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2024 QUANTUM INFORMATION SCIENCE APPLICATIONS ROADMAP

For the U.S. Department of Energy

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Sandia National Laboratories

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U.S. Department of ENERGY NNSA National Nuclear Security Administration

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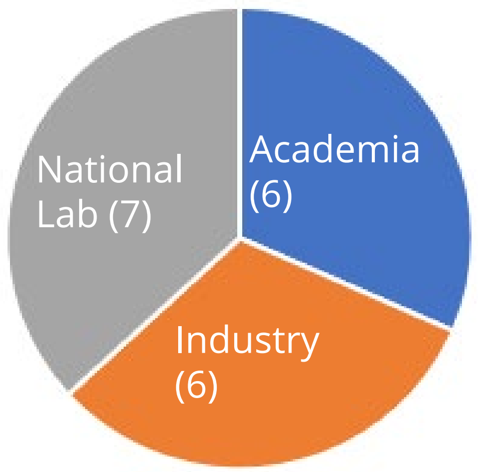
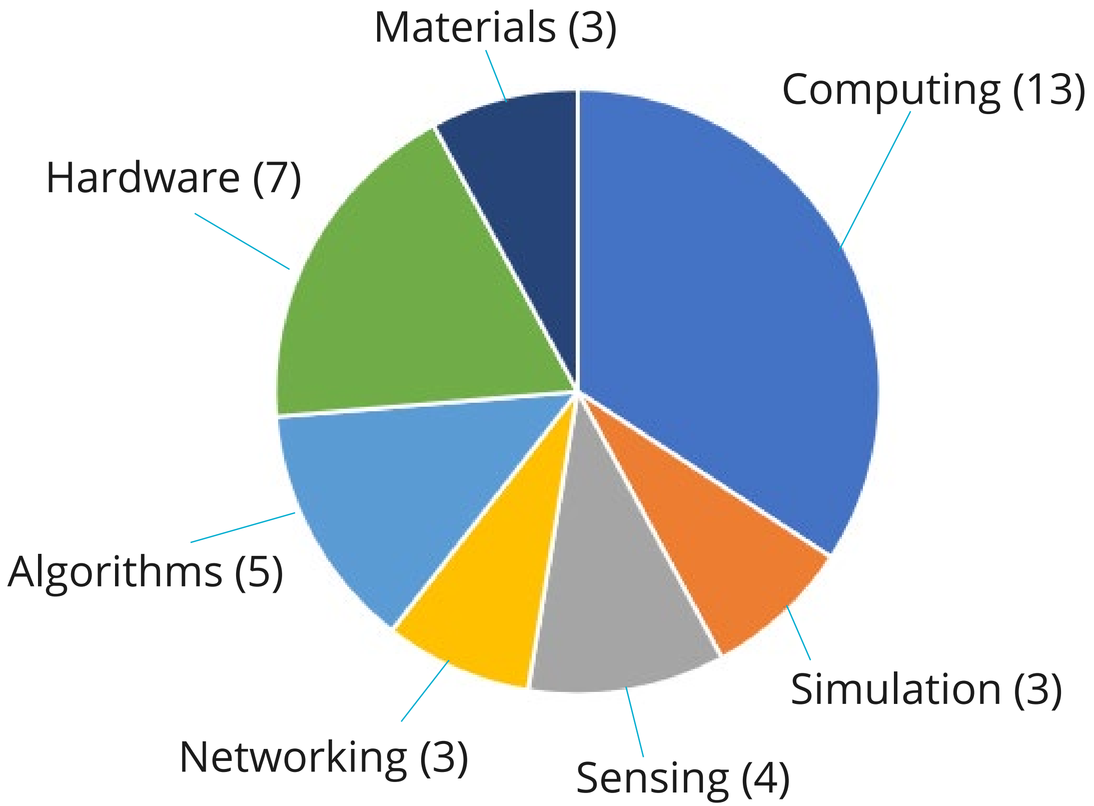
In March 2024, a diverse committee of 19 quantum experts was formed to write application roadmaps

Workplace



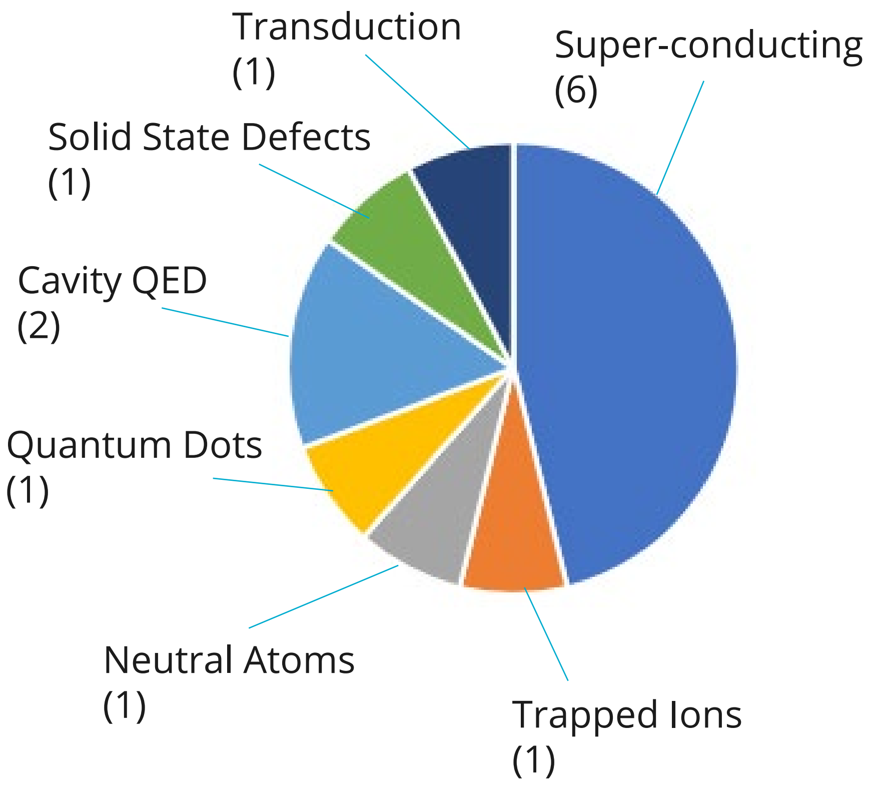
Quantum expertise

(self reported, could chose more than one, 4 did not report)



Quantum Platform

(self reported, could chose more than one, 4 did not report)



To further broaden our expertise, we interviewed 16 additional experts for their thoughts on promising quantum applications

Broke into separate subgroups for each application roadmap

4 months later, we submitted our report to the DOE

Another 4 months later, it was published on the DOE website

https://science.osti.gov/Initiatives/QIS/Community-Resources/SC-Sponsored-Reports

The results: We're still excited about quantum!

Quantum information science will allow us to better understand the world we live in

Quantum Computing is fundamentally different from classical computing for solving various classes of problems, but to be useful the computer must have many qubits and be fault-tolerant. We're particularly excited about prospects for using quantum computers for physics and materials simulations.

Quantum Sensing may be the best near term application of quantum information science, though there is still lots of research to do to effectively harness quantum properties of these sensors. We are looking forward to using quantum sensors to measure fundamental constants and as biomedical imaging devices

Quantum Networking's ability to provide entanglement between any two points is a service that isn't necessarily application specific, similar to the internet. However, they can also be used to enhance the abilities of our quantum computers and sensors.

We generated 3 application roadmaps, each with several concrete examples

Quantum Computing to Extend the Frontiers of Computation

- Simulating dynamics of the strong force
- More accurate chemical and material simulations
- Enhancing scientific computing applications
- Enabling more efficient management of infrastructure, logistics, and commerce

Quantum Sensing to Enable Unprecedented Precision and New Discoveries

- Precision measurements for new physics
- Sensitive and high-resolution probes to understand materials
- Robust and deployed sensors
- Biological, chemical, and biomedical sensing

Quantum Networks to Harness the Power of Linked Quantum Resources

- Linking sensors for increased resolution
- Linking sensors to quantum processors for finding rare or small signals
- Linking quantum computers to increase processing power

Quantum Computing to extend the frontiers of computation

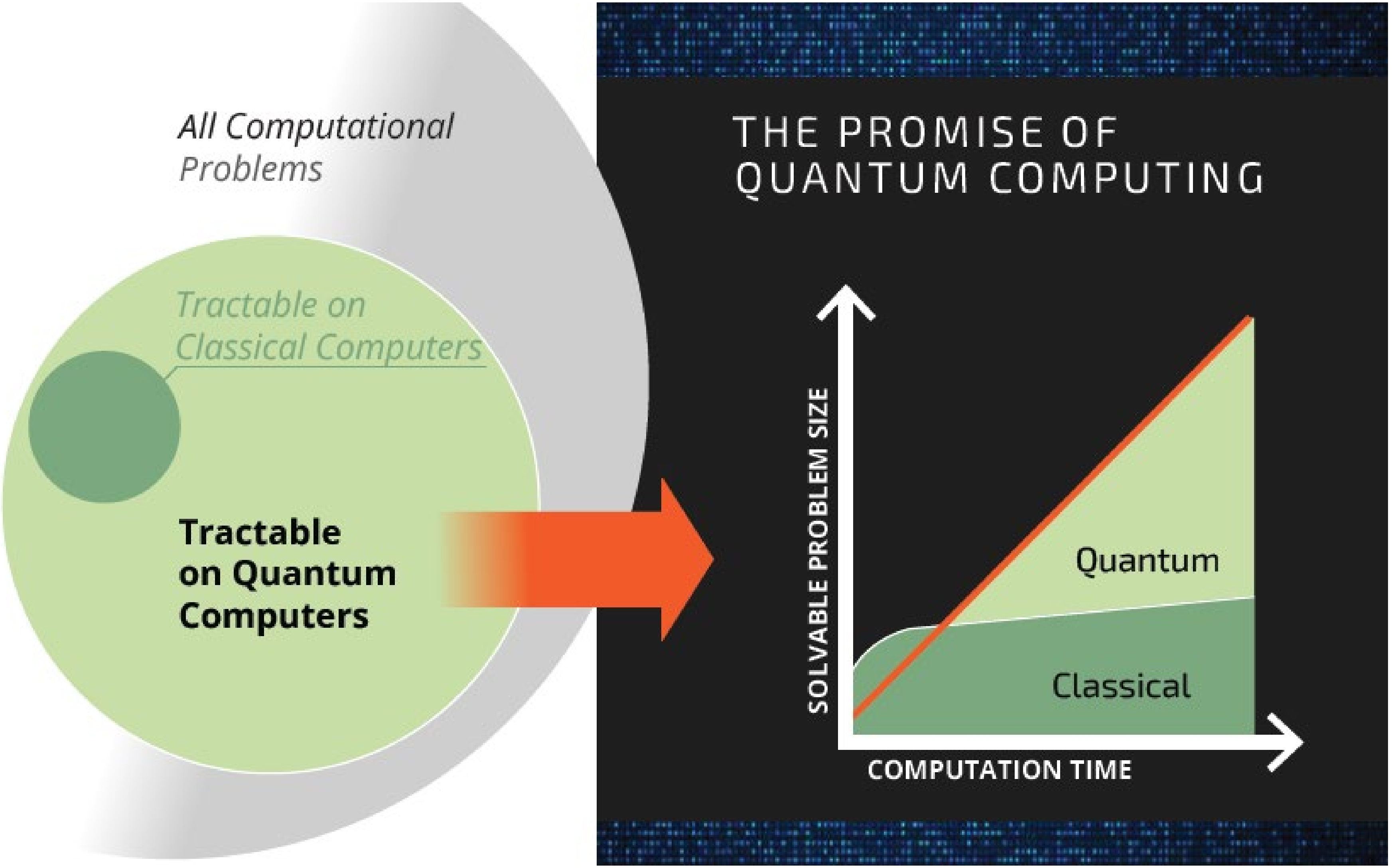


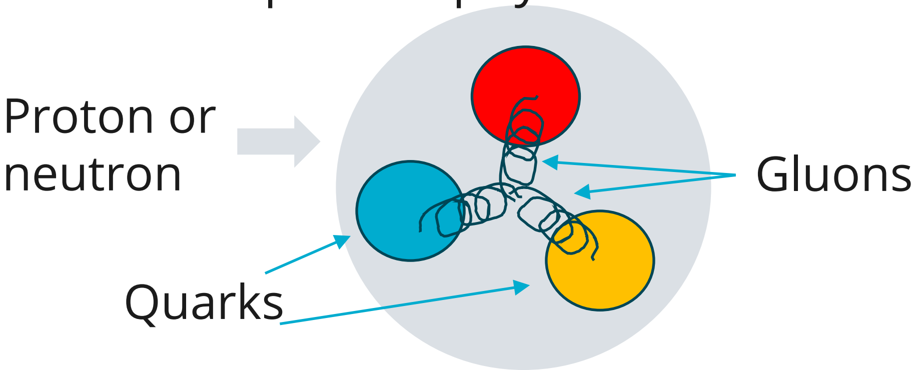
Fig. 1, the promise of quantum computing

Note: classical computing includes:

- Supercomputers
- Artificial intelligence
- GPU-based computing

Examples of things we'd like to compute, but can't now, #1

- **Simulating the dynamics of the strong force:**
  - Strong force binds quarks together to form protons and neutrons (carried by gluons) and described by quantum chromodynamics (QCD)
  - Coupling between particles (in this case quarks) grows with distance, making it impossible to calculate the properties of protons and neutrons with standard techniques, requiring approximations whose accuracy is unknown
  - Understanding these properties will allow us to:
    - Better understand the evolution of the universe shortly after the Big Bang
    - Better use our facilities (Large Hadron Collider, Electron Ion Collider, etc) to search for new fundamental interactions or particles
  - With a large, fault-tolerant quantum computer and continued advances in algorithms, we can numerically simulate QCD dynamics in general, which provides numerical access to a wide variety of problems in nuclear and particle physics.



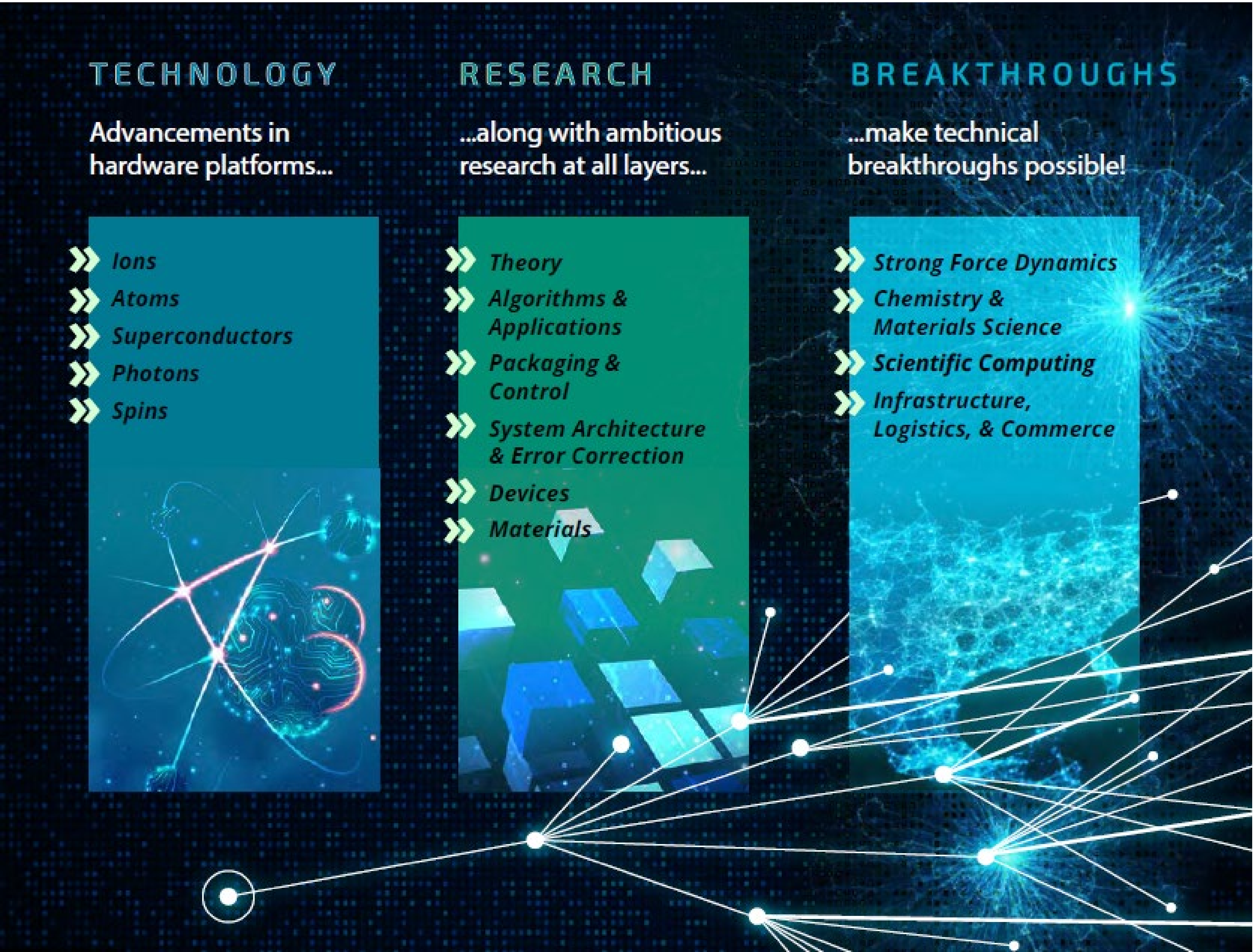
Examples of things we'd like to compute, but can't now, #2

- **More accurate chemical and materials simulations**
  - Problems ranging from
    - Catalysis
    - Energy storage
    - Drug discovery
    - Quantum materials
  - Simulating on a classical computer is possible, well-researched, and widely done, but requires sacrificing accuracy or efficiency
  - With a fault-tolerant quantum computer and advances in algorithms, we could do much larger simulations without sacrificing accuracy

Examples of things we'd like to compute, but can't now, #3 & #4

- **Enhancing scientific computing applications**
  - Many physics simulation applications (plasma physics, fluid dynamics, structural mechanics, and astrophysics) rely on solving ordinary and partial differential equations
  - Simulating on a classical computer is possible, well-researched, and widely done
  - A fault-tolerant quantum computer is predicted to solve these types of problems faster
- **Enabling more efficient management of infrastructure, logistics and commerce**
  - There is a large class of problems that requires optimization over many variables, for example
    - Management of supply chain uncertainties
    - Determining best shipping routes
    - Allocation of resources in power grids
    - Improving manufacturing processes
  - Optimization is well-studied classically, and many mature software packages exist. However, runtime grows exponentially with problem size
  - It is possible that quantum computers may help, but more research is necessary to establish speedup guarantees and tabulate resources estimates

Computing applications hinge on a fault-tolerant quantum computer



How to best build one?

How to best use one?

Fig 2.3, quantum computers can possibly be built with a variety of technologies. Research in all layers of each technology will speed up the arrival of useful quantum computations

Timeline and milestones for realizing a fault-tolerant quantum computer

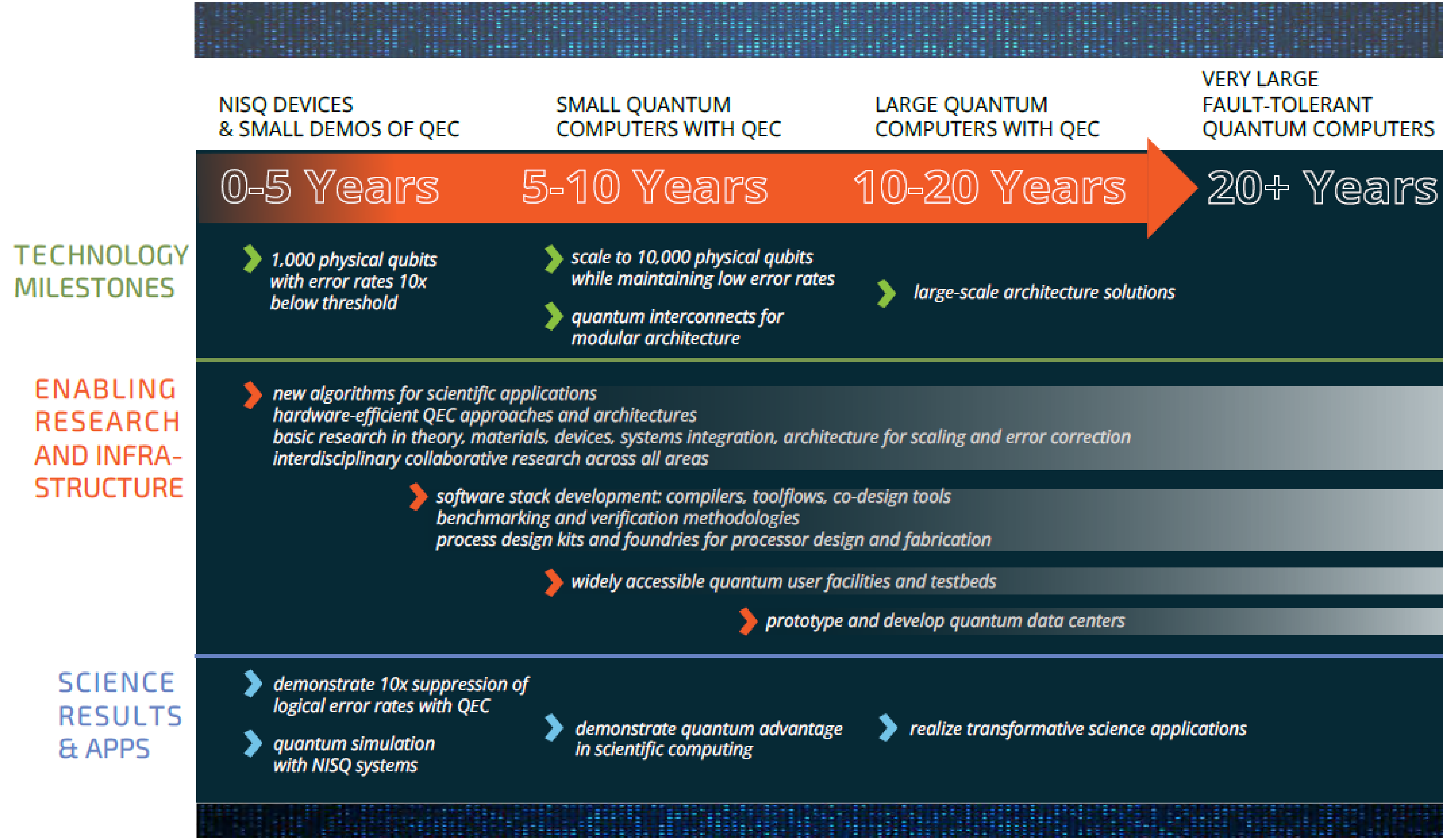


Fig. 2.2 shows necessary developments and predicted order and timeline

While the roadmap emphasizes number and fidelity of qubits, there are many ways that working with small numbers of noisy qubits can lead to breakthroughs that accelerate progress

On to Quantum Sensing!

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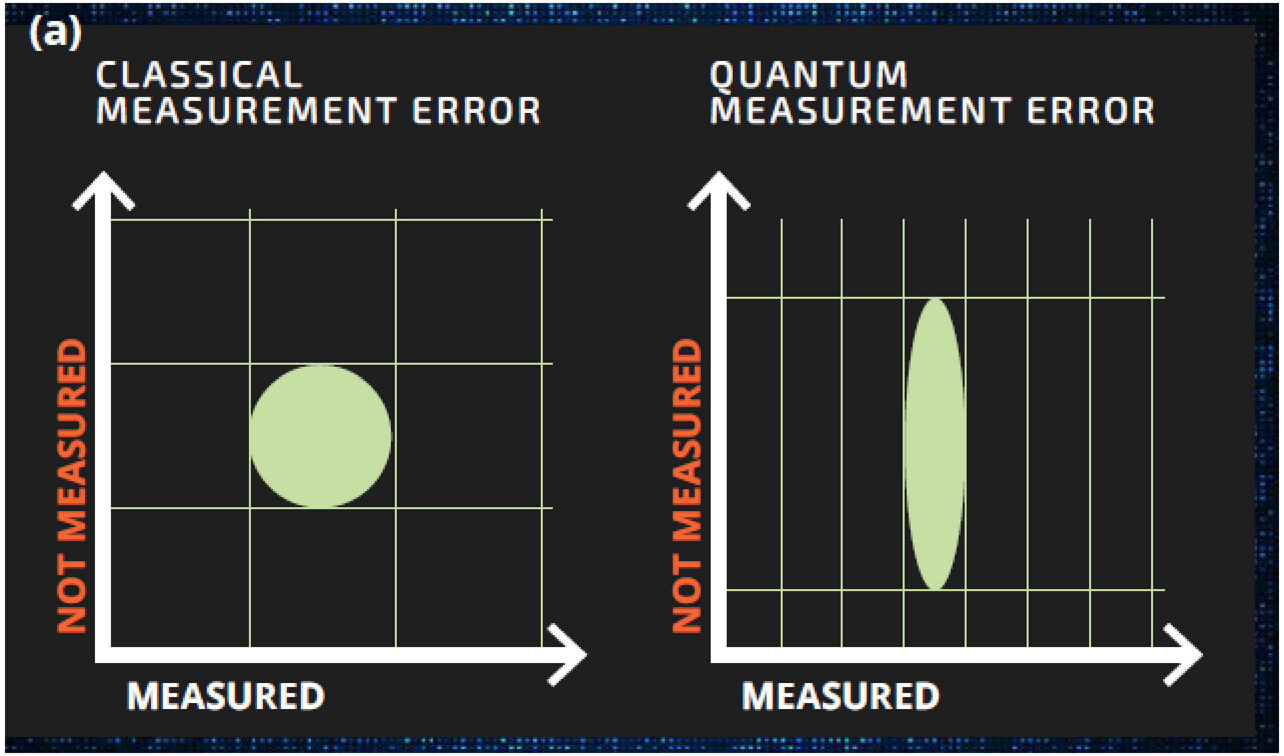
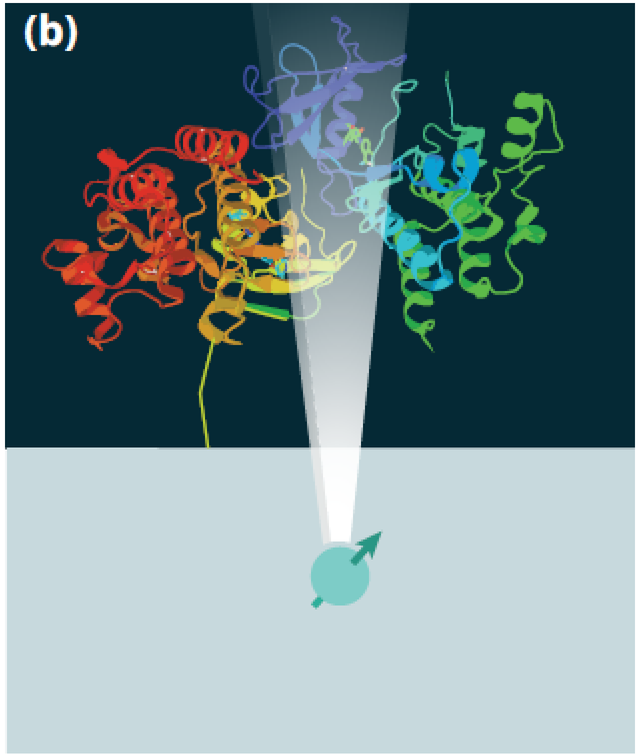
Quantum Sensing to Enable Unprecedented Precision and New Discoveries

Quantum sensors allow more accurate measurements by reallocating measurement uncertainty



Quantum sensors can increase spatial resolution because they can be small



#1, Precision measurement for new physics

- Historically, scientific discovery has been propelled by new measurement techniques
- New and better quantum sensors, given their small size and excellent accuracy, will allow us to probe limits of physics that we currently cannot access
  - Faster searches for dark matter over a large frequency range (crucial for understanding structure and formation of galaxies)
  - Testing the weak equivalence principle, which may expand the theory of general relativity
  - Increasingly precise measurements of the fine structure constant, which tests the Standard Model, potentially revealing new particles or phenomena

#2, Sensitive and high-resolution probes to understand materials

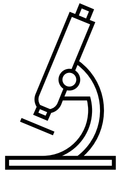
- Our ability to create, enhance, and produce technologies is fundamentally linked to our understanding of materials.
- Quantum sensors have the potential to be small and accurate enough to perform measurements of materials with higher resolution than can currently be achieved
  - Miniscule magnetic and electric fields
  - Local temperatures and pressures within a solid
- Large scale entanglement of sensors increases their sensitivity

#3, Robust and deployed quantum sensors

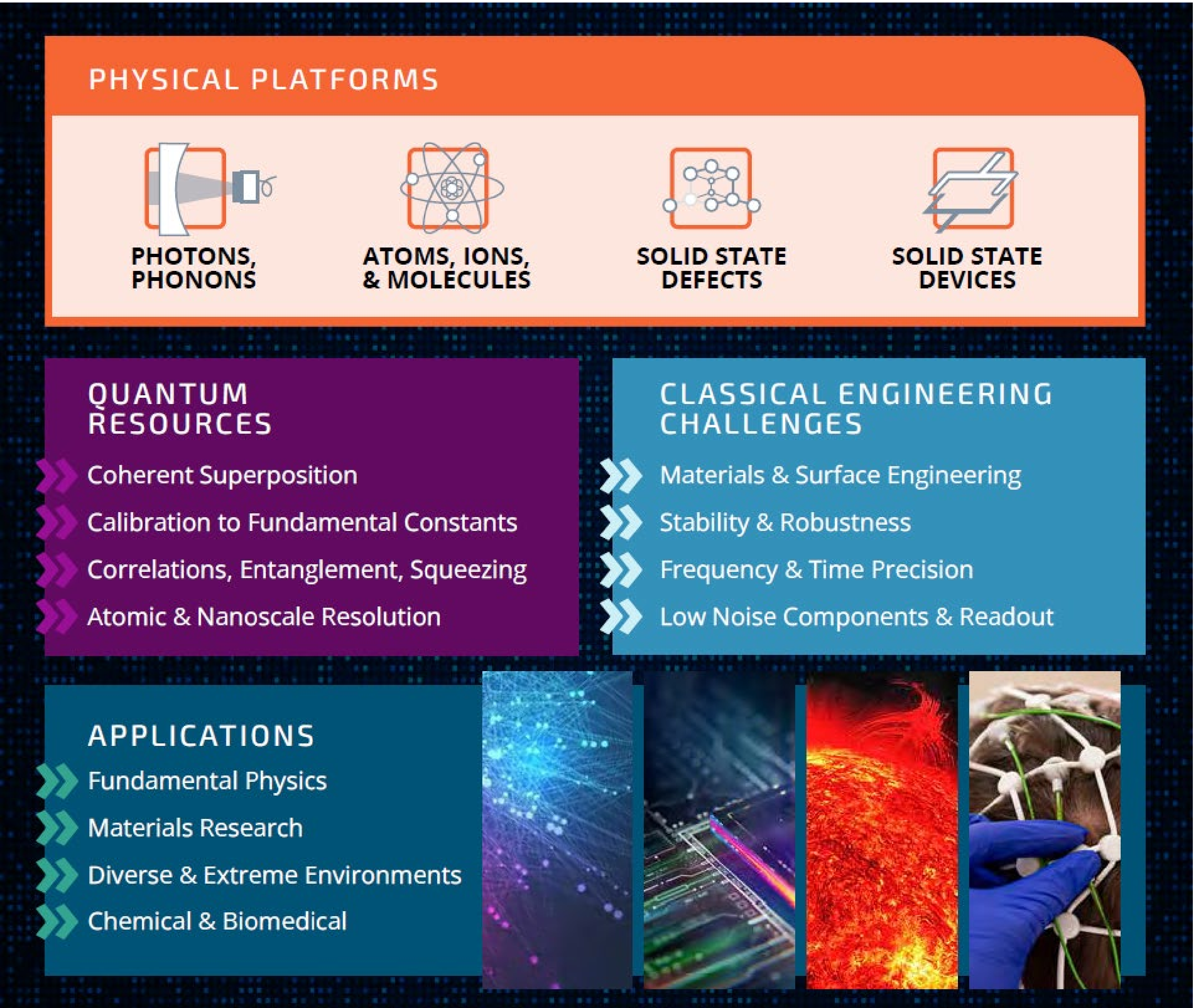
- Quantum sensors come pre-calibrated to physical constants and can be naturally robust
  - Single atoms are identical and calibrated to physical constants making them ideal for extreme environments, like space, plasmas, and ion beam sources
  - Small size makes them less likely to absorb harmful radiation, which may make them suitable as sensors inside fusion plants
  - Quantum gravity and gradient sensors can leverage the inherent stability of individual atoms to enable low-noise, low-drift measurements of the Earth’s shape and density variations.
- However, details of sensor design, material synthesis, device fabrication, and quantum sensing protocol research is needed to harness these advantages

#4, Biological, chemical, and biomedical sensing

- Our understanding of biology, disease, and human health depends on technology to detect very small signals and minute concentrations of molecules, sometimes from deep within a living organism such as a human body.
- Quantum sensors can be small and sensitive enough to perhaps:
  - Detect and localize small magnetic fields inside the body – crucial for higher resolution MRIs or monitoring heart and brain activity
  - Ultra-sensitive detection in microfluidic assays can aid drug discovery, screening for infectious diseases, early detection of chronic disease
  - Quantum light sources producing entangled or squeezed light can enhance microscopy resolution and would allow us to study light-sensitive organisms without damaging them



Combining quantum resources with improved classical engineering will allow us to realize these applications



Classical engineering is crucial to eliminate noise to the point that the quantum resources are effective at improving sensing ability

Quantum sensing is a near team realizable application from quantum information sciences

	1-5 Years	5-10 Years	10+ Years
PRECISION MEASUREMENT FOR NEW PHYSICS	*Quantum control techniques to extend searches for new physics with quantum sensors* *Develop new precision measurement platforms for next-gen searches for new physics*	*Next-gen quantum sensing searches for new physics, targeting parameter space with highest potential for new discoveries* *Entanglement enhanced searches for new physics with beyond-classical capabilities*	*Quantum sensors and sensor networks for axion and ultralight dark matter search over large parameter space.* *Use quantum sensors to explore interface between relativity and quantum mechanics.* *Integrate quantum sensors with particle accelerators and detectors to enhance their performance.*
SENSITIVE HIGH-RESOLUTION PROBES FOR MATERIALS ANALYSIS AND DESIGN	*Ultrahigh sensitivity magnetometers near the quantum noise limit,* *Discovery of new qubits for sensing* *Nanometer resolution magnetic imaging of currents, magnetic phases* *Noise sensing for dynamics*	*Integrated probes and instruments for high-throughput materials science* *Measure correlation functions in materials* *Exploit many-body physics, squeezing, entanglement for better sensitivity*	*User facilities with quantum sensors* *Commercial deployment of materials analysis tools* *Nanoscale sensors with quantum advantage*
ROBUST AND DEPLOYED SENSING RESULTS	*Improvements in size, weight & power, component integration, robustness to bring state-of-the-art quantum sensors into the field* *Materials development for radiation, thermal, and chemical resilience*	*Demonstrate prototypes in the field* *Demonstrate sensors in fusion environments*	*Mid-scale and large-scale manufacturing and deployment for scientific applications* *Technology translation to commercial partners*
BIOLOGICAL, CHEMICAL, AND BIOMEDICAL SENSING	*Sensor integration with relevant geometry for biological and chemical sensing and imaging, materials development and surface functionalization* *New protocols for measuring dynamics and small signals*	*Translation to bioenergy, capture of CO_2, biomedical and clinical applications* *Quantum sensing and imaging in physiologically relevant conditions* *Demonstrate high-throughput, high-sensitivity chemical sensing*	*Technology transfer to clinical settings, bioenergy and a bioeconomy* *Wide-scale deployment of biological and chemical assays*

Report outlines the steps and milestones necessary to realize each concrete example

On to Quantum Networks!

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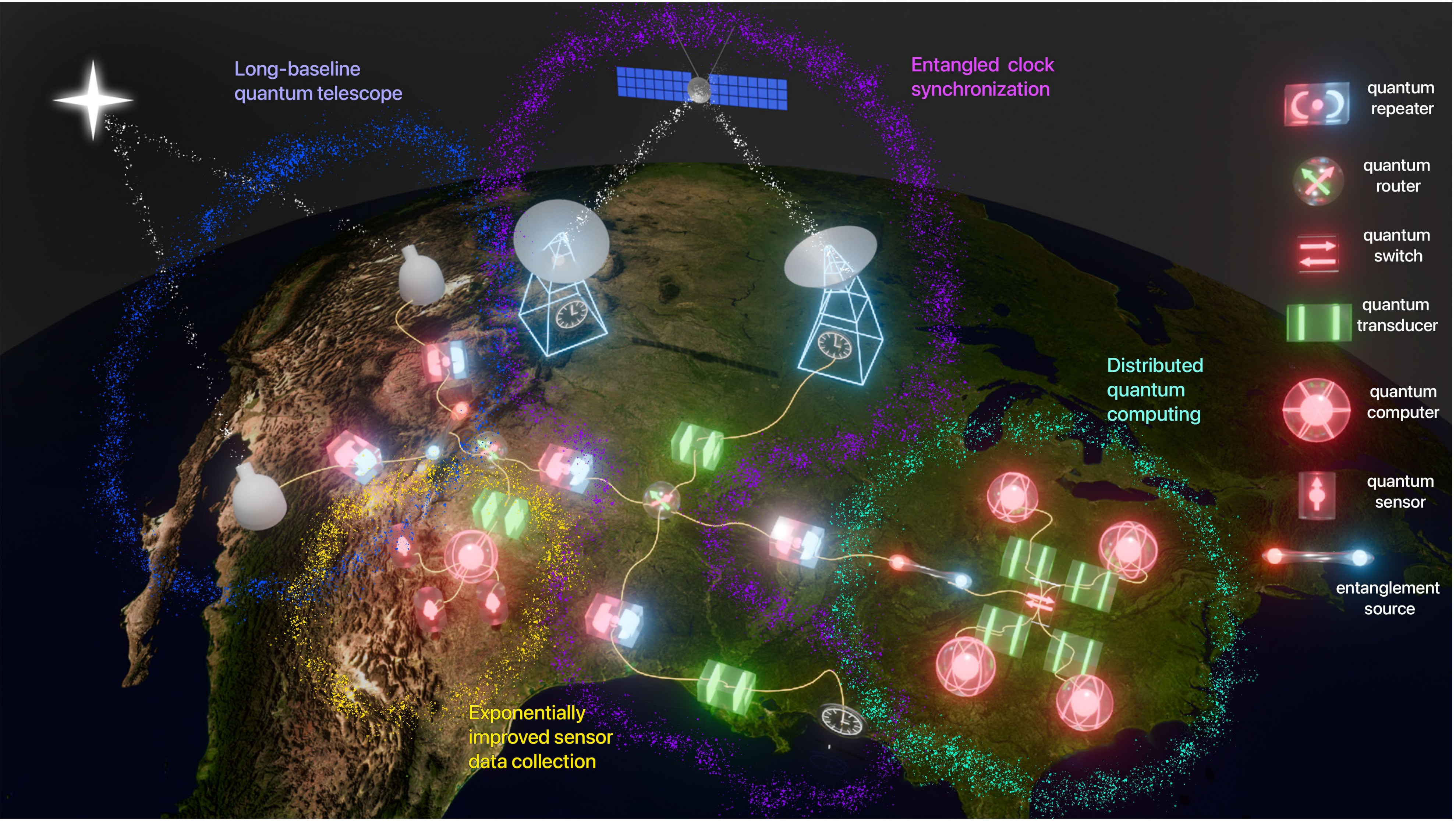
The vision of large-scale quantum networks requires the development of specific quantum networking tools

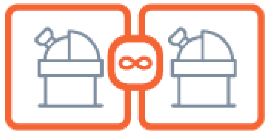


Network "core" needed for sending and routing photons

Network "edge" needed for utilizing the generated entanglement

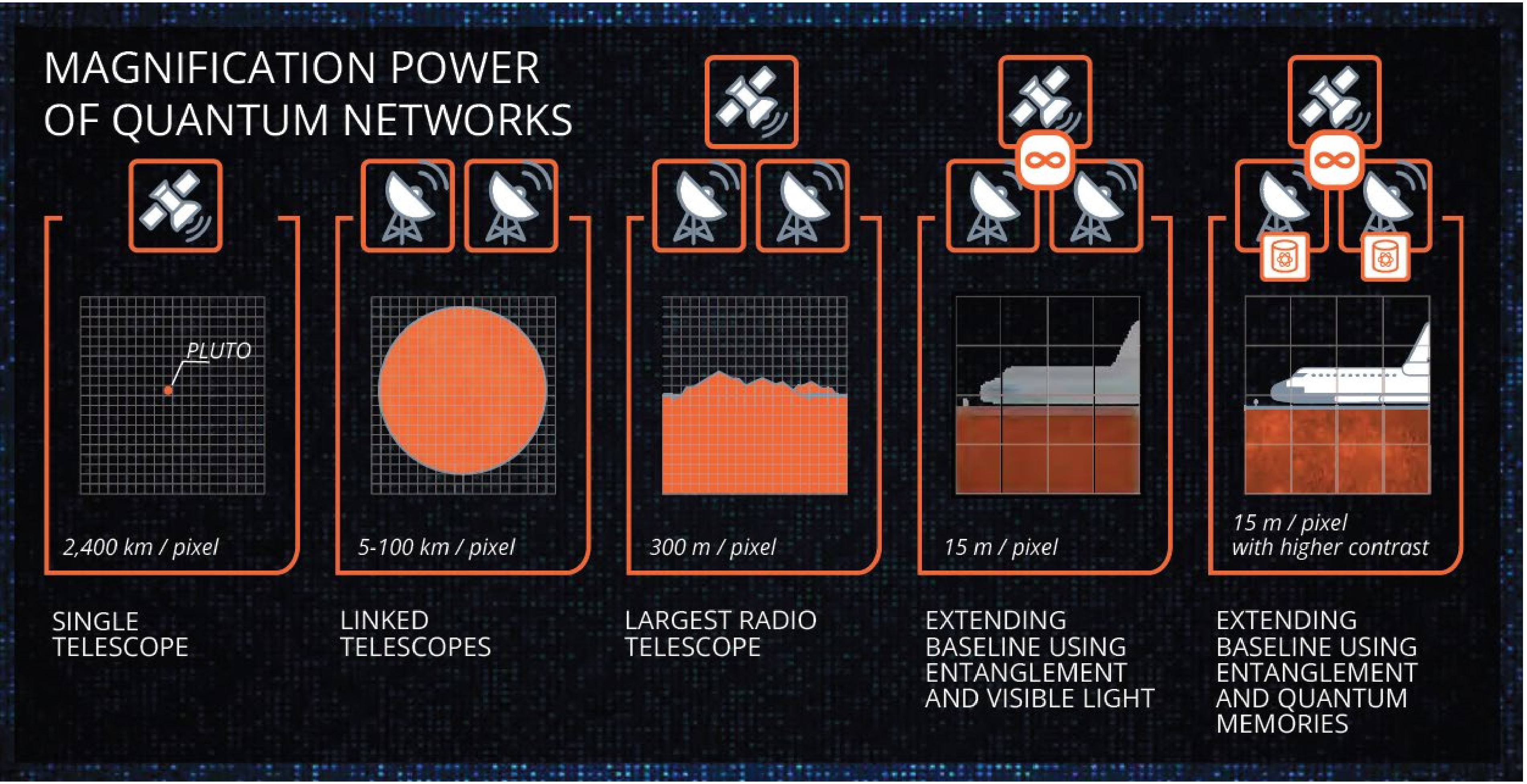
#1, Linking sensors for increased resolution

- **Increasing telescope resolution allows us to study more of the universe**
  - Viewing starspots to learn how a star's magnetic field affects temperature
  - Viewing topological features on exoplanets to learn about planetary formation
  - Viewing very faint stars, important for benchmarking galactic distances
  - Viewing environments around massive stars to understand mass loss and transfer in rotating systems



- **Linking atomic clocks allows for more precise timekeeping, useful for:**
  - Imposing tighter constraints on fundamental constants
  - Detecting dark matter
  - Detecting small shifts relative to Earth's gravitational field that may indicate underground volcanic processes

To drive home the advantages of networked quantum sensors, a back of the envelope calculation of resolution improvements of different types of telescopes

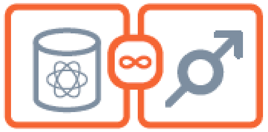


Telescope resolution is improved by spacing telescopes further from each other or using shorter wavelength light

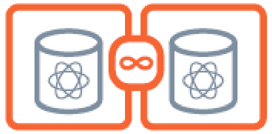
Linked via a quantum network, telescopes with shorter wavelengths could be spaced further apart

#2 & #3 Linking quantum processors to sensors or other quantum processors

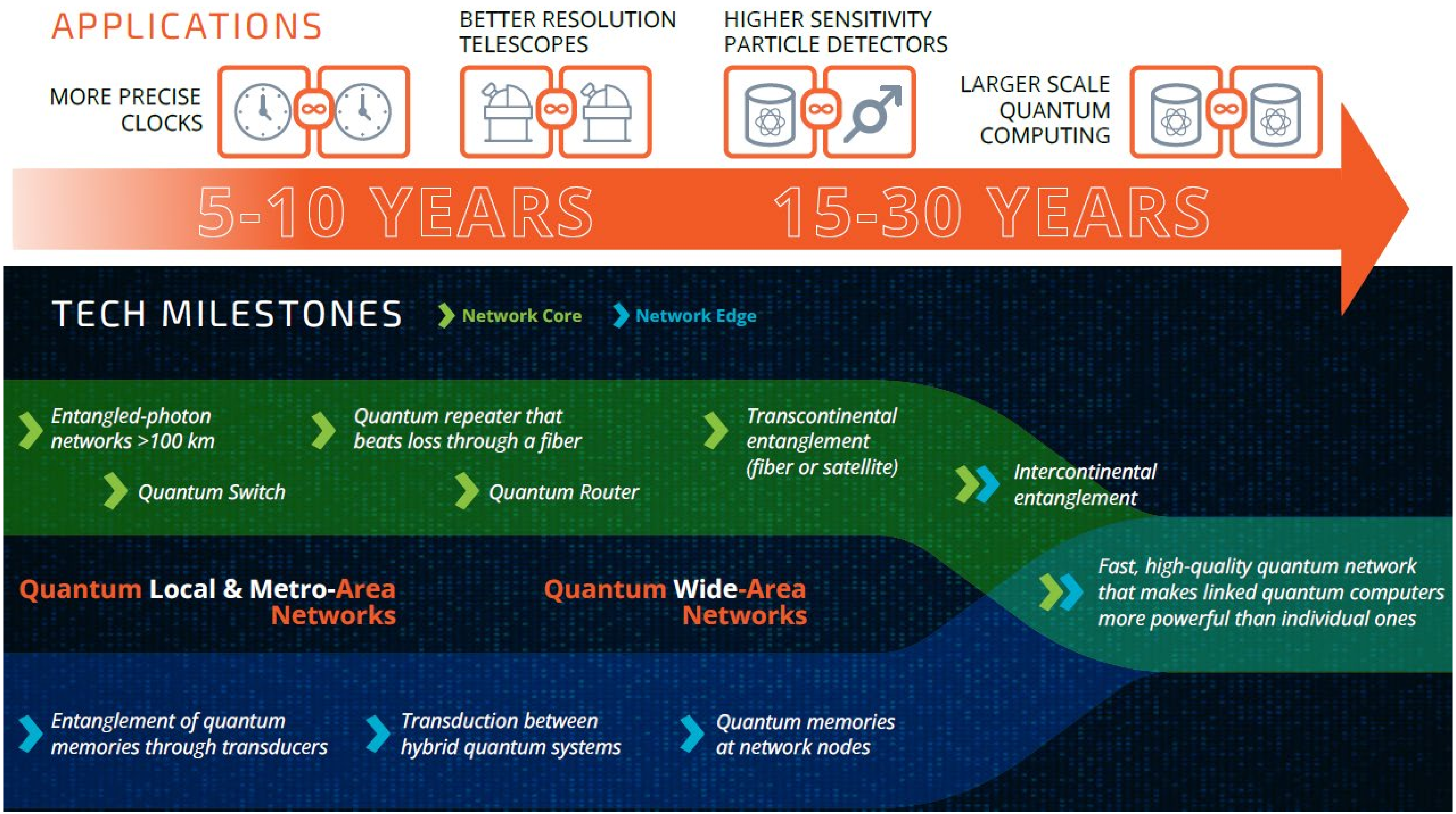
- **Linking sensors to quantum processors for finding rare or small signals**
  - Usually information from quantum sensors is measured immediately to put it in a classical state that can be easily stored
  - By using a quantum memory to manipulate the information from the sensor before converting to classical information, new enhancements are possible



    - Can learn the state of a physical system with exponentially fewer measurements
    - Can extract small signals from a noisy background, for example detecting rare or small signals in particle accelerator outputs
- **Linking quantum computers to increase processing power**
  - Similar to classical computers, quantum computers can be linked to increase their overall processing power – but via a quantum link that allows for state or gate teleportation
  - Quantum links between quantum computers also reduce communication overhead – the same information sent using $>10^{18}$ classical bits could be sent with only tens of qubits



Possible roadmap for realizing quantum networking applications



Quantum repeaters and transducers are critical developments necessary for quantum networks

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Quantum information science will allow us to better understand the world we live in

Quantum Computing requires fault tolerance, but there are many steps to fault tolerance using small noisy quantum systems

Quantum Sensing requires classical engineering to make the sensors useful, and investigation using new quantum materials as sensors

Quantum Networking requires repeaters and transducers to send fragile signals long distance and manipulate them at the nodes.