



Faster Computational Docking

Objective: Develop a faster version of a valuable molecular modeling technique known as protein-ligand docking

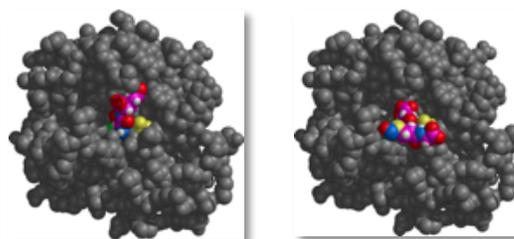
Implications: Could speed development of new drug treatments and other products.

Accomplishments: Developed an MPI-parallel method to scan the most widely-used molecular database (Autodock4).

- Allows rapid protein docking at unprecedented scale.
- Could provide a “missing link” between supercomputers and huge molecular databases like the Human Genome Project

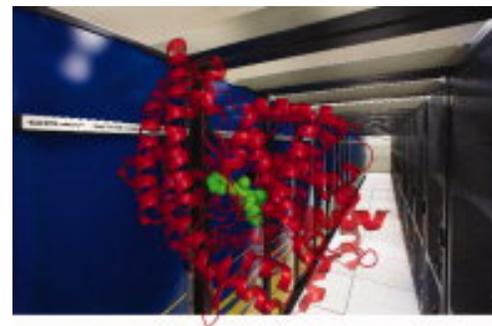
- **NERSC:** 3.7M early user Hopper hours were used for high-throughput screening of an EPA database to identify environmental pollutants that may have estrogenic properties; used 16 – 65k cores.

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Conceptual view of a protein showing two possible docking orientations for a ligand.

Docking programs try to identify the best of all possible orientations.



An illustration of a protein structure superimposed on NERSC's Franklin system, which was used to understand the scalability of the newly parallel Autodock method. This image appeared in the journal's table of contents.

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