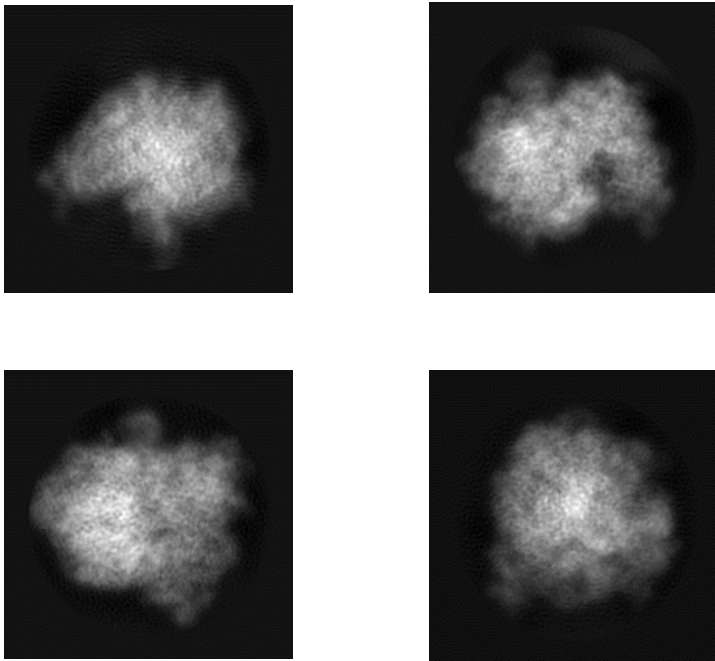# Bridging Structure and Evolution

Evolutionary Discovery of Molecular Structures
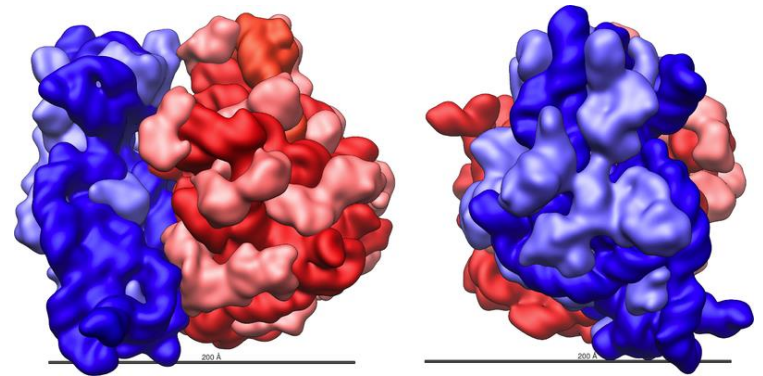
Kyle Harrington
DEMO Lab, Computer Science
Brandeis University

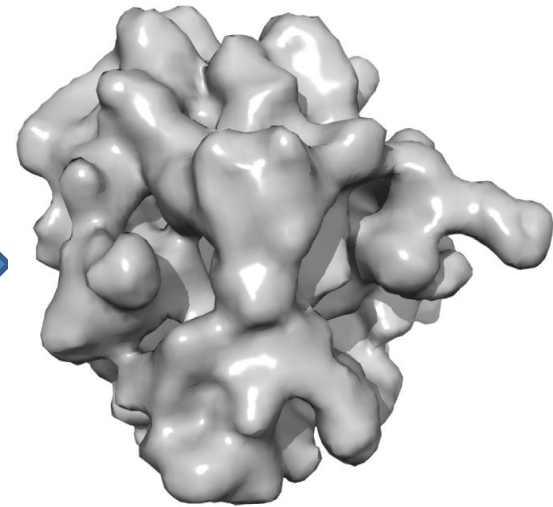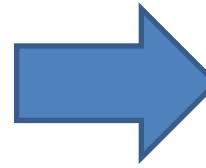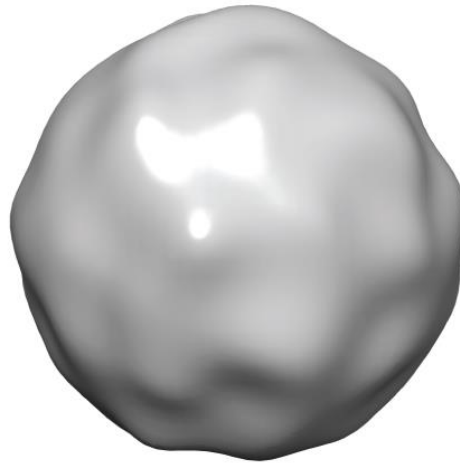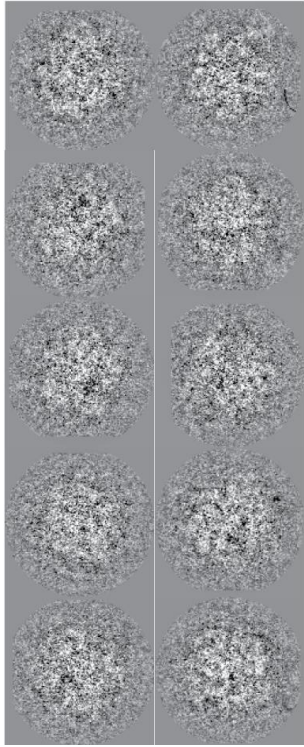# Micrographs to 3D structures

Rendering of experimentally-derived ribosome structure

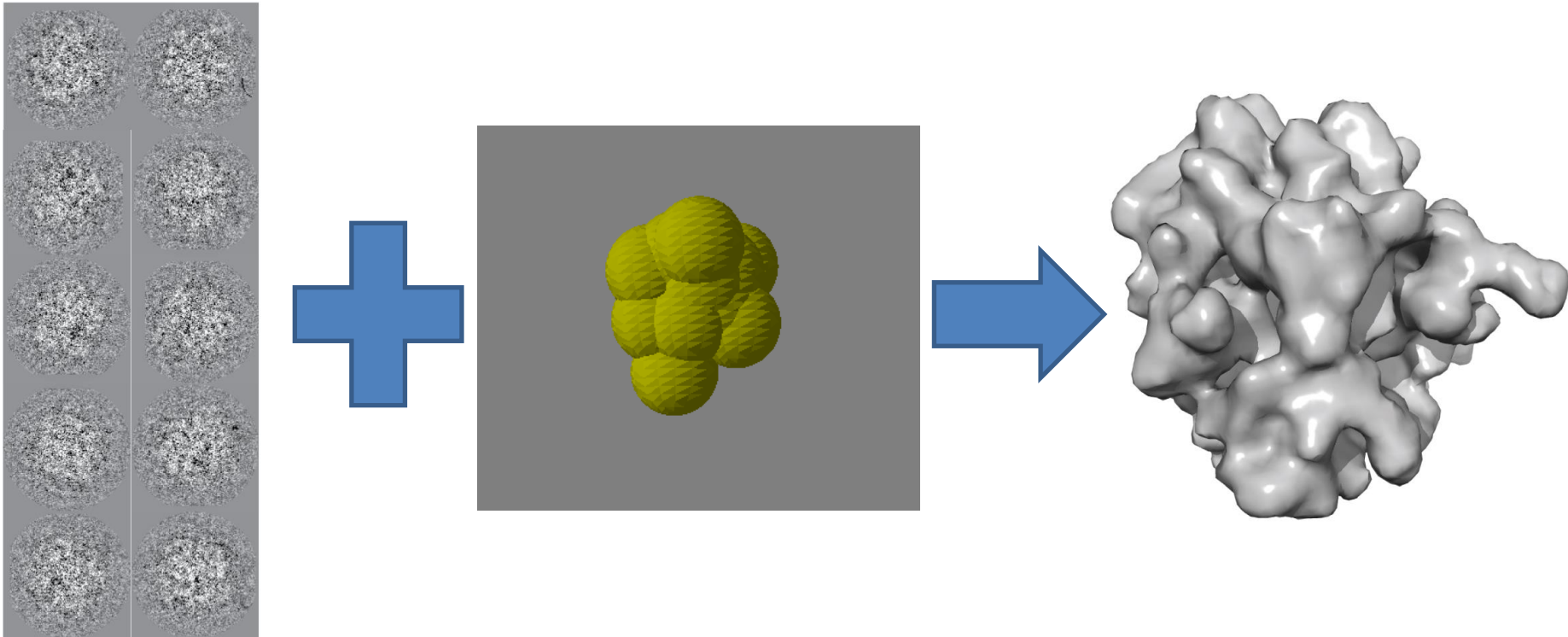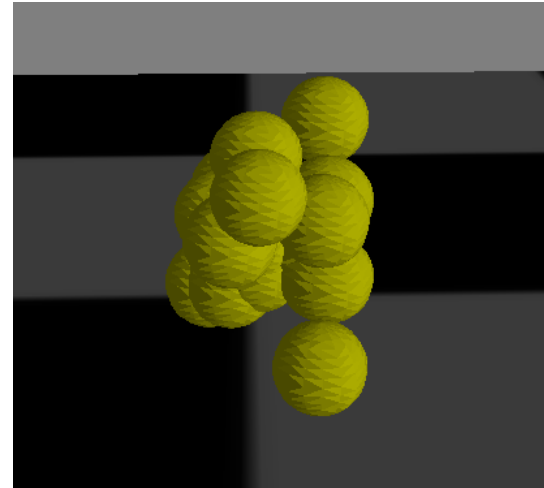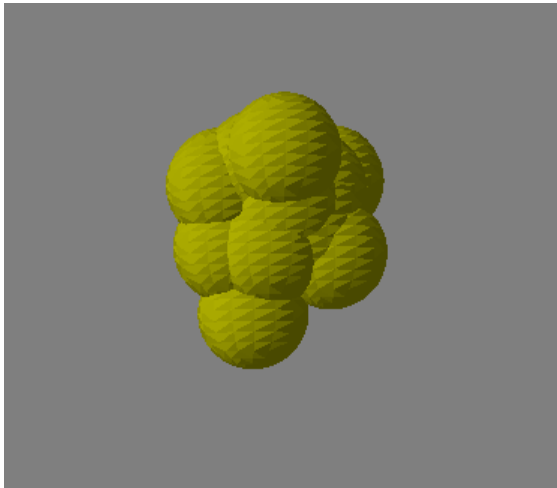3D reconstruction

Projection Matching Methods
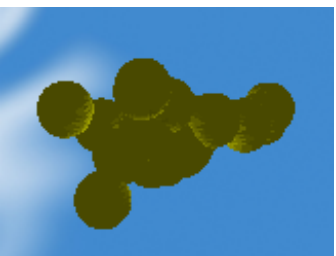
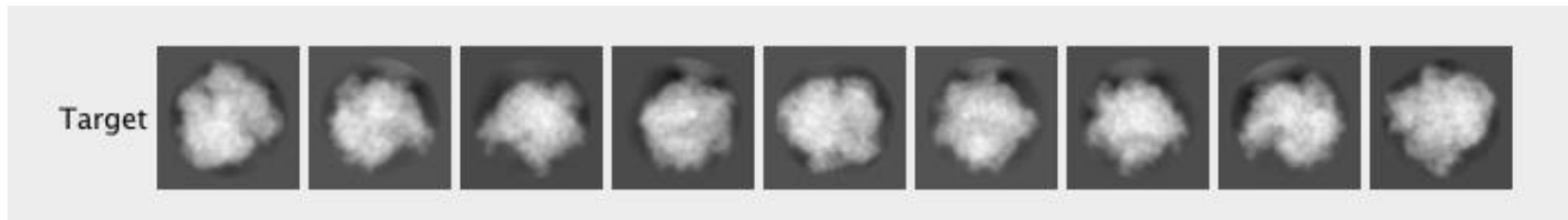# BEADS Evolutionary Automated Discovery of Structures

Our Representation

- Volumes of density as spheres
  - Variable number of spheres
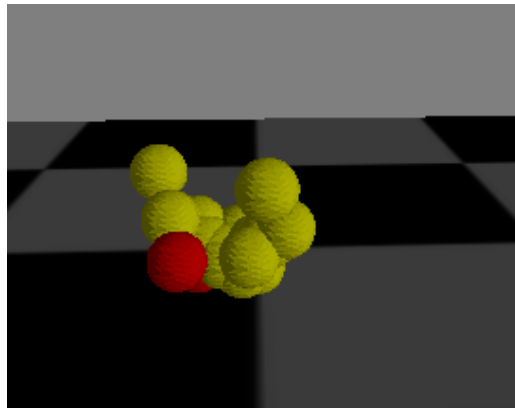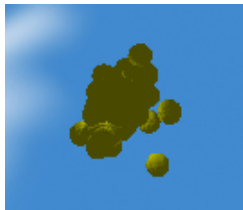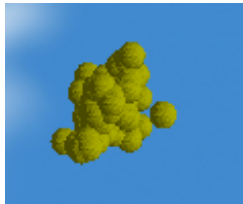 - Variable radius

Evaluating a candidate model

- Computing fitness of a model
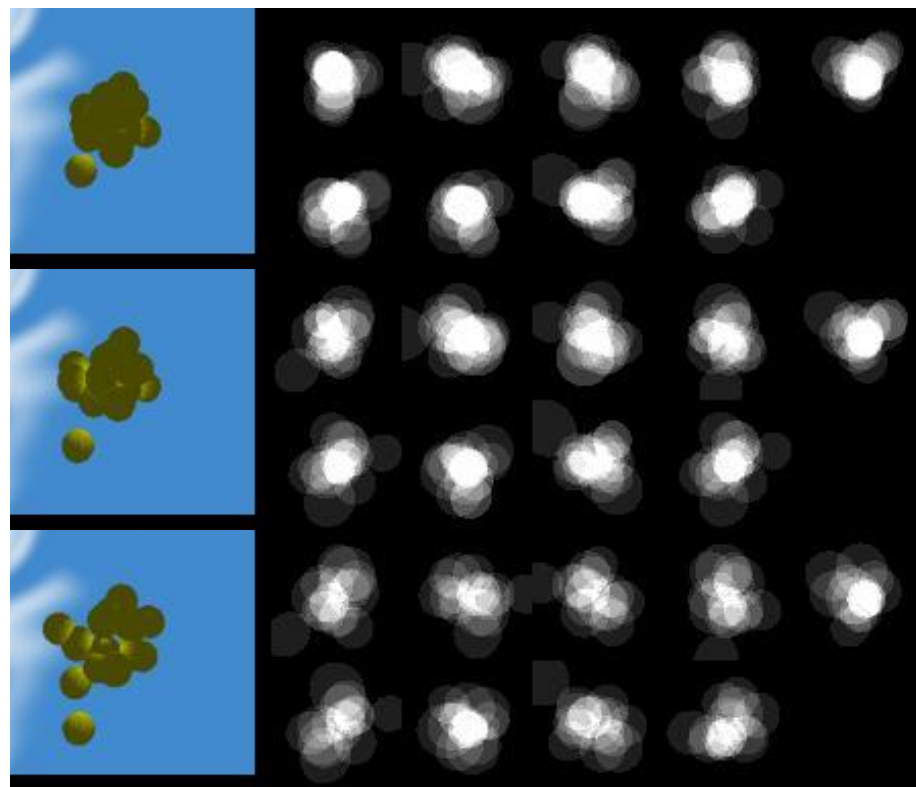 - Simulate microscope imaging
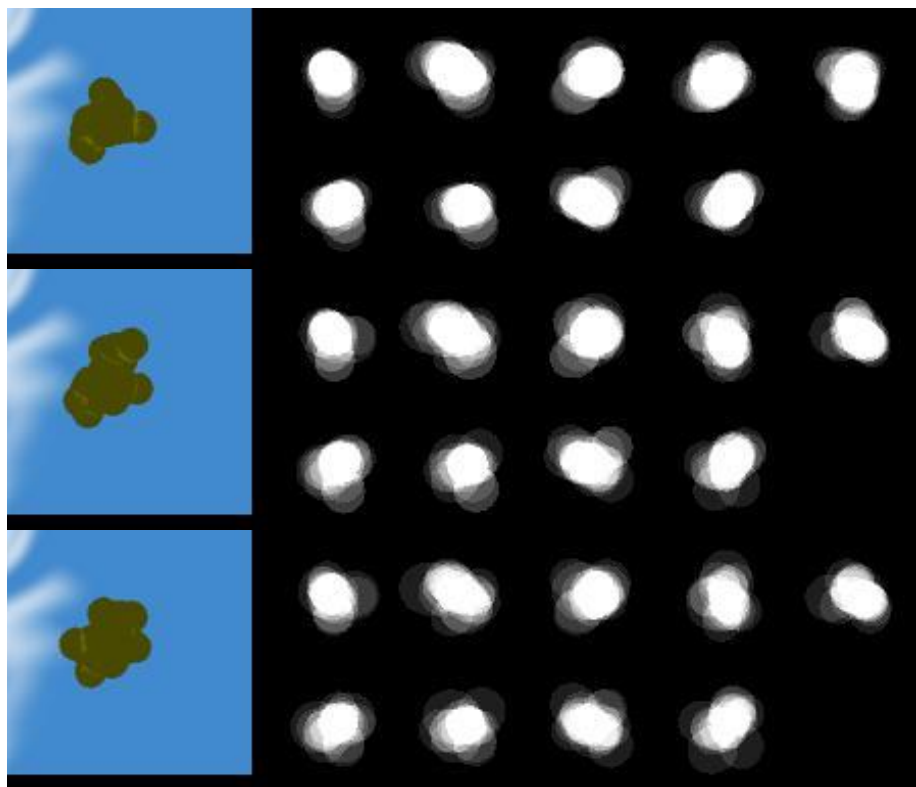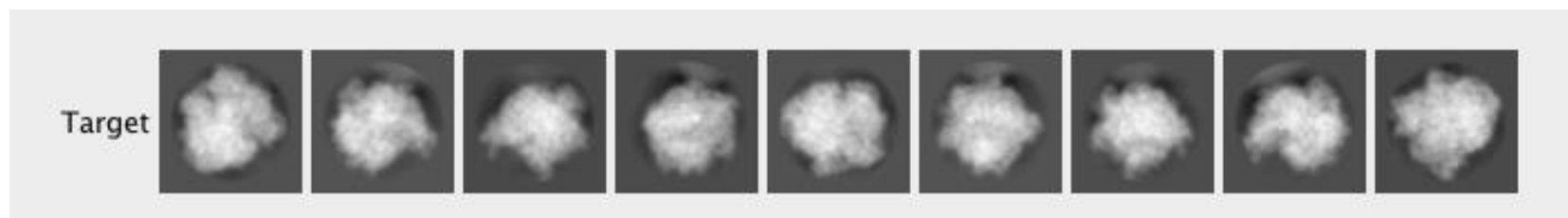 - Ray-trace from imaging plane

Mutation

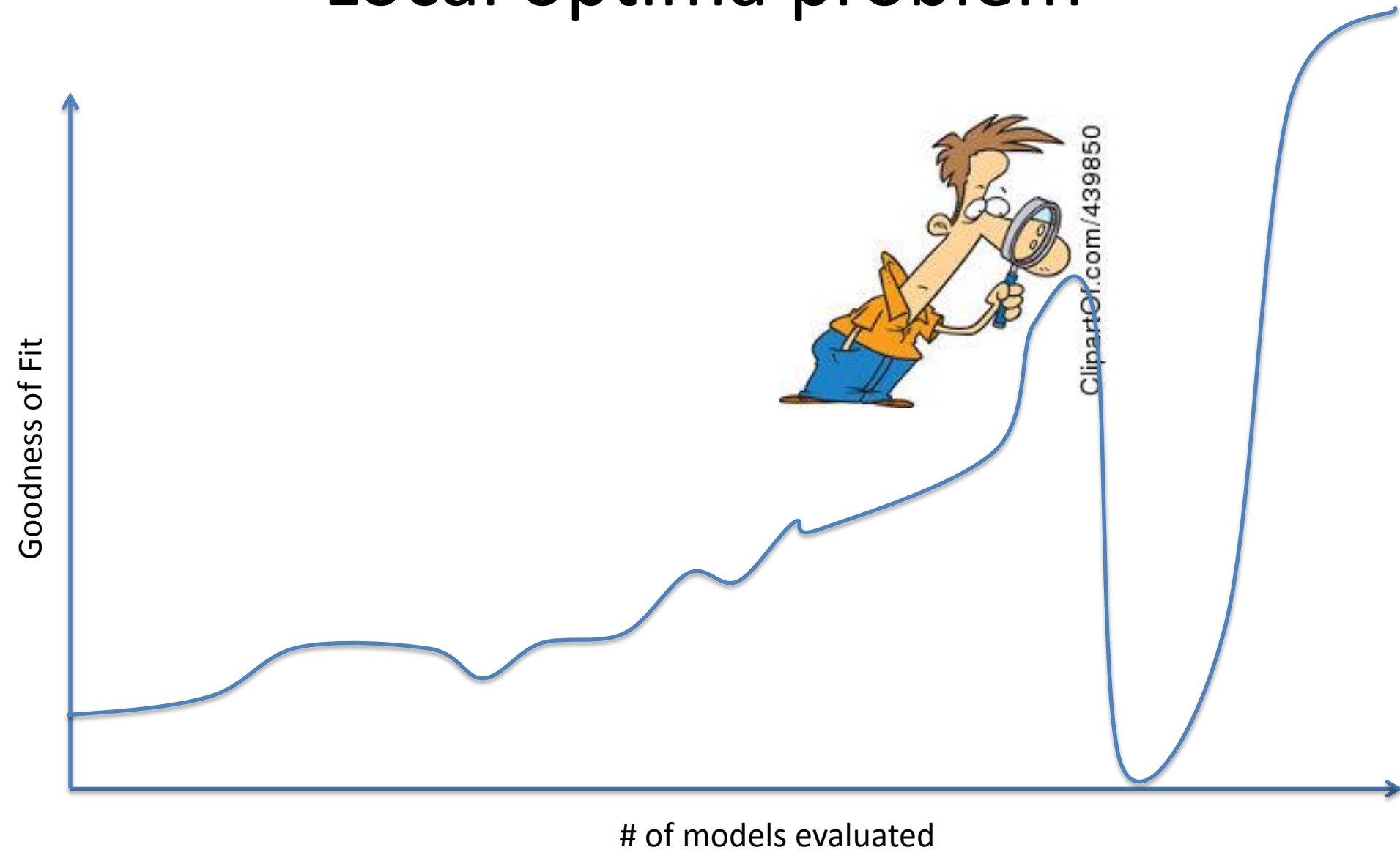- Mutation randomly perturbs candidate model

Example: Structure Search

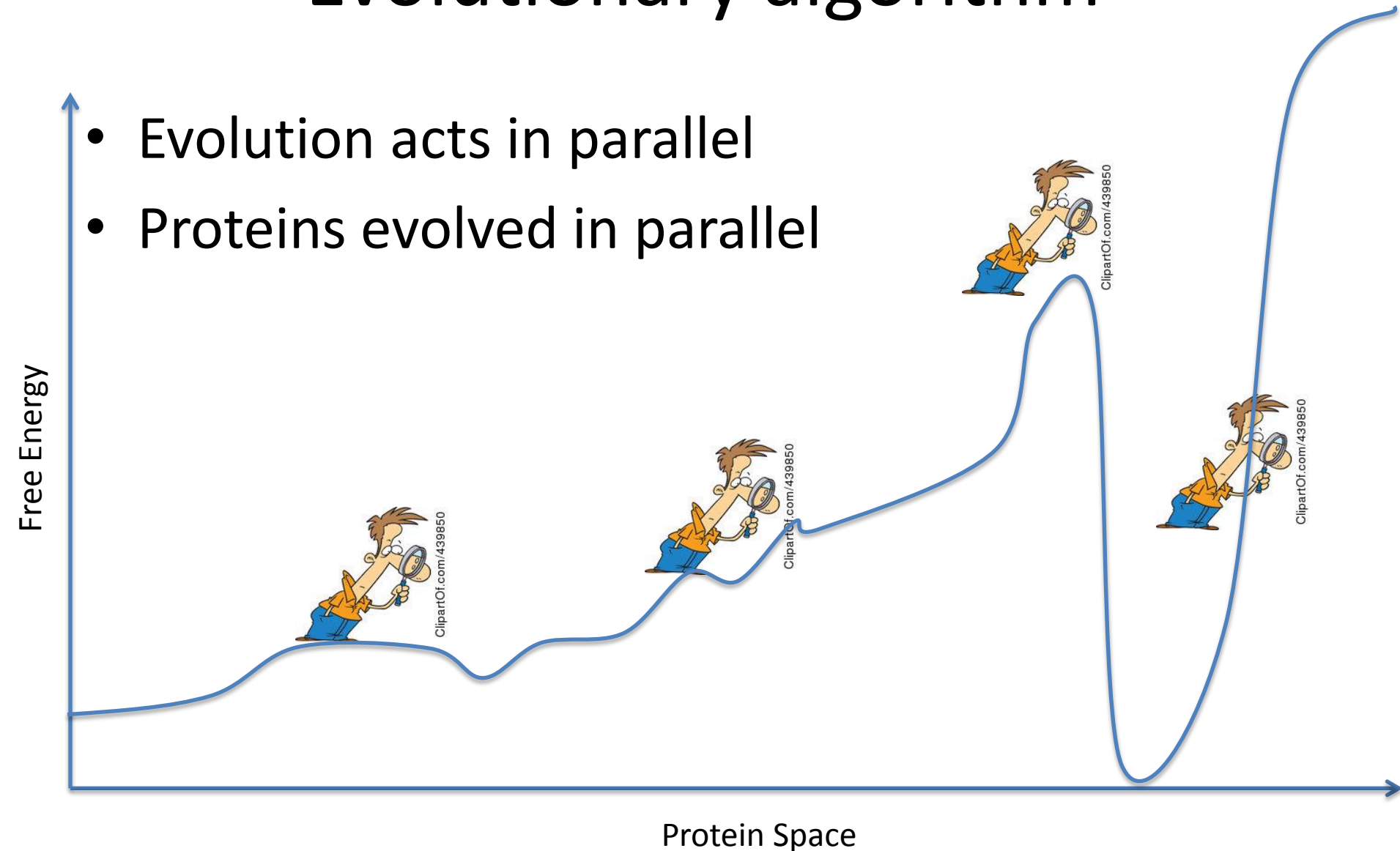# Local optima problem

Goodness of Fit

# of models evaluated
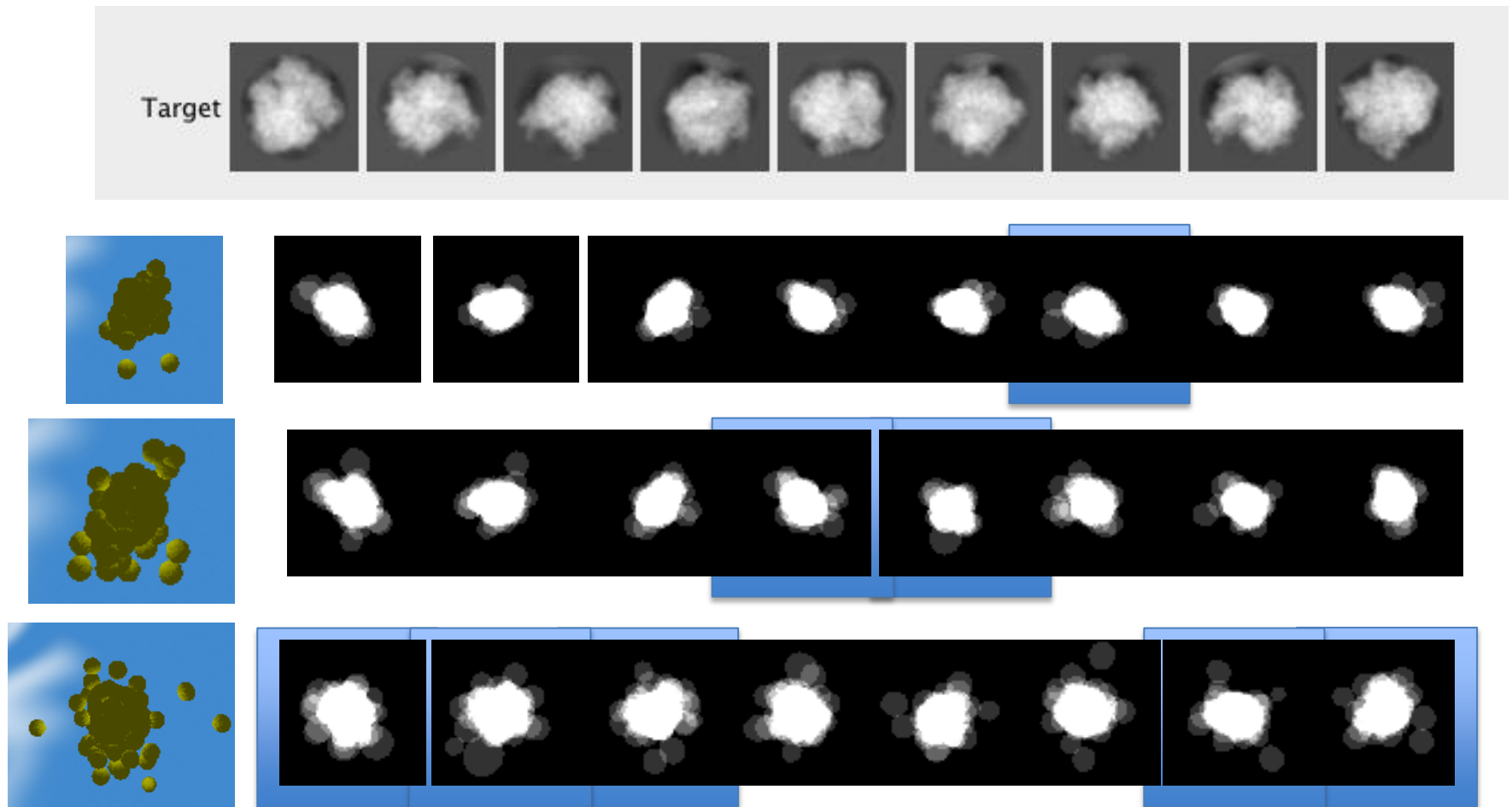
ClipartOf.com/439850

Evolutionary algorithm

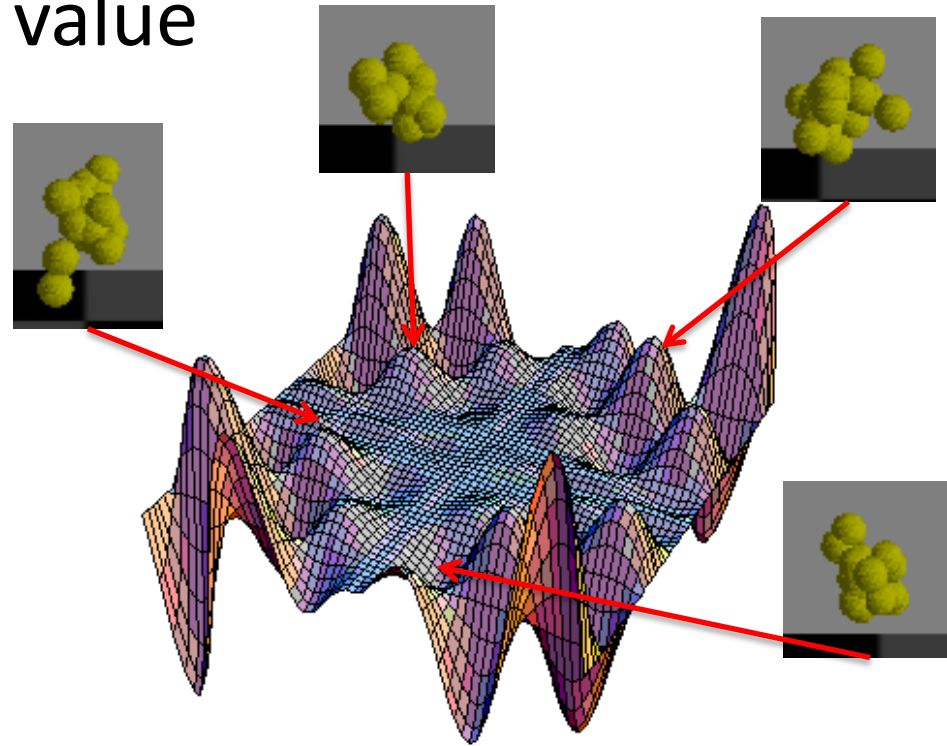- Evolution acts in parallel
- Proteins evolved in parallel

Populations of models

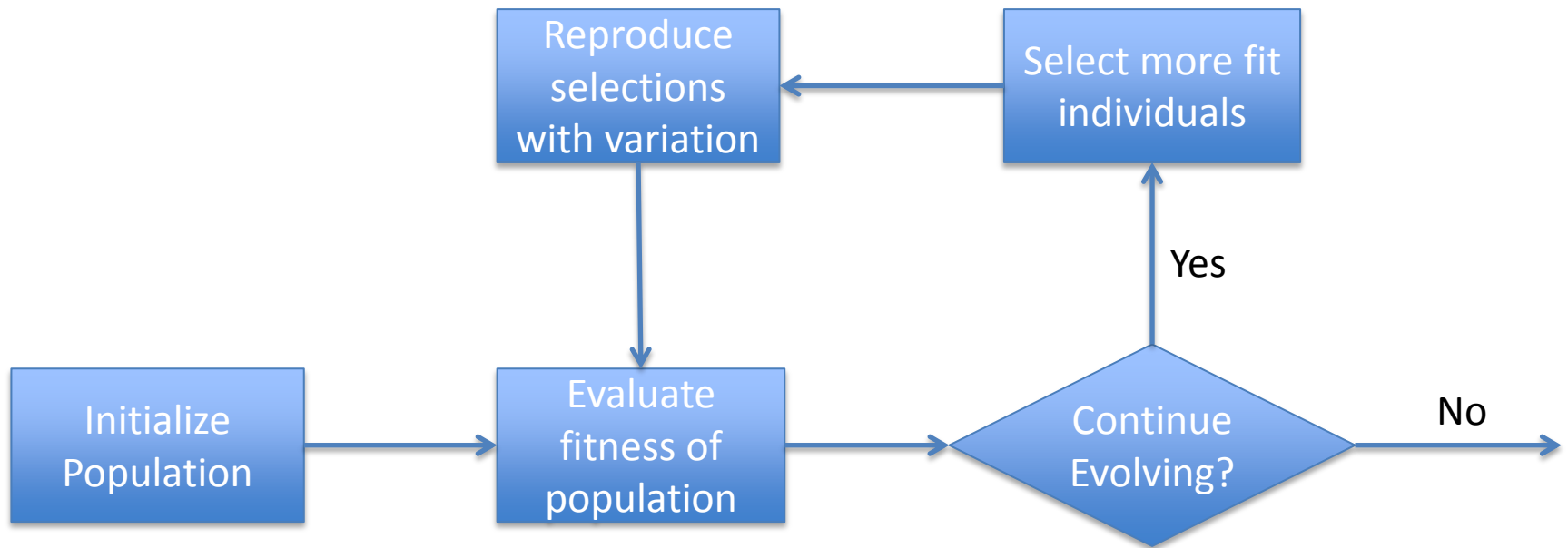- Individual models may favor different features

Fitness Landscapes

- Fitness landscape describes the distribution of phenotypes by fitness value

- Local optima

- Multiple peaks

- Deceptive optima

Evolving Structural Models

Thank you

- Jordan Pollack
- Jeff Gelles and Jane Kondev
- QB program
- Audience

Brevis

- http://brevis.golemics.org
- New standalone IDE