Bacteriophage

100-parts autonomous machine to search for, recognize & land on a target cell, drill a hole, & inject DNA, which is self-assembled!

None of the methods we have learned can simulate this
White Blood Cell Chases Bacteria

Long-time dynamics via a series of rare events

Yes, it’s called accelerated dynamics

http://www.youtube.com/watch?v=HnbMYzdjuBs&feature=related
Accelerated Molecular Dynamics

- **Hyperdynamics**  

- **Parallel replica dynamics**  

- **Temperature accelerated dynamics**  

- **Markov state model**  

- **Metadynamics**  

- **Paradynamics**  

...
Divide-Conquer-Recombine KMC

Divide

Conquer

Recombine

Molecular Dynamics

Quantum Molecular Dynamics

Amorphous DPT

Experimental Length & Time Scales

Δt = 10^{-15} s

t = 10^{-9} s or longer

Roberts et al., JACS (’12)

Mou et al., APL (’13)

Excitation population

Time (ps)

0.01 0.1 1 10 100 1000

0 0.5 1 1.5 2

Singlet

Triplet

10^6 excitations/μm^3

Time (ps)

0.01 0.1 1 10 100 1000

0 0.5 1 1.5 2
Directed evolution


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**Parent selection**
- Best starting point or points out of natural or synthetic sequences

**Sequence diversification**
- Error-prone PCR, recombination or computer-guided mutagenesis

**Functional assay**
- High-throughput screen or selection

**Application**
- Medical, agricultural, environmental, industrial or energy uses

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Accelerating directed evolution to design new materials *in silico*?
Abstract. Living organisms function in accordance with complex mechanisms that operate in different ways depending on conditions. Darwin's theory of evolution suggests that such mechanisms evolved through variation guided by natural selection. However, there has existed no theory that would explain quantitatively which mechanisms can so evolve in realistic population sizes within realistic time periods, and which are too complex. In this article, we suggest such a theory. We treat Darwinian evolution as a form of computational learning from examples in which the course of learning is influenced only by the aggregate fitness of the hypotheses on the examples, and not otherwise by specific examples. We formulate a notion of evolvability that distinguishes function classes that are evolvable with polynomially bounded resources from those that are not. We show that in a single stage of evolution monotone Boolean conjunctions and disjunctions are evolvable over the uniform distribution, while Boolean parity functions are not. We suggest that the mechanism that underlies biological evolution overall is "evolvable target pursuit", which consists of a series of evolutionary stages, each one inexorably pursuing an evolvable target in the technical sense suggested above, each such target being rendered evolvable by the serendipitous combination of the environment and the outcomes of previous evolutionary stages.