Computational Knowledge meets Quantum Chemistry

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Density Functional Theory

Computational Knowledge

Wolfram Language™

Chemistry

Drug Design

Molecular Biology

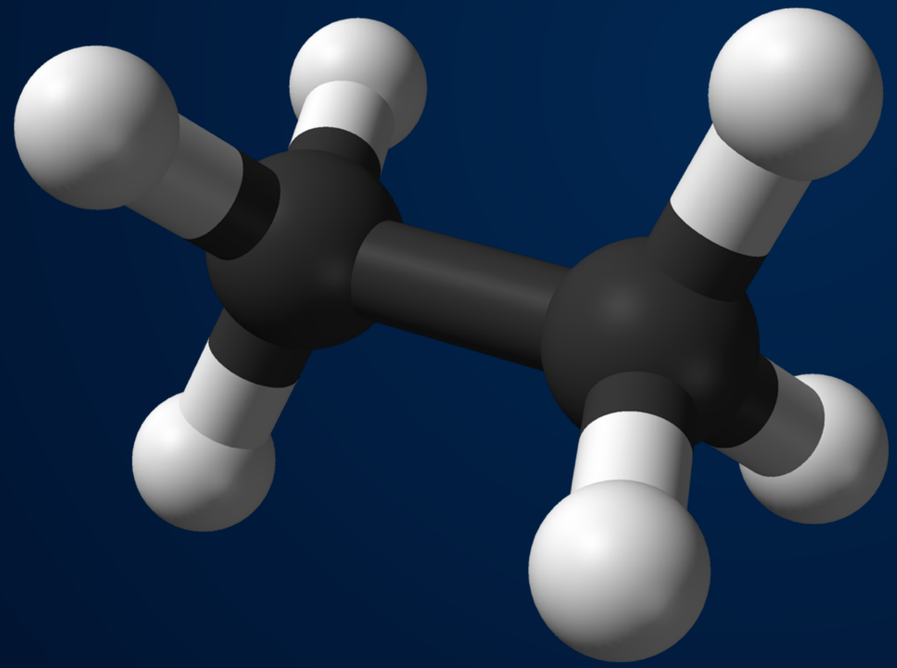
$$H\psi = E\psi$$

Material Science
(Steel production down to nanotechnology)

Semiconductor technology

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

Ethane (C_2H_6)



30 electrons

$$\psi(x_1, y_1, z_1, x_2, y_2, z_2, \ldots, x_{30}, y_{30}, z_{30})$$

20 grid points per coordinate ⟶ **needs 8 20^{90} bytes**

Ultimate storage medium (hypothetical): 1 byte per atom…

← 10^9 Petabyte!

Volume to store 8 20^{90} bytes?


About 1.6 10^{39} ly^3
(yes, cubic light-years)
Roughly ~ 1 Million x
size of the universe

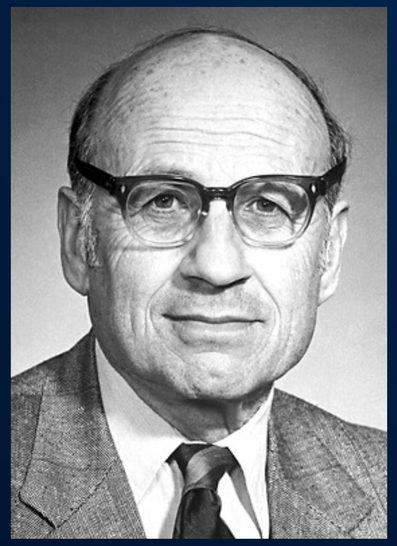
Density Functional Theory

("DFT")

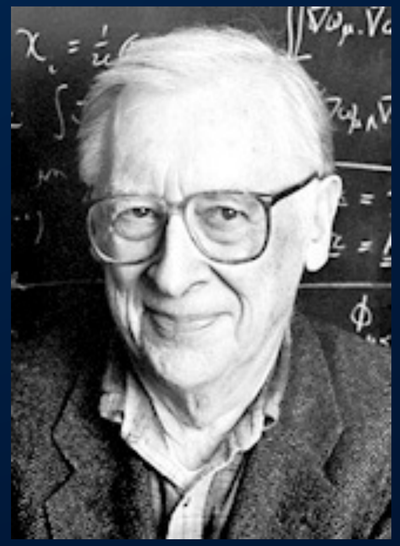
Approximation to the *ground state* of the system

Based on two theorems by Pierre C. Hohenberg and Walther Kohn (1964)

Pierre C. Hohenberg



Walther Kohn
(nobel laureate
chemistry 1998)

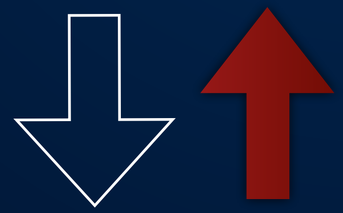


John A. Pople
(nobel laureate
chemistry 1998)

Hohenberg-Kohn 1: “The density is special”

Whole information on ground state is
“*in principle*” contained in the density alone!

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$ (Millions of universes…)



$$\rho(\mathbf{r})$$ (100 kB … 100 MB)

(existence theorem alert !)

Everything depends on the density ***alone***!

“Everything is a ***functional*** of the density”

$$E = E[\rho]$$

Hohenberg-Kohn 2: “The energy is special”

The ground state density minimises the energy functional

$$E[\rho \neq \rho_0] \geq E[\rho_0] = E_0$$

Existence theorem alert:
we still *don’t know* the exact energy functional

Minimize **approximations** to the energy functional
(50 years of experience in finding good approximations)

Calculations: Demanding, but doable

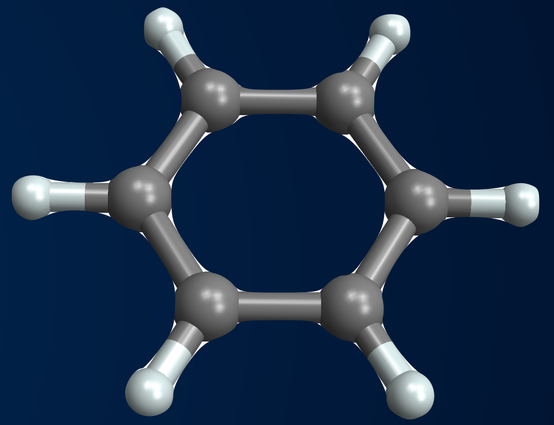
	CPU time (core hours)	Memory
Ethane (30 electrons)	seconds	few megabytes
Fullerene (C60) (240 electrons)	5 core-h	few gigabytes
Si Nanowire (~57000 electrons)	1.1 Mio. core-h	few TB (?)

Show me what you can do!

Example 1:
Quantum Dots

Example 2: Nuclear Magnetic Resonance

Benzene Molecule



Calculation Input:

- 6 Carbon
- 6 Hydrogen
- rough structure

chem. structure

NMR spectrum

DFT and the Wolfram Language

Why Wolfram Language

- Traditional languages: Fortran, C++
  - How do they compare?
- Rapid Development, framework that makes it easy to try out new ideas
- Use it as a “computational knowledge tool” (more later …)

Disclaimer:

This is a very rough, qualitative, anecdotal, largely inadequate comparison.
It’s a “user story”, not a benchmark.

Only orders of magnitude count !
(i.e. a factor of 2 is not a big deal - a factor of 100 might be significant)

Efficiency: Runtime

Disclaimer: Very different Algorithms!
(only orders of magnitude count)

Mathematica code roughly ~ C++ code

	C++ Code	Mathematica
Harmonic Oscillator	4.1s	4.5s
Fullerene (C60) Full calculation	5h 35m	5h 55m

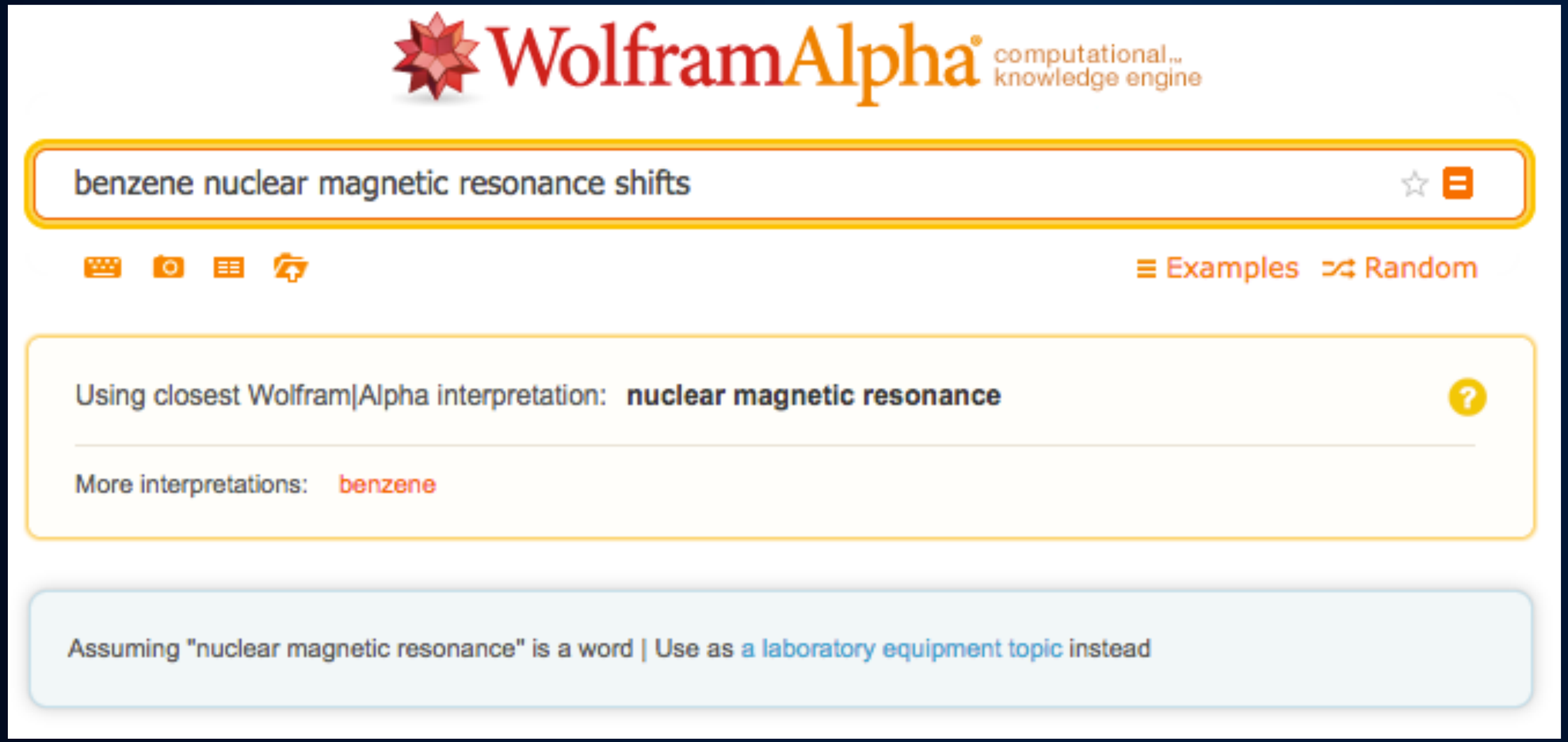
Efficiency: Development

	Language	SLOC	person years	Features	Features
LiMeReC	Fortran	50,000	3-4 years	100%	2D+3D, FD, Pseudopotentials
PEST	C++	20,000	1.5 years	80%	2D + 3D, FD, Magnetic Fields
Mathematica DFT	Wolfram	300 (DFT) + 860 (FEM)	70hrs	50%	2D+3D, FEM

DFT and Computable Knowledge

- Chemical Space (“all possible compounds that can be produced by elements from the periodic table”) is huge
- no way to get empirical (experimental) data on all that
- At least a subset of that can be made **computable** (from just the knowledge of the chemical structure)

Vision: Quantum Chemistry and Computational Knowledge



Thank You!

Questions?