OAK RIDGE National Laboratory

Update on Second Target Station Instrument Selection

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Webinar

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https://neutrons.ornl.gov/sts

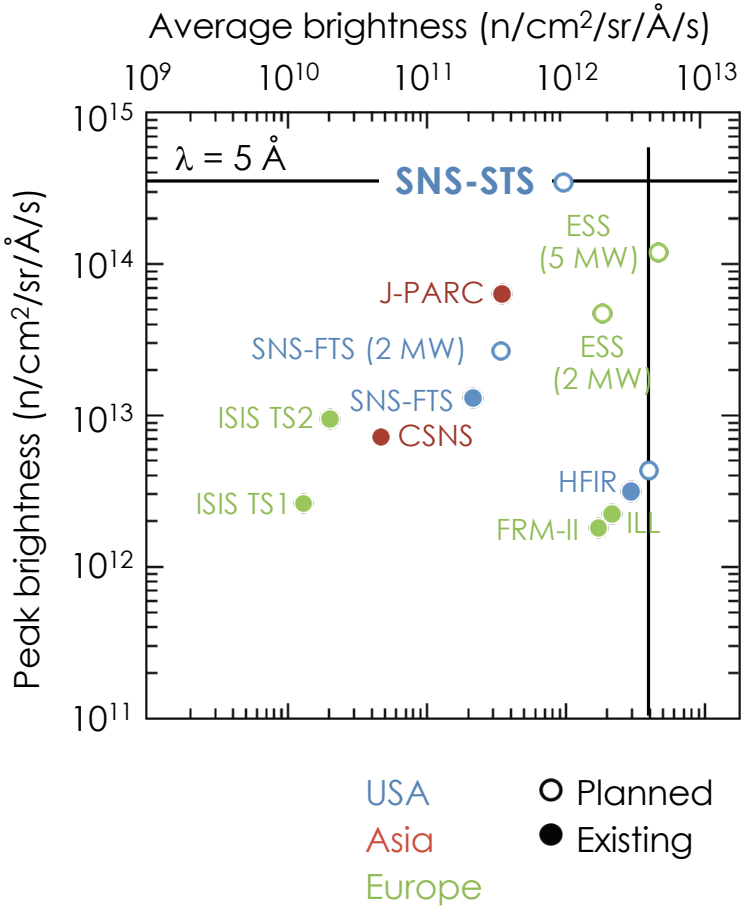
ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

STS at SNS will be a high peak brightness pulsed source for cold neutrons

STS will deliver beams of cold neutrons with higher peak brightness and broader ranges of neutron energies that are needed to meet challenges at the frontiers of matter and energy:

- Simultaneous measurement of hierarchical architectures across unprecedented ranges of length scales
- Time-resolved measurements of kinetic processes and beyond-equilibrium matter
- Characterization of smaller samples and matter under more extreme conditions
- Applications for developing next-generation materials for energy, security, and industrial applications



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Conceptual design scope supports case for achieving world-leading capability

Accelerator

- Transport protons to STS
- Independent operation of FTS and STS

Target

- Solid rotating tungsten target
- 2 high brightness, supercritical H_2 moderators

Instruments

- Provide capability for 22 beam line instruments
- 8 (of 22) instruments included in STS

Expect 8 instruments to be selected in June 2021

Conventional facilities

- 9 new buildings (350k square feet)
- 40 m, 50 m, and 90 m instrument halls

Integrated controls

- Control systems and computing infrastructure
- Data acquisition for neutron scattering instruments

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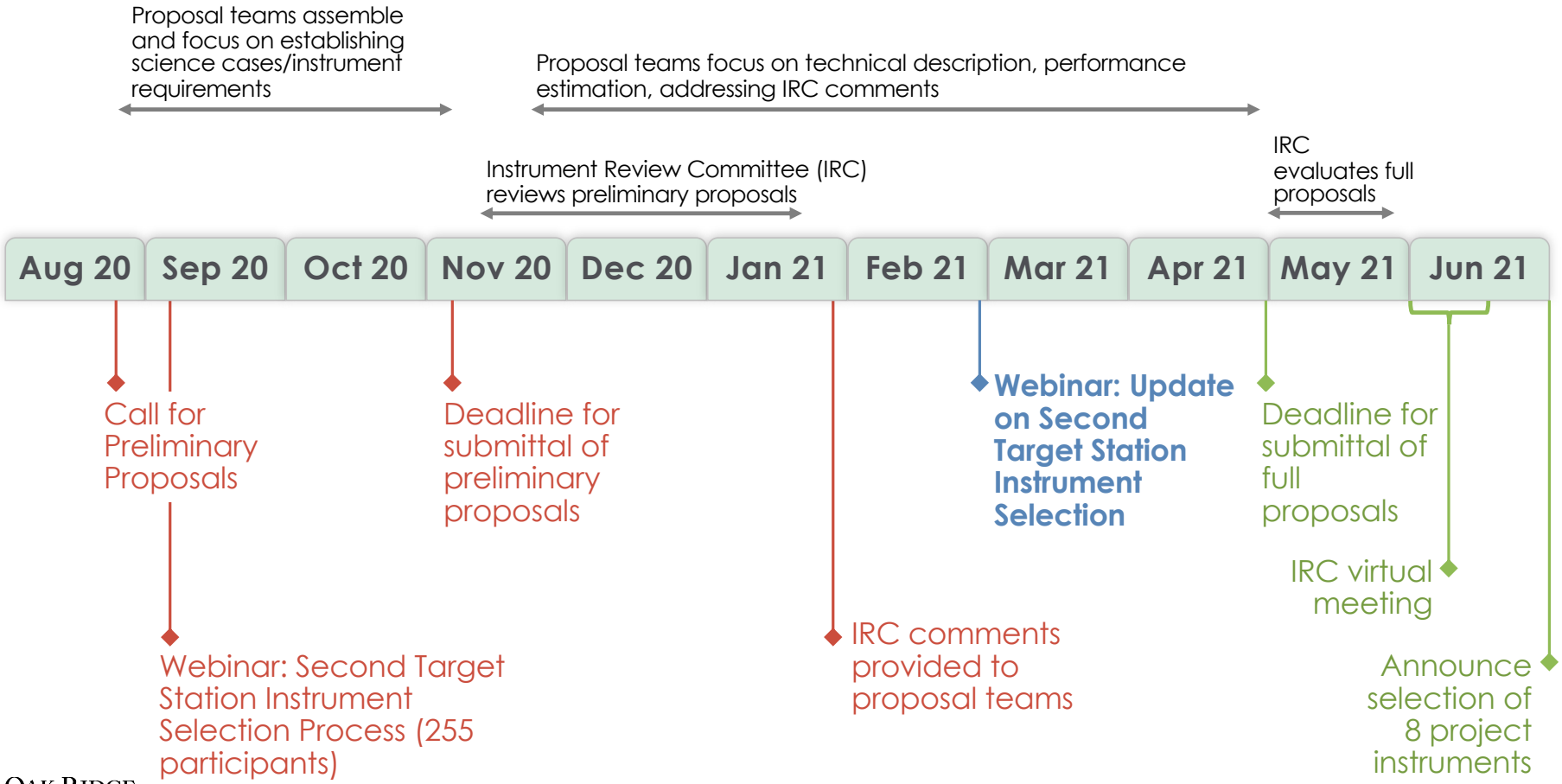
Selection criteria guide prioritization for instrument construction

- Scientific importance and impact
  - Will the proposed instrument advance the frontiers of knowledge?
  - What are the broader societal impacts of the proposed science case?
  - Does the science case identify grand challenges from national studies and reports?
  - Does the science case include a sufficiently wide application area?
  - What is the potential for high impact publications?
- Strength of the relevant user community
  - What is the predicted demand?
  - What research communities will use this instrument? Does this instrument have the potential to expand the neutron user community?
  - Will inclusion of this instrument maintain a balanced science portfolio across the ORNL neutron sources?
- Uniqueness of STS source capabilities (cold neutrons, broad bandwidth, high brightness)
  - Does this instrument take maximal benefit of STS unique source capabilities?
  - Would the capabilities of this instrument be better enabled at another of the ORNL neutron sources?
  - Does this instrument complement the capabilities of existing instruments at ORNL?
- Quality of the proposed instrument (world-leading, competitive, other)
- Feasibility of instrument concept *(only for full proposals)*
  - Is there a high degree of certainty that the proposed instrument will achieve its performance goals?
  - Is there R&D required before the instrument can achieve its goals?
  - Can the instrument be built within the budget and schedule constraints of the STS project?

Instrument selection timeline finishes with announcement of 8 project instruments



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12 instrument preliminary proposals were submitted last November

Proposed instruments address the science areas discussed in the First Experiments Report and in User Workshops

	Science Themes/Grand Challenge Areas					
	*Polymers & Soft Materials	*Quantum Materials	*Materials Synthesis & Energy Materials	*Structural Materials	*Biology & Life Sciences	Environmental & Earth Sciences
Concept Instrument	†Hierarchical & Beyond-equilibrium	†Coherence in Matter	†Heterogeneity Interfaces & Disorder	†Heterogeneity Interfaces & Disorder	†Hierarchical & Beyond-equilibrium	†Heterogeneity Interfaces & Disorder
Diffractometers						
EWALD – macromolecular single-crystal					✓	
PIONEER – polarized single-crystal		✓	✓			✓
VERDI – polarized powder/single-crystal		✓				
Spectrometers						
BWAVES – broadband, indirect geometry	✓		✓		✓	
CHESS – cold neutron chopper spectrometer for weak signals	✓	✓	✓		✓	
EXPANSE – wide-angle neutron spin echo	✓	✓			✓	
Large Scale Structures						
CENTAUR – SANS&WANS with inelastic	✓	✓	✓		✓	✓
M-STAR – focused, polarized reflectometer	✓	✓	✓			
QIKR – kinetics reflectometer	✓	✓	✓		✓	✓
Multimodal						
MENUS – multi-modal engineering beamline			✓	✓		
TITAN – multi-modal characterization of materials at extreme conditions		✓	✓	✓		✓
Imaging						
CUPI^{2}D – imaging of fast dynamic processes in natural/engineered materials			✓	✓	✓	✓

Instrument proposal abstracts are on the STS website

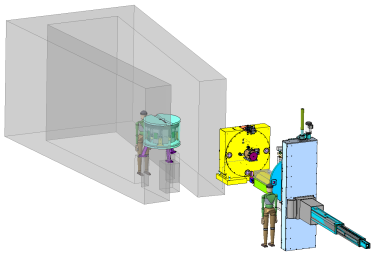
*Chapters in the First Experiments Report
†Themes from BESAC Grand Challenges Report

Instrument proposal teams include spokesperson, ORNL point-of-contact(s), and other researchers contributing to the science case and technical descriptions

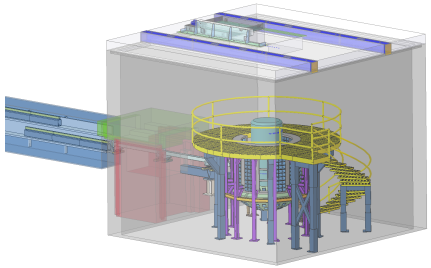
Instrument Name	Instrument Description	Spokesperson(s)	ORNL Point-of-Contact(s)
Diffractometers			
EWALD	Macromolecular single-crystal diffractometer	Gloria Borgstahl (University of Nebraska)	Leighton Coates
PIONEER	High-resolution polarized single-crystal diffractometer	Stephan Rosenkranz (Argonne National Laboratory)	Huibo Cao & Yaohua Liu
VERDI	Polarized Powder/single-crystal diffractometer	Stephen Wilson (University of California, Santa Barbara)	Stuart Calder & Ovidiu Garlea
Spectrometers			
BWAVES	Indirect geometry spectrometer with very broad range of energy transfers	Alexei Sokolov (University of Tennessee – Knoxville & ORNL)	Eugene Mamontov
CHESS	Cold neutron chopper spectrometer optimized for weak signals	Martin Mourigal (Georgia Institute of Technology)	Gabriele Sala
EXPANSE	Wide-angle neutron spin echo	Yang Zhang (University of Illinois Urbana-Champaign)	Changwoo Do
Large Scale Structures			
CENTAUR	SANS/WANS with inelastic capabilities	Rachel Segalman (University of California, Santa Barbara)	Shuo Qian (Wei-Ren Chen original)
M-STAR	Polarized reflectometer optimized for magnetism	Kang Wang (University of California, Los Angeles) & Tim Mewes (Alabama University)	Valeria Lauter
QIKR	Kinetics reflectometer	Eugenia Kharlampieva (University of Alabama-Birmingham)	John Ankner
Multimodal			
MENUS	Multi-modal engineering materials beamline for large unit/cell complex materials	Brent Heuser (University of Illinois Urbana-Champaign)	Ke An
TITAN	Extreme environments (H,P,T) multi-modal instrument emphasizing spectroscopy and diffraction	Collin Broholm (Johns Hopkins University)	Barry Winn
Imaging			
CUPI^{2}D	Imaging of fast dynamic processes in natural and engineered materials	Adrian Brügger (Columbia University)	Hassina Bilheux

Engineering models are being developed for the 12 instruments to define geometry and equipment and support cost estimates

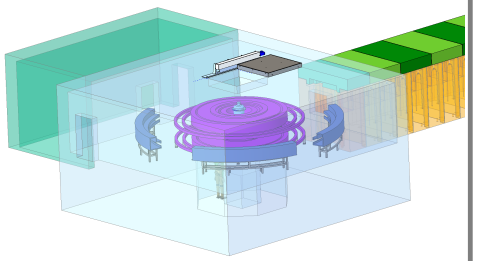
BWAVES



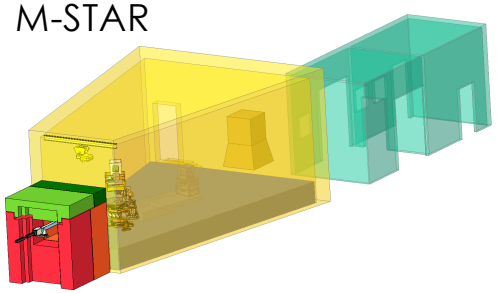
PIONEER



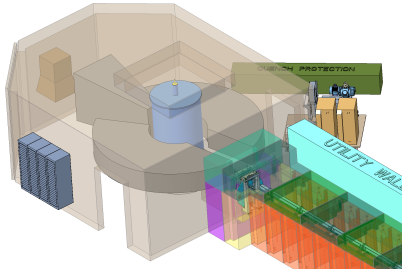
EXPANSE



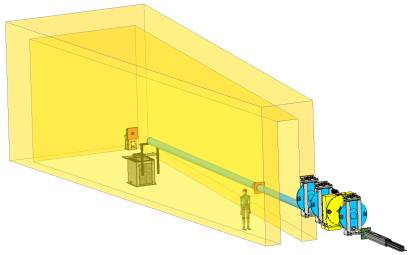
M-STAR



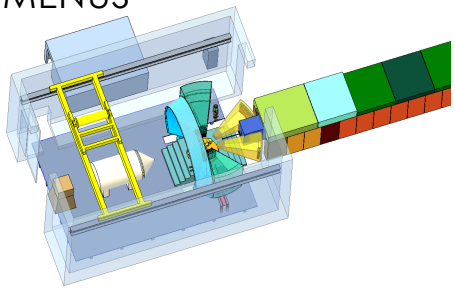
TITAN



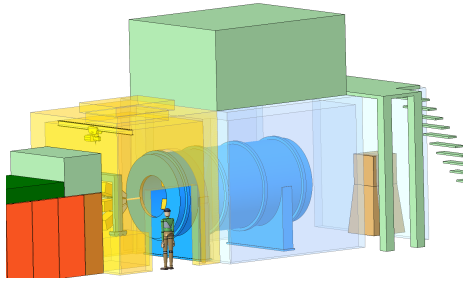
CUPI²D



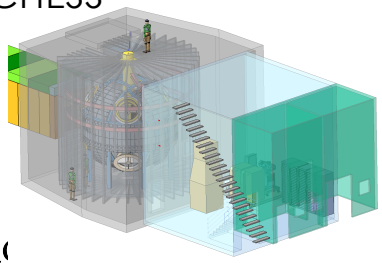
MENUS



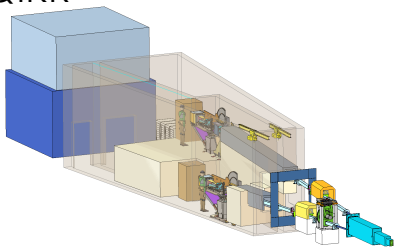
CENTAUR



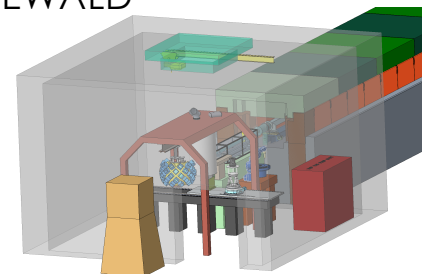
CHESS



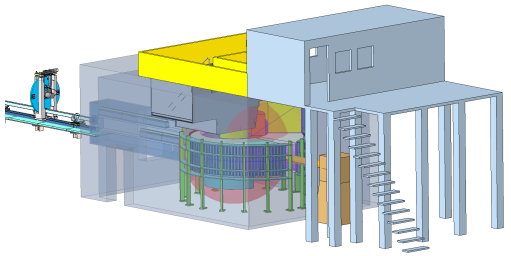
QIKR



EWALD

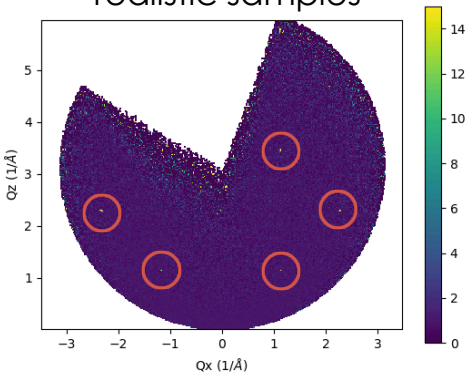


VERDI

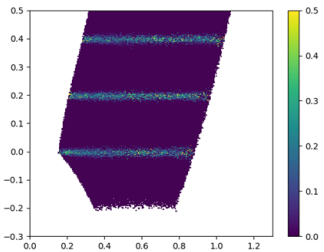


Monte Carlo models supporting instrument performance estimates are being developed

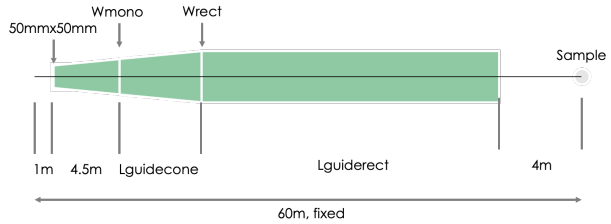
MCViNE is being used to simulate realistic samples



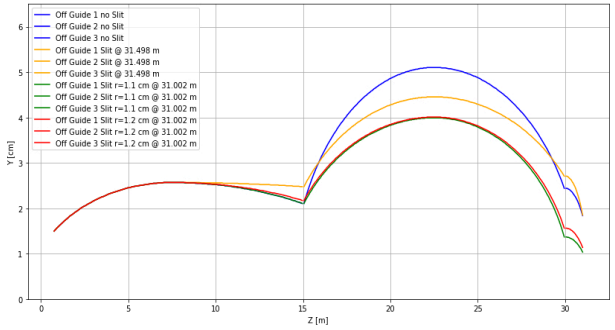
PIONEER simulation of single crystal Si sample



BWAVES needed a new component for the WAVES chopper that has identified parameters for the desired 0.02 meV resolution

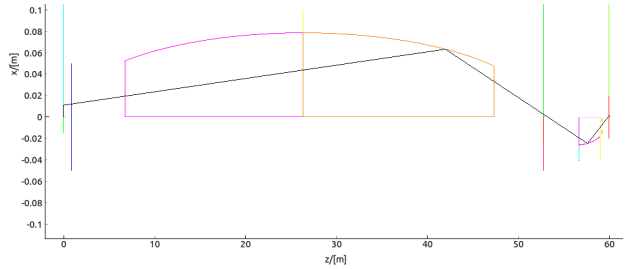


EXPANSE has optimized a guide that must stop outside the precession field, 4 m upstream of the sample

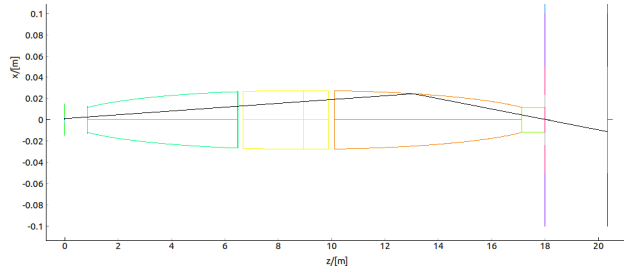


CHESS has used an automated workflow to optimize final guide shapes beyond initial analytic forms

Elliptical guide and mirror elements form the basis of several concepts



PIONEER guide uses elliptical mirrors to optimize divergence and beam size at the sample position with flux of 4.5e8 n/cm^2/s integrated over 2 Å to 6 Å, 5 mm x 5 mm max sample size



CUPI^{2}D guide creates a virtual source L/D resolution has flux of 9e8 n/cm^2/s integrated over 1.7 Å to 14 Å (white beam), 4 cm x 4 cm field-of-view

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Support team: Matt Frost, Thomas Huegle, Jiao Lin, Ducu Stoica

Full proposal template provides guidance to address the selection criteria

- Cover Page
  - Title, team spokesperson name, affiliation, contact information, team member names, proposal role and affiliation, and an abstract of 200 words or less.
- Science Case
- Anticipated User Community
- Instrument Description
  - Discussion of the physics parameters and design of the instrument and how they support the capability requirements derived from the science case.
  - An engineering concept illustrated through drawings that describe the geometry, desired location, and footprint of the instrument.
  - A table of key instrument components and their locations (this table will be provided by STS engineering staff).
  - Evaluation of the instrument performance typically demonstrated by Monte Carlo simulations modeling neutron transport and scattering from a prototypical sample. Analysis may also include scaling arguments based on existing instrument performance and projected source parameters.
  - Analysis of the feasibility of the instrument concept that discusses the use of existing technology and any need for R&D to realize the full capability of the instrument design.
- Use of Unique STS Source Characteristics
- Estimate of Instrument Cost (This section will be provided by STS Project staff)
- References and Team Members Biographical Sketches
- Supporting letters from researchers who intend to use the instrument

Next steps

- Proposal teams complete full proposals and submit by April 30
- Instrument Review Committee (IRC) evaluates full proposals during May
- Virtual meeting of IRC is being finalized for a time in the first half of June
  - Proposal teams will present instrument
  - IRC will formulate recommendation for instrument priorities
- Management and stakeholder discussions in mid- to late-June
- Proposal teams notified of final outcomes and announcement made to the user community at the end of June

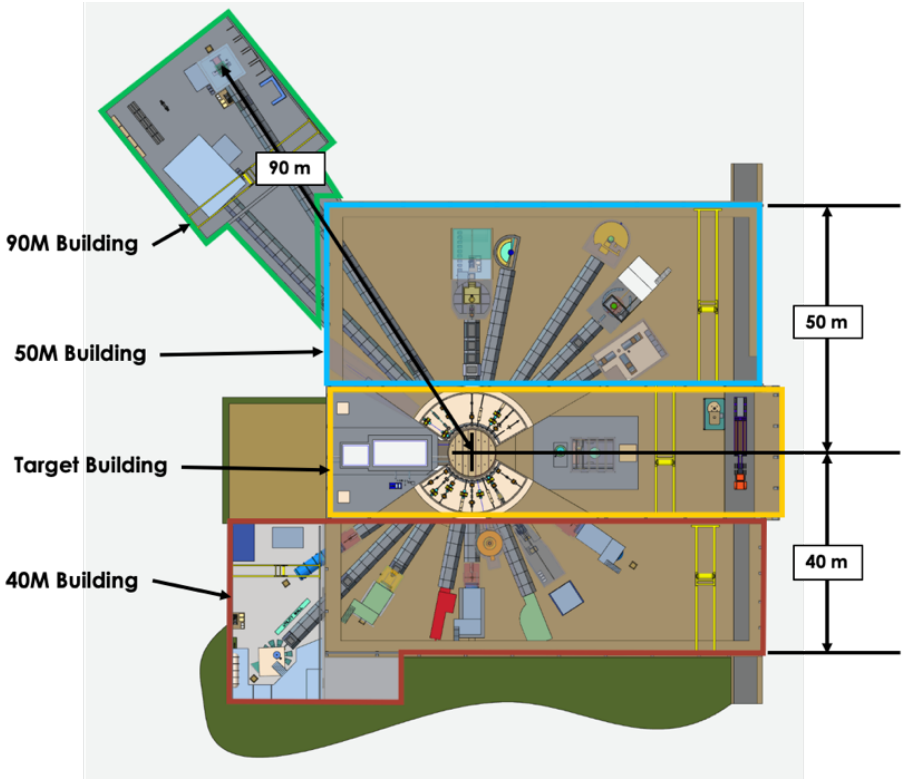
Questions

STS website: https://neutrons.ornl.gov/sts

Backup material

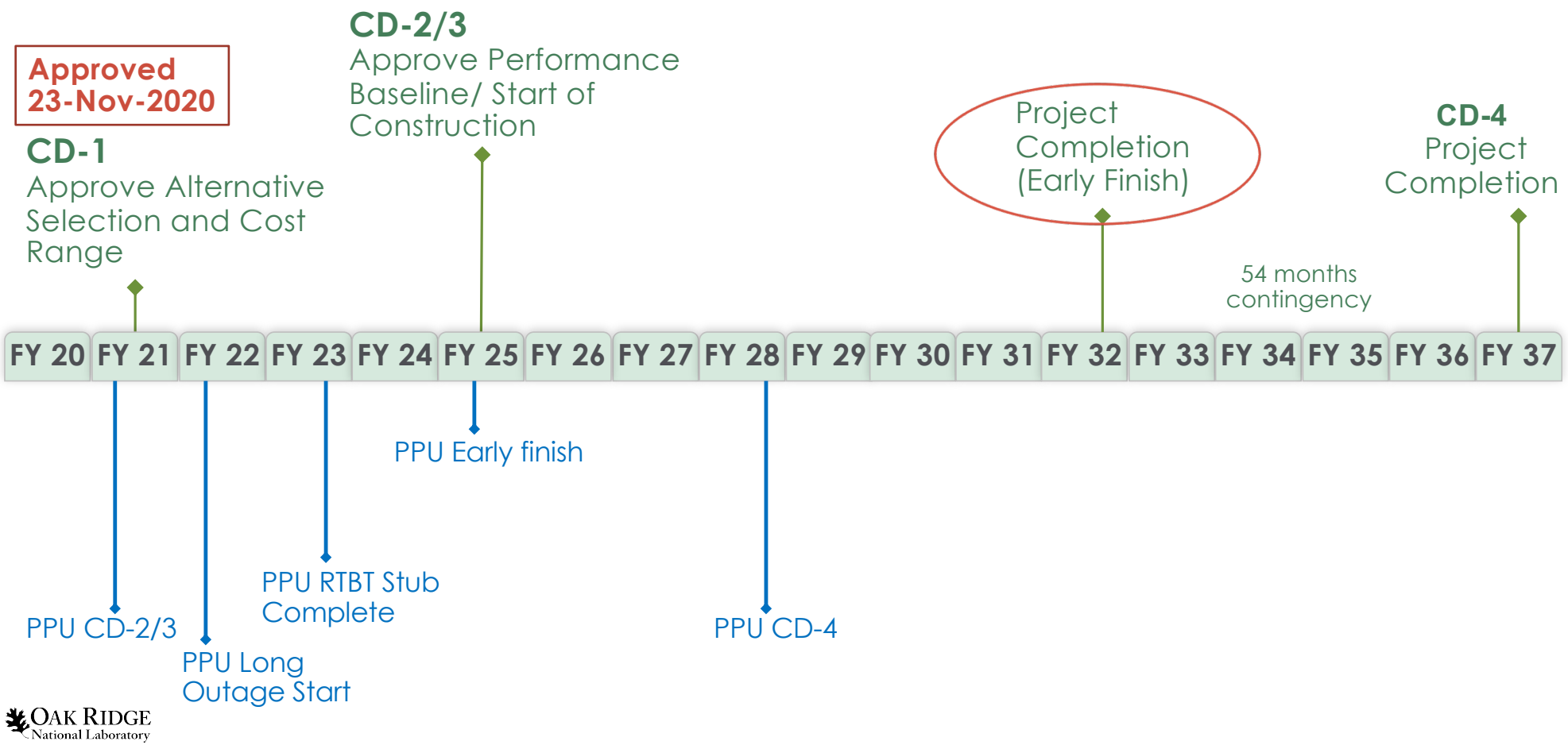
STS Instrument Systems will complete 8 world-class instruments ready to begin commissioning with neutron beams

- STS will have the capacity for 22 beamlines
- Instrument Systems includes Scientific Software that extends current reduction/analysis software to support 8 new STS instruments
- Instrument Systems includes an initial suite of sample environment equipment to support the early science programs
- Instrument Systems includes bunkers as a near-monolith, integrated shielding solution



Schematic view of the Target Building and Instrument Halls with 16 notional instruments illustrated.

STS Critical Decision (CD) dates with PPU milestones



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The roles of proposal team members are aligned with the principles for instrument selection

- Spokesperson(s) – coordinate development of the science case and definition of the instrument science capability requirements, submit proposal to STS, discussions with the STS Instrument Review Committee
- ORNL Point-of-Contact – coordinate development of the instrument technical/concept development and access to ORNL resources (e.g., engineering and modeling support), discussions with the STS Instrument Review Committee
- Proposal team members – contribute to the science case and technical descriptions as appropriate
- Engage with STS throughout the project to provide science and technical advice at key decision points (e.g., review of the design criteria document, selection of sample environment equipment, software validation, planning for and participating in the early science commissioning of the instrument)