Computing for Creation of Clean Energy Catalysts

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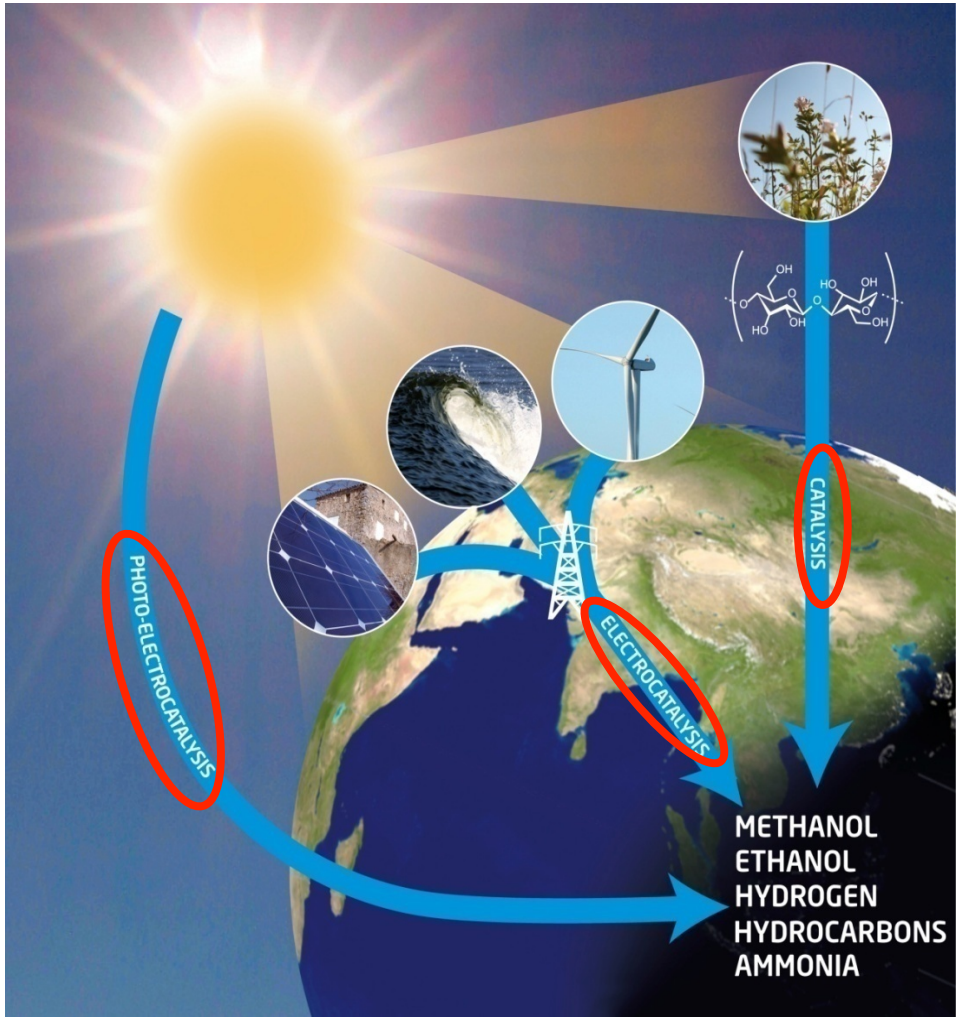


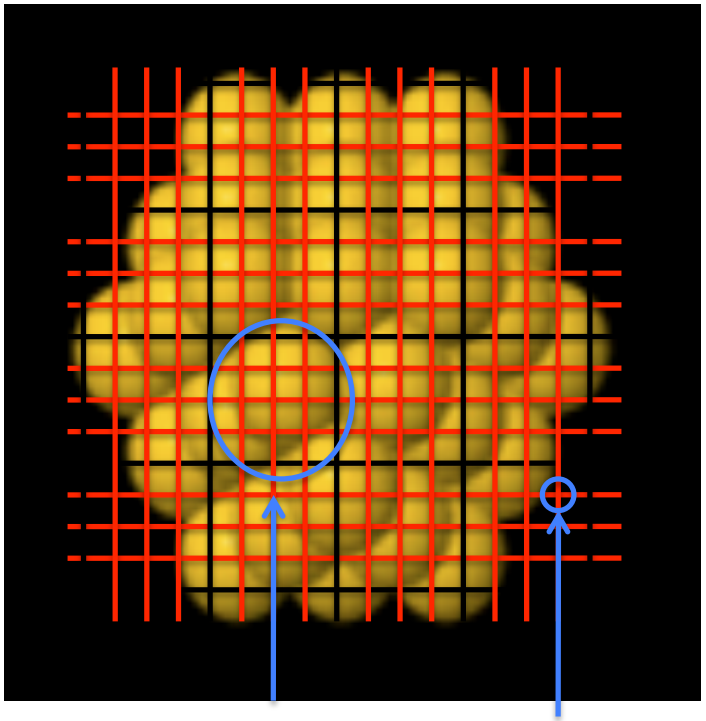
The SUNCAT Cluster

- Trying to invent energy-related catalysts computationally

- 260 dual quad-core 2.67GHz Nehalem 5550 (2080 cores)
- 24GB DDR3 RAM
- Memory-bandwidth limited
- 1-Gbit Ethernet MPI interconnect (relatively little network communication) although channel-bonding improves performance by few percent

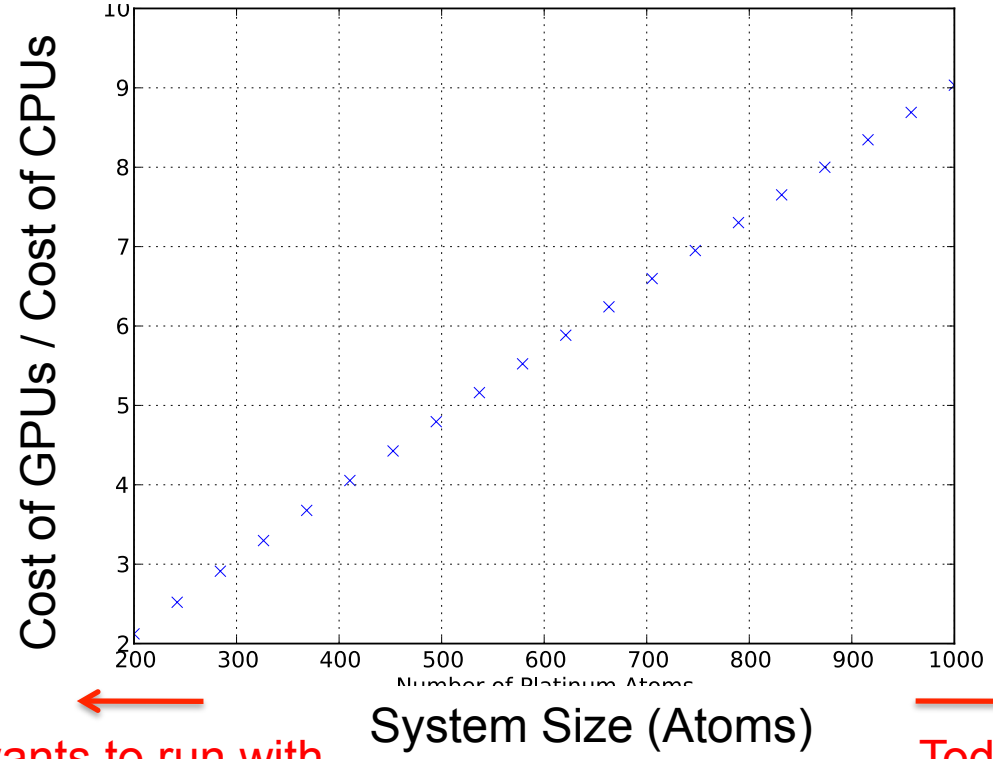
How Does SUNCAT Software Solve Schrodinger Equation?

- 200K C/Python code written in Denmark
- Grid turns quantum differential equations into difference equations
- 1 node: Cube is $n \times n \times n$
- 1 node: calculations scale $O(n^3)$ (cube volume)
- Communication scales $O(n^2)$ (cube surface area)
- Should be good for MPI, but typically n~200, so difficult to scale past ~64 cores for typical systems.
- Calculations take weeks



The Future: GPUs vs. CPUs?

Preliminary study comparing SUNCAT CPU code to Todd Martinez GPU code



SUNCAT wants to run with these system sizes

Todd has optimized for these system sizes

Have applied for LDRD money to see if GPUs can get “factor of 10” for SUNCAT