Quantum Technologies for Nuclear Engineering

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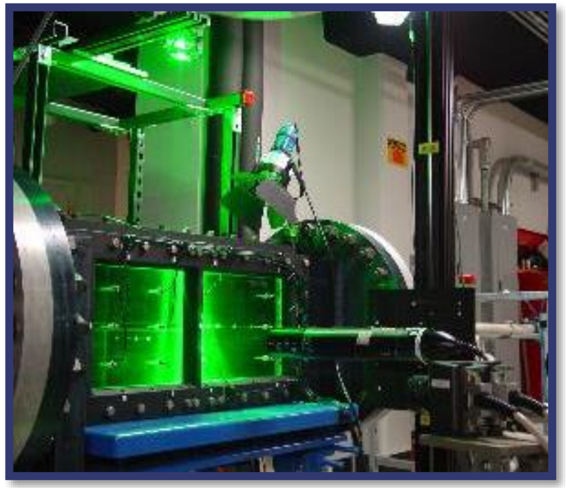
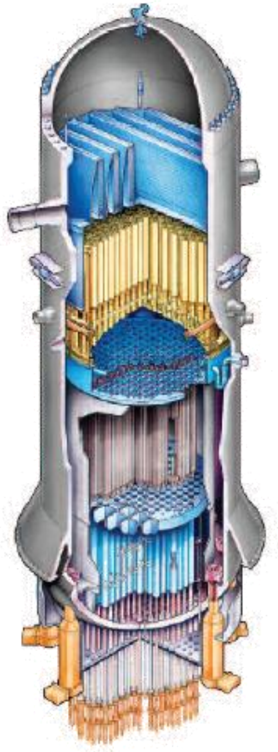
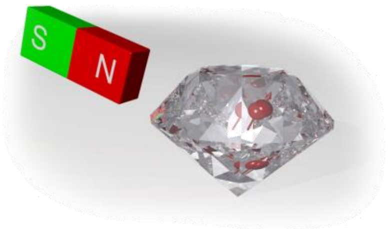
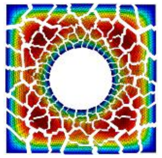
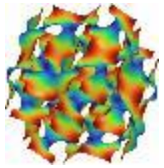
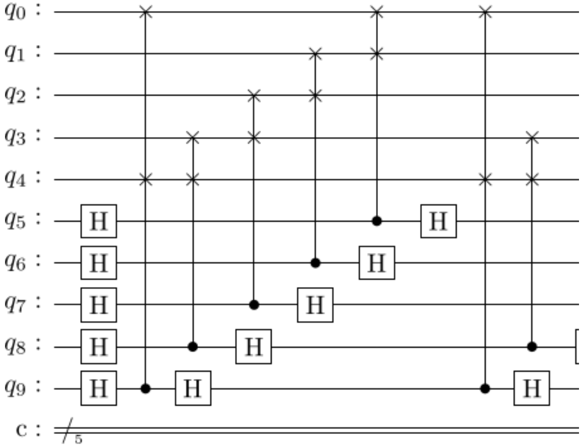
July 24, 2023

Womanium Quantum 2023 Summer Program

Talk Overview

- Introduction
- Nuclear Engineering Overview
  - Ecosystem
  - Nuclear Power Basics
- Quantum Technology Applications
  - Computing
  - Sensing
- Workforce Development

About Me

- 2000: “Discovered” Quantum Computing
  - April 2000 issue of Scientific American
  - “The Quantum Adventures of Alice and Bob”
- 2003-2006: Nuclear Fusion
  - Farnsworth Fusor → “Hobbyist” fusion reactor
  - Built mostly with surplus parts
- 2006-2016: Nuclear Engineering @ RPI
  - Designed and built specialized instruments for neutron physics experiments
  - Licensed research reactor operator
- 2016-Now: R&D Engineer at NNL
  - Scientific computing and emerging technologies
  - Quantum Technology Lead since 2017
  - Motivated by Oak Ridge “Deuterium Paper”
  - “Zero-to-One” Integration


Surprisingly Modern Neandertals • National Medal of Technology

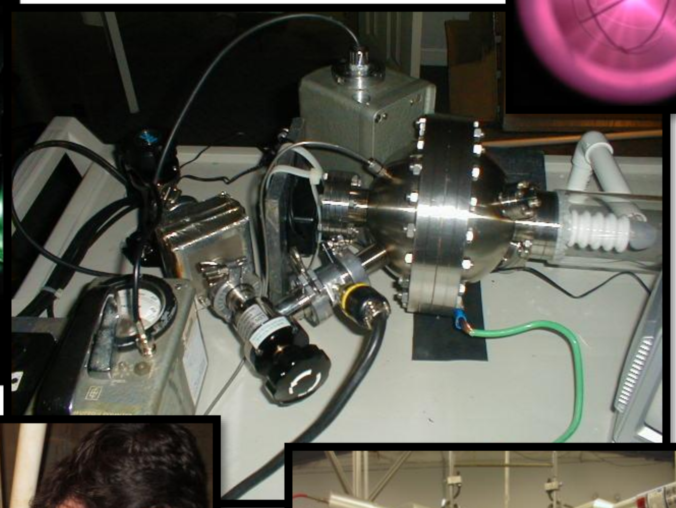
SCIENTIFIC AMERICAN

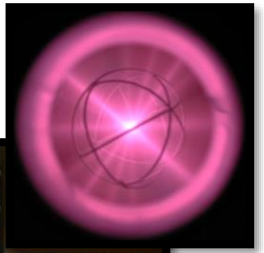
QUARK SOUP
CERN cooks up a new state of matter
see page 16

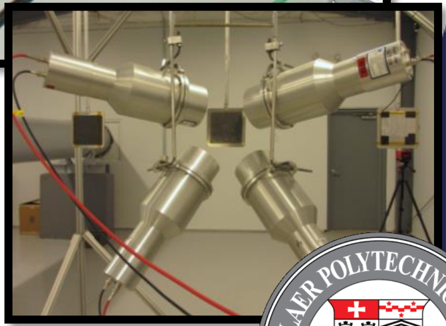
QUANTUM Teleportation
The Future of Travel? Or of Computing?

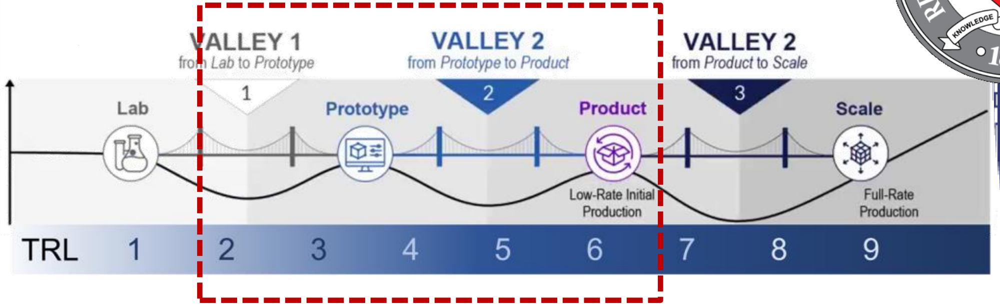
Of Mice and Men
Genetic formula for a smarter mouse

Brown Dwarfs
Stars that fizzled fill the galaxy



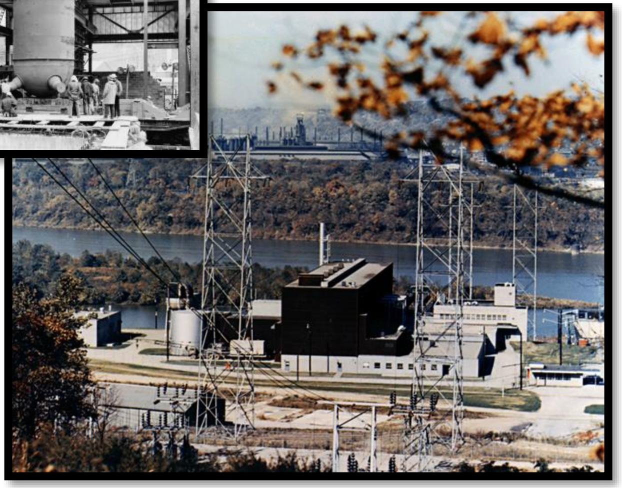






NNL History

- Founded in 1946 by Admiral Rickover
  - Government-owned: US Naval Nuclear Propulsion Program
  - Contractor-operated: Fluor Marine Propulsion
- Full life-cycle responsibility for US Naval Nuclear Reactors
  - Full-stack nuclear engineering
  - Research, design, testing, maintenance and disposal
- Deployed the first practical nuclear power reactors
  - USS Nautilus → First nuclear-powered submarine
  - USS Enterprise → First nuclear-powered aircraft carrier
  - Shippingport PWR-1 → First commercial grid-scale reactor
  - Shippingport PWR-3 → thorium-cycle breeder reactor



NNL Today

- ~8000 People at 5 primary locations
- More than 80 reactors in service
  - ~70 submarines
  - ~10 aircraft carriers
- Over 7500 reactor-years of safe operation
  - 2-3 new reactors every year
  - 171 million ship-miles traveled

Bettis Laboratory
Pittsburgh, PA

Moored Training Ships at Nuclear Power Training Unit
Charleston, SC

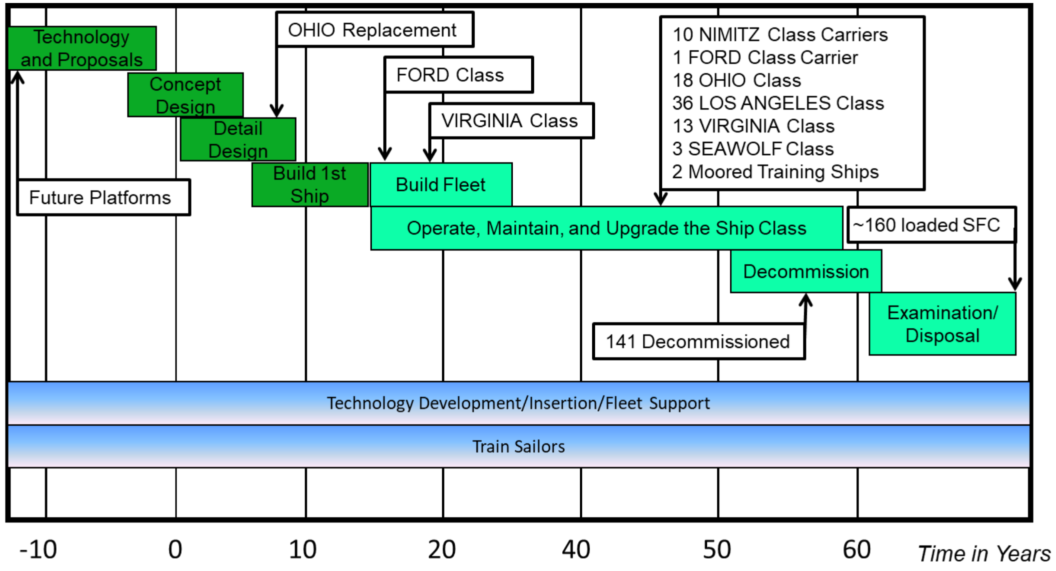
Kesselring Site
West Milton, NY

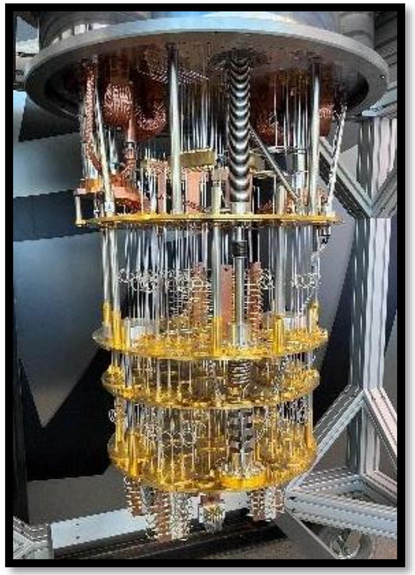
Knolls Laboratory
Schenectady, NY

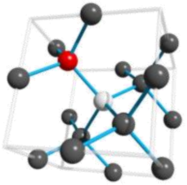
Naval Reactors Facility
Idaho Falls, ID

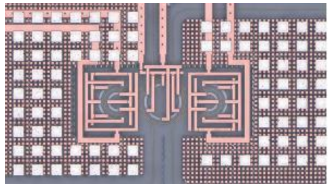
Quantum at NNL

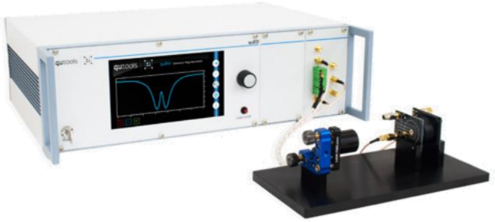
- Long-term focus on technology
  - Deep time → Approaching 100 years for some ship classes
  - Emerging technologies matter on these timescales
- Quantum Applications Team
  - Started in 2015 to look at quantum computing applications
  - Expanded in 2019 to include sensing, materials and energy technologies
  - Current projects in algorithm development, diamond NV centers
- Team Objectives
  - <u>Identify</u> impactful quantum technologies.
  - <u>Develop</u> internal expertise and use cases in quantum technologies.
  - <u>Engage</u> external partners to jointly develop and deploy quantum technologies.
  - <u>Educate</u> the current and future workforce to be quantum-aware.









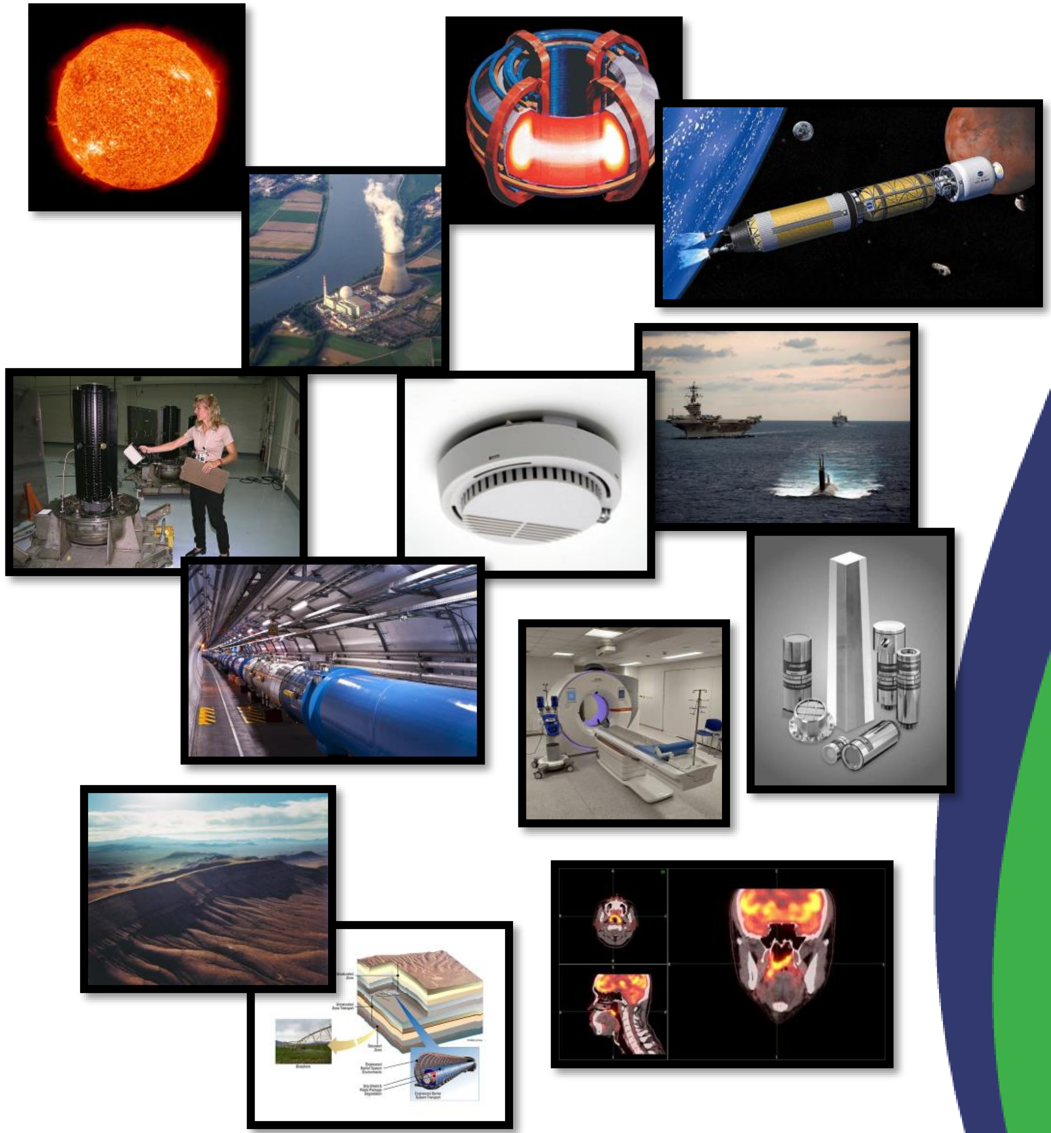


The Nuclear Engineering Landscape

- Nuclear technology can be considered a “first-generation” quantum technology.
  - Nuclei have an inherently quantum mechanical description.
  - Nuclear interactions are probabilistic.
  - Macroscopic behavior is determined by quantum processes.

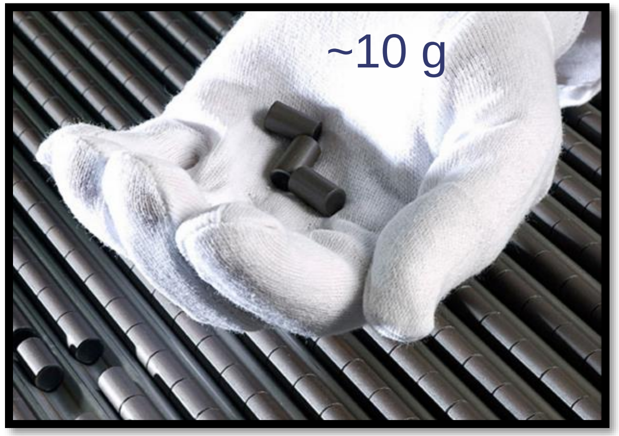
- Nuclear engineering harnesses nuclear phenomena for useful applications.
  - Energy → Fission & Fusion
  - Medicine → Imaging & Therapy
  - Safety & environmental protection
  - Safeguards & nonproliferation
  - Instrumentation & measurement
  - Fundamental science & astrophysics

- Nuclear engineers use many advanced tools and methods.
  - Supercomputer clusters
  - Particle accelerators
  - Research reactors
  - Radiation and particle detectors
  - Fluid test loops
  - Material synthesis and characterization
  - …

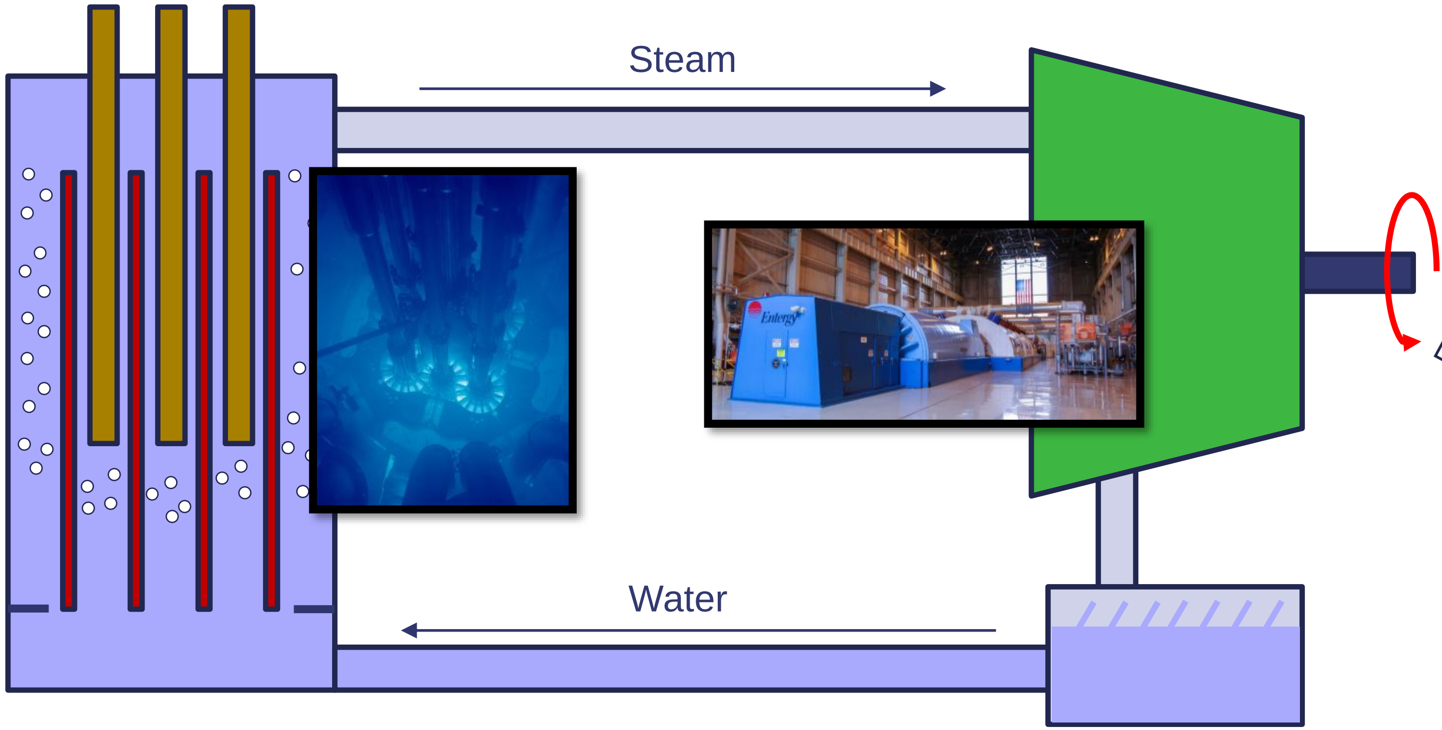


Why Nuclear Energy?

- Energy dense
  - 100 million times more energy per gram than fossil fuels
  - Compact facilities and land usage
- Combustion-Free
  - Zero CO_2 emissions during operation
  - No oxygen required → works underwater and in space
- High availability
  - 90% capacity factors → always on
  - 1.5-30 years without refueling

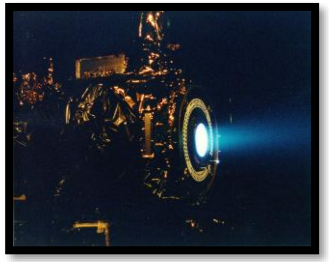


Nuclear Energy Production



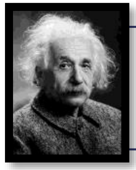
Land

Sea



Space

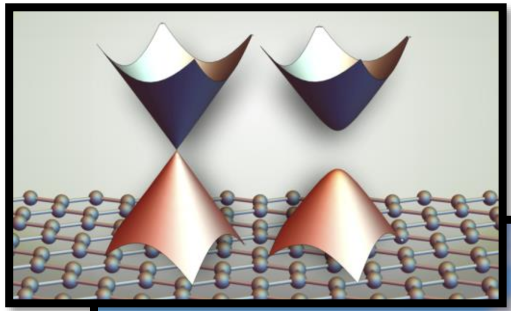
Fuel → Sustain fission and generate heat
Control Rods → Absorb neutrons to control the reaction
Moderator → Slow down neutrons to increase their probability of causing fission
Coolant → Remove heat energy from the fuel
Turbine → Convert heat energy in the coolant into useful work



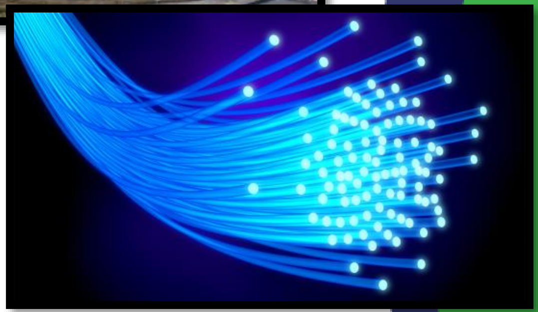
"…a hell of a way to boil water"
- *Albert Einstein*

Nuclear + Quantum?

- The intersection of nuclear and quantum technologies is relatively underexplored!
- Quantum Computing
  - Engineering design & simulation
  - Chemistry
  - Nuclear physics
- Quantum Sensing
  - Laboratory, manufacturing & plant process monitoring
  - Safeguards & nonproliferation
- More research is needed!





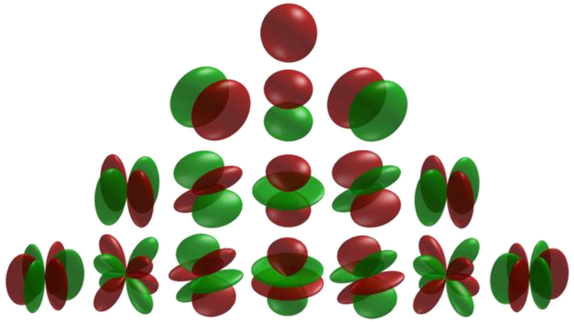


Quantum Computing

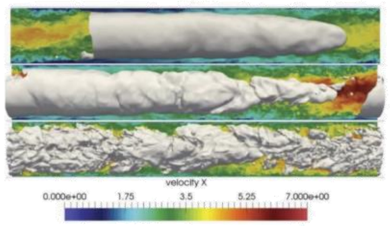
Quantum Computing

- Quantum computers can enable scaling improvements for problems used in nuclear engineering:
  - Engineering simulations (e.g., FEA, CFD, general PDE solving)
  - Probabilistic algorithms (e.g., Monte Carlo, Bayesian statistics, machine learning)
  - First-principles simulations (e.g., materials science, nuclear physics, chemical reactions)

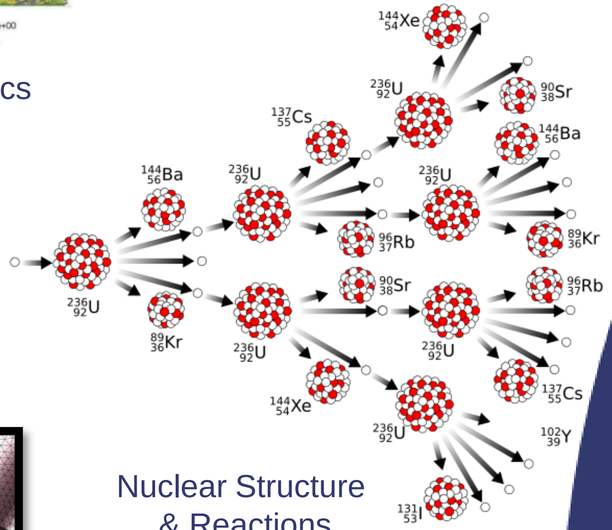
- NNL is conducting multiple R&D efforts.
  - University of Pittsburgh collaboration for PDE algorithm development.
  - Womanium Launchpad Project



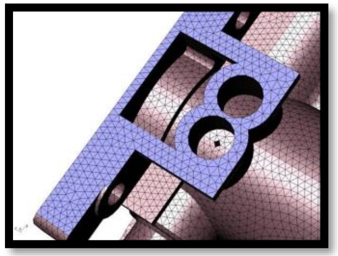
Electronic Structure



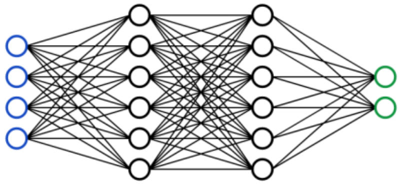
Boiling Fluid Dynamics



Nuclear Structure & Reactions



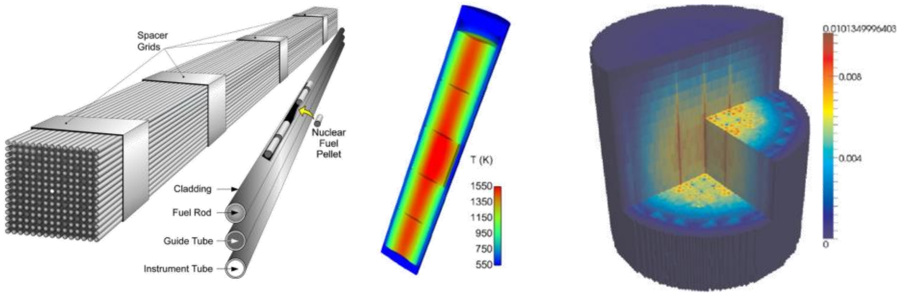
PDE Solving



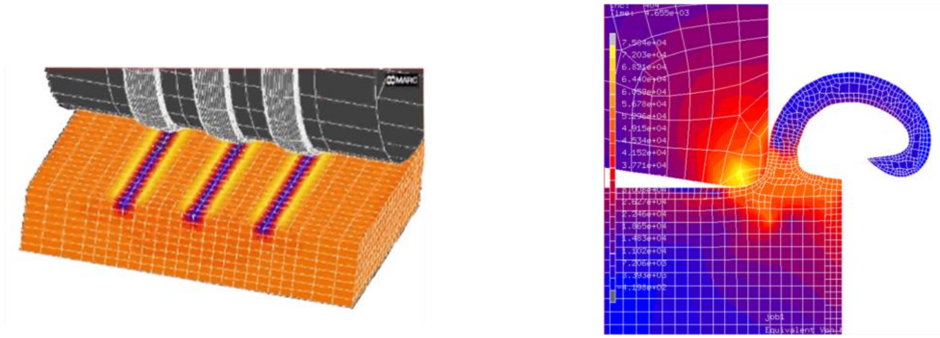
Surrogate Model Training & UQ

Engineering Simulations

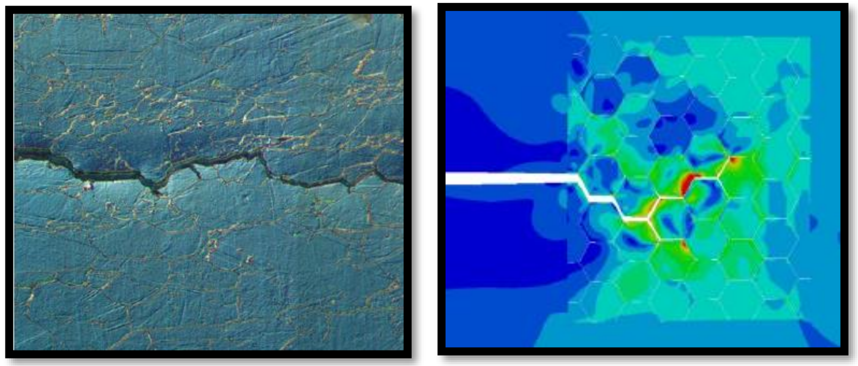
- Computer simulation is essential for reactor design and maintenance.
- Simulations can be expensive!
  - Detailed fluid dynamics
  - Neutron-by-neutron simulation
  - Multi-physics coupling
  - Complex materials and interactions
- Many simulations are needed to determine the design landscape.
- Quantum computing may be able to speed up bottlenecks.
  - Nuclear applications of quantum computing are not well-studied.
  - More research is needed!



Reactor Performance



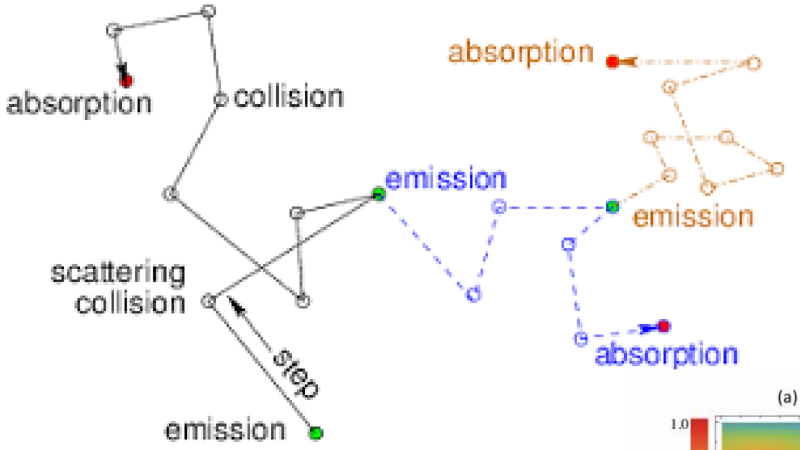
Manufacturing Processes

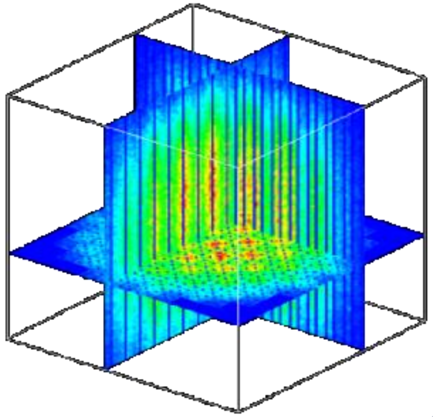


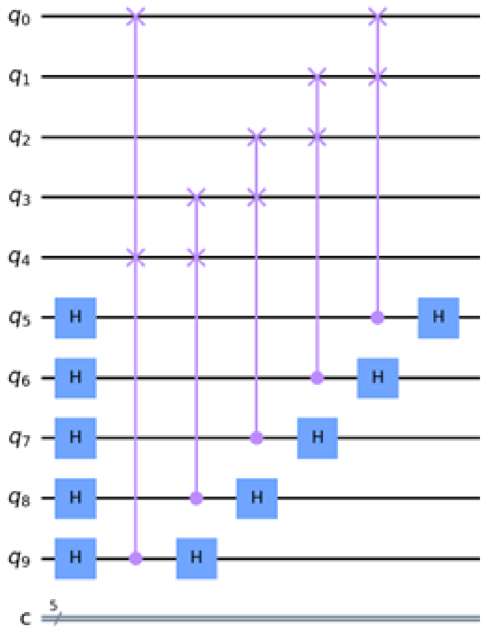
Material Corrosion & Degradation

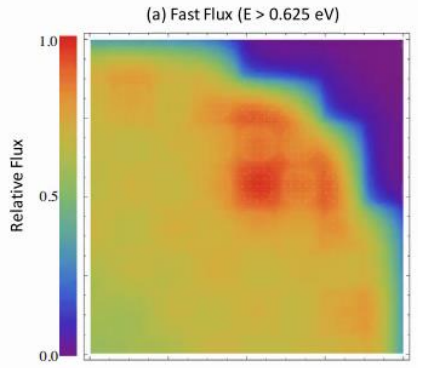
Radiation Transport

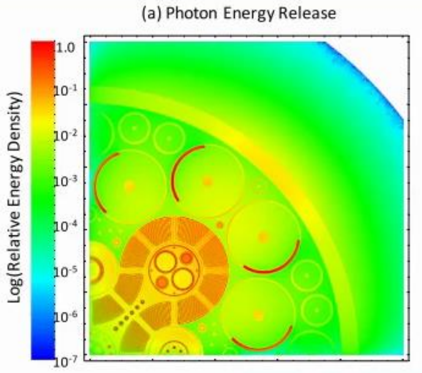
- We need to know how radiation moves and interacts in various systems.
  - Power & heat production
  - Fuel consumption
  - Shielding
- The Monte Carlo method is the "gold standard."
  - Nuclear and particle interactions are probabilistic
  - Track radiation particle-by-particle
  - Tally reactions and energy deposition
- Early computers were built specifically for solving this problem!
- <u>Quantum should provide a scaling advantage.</u>
  - Evidence of speedup from other domains (e.g., finance)





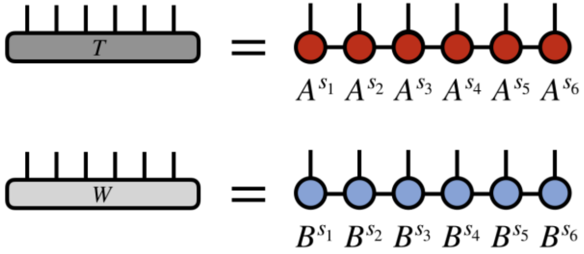


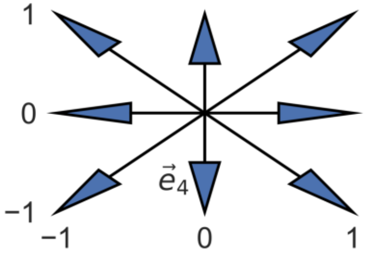


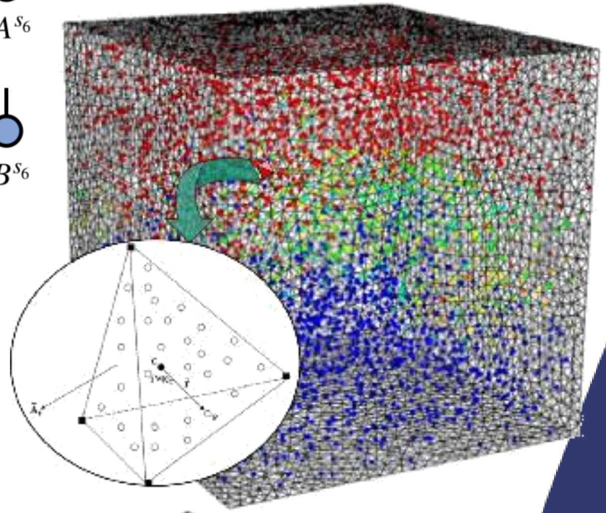


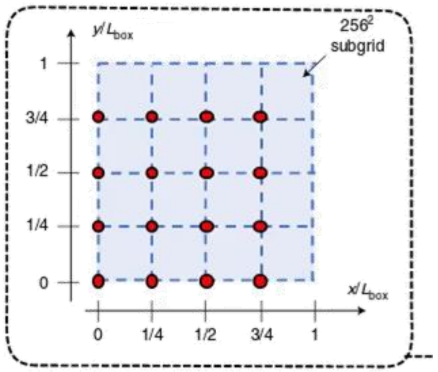
Fluid Dynamics

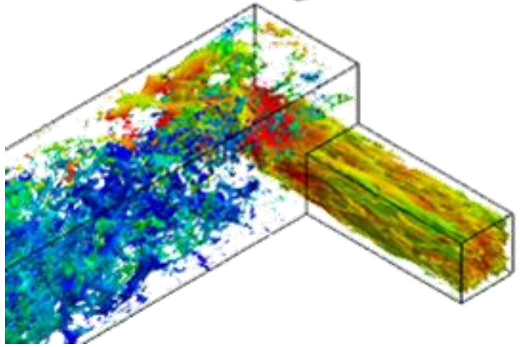
- A working fluid is used to extract the heat energy produced by the nuclear fuel.
  - Water, helium, CO_2, sodium, molten salt, …
  - Phase changes (e.g., boiling & condensation)
  - Feedback effects with power production
- Accurate knowledge of fluid dynamics is needed.
  - Directly determines safety limits
  - Impacts efficiency
- Quantum can improve the performance of complex fluid dynamics calculations.
  - Tensor network methods
  - Lattice Boltzmann methods

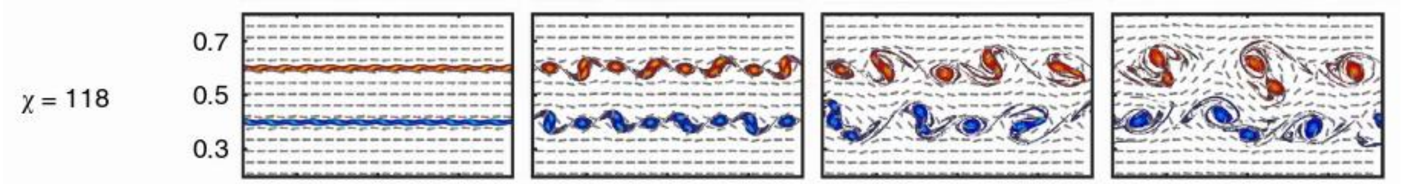










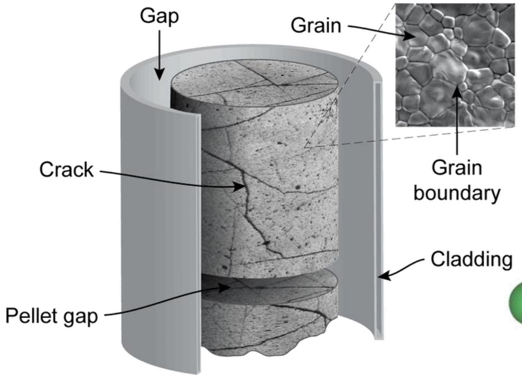


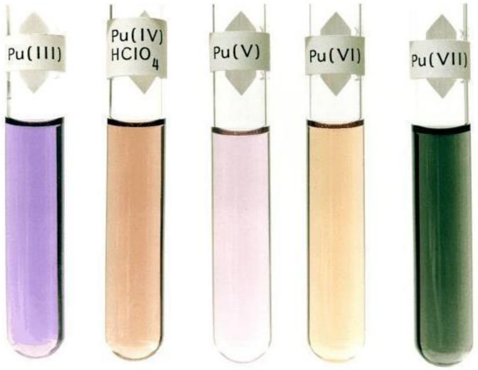
Materials Science & Simulation

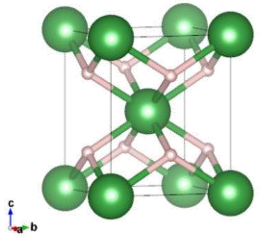
- Understanding material properties is essential for safety, reliability, and efficiency.
  - Inherently safe, high-performance fuel systems
  - Corrosion-resistant alloys
  - Robust and resilient waste forms

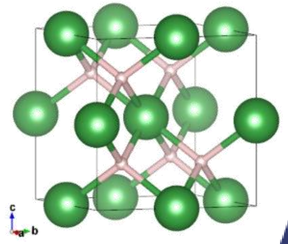
- Accurate, first-principles simulations and experiments on nuclear-relevant materials are challenging.
  - *d* and *f* orbitals in actinide materials (e.g., Th, U, Np, Pu…) have strongly entangled, highly relativistic electrons.
  - Materials are expensive, radioactive, and require specialized facilities
  - Typically need expensive computational methods, limiting scalability.

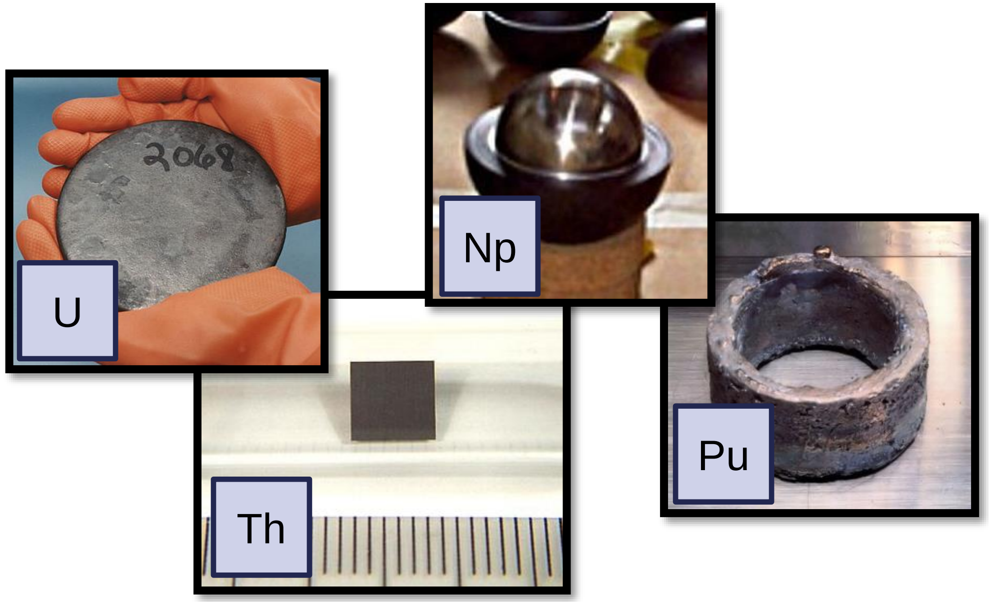
- Quantum computing may be able to help.
  - Embedding Methods
  - Tensor Networks
  - …





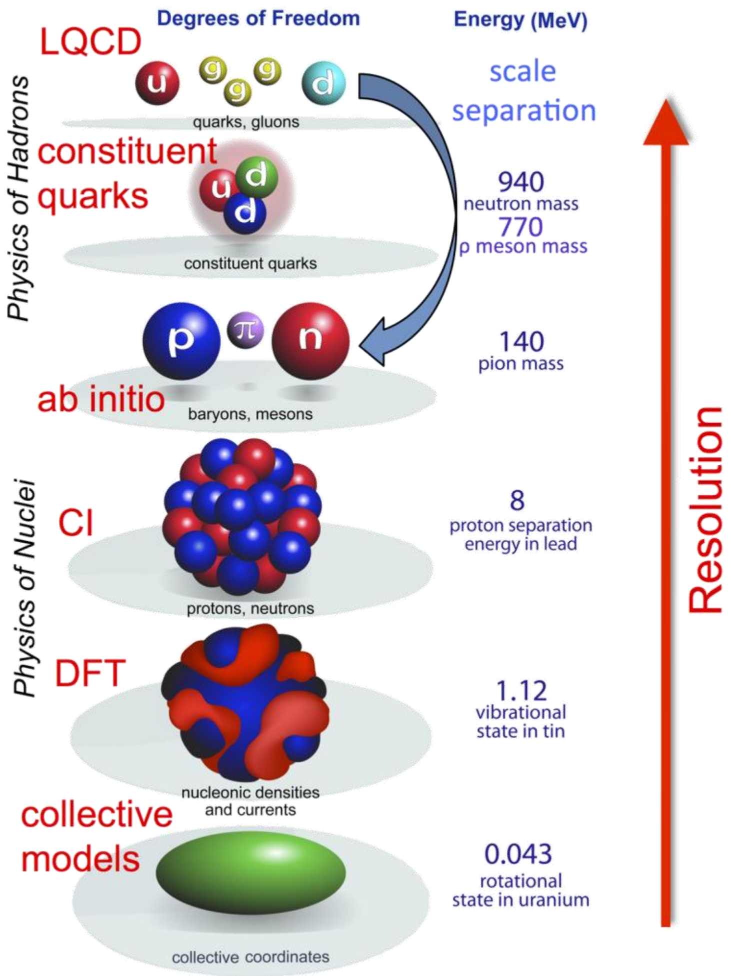


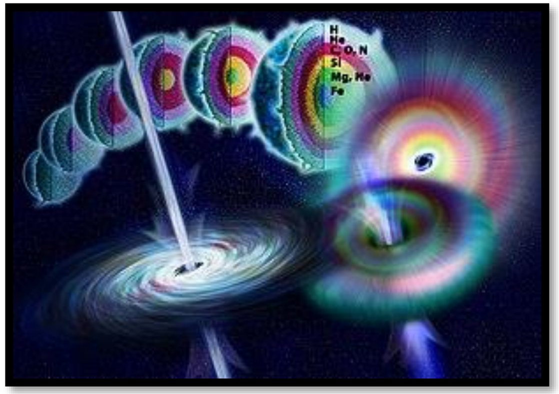


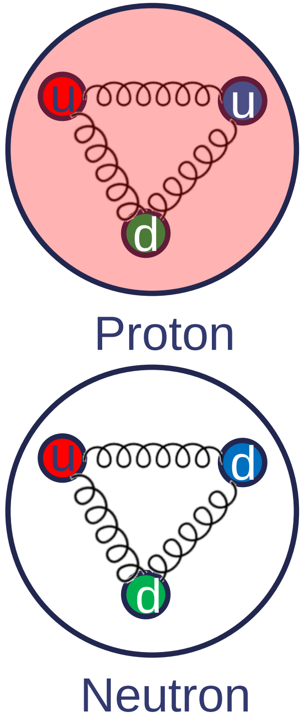


Fundamental Nuclear Physics

- Nuclear energy, astrophysics and nuclear medicine need accurate nuclear data.
  - Genesis of the heavy elements
  - Behavior of nuclear energy systems
- Experiments aren't always practical.
  - Rare & expensive isotopes
  - Highly radioactive, short-lived samples
- Nuclei are too complex to simulate from first-principles.
  - Many degrees of freedom per nucleon
  - Strong entanglement between nucleons
  - Incomplete theories of bound quarks and gluons
- **Quantum computing is <u>required!</u>**
  - First-principles calculations are intractable for elements heavier than oxygen.



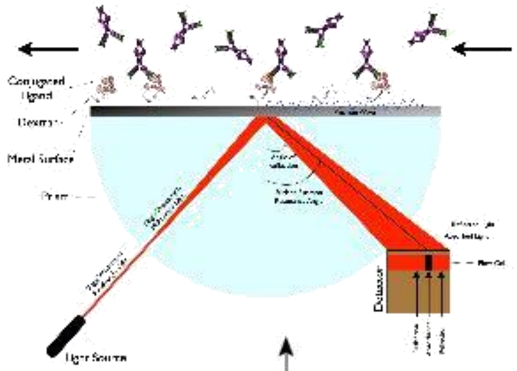




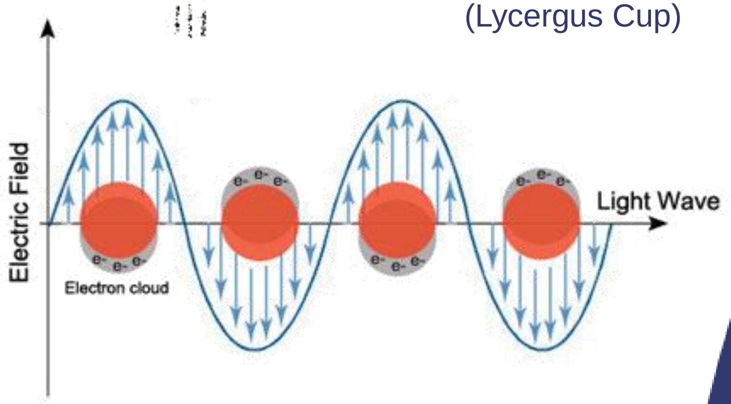
Quantum Sensing

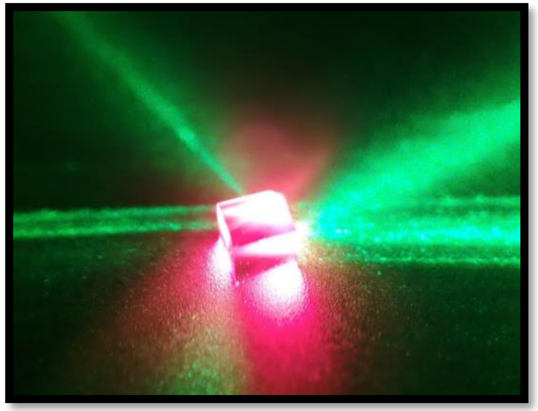
Quantum Sensing

- Qubits are very sensitive to environmental effects.
  - Makes fault-tolerant computing challenging!
  - Makes sensing applications attractive!
- Nuclear plants have thousands of sensors.
  - Needed for safe and reliable operation
  - Need to last many years under harsh conditions
- Laboratory experiments and manufacturing processes require very precise sensors and detectors
- **Photonic** quantum sensors may offer advantages
  - Diamond NV centers
  - Plasmonic sensors
  - Photons & fiber optics

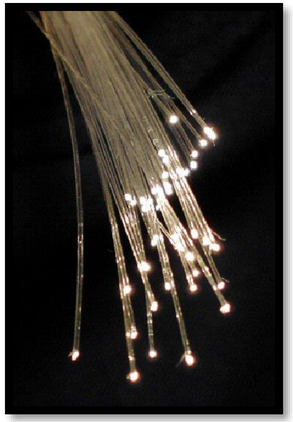


Plasmonic Dichroism (Lycergus Cup)





Diamond NV Center ODMR (Element Six)

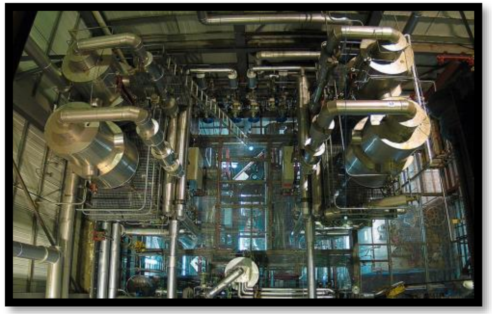


Process Monitoring

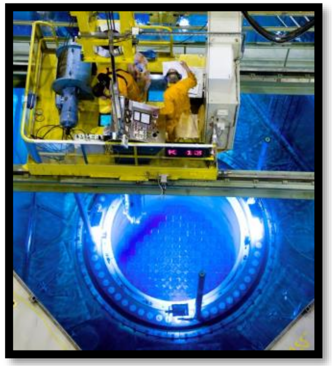
- Quantum sensors can improve monitoring of many processes common in engineering applications:
  - Laboratory studies
  - Manufacturing
  - Plant operations
- Quantum sensors can measure many quantities of interest
  - Temperature
  - Pressure
  - Mechanical stress & vibration
  - Fluid chemistry

Pump & Motor Fatigue

AP1000 PWR (Westinghouse)



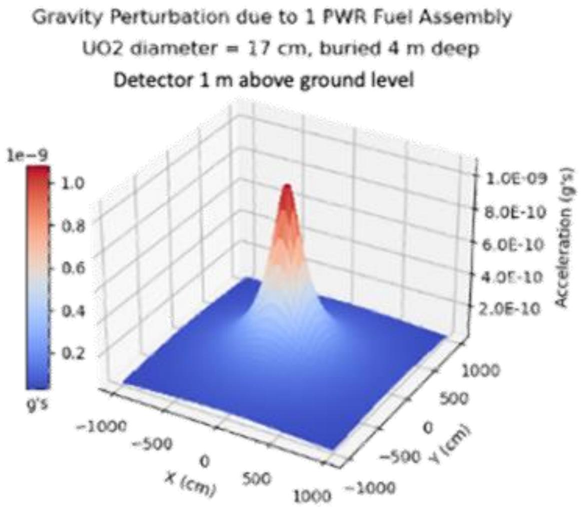
Steam Generator Inspection



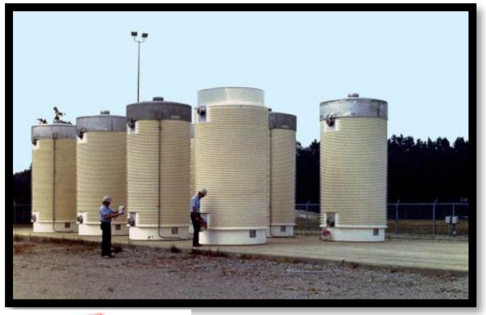
Cooling Water Chemistry

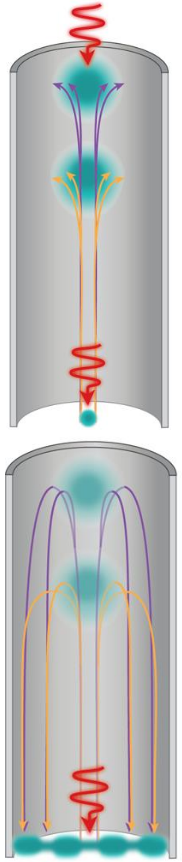
Physics Experiments (NIST)

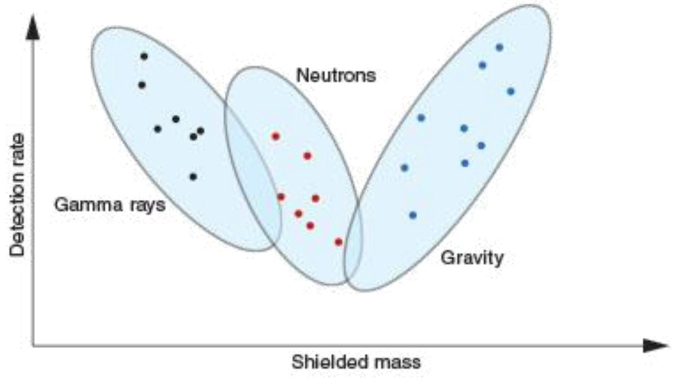
Safeguards & Nonproliferation

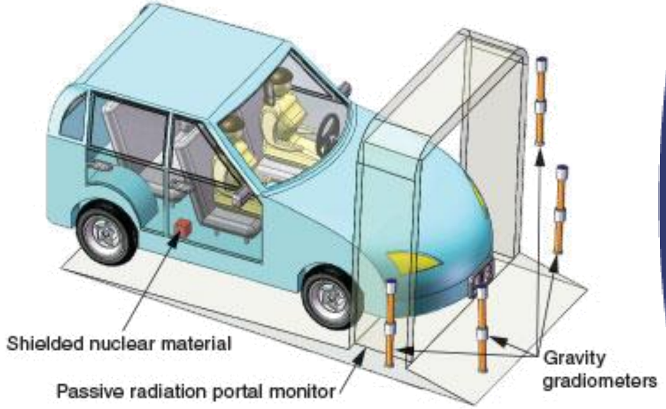


- Tracking and securing nuclear materials is critically important.
  - Nonproliferation treaties require monitoring to ensure compliance.
  - Detection is difficult, radiation is easily shielded.
- Cold atom interferometers can be used for material verification and nuclear forensics.
  - Tamper-proof scanning of spent nuclear fuel
  - Detection of smuggling at ports-of-entry
- Mass anomalies are detectable by their gravitational pull on the atoms!
  - Nuclear materials are very dense: 15-20 g/cm^3
  - Multiple detectors can measure gravitational gradients.
- Data fusion with radiation measurements can increase confidence and reduce false-positives.









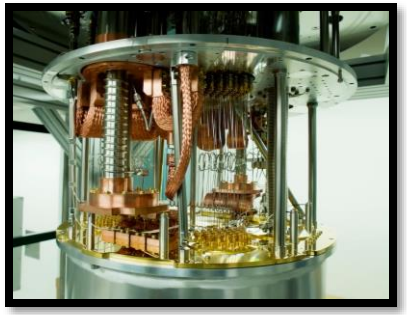
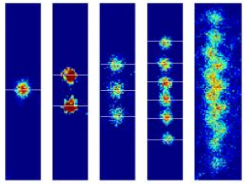
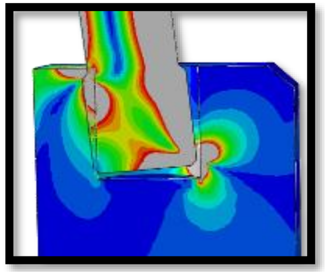
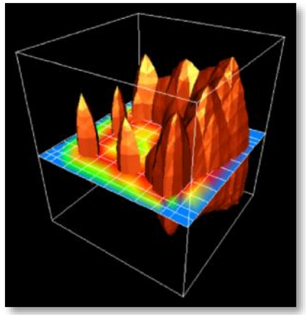
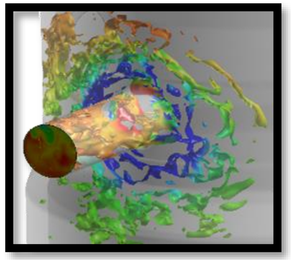
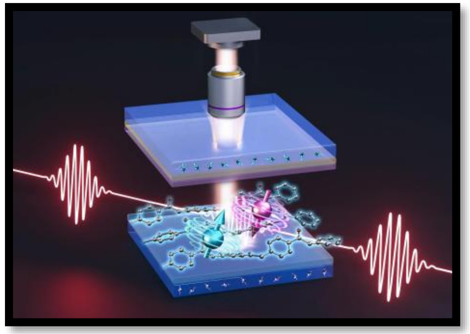
Workforce Development

Workforce Development

- Non-quantum organizations need a quantum-literate workforce.
  - Core team of experts to understand and match technologies with use cases
  - Broad base of user and support communities
  - Informed decision-making on new technologies
- Early-stage quantum efforts require multidisciplinary people and teams.
  - “All hands on deck”
  - Strong understanding of company’s core business
  - Strong understanding of quantum technologies
  - Strong support in enabling technologies
- Strive for excellence in quantum technology **<u>AND</u>** another subject matter domain!
- **<u>There’s room for everyone!</u>**

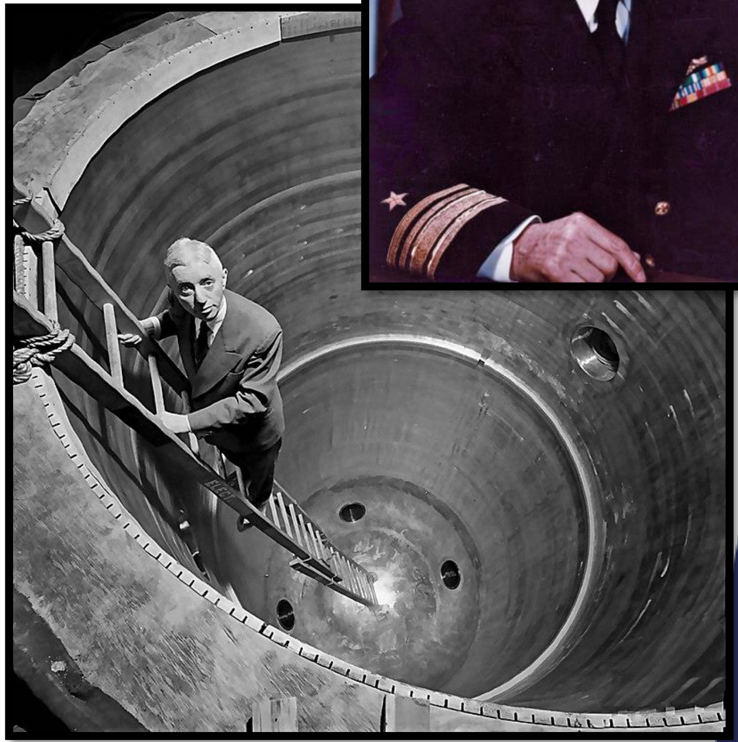
Summary

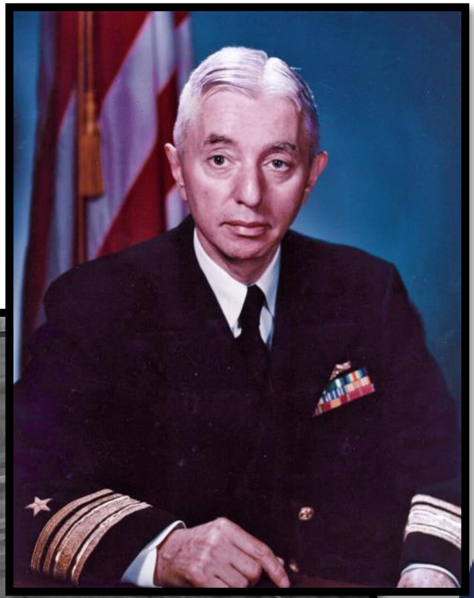
- There are numerous greenfield opportunities for quantum technology within the nuclear engineering field.
- Quantum computing may potentially enable step changes in simulation capabilities for design and maintenance.
- Quantum sensing will enable smaller, more durable and more precise instrumentation across the industry.
- All engineering organizations will require a quantum-literate workforce.

Final Words

- “Good ideas are not adopted automatically. They must be driven into practice with courageous impatience.”
- “Sit down before fact with an open mind. Be prepared to give up every preconceived notion. Follow humbly wherever and to whatever abyss Nature leads, or you learn nothing.”
- “The tools of the academic designer are a piece of paper and a pencil with an eraser. If a mistake is made, it can always be erased and changed. If the practical-reactor designer errs, he wears the mistake around his neck; it cannot be erased. Everyone sees it.”
- “The Devil is in the details, but so is salvation.”





Paper Reactors, Real Reactors (June 5, 1953)

https://en.wikiquote.org/wiki/Hyman_G._Rickover

Thank You!

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https://linkedin.com/in/brianjm-nnl

We’re hiring! navalnuclearlab.energy.gov

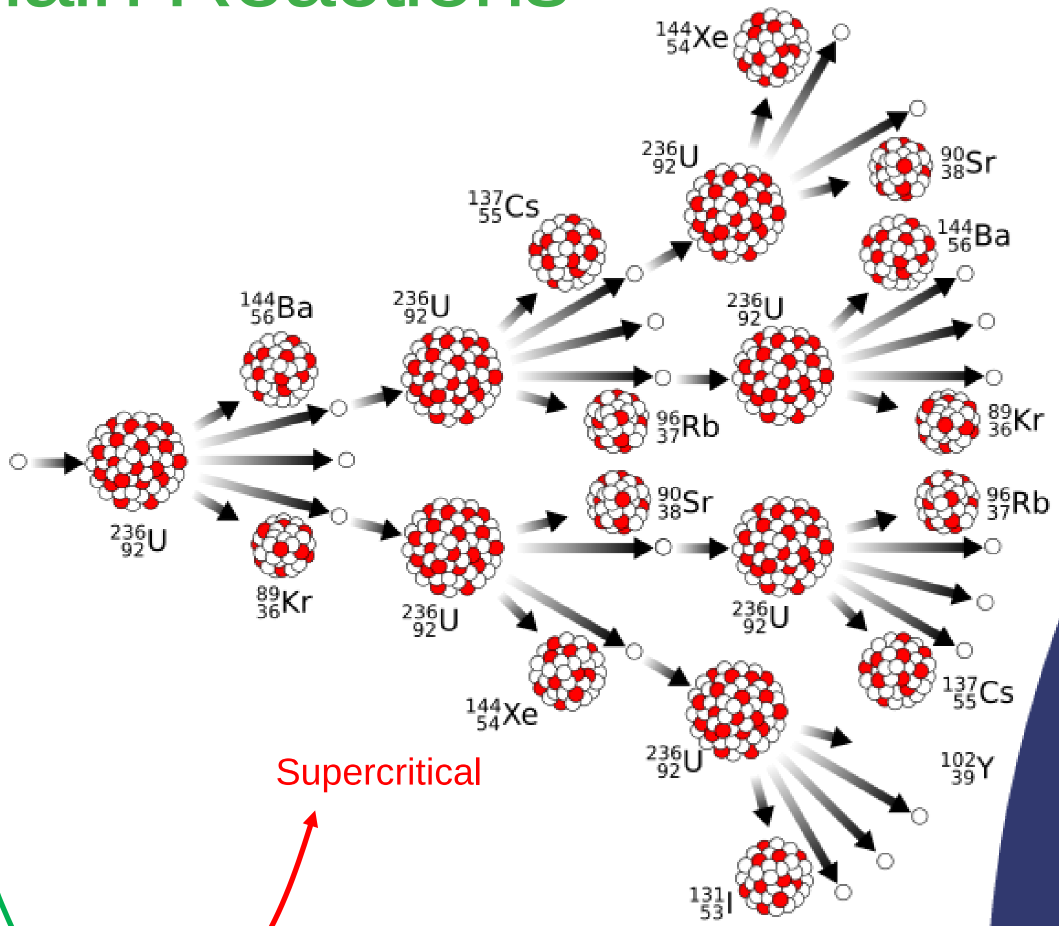
Recommended Reading

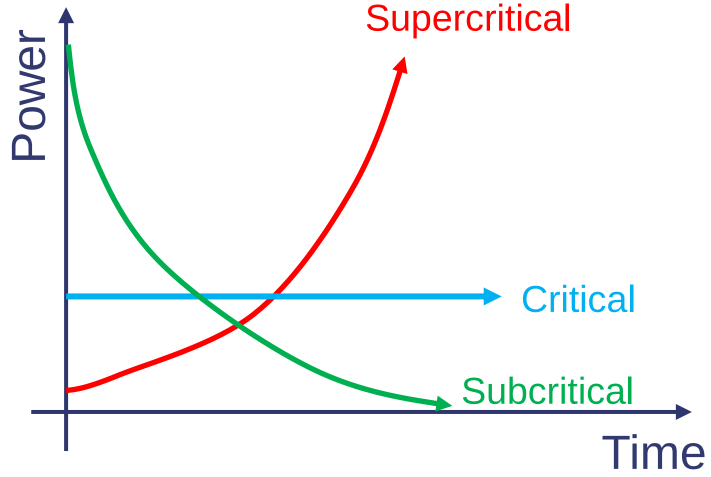
- Glasstone, S. *Sourcebook on Atomic Energy*, D. Van Nostrand Co., 1967.
- Paudel, H. et al., *Quantum Computing and Simulations for Energy Applications: Review and Perspective,* ACS Engineering Au, 2022 **2** (3), 151-196 Online: https://doi.org/10.1021/acsengineeringau.1c00033
- Crawford, S. et al., *Quantum Sensing for Energy Applications: Review and Perspective*, Adv. Quantum Technol. **4**: 2100049. 2021, Online: https://doi.org/10.1002/qute.202100049
- Carlson, J., *Quantum Computing for Theoretical Nuclear Physics*, Institute For Nuclear Theory Report 18-008, Online: osti.gov
- Degen, C. et al., *Quantum Sensing*, Rev. Mod. Phys. **89**, 035002 (2017).
- Libby, S. et al., *Feasibility Study of a Passive, Standoff Detector of High Density Masses with a Gravity Gradiometer Based on Atom Interferometry*, Technical Report LLNL-TR-465878, Lawrence Livermore National Laboratory, January 2011. Online: osti.gov
- Farley, D., *Quantum Sensing and its Potential for Nuclear Safeguards*, Technical Report SAND2021-13677, Sandia National Laboratories, October 2021. Online: osti.gov

Supplemental Slides

Nuclear Energy: Chain Reactions

- **Fissile** materials are the key ingredient
  - ^{233}U, ^{235}U, ^{239}Pu
- A fissile nucleus absorbs a neutron, then breaks apart.
  - Two **fission fragments** carry away most of the energy.
  - ~2.5 new neutrons are emitted
- In the right configuration, this process is self-sustaining → **Critical**
- We can control the reaction rate with neutron absorbers (poisons)
  - Control rods
  - Fixed poisons
  - Dissolved poisons



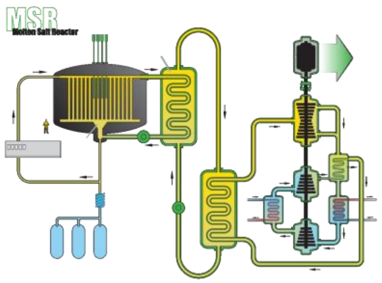


The Reactor Zoo

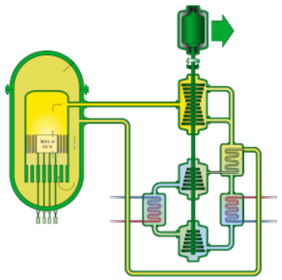
Coolants
- Water (H_2O)
- Heavy Water (D_2O)
- Helium
- CO_2
- Sodium
- Lead
- Molten Salt

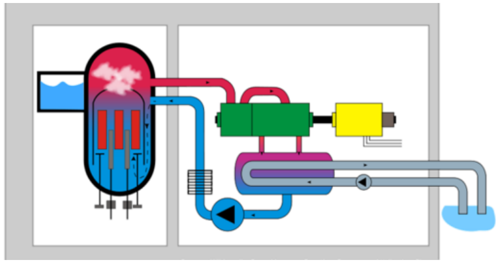
Moderators
- Water (H_2O)
- Heavy Water (D_2O)
- Graphite
- None (Fast Reactors)

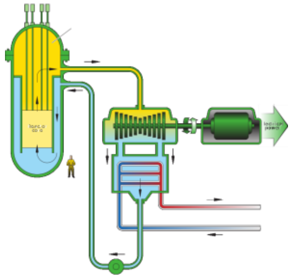
Fuels
- Uranium ($^{235}U/^{238}U$)
- MOX ($^{235}U/^{239}Pu$)
- Thorium ($^{232}Th/^{233}U$)

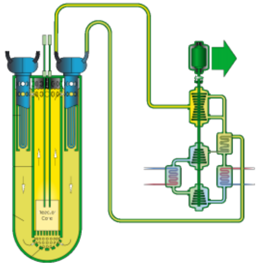


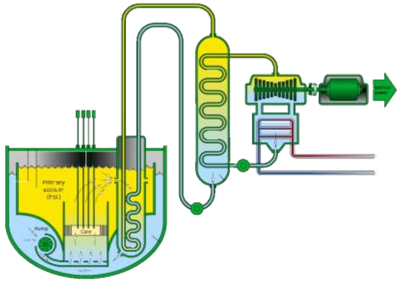
Molten Salt

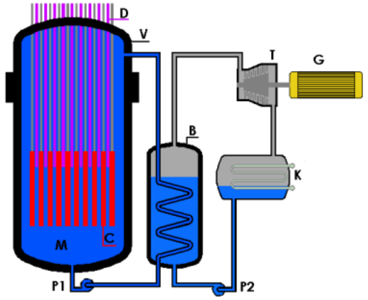

Helium-Cooled


Boiling Water

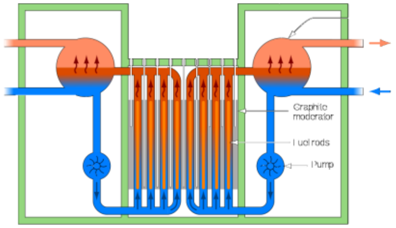

Supercritical Water


Lead/Bismuth-Cooled

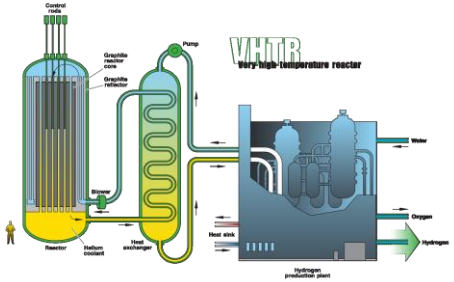

Sodium-Cooled



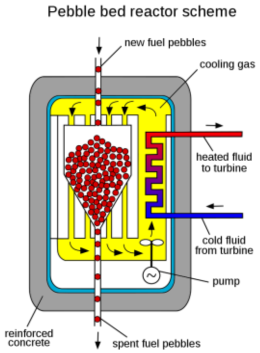
Pressurized Water



Water-Cooled, Graphite Moderated (RBMK)



Very High Temperature



Pebble Bed