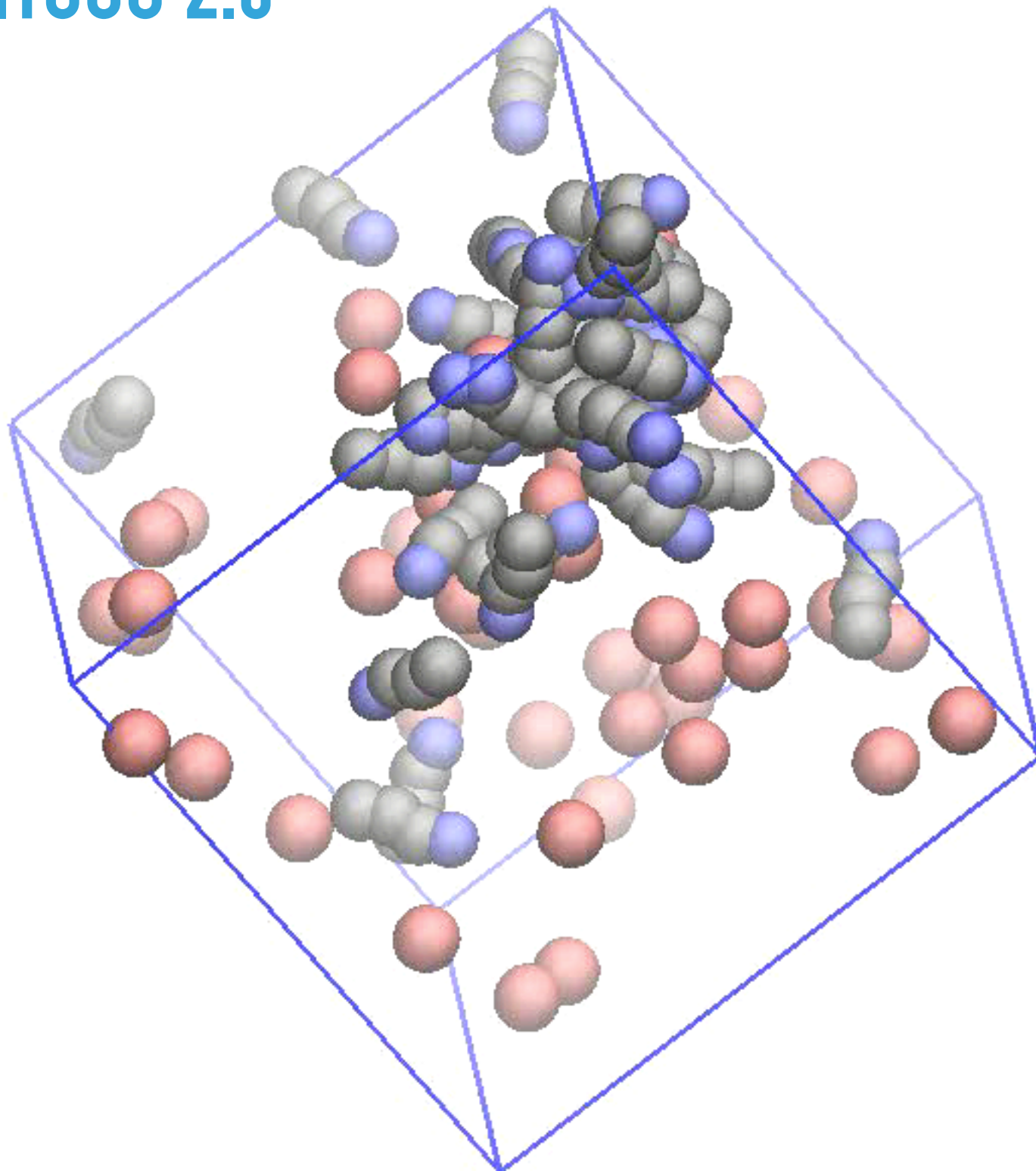
- ▶ C++
- ▶ Parallelised with MPI
 - Over scattering calculation for each population member
- ▶ Population of structures
- ▶ Centre-of-mass and orientation are parameters that are optimised
- ▶ Relatively straightforward to try different algorithms
- ▶ Really not ready for people to use but if you know what you are doing feel free
 - Open-source on Github

How is the scaling?

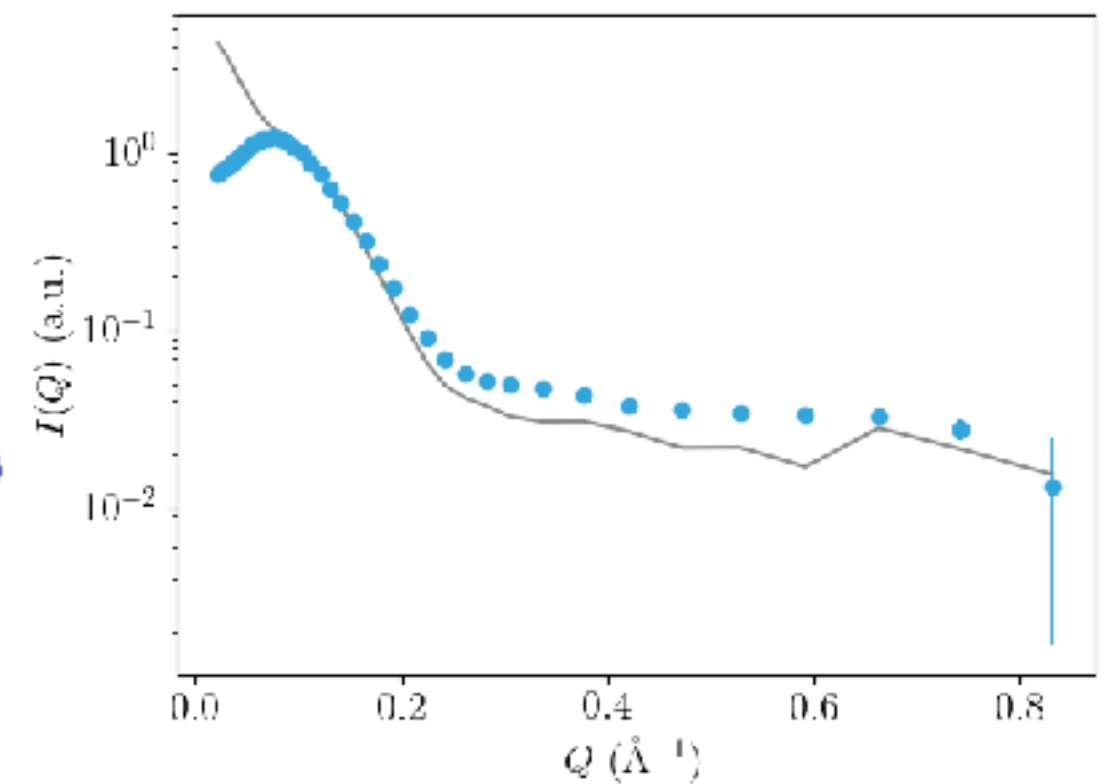




FIT00G 2.0



population size = 10000
number of steps = 10000



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Sadie