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Exploring Quantum Computing for O&G industry application

INTRODUCTION

EXPLORATION-PRODUCTION @ TOTAL AND HPC A SUCCESSFUL PARTNERSHIP

COMPUTE REQUIREMENTS CONTINUE TO GROW AN THERE'S MORE WE WANT TO DO

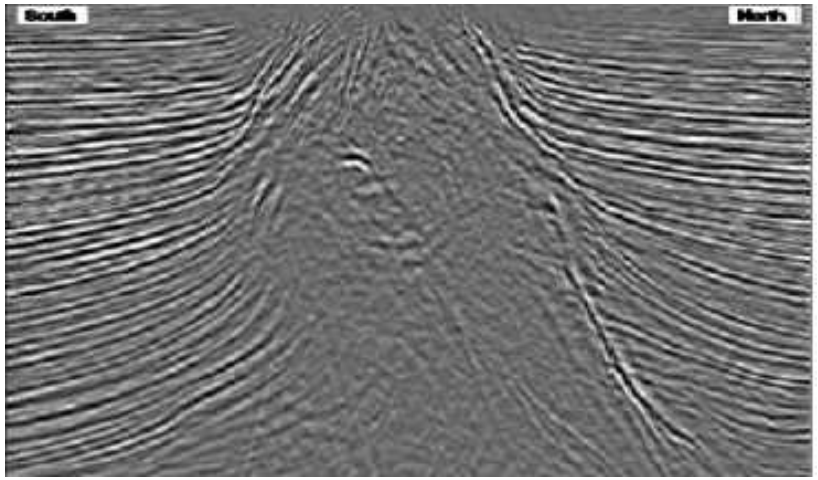
EXPLORE ALTERNATIVE HPC TECHNOLOGIES: QUANTUM COMPUTING

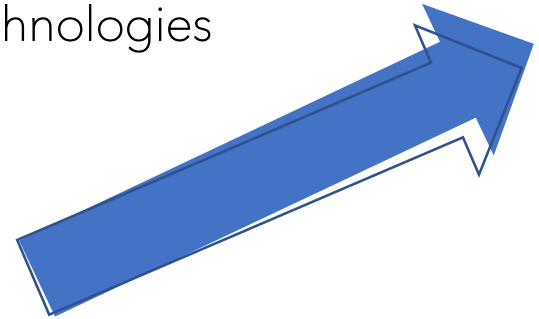
CONCLUSION

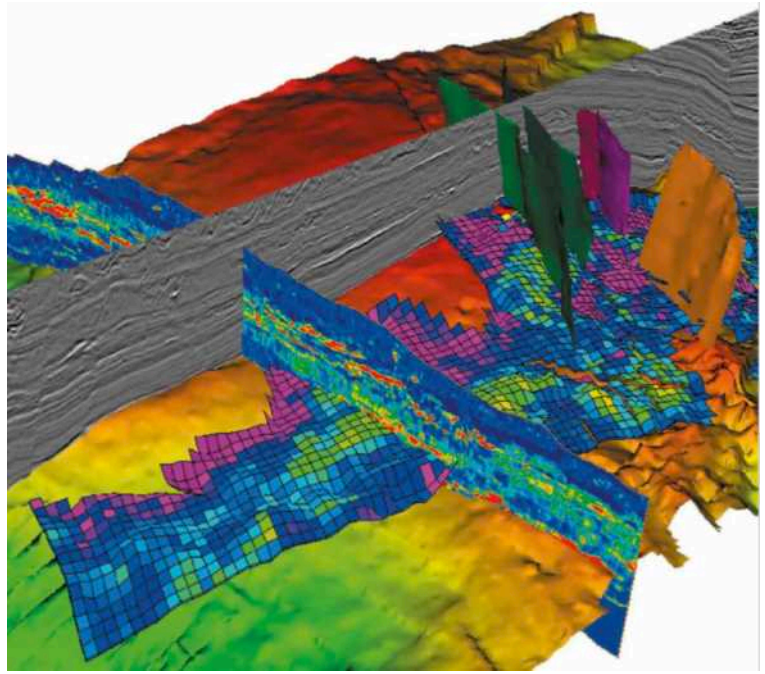
More than 30 years of R&D and innovation

O&G E&P, a challenging environment:

- ✓ Reduce Risks, Reduce Cost
- ✓Open new frontiers
  - ➔Improve technology
  - ➔Increase Know How
  - ➔Integrate more advanced technologies







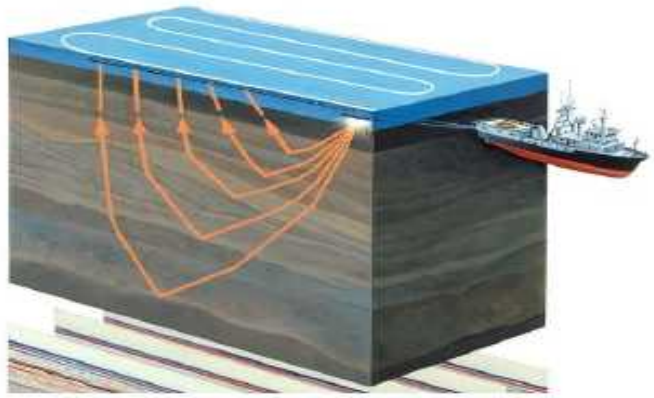
HPC is one of the key element for the integration of:

- ✓ More physics,
- ✓ More complex algorithm
- ✓ More data from different sources.
- ✓ …

TOTAL

O&G E&P, in one slide

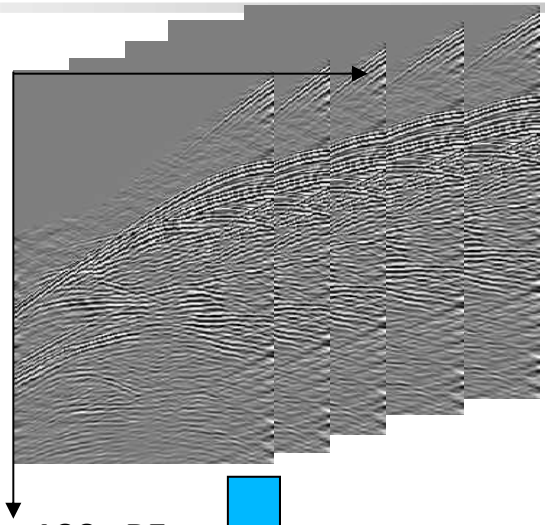
$100s M



1000's Km^2 surface acquisition

Seismic acquisition

100s TB data



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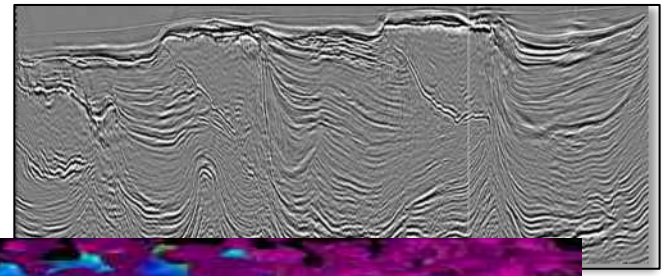
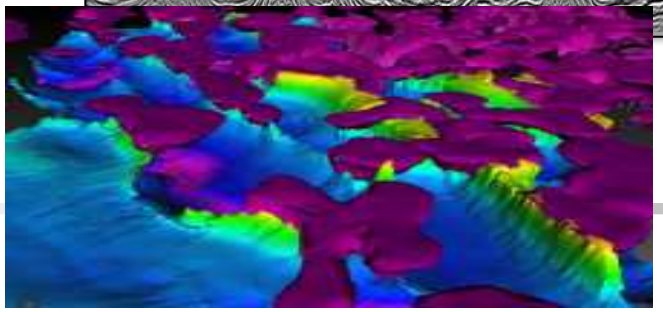
Seismic Depth Imaging

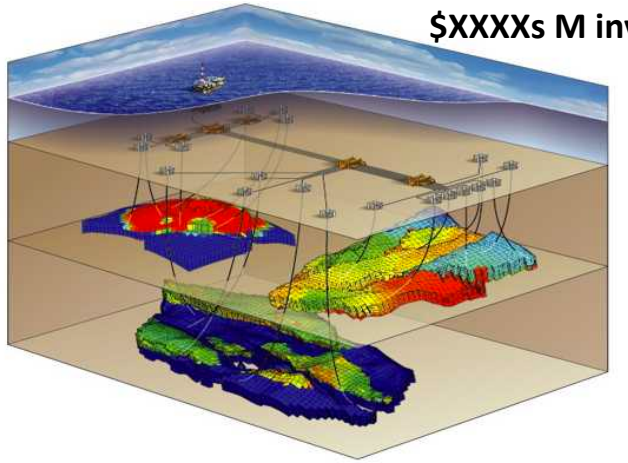




Reservoir appraisal

$XXXXs M investment

XXXs Gboe

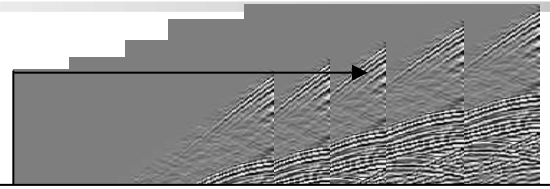


Production Forecast and optimization

TOTAL

O&G E&P, in one slide

Seismic acquisition

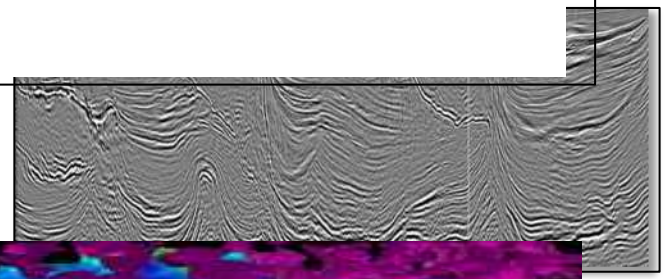


$100s M

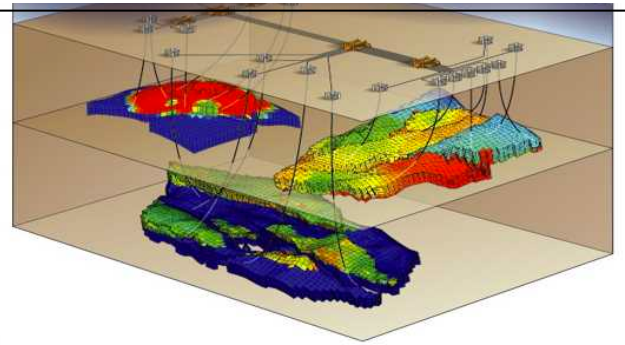
Improving process:

- ➔ More physics
- ➔ More complex Algorithm
- ➔ More integration of different technologies
- ➔ More R&D
- ➔ More HPC.

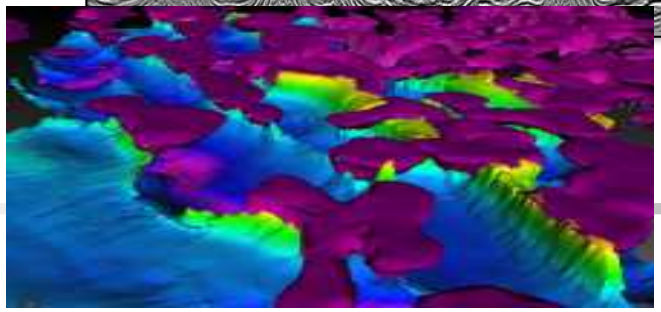
maging



XXXs Gboe



Production Forecast and optimization



TOTAL

Seismic depth imaging technology key dates

More physics, more accurate images
More complex optimization process:
Non linear inverse problem (FWI)

3D full wave equation depth imaging

Emergence of 3D seismic depth imaging

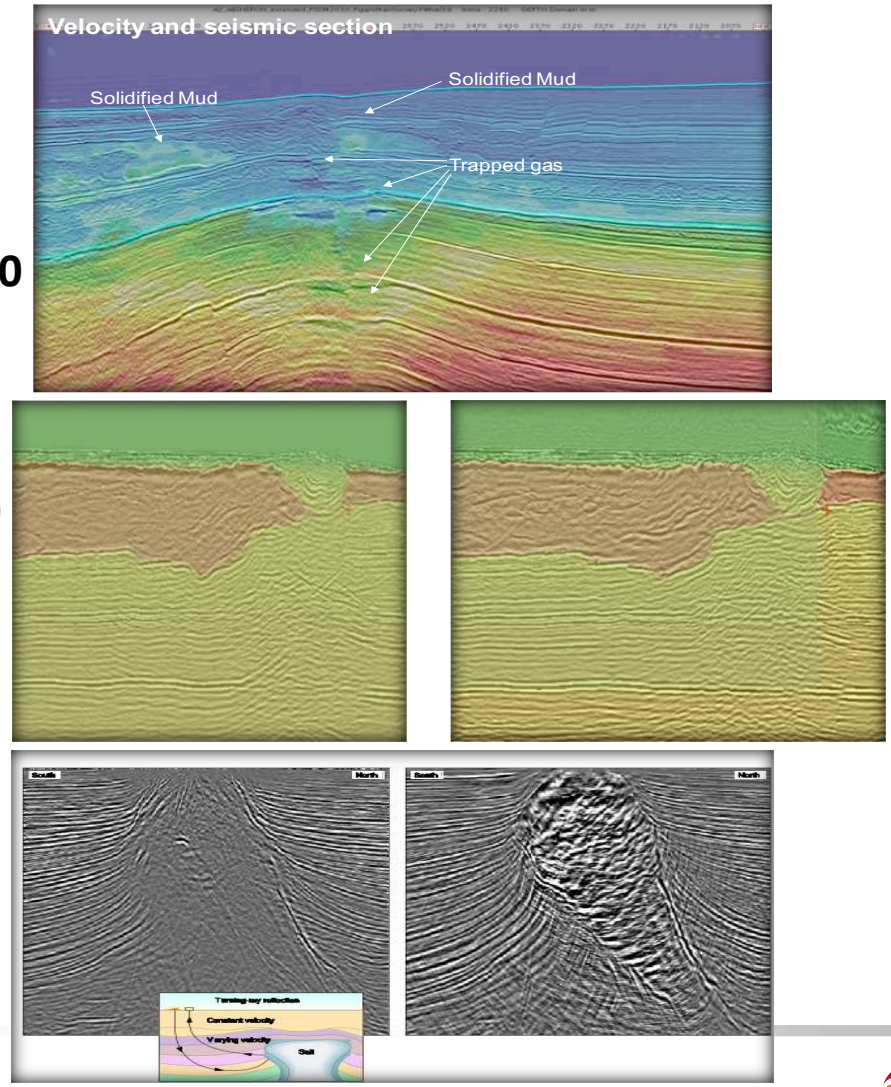
The 2D space Era

1980

1990

2000

2010



Seismic depth imaging and HPC a successful partnership

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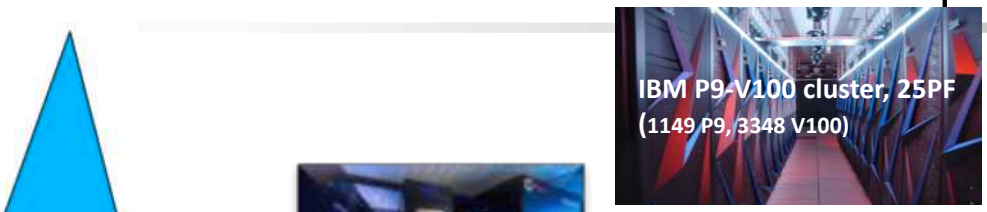
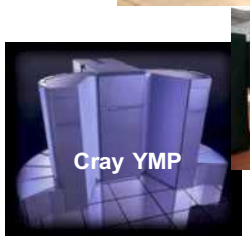




Accelerated Cluster

CPU Cluster

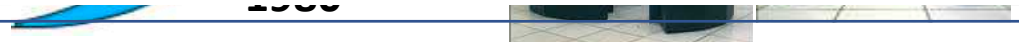
CPU SMP

Vector HPC

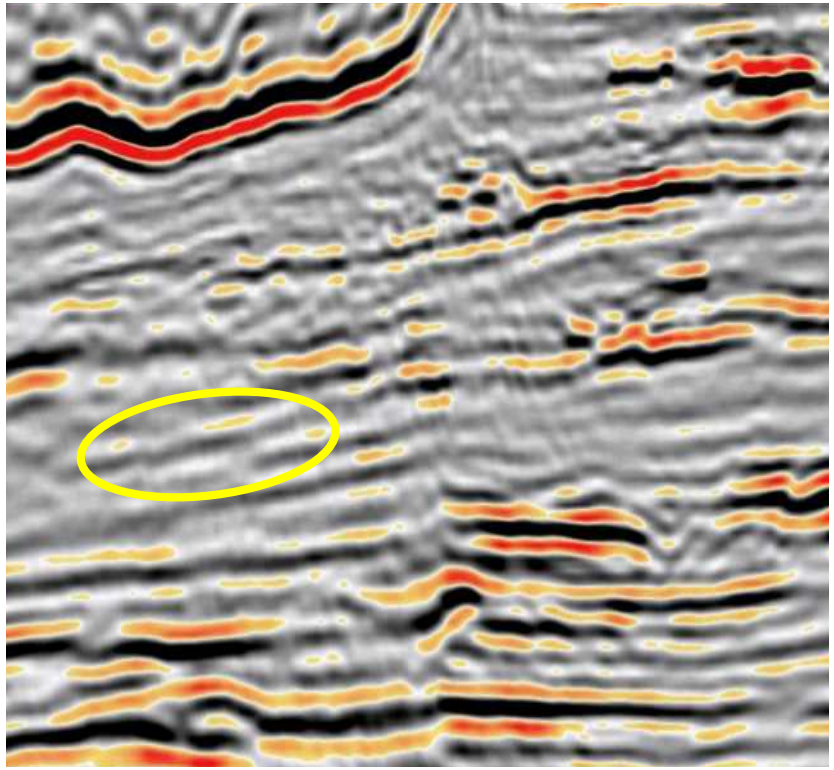
TOTAL

Seismic depth imaging and HPC a successful partnership

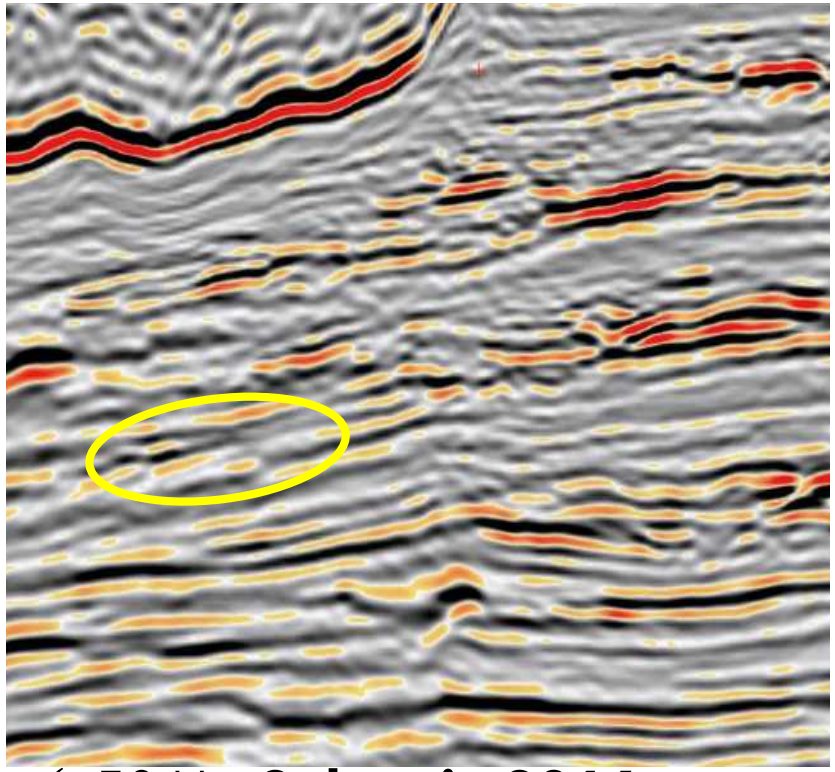
- Reduce Risks
  - Be more precise and selective
  - Run faster and see better
  - Optimize seismic depth imaging workflow
- Reduce Cost
  - Optimize acquisition design
  - Better production forecasting, improve EOR
- Open new frontiers
  - Better appraisal of new exploration domains



Run faster, see better



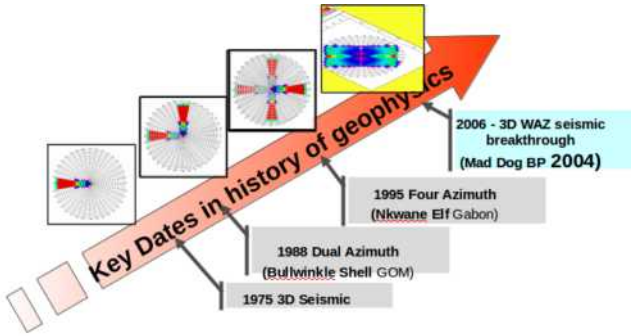
- ✓ 35 Hz, **30 days in 2012**
- ✓ … where is the turbiditic lobe?

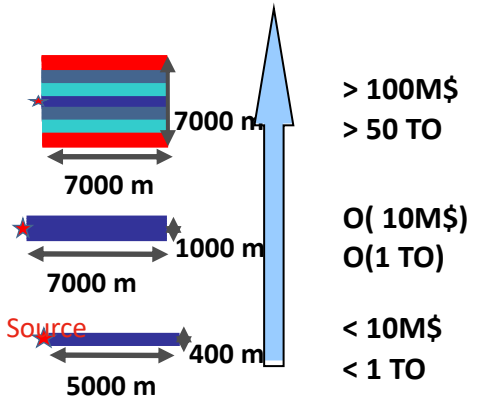


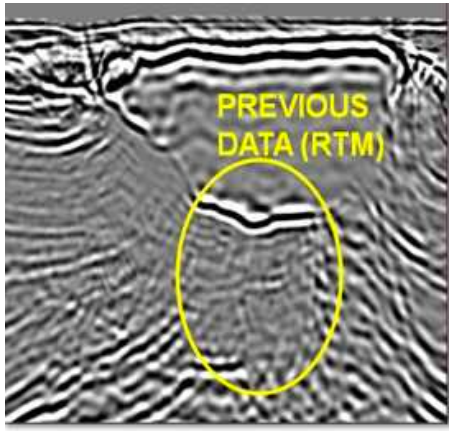
- ✓ 50 Hz, **3 days in 2016**
- ✓ … Lobe can be seen !

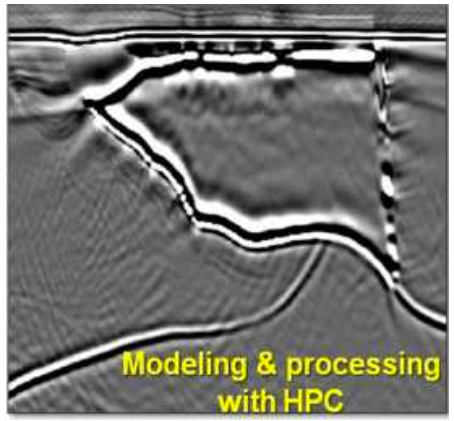
Accessing more reserves, previously unseen / undevelopable

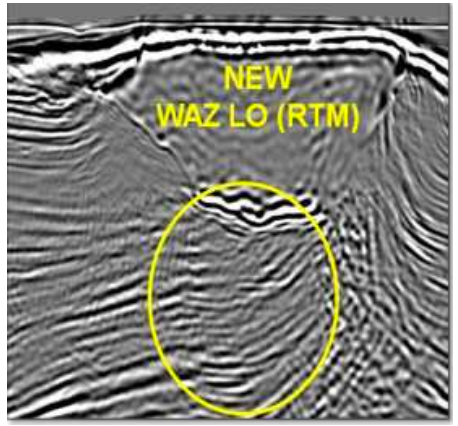
Reduce Risk and Cost









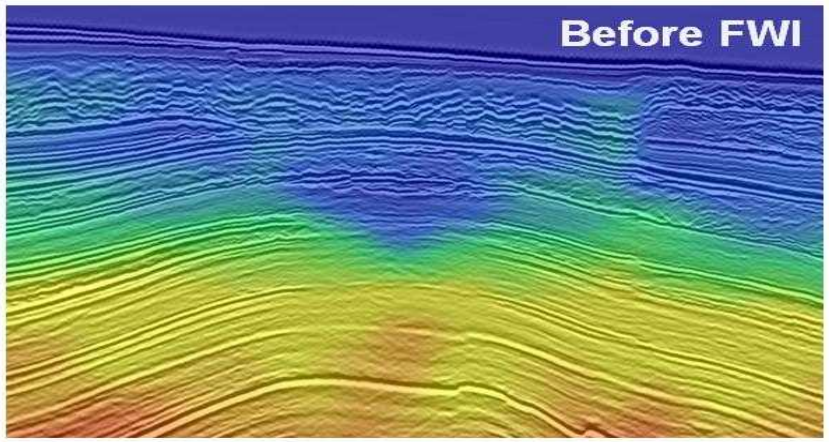


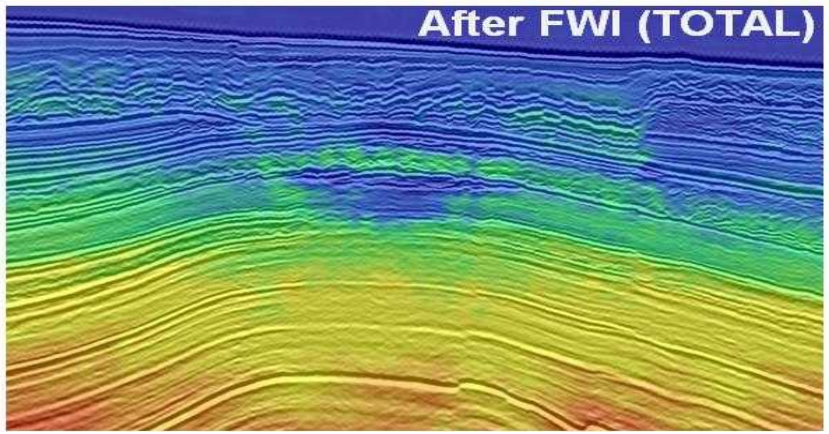
✓ Better illumination of complex geological structures

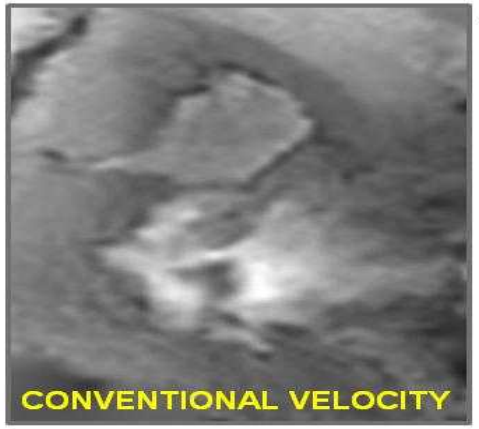
✓ Improves imaging process

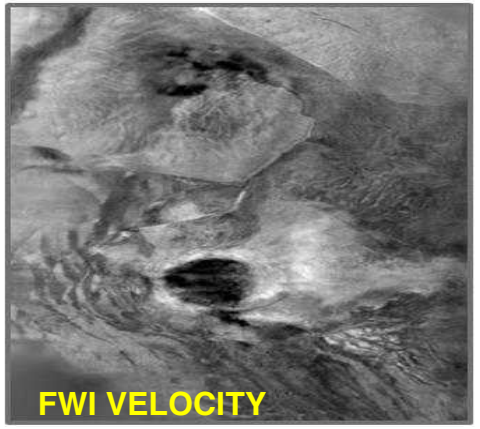
➔ saving > $20 M of exploration budget while matching expected quality

Reduce Risk and accelerate appraisal









Improved resolution of seismic velocities

↓

Hazards & Pore Pressure prognosis

Reliable structure

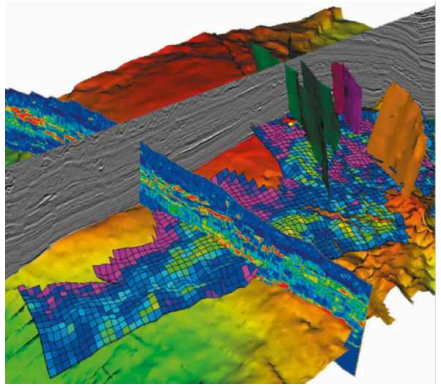
Full wave form inversion of seismic velocities

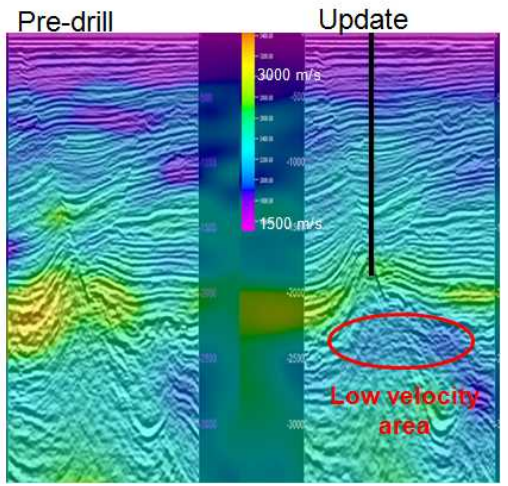
➔ sharper imaging, hazards identification, increased reliability of discovered volumes

➔ accelerate appraisal & reduce its cost

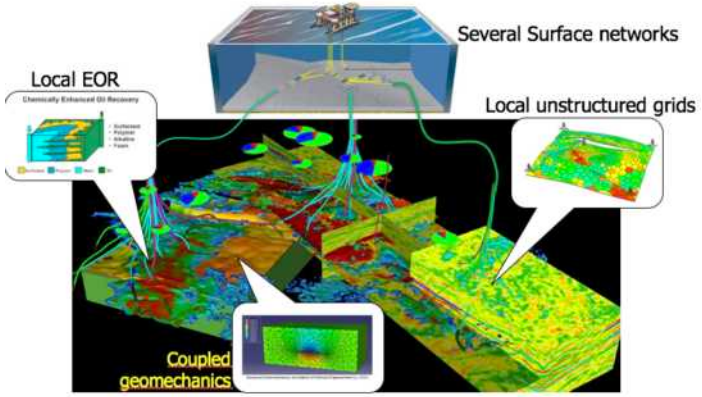
Compute requirement continue to grow

- ✓ Seismic depth imaging:
  - ✓ compute better, faster
  - ✓ More physics
  - ✓ More data integration
  - ✓ Uncertainty quantification





- ✓ Reservoir simulation:
  - ✓ Compute faster
  - ✓ Better predictability



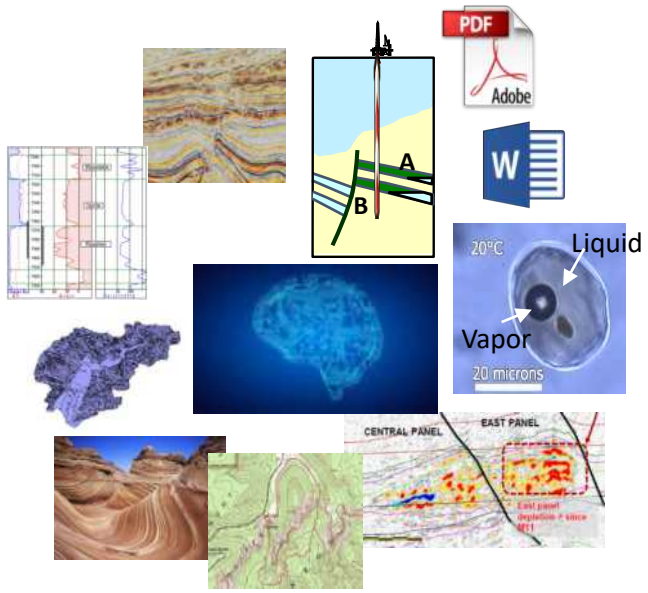
- ✓ Multi real time simulations
  - ✓ Inversion of subsurface models
  - ✓ operations optimization,
  - ✓ cost and risk reduction

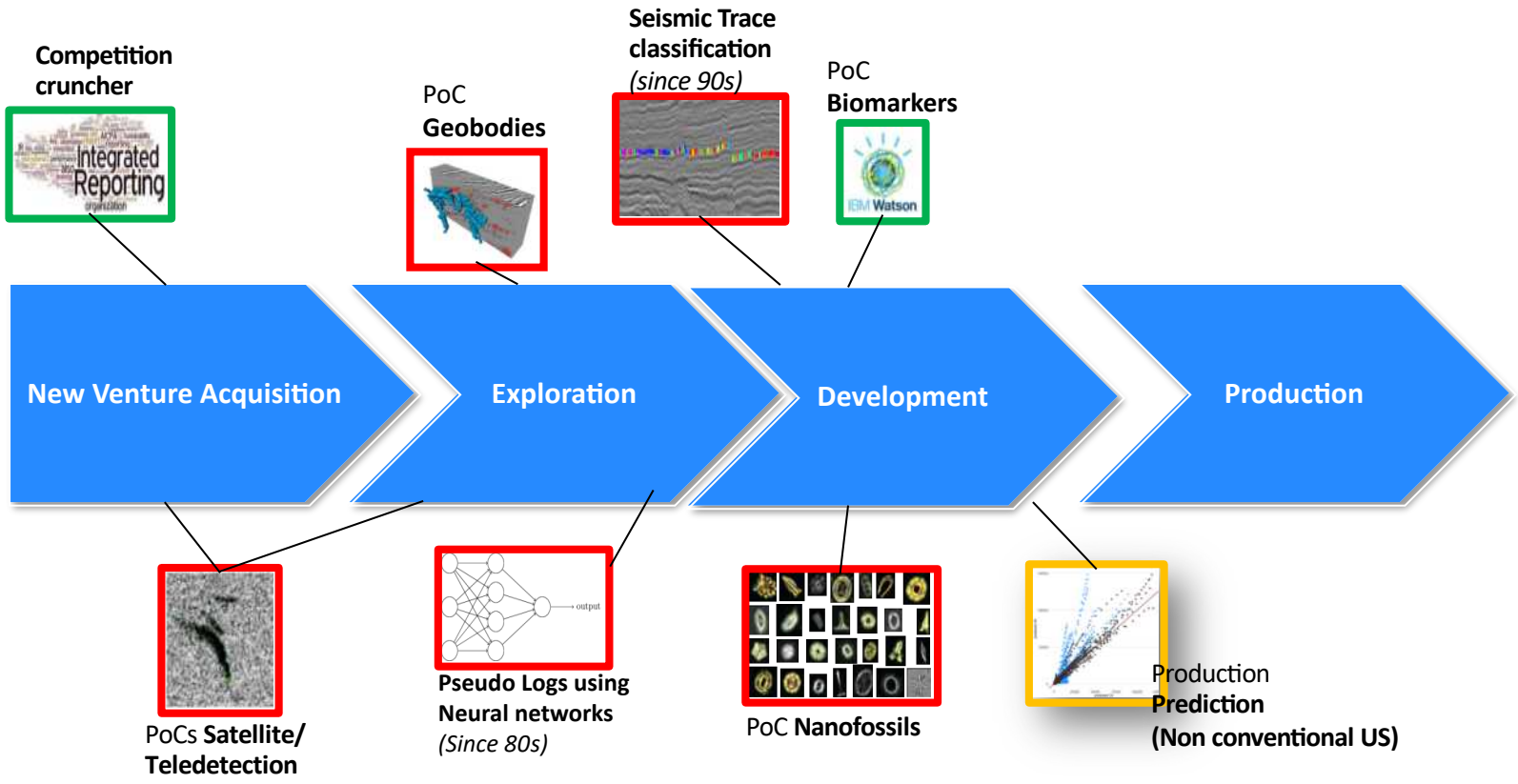
- ✓ More complex targets:
  - ✓ strong geological heterogeneity – several reservoirs
- ✓ Massive simulations:
  - ✓ history matches; uncertainty Mgt on huge models
- ✓ New physics for EOR & integration of different processes incl. geomechanics

And there is more we want to do

Machine learning, HPDA

- ✓ Development of new training set and algorithms
- ✓ Classification and sampling of large dataset
- ✓ Physics-constrained neural nets…





- ✓ 20 years of "routine" application of neural networks for seismic image analysis
- ✓ Competency update in the past 2 years through R&D and Digital "small scale" projects

TOTAL

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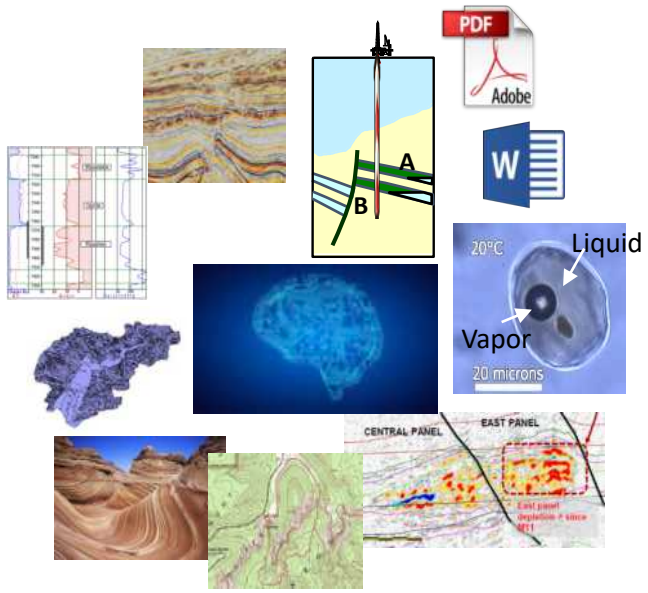
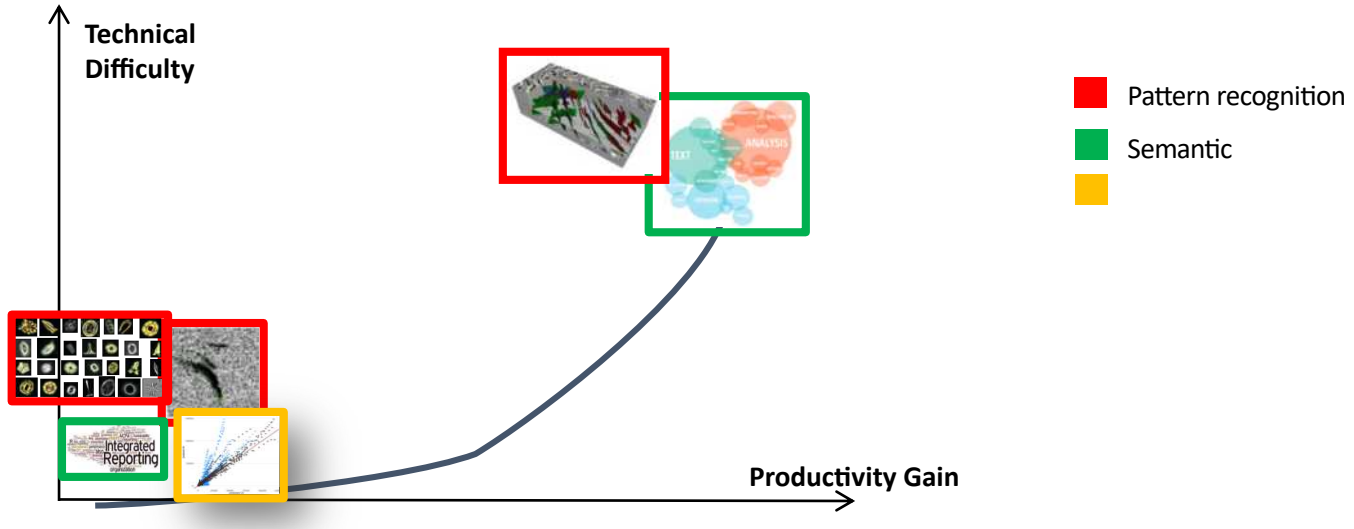




Exploration Workflow

IA — *Reduction of time to get the right information*

Seismic Acquisition — 6 months prep, 2 months acq

Processing & Imaging — 3-12 months

Interpretation — 3-6 months

IA — *Reduction of manual tasks & automated feature extraction*

Well Preparation — 8-12 months

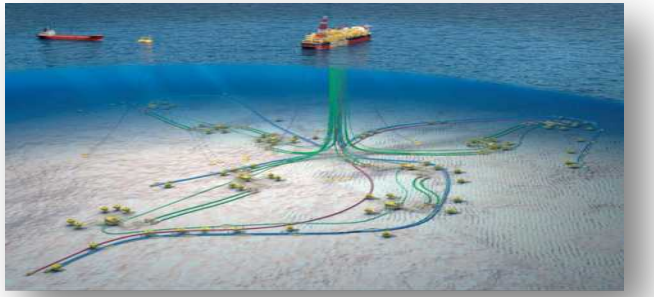
Drilling — 2-4 months

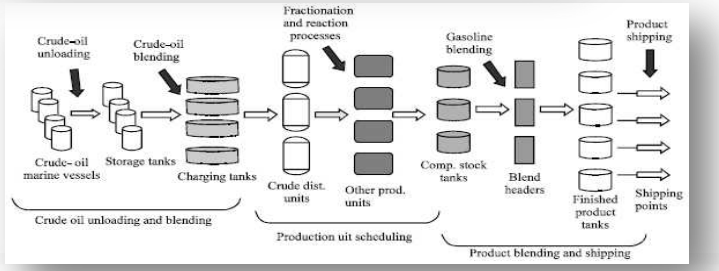
TOTAL

And there is more we want to do

Combinatorial optimization

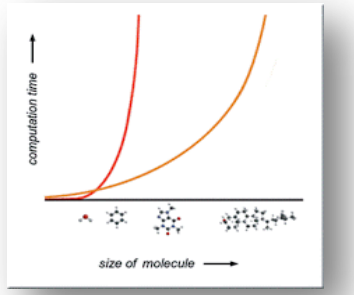
- ✓ MINLP (Mixed Integer Non Linear programming) problems in general including:
  - ✓ Refinery blending,
  - ✓ Scheduling, production, shipping.
  - ✓ Oil field/reservoir optimization
  - ✓ ….

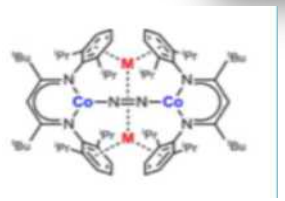




Computational material science

- ✓ The ability to accurately model ground states of fermionic systems would have significant implications for many areas of chemistry and materials science:
  - ✓ Catalysis, Solvents, Lubricants, batteries…
  - ✓ CO_2 capture
  - ✓ …





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Computational mate

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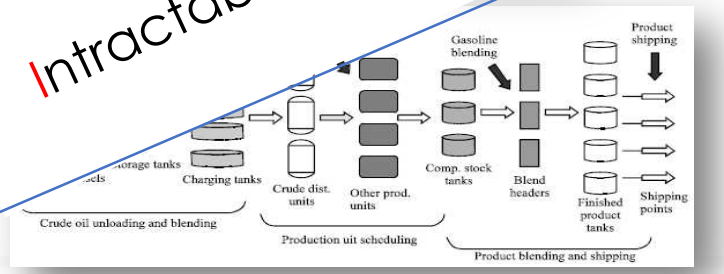
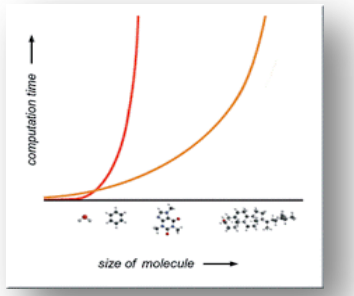
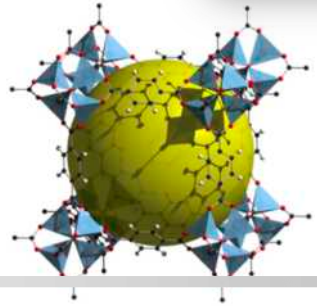
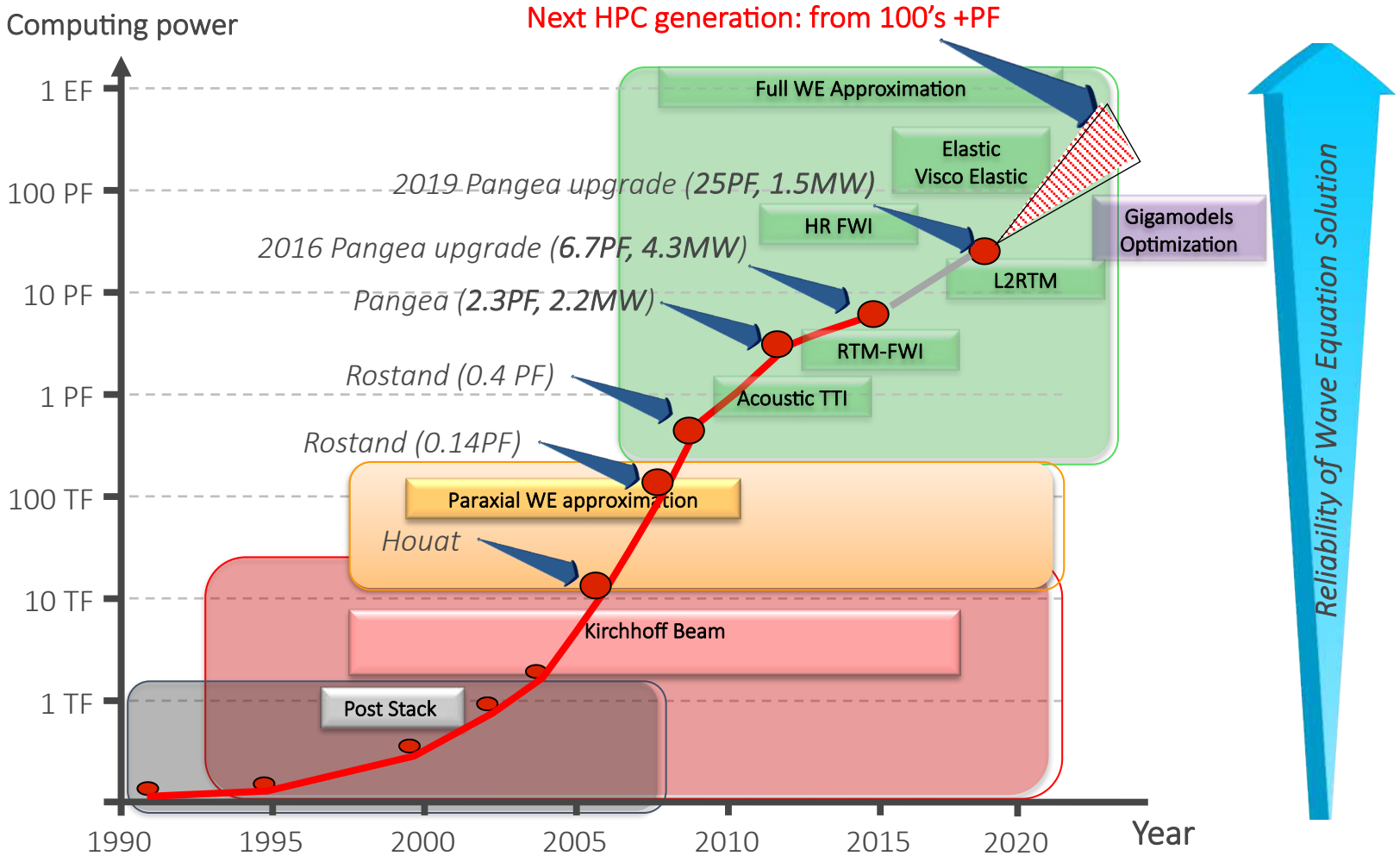
Intractable problems on classical High Performance Computing





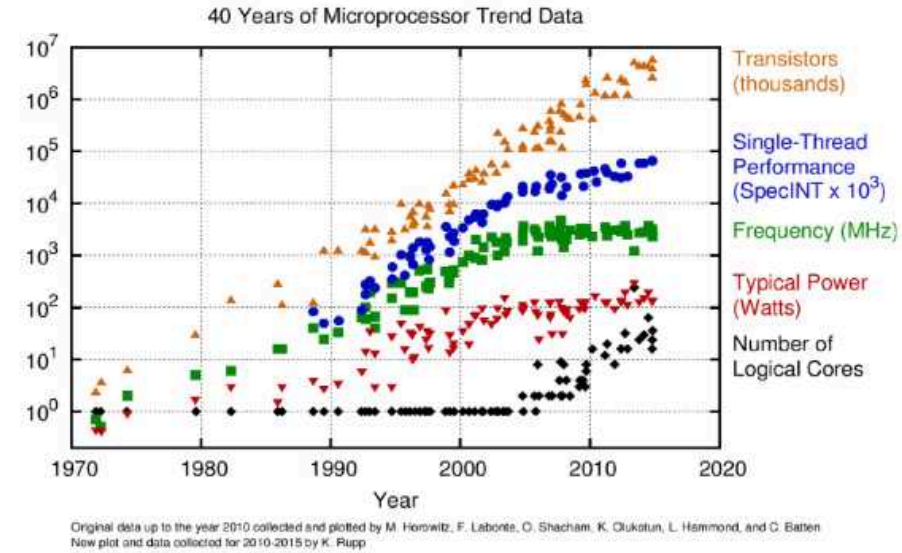


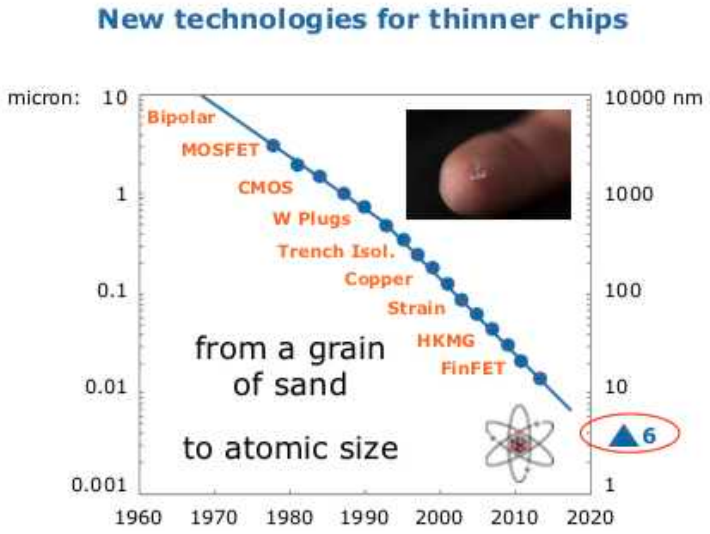
Compute Power and seismic imaging methods evolution

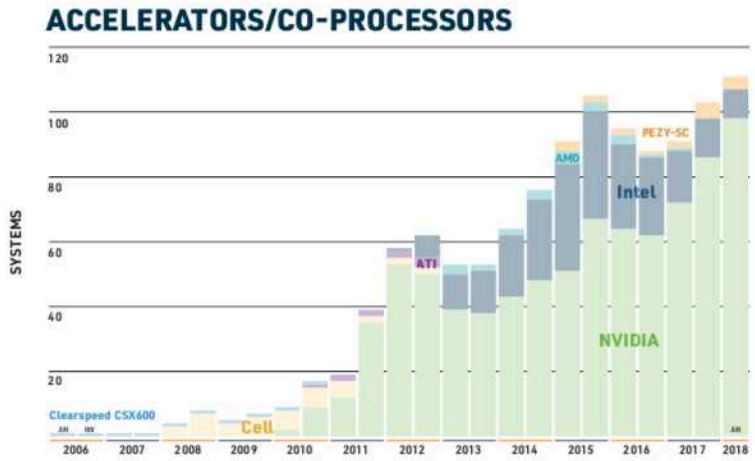


Toward complex classical HPC systems

- ✓ Classical computers have fundamental limits:
  - Transistor scaling
  - Energy consumption
- ✓ HPC systems are likely to become much more heterogeneous and massively-parallel systems
  - Parallelism limitations: Adhams'law
- ✓ End of Moore's law is expected by around 2025 !!

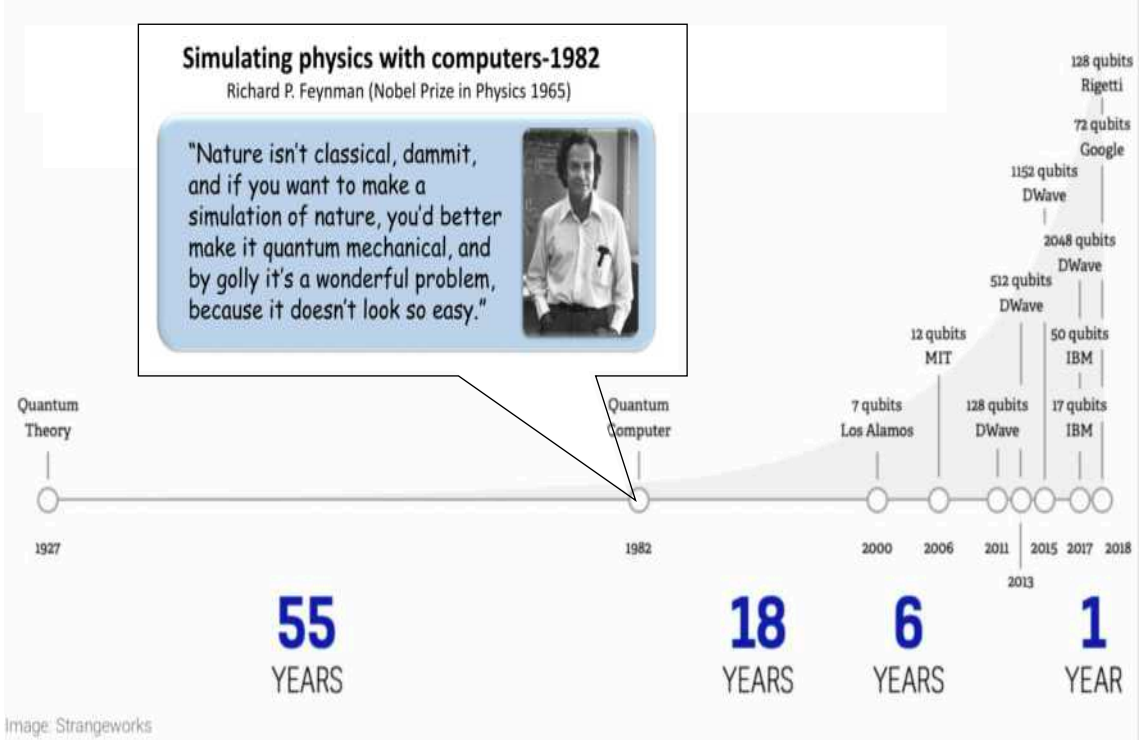






Quantum Computing a groundbreaking new approach

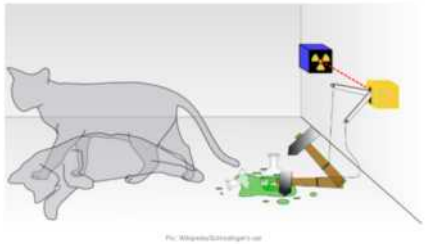
Quantum computation exploits the rules of quantum mechanics to process information

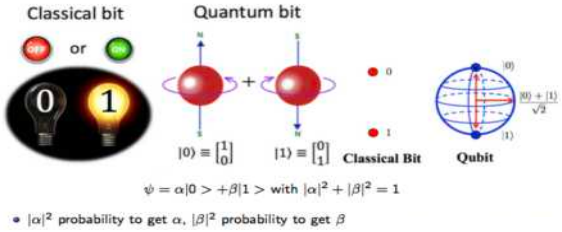


Quantum hardware development is accelerating

Superposition:

- 2 different states simultaneously until … measurement





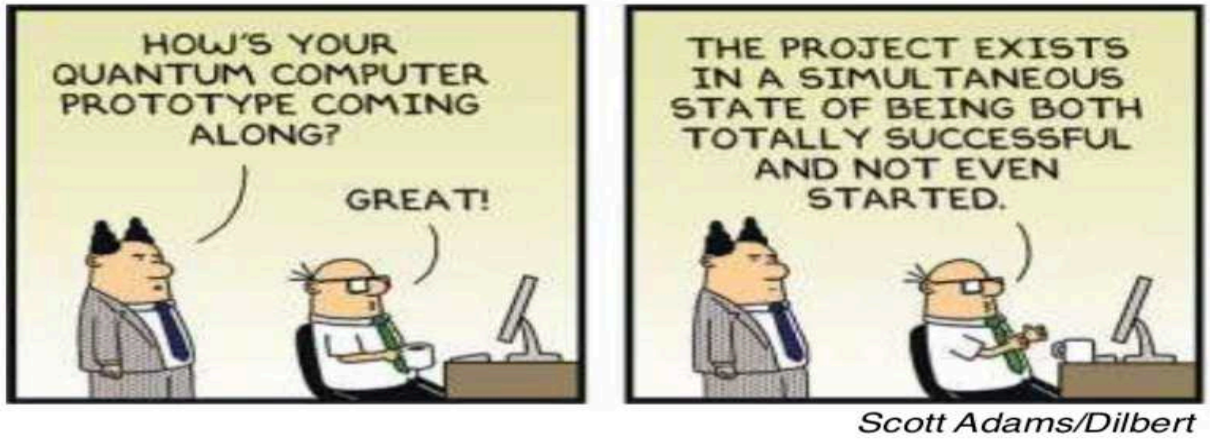
- N particles in superposition can carry out 2^N numbers a quantum computer can manipulate in parallel

Entanglement:

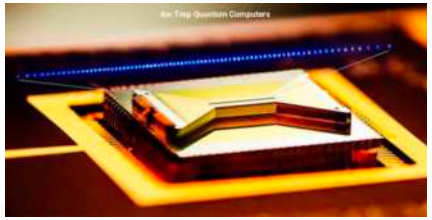
A very challenging technology

✓Quantum computing is a huge paradigm shift and Quantum algorithmics is a brand new science
✓Quantum Hardware comes in many forms (supra-conductors, ion trap, photonics…).
✓ Still limited to few ten's of qubits NISQ (Noisy Intermediate scale Quantum device).

IBM



Rigetti



IONQ

XANADU

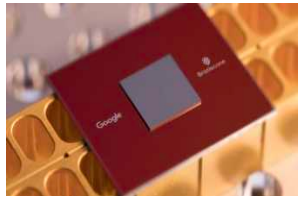
Google

Objectives

✓ Understand Quantum Computers technology evolution

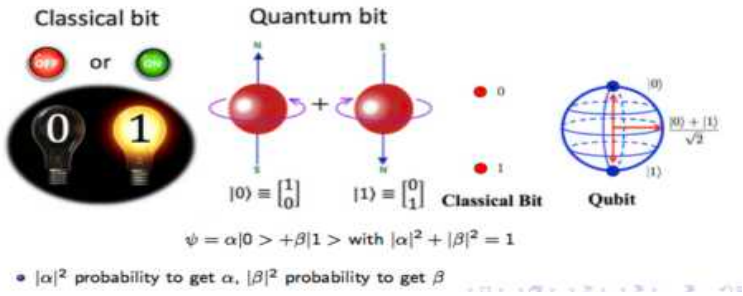
D'WAVE computer

IBM Q

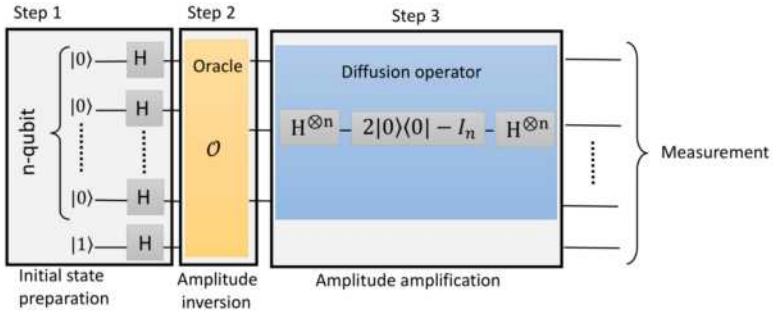


Google: bristlecone

Rigetti : 16Q Aspen



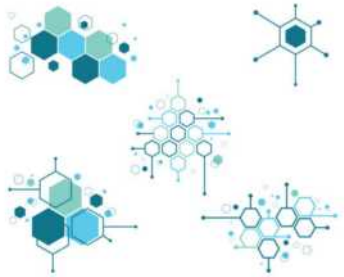
✓ Accelerate and build in-house competencies skill set with research partners and hardware providers ecosystem to develop algorithms for Total business use cases



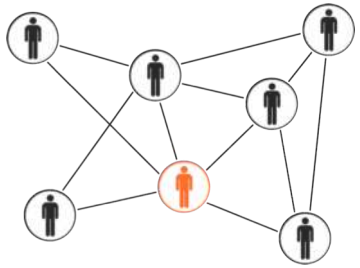
✓ Take advantage of NISQ technology and be ready when industrial quantum computers become available.

Anticipated impact (what we expect)

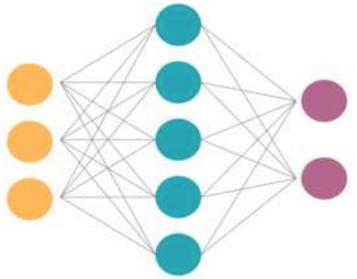
- ✓ Compute better, compute faster
- ✓ Open new frontiers in R&D for Chemistry, material science, optimization, machine learning,….



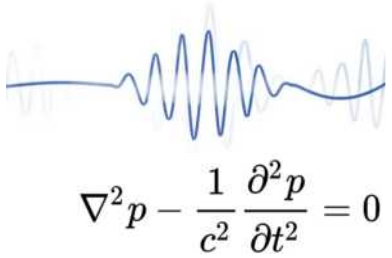
Quantum chemistry



Quantum combinatorial optimization



QML



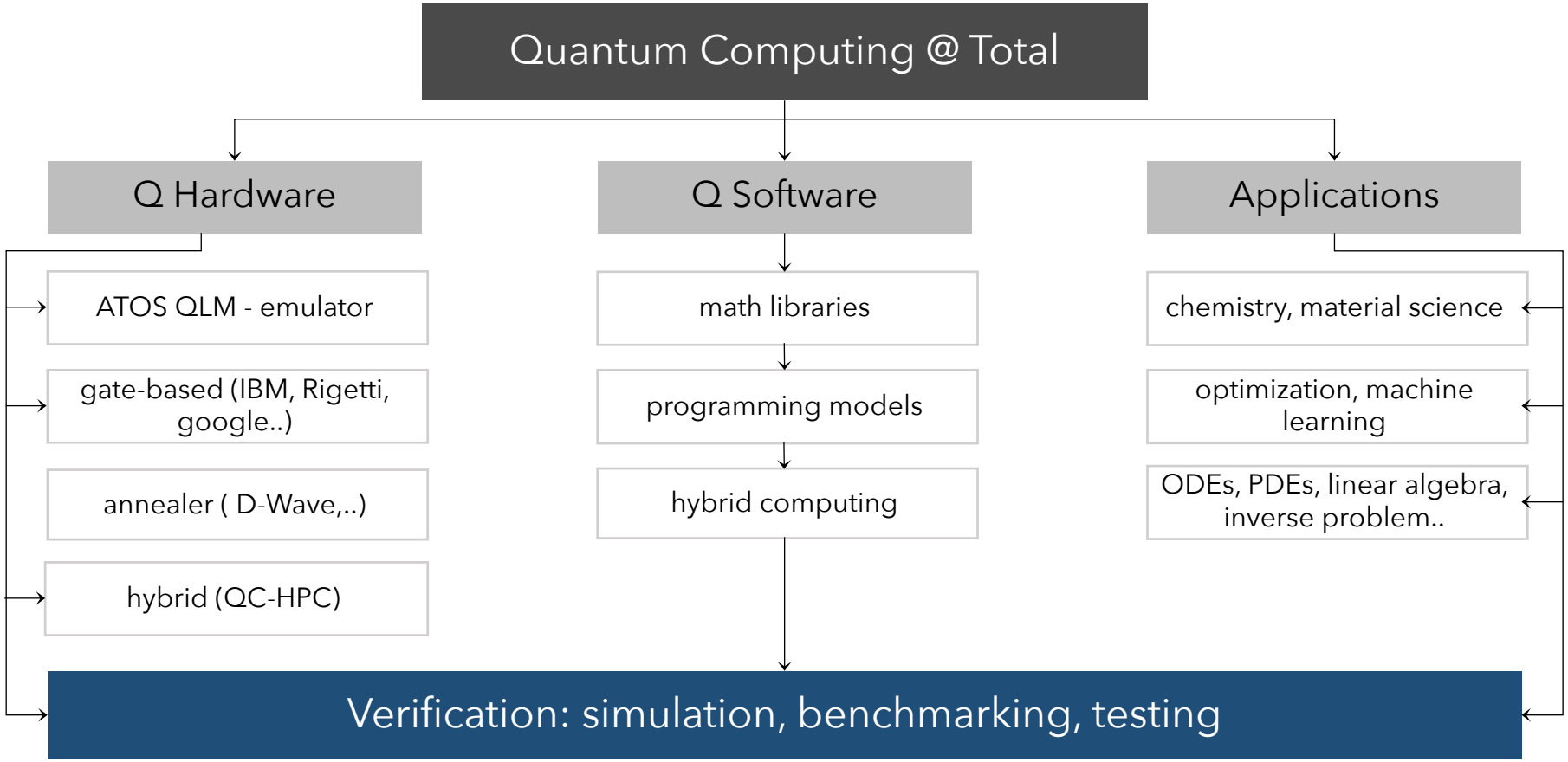
Linear algebra (ODEs, PDEs, inverse problems)

NISQ device ~ (10^2 qubits) 3-5 years

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

TOTAL

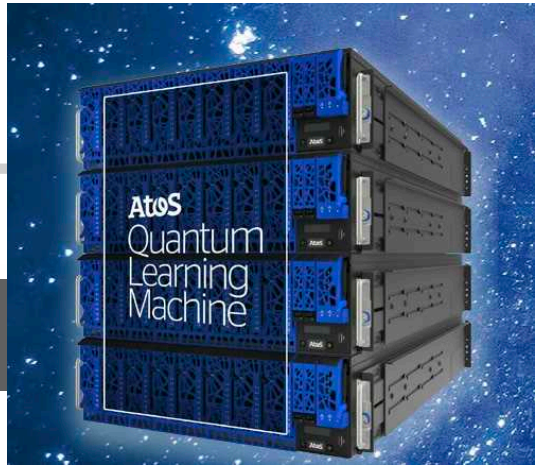
Global program overview



Industrial & academic network

TOTAL

ATOS 30 and 35 qubit QLM



ATOS Quantum Learning Machine functional scope

Programming

- **AQASM** — Assembly language to build quantum circuits
- **pyAQASM** — Python extension to AQASM
- **CIRC** — Binary format of quantum circuits
- **QLIB** — AQASM & pyAQASM libraries
- **INTEROP** — Connections with other frameworks

QPU

- **QPU** — Quantum processing unit emulation

Optimization

- **PBO** — Pattern based optimizer
- **Circuit Optimizer** — Generic circuit optimizer
- **NNIZER** — Topology constraint solver

Simulation

- **SIMULATORS** — Simulation modules
- **SIM OPTIMIZER** — Best Simulator dynamic selection
- **PHYSICS** — Physical Noise models

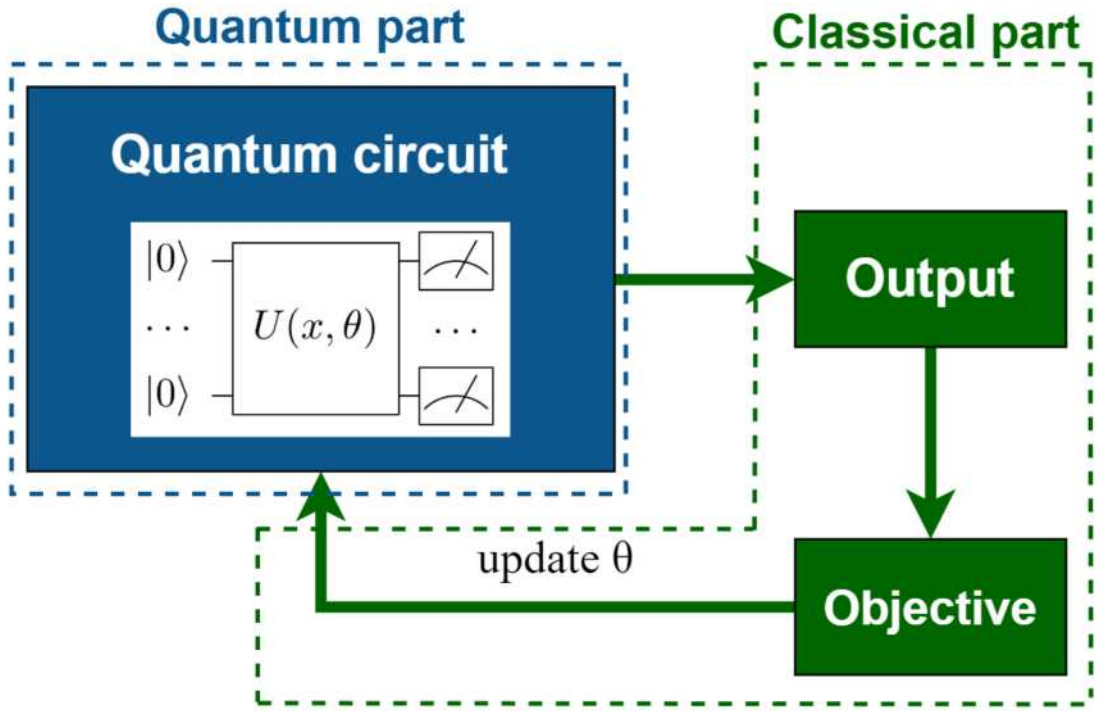
Bull Atos technologies (2018)

TOTAL

Variational Quantum Computing Algorithms

- ✓ Conventional Quantum Algorithms, generally, require long depth circuit:
  - ➔ Fault tolerant quantum computer
  - ➔ Challenging with existing NISQ technology

- ✓ Employ variational hybrid quantum computing to reduce quantum circuit depth at the expense of classical optimization:



- ✓ Variational Algorithms
  - ✓ VQE: Quantum Chemistry Application
  - ✓ QAOA: Combinatorial optimization
  - ✓ VQSD: Eigen Value Estimation
  - ✓ VQLS: Linear solver
  - ✓ VQNN: Quantum Neural Network
  - ✓ …

From Dawid Kopczyk

TOTAL

Molecular modeling with VQE

VQE – Variational Quantum Eigensolver, by Peruzzo, McClean et al. 2014

Problem definition:
Find the ground state energy of many-body interacting fermionic Hamiltonian, that corresponds to the molecular potential energy surfaces (intractable by classical computer in case of complex molecular systems with large number of particles

Finding the ground state energy = solving an eigenvalue problem

$$\hat{H}|\Psi(\mathbf{R})\rangle = E(\mathbf{R})|\Psi(\mathbf{R})\rangle$$

intractable problem in general!

TOTAL

VQE | from fermions to qubits

I. Fermionic Hamiltonian

$$\hat{H}|\Psi(\mathbf{R})\rangle = E(\mathbf{R})|\Psi(\mathbf{R})\rangle$$

II. Second quantization

$$\hat{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

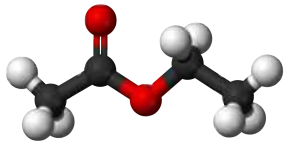
III. Mapping from fermions to qubits – qubit Hamiltonian
(Jordan-Wigner or Bravyi-Kitaev transformation)

$$H_q = \sum_\alpha h_\alpha P_\alpha \,, \qquad P_\alpha = \sigma_1^{\alpha_1} \otimes \sigma_2^{\alpha_2} \otimes \ldots \sigma_N^{\alpha_N}$$

TOTAL

VQE | design

fermionic problem



qubit Hamiltonian

$$H_q = \sum_\alpha h_\alpha P_\alpha$$

optimize

prepare trial state — QPU

$$|\Psi(\boldsymbol{\theta})\rangle$$

measure expectation value

$$h_\alpha \langle \Psi(\boldsymbol{\theta}) | P_\alpha | \Psi(\boldsymbol{\theta}) \rangle$$

calculate energy — CPU

$$E_q(\boldsymbol{\theta}) = \langle \Psi(\boldsymbol{\theta}) | H_q | \Psi(\boldsymbol{\theta}) \rangle = \sum_\alpha h_\alpha \langle \Psi(\boldsymbol{\theta}) | P_\alpha | \Psi(\boldsymbol{\theta}) \rangle$$

adjust parameters

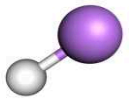
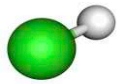
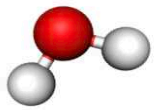
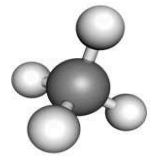
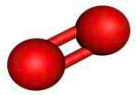
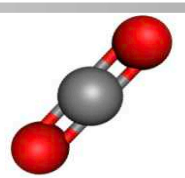
$$(\boldsymbol{\theta})$$

solution

$$E_q^{\min}$$

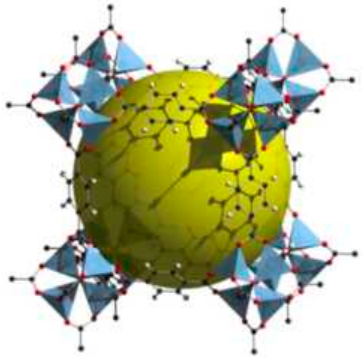
VQE | applications

Molecular benchmark suite definition

configuration						
	LiH	BeH	H2O	CH4	O2	CO2
num_orbitals	6	6	7	9	10	15
num_qubit	12	12	14	18	20	24*
num_shots	500	500	500	500	500	500
maxiter	350	350	350	350	350	350

From Elvira Shishenina (elvira.shishenina@total.com)

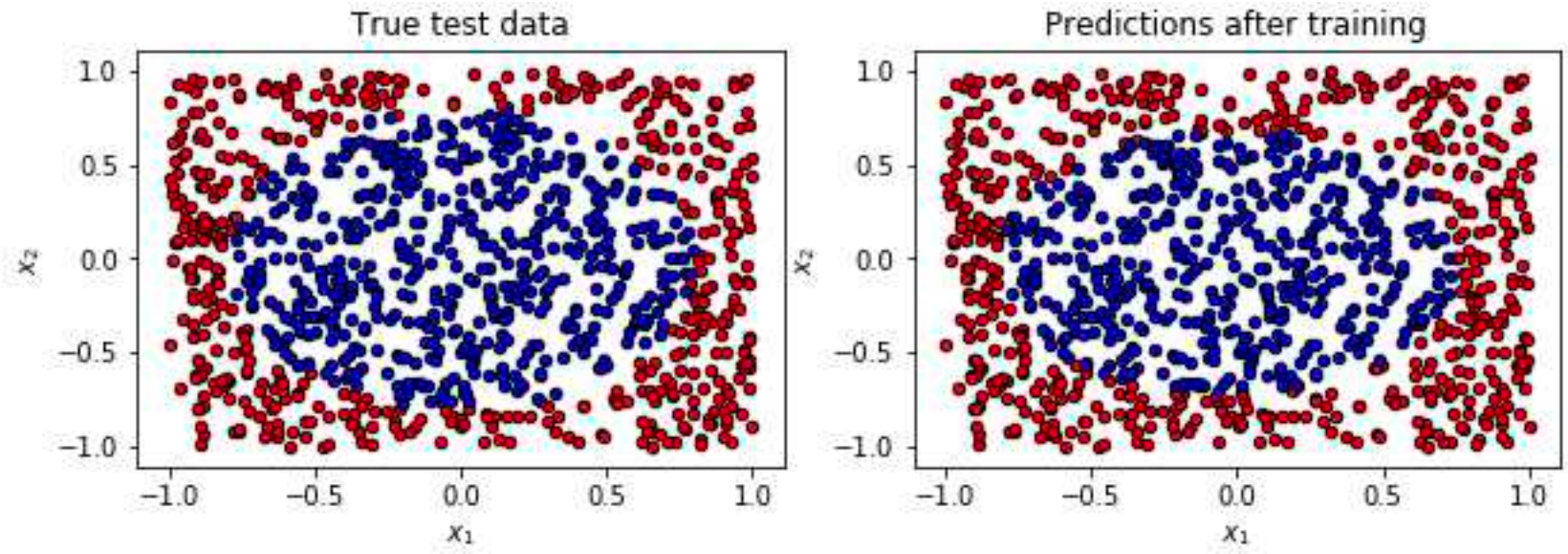
Potential use case: Quantum Computing at Adsorption-based CO2 recovery



TOTAL

VQNN| 1st example

Explore Variational quantum computing for Neural Network implementation

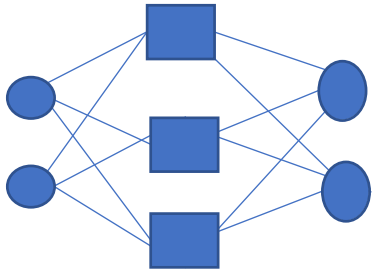


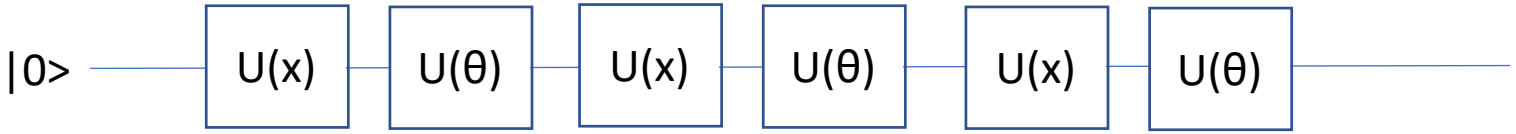
Example: 1 qubit VQNN classifier

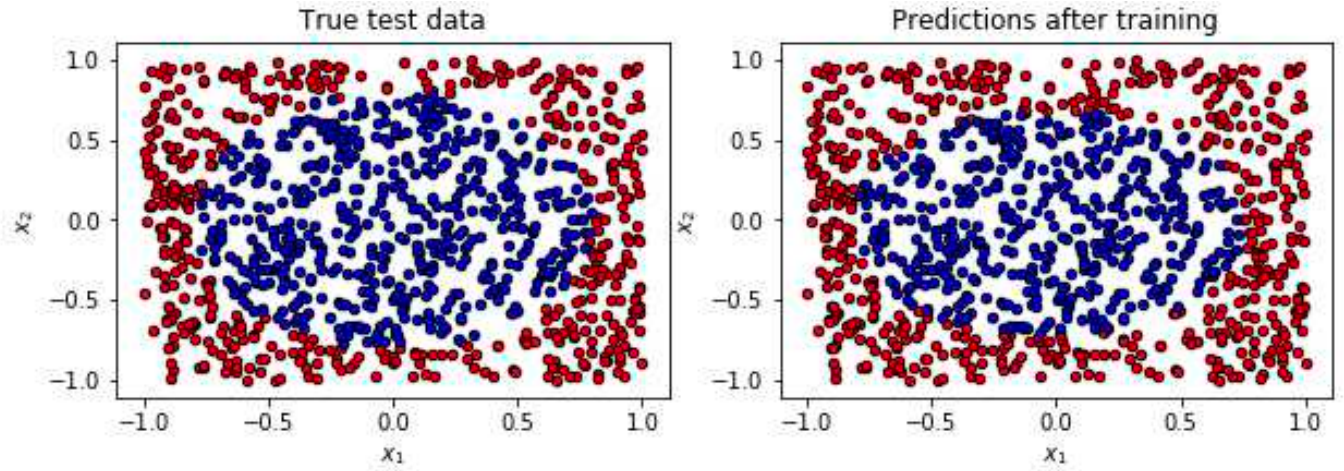
From **Data re-uploading for a universal quantum classifier (Adrián Perez-Salinas arXiv:1907.02085), a simple 1 qubit classifier neural network implemented on the ATOS QLM**

VQNN| 1st example

Explore Variational quantum computing for Neural Network implementation







Example: 1 qubit VQNN classifier

From **Data re-uploading for a universal quantum classifier (Adrián Perez-Salinas arXiv:1907.02085), a simple 1 qubit classifier neural network implemented on the ATOS QLM**

TOTAL

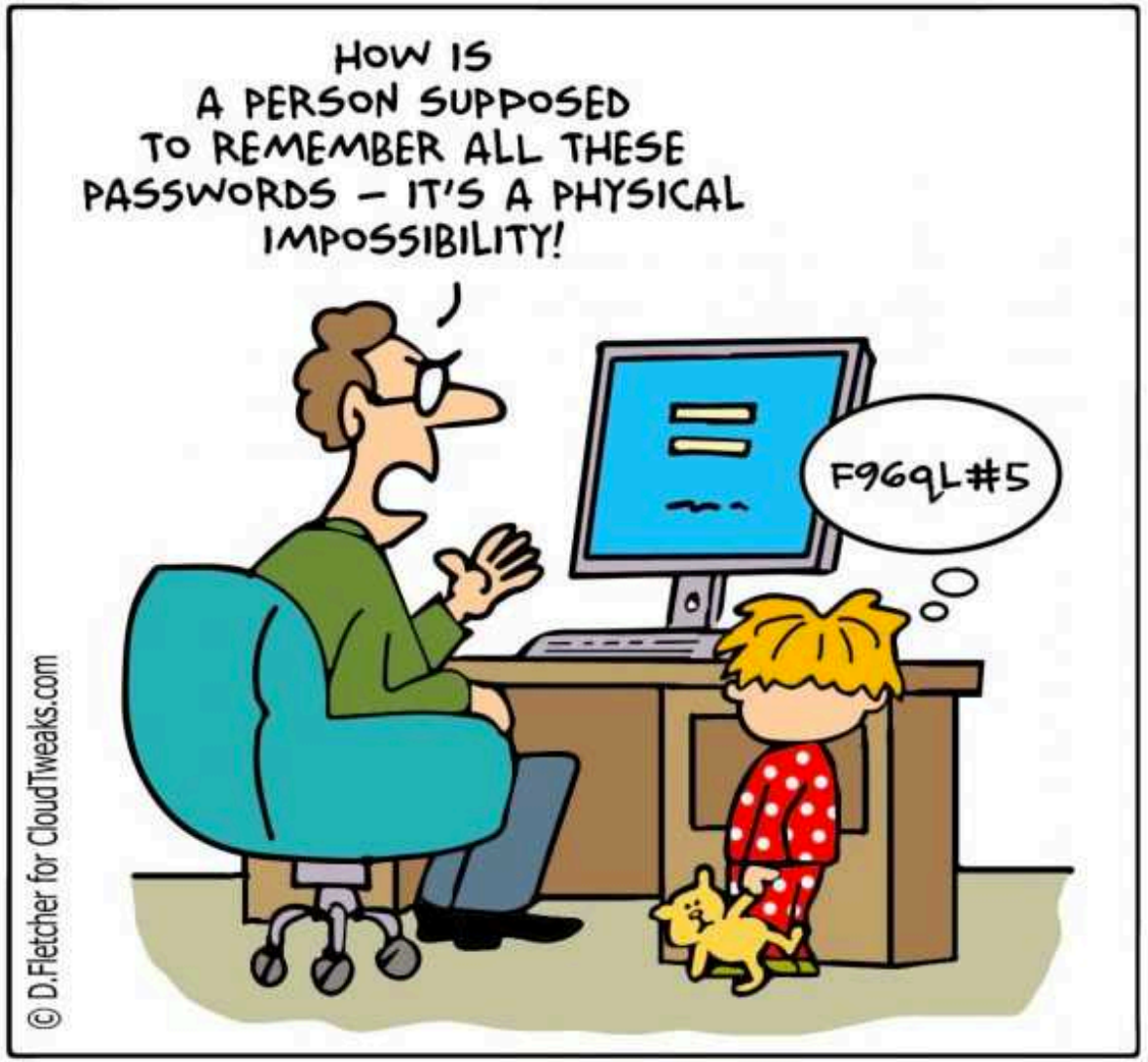
Conclusion

- ✓ Innovation has always been the core of our business
- ✓ R&D and Technology integrator, a key competitive add for Total
- ✓ Compute requirement continue to grow and there is more we want to do:
  - ✓ Compute better, compute better
  - ✓ Machine learning, big data a new revolution for our industry
  - ✓ Explore new opportunities still intractable on classical HPC
- ✓ Quantum computing is a huge paradigm shift and Quantum algorithmics is a brand new science
- ✓ Quantum computing can provide new opportunities, opening new frontiers in R&D in many fields of applications for TOTAL.

GROVER ALGORITHM

TOTAL

Conclusion


HOW IS A PERSON SUPPOSED TO REMEMBER ALL THESE PASSWORDS – IT'S A PHYSICAL IMPOSSIBILITY!
F96QL#5
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