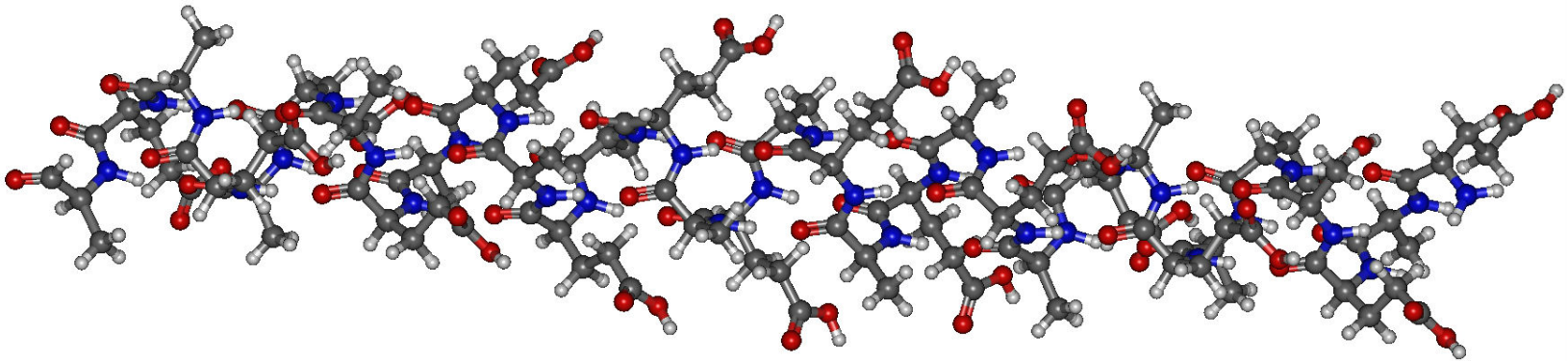
Large scale electronic structure calculations



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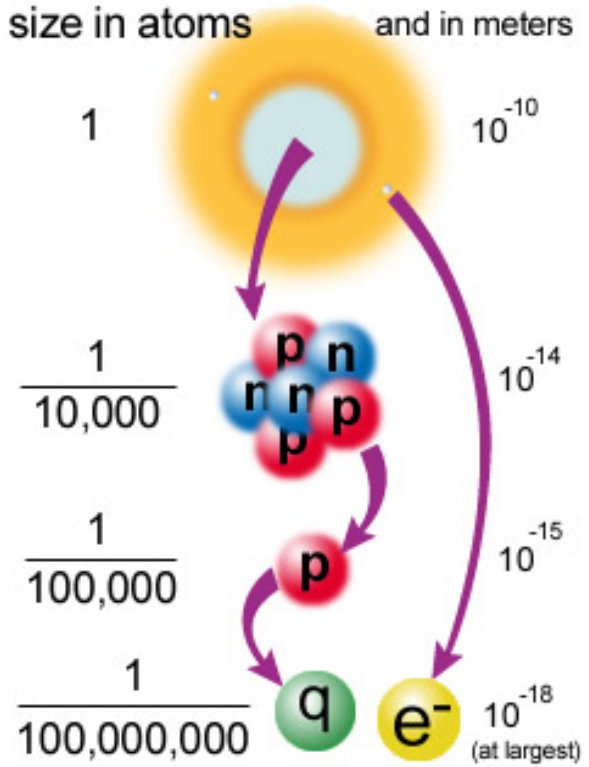
What is quantum chemistry?

Quantum chemistry - understanding properties of matter at a subatomic scale.

Which scales we are talking about:

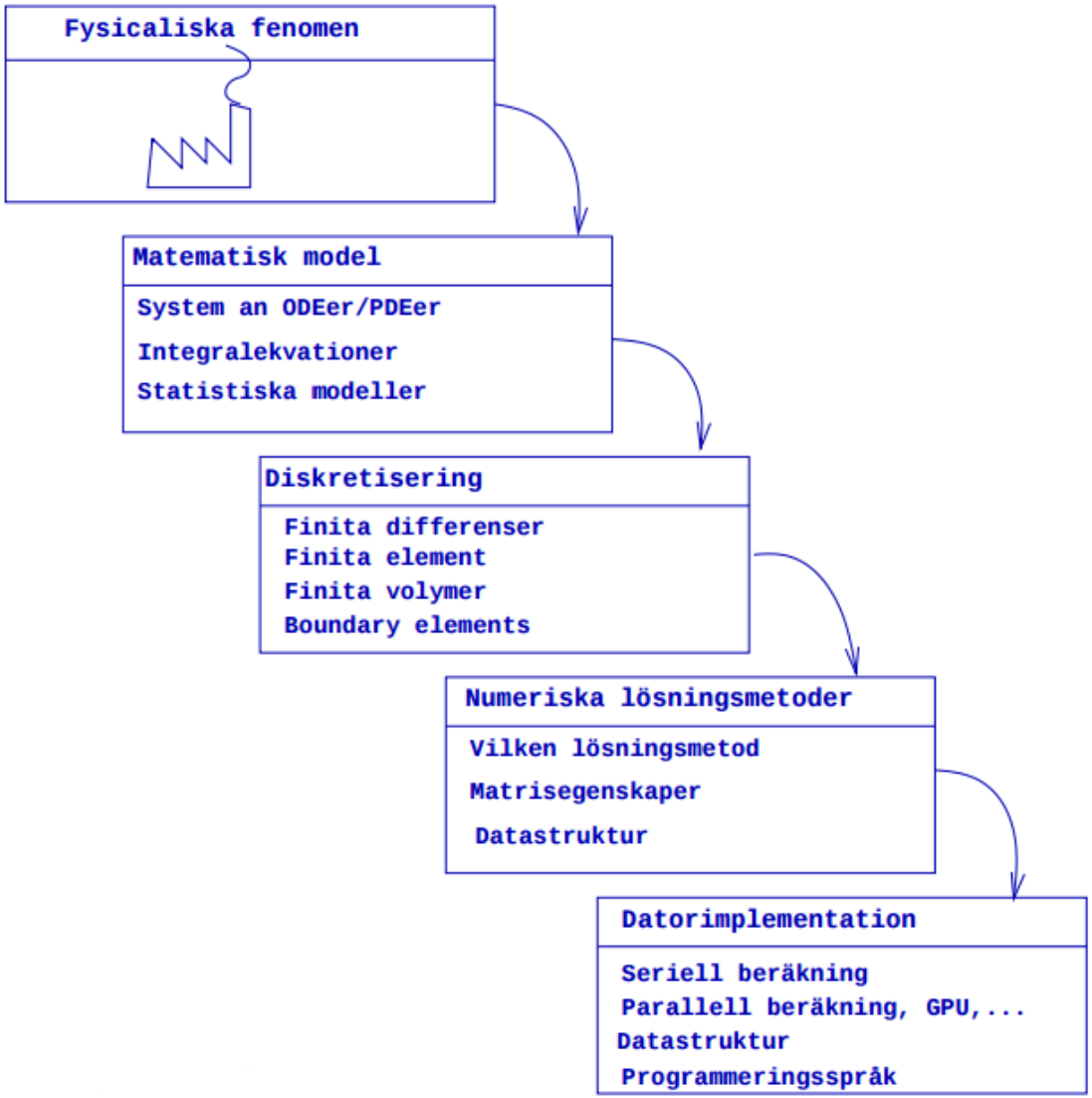
- electronic cloud of an isolated atom: 1 Å $= 10^{-10}$ m
- size of the nucleus: 10^{-14} m (10000 times smaller!)
- vibration period of the molecular bond: 1 fs $= 10^{-15}$ s



(http://www.particleadventure.org/)

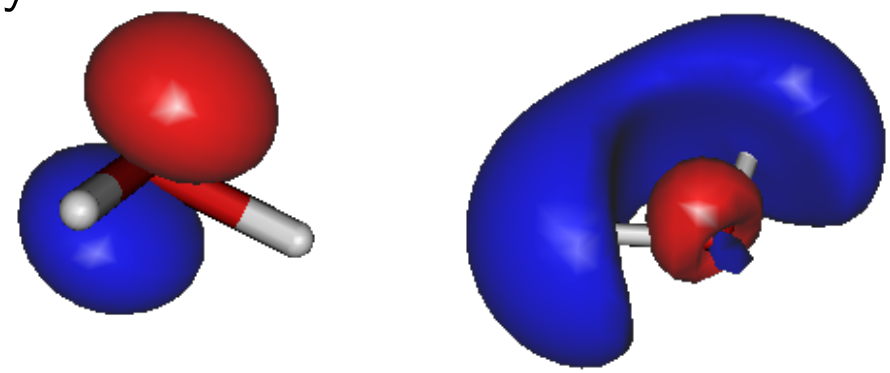
Quantum chemistry calculations:
modelling very small size systems during very short time

Modelling steps



Applications

- modelling complex biological systems (DNA studies)
- drug design (preselecting molecules as potential good candidates)
- materials industry (selecting materials with the right properties)
- chemical industry
- food industry
- . . .



Mathematical model

The **Schrödinger equation** rules the interactions between nuclei and electrons.

Non-relativistic time independent form (eigenvalue problem):

- Ground-state energy
- Hamiltonian operator

$$H\,\Phi = E\,\Phi$$

- Many-body wavefunction:
  $\Phi = \Phi(\text{coord. of nuclei}, \text{coord. of electrons})$

Mathematical model

Born-Oppenheimer approximation:
Assume that nuclei are fixed and do not move. Compute electronic wavefunction.

Then the total ground state energy is

$$E = E_{electrons} + E_{nuclei}$$

Electronic structure is the state of motion of electrons in an electrostatic field created by stationary nuclei.

Electronic structure calculations: numerically determination of electronic structure and predicting properties of matter from it.

Mathematical model

$E_{electrons} - ?$

Electronic Schrödinger equation:

$$H_{el}\Phi = E\Phi, \quad \Phi = \Phi(\text{coord. of electrons})$$

Mathematical model

$E_{electrons} - ?$

Electronic Schrödinger equation:

$$H_{el}\Phi = E\Phi, \quad \Phi = \Phi(\text{coord. of electrons})$$

Another approximation:
assume the form of the wavefunction – Φ expressed using single-particle wavefunctions ψ_i

Numerical discretization

Discretization of the single-particle wavefunction ψ_i

- Finite difference
- Finite elements; localized basis functions

Chosen basis set $\{\chi_j\}_{j=1}^{m}$

$$\psi_i = \sum_{j=1}^{m} C_{ji}\chi_j, \quad i = 1, \ldots, N$$

Solution method

Our non-linear eigenvalue problem:

$$\widehat{H}(C)C = EC$$

(1) fix C, compute $\widehat{H}$
(2) solve $\widehat{H}C = EC$ to get new C
(3) if not converged, return to step (1)

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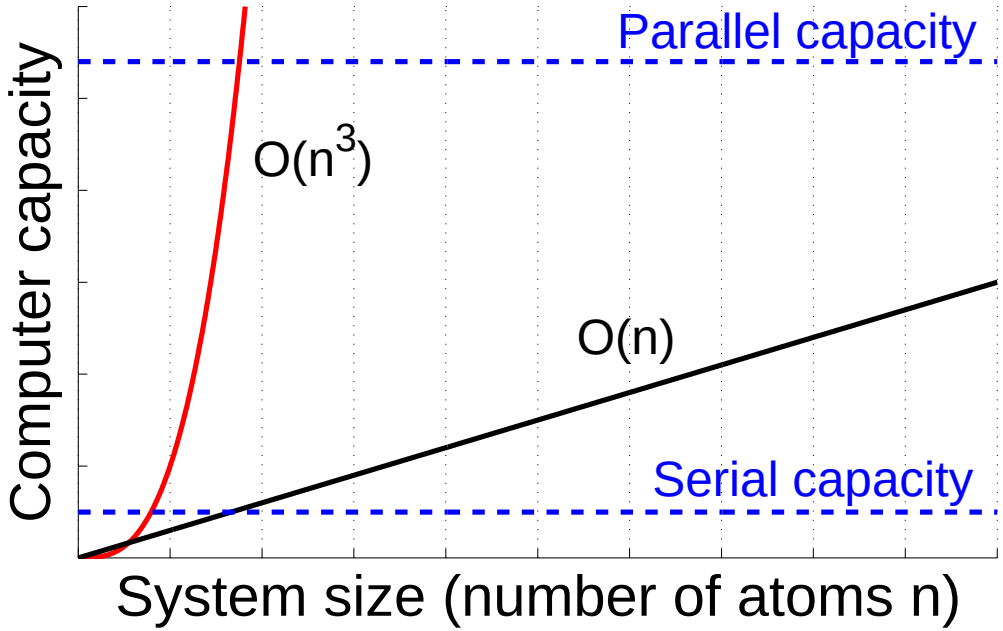
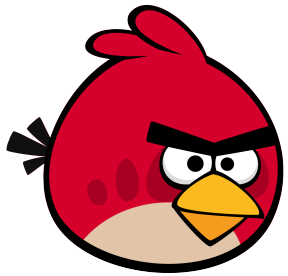
Direct diagonalization is too expensive!
We want linear scaling!

Implementation



- quantum chemistry program "Ergo"
- Chunks and Tasks programming model

Plans and goals



- Parallelize Ergo using Chunks and Tasks
- Controlling errors due to approximations, only one threshold value!

Thank you for your attention!