# Quantum Computing for High Energy Physics Applications

PhD course on Quantum Computing

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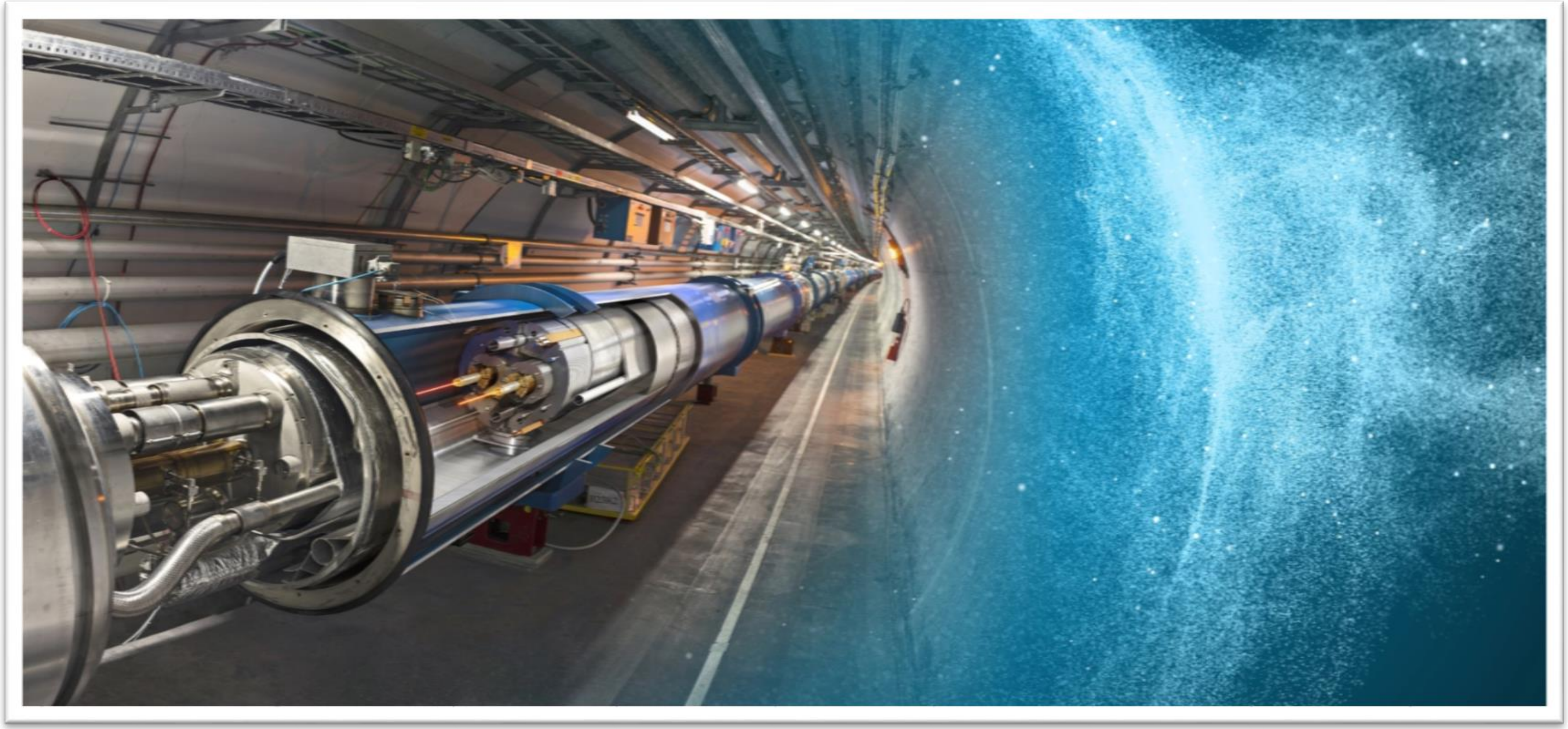
February 21st, 2019

# CERN: A UNIQUE ENVIRONMENT

*Pushing technologies to their limits*



# CERN

"Science for peace"

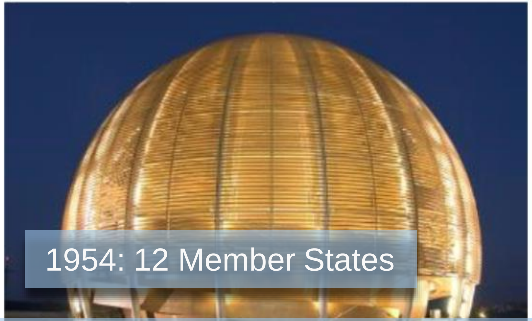
International organisation close to Geneva, straddling Swiss-French border, founded 1954

Facilities for fundamental research in particle physics

22 member states,
1.1 B CHF budget

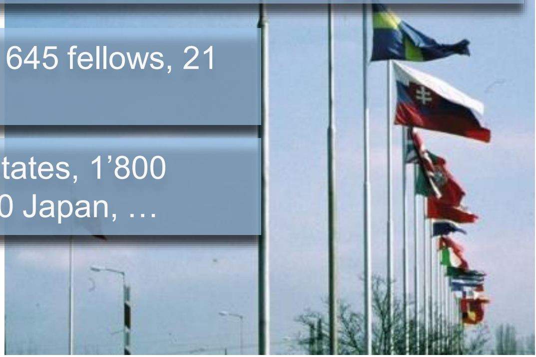
3'197 staff, fellows, apprentices, …

13'128 associates



1954: 12 Member States

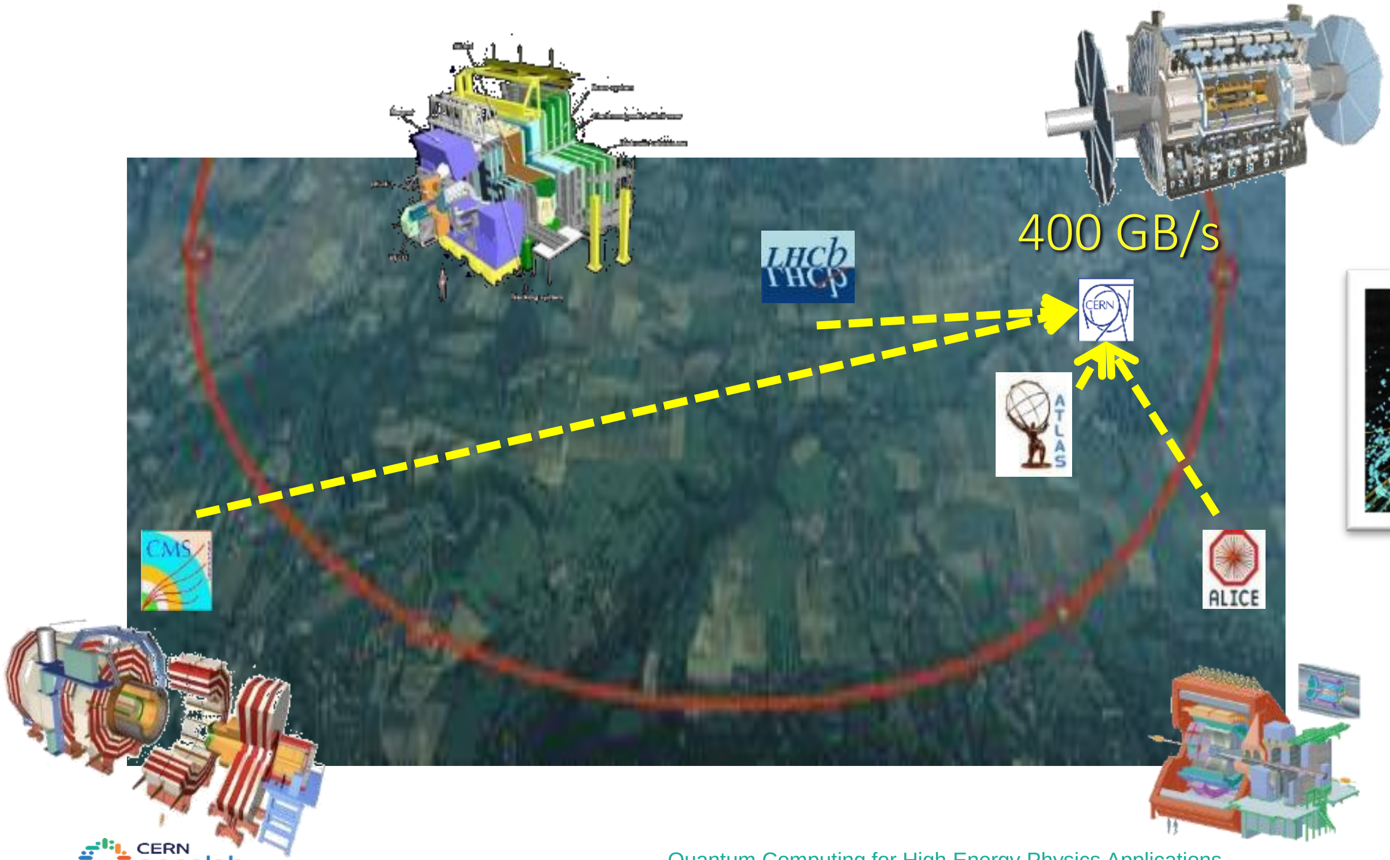
**Members**: Austria, Belgium, Bulgaria, Czech republic, Denmark, Finland, France, Germany, Greece, Hungary, Israel, Italy, Netherlands, Norway, Poland, Portugal, Slovak Republic, Spain, Sweden, Switzerland, United Kingdom
**Candidate for membership**: Cyprus, Serbia; Slovenia
**Associate members:** India, Lithuania, Pakistan, Turkey, Ukraine
**Observers**: EC, Japan, JINR, Russia, UNESCO, United States of America
Numerous **non-member states with collaboration agreements**

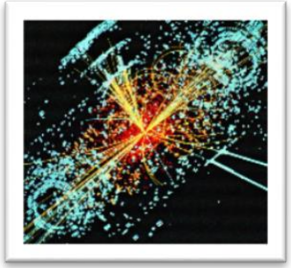


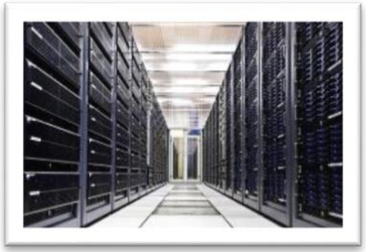
2'531 staff members, 645 fellows, 21 apprentices

7'000 from member states, 1'800 USA, 900 Russia, 270 Japan, …

# The Large Hadron Collider (LHC)





Standard Model of

# FUNDAMENTAL PARTICLES AND INTERACTIONS

The Standard Model summarizes the current knowledge in Particle Physics. It is the quantum theory that includes the theory of strong interactions (quantum chromodynamics or QCD) and the unified theory of weak and electromagnetic interactions (electroweak). Gravity is included on this chart because it is one of the fundamental interactions even though not part of the "Standard Model."

## FERMIONS

matter constituents
spin = 1/2, 3/2, 5/2, ...

**Leptons** spin = 1/2

| Flavor | Mass GeV/c² | Electric charge |
|---|---|---|
| $\nu_e$ electron neutrino | $<1\times10^{-8}$ | 0 |
| e electron | 0.000511 | –1 |
| $\nu_\mu$ muon neutrino | <0.0002 | 0 |
| $\mu$ muon | 0.106 | –1 |
| $\nu_\tau$ tau neutrino | <0.02 | 0 |
| $\tau$ tau | 1.7771 | –1 |

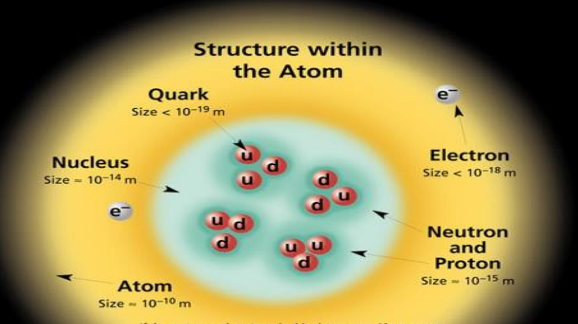
**Quarks** spin = 1/2

| Flavor | Approx. Mass GeV/c² | Electric charge |
|---|---|---|
| u up | 0.003 | 2/3 |
| d down | 0.006 | –1/3 |
| c charm | 1.3 | 2/3 |
| s strange | 0.1 | –1/3 |
| t top | 175 | 2/3 |
| b bottom | 4.3 | –1/3 |

**Spin** is the intrinsic angular momentum of particles. Spin is given in units of ħ, which is the quantum unit of angular momentum, where $\hbar = h/2\pi = 6.58\times10^{-25}$ GeV s $= 1.05\times10^{-34}$ J s.

**Electric charges** are given in units of the proton's charge. In SI units the electric charge of the proton is $1.60\times10^{-19}$ coulombs.

The **energy** unit of particle physics is the electronvolt (eV), the energy gained by one electron in crossing a potential difference of one volt. **Masses** are given in GeV/$c^2$ (remember $E = mc^2$), where 1 GeV = $10^9$ eV = $1.60\times10^{-10}$ joule. The mass of the proton is 0.938 GeV/$c^2$ = $1.67\times10^{-27}$ kg.




If the protons and neutrons in this picture were 10 cm across, then the quarks and electrons would be less than 0.1 mm in size and the entire atom would be about 10 km across.

## BOSONS

force carriers
spin = 0, 1, 2, ...

**Unified Electroweak** spin = 1

| Name | Mass GeV/c² | Electric charge |
|---|---|---|
| $\gamma$ photon | 0 | 0 |
| $W^-$ | 80.4 | –1 |
| $W^+$ | 80.4 | +1 |
| $Z^0$ | 91.187 | 0 |

**Strong (color)** spin = 1

| Name | Mass GeV/c² | Electric charge |
|---|---|---|
| g gluon | 0 | 0 |

### Color Charge

Each quark carries one of three types of "strong charge," also called "color charge." These charges have nothing to do with the colors of visible light. There are eight possible types of color charge for gluons. Just as electrically-charged particles interact by exchanging photons, in strong interactions color-charged particles interact by exchanging gluons. Leptons, photons, and **W** and **Z** bosons have no strong interactions and hence no color charge.

### Quarks Confined in Mesons and Baryons

One cannot isolate quarks and gluons; they are confined in color-neutral particles called **hadrons**. This confinement (binding) results from multiple exchanges of gluons among the color-charged constituents. As color-charged particles (quarks and gluons) move apart, the energy in the color-force field between them increases. This energy eventually is converted into additional quark-antiquark pairs (see figure below). The quarks and antiquarks then combine into hadrons; these are the particles seen to emerge. Two types of hadrons have been observed in nature: **mesons** $q\bar{q}$ and **baryons** $qqq$.

### Residual Strong Interaction

The strong binding of color-neutral protons and neutrons to form nuclei is due to residual strong interactions between their color-charged constituents. It is similar to the residual electrical interaction that binds electrically neutral atoms to form molecules. It can also be viewed as the exchange of mesons between the hadrons.

## PROPERTIES OF THE INTERACTIONS

| Property \ Interaction | Gravitational | Weak (Electroweak) | Electromagnetic (Electroweak) | Strong: Fundamental | Strong: Residual |
|---|---|---|---|---|---|
| Acts on: | Mass – Energy | Flavor | Electric Charge | Color Charge | See Residual Strong Interaction Note |
| Particles experiencing: | All | Quarks, Leptons | Electrically charged | Quarks, Gluons | Hadrons |
| Particles mediating: | Graviton (not yet observed) | $W^+$ $W^-$ $Z^0$ | $\gamma$ | Gluons | Mesons |
| Strength relative to electromag for two u quarks at: $10^{-18}$ m | $10^{-41}$ | 0.8 | 1 | 25 | Not applicable to quarks |
| Strength relative to electromag for two u quarks at: $3\times10^{-17}$ m | $10^{-41}$ | $10^{-4}$ | 1 | 60 | Not applicable to quarks |
| for two protons in nucleus | $10^{-36}$ | $10^{-7}$ | 1 | Not applicable to hadrons | 20 |

**Baryons qqq and Antibaryons $\bar{q}\bar{q}\bar{q}$**
Baryons are fermionic hadrons.
There are about 120 types of baryons.

| Symbol | Name | Quark content | Electric charge | Mass GeV/c² | Spin |
|---|---|---|---|---|---|
| p | proton | uud | 1 | 0.938 | 1/2 |
| $\bar{p}$ | anti-proton | $\bar{u}\bar{u}\bar{d}$ | –1 | 0.938 | 1/2 |
| n | neutron | udd | 0 | 0.940 | 1/2 |
| $\Lambda$ | lambda | uds | 0 | 1.116 | 1/2 |
| $\Omega^-$ | omega | sss | –1 | 1.672 | 3/2 |

**Mesons $q\bar{q}$**
Mesons are bosonic hadrons.
There are about 140 types of mesons.

| Symbol | Name | Quark content | Electric charge | Mass GeV/c² | Spin |
|---|---|---|---|---|---|
| $\pi^+$ | pion | $u\bar{d}$ | +1 | 0.140 | 0 |
| $K^-$ | kaon | $s\bar{u}$ | –1 | 0.494 | 0 |
| $\rho^+$ | rho | $u\bar{d}$ | +1 | 0.770 | 1 |
| $B^0$ | B-zero | $d\bar{b}$ | 0 | 5.279 | 0 |
| $\eta_c$ | eta-c | $c\bar{c}$ | 0 | 2 .980 | 0 |

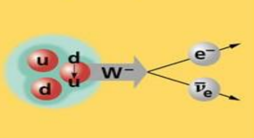
### Matter and Antimatter

For every particle type there is a corresponding antiparticle type, denoted by a bar over the particle symbol (unless + or – charge is shown). Particle and antiparticle have identical mass and spin but opposite charges. Some electrically neutral bosons (e.g., $Z^0$, $\gamma$, and $\eta_c = c\bar{c}$, but not $K^0 = d\bar{s}$) are their own antiparticles.

### Figures

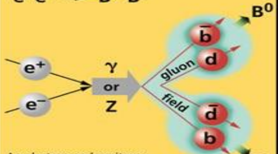
These diagrams are an artist's conception of physical processes. They are *not* exact and have *no* meaningful scale. Green shaded areas represent the cloud of gluons or the gluon field, and red lines the quark paths.

$n \rightarrow p\, e^- \,\bar{\nu}_e$



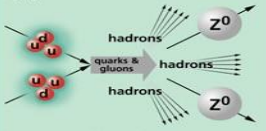

A neutron decays to a proton, an electron, and an antineutrino via a virtual (mediating) W boson. This is neutron β decay.

$e^+e^- \rightarrow B^0\, \bar{B}^0$




An electron and positron (antielectron) colliding at high energy can annihilate to produce $B^0$ and $\bar{B}^0$ mesons via a virtual Z boson or a virtual photon.

$p\,p \rightarrow Z^0Z^0$ + assorted hadrons




Two protons colliding at high energy can produce various hadrons plus very high mass particles such as Z bosons. Events such as this one are rare but can yield vital clues to the structure of matter.

### The Particle Adventure

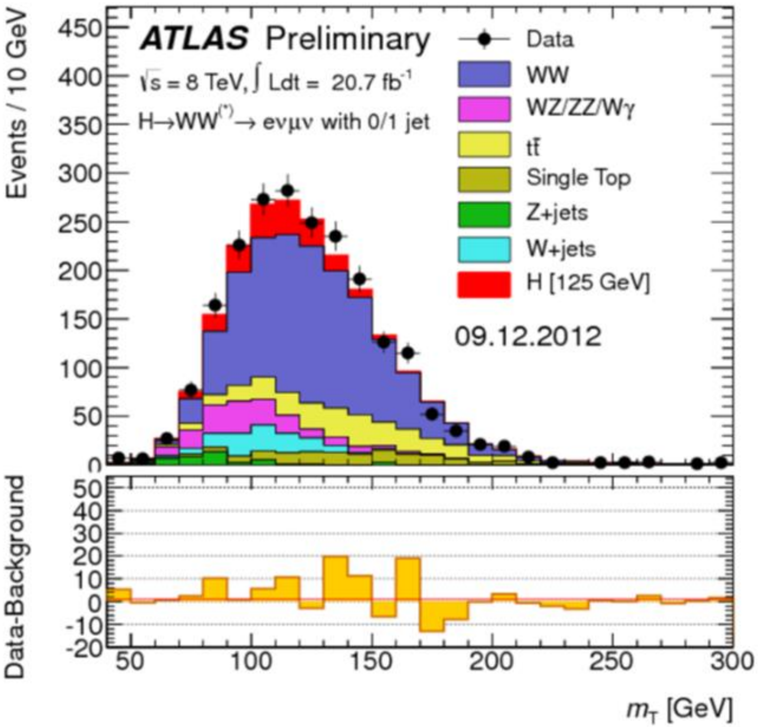
Visit the award-winning web feature *The Particle Adventure* at
**http://ParticleAdventure.org**


**This chart has been made possible by the generous support of:**
U.S. Department of Energy
U.S. National Science Foundation
Lawrence Berkeley National Laboratory
Stanford Linear Accelerator Center
American Physical Society, Division of Particles and Fields
**BURLE** INDUSTRIES, INC.

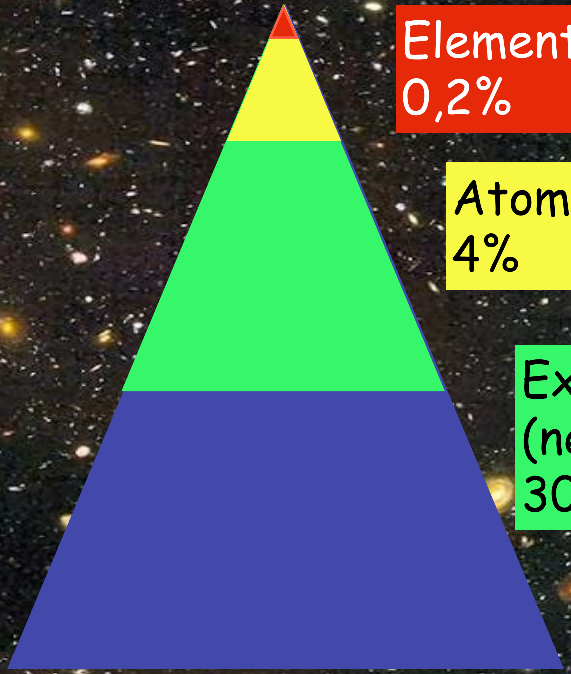



**http://CPEPweb.org**

# The Higgs Boson




# What is the place of matter in the universe



Elementary particles
0,2%

Atoms, stars, diffused gas
4%

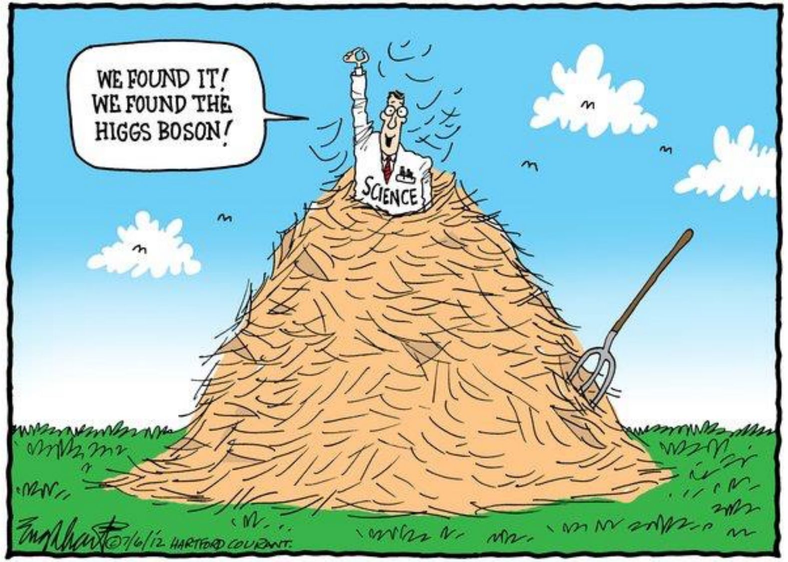
Exotic dark matter
(neutrinos, neutralinos,…)
30%

Dark energy
(Vacuum energy,…)
66%

Whe ignore most things about the 4% of the Universe

But we do not even know of what the remaining 96% is made of

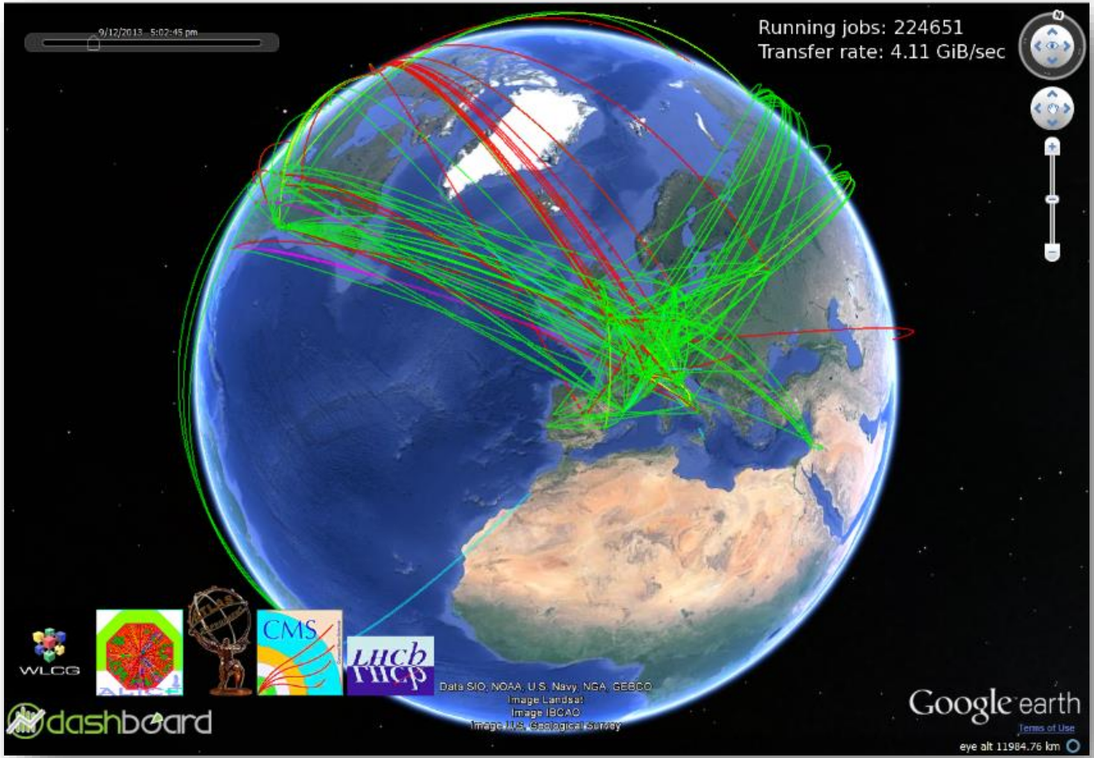
# From ridiculously difficult…

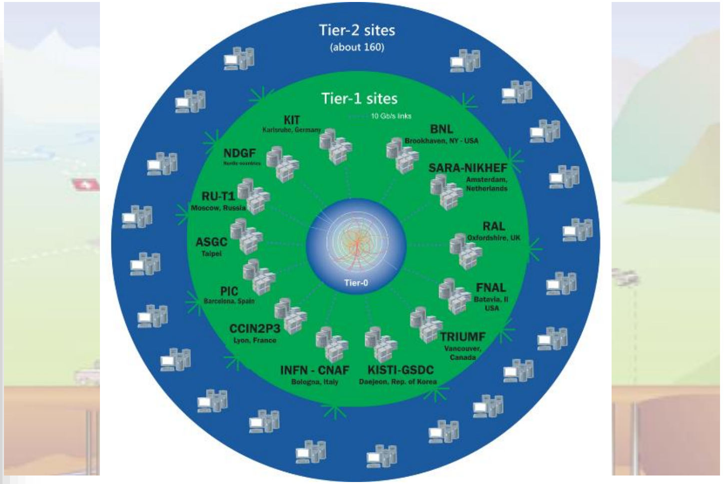




# …to almost impossible

# Worldwide LHC Computing Grid



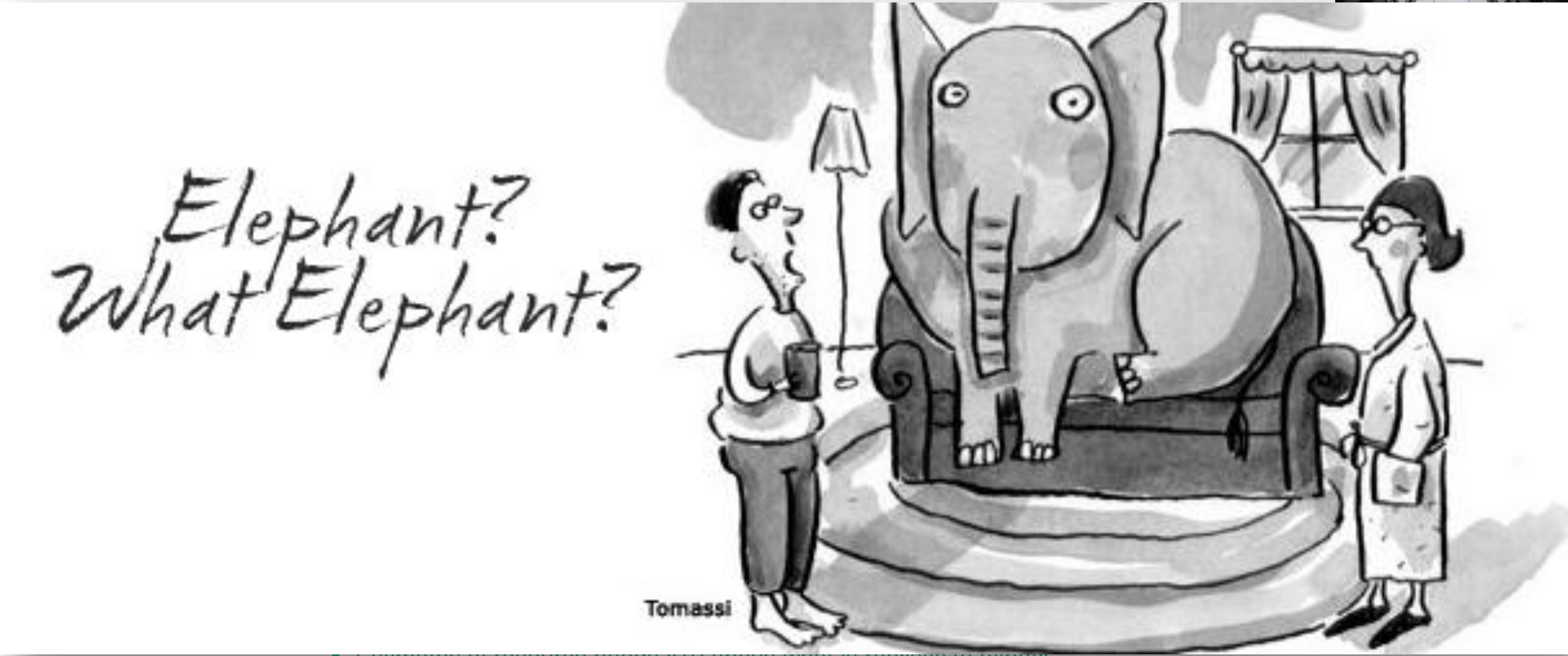

Tier-0 (CERN):
- Data recording
- Initial data reconstruction
- Data distribution

Tier-1 (14 centres):
- Permanent storage
- Re-processing
- Analysis

Tier-2 (72 Federations, ~149 centres):
- Simulation
- End-user analysis

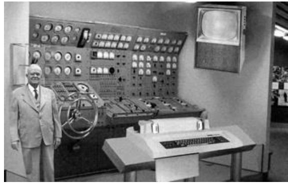
- 760,000 cores
- 700 PB

# HL-LHC: data volume

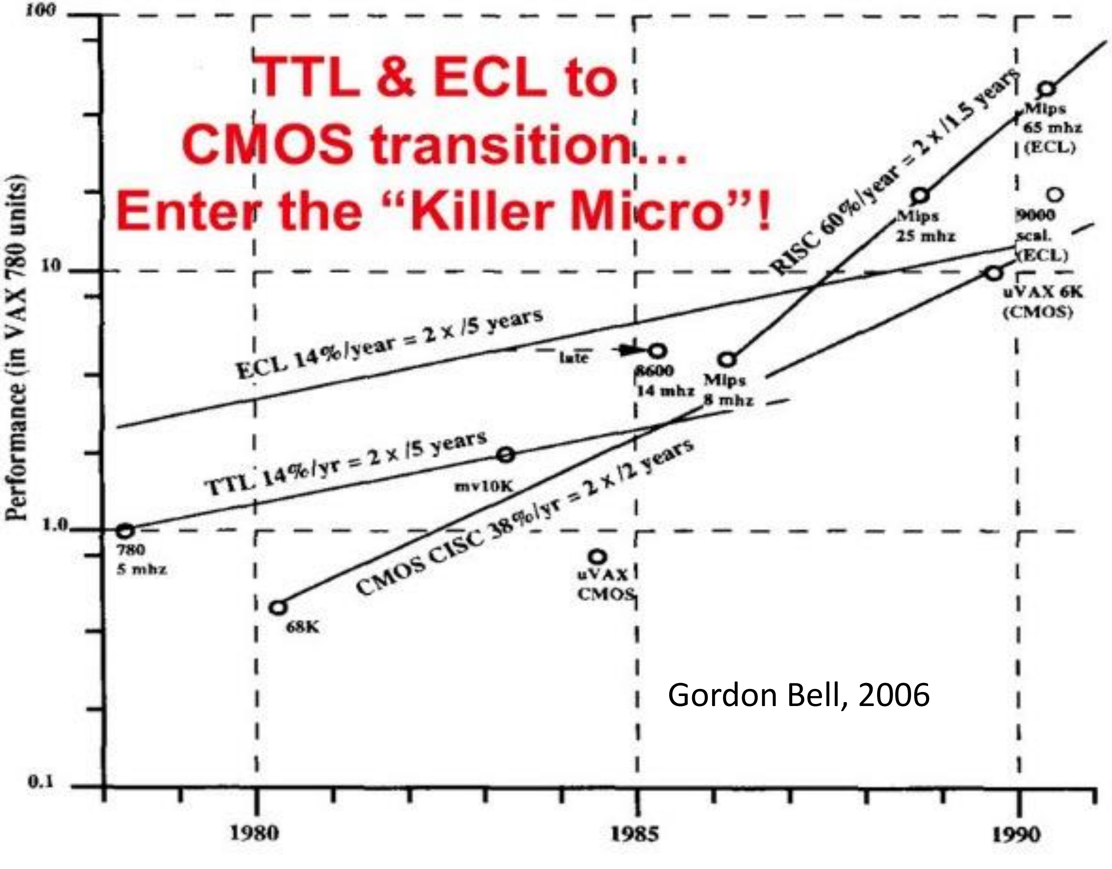



- Estimates of resource needs x10 above what is realistic to expect

# History – LEP



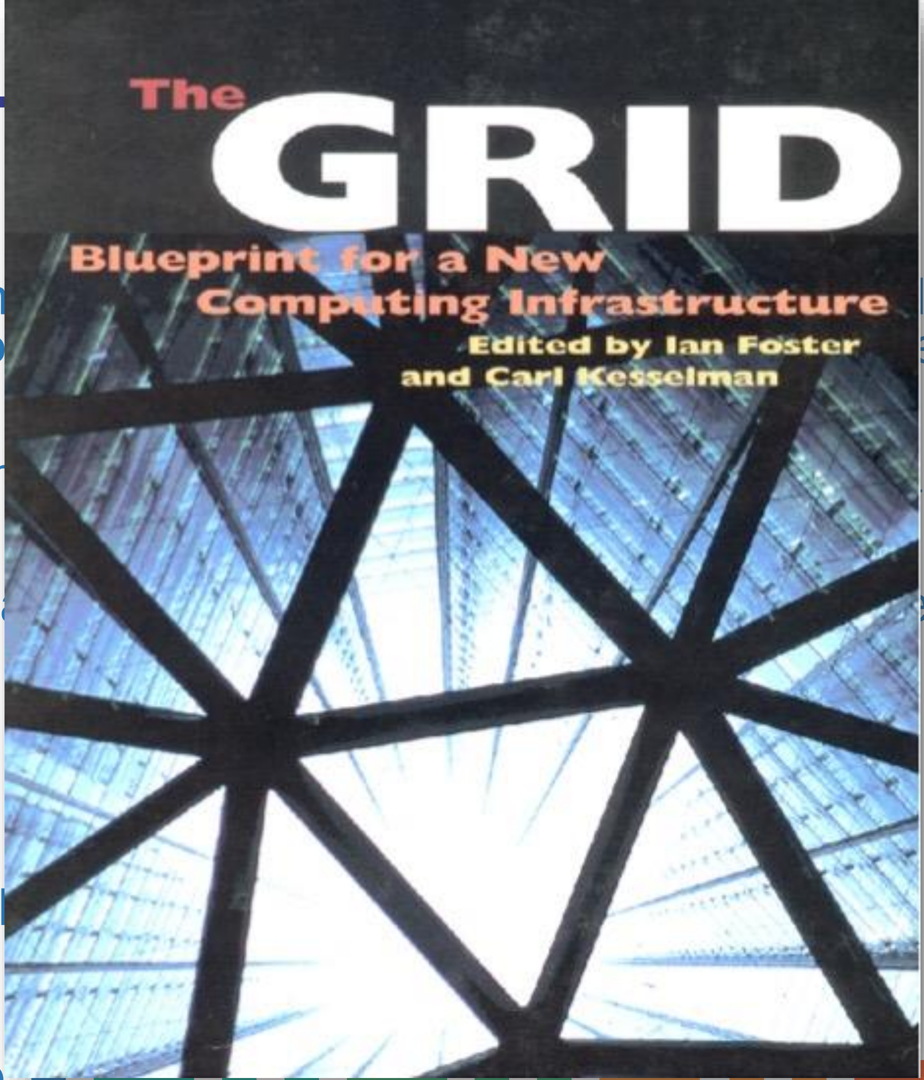
- The es… contai… throug… …e
- It was… …with mainfr…




- Here c…

# History -

- The LHC com… out in 2000-2001 (the "Ho… committee was accused
- Putting this ar… ilable, would have created
- Working with … Fiction
- Here comes t…

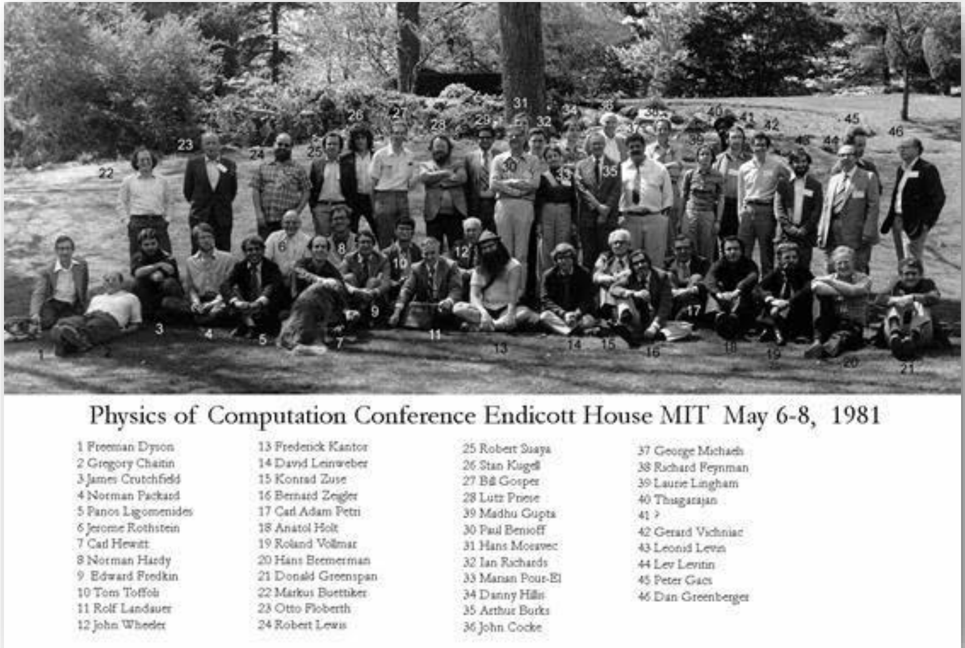


# History – conclusions

*Moral of the story*

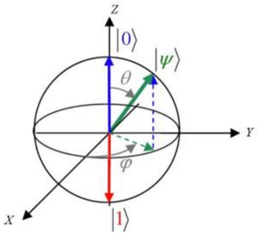

- HEP has regularly faced “computer requirement walls” and the associated scaremongering
  - It reminds me a bit of the Y2K story… if you are old enough to remember it
- We have been very good to “seize the opportunity” and turn emerging technologies into production facilities
- This has allowed us to survive (indeed very well) at a reasonable cost
- This has also provided a productive dialogue with the ICT community
- One essential element of the success is that we had people already investigating the field within HEP, i.e. the “seeds” were already there
- The only question (!) is what will be the next “savior(s)”

# Quantum Computing?



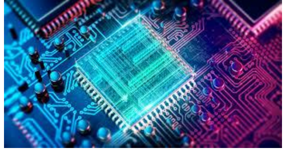

**"Nature is quantum, goddamn it! So if we want to simulate it, we need a quantum computer."**
**R.Feynman, 1981, Endicott House, MIT**

Use qubits instead of bits…
e.g. bits that exhibit quantum behavior




`Bloch's sphere

# Quantum Computing in perspective

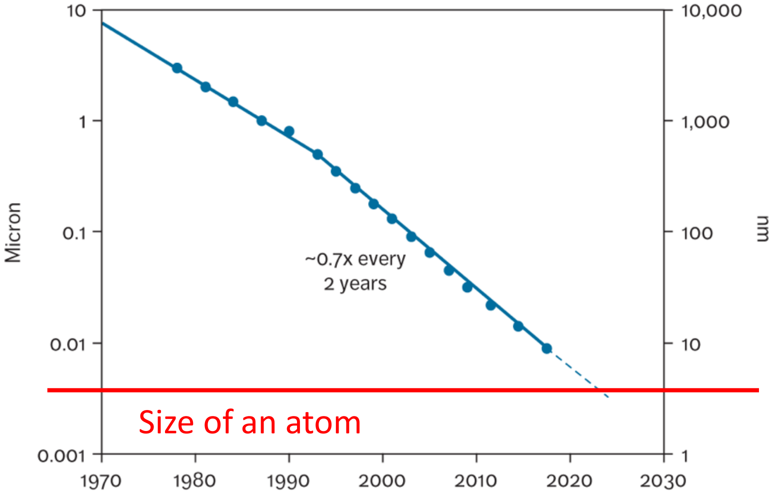


## The three frontiers

- Short distance -> High Energy Physics
- Long distance -> Cosmology
- Entanglement (i.e. complexity) -> Quantum Information Technology

## Since Turing it was believed that the “hardness” of a problem was intrinsic to it

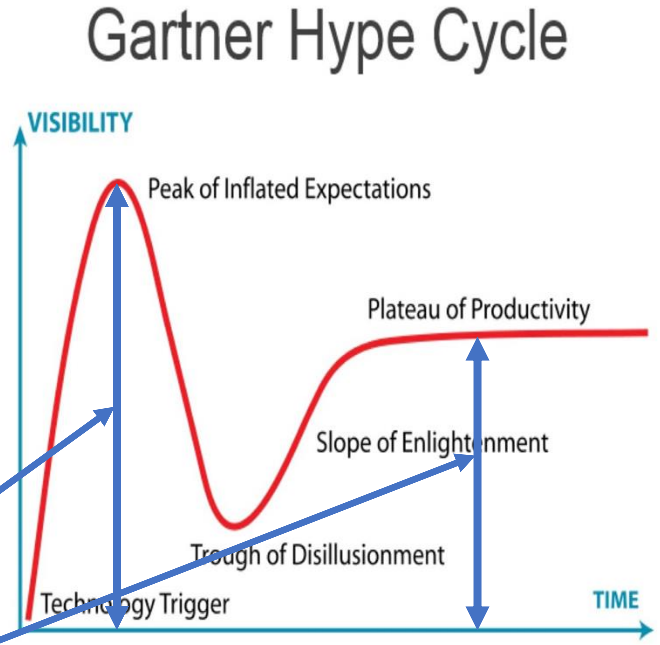
## Quantum Computing is now challenging this




We could argue that Quantum Computing is a natural consequence of Moore’s law

# … and money is flowing in…

- EU Quantum Flagship – large-scale initiative
  - funded at the 1b € level on a 10 years timescale.
- US-DoE Quantum Information Science Enabled Discovery (QuantISED) for High Energy Physics
  - Up to $13M total of awards in FY 2018 (FOA+LAB)
- US-DoE Quantum Information Science in FY 2019 HEP
  - President's Budget Request: $27.5M




**What people laugh about**

**What matters at the end**

# Just for the skeptical

I think there can be a world market for maybe five computers. (Thomas Watson, CEO of IBM, 1943)

There is no reason for an individual to have a computer at home . (Ken Olsen , president, director and founder of Digital Equipment Corp., 1977)

I think that this thing that Tim (Berners-Lee) has shown me has no future (F.Carminati, 1989)

# CERN OPENLAB'S MISSION


**Evaluate and test** state-of-the-art technologies in a challenging environment and improve them in collaboration with industry.

You make it, we break it

...and you better fix it fast...

and exchange
ith other
munities to create
knowledge and
innovation.


**Communic**
demon
and

**Train** the next generation of engineers/researchers, **promote** education and cultural exchanges.

# Research paths in QC

- Get access to emulators and simulators to start assessing development tools and methodology, develop proof-of-concept algorithms for HEP workloads
- Get access to real devices, benchmark, compare results
- Investigate and collaborate in the development of APIs and user interfaces to access QC systems
- Discuss collaboration on engineering aspects of QC installation, primarily cryogenics and material science
- Understand the role that CERN can play as part of broader QC development initiatives

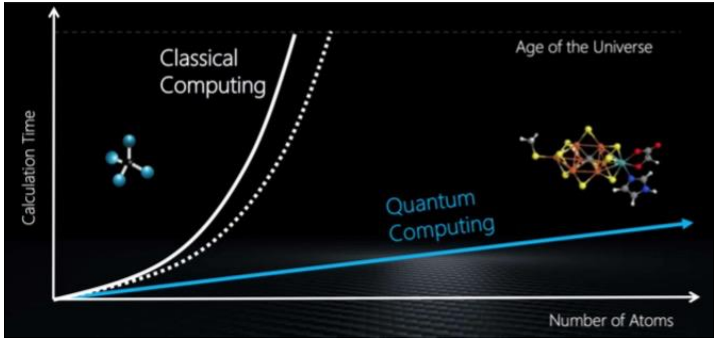
# The “seeds” are already there

- Most of what we do is optimisation / fitting / minimisation (superpolynomial speedup!)
  - https://www.nature.com/news/quantum-machine-goes-in-search-of-the-higgs-boson-1.22860
- Training of Deep Learning is revealing a bottleneck, Quantum Computing can help
  - https://www.datasciencecentral.com/profiles/blogs/quantum-computing-deep-learning-and-artificial-intelligence
- Combinatorial searches can be speeded up
  - e.g. track reconstruction
- We can simulate basic interactions with QC
  - https://www.nature.com/news/quantum-computer-makes-first-high-energy-physics-simulation-1.20136
  - https://mappingignorance.org/2017/01/27/simulating-particle-physics-quantum-computer/
- Lattice QCD calculations
  - https://mappingignorance.org/2017/01/27/simulating-particle-physics-quantum-computer/
- Very fast random number generators can be built
  - https://www.osapublishing.org/viewmedia.cfm?r=1&uri=ICQI-2007-JWC49&seq=0
- Quantum Detectors combined with Quantum Computing for online

# Quantum Computing for Theoretical Particle Physics

*Quantum on Quantum*

- QC can be used to solve *directly* Quantum Many Body and Quantum Field Theory problems
- In chemistry we already have variational calculations of atomic orbital configurations
  - Complex molecules are the ”killing app” here
- Similarly for Nuclear Physics the challenge will be to describe nuclei and their scattering and interactions
- This is well beyond exascale computing and current theoretical understanding



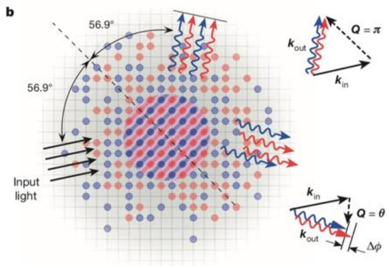
# Two approaches to QoQ

*Analog quantum simulations*

- Use interactions between quantum elements to simulate the continuous-time evolution governed by a given Hamiltonian.
- Same equations - same physics
- Direct implementation of Schrödinger's equation.
- Usually special purpose systems

# Analog Quantum Simulation

*One important example*




Ultracold atoms in optical lattices to describe many-body physics & high-temperature superconductivity
Hart et al., Nature 519:211 2015

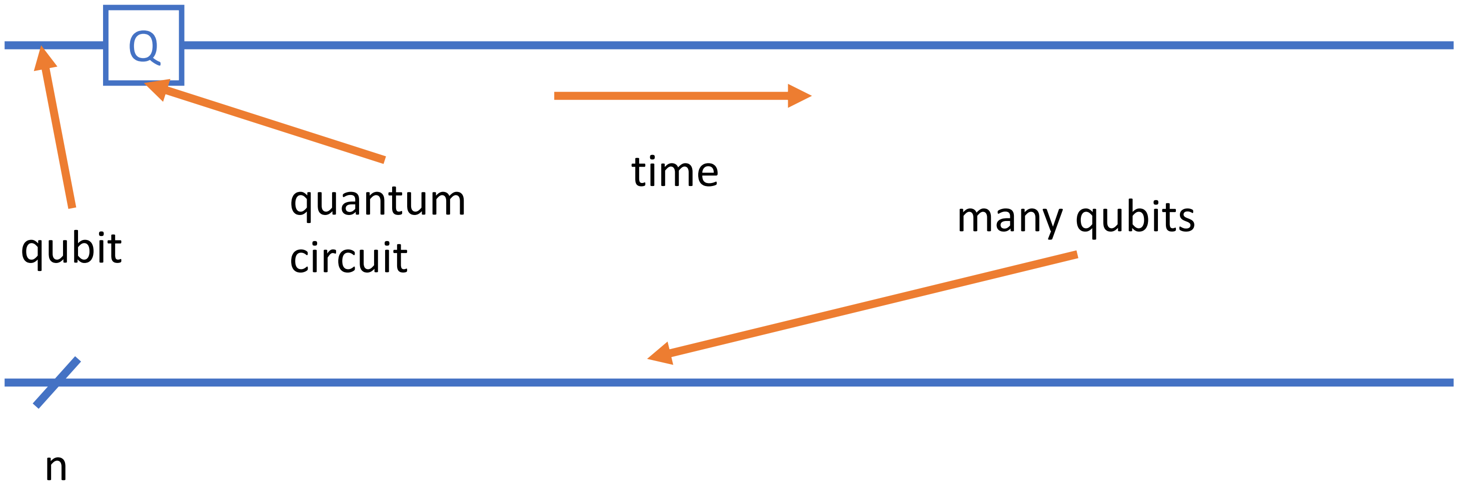
- Study of quantum phase transitions
- Quantum magnetism
- High-temperature superconductors
- Quantum Hall effect
- Address problems in quantum filed theory

# Two approaches to QoQ

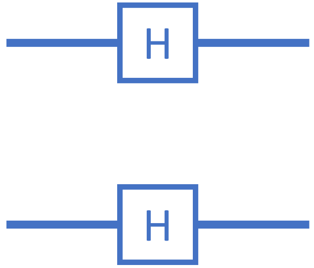
*Digital Quantum Simulation*

- Digital Quantum Simulation which can solve the Schrödinger equation using a discretized approximation of the time-evolution operator.
- Use efficient methods for constructing the system Hamiltonian and then decompose the time-evolution operator into a sequence of well-defined instructions
- These instructions are applied to the register in order to carry out a specific simulation sequence
- All this in a “generic” quantum computer

# Recalling a bit of notation



# Recall – the Hadamard gate



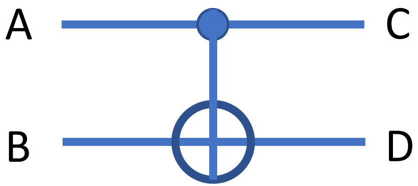

$|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

$|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \langle 0|\psi\rangle \\ \langle 1|\psi\rangle \end{pmatrix}$$

# Recall -- C-not gate

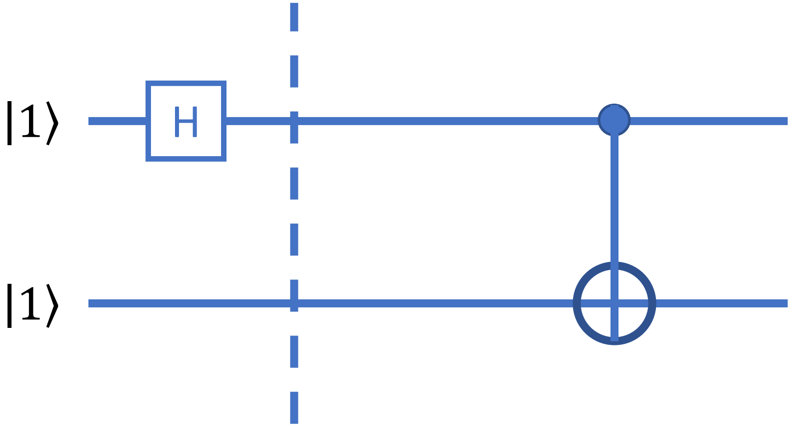
- Remember the c-not gate?




$$\begin{bmatrix} 1000 \\ 0100 \\ 0001 \\ 0010 \end{bmatrix} \quad \begin{bmatrix} \langle 00|\psi\rangle \\ \langle 01|\psi\rangle \\ \langle 10|\psi\rangle \\ \langle 11|\psi\rangle \end{bmatrix}$$

| A | B | C | D |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 1 | 0 | 1 |
| 1 | 0 | 1 | 1 |
| 1 | 1 | 1 | 0 |

# Producing entangled states




$$\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

$$\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)|1\rangle$$

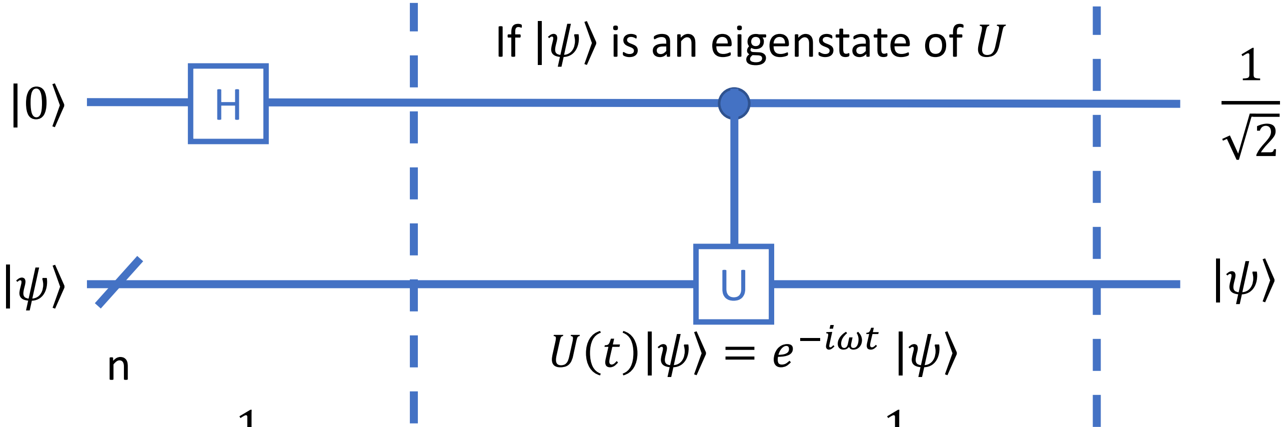
A c-not gate is a unitary operator just like the time evolution operator

$$U(t)|\psi\rangle = e^{-i\frac{H(t)}{\hbar}}|\psi\rangle$$

# Controlled Unitary Evolution

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & U_{11} & U_{12} \\ 0 & 0 & U_{21} & U_{22} \end{bmatrix} \begin{bmatrix} \langle 00|\psi\rangle \\ \langle 01|\psi\rangle \\ \langle 10|\psi\rangle \\ \langle 11|\psi\rangle \end{bmatrix}$$

If $|\psi\rangle$ is an eigenstate of $U$




$$\frac{1}{\sqrt{2}}\left(|0\rangle + e^{-i\omega t}|1\rangle\right)$$

$$|\psi\rangle$$

$$U(t)|\psi\rangle = e^{-i\omega t}\,|\psi\rangle$$

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|\psi\rangle$$

$$\frac{1}{\sqrt{2}}\left(|0\rangle|\psi\rangle + e^{-i\omega t}|1\rangle|\psi\rangle\right)$$

Eigenstate does not change but the control bit oscillates!

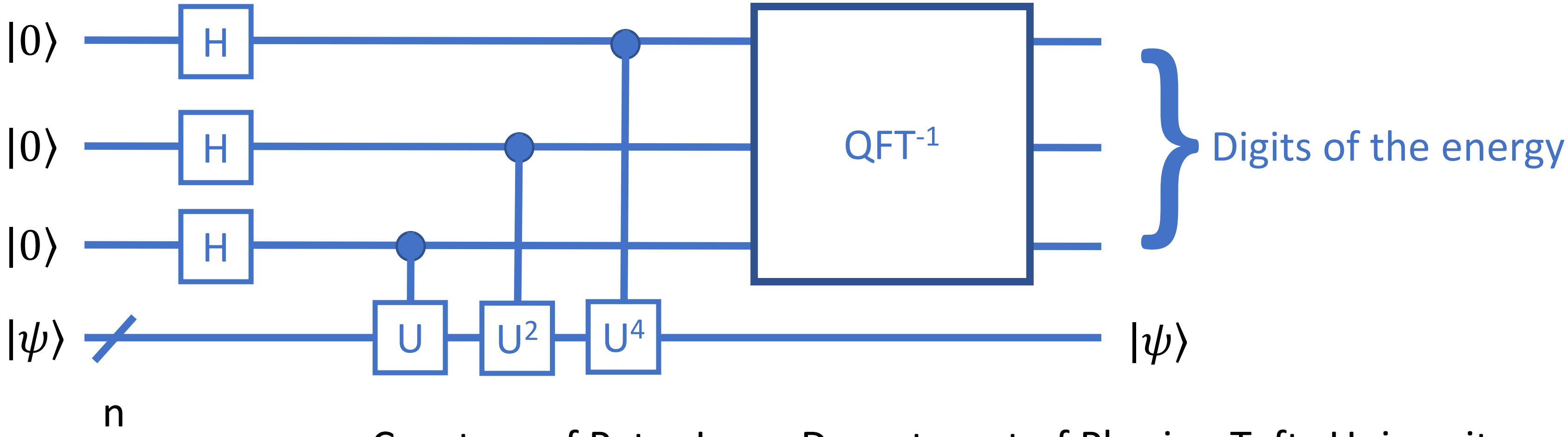
# How to measure the phase?

$$\frac{1}{\sqrt{2}}\left(|0\rangle + e^{-i\omega t}|1\rangle\right)$$


$$e^{-i\omega t/2}(\cos(\omega t/2)|0\rangle + \sin(\omega t/2)|1\rangle)$$

…and voila, the phase is an amplitude…

…but we still need $U(t)$…




Courtesy of Peter Love, Department of Physics, Tufts University

# Getting serious about it

*Simulating QCD processes*

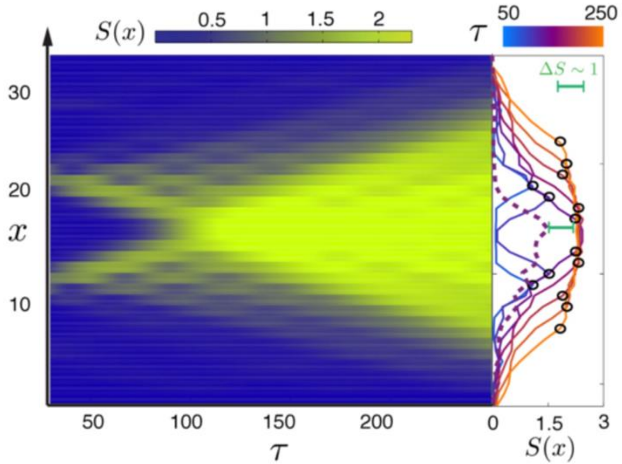
- For high-energy processes in small volumes of space- time, QCD can be solved by expansions
- Conversely, the only technique for solving QCD in the intermediate regime is Lattice QCD (LQCD), in which space-time is discretized on a grid and the theory is solved numerically
- But these calculations are affected by the “sign problem”
  - Which also affect the weights of path integral solutions!
- Real-time evolution of strongly interacting quarks and gluons cannot be determined with current computers and algorithms
  - Fragmentation, QGP, matter in extreme conditions and the origin of the universe, star structures, supernovae

# Simulating QCD

- Quantum computer can naturally manipulate complex amplitudes and thus does not suffer from sign or complex weight problems
- New approaches such as the Tensor Networks representation of the wave function in LGT and Quantum Link Model formulation of LGT are particularly suited for Quantum Computers

# One example

- Dashed line is single meson moving through the lattice
- Colored lines are cuts of the entanglement entropy at different times
- A singlet state has been created between the two indistinguishable mesons
- The entropy has increased by one ebit because the information of the fate of the two mesons (bouncing back or continue traveling) is lost due to the superposition state
- This kind of calculations are particularly suited for digital or analog quantum computers



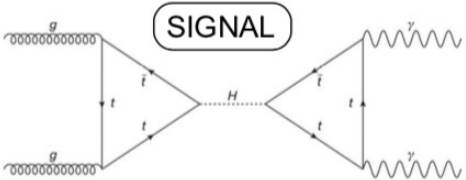

Entanglement entropy in the scattering of two mesons in the Schwinger model calculated using tensor networks.

T Pichler, *et al.* *Phys. Rev. X.*, vol. 6, p. 011023, 2016.

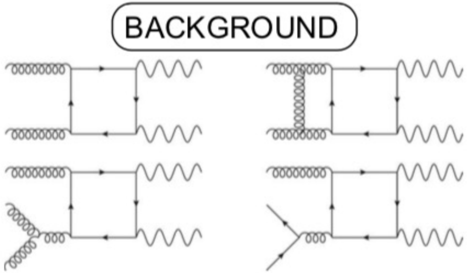
# QC and Higgs Analysis

*Mott A et al. Nature 2017, 550:175*

- Problem: distinguish signal from background




Generated with PYTHIA 6.4 at 8TeV proton-proton c.o.m energy

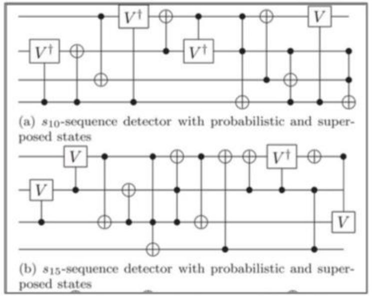



Generated with SHERPA at 8TeV proton-proton c.o.m energy

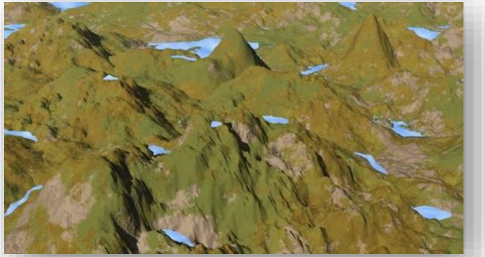
- Photon pT of 32 GeV and 25 GeV for realistic trigger selection
- Di-photon mass [122.5, 127.5] GeV
- Higgs candidate $|\eta|<2.5$

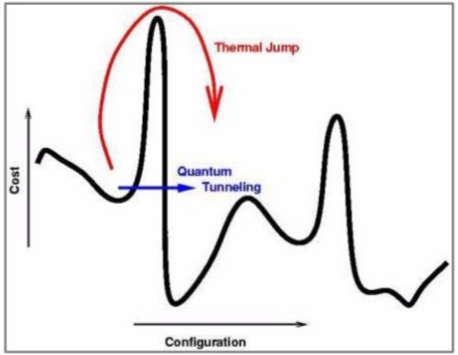
# Take 1 – Quantum Annealing

- The D-Wave system




Quantum Circuit






Quantum Annealer

D-Wave 2XTM

1098 qubits

Operates @ 15mK

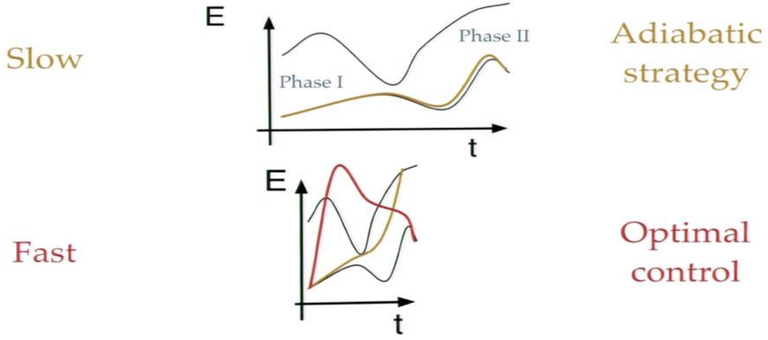
Anneals in 5-20μs

# Take 1 – Quantum Annealing

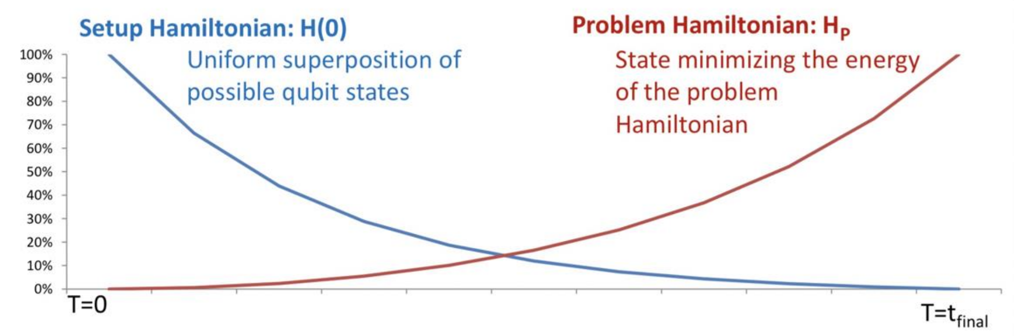
*How does it work*

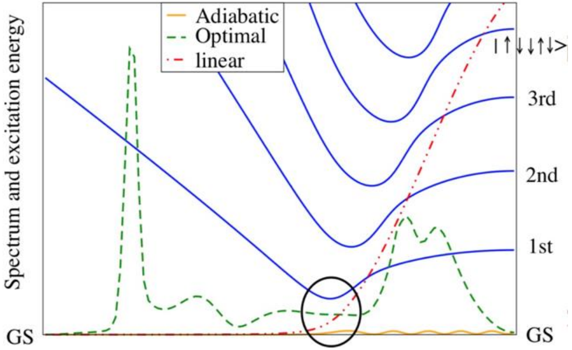
- Setup with trivial $H_0$ and evolve to target $H_p$ in the ground state

$$H(t) = A(t)H_0 + B(t)H_p$$




*T.Caneva et al. PRA (2014)*




https://arxiv.org/abs/quant-ph/0001106
https://arxiv.org/abs/quant-ph/0104129

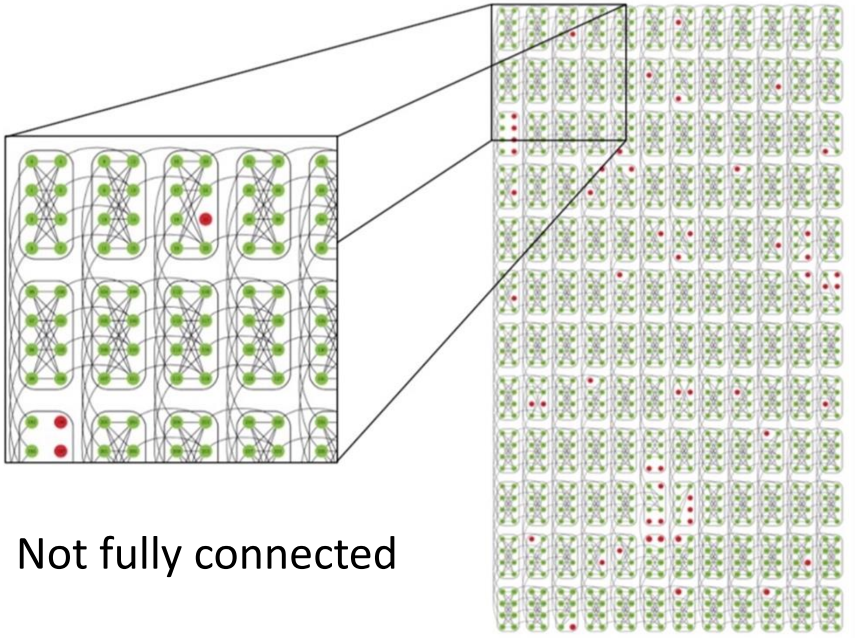
# D-Wave qubit connectivity

Ising Hamiltonian

$$H_{Ising} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

External Field

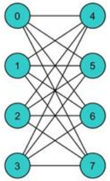
Interactions

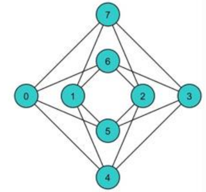


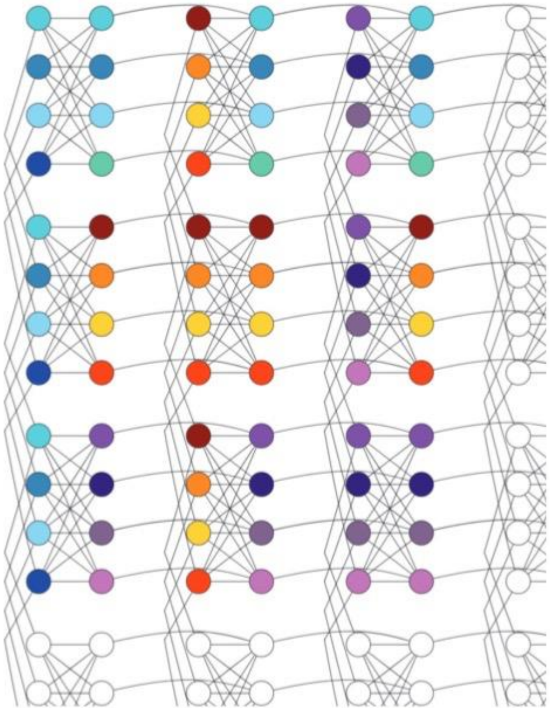
Not fully connected

But what if we do not have all connections?

# D-Wave Chimera network



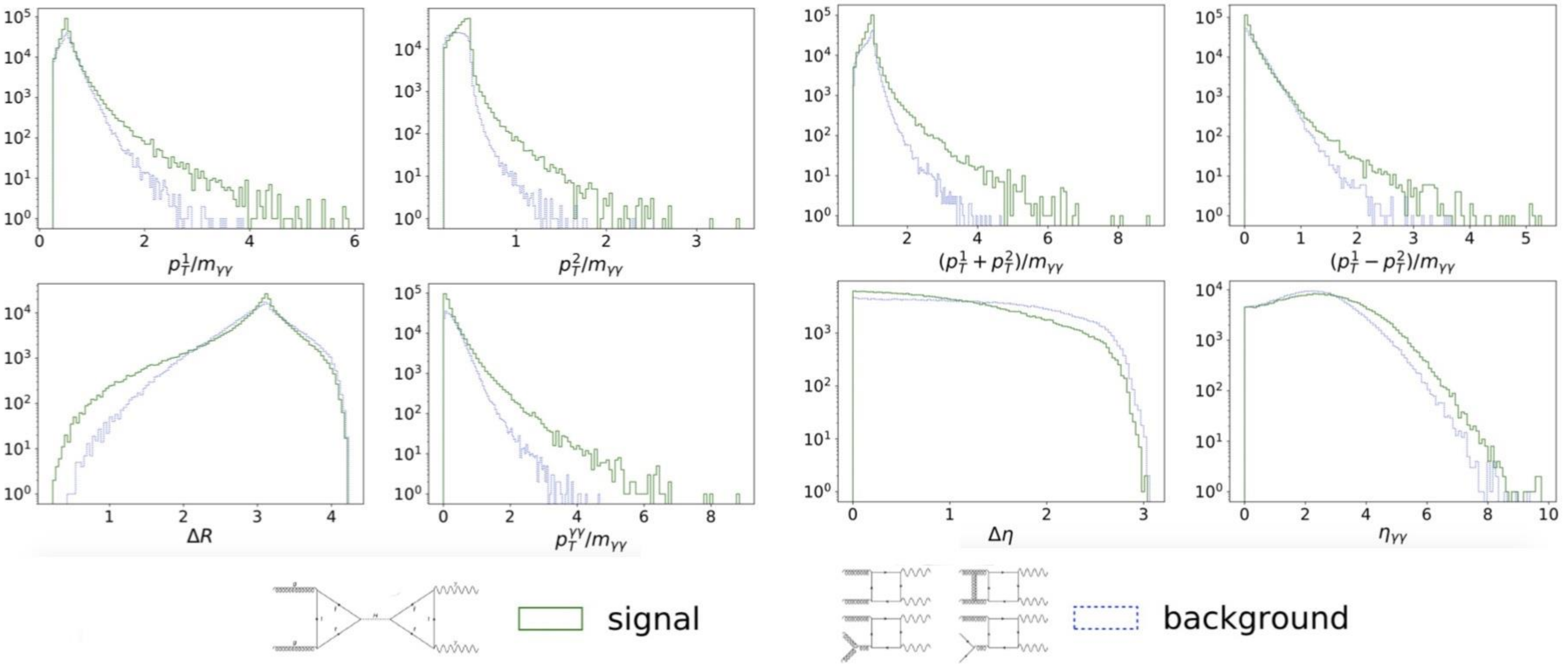



- Realize full Ising via spin chains by the Chimera graph
- Split local fields across all qubits in the chain
- Tightly intra-chain coupling ($J_F$ up to 6)
- Non-unique, heuristic embedding
- Post-process to correct broken chains
- Majority vote
- Approximately 40 spins full Ising Model

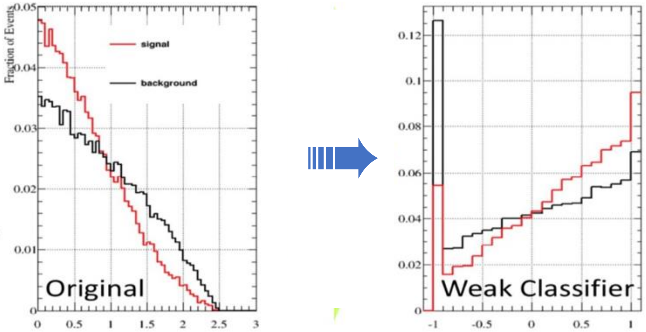
https://arxiv.org/abs/1210.8395

# Now let’s do this…!



# Weak → Strong classifier

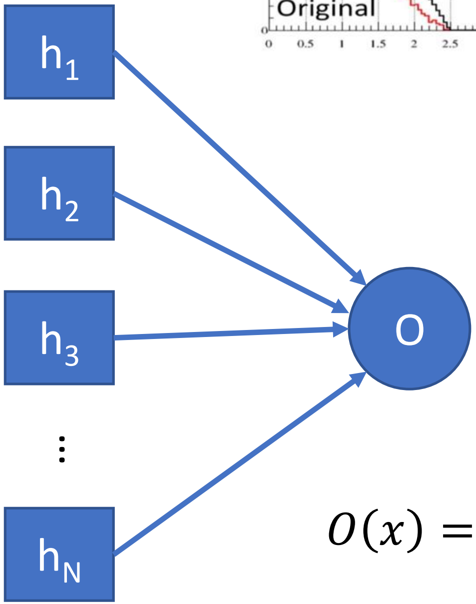
*How to obtain a strong classifier*




- $h_i(\boldsymbol{x}) \in [-1,1]$ are functions of the variables such that
- $P(S|h_i>0) > P(B|h_i>0)$
- $P(B|h_i<0) > P(S|h_i<0)$

i.e.

- $h_i>0$ probably Signal
- $h_i<0$ probably Background




$$O(x) = \sum_i w_i h_i(x)$$

# The gory details…

- Since we have a MC, we can define a precise target

$$y(x) = \begin{cases} +1, if\ x \in S \\ -1, if\ x\ \in B \end{cases}$$

- So the error per event is

$$E_s = E(x_s) = y(x_s) - \sum_{i=1}^{N} w_i h_i(x_s)$$

- And the total error is

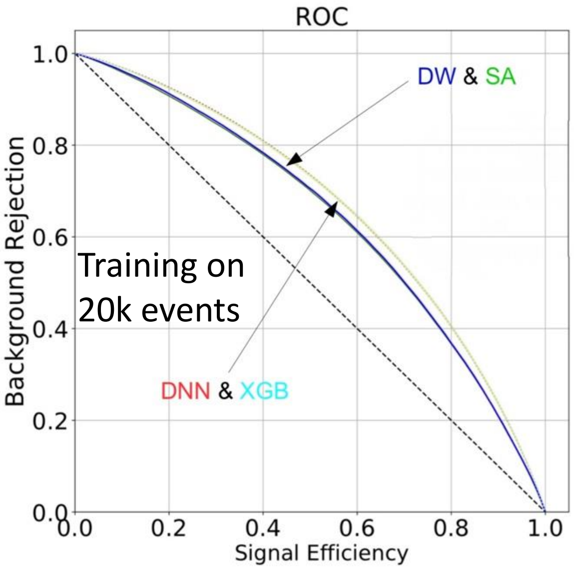
$$\delta(x) = \sum_s E_s^2 = |y_s|^2 + \sum_{i,j=1}^{N} C_{ij} w_i w_j - 2\sum_{i=1}^{n} C_{yi} w_i \qquad C_{ij} = \sum_s h_i(x_s) h_j(x_s) \qquad C_{yj} = \sum_s h_i(x_s) y_s$$

$$\delta'(x) = \sum_{i,j=1}^{N} C_{ij} w_i w_j + 2\sum_{i=1}^{N} (\lambda - C_{yi}) w_i$$

+ sparsity penalty (λ, Hamming weight)
– constant ($|y_s|^2$)

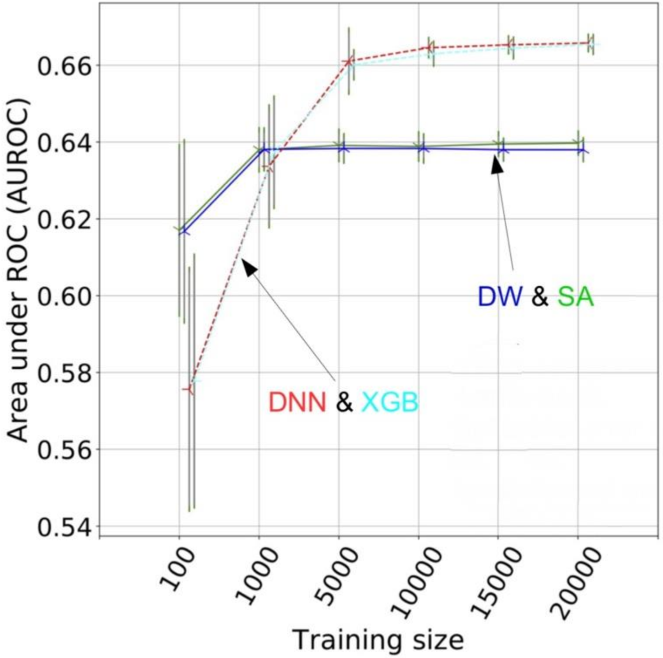
# So here we are!

$$\delta'(x) = \sum_{i=1}^{N} 2(\lambda - C_{yi})w_i + \sum_{i,j=1}^{N} C_{ij}w_iw_j \quad \Rightarrow \quad H_{Ising} = \sum_i h_i\sigma_i^z + \sum_{ij} J_{ij}\sigma_i^z\sigma_j^z$$




DNN & XGB
- Classical ML

DW & SA
- D-Wave annealing



# For reference

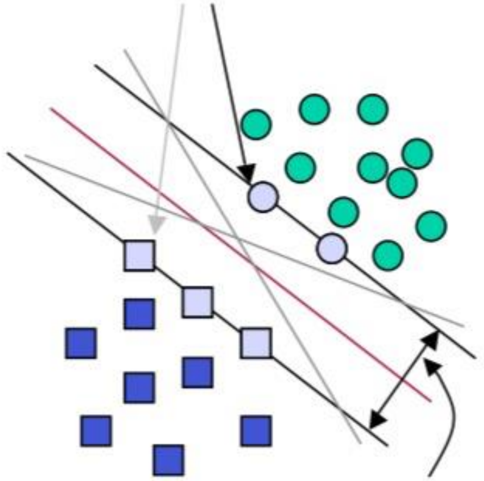
- XGBoost (XGB)
  - Extremely efficient library for training decision trees (http://xgboost.readthedocs.io)
  - Discovered during the higgs-ml challenge (https://www.kaggle.com/c/higgs-boson)
  - Moderately optimize the hyper-parameters
- Deep Neural Network (DNN)
  - Simple fully connected model 2 layers 1000 nodes
  - https://keras.io/ http://deeplearning.net/software/theano/
  - Moderately optimize the hyper-parameters

# Take 2 – Quantum Circuits

*The IBM Q-machine*

- Same problem – different take
- Analysis done with Support Vector Machine
- Separate two sets of points with the widest possible margin
- The decision function is fully specified by a (usually very small) subset of training samples, the support vectors.
- The solution is fully specified by a (usually small) subset of training samples, the support vectors.
- If there is an hyperplane that divides the points it is a simple quadratic optimization

Support Vectors



Maximize margin

Support Vectors: vectors that “support” the dividing planes

# *Almost* a DNN

- Input: set of training pair samples with a result function $y(x_i) \in [-1,1]$;
- Output: set of $w_i$ whose linear combination predicts the value of $y(x_i)$
- Important difference: optimization has two objectives: maximize the margin ("street width") **and** reduce the number of weights to the (usually few) support vectors

# One word on how SVM works

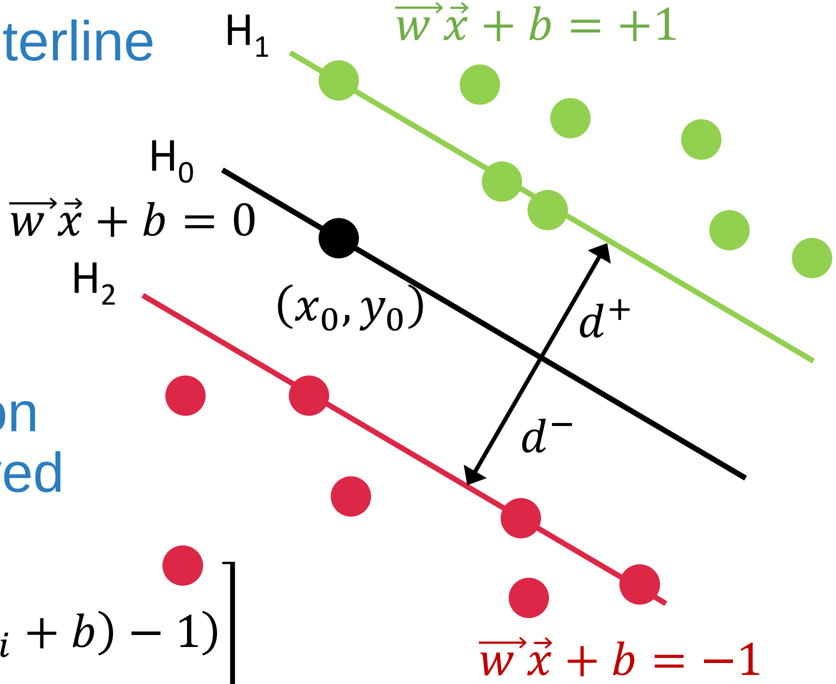
- Distance from support point to centerline

  $d = |\vec{w}\vec{x} + b| / |\vec{w}| = 1/|\vec{w}|$

- We have to minimize $|\vec{w}|$ and impose no points "in between"

  $y_i(\vec{w}\vec{x}_i + b) \geq 1$

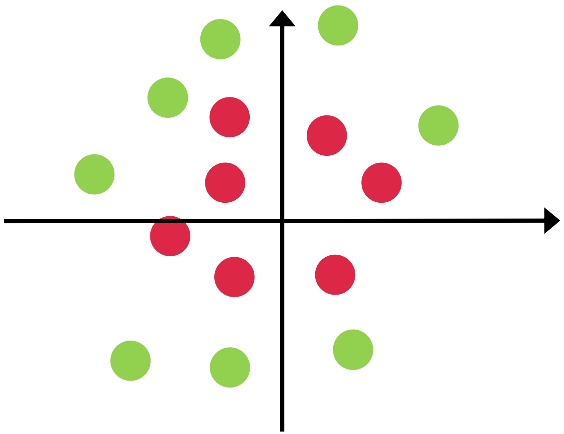
- Well defined quadratic minimization problem with linear constraint solved with Lagrangian multipliers



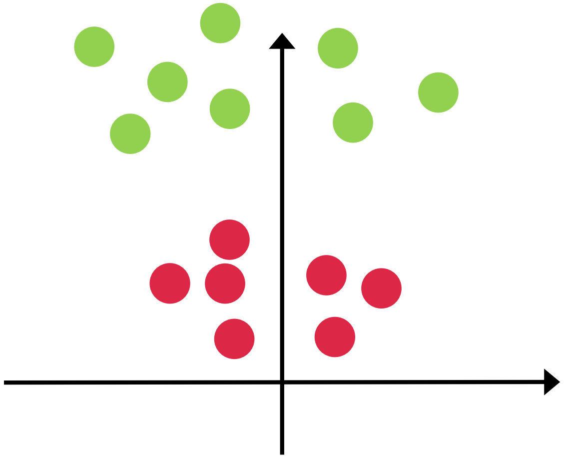

$$\min_{\vec{w},b} \mathcal{L}(\vec{x}, \vec{a}) = \min_{\vec{w},b} \left[ 1/2|\vec{w}| + \sum_i a_i(y_i(\vec{w}\vec{x}_i + b) - 1) \right]$$

# This is great but…

- What about this?



$$x_i' = x_i$$
$$y_i' = \sqrt{x_i^2 + y_i^2}$$



- With the bonus of the Kernel Trick

We do not need $\overrightarrow{x'} = \Phi(\vec{x})$ but just $\mathrm{K}\left(\overrightarrow{x_i}, \overrightarrow{x_j}\right) = \Phi(\overrightarrow{x_i}) \cdot \Phi\left(\overrightarrow{x_j}\right)$!

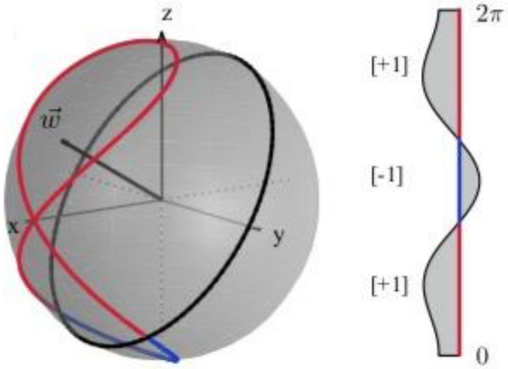
# Now on Quantum

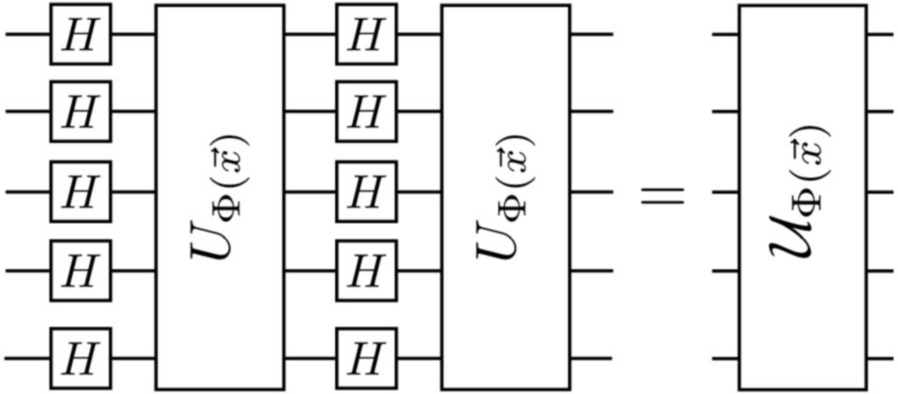
- Step 0: Build a classifier like before
- Step 1: Feature-map the data to a much larger dimensional space
- Step 2: Train a the weights
- Step 3: Apply Quantum Classification

# Step 1

- Feature-map to a high-dimensional space (with entanglement)

$$\mathcal{U}_{\Phi(\vec{x})} = U_{\Phi(\vec{x})} H^{\otimes n} U_{\Phi(\vec{x})} H^{\otimes n}$$



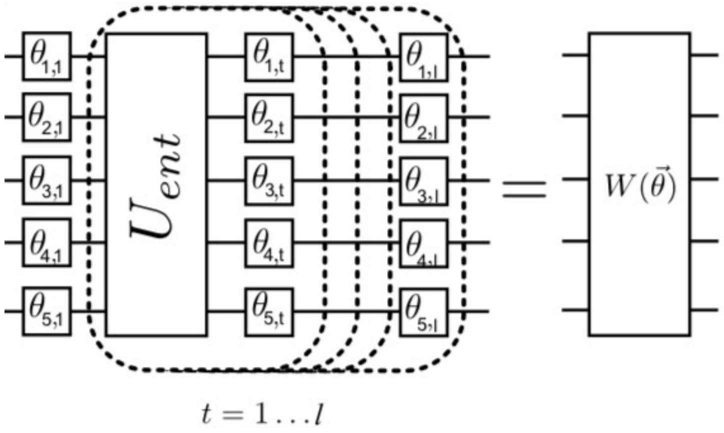



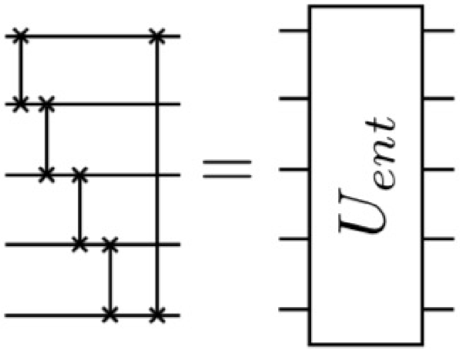

Single qubit mapping with phase gate $U_{\Phi(x)} = \begin{bmatrix} 1 & 0 \\ 0 & e^{ix} \end{bmatrix}$

$$U_{\Phi(\vec{x})} = \exp\left( i \sum_{S \subseteq [n]} \phi_S(\vec{x}) \prod_{i \in S} Z_i \right)$$

# Step 2a

- Define the training network as a short-depth quantum circuit made of layers of single-qubit unitaries and entangling gates

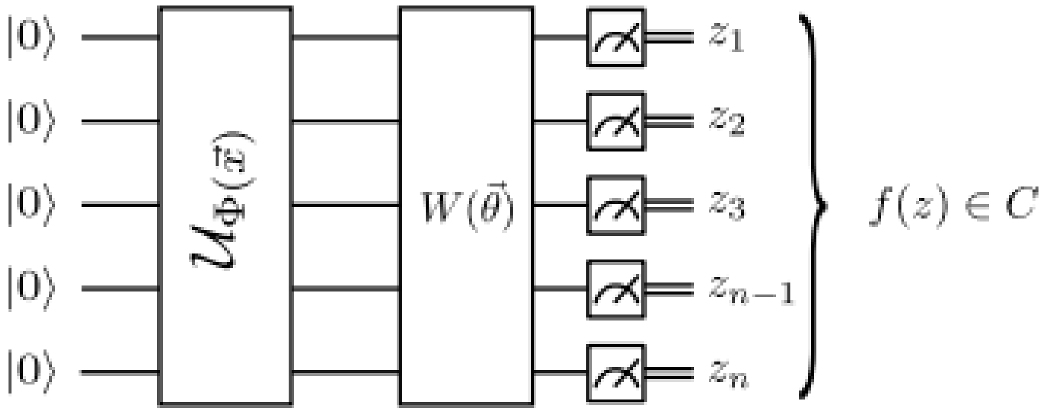



$$W(\vec{\theta}) = U_{loc}^{(l)}(\theta_l)U_{ent} \cdots U_{loc}^{(2)}(\theta_2)U_{ent}U_{loc}^{(1)}(\theta_1)$$

# Step 2b

- Apply a binary measurement $\{M_y\}$ to get the classifier and measure the probability of the foreseen outcome




$$p_y(\vec{x}) = \left\langle \Phi(\vec{x}) \middle| W^\dagger(\vec{\theta}) M_y W(\vec{\theta}) \middle| \Phi(\vec{x}) \right\rangle$$

# Step 3

- Train the network
- Obtain the empirical distribution $\hat{p}_y$
- Assign label $\tilde{m}(\vec{x}) = y \quad iff \quad \hat{p}_y(\vec{x}) > \hat{p}_{-y}(\vec{x}) - yb$
- Use cost $R_{emp} = \frac{1}{|T|}\sum_{\vec{x}\in T} Pr\left(\tilde{m}(\vec{x}) \neq m(\vec{x})\right)$ on training set
- Optimize for $\left(\vec{\theta}, b\right)$

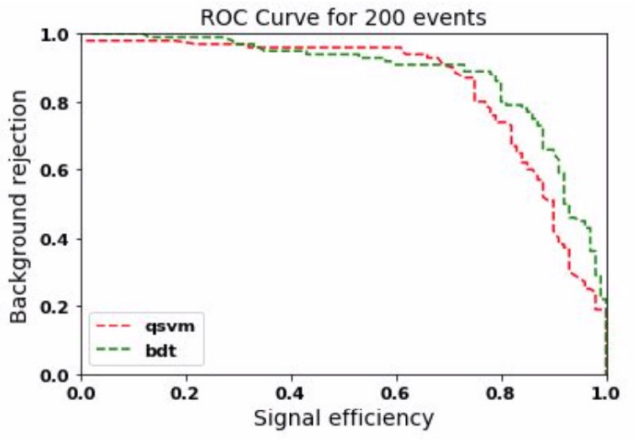
# Apply to data – simulator

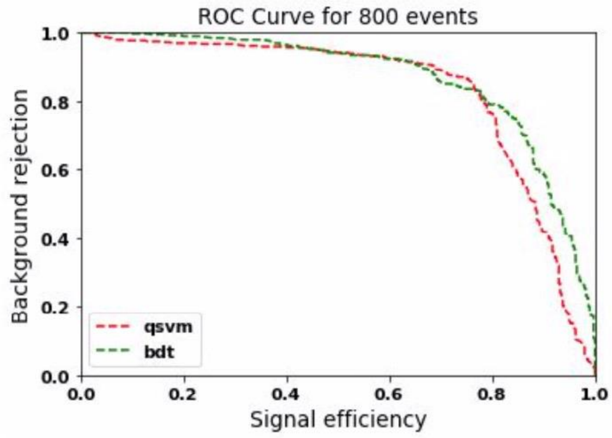
- Results

| ttH(H->$\gamma\gamma$) accuracy | 200 | 800 | 3200 |
|---|---|---|---|
| QSVM | 0.775 | 0.798 | 0.774 |
| BDT | 0.810 | 0.796 | 0.781 |

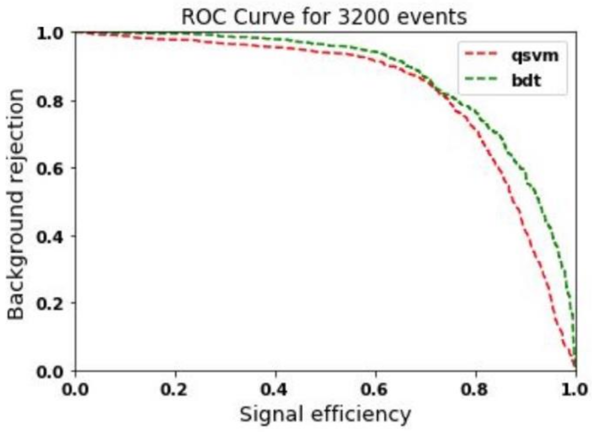
| ttH(H->$\gamma\gamma$) auc | 200 | 800 | 3200 |
|---|---|---|---|
| QSVM | 0.849 | 0.834 | 0.826 |
| BDT | 0.880 | 0.867 | 0.869 |

# Apply to data – simulator



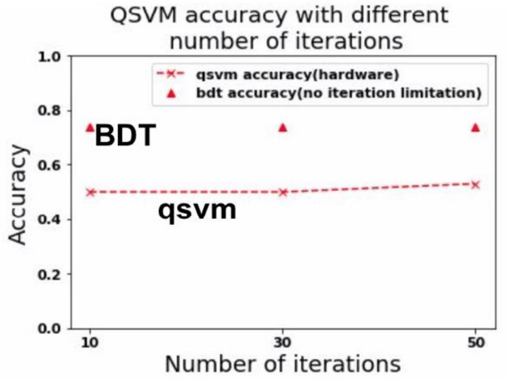



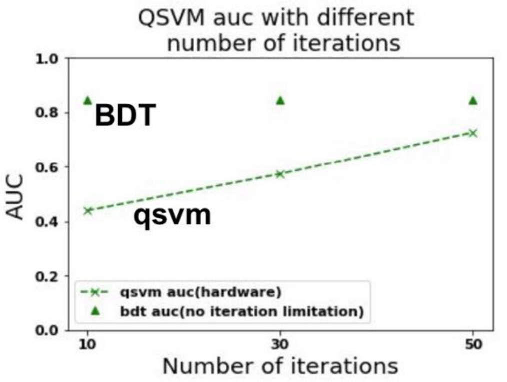

ROC = Receiver Operating Characteristic



# Apply to data -- hardware

- Accuracy and AUC with different number of iterations.
- QSVM accuracy increases with iterations
- QSVM AUC increases rapidly with iterations
- We plan to run the test with many more iterations if possible

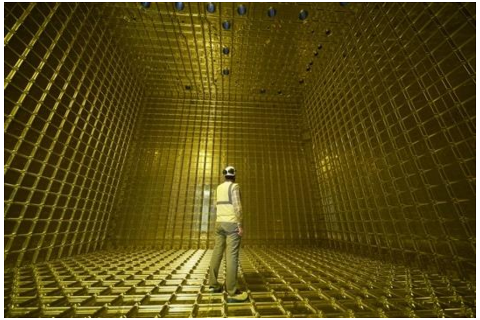


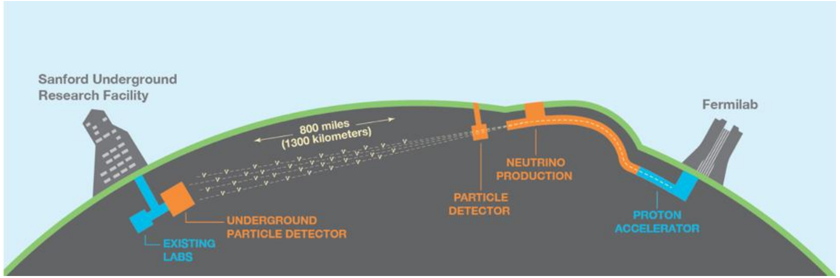



# Other examples – 1

*DUNE experiment*

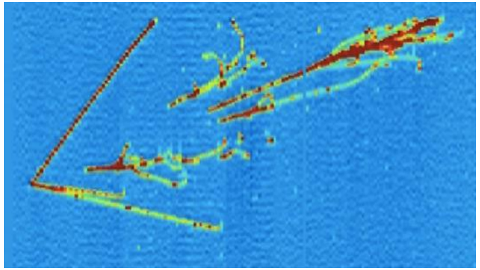
- Origin of Matter
- Unification of forces
- Black hole formation






- Supervised Quantum Learning to reconstruct neutrino interactions with a Quantum Computer

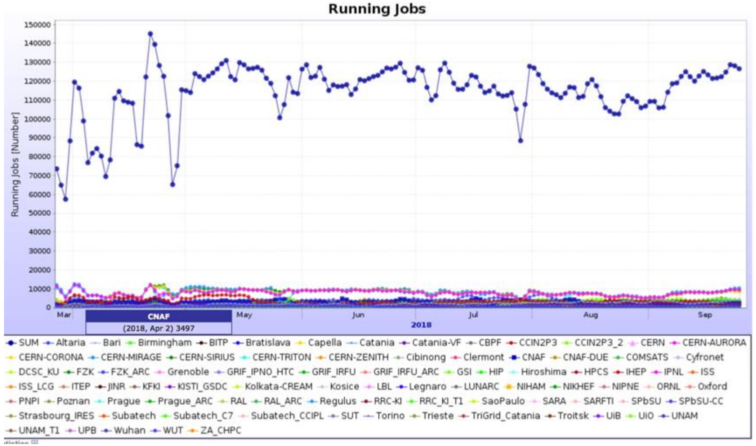
- Unsupervised learning to analyze the simulated and real event structures

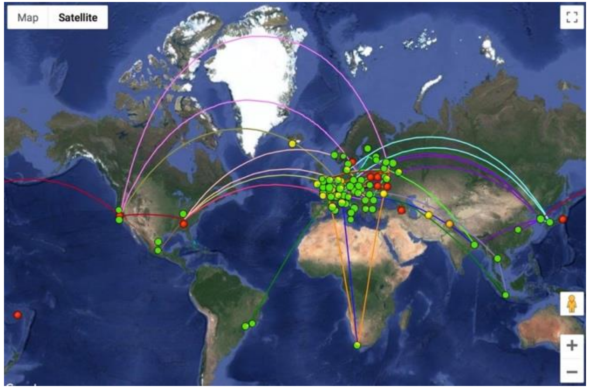


# Other examples – 2

*Optimize Grid workflow*

- ALICE Grid
  - 70 computing centres in 40 countries
  - 150,000 CPU cores and 120 PB of storage
  - ~140.000 jobs running 24 x 7 x 365



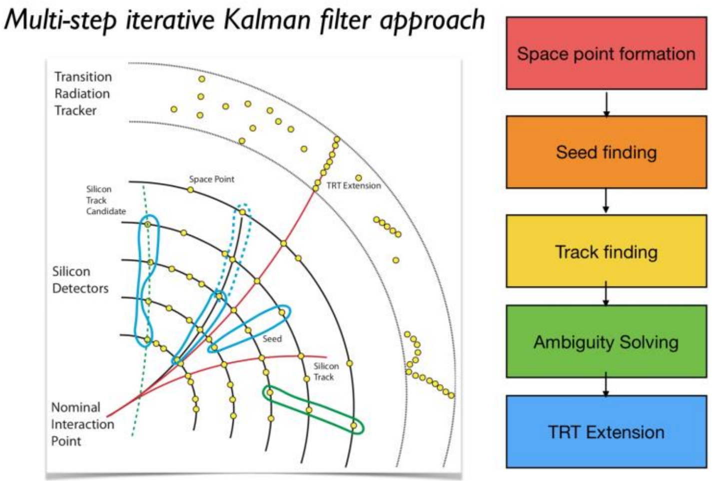



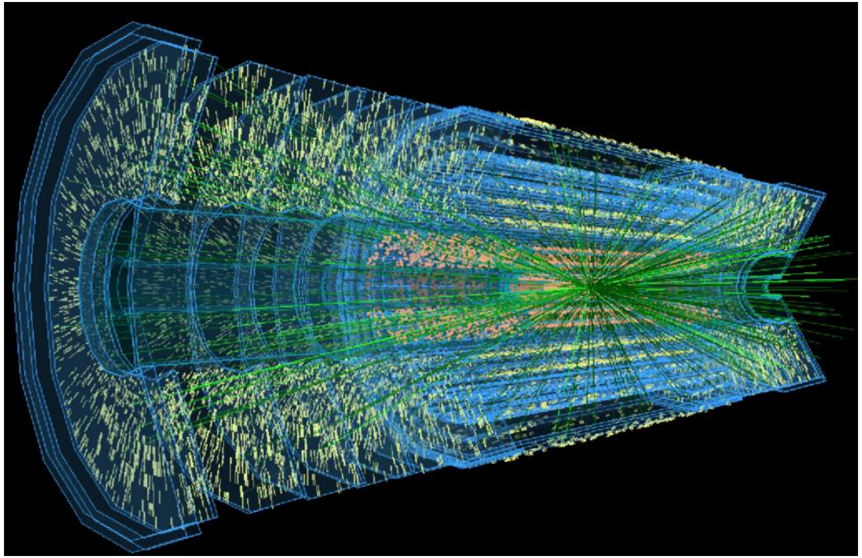

- Optimize storage location and job workflow
- Use Quantum Computing algorithms to find best distribution in a dynamic environment

# Other examples –

*Track reconstruction in dense environments*

- Track candidates are identified via combinatorial search
- And then “followed” via Kalmnan filters
- The track is no better than its seeds!



- Use Quantum Computing to speed up combinatorial searches
- And Genetic Algorithms to quickly optimize the search

# Quantum Computing Initiatives

- CERN openlab has organized a kick-off event of its Quantum Computing initiative on **November 5th-6th**
  - https://indico.cern.ch/event/719844/
- > 400 registered participants from the HEP physics community, companies and worldwide research laboratories and beyond
- Create a database of QC projects to foster collaborations between interested user groups, CERN openlab and industry
- Continue to seek funding opportunities for QC projects

# Conclusions


- CERN openlab is a unique public – private infrastructure fostering collaboration between research and ICT industry
- We have presented two specific fields of investigation that have a high relevance both for fundamental research and for society at large
- Deep Learning has emerged in recent years as a very interesting discipline that has already proved its worth in many fields, but that is still an active domain of research and investigation
- While still not a ready for prime-time production, Quantum Computing holds the promise to herald a revolution in ICT
- CERN openlab intends to investigate the opportunities offered by these and other advanced ICT fields, fostering collaborations between scientists and industry

# Thanks for your attention!

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