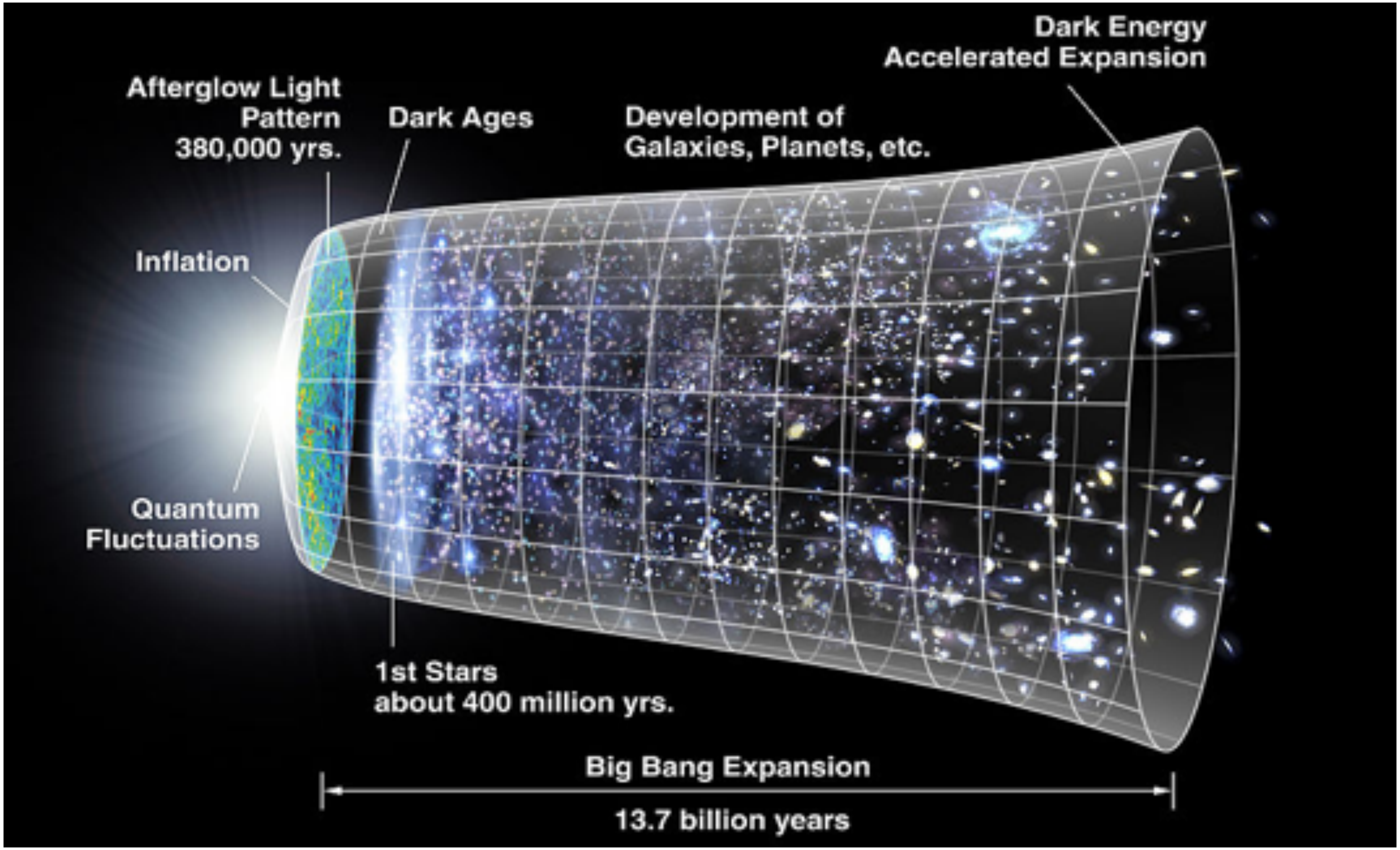


Computing for Big Science in the next Decade, plus HEP and Quantum Computing

Liz Sexton-Kennedy
CoDaS-HEP, 24-July-2018

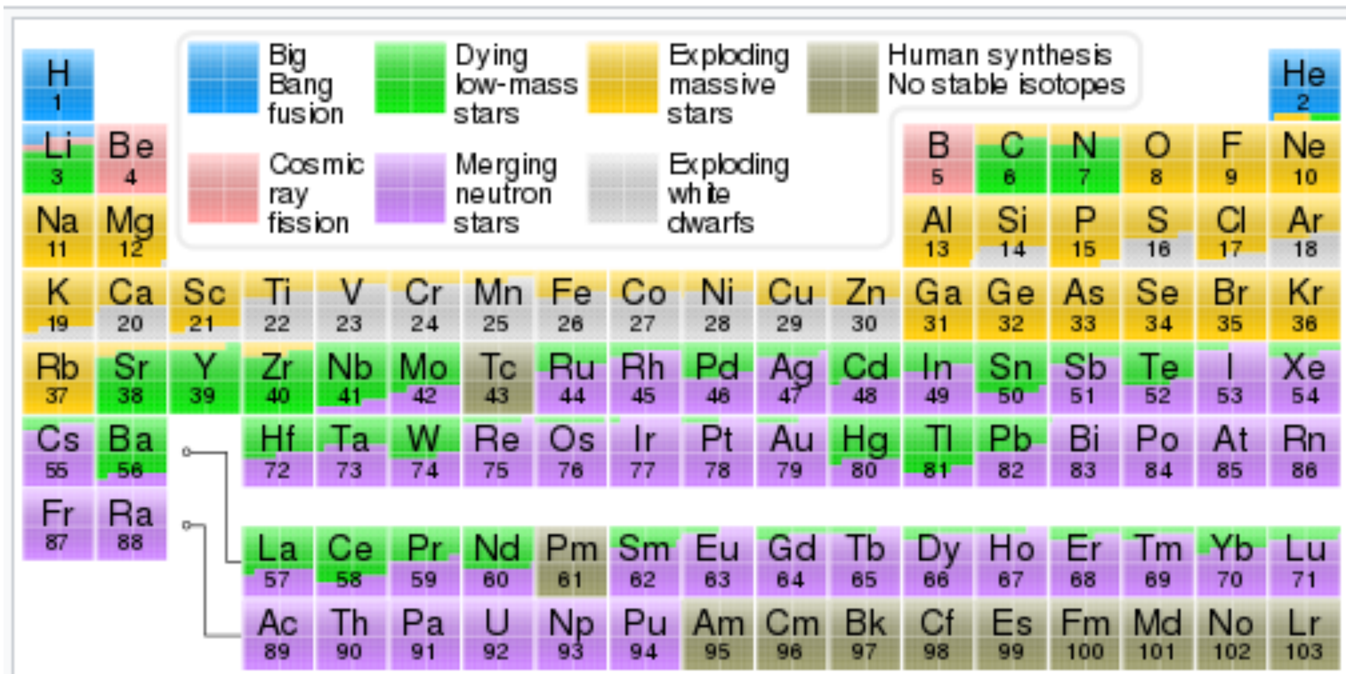
The Big Questions and Where They Lead us Today

- What are we? and How did we get here?

- These questions are at the heart of the sciences. For HEP they are particle, astro-particle, and cosmology questions.

- r-process nucleosynthesis

- cosmic evolution



Periodic table showing the cosmogenic origin of each element. The elements heavier than iron with origins in supernovae are typically those produced by the *r*-process, which is powered by supernovae neutron bursts

Science Drivers

- Concentrating on the decadal drivers, we have:
  - Fully exploit the Higgs using it as a tool for further discovery, electroweak and flavor physics
  - Investigate the neutrino mass and hierarchy
  - Investigate dark matter and it's role in cosmic evolution
  - Investigate cosmic acceleration, dark energy, quantum gravity
  - Explore the unknown

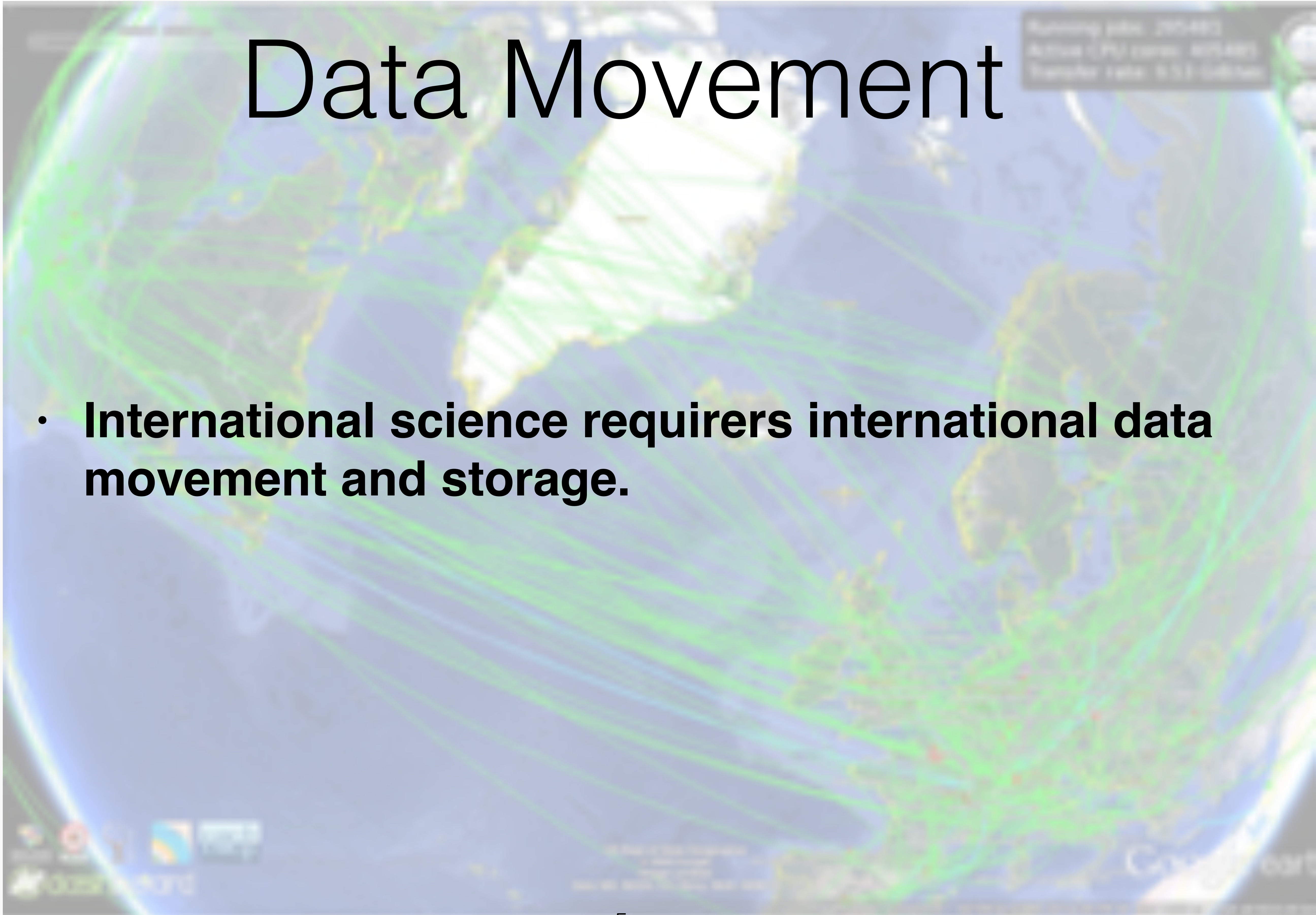
Instrumentation

- **Large scientific achievements in the past decades have been enabled by large advances in in instrumentation.**

- **Large silicon detectors and cameras with high granularity are driving us to large computing and data challenges.**

- **Large costs of these projects require an international scope.**

Data Movement

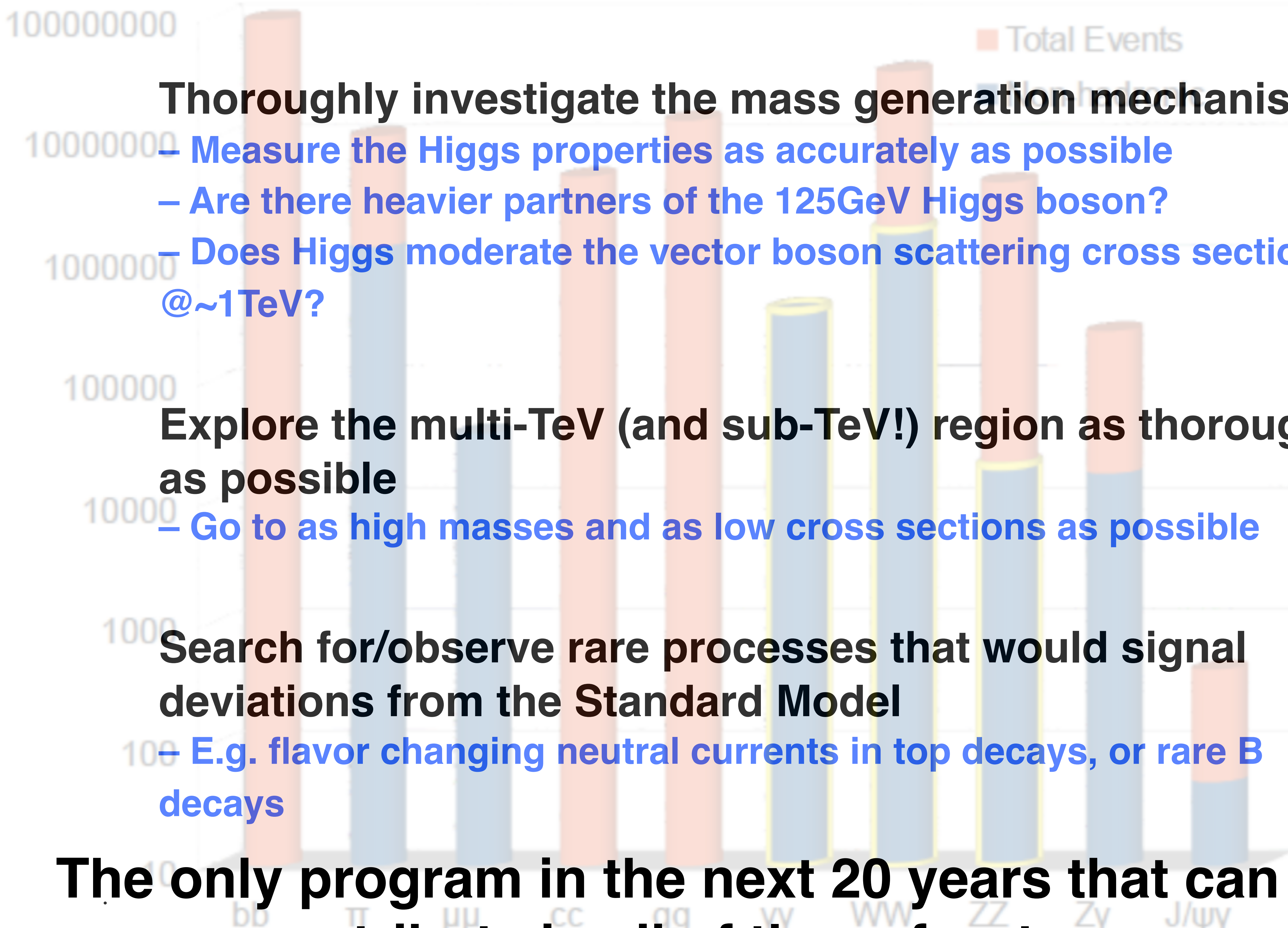


- **International science requirers international data movement and storage.**

International Big Data Science

- LHC, SKA, DUNE, LIGO, LSST
  - For each of these I will have one slide on the science case and one slide on the data needs
  - While we know the computing challenges are equally large, others outside of HEP are planing to build exescale compute
  - Most likely our community will have to build exescale data along with our partners.

HL-LHC Science



Thoroughly investigate the mass generation mechanism
- Measure the Higgs properties as accurately as possible
- Are there heavier partners of the 125GeV Higgs boson?
- Does Higgs moderate the vector boson scattering cross section @~1TeV?

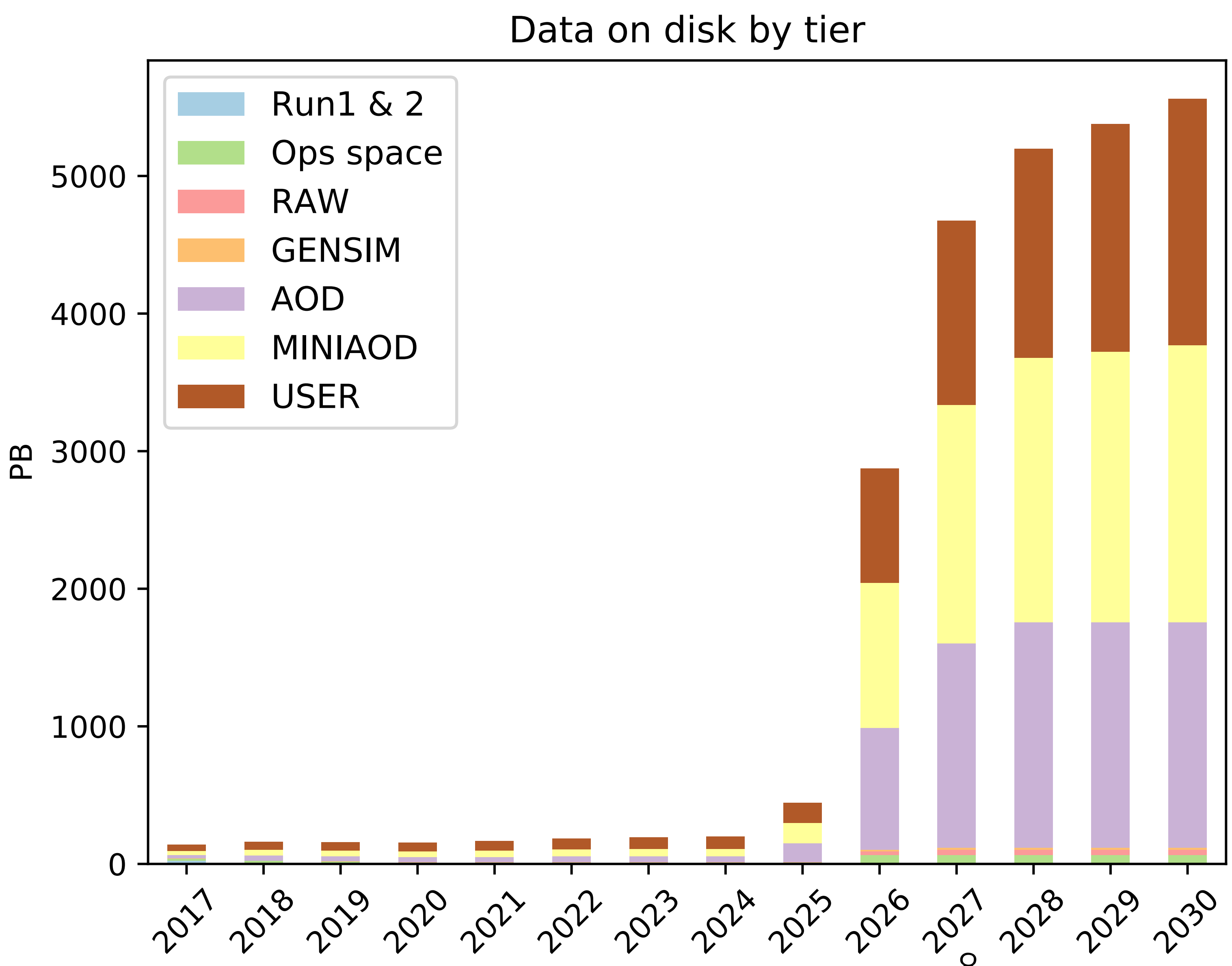
Explore the multi-TeV (and sub-TeV!) region as thoroughly as possible
- Go to as high masses and as low cross sections as possible

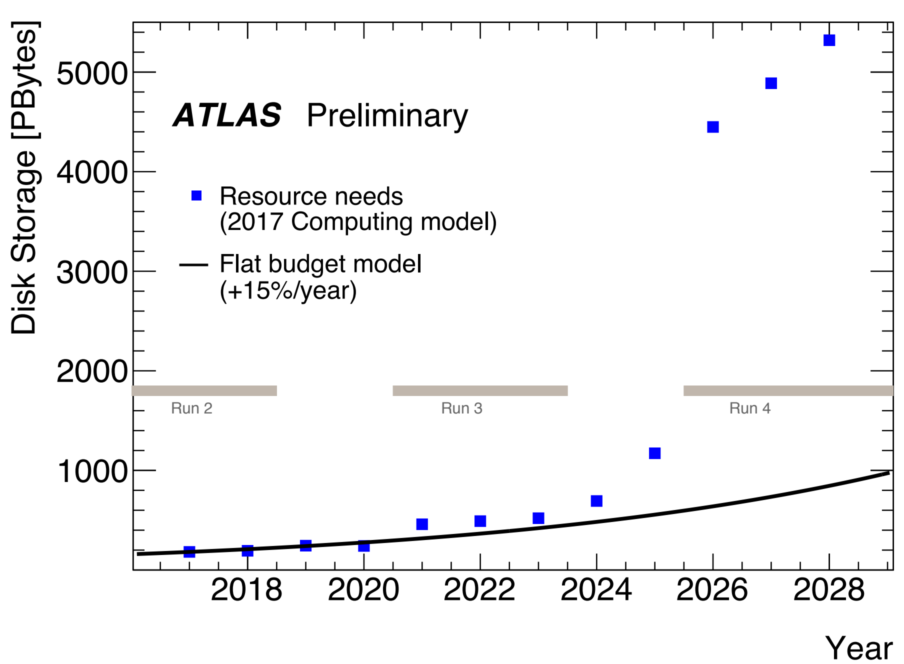
Search for/observe rare processes that would signal deviations from the Standard Model
- E.g. flavor changing neutral currents in top decays, or rare B decays

The only program in the next 20 years that can contribute in all of these fronts.

LHC Current Data Projections

- From the HEP Community White Paper
- The step from LHC to HL-LHC is clear challenge. The plots themselves show that data models have to change.

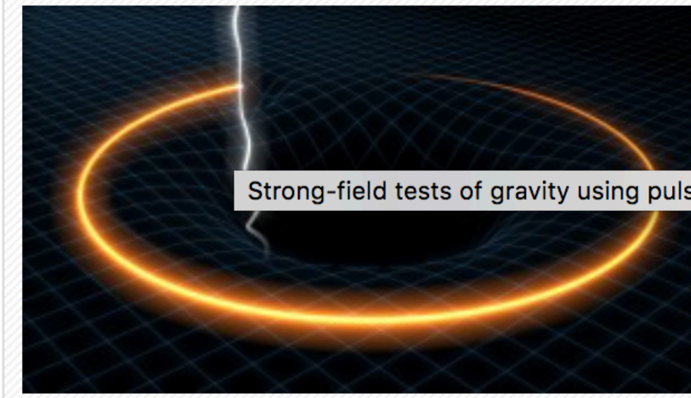




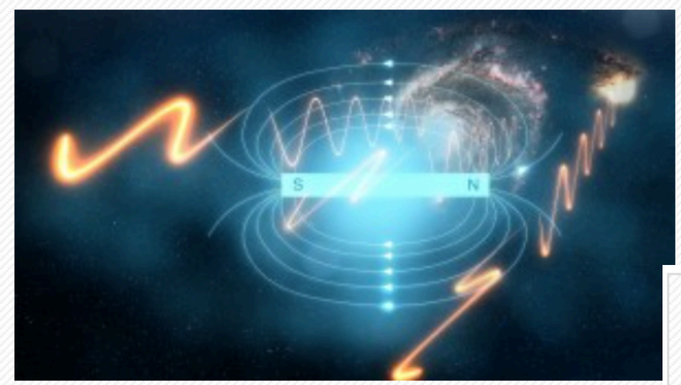
SKA Science

- The SKA will investigate this expansion after the Big Bang by mapping the cosmic distribution of hydrogen.
- SKA will investigate the nature of gravity and challenge the theory of general relativity
- SKA will create three-dimensional maps of cosmic magnets to understand how they stabilize galaxies, influence the formation of stars and planets, and regulate solar and stellar activity.
- SKA will look back to the Dark Ages, a time before the Universe lit up, to discover how the earliest black holes and stars were formed.
- SKA will be able to detect very weak extraterrestrial signals and will search for complex molecules, the building blocks of life, in space.

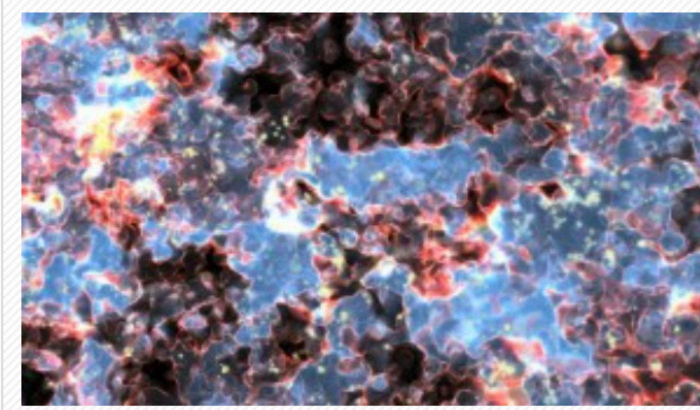
Galaxy evolution, cosmology and dark energy



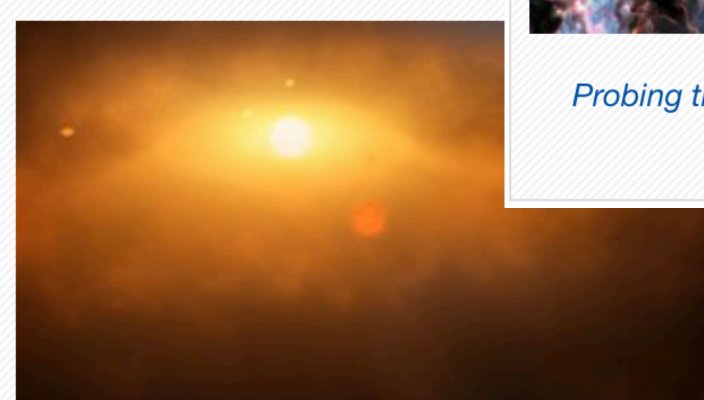
Strong-field tests of gravity using pulsars and black holes



Investigating the origin and evolution of cosmic magnetism



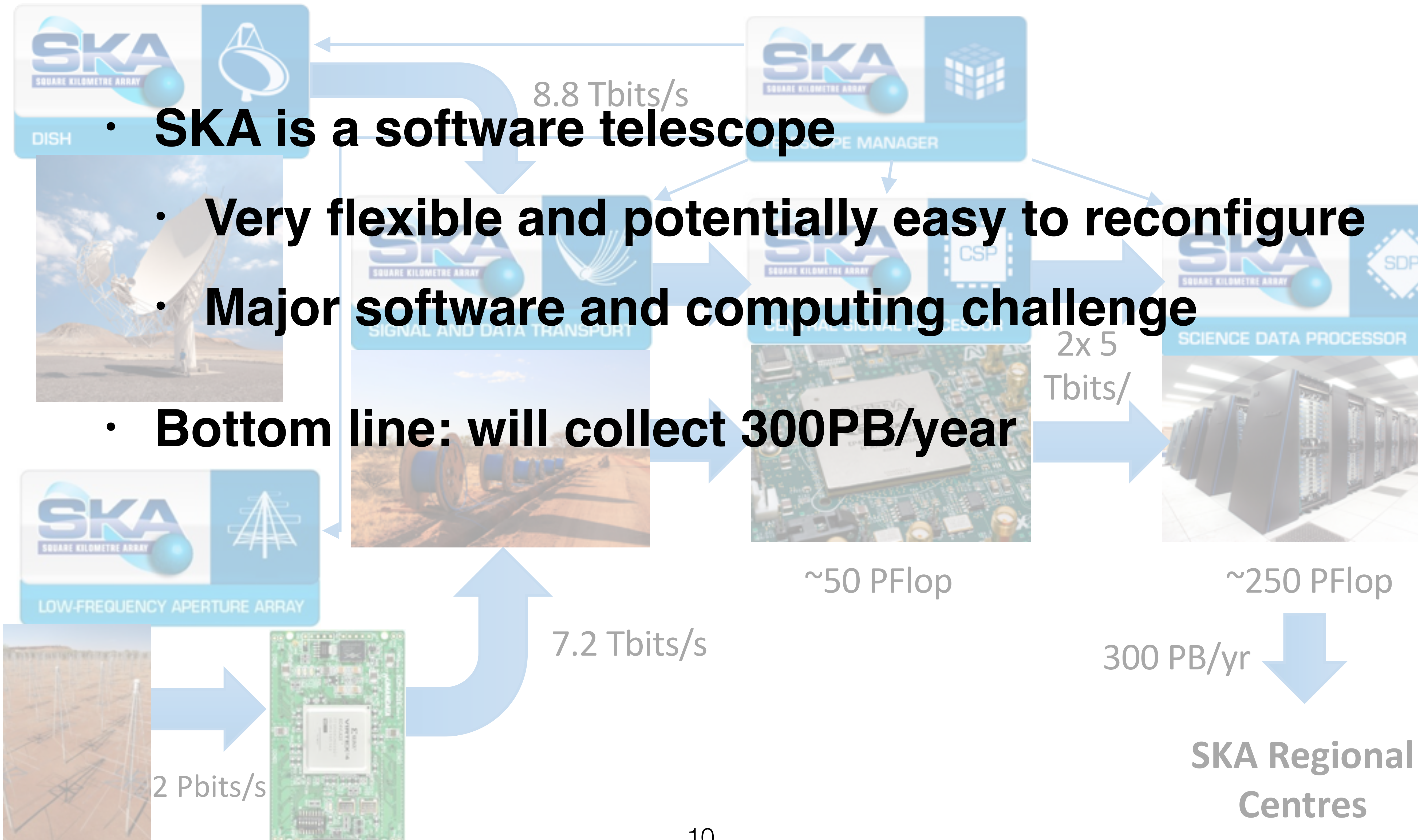
Probing the dark ages – the first black holes and stars



The cradle of life searching for life and planets

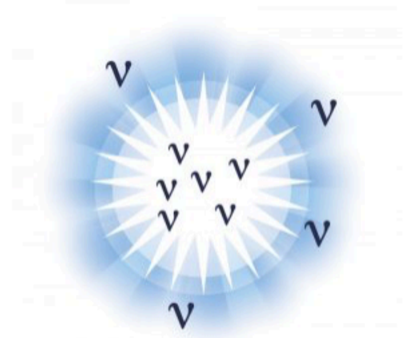
SKA Data

- **SKA is a software telescope**
  - **Very flexible and potentially easy to reconfigure**
  - **Major software and computing challenge**
- **Bottom line: will collect 300PB/year**



DUNE Science

Aiming for groundbreaking discoveries



Origin of Matter Neutrino Oscillations

Could neutrinos be the reason that the universe is made of matter rather than antimatter? By exploring the phenomenon of neutrino oscillations, DUNE seeks to revolutionize our understanding of neutrinos and their role in the universe.

Unification of Forces Proton Decay

With the world's largest cryogenic particle detector located deep underground, DUNE can search for signs of proton decay. This could reveal a relation between the stability of matter and the Grand Unification of forces, moving us closer to realizing Einstein's dream.

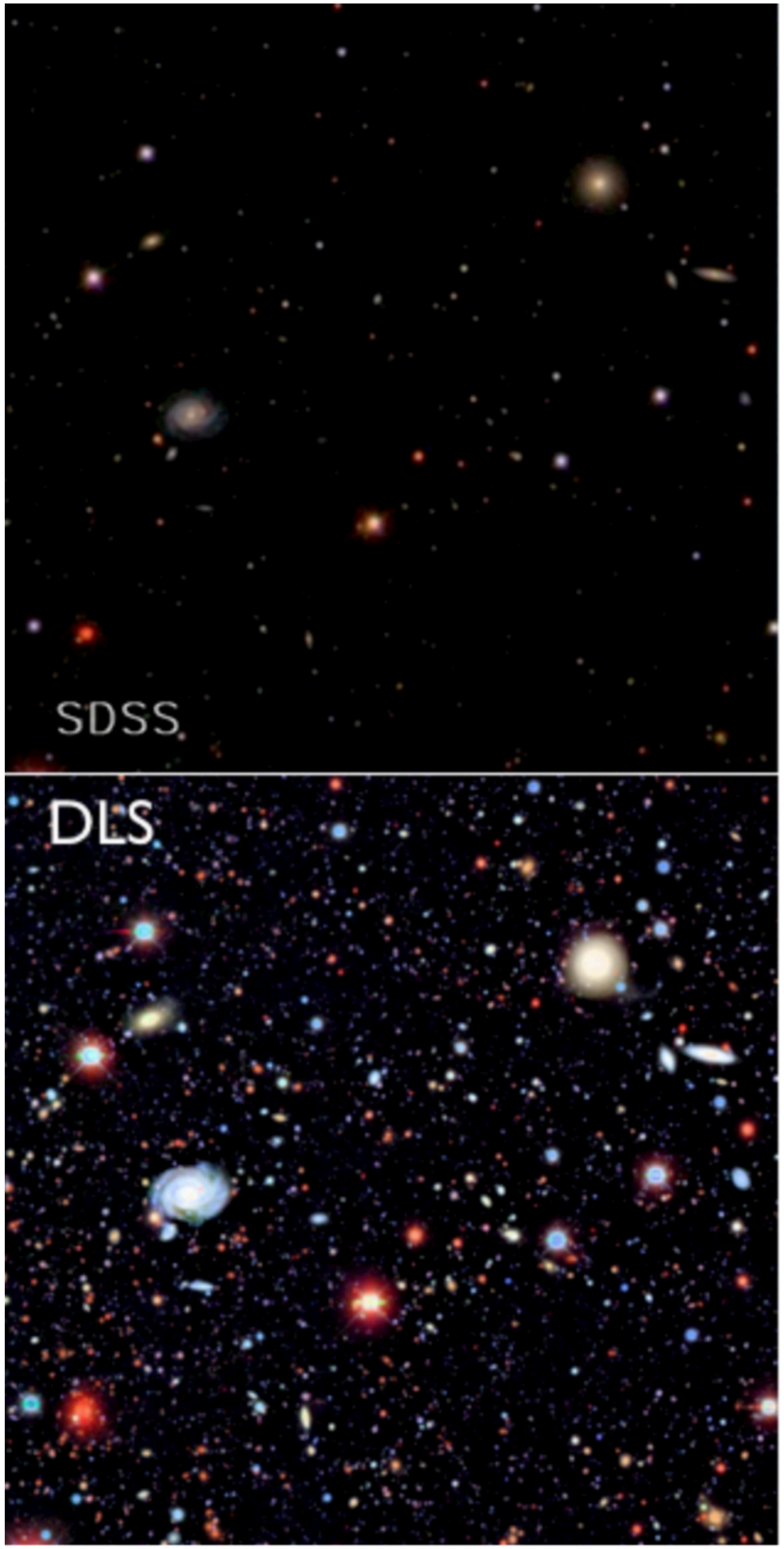
Black Hole Formation Neutrino Astrophysics

DUNE's observation of thousands of neutrinos from a core-collapse supernova in the Milky Way would allow us to peer inside a newly-formed neutron star and potentially witness the birth of a black hole.

DUNE Data

- Full Stream Data for DUNE is impossibly large, order 150EB/year
  - Much of the detector research will go into reducing that to reasonable levels
  - suppression of ^{39}Ar decay, cold electronics noise, space charge effects, argon purities all play a role
  - above means that most challenging data needs for DUNE are during it's prototyping phase - now untill 2020
  - Needs proposed at review: low/high = 4/59 PB, most probable 16PB

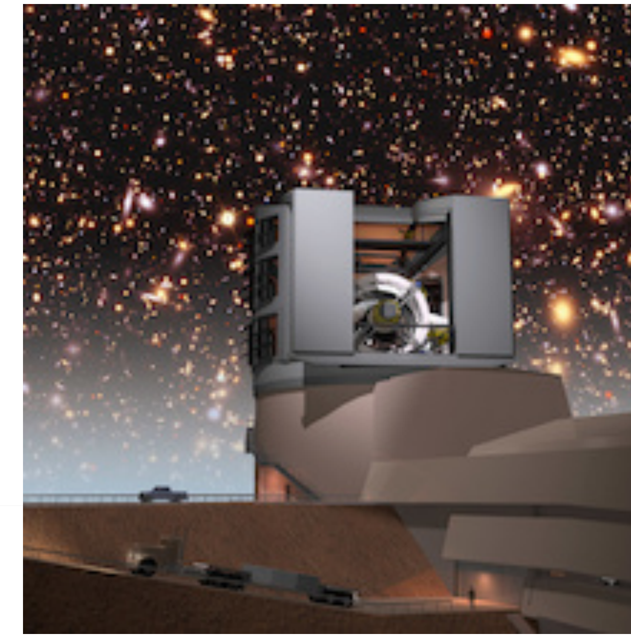
Year	CPU (10^6 Hr)	Storage (TB)	Tape (PB) low/high
FY18	9.25	703	0.8/5.9
FY19	28.6	1938	3/49.8
FY20	12.5	237	0.04/3.4



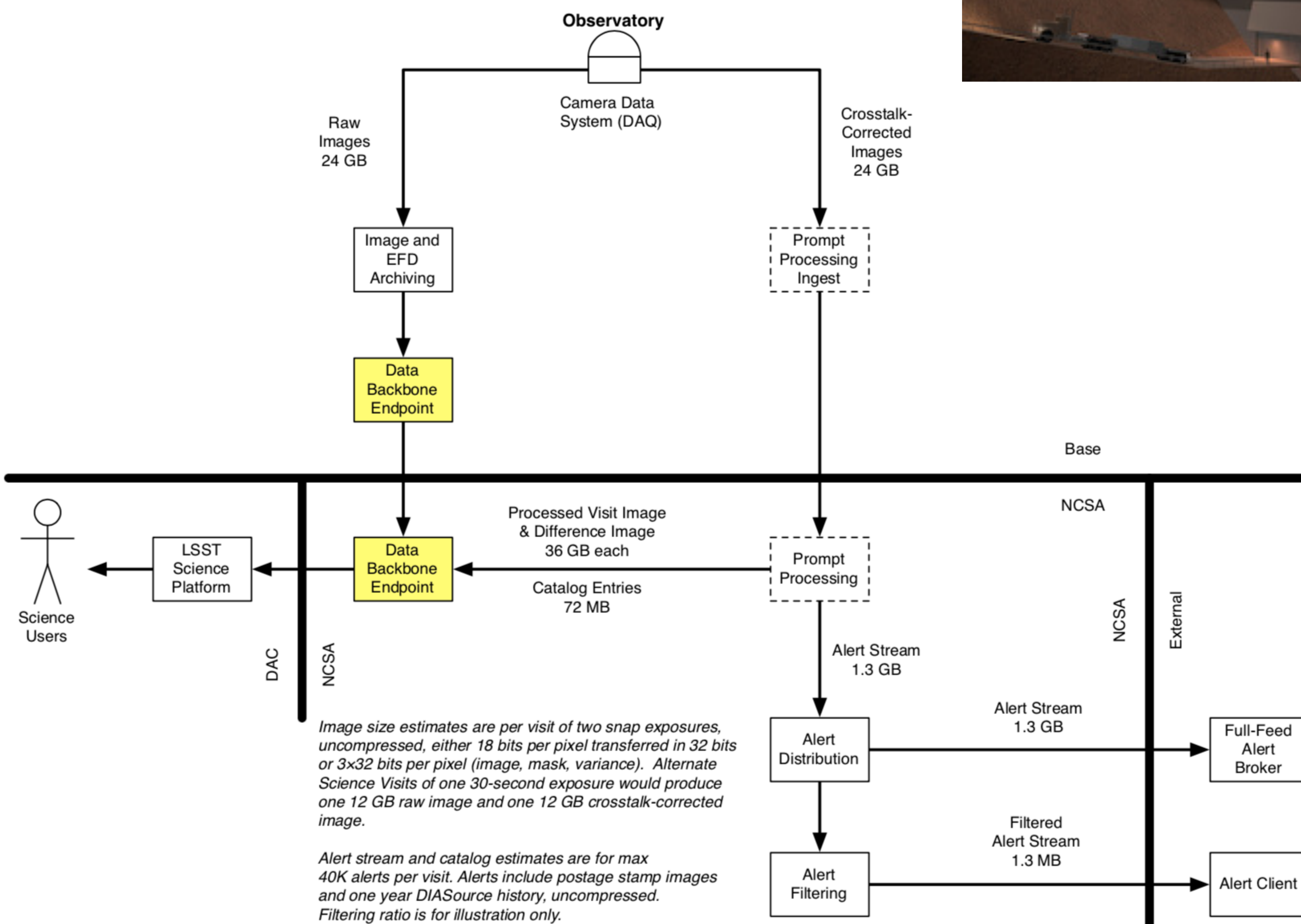
LSST Science

- LSST will conduct a deep survey with a frequency that results in taking repeat images of every part of the sky every few nights in multiple bands for ten years.
  - Milky Way Structure & Formation: by creating a map 1000 times the volume of past surveys, cataloging the colors and brightnesses of billions of new stars.
  - Probe the nature of dark matter and dark energy using several billion galaxies
  - Exploring the Changing Sky and Cataloging the Solar System

LSST Data



- LSST will collect 50PB/ year of data



LIGO Science

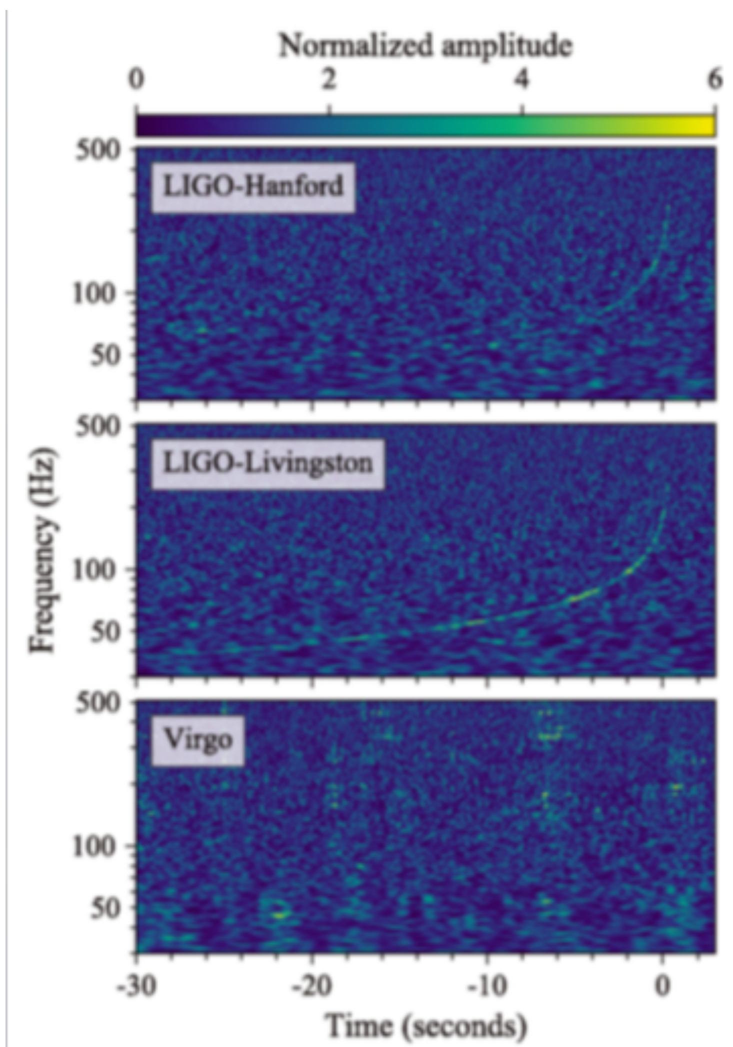
Is general relativity the correct theory of gravity?
How does matter behave under extreme densities and pressures?
How abundant are stellar-mass black holes?
What is the central engine driving gamma ray bursts?
What happens when a massive star collapses?

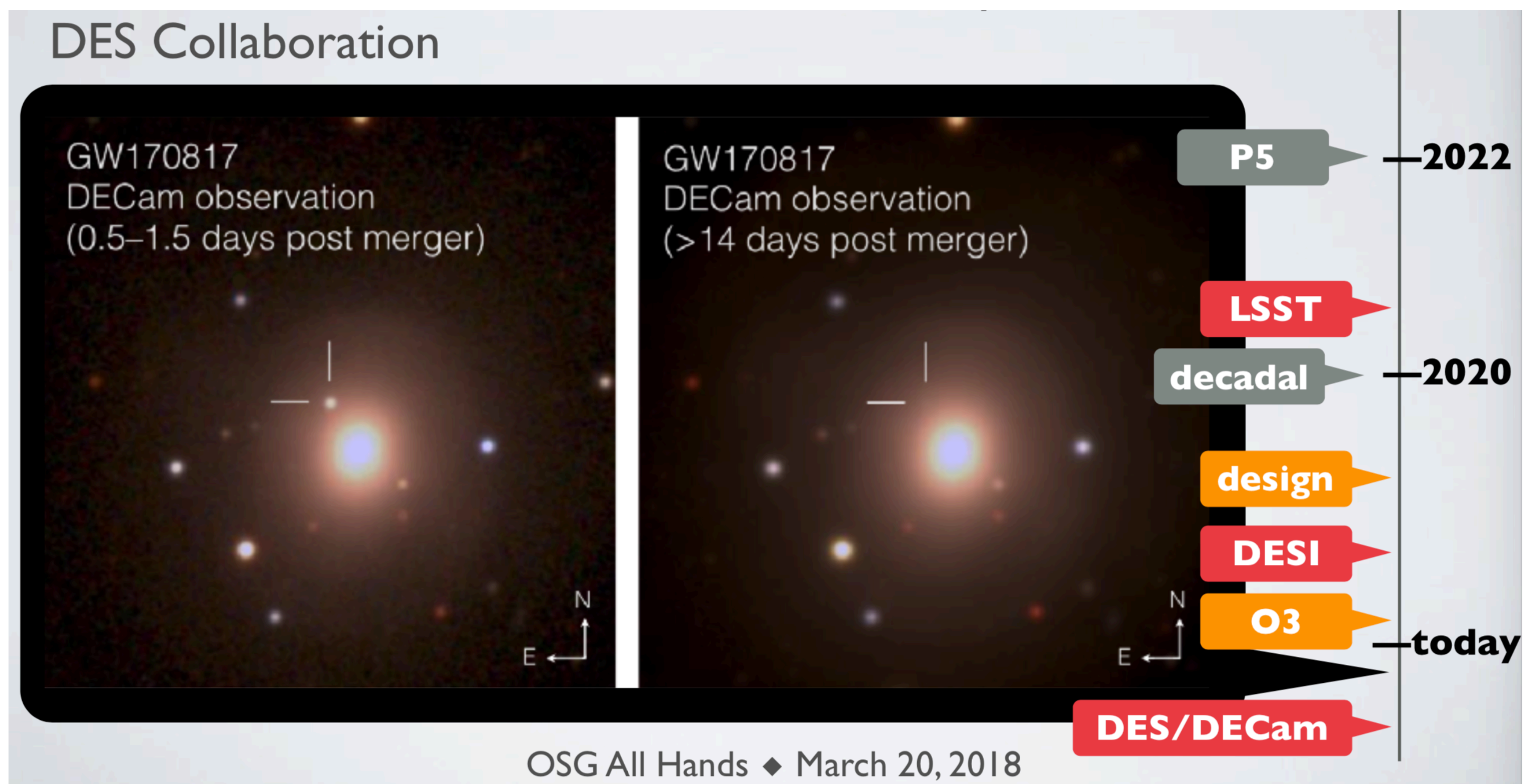
- With the discovery of gravitational waves LIGO has ushered in a new branch of astronomy

MULTI-MESSENGER ASTRONOMY

- Data science is not just about the large size of datasets it is also about the needed velocity of processing.

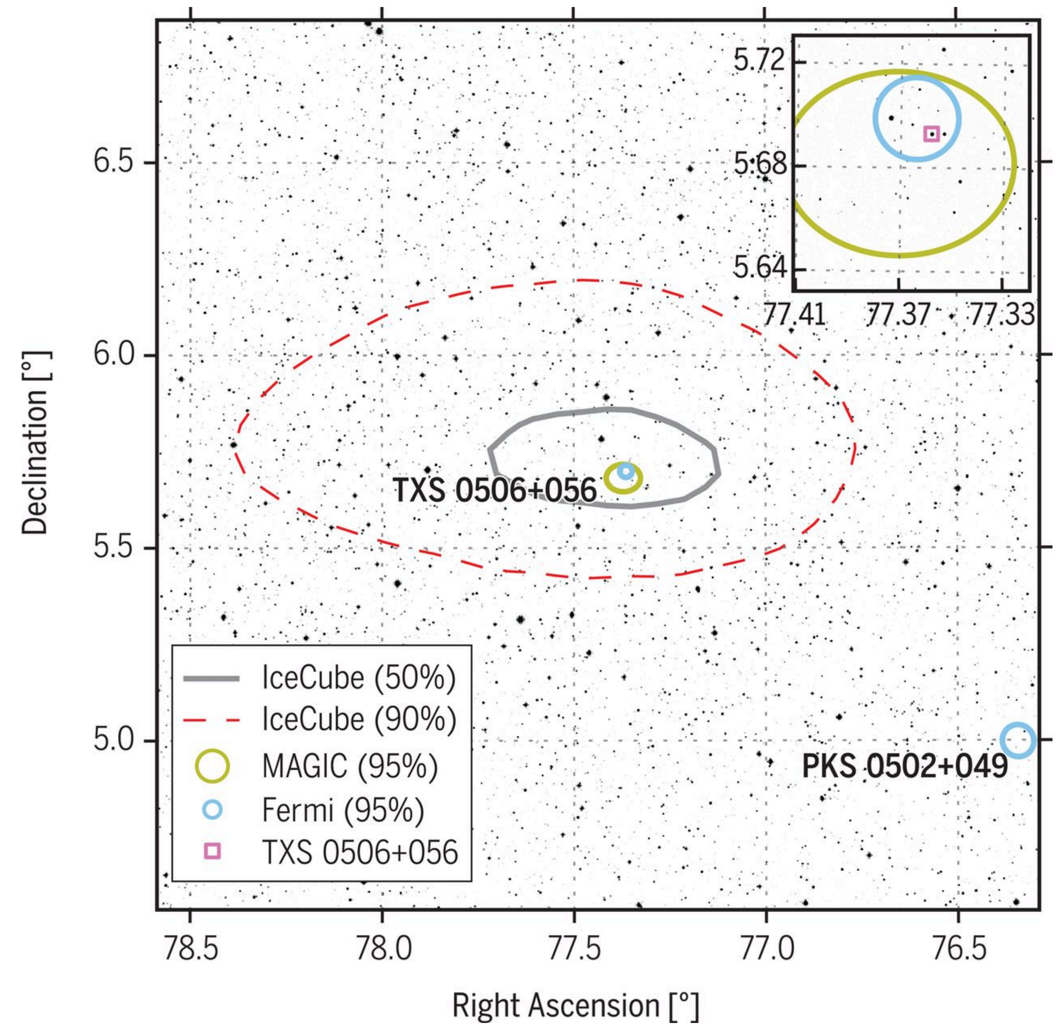
- Grid resources were used to search for the EM counterparts of GW events enabling the witnessing of **r-process nucleosynthesis**





MULTI-MESSENGER NEUTRINO ASTRONOMY

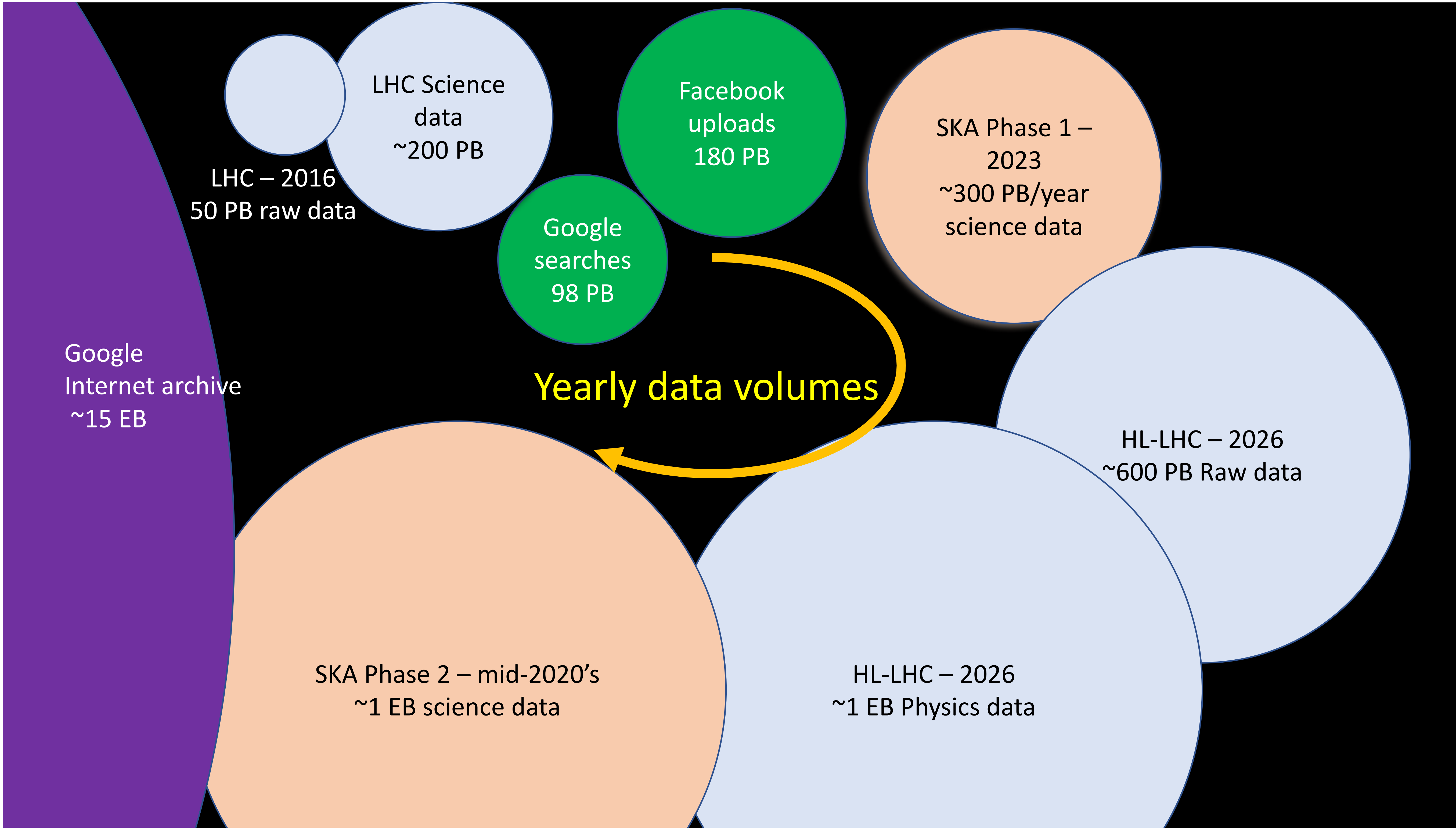
Globally coordinated observations of cosmic rays, neutrinos, gravitational waves, and electromagnetic radiation across a broad range of wavelength of the em-spectrum opens up new understanding of the Universe



- **The IceCube Collaboration, *Fermi*-LAT, MAGIC, *AGILE*, ASAS-SN, HAWC, H.E.S.S., *INTEGRAL*, Kanata, Kiso, Kapteyn, Liverpool Telescope, Subaru, *Swift/NuSTAR*, VERITAS, VLA/17B-403 teams**

The energies of the γ-rays and the neutrino indicate that blazar jets may accelerate cosmic rays to at least several PeV. The observed association of a high-energy neutrino with a blazar during a period of enhanced γ-ray emission suggests that blazars may indeed be one of the long-sought sources of very-high-energy cosmic rays, and hence responsible for a sizable fraction of the cosmic neutrino flux observed by IceCube.

International Data Needs



Conclusions

- The data and compute challenges of the next decade are large, even daunting.
- In order to satisfy the scientific needs of our community, we will need to build unprecedented scientific facilities and capabilities
- The scientific harvest that is arriving with this new era of big data science, is extremely compelling.

Special thanks to Ian Bird, Ken Herner & Marcelle Soares-Santos, and others who contributed to the slide content

Quantum Computing for HEP?

- What is all of this about?
- Why might it eventually be useful?
- Why should HEP be involved.
- How is Fermilab planning on participating.

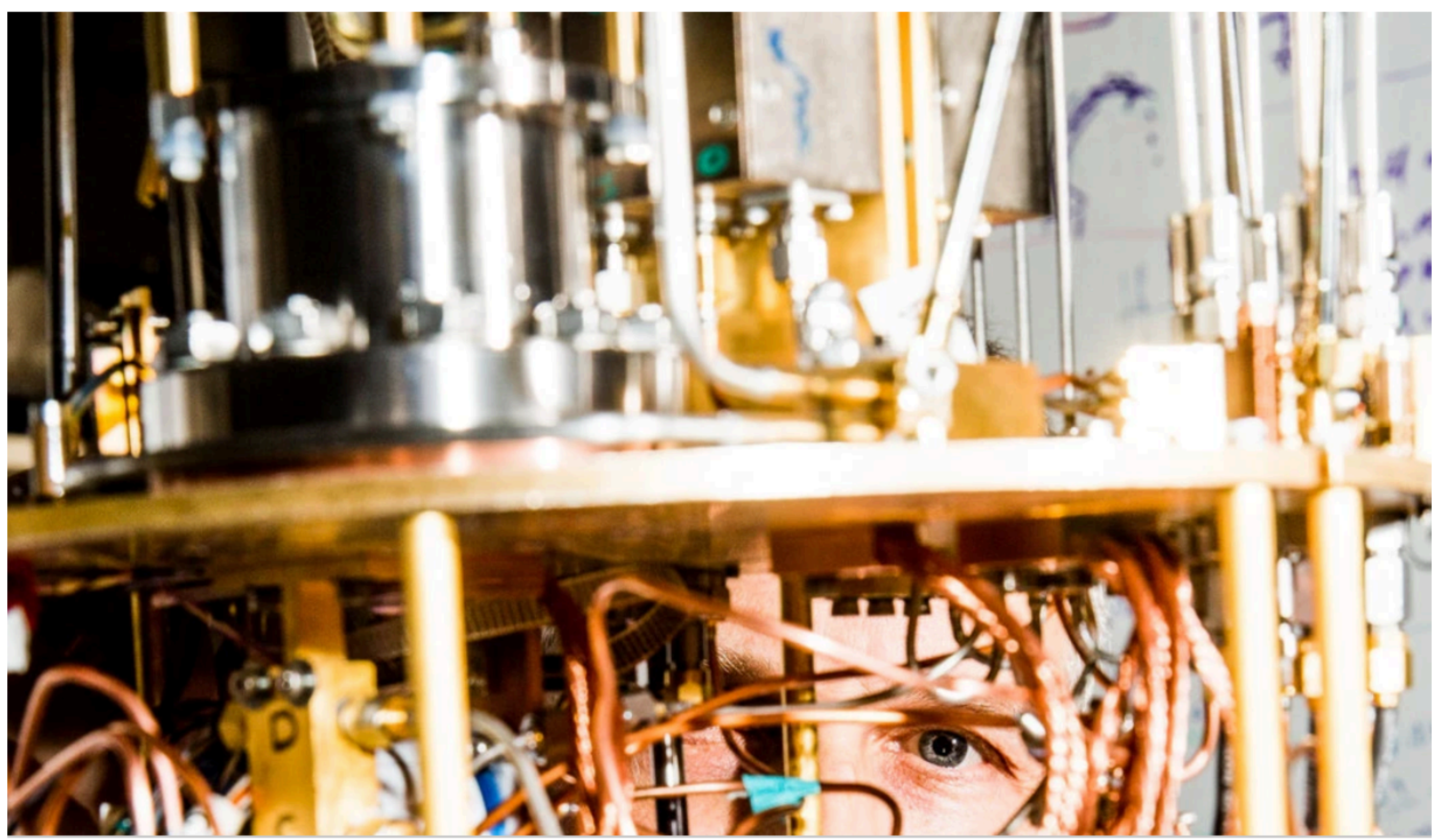
https://www.smbc-comics.com/comic/the-talk-3

Quantum Computing Excitement

The New York Times

Yale Professors Race Google and IBM to the First Quantum Computer

Nov. 13, 2017



More Quantum Computing Excitement

October 16, 2017

THE WALL STREET JOURNAL.

Europe is not Immune

January 30, 2018

ZEIT ONLINE

Suche

Politik Gesellschaft Wirtschaft Kultur Wissen Digital Campus Arbeit Entdecken Sport ZEITmagazin mehr #D18

AUS DER SERIE
Die Zumutung

Technologie

Wie funktioniert ein Quantencomputer?

Zwanzig Jahre lang waren Quantencomputer eine fixe Idee von Grundlagenforschern. Nun investieren Google, IBM und Microsoft, die EU und China, Geheimdienste und sogar Volkswagen in die mysteriöse Technologie. Warum?

Von **Max Rauner**

"For twenty years, quantum computers were a fixture of basic research. Now Google, IBM and Microsoft, the EU and China, intelligence agencies and even Volkswagen invest in the mysterious technology. Why?"

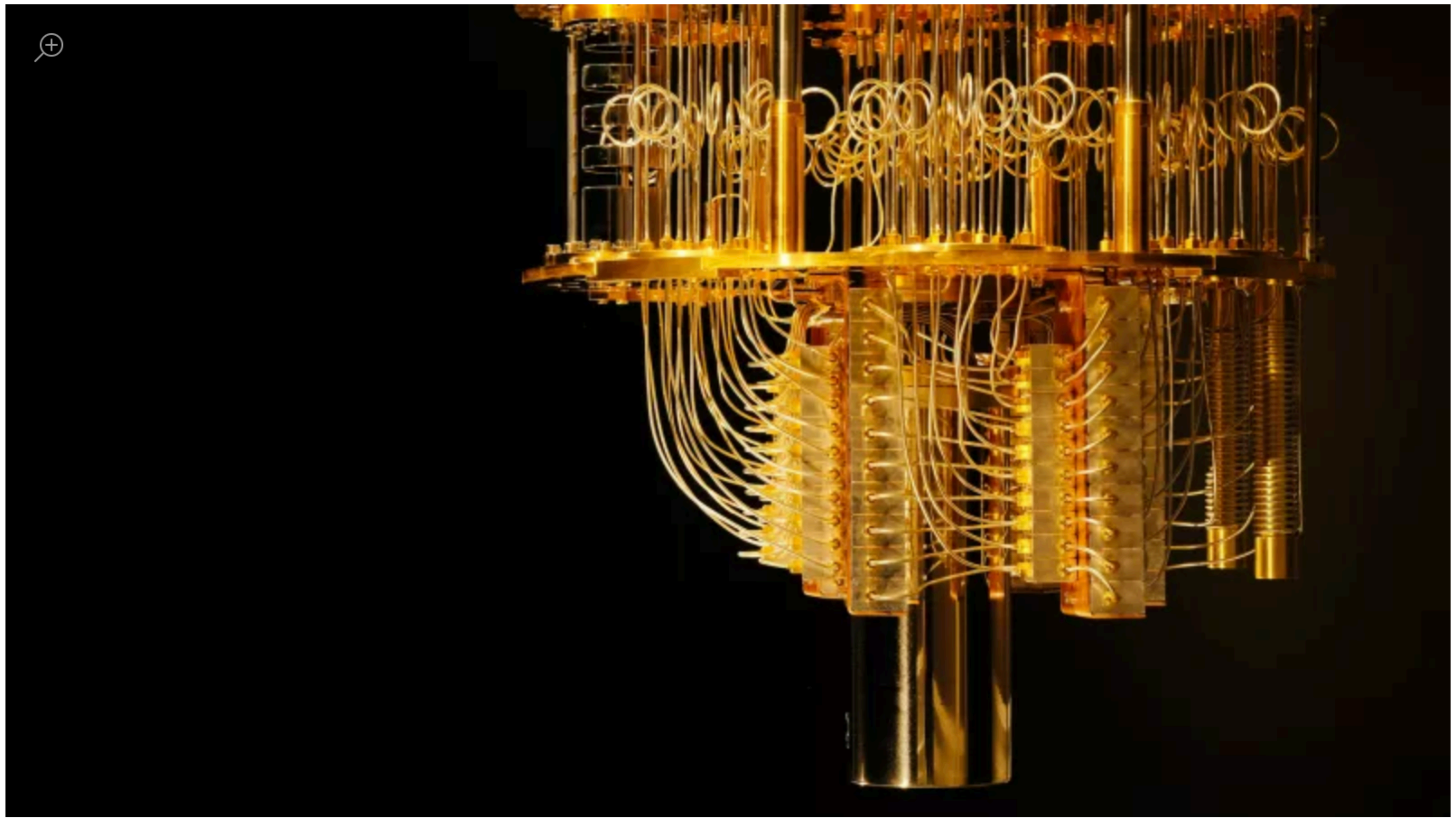
Quantum Computing Excitement Has Reached the U.S. Congress

Two Quantum Computing Bills Are Coming to Congress

Ryan F. Mandelbaum
6/08/18 5:26pm • Filed to: QUANTUM COMPUTING

27.7K 21 4

June 8, 2018



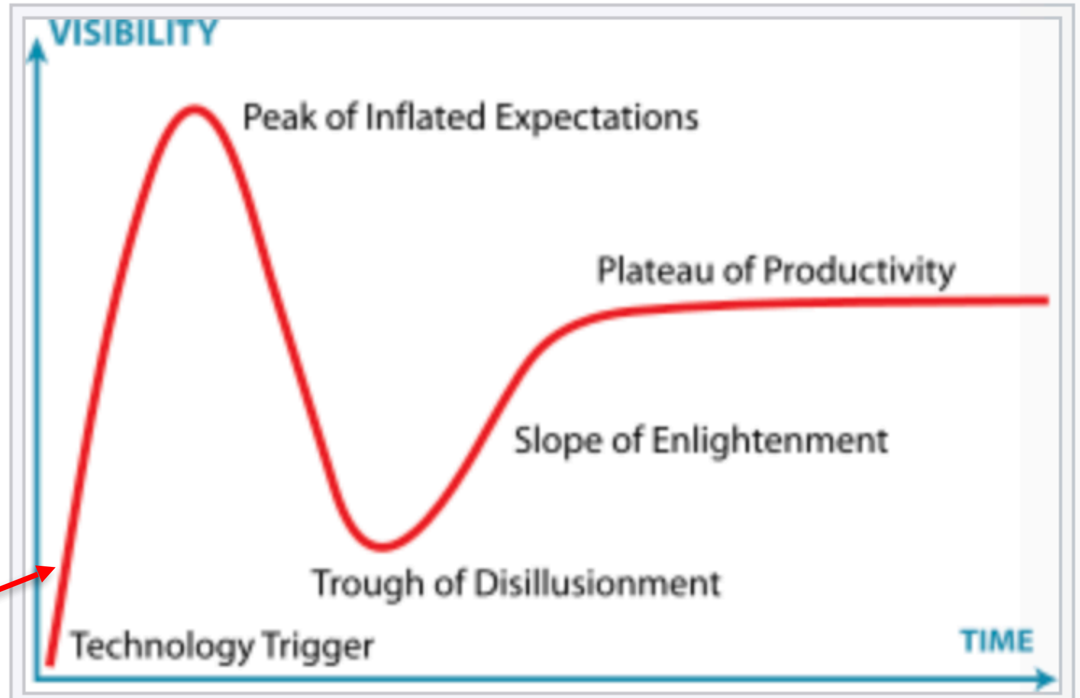
A dilution refrigerator from an IBM quantum computer.
Photo: IBM Research (Flickr)

...and Congress Appropriates money

It's Just Beginning

- Where are we on the Hype Curve?
- According to Wikipedia:

Technology Trigger: A potential technology breakthrough kicks things off. Early proof-of-concept stories and media interest trigger significant publicity. Often no usable products exist and *commercial viability is unproven.*



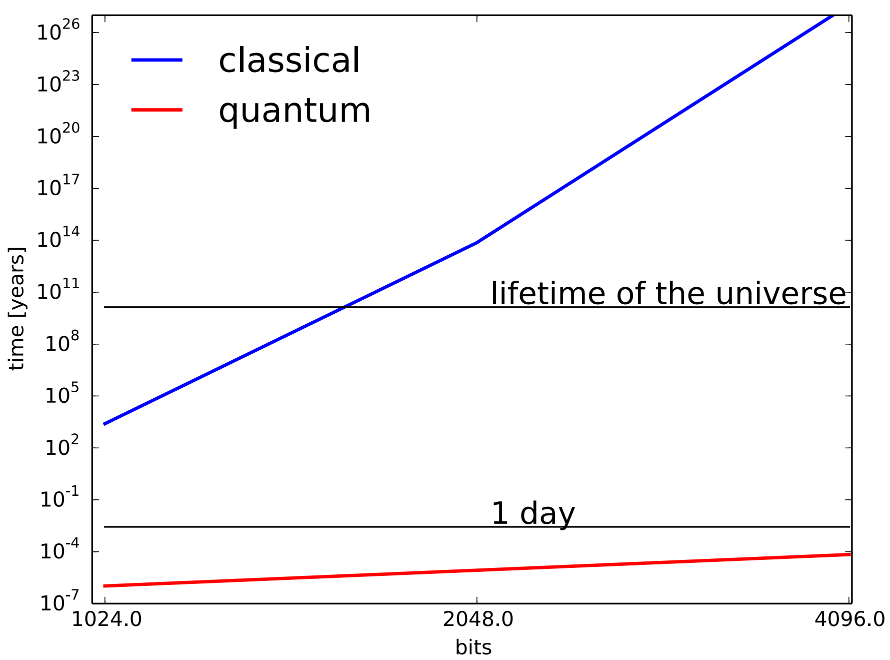
Hype cycle

Where the Excitement Started

- Peter Shor: A general-purpose quantum computer could be used to efficiently factor large numbers
- Shor's Algorithm (1994)
- Resource estimates from LA-UR-97-4986 "Cryptography, Quantum Computation and Trapped Ions," Richard J. Hughes (1997)

num size	1024 bits	2048 bits	4096 bits
qubits	5124	10244	20484
gates	3×10^{10}	2×10^{11}	2×10^{12}

Analog of clock cycles in classical computing



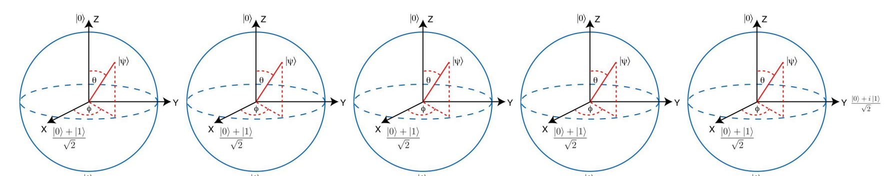
n.b. This is an old estimate; improvements have been made in the meantime.

Quantum Information

n classical 2-state systems: n bits of information
$b_1 \ldots b_n$

b_1 b_2 b_3 ... b_n

n quantum 2-state systems: 2^n “bits” of information
$a_1 \ldots a_k$ where $k = 2^n$



$$|\psi\rangle = a_1|0\ldots00\rangle + a_2|0\ldots01\rangle + a_3|0\ldots10\rangle + \ldots + a_k|1\ldots11\rangle$$

https://indico.cern.ch/event/587955/contributions/2935787/attachments/1683174/2707552/CHEP2018.QPR.HEP.pdf

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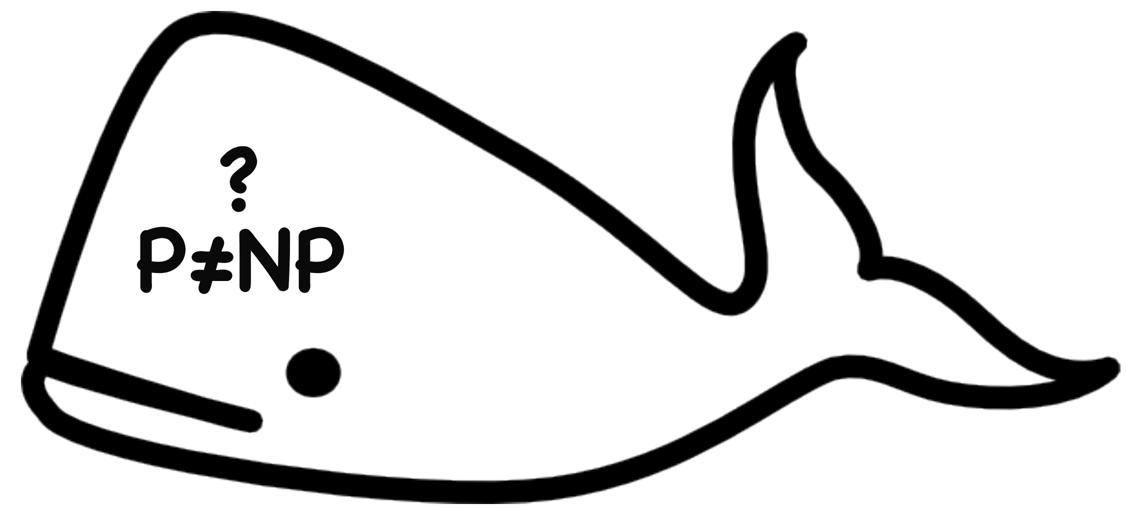
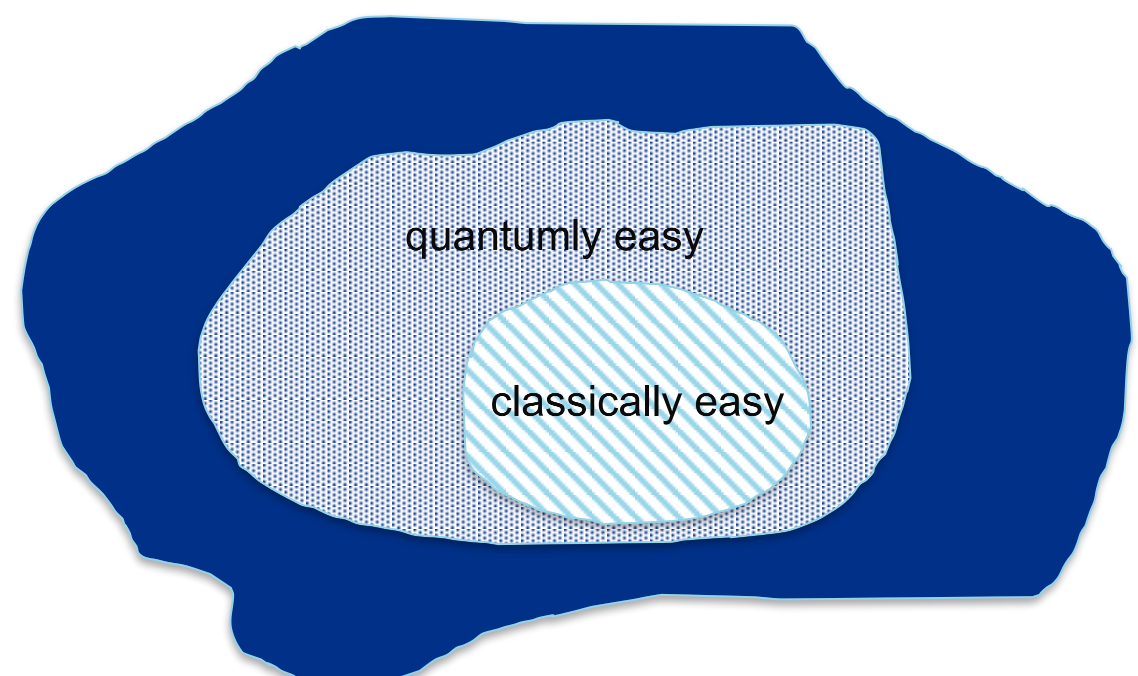
Theoretical Computer Science

- **Classical Computing**
  - "Easy" problems can be solved in "polynomial time" (**P**)
  - "Hard" problems require "nondeterministic polynomial time" (**NP**)
    - Proving P ≠ NP is a great unsolved problem in computer science



- **Quantum Computing**
  - Some problems are easy in quantum computing, but hard in classical computing -> quantum complexity classification
  - Some problems appear to be hard either way



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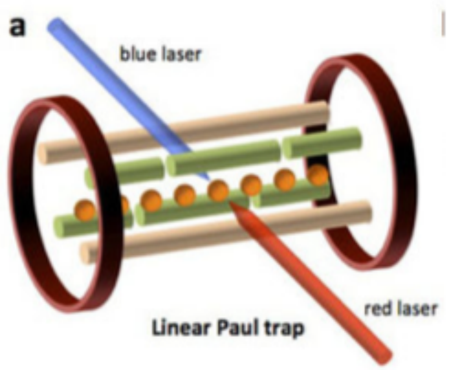
Quantum Algorithms

- Shor's Algorithm: factorization -- Speedup: Superpolynomial
- Grover's Algorithm: search -- Speedup: Polynomial
- If there exists a positive constant α such that the runtime C(n) of the best known classical algorithm and the runtime Q(n) of the quantum algorithm satisfy $C=2^{\Omega(Q^{\alpha}))}$ then the speedup is superpolynomial, otherwise it's polynomial.
- Many more available at the Quantum Algorithm Zoo https://math.nist.gov/quantum/zoo/
  - **A catalog of 60 quantum Algorithms in 3 categories:**
    - **Algebraic and Number Theoretic Algorithms -> cryptography**
    - **Oracular Algorithms→ optimization and machine learning**
    - **Approximation and Simulation Algorithms -> quantum physics and chemistry**

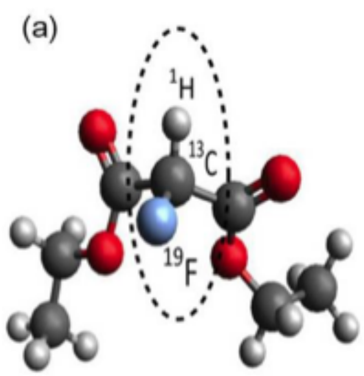
Current and Near-term Quantum Hardware

Ion trap



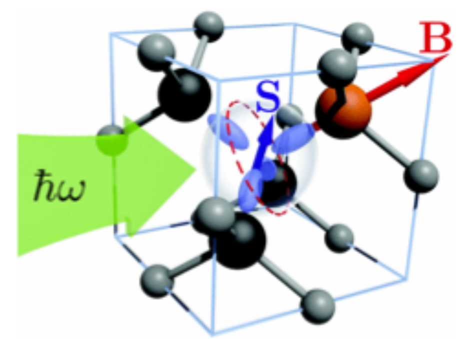
Scientific Reports 4, 3589 (2014)

NMR



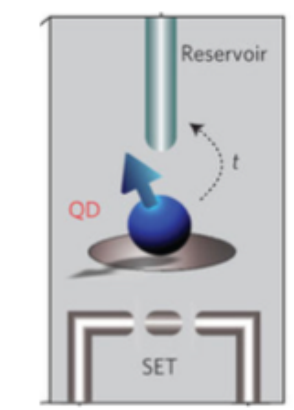
Sci. China Phys. Mech. Astron. 59:630302 (2016)

NV center



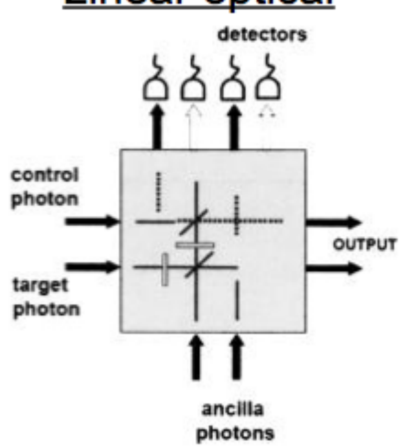
Phys. Rev. B 86, 125204 (2012)

Quantum dot



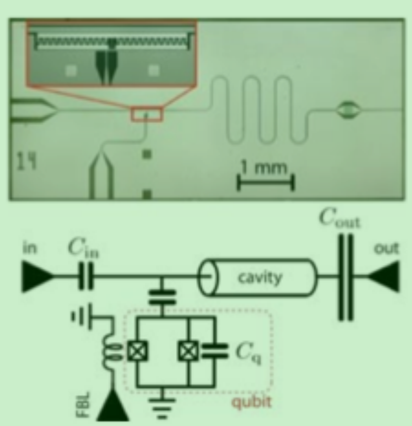
4 Nature Nanotechnology 9, 981–985 (2014)

Linear optical



J. Opt. Soc. Am. B, 24, 2, 209-213 (2007)

Superconducting



Ann. Phys. (Berlin) 525, 6, 395–412 (2013)

… many more

- Thanks to Andy Li
  - Fermilab Scientific Computing Division's first quantum computing postdoc!

- Superconducting is the most prominent commercial HW and was presented at CHEP2016

Current Commercial Quantum Computing Efforts

- Many companies have announced that they have produced small quantum computers in the 5-72 qubit range
  - Google, IBM, Intel, Rigetti ←use superconducting Josephson Junction technology
  - IonQ ←use ion traps
  - Other companies…
  - Academic efforts…
  - D-Wave
    - Quantum Annealing machine
      - Subject of a much longer talk
- IBM's machine is available on their cloud

Counting Qubits is Only the Beginning

- The number of gates that can be applied before losing quantum coherence is the limiting factor for most applications
  - Current estimates run few thousand
  - Not all gates are the same
    - The real world is complicated
- IBM has a paper proposing a definition of "Quantum Volume"
  - Everyone else seems to dislike the particular definition
  - The machines with the largest number of qubits are unlikely to have the largest quantum volume

num bits	1024 bits	2048 bits	4096 bits
qubits	5124	10244	20484
gates	$3x10^{10}$	$2x10^{11}$	$2x10^{12}$

- "Logical qubits" incorporating error correction are the goal
  - Probably require ~1000 qubits per logical qubit
    - Minimum fidelity for constituent qubits is the current goalpost

Fermilab Quantum Efforts

- Fermilab has a mixture of on-going and proposed work in quantum computing in four areas:
    - Quantum Computing for Fermilab Science
    - HEP Technology for Quantum Computing
    - Quantum Technology for HEP Experiments
    - Quantum Networking

Quantum Computing for Fermilab Science

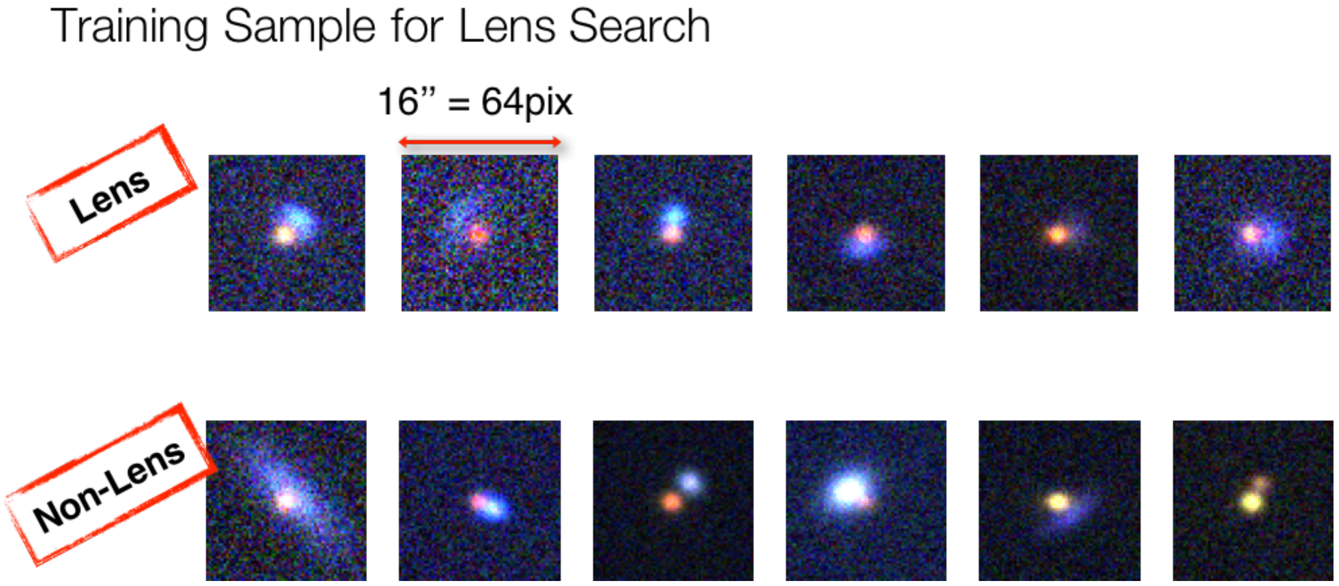
- Three promising areas for quantum applications in the HEP realm
  - Optimization
    - Area under active investigation in the quantum world
    - NP-hard problems
    - Quantum Approximate Optimization Algorithm (QAOA)
      - Farhi, Goldstone and Gutmann xarg
      - proposed for finding approximate solutions to combinatorial optimization problems.
  - Machine Learning
    - Computationally intensive
    - Also under active investigation in the quantum world
  - Quantum Simulation
    - Good reason to believe that quantum systems should be well-suited to quantum computation

Fermilab Quantum Applications

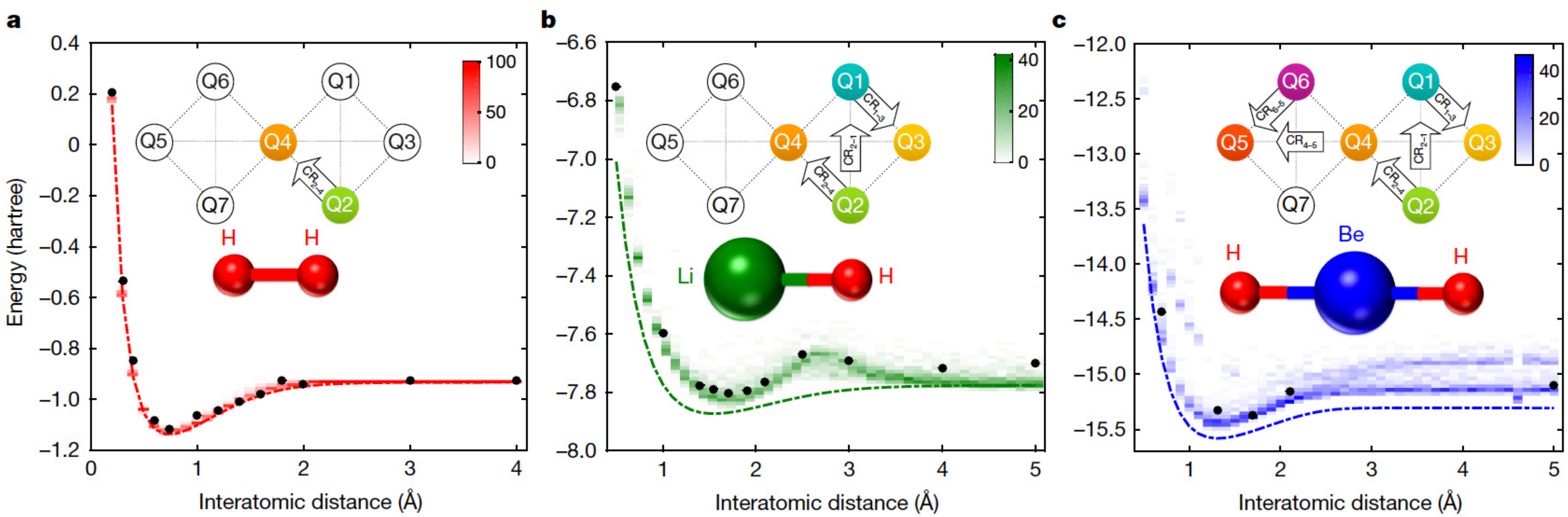
- Quantum Optimization and Machine Learning
  - Proposed work by Gabe Perdue, et al.
- Quantum Information Science for Applied Quantum Field Theory
  - Marcela Carena, et al., including JFA (Amundson)
  - Scientific Computing Division/Theory Department collaboration
    - FNAL: James Amundson, Walter Giele, Roni Harnik, Kiel Howe, Ciaran Hughes, Joshua Isaacson, Andreas Kronfeld, Alexandru Macridin, Stefan Prestel, James Simone, Panagiotis Spentzouris, Dan Carney (U. Maryland/FNAL)
    - Also includes University of Washington (David Kaplan and Martin Savage) and California Institute of Technology (John Preskill)
  - First effort from Fermilab: Digital quantum computation of fermion-boson interacting systems

Quantum Optimization and Machine Learning

- Partnering with Lockheed Martin to bring quantum computing to bear on a machine learning project in astrophysics.
- Several exploratory projects leveraging a D-wave annealer: star / galaxy classification, anomaly detection, and autoencoders (possibly for compression or simulation).
- Large focus on exploring data representations (flexible resolution requirements, and multiple sorts of data available for each object), matching data representation to hardware, and building workflows.
- Astrophysics chosen over some other domains (e.g. neutrino physics) because we have scientifically interesting data that is low enough in dimensionality to be compatible with modern quantum hardware.
- Gabe Perdue and Brian Nord



Successful Quantum Simulation



- Quantum Chemistry has the first big successes in quantum simulation.
- GitHub has a project for general simulations of interacting fermions.
- However, interesting HEP systems, e.g., QCD, also require boson-fermion interactions.

OpenFermion

https://github.com/quantumlib/OpenFermion

Digital Quantum Computation of Fermion-Boson Interacting Systems

- Previous encoding schemes for bosons on quantum computers had errors of $O(n_{occupation}/n_{qubits})$
- Alexandru Macridin, Panagiotis Spentzouris, James Amundson, Roni Harnik
  - Digital quantum computation of fermion-boson interacting systems
    - **arXiv:1805.09928**
    - Accurate and efficient simulation of fermion-boson systems; *simple enough for use on near-term hardware*
  - Electron-Phonon Systems on a Universal Quantum Computer
    - **arXiv:1802.07347**
    - First application was to polarons – electron dressed by phonons. Cross-disciplinary interest.

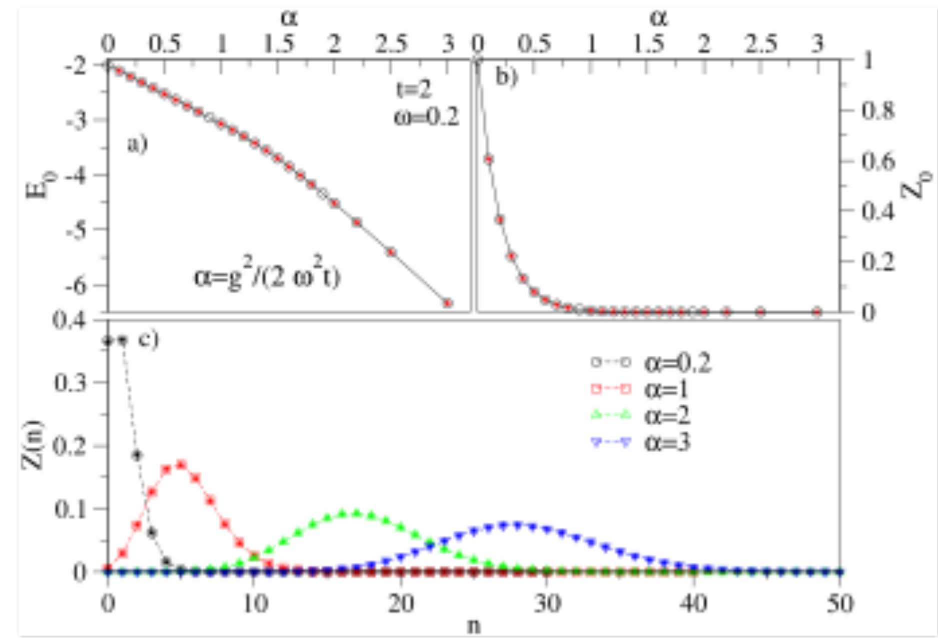


FIG. 4. $n_x = 6$ qubits per HO. The energy (a) and quasiparticle weight (b) for the 2-site Holstein polaron versus coupling strength. (c) The phonon number distribution for different couplings. The open (full) symbols are computed using exact diagonalization (QPE algorithm on a quantum simulator).

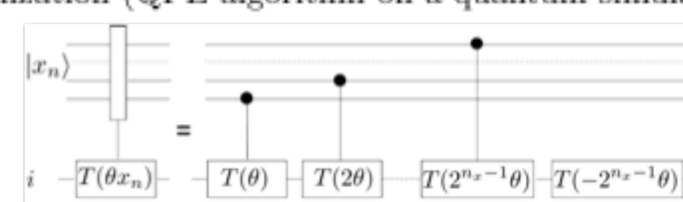
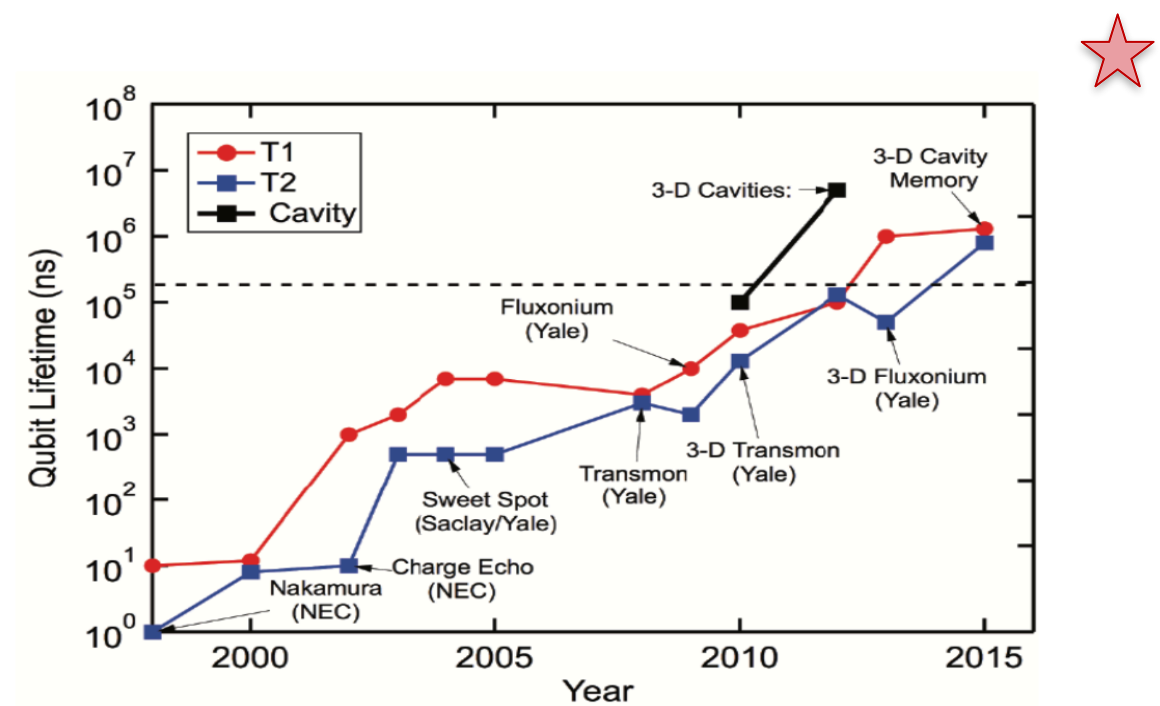


FIG. 3. Circuit for $\exp(-i\theta c_i^\dagger c_i \tilde{X}_n)|i\rangle \otimes |x_n\rangle$. The phase shift angle is $\theta(x_n - N_x/2) = \theta \sum_{r=0}^{n_x-1} x_n^r 2^r - \theta 2^{n_x-1}$, where $\{x_n^r\}_{r=\overline{0,n_x-1}}$ take binary values.

HEP Technology for Quantum Computing

- Ultra-High Q Superconducting Accelerator Cavities for Orders of Magnitude Improvement in Qubit Coherence
  – Alex Romanenko, et al.

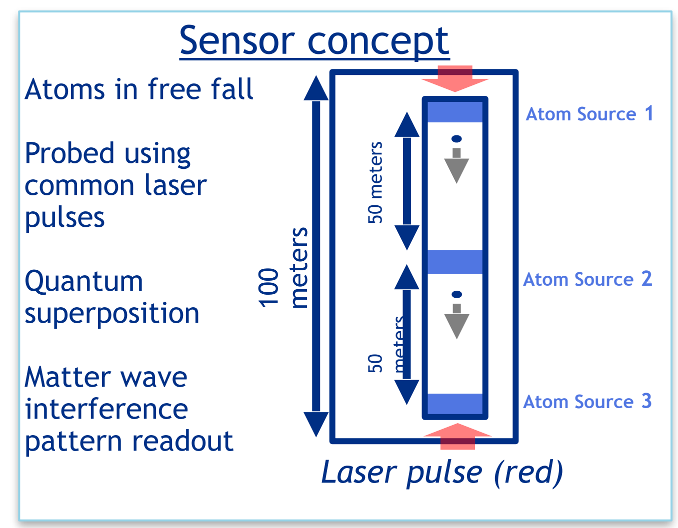
SRF resonators

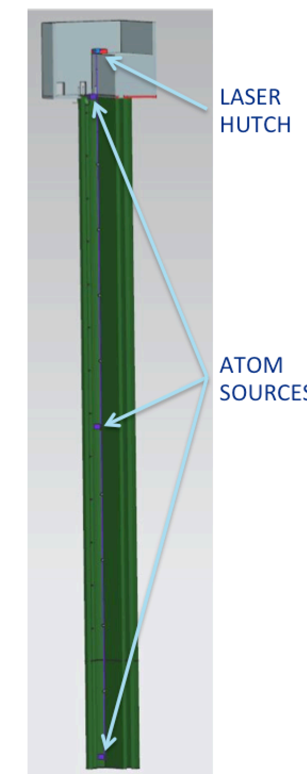


- Novel Cold Instrumentation Electronics for Quantum Information Systems
  – Davide Braga, et al.

Quantum Technology for HEP Experiments

- Matter-wave Atomic Gradiometer Interferometric Sensor
  (MAGIS-100)
  – Robert Plunkett, et al.
- Skipper-CCD: new single photon sensor for quantum imaging
  – Juan Estrada, et al.
- Quantum Metrology Techniques for Axion Dark Matter Detection
  – Aaron Chou, et al.





CAD model of detector in 100-meter MINOS shaft)

https://indico.cern.ch/event/686555/contributions/2977589/attachments/1681093/2700822/magis-100-ICHEP_2018.pdf

Conclusions

- Quantum computing holds the promise of remarkable new computational capabilities
  - The future is not here yet
    - … but we are getting there
- Fermilab has quantum computing efforts on many fronts
  - Quantum Applications
  - HEP technology for QC
  - QC technology for HEP experiments
  - and more…