

Amount of Physical Detail \uparrow

$$H\Psi = E\Psi$$

100 fs, 30 atoms:
photochemistry



Correlated methods
(MP2, CCSD, CI)

Density Functional Theory

100 ps, 100 atoms:
fast chemical reactions



Hartree-Fock

1 μ s–1 ms, 100k atoms:
protein dynamics,
drug binding



Atomistic MM

1 ms+, 1 million atoms:
folding of large proteins,
virus capsids



Coarse-grained simulations

Continuum mechanics

Cost of Calculation \rightarrow

Molecular Mechanics

Chao Zhang



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