Solving Inverse Problems

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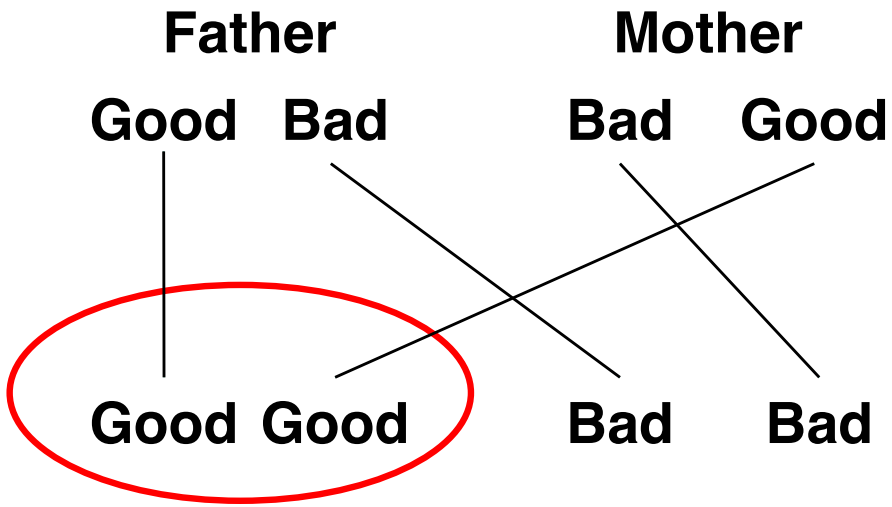
Key concept: An ensemble (outer loop: desired property → solution structure) of forward solutions (inner loop: given structure → property)

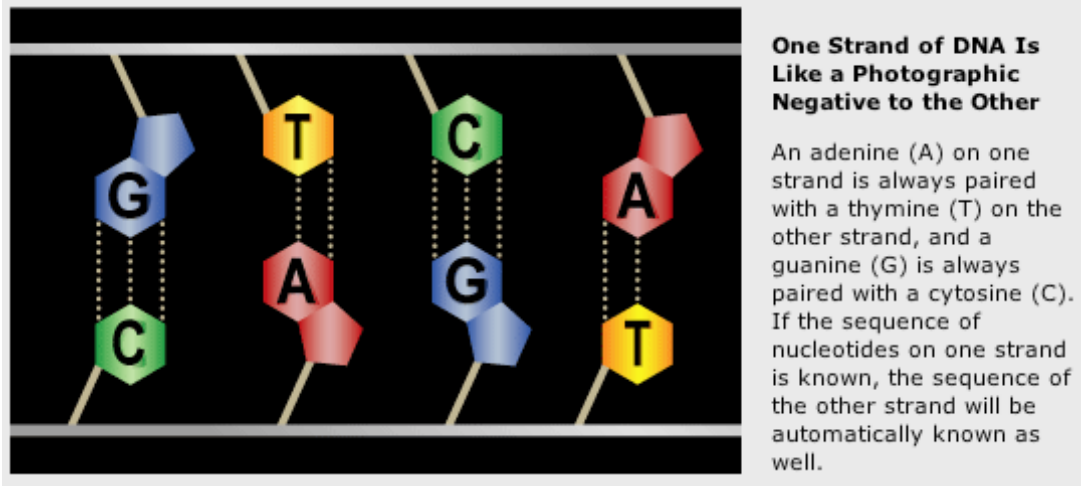
Genetic Algorithm

1D Ising model ↑ – ↓ – ↓ – ↑ – ↑ – ↑ – ↑ – ↓

Gene = bit string = (10011110)

- **Population in the solution space: Multiple chains, diversity**
- **Selection: Elitist strategy = survival of the fittest**
- **Crossover**



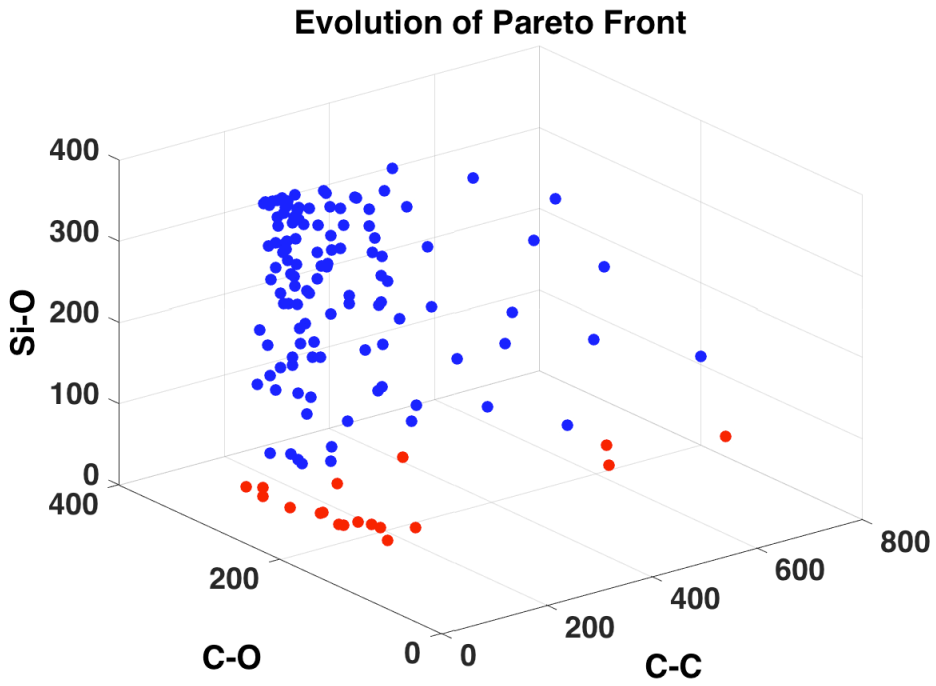


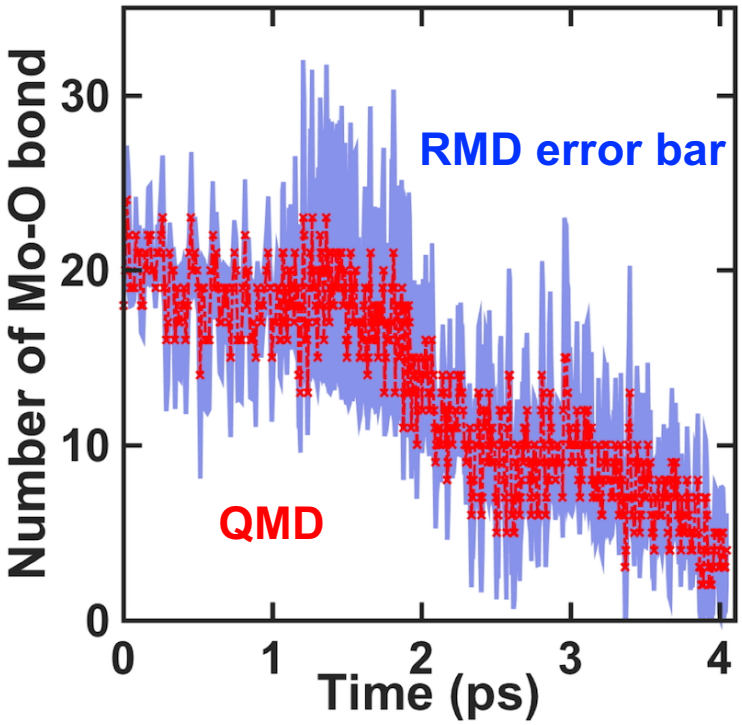
One Strand of DNA Is Like a Photographic Negative to the Other

An adenine (A) on one strand is always paired with a thymine (T) on the other strand, and a guanine (G) is always paired with a cytosine (C). If the sequence of nucleotides on one strand is known, the sequence of the other strand will be automatically known as well.

Pareto-Frontal Uncertainty Quantification

- **Train reactive force-field parameters by dynamically fitting reactive molecular dynamics (RMD) trajectories to quantum molecular dynamics (QMD) trajectories on-the-fly**
- **Pareto optimal front in multiobjective genetic algorithm (MOGA) provides an ensemble of force fields to enable uncertainty quantification (UQ)**





- **Pareto-optimal solutions during genetic training (RMD errors for three quantities-of-interest)**
- **Converged Pareto-optimal front**

A. Mishra *et al.*, *npj Comput. Mater.* **4**, 42 ('18)

Replica Exchange MC

JOURNAL OF CHEMICAL PHYSICS VOLUME 118, NUMBER 14 8 APRIL 2003

Replica-exchange multicanonical and multicanonical replica-exchange Monte Carlo simulations of peptides. I. Formulation and benchmark test

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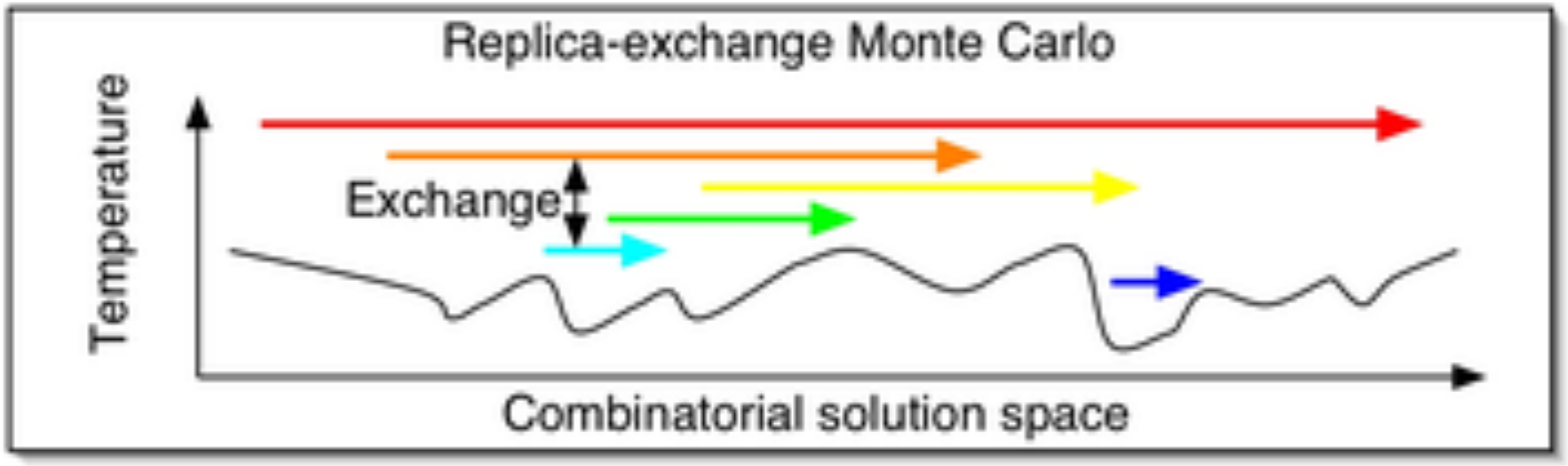
J. Chem. Phys. **118**, 6664 ('03)

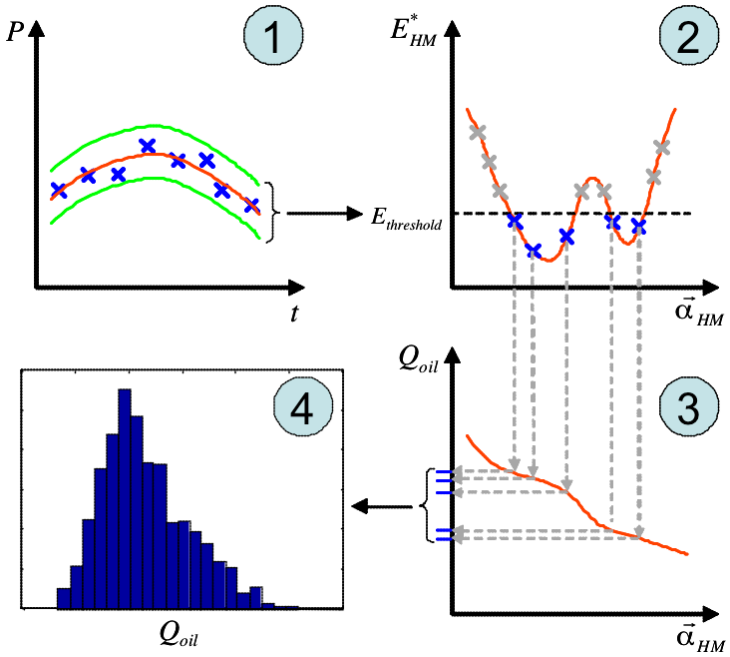
Multiple Markov chains at different temperatures

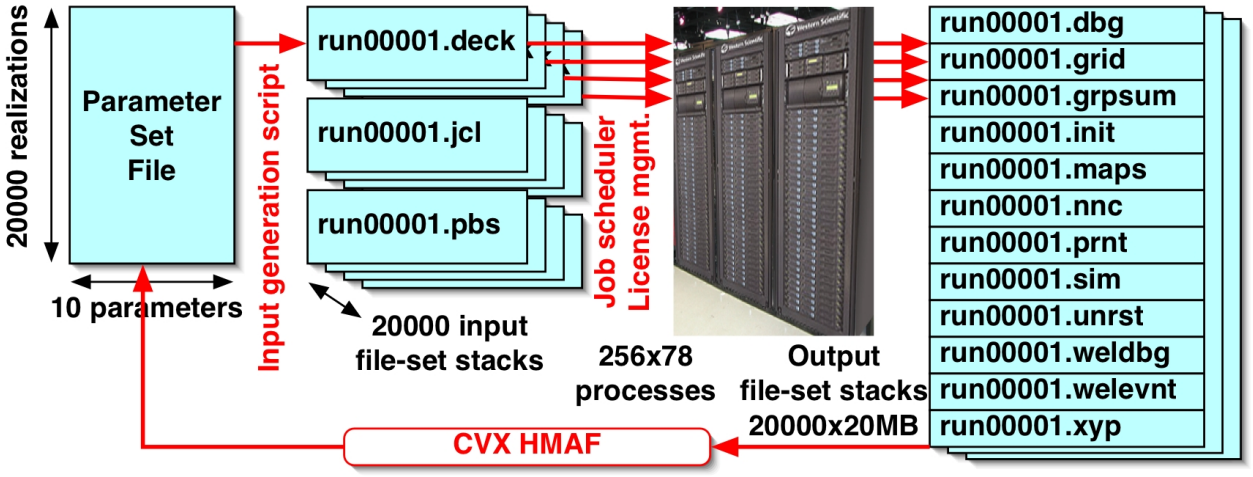


Parallel History Matching

- **Provide USC's parallel computing environment to demonstrate parallel execution of CVX's history match & associated forecast (HMAF) framework.**
- **History matching of a real field case (offshore Africa, North Sea & Gulf of Mexico) with 10,000-20,000 forward simulation runs on CACS high performance computing resources.**

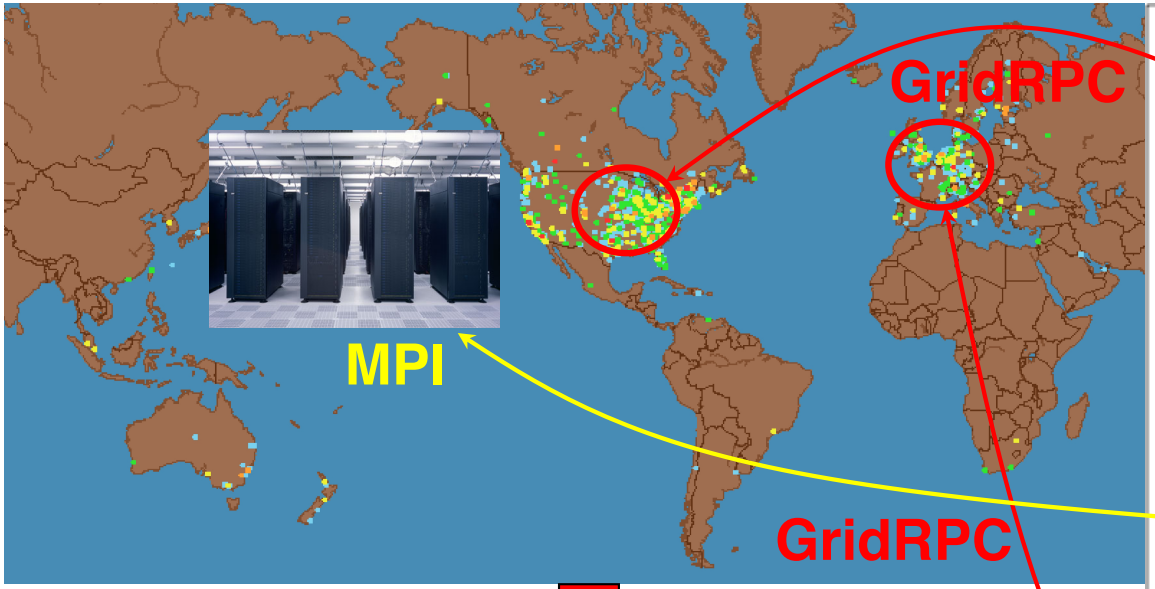
http://cisoft.usc.edu

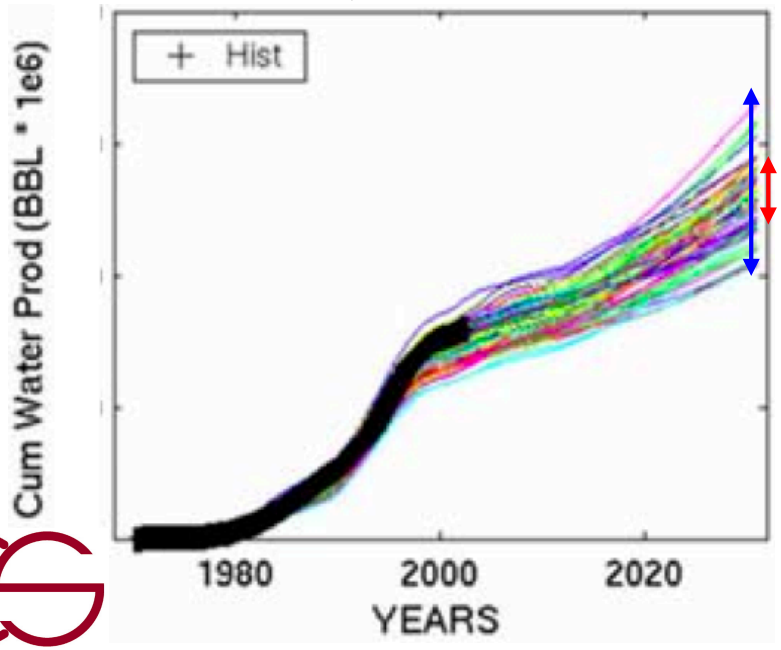


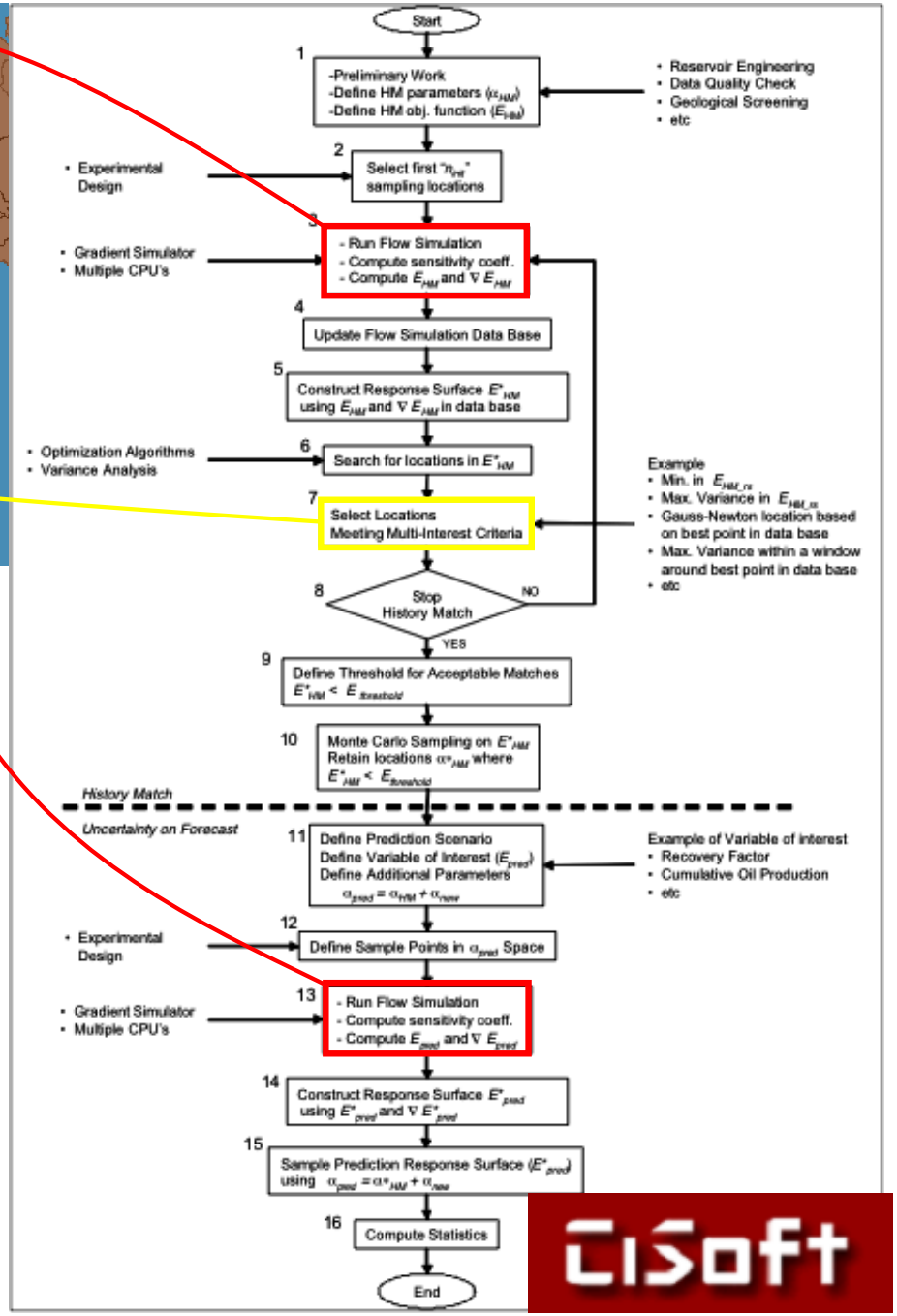


K. Nomura *et al.*, *J. Supercomputing* **41**, 109 ('07)

Opportunity: Overnight HMAF on a Grid

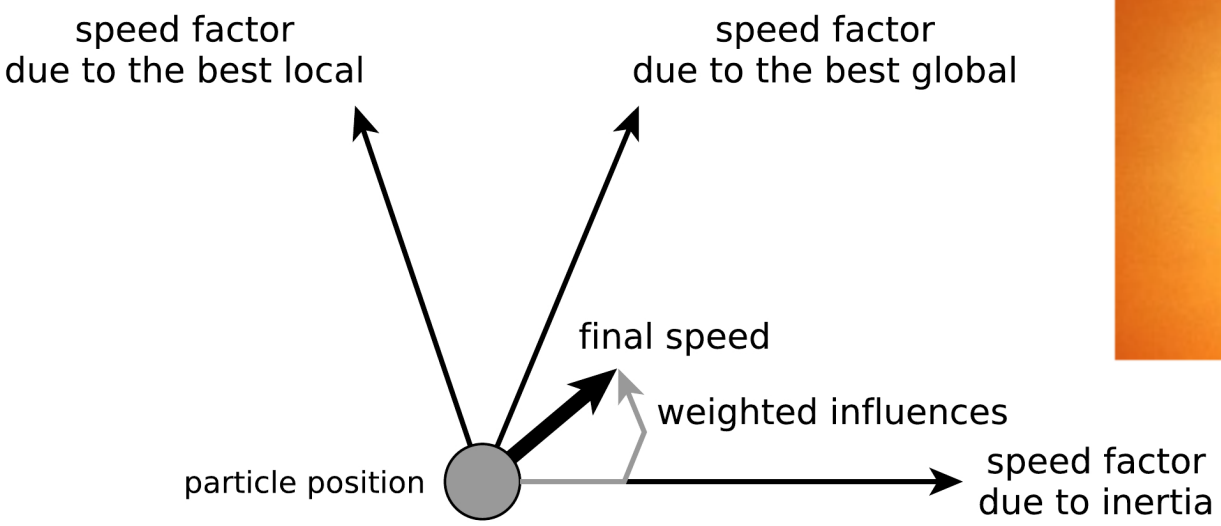






Particle Swarm Optimization

An ensemble of interacting particles in the solution space explores the optimal solution: Each particle's movement is guided toward the best known positions in the search space, which are updated as better positions are found by other particles.



J. Kennedy & R. Eberhart, *IEEE Int'l Conf. Neural Networks* ('95)
CALYPSO (particle-swarm structural prediction): http://www.calypso.cn

Particle Swarm for Inverse Rendering

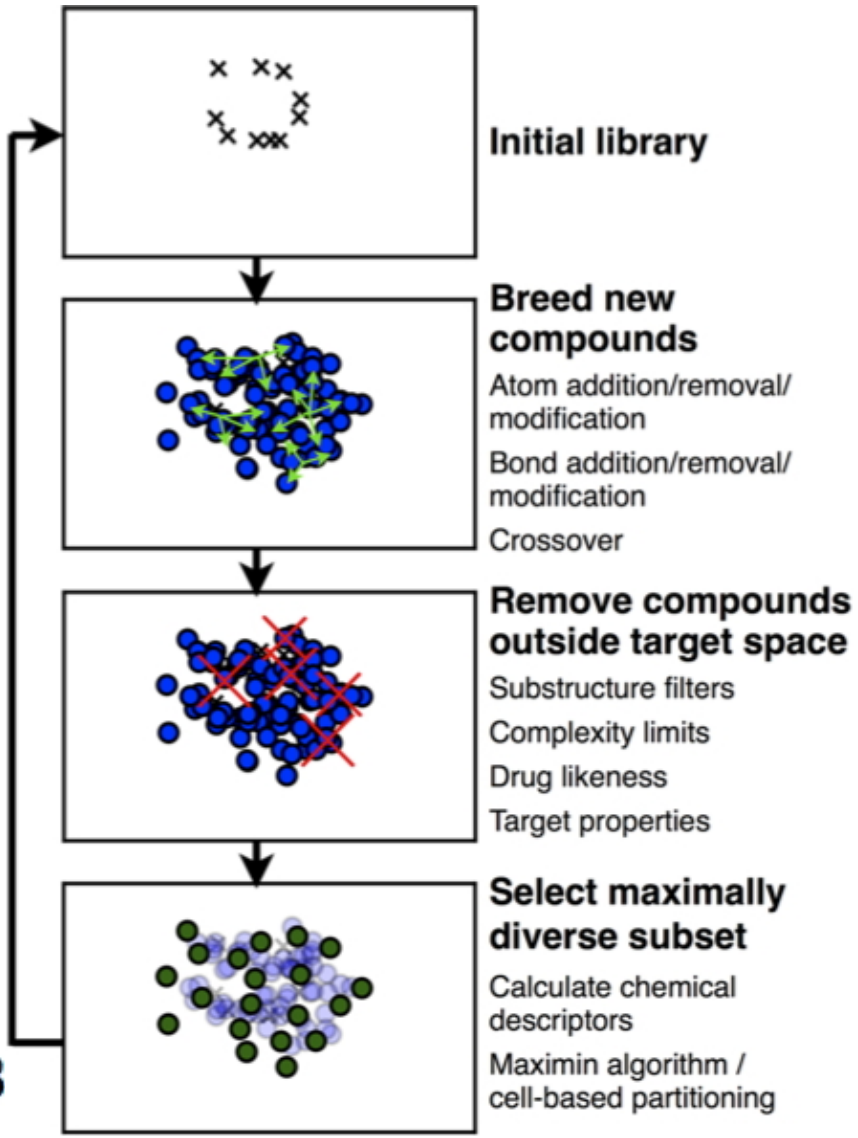
K. Nagano *et al.*, *J. Vis.* **20**, 195 ('17)

Large Search-Space Exploration

Stochastic Voyages into Uncharted Chemical Space Produce a Representative Library of All Possible Drug-Like Compounds

Aaron M. Virshup,[†,§] Julia Contreras-García,[†,§,#] Peter Wipf,[‡,§] Weitao Yang,[*,†,§] and David N. Beratan[*,†,§]

Explore the set of 10^{60} molecules (< 500 Da) by a maximally diverse ensemble



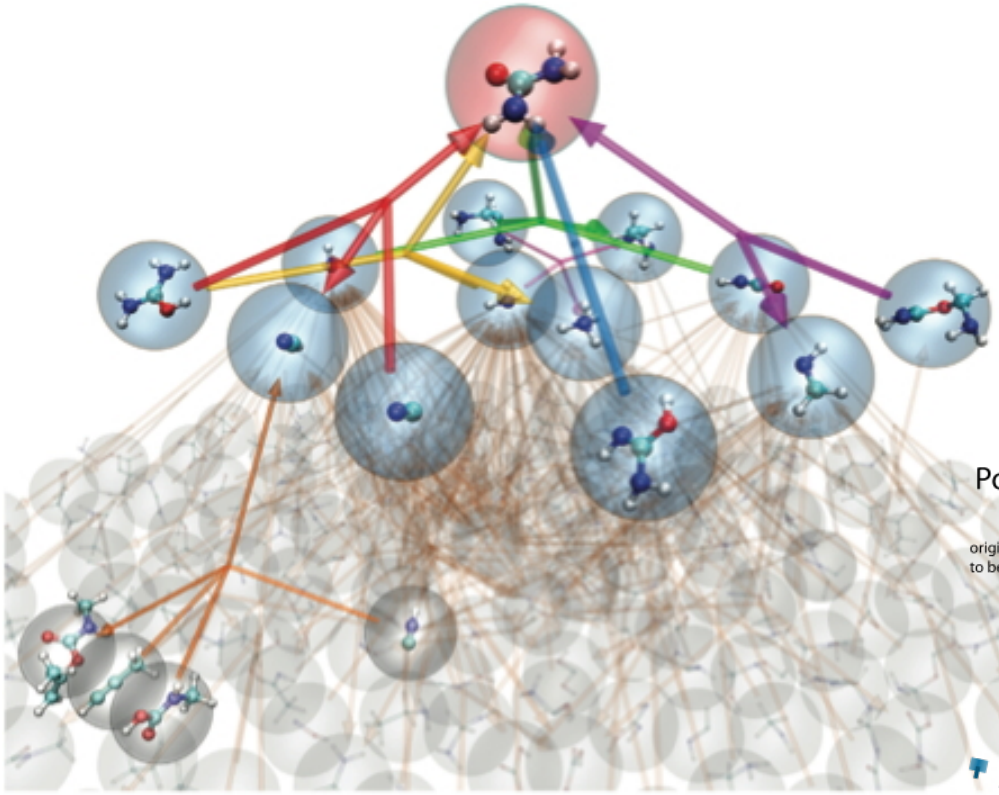
J. Am. Chem. Soc. 2013, 135, 7296–7303

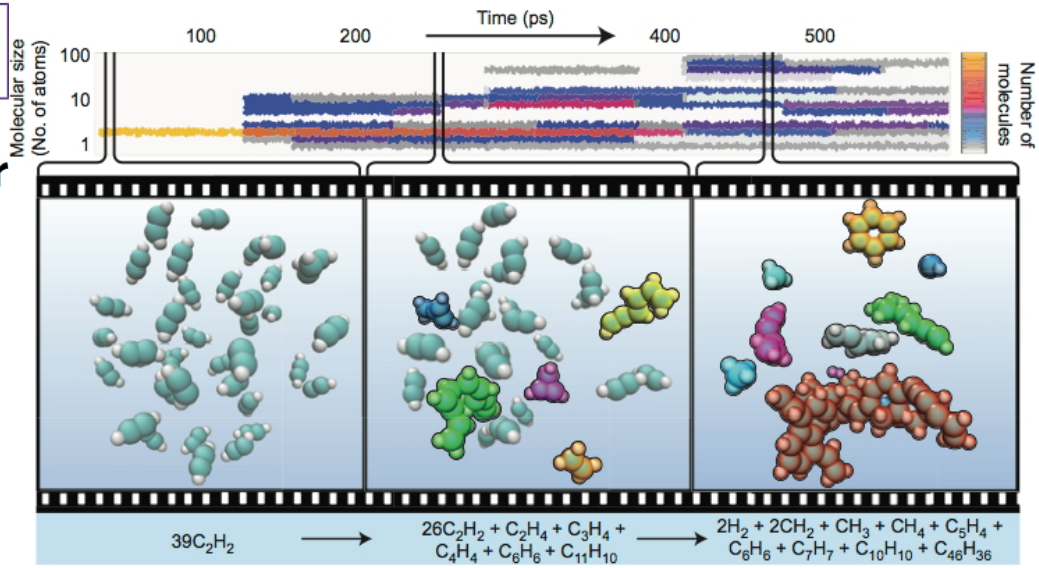
Simulated PCR?

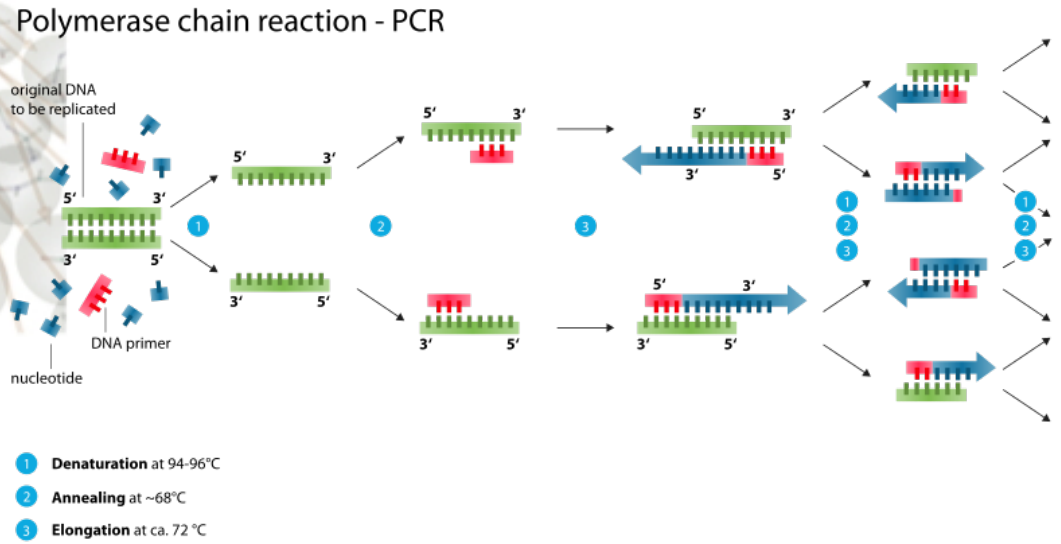
ARTICLES
PUBLISHED ONLINE: 2 NOVEMBER 2014 | DOI: 10.1038/NCHEM.2099
nature chemistry

Discovering chemistry with an *ab initio* nanoreactor

Lee-Ping Wang[1,2], Alexey Titov[1,2†], Robert McGibbon[2], Fang Liu[1,2], Vijay S. Pande[2] and Todd J. Martínez[1,2,3*]



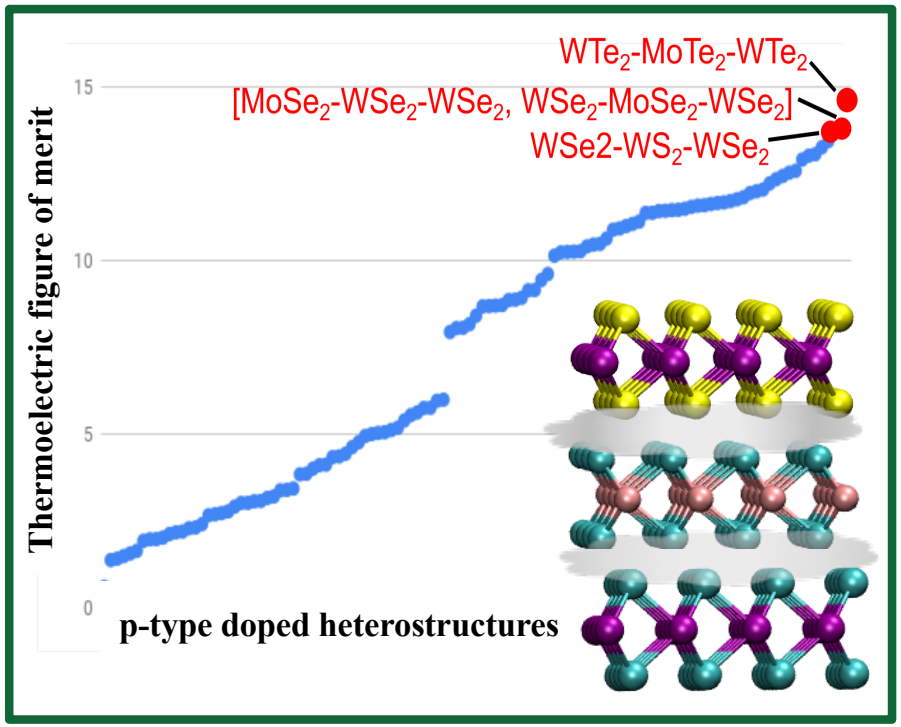


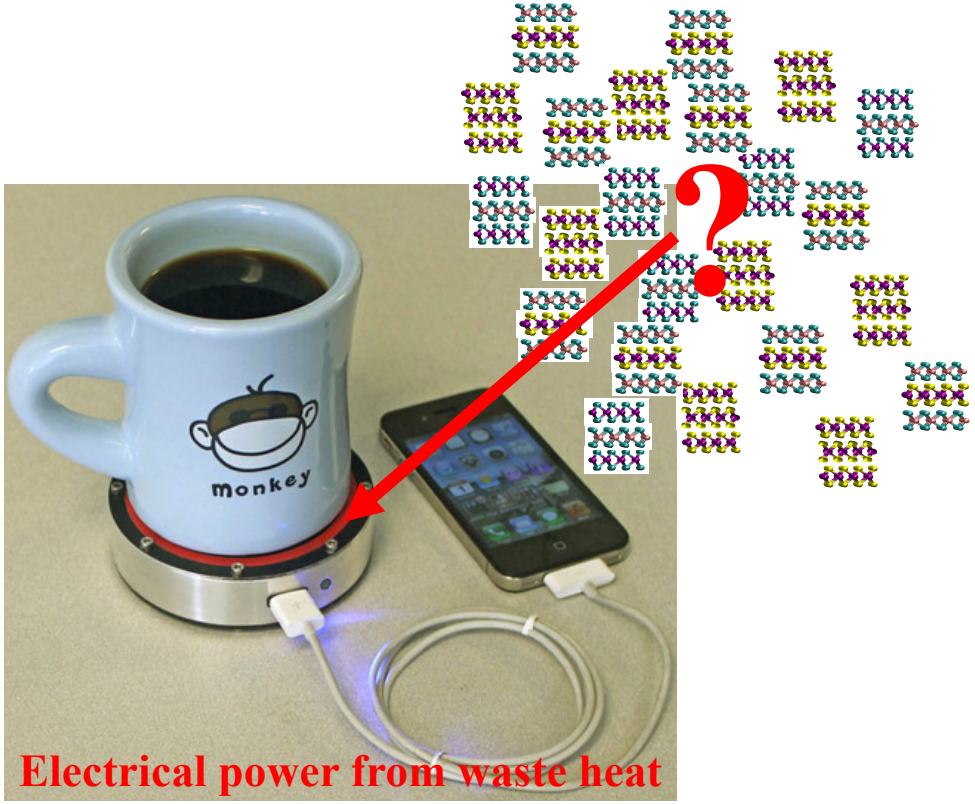


- Pressure to temperature cycling
- Primer?

Active Learning of Optimal Materials

- **Bayesian optimization balances exploitation & exploration to find a structure with the desired property with a minimal number of quantum-mechanical calculations**
- **Predicted three-layered transition-metal chalcogenide (TMDC) heterostacks with the largest thermoelectric figure-of-merit**

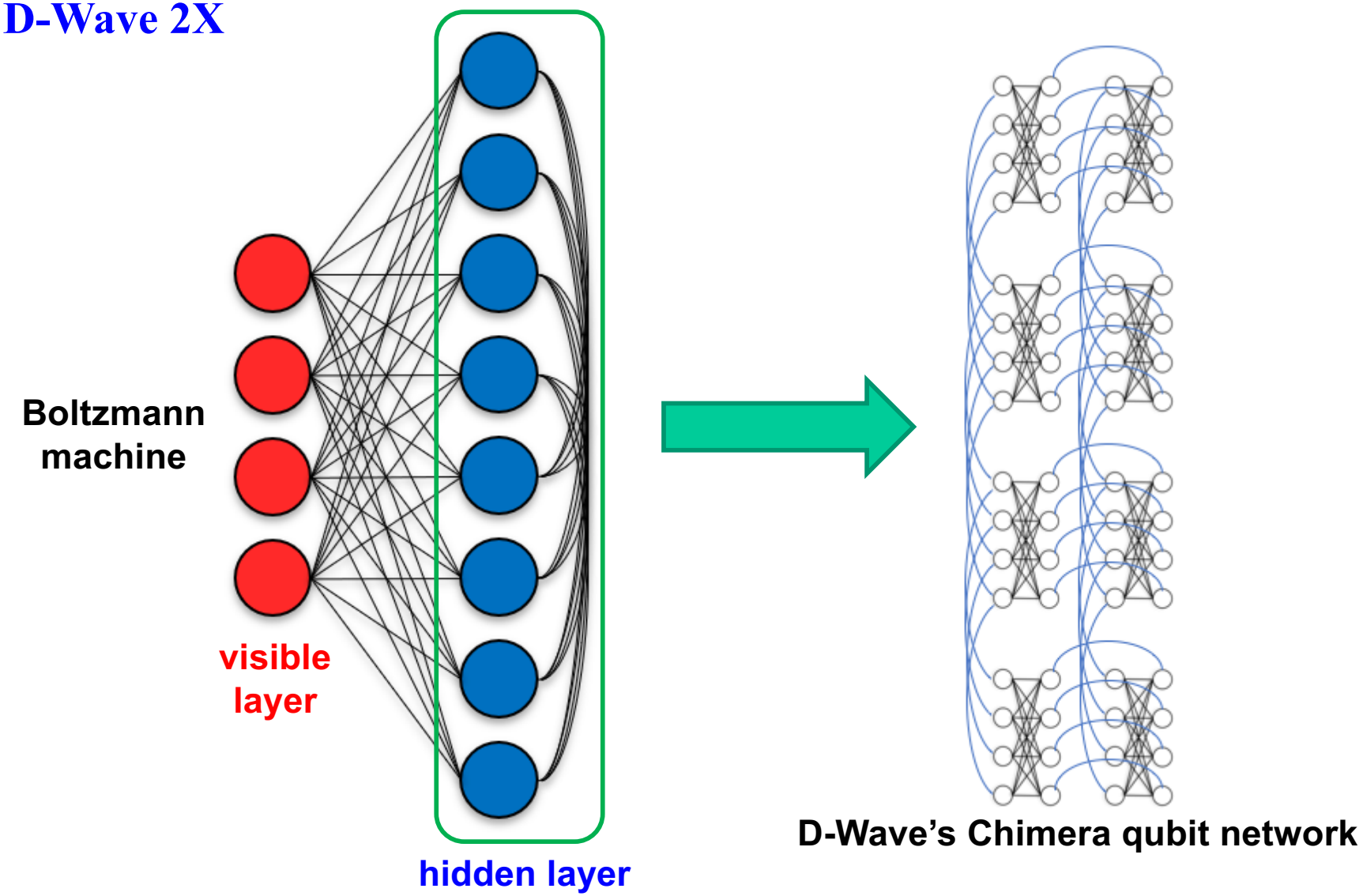




L. Bassman *et al.*, *npj Comput. Mater.* **4**, 74 ('18)

Quantum-Classical Boltzmann Machine

- **Offload a hard machine-learning task to a 1,098-qubit quantum annealer, D-Wave 2X**



J. Liu *et al.*, *Comput. Mater. Sci.* **173**, 109429 ('20)