



Quantum Computing at Total

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 project leader researcher scientific advisor
 + PhD students, postdocs, interns

The background features a collage of scientific and mathematical content:

- Top Left:** TOTAL logo.
- Top Center:** Vector calculus identities:

$$\begin{aligned} \nabla \cdot (\psi \nabla \chi) &= (\nabla \psi) \cdot \nabla \chi + \psi \nabla^2 \chi \\ \nabla \cdot (\chi \nabla \psi) &= (\nabla \chi) \cdot \nabla \psi + \chi \nabla^2 \psi \\ \nabla \cdot (\psi \nabla \chi) - \nabla \cdot (\chi \nabla \psi) &= (\nabla \psi) \cdot \nabla \chi - (\nabla \chi) \cdot \nabla \psi \\ \nabla \psi \times \nabla \chi &= -\nabla \chi \times \nabla \psi \end{aligned}$$
- Top Right:** Quantum wavefunction equations:

$$\begin{aligned} \nabla^2 \psi + k^2 \psi &= 0 \\ \psi_0(x) &= e^{i\frac{1}{2}kx} \sin 2x \\ \psi_{sc}(x) &= e^{i\frac{1}{2}kx} \sin 2x (\cos x + \sigma \sin x) \end{aligned}$$
- Middle Left:** A graph showing a sinusoidal wave $y_0(x)$ on a coordinate system.
- Middle Right:** A 3D sphere with axes labeled a, b, and c.
- Center:** A logic flow diagram with nodes: TRUE, FALSE, P & Q, P & ~Q, ~P & Q, P & ~P, Q & ~Q, P & Q & ~Q, ~P & Q & ~Q, P & Q & P, ~P & Q & P, P & Q & P & Q, ~P & Q & P & Q, P & Q & P & Q & ~Q, ~P & Q & P & Q & ~Q.
- Bottom Left:** Chemical structures including a carbocation $K^+ O=N^+ H-O-CH_2-CH_3$ and a complex organic molecule.
- Bottom Center:** A graph of a domain with points a and b on the x-axis.
- Bottom Right:** A 3D coordinate system with axes dx, dy, dz and a vector field.

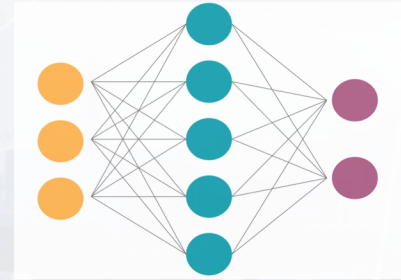
Roadmap & potential use cases



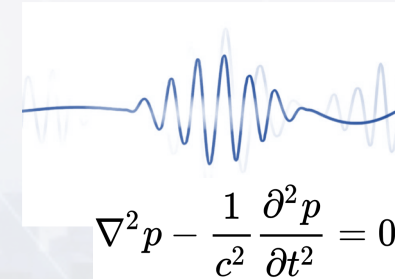
Quantum chemistry



Quantum combinatorial optimization



QML

A blue waveform representing a signal, with the partial differential equation $\nabla^2 p - \frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} = 0$ written below it.

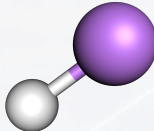
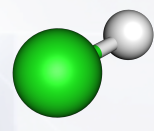
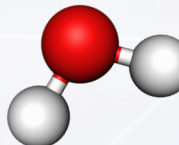
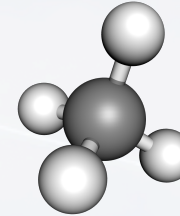
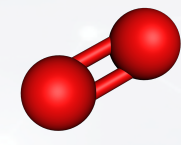
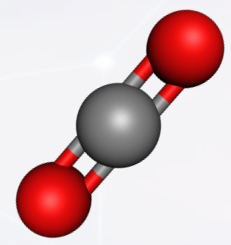
Linear algebra (ODEs, PDEs, inverse problems)

NISQ device $\sim (10^2)$ qubits) 3-5 years

(pre)-QEC device $\sim (10^{3(-6)})$ qubits) 5++ years

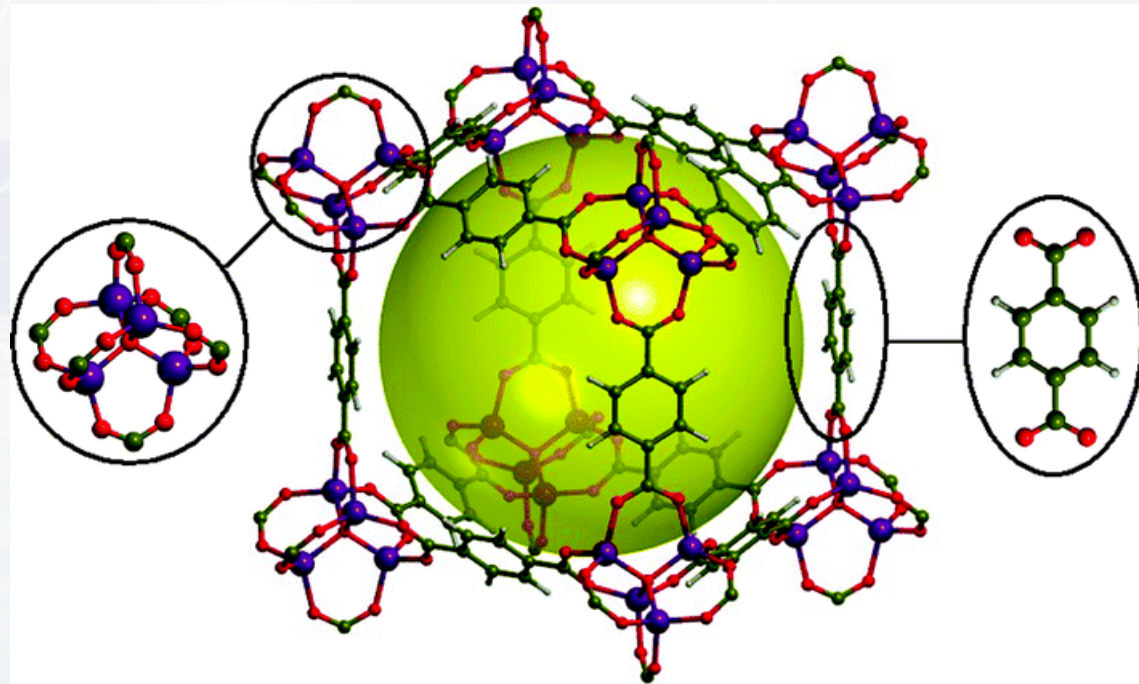
Quantum Chemistry ground state problem with VQE

ATOS 35 qubit simulator

ground state energies						
	LiH	BeH	H2O	CH4	O2	CO2
VQE Total	-7.76	-14.44	-72.91	-38.97	-144.28	-179.93
VQE Atos	-7.79	-14.60	-73.15	-39.12	-144.15	-180.92
FCI OpenFermion	-7.87	-14.96	-74.99	-39.81	-147.74	-185.23

1 - 3 % difference with respect to classical algorithms

Quantum Chemistry ground state problem with VQE

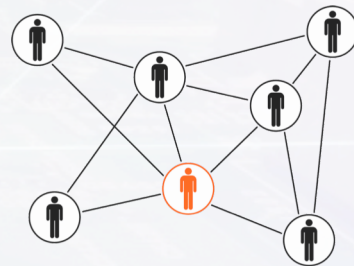


CrystEngComm, 8, 364-371 (2006)

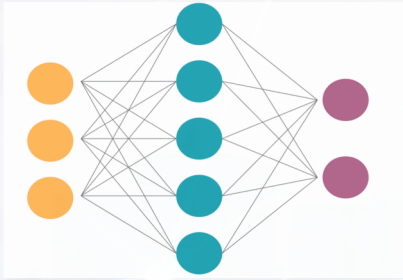
Quantum Combinatorial Optimization

with V. Dunjko and C. Moussa from Leiden

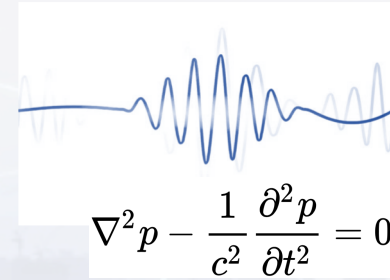
- **Knapsack problem** - Function Maximization with Dynamic Quantum Search. In International Workshop on Quantum Technology and Optimization Problems (pp. 86-95). Springer, Cham.
- **MaxCut** (comparison between GW and QAOA for graph cuts)
- **Scheduling, Traveling Salesman, Mesh segmentation**



ML and PDE's




Hydrocarbon well modelling



Seismic depth imaging (sesmic wave Eq.)

Quantum computing in 2020 at TOTAL

- Investigating the scalability of VQE + investigate further algorithms for chemistry 
- Continue investigating combinatorial optimization (traveling salesman)
- Pursue exciting avenues to explore with quantum computing: differential equations, machine learning (pattern recognition)
- Run algorithms on actual hardware

Quantum computing in the next 5 years

- TOTAL is the global leader in quantum algorithm design