2019 National School on Neutron and X-ray Scattering

June 16-29, Argonne and Oak Ridge National Laboratory

PROPOSAL WRITING TIPS

STEPHAN ROSENKRANZ
Neutron and X-ray Scattering Group
Materials Science Division
Argonne National Laboratory

U.S. DEPARTMENT OF ENERGY
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

Argonne NATIONAL LABORATORY

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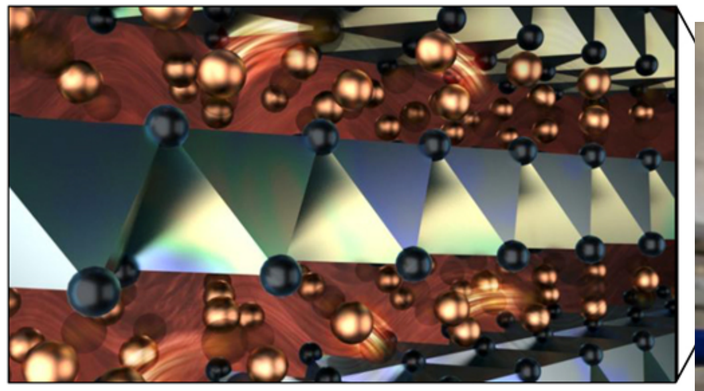
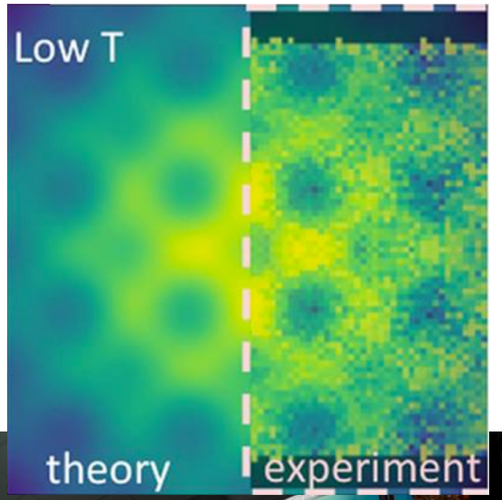
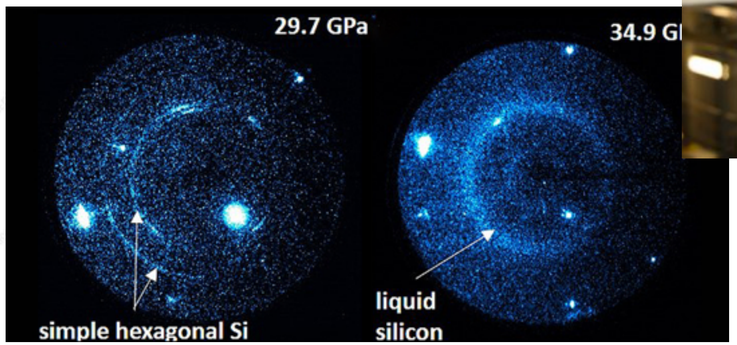
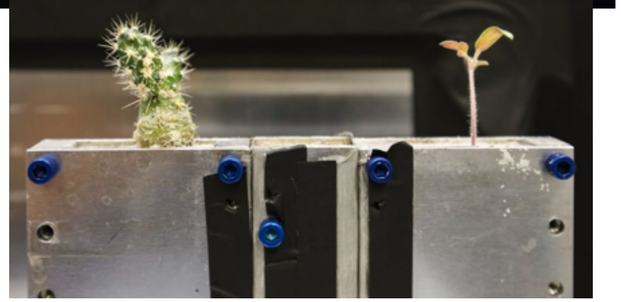
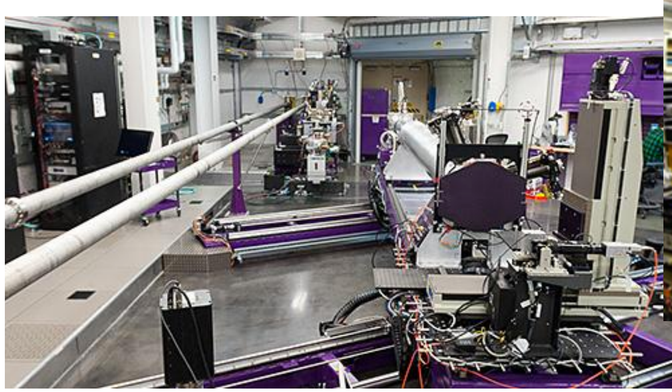
WHAT DO SCIENTISTS WANT?





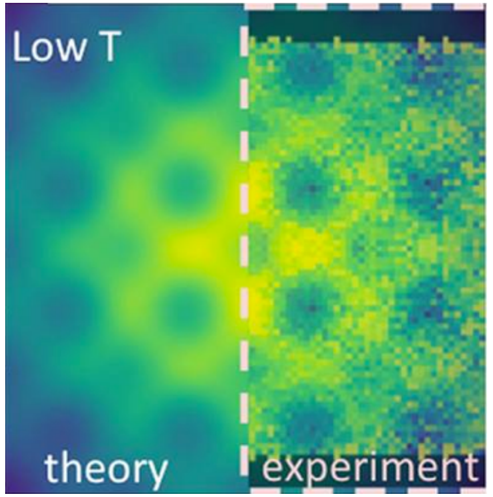






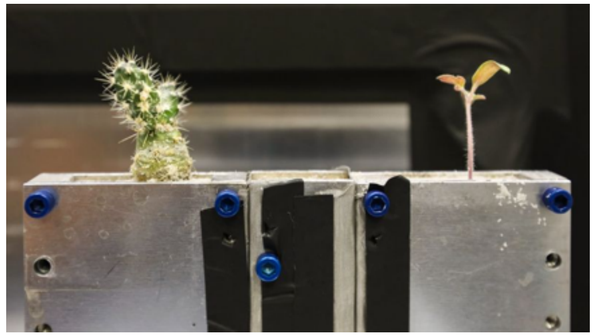
WHAT DO SCIENTISTS DO?

- Need to get funding, beamtine
- Call for proposals
  - write proposals
  - review proposals
  - give presentations
  - (try to) get (more) funding, beamtime



"Still nothing. You sure this is the best computer we have?"

Neutrons Investigate Tomatoes for Insights Into Interplant Chatter



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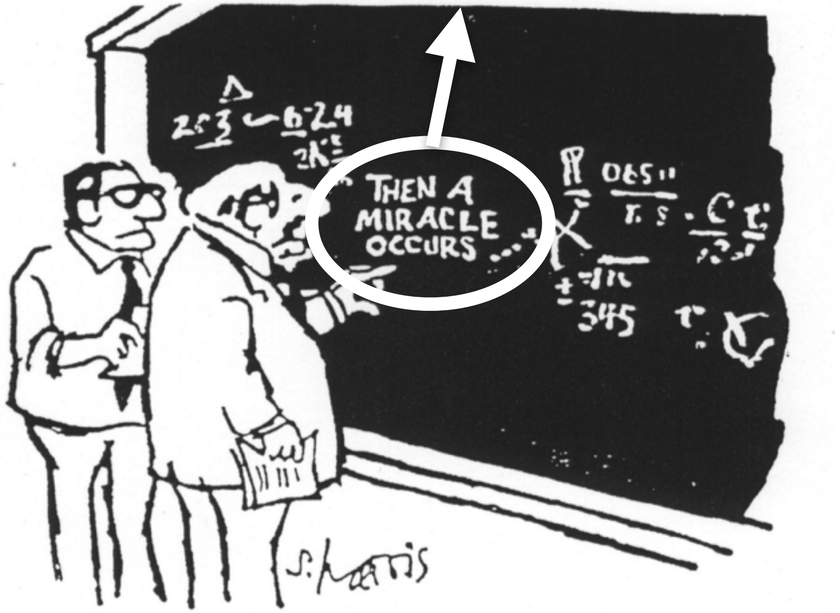

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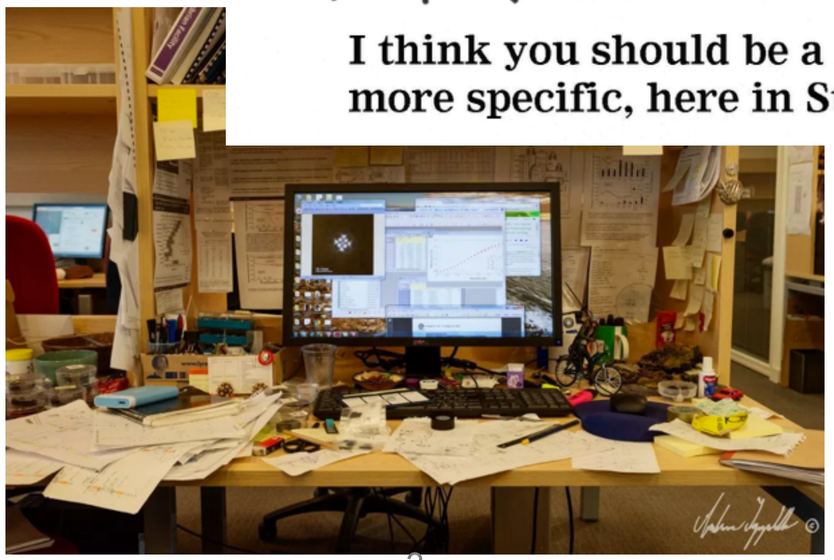


X-RAY AND NEUTRON SOURCES AVAILABLE WORLDWIDE

- **Light Sources summarized at www.lightsources.org**

  ~61 facilities: 48 synchrotrons + 13 free electron lasers (FELs)

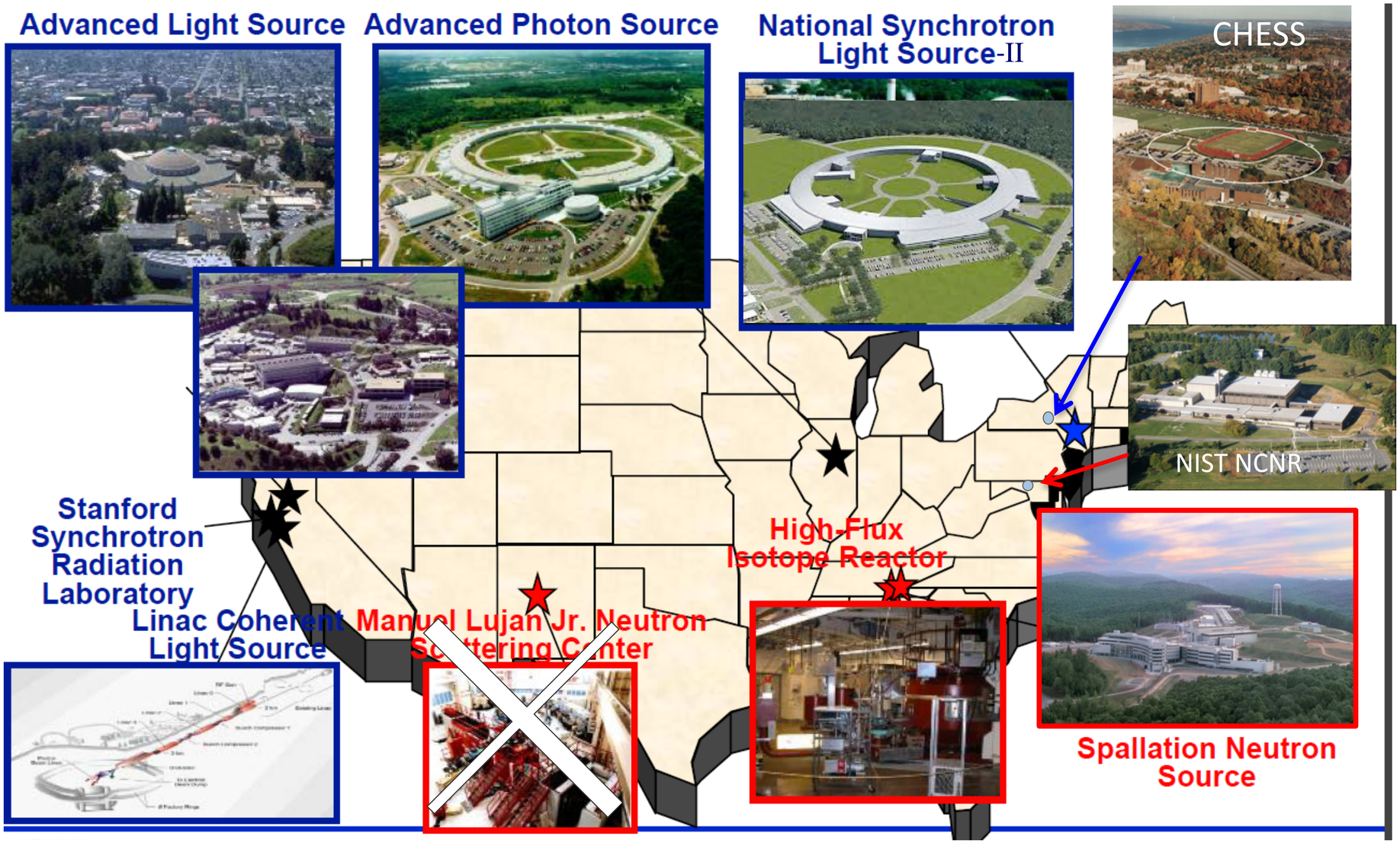
  - European Synchrotron Radiation Facility (ESRF), Grenoble, France
  - SPRING-8, Japan
  - PETRA III, Germany
  - CLS, SLS, Shanghai, DIAMOND, BESSYII, SOLEIL, Taiwan, Pohang, …
  - XFEL.EU, SACLA, FLASH, …

- **Neutron Sources summarized at www.neutronsources.org**

  ~50 research centers:

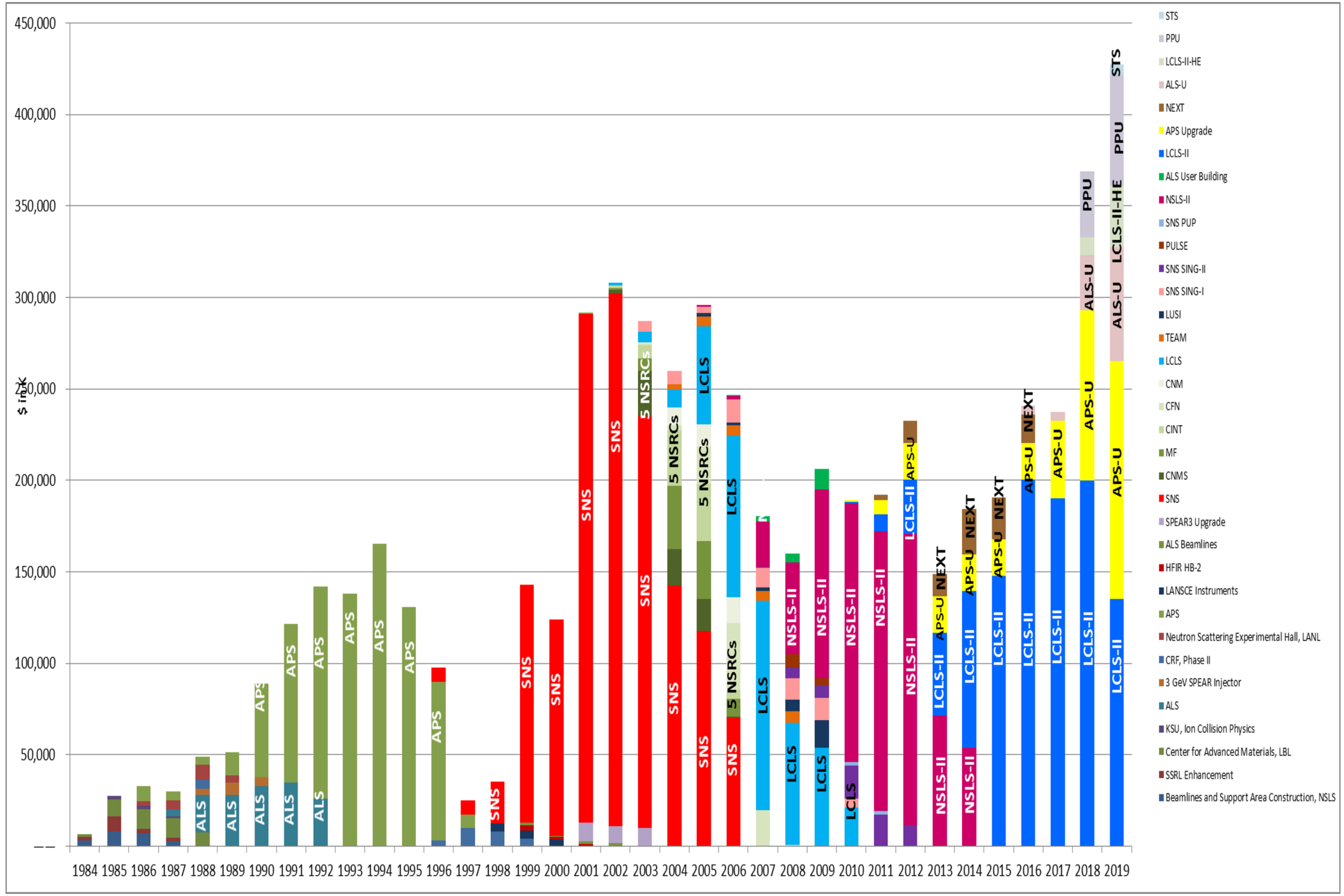
  - Institut Laue-Langevin (ILL), Grenoble, France
  - ISIS UK
  - JSNS at J-PARC, Japan
  - China Spallation Neutron Source, Dongguan (~2018)
  - European Spallation Source (ESS), Lund, Sweden (~2019)

U.S. X-RAY AND NEUTRON SOURCES (MOST DOE-BASIC ENERGY SCIENCES)



Also
5 DOE Nanoscience Centers (BNL, SNL/LANL, ORNL, ANL, LBNL)
3 DOE Electron Microscopy Centers (ANL, LBNL, ORNL)

BES Construction/MIE Funding Profile 1984 – 2019



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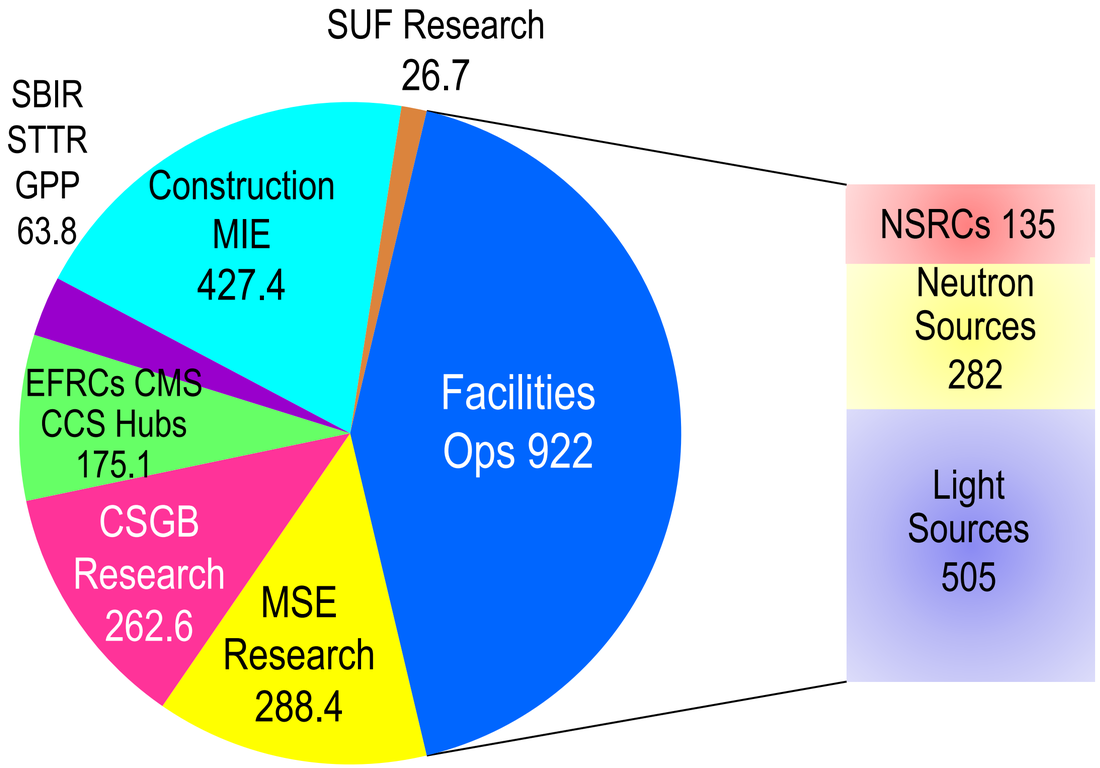
FY 2019 BES Budget:
$2166.0M (+$76M or +3.6% from FY 2018)

Research programs

- Core Research will emphasize quantum information science, data science for discovery, and BRN topics ($551M).
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($110M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).



Scientific user facilities

- Operations of 12 facilities at nearly 100% optimal level ($922M; **Δ=+$23.4M**)

Construction/MIE* **Δ=+$58.4M**

- Last year of funding, LCLS-II ($135.4M)
- APS-U ($130M), LCLS-II-HE ($34M), ALS-U ($62M), PPU ($60M)
- One new start: STS ($6M)

*includes OPC

Research at APS Contributes to 2018 Chemistry Nobel Prize

Scientific Achievement

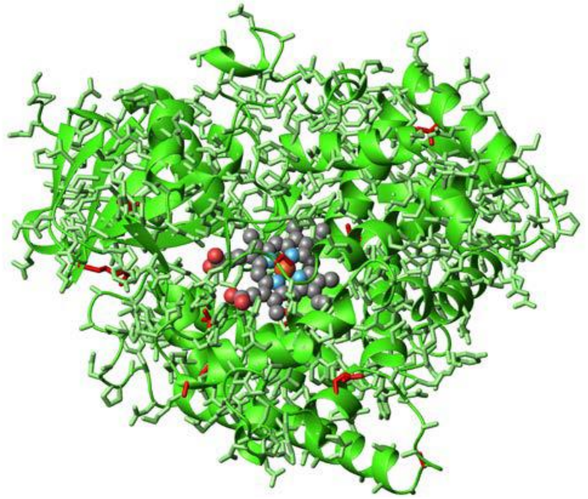
Dr. Frances Arnold (California Institute of Technology) was 1 of 3 2018 Chemistry Nobel awardees for work showing how “directed evolution” can be used to develop proteins or enzymes that have desired enzymatic activity, which can be used to produce chemicals, biofuels, and pharmaceuticals.

Significance and Impact

“The structures were critically important to advancing and understanding the overall evolutionary design successes for which Dr. Arnold has been recognized,” said Matthew Redinbo, William R. Kenan Distinguished Professor of Chemistry, Biochemistry, Microbiology, and Genomics at the University of North Carolina at Chapel Hill, who collaborated on the study.

Research Detail

As part of this research, samples of the enzymes that were created were studied utilizing the General Medical Sciences and Cancer Institutes beamline 23-ID-D at the Advanced Photon Source (APS), a U.S. Department of Energy Office of Science User Facility.



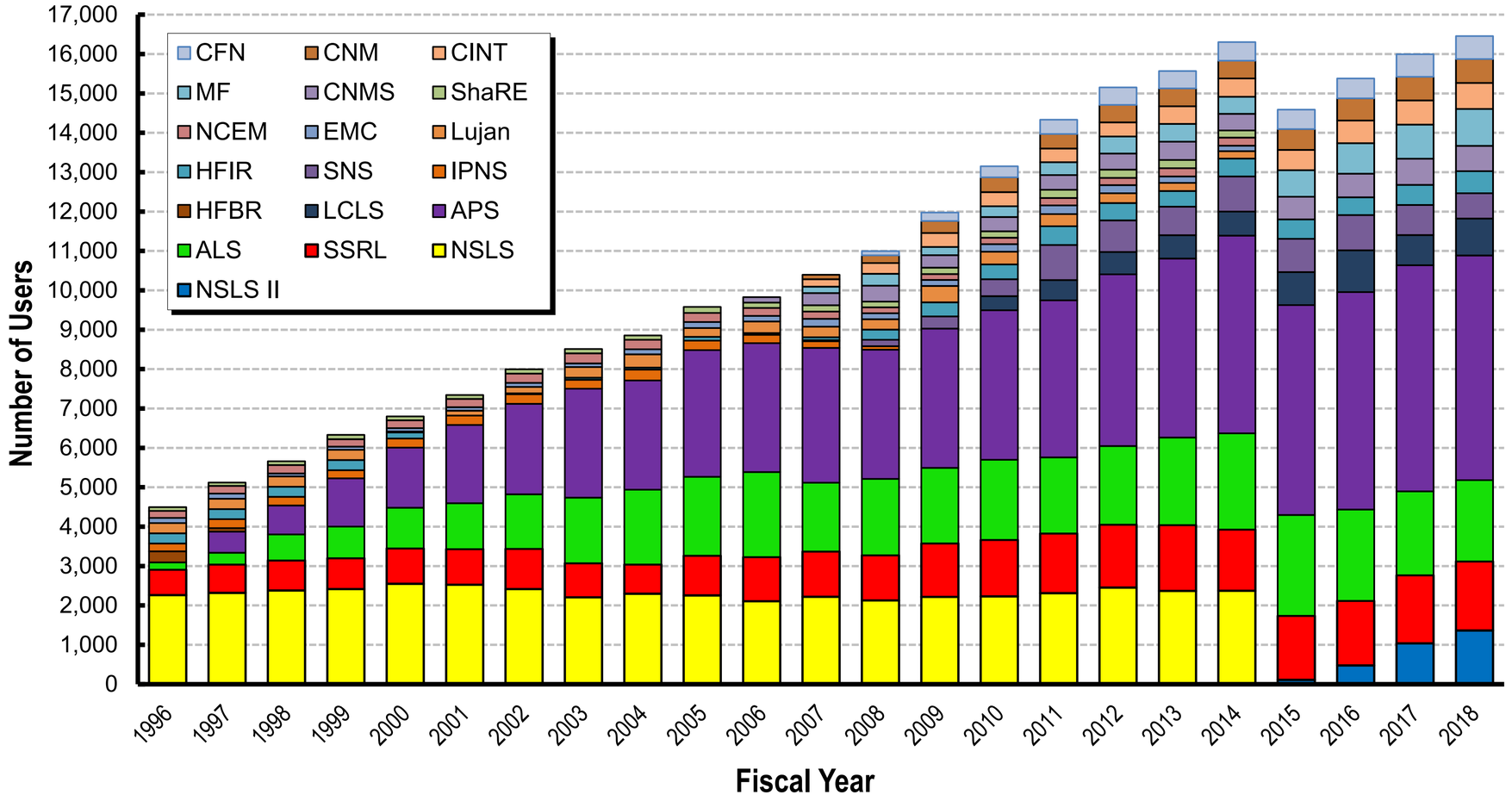
Structure of an evolved biocatalyst for cyclopropanation, determined at the APS.

See: P.S. Coelho et al., Nat. Chem. Biol. **9**, 485 (2013). DOI: 10.1038/nchembio.1278
Contact: frances@cheme.caltech.edu

Scientific Background on the Nobel Prize in Chemistry 2018, “DIRECTED EVOLUTION OF ENZYMES AND BINDING PROTEINS,” 3 OCTOBER 2018, https://www.nobelprize.org/uploads/2018/10/advanced-chemistryprize-2018.pdf

Work performed at Argonne National Laboratory

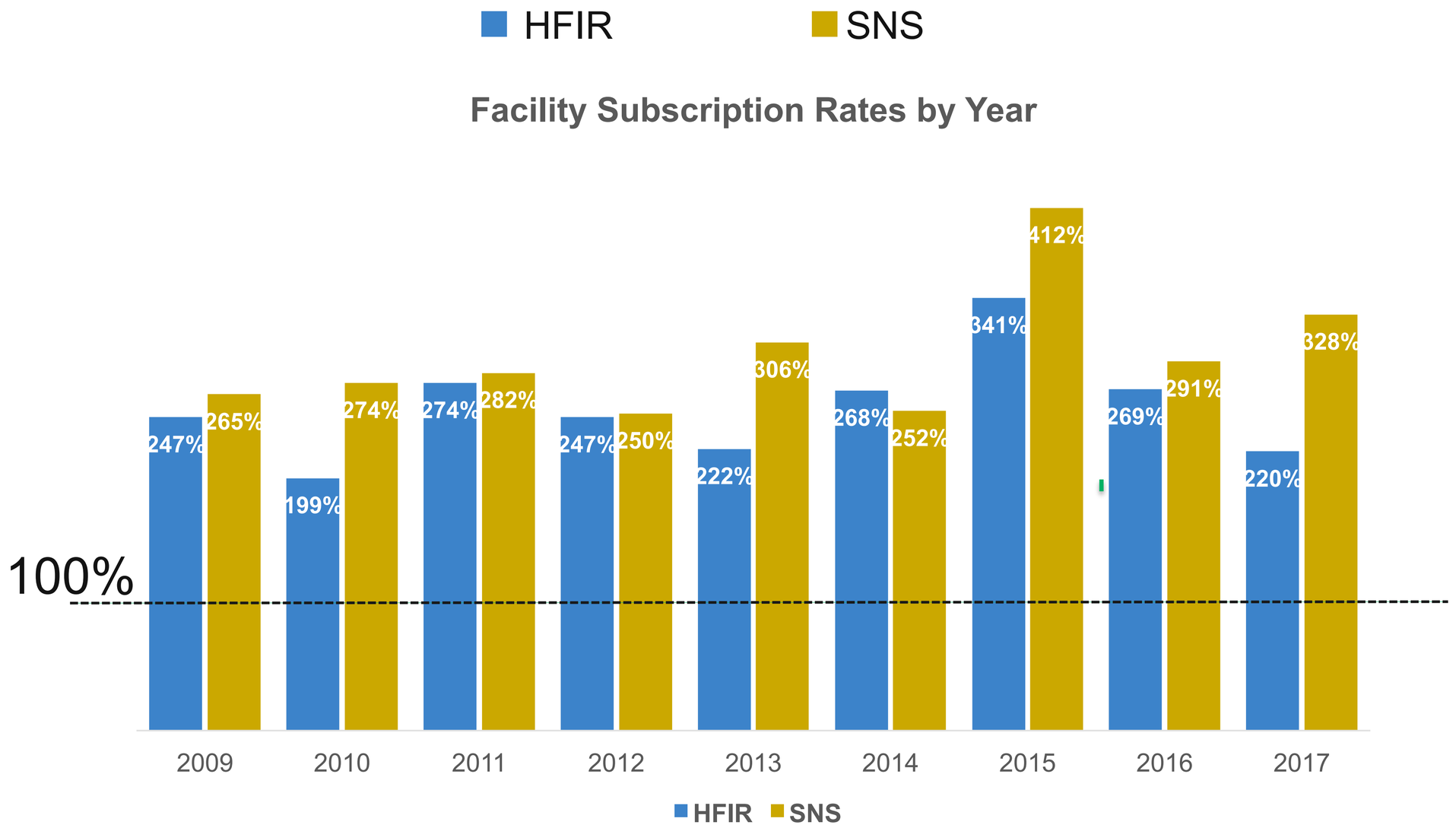
BES User Facilities Hosted >16,000 Users in FY 2018



More than 300 companies from various sectors of the manufacturing, chemical, & pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

BOTH SNS AND HFIR ARE OVERSUBSCRIBED

Getting beam time is not guaranteed



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BASICS OF THE FACILITY PROPOSAL SYSTEMS

How do I get beam time at a User Facility?

- All DOE, NIST, and NSF neutron and x-ray sources offer access to beam time through an experimental proposal system. “General Users (GU)”.

- Proposal submission is done through a web-based application. When and how often proposals are submitted varies by facility.
  - APS, NSLS-II three times (“cycles”) per year.
  - SNS/HFIR, ALS, LCLS two times per year

- All proposals are peer-reviewed and rated, and beam time is allocated based on the scores of these reviews. Once time has been allocated, the beamline staff schedule the proposals.

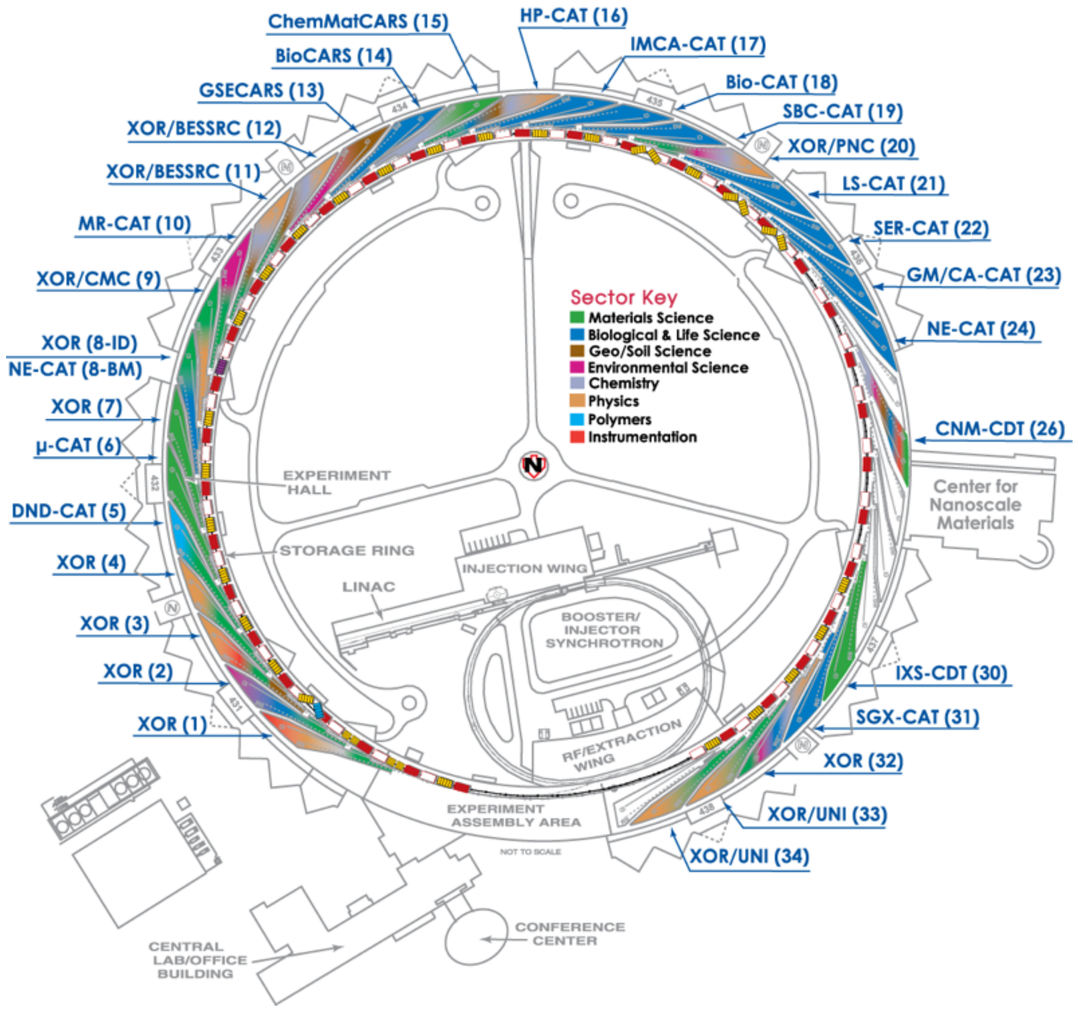
AMOUNT OF GENERAL USER TIME AVAILABLE

APS/NSLS/SSRL/ALS

- ✓ All beamlines offer GU beam time.
- ✓ Most DOE/NSF funded beamlines provide 80-100% of their time to general users.

SNS/HFIR

- ✓ Amount varies by instrument.
- ✓ ~75% of time will be for general users.



For most, you can search facility websites by technique or by beamline. Quality of proposal websites varies.

PROPOSAL DEADLINES

X-ray sources (cycles/yr)	Deadlines
APS (3)	July 5, 2019 (every 4 months)
ALS (2)	Sept 4, 2019 (every 6 months)
NSLS-II (3)	Sept 30, 2019
LCLS (~2)	down for upgrade
SSRL (3)	May 1, Aug 1, Nov 1
CHESS	July 8, 2019 (8 am)

Neutron sources	
HFIR (2)	currently not operational
SNS (2)	soon
NIST-NCNR (2)	~ October and April

- These are hard deadlines.
- APS at Friday midnight, central time (12:01 → next cycle)

Get Started with Assistance From the Instrument Scientists

- Study facilities and instrument web pages
- **Contact an Instrument Scientist to discuss your research**
  - What is the research problem?
  - Which instrument(s) are appropriate? (scores?)
  - How mature is the research project (risk, size)?
  - What is the material – sample composition, form, size, availability?
  - What are the experimental conditions
    - temperature, pressure, magnetic field, *etc* ?
  - What will be measured?
  - Probability of success? Impact? Significance?
  - How will results be presented and to whom?
  - What is the timeline?

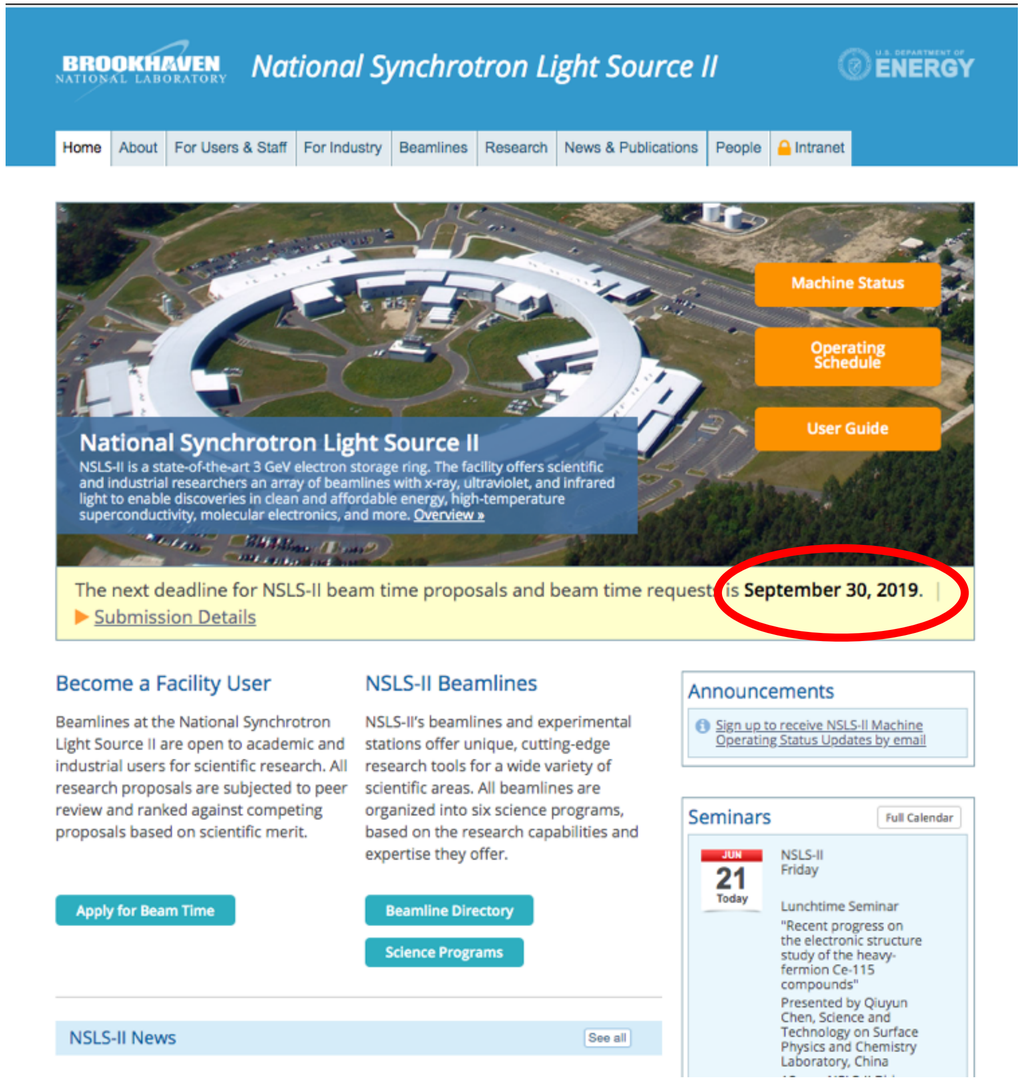
Instrument Scientists Assist First-time and Returning Users

- **Provide technical advice, guidance, and assistance**
  - **Instrument options**
  - **Sample and experiment preparation**
  - **Number of experiment days**
  - **Logistics (scheduling, transporting and storing samples)**
  - **Proposal preparation tips and assistance**
  - **Experiment team members**
  - **Data analysis**
  - **Publication considerations**
- **Consider beamline staff as collaborators**

Submitting a proposal

Facilities generally have link on home page

NSLS-II



Submitting a proposal

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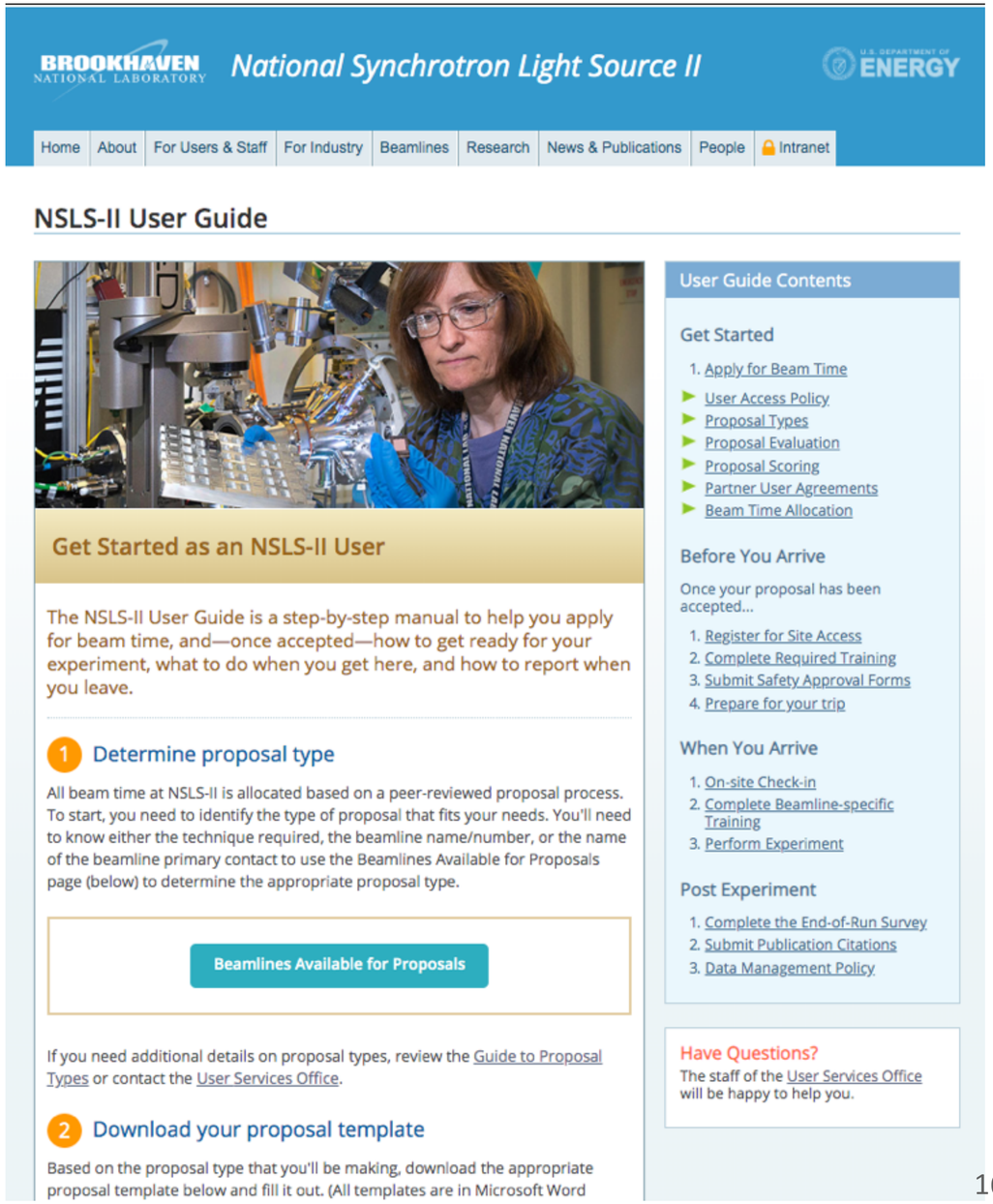
NSLS-II



Submitting a proposal

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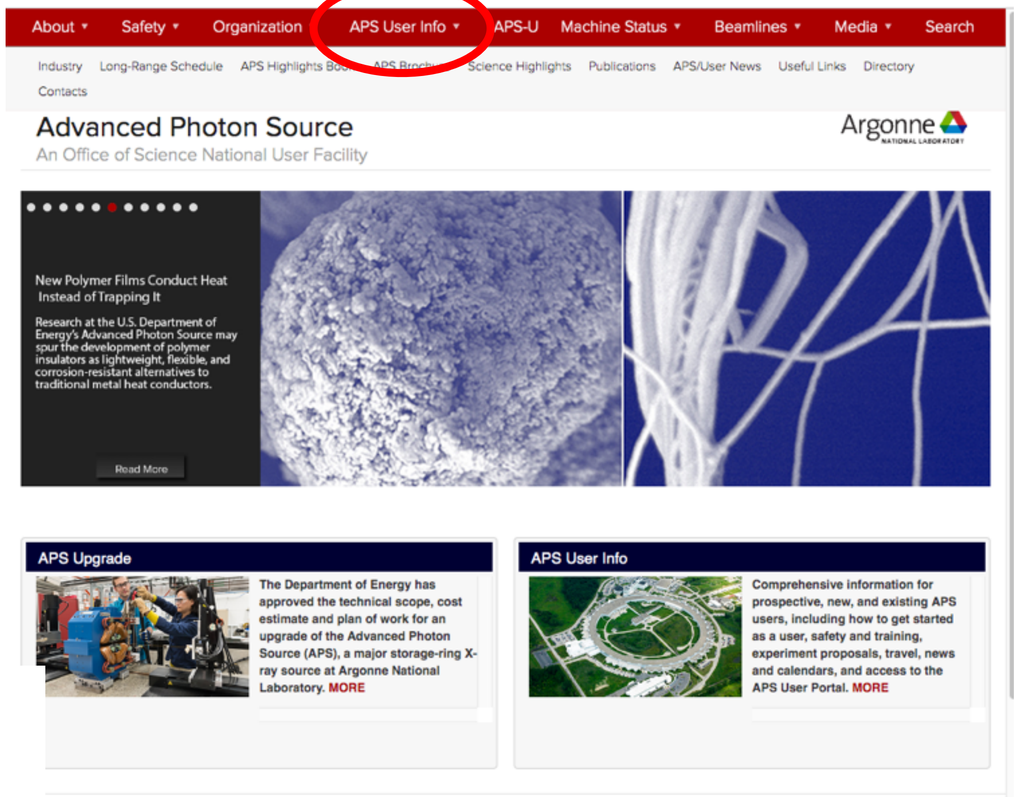
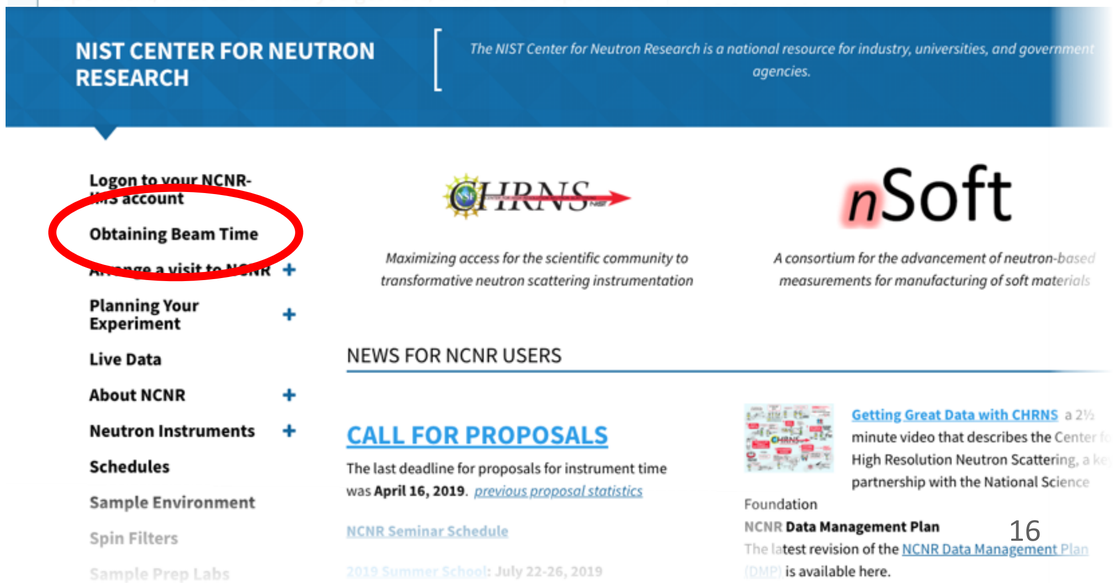
NSLS-II

APS



NIST



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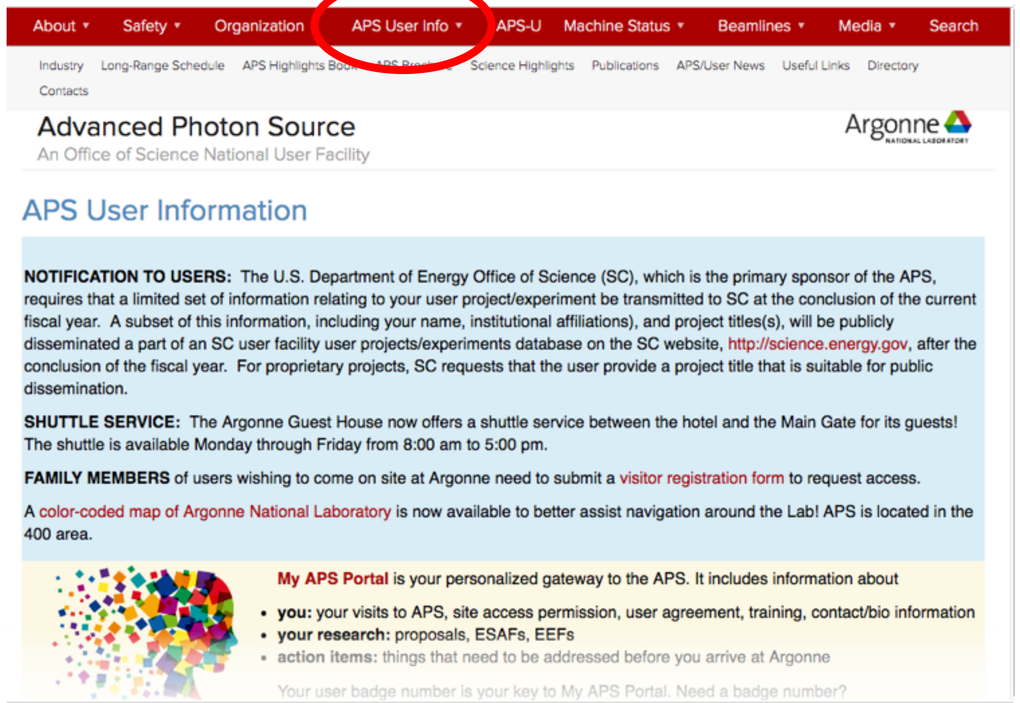
Submitting a proposal

Facilities generally have link on home page

NSLS-II

APS



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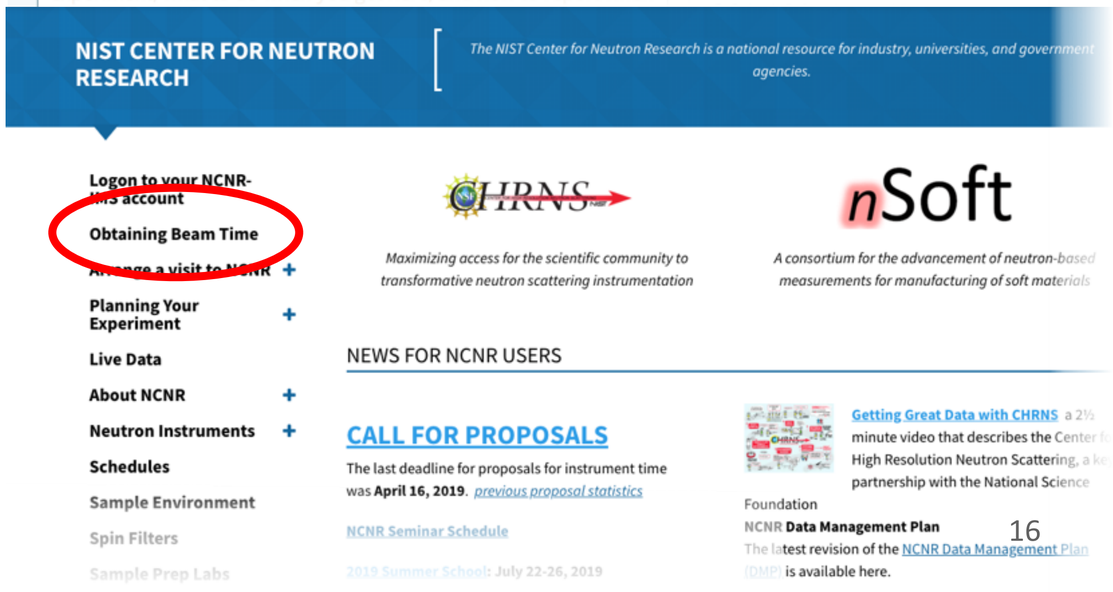
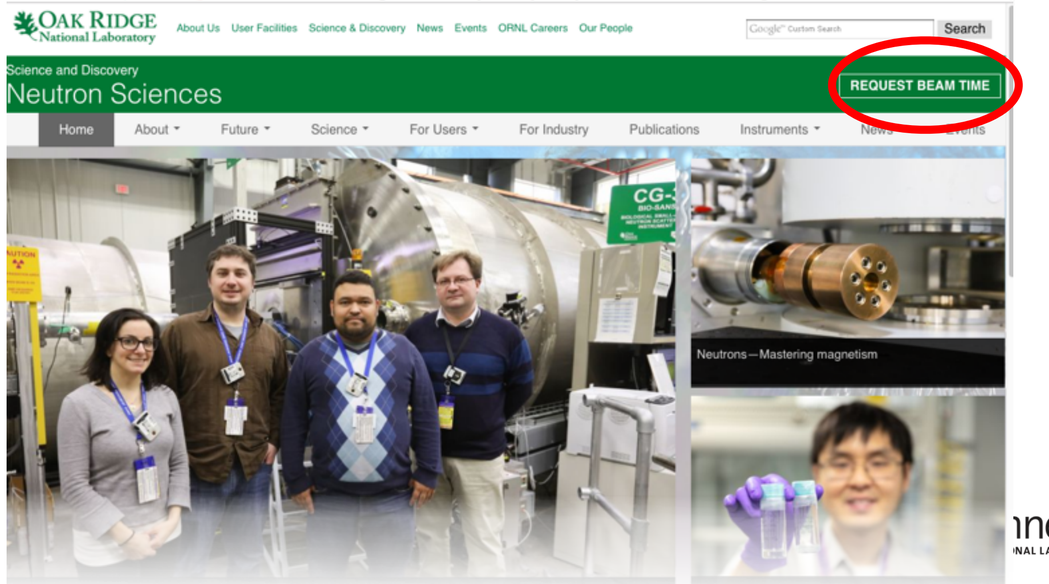


SNS
HFIR



Different types of proposals allow facility flexibility

Each facility has particular systems or proposal modes:

APS

GUP - General User Proposal are valid for two years or until recommended shifts are fully used. A beam time request has to be submitted for each cycle for which the proposal is to be considered.

PUP – Partner User Proposal - Groups whose work involves a greater degree of collaboration with the APS. (e.g. major new instrumentation or technique).

Rapid Access Mail in Powder Diffraction for 11-BM, 11-ID, 17-BM. Very easy , they send you capillary tubes.

Rapid Access General User Proposal is valid for a single cycle, single Beam Time Request

CHESS – Cornell

Standard Proposal is good for two years from the date of review and acceptance. After a proposal has been reviewed and accepted, it generates its first beam time request. A Beam Time Request (BTR) must be submitted for every following cycle for which a user requests beam time.

Fesibility study proposals are only granted for one time access to test something never done before.

NIST Center for Neutron Research

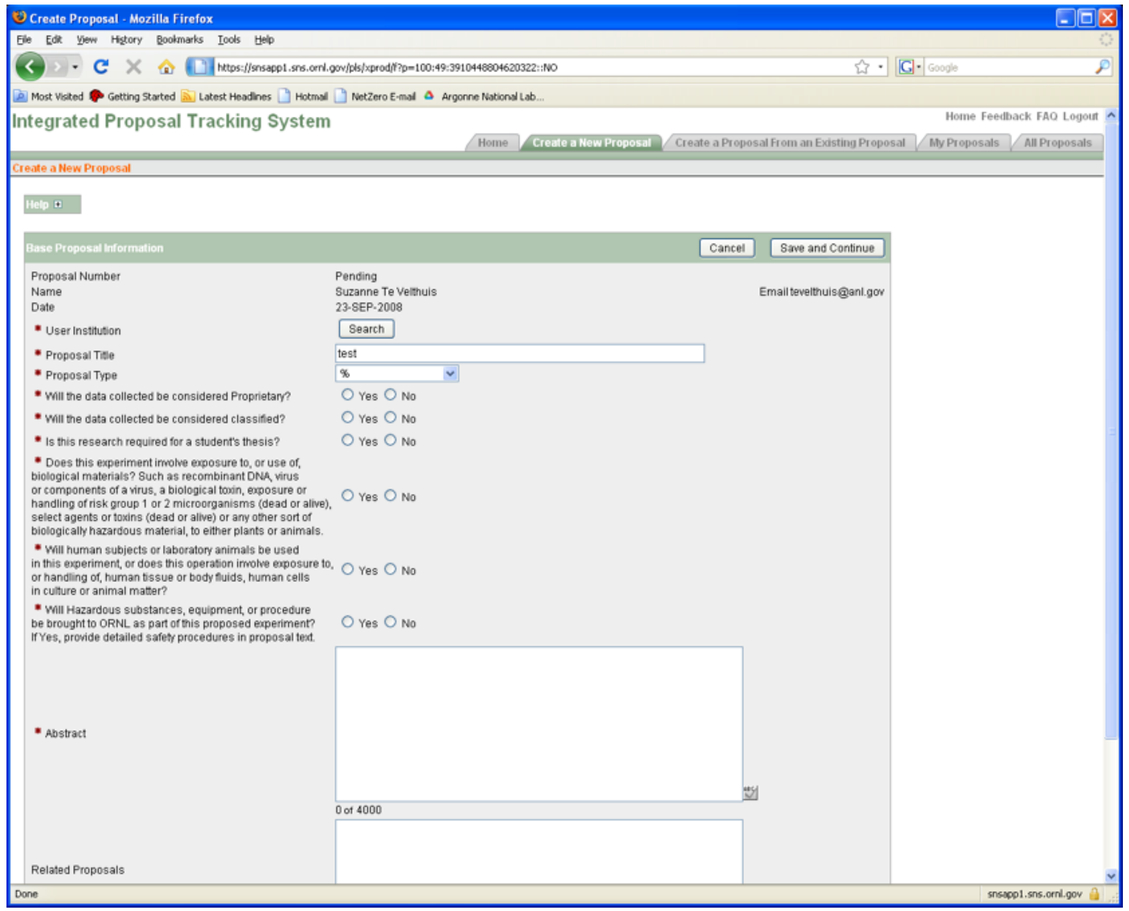
New Proposal Regular proposal (including continuation) for one beam time access, reviews by Committee (BTAC)

Quick Access Proposal for experiments that cannot be delayed. Reviewed by BTAC but held to higher standard

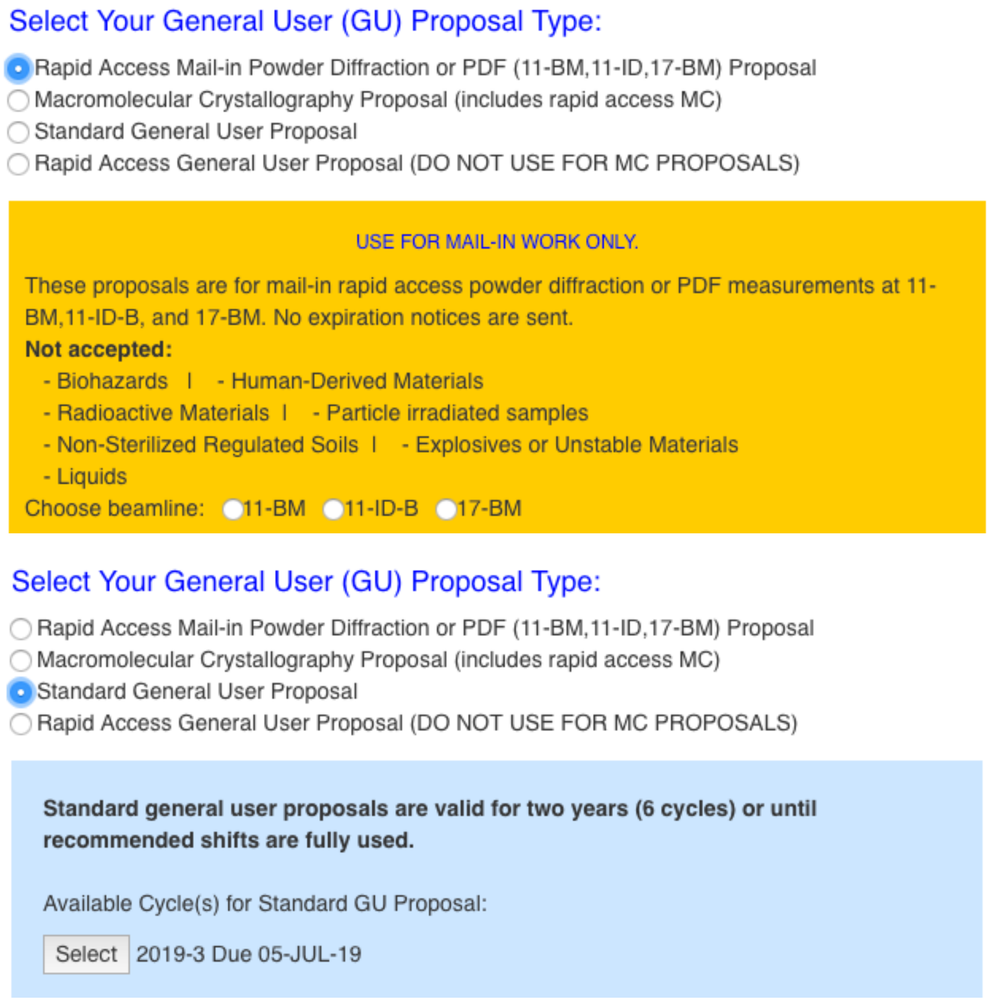
Beam Time Request is a request for part of the instrument time reserved for NIST internal research programs. Such requests may be made by external users through collaborative research projects with a NIST Staff member

Proposal forms at SNS and APS

SNS/HFIR



APS



Each proposal system will ask very similar questions

Proposal forms at SNS and APS

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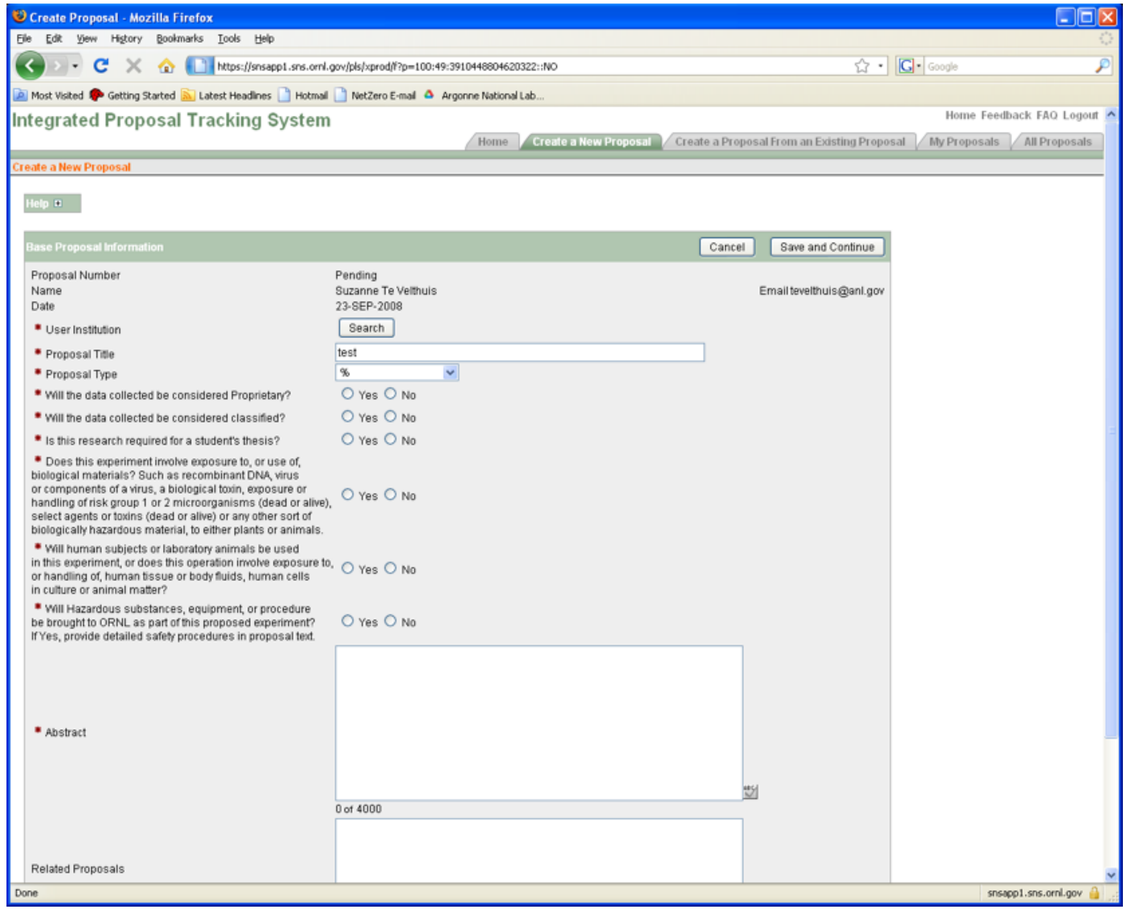

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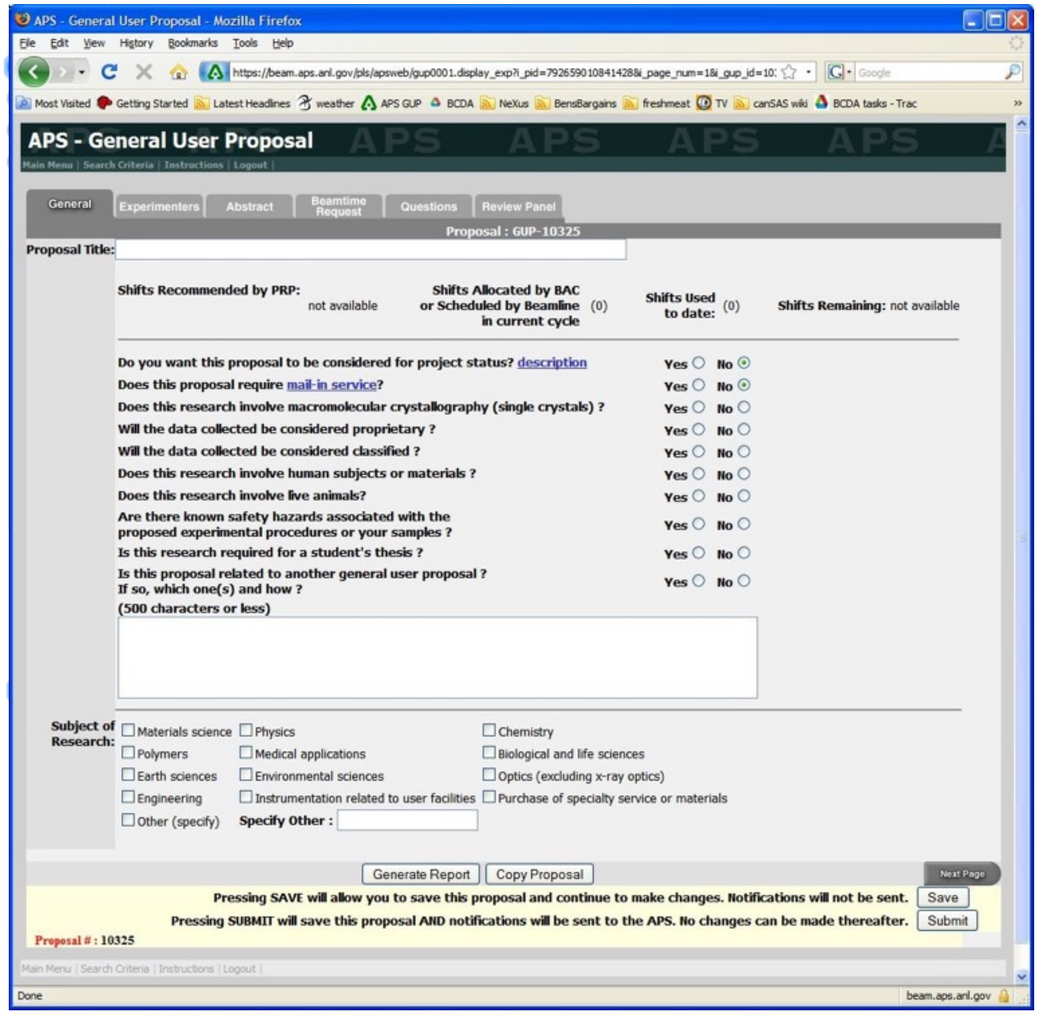
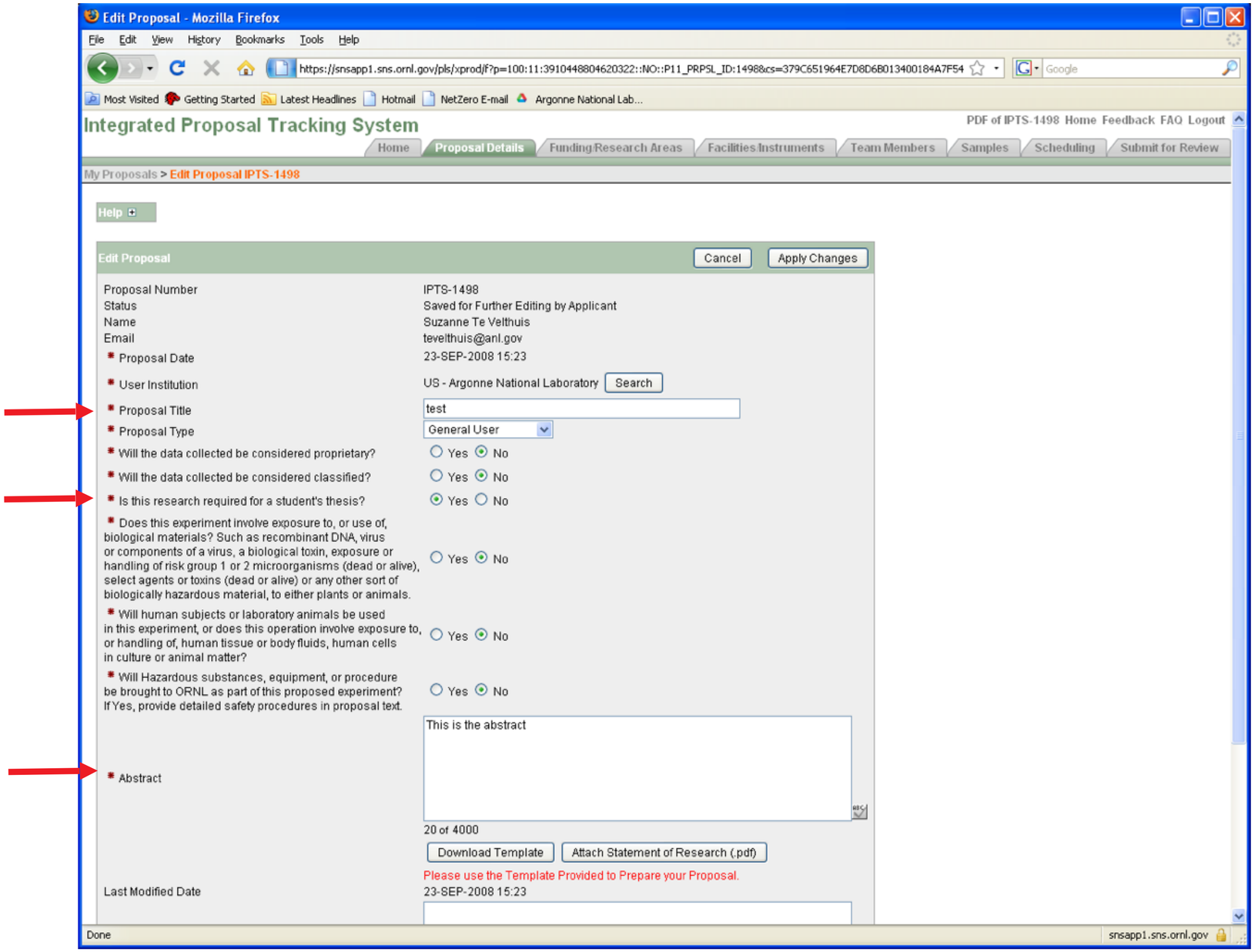


Each proposal system will ask very similar questions

Questions asked

- Proposal Title
- General Info (Title, Experimenters, Funding source, etc.)
- Abstract - What is the ***scientific importance*** of the proposed research?
- Why do you need the facility to do this research?
  - (Neutron vs. X-rays) or (Neutrons + X-rays)?
  - Why do you need an insertion device beamline instead of a bending magnet?
  - Spallation source vs. reactor source
  - Hard X-rays vs. Soft X-rays
- Why do you need the beam line (and/or instrument)?
  - Particular technique or sample environment
- What previous experience / sample characterization / results do you have (pubs important)?
- Describe the proposed experiment(s), including samples and procedures. Show that you're prepared.
- Justification of the amount of time requested. Don't be greedy or unrealistic about time needed. Ask beamline staff if not known from previous experience.

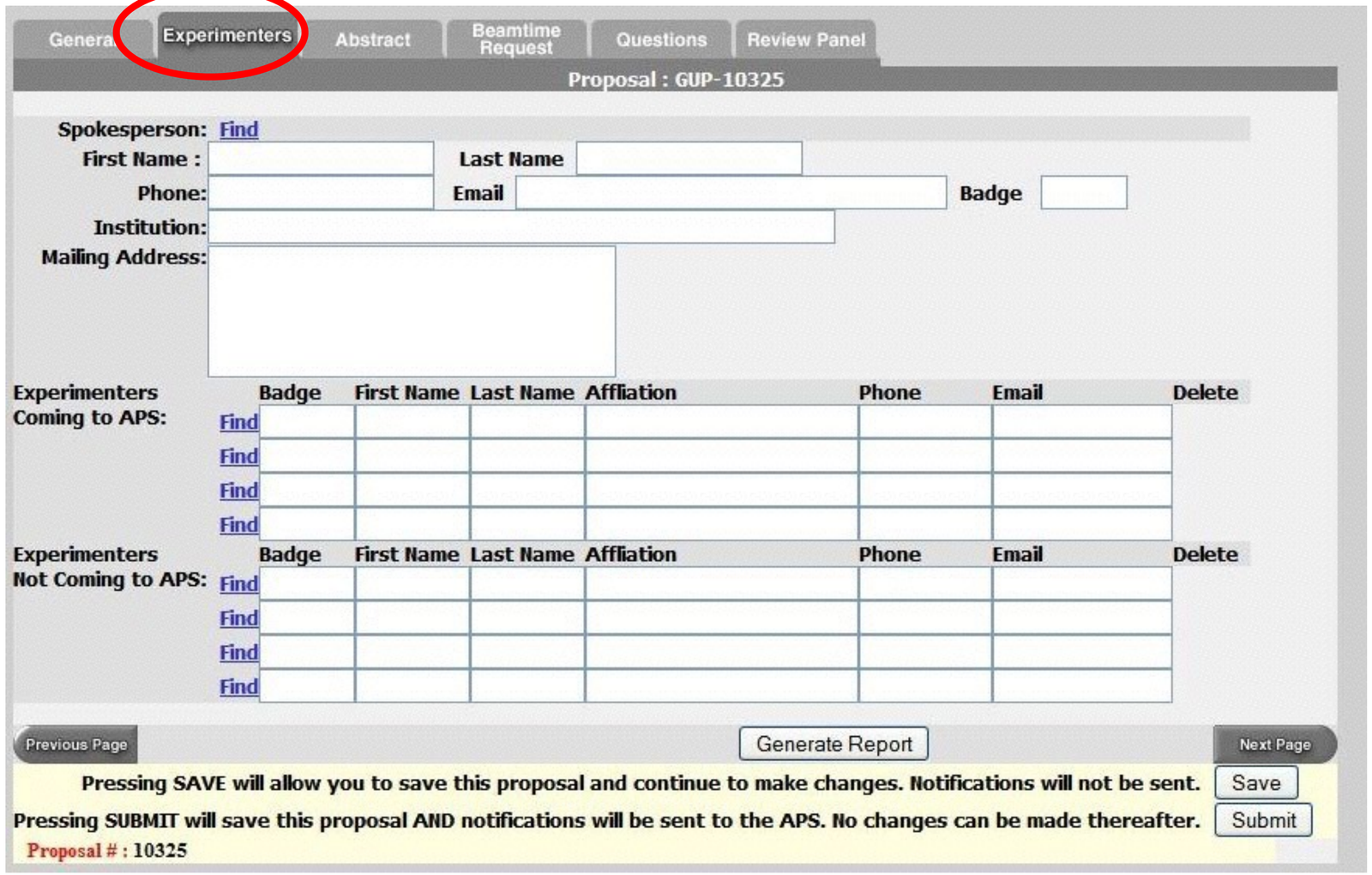
General Information



Proposal: General information

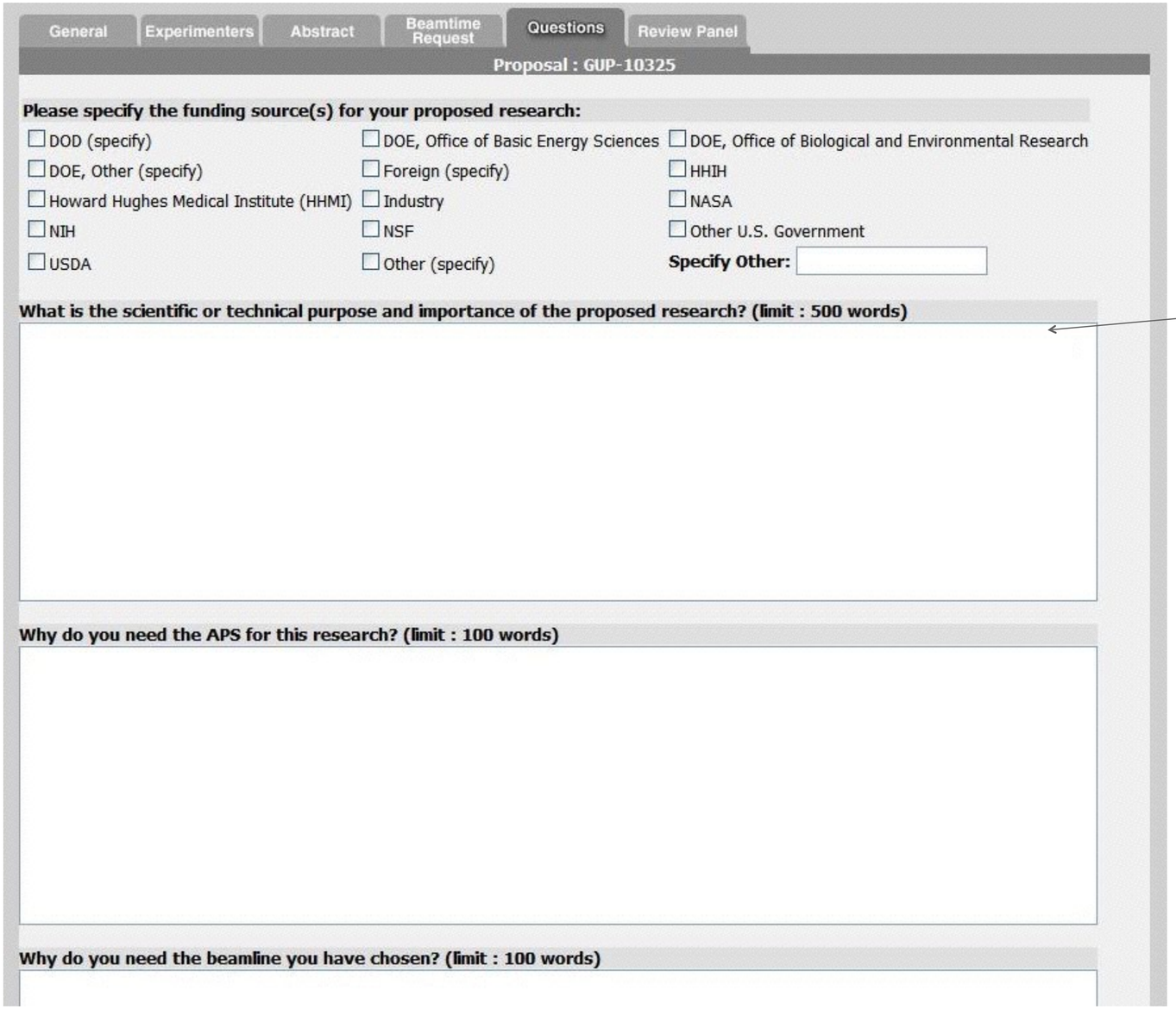
- Pick a good title. Specific and to the point is better than spectacular and vague. Spectacular and specific is fine if credible.
  - Good: “XAS study of Fe valence in CaFe2As2 under pressure ”
  - Bad: “Understanding superconductivity in superconductors”
- Is it thesis related? Is there a deadline?
  - May push your proposal up if scores are close
- Fill in the abstract - this is where the reviewer develops first impression.
  - Do not just upload a PDF document! Creates more work for reviewer.
  - Scientific merit in abstract is most important criteria for the score.
- Do upload a figure from previous work
  - shows how you made use of previous beamtime
  - Do NOT upload 20 pages of supplemental materials. Only a few figures to help your scientific case

Proposal: Experimenters page



- Use the “find” feature
- List everyone involved in experiment
- Even theorists are useful to show impact / readiness of the team to interpret results

Experiment Description



Note guidance!

Don't write one sentence or 1000 words.

Do not use undefined jargon or acronyms that could frustrate reviewer!

Experimental Details

- Give background information why it is important.
  - Science at facilities is very diverse. Reviewer is not necessarily an expert on your subject. Try to capture imagination of reviewer with basic idea.
  - Each committee gets many proposals each cycle. Proposal needs to be clear and concise.

- Clearly state what you want to measure and how
  - Give some details. Temperature range, X-ray Energy, Sample geometry
  - What sample characterization has been done already (XRD, SEM, etc.)? Is there preliminary data?
  - Can you provide a calculation to show sensitivity is there ?
  - Reviewer needs to judge if experiment is feasible

  ➡ Does x-ray energy match laser penetration depth

  ➡% of dilute atoms OK for fluorescence measurements

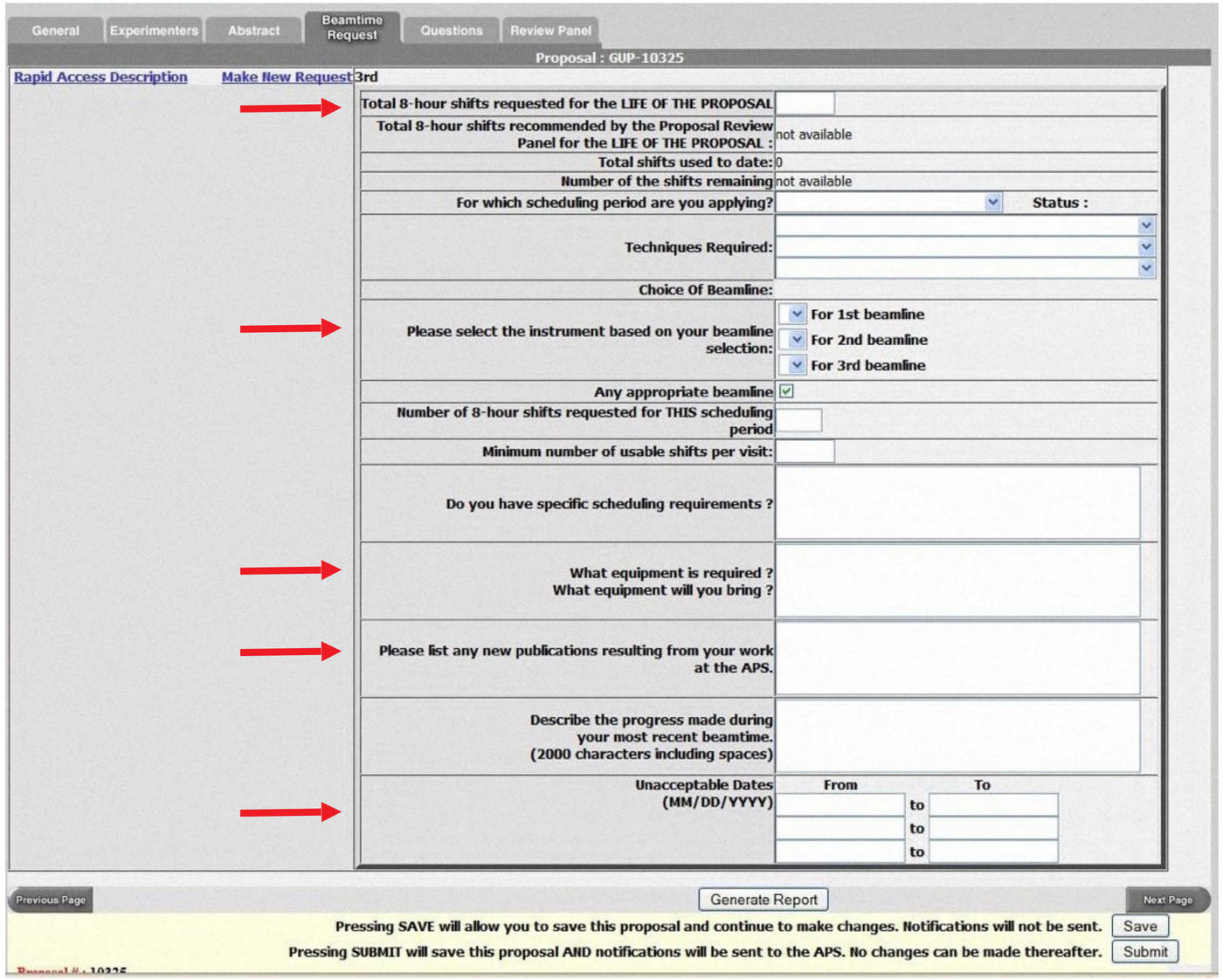
Experimental Details

- Why use x-rays or neutrons?
  - Neutron vs. X-rays OR Neutron + X-rays?
  - TEM, Mössbauer, Laser Raman, etc. (Have you done your homework?)

- Justify the amount of beam time requested (ask instrument scientist!)
  - Be reasonable.

- How will you analyze your data?
  - Don’t count on a Miracle to occur

Beamtime Request



- APS proposals are valid for two years, but need to put in beam time request each cycle.
- Chose multiple beamlines.
  - SAXS (12-ID, 5-ID, 15-ID)
  - XAFS (20-BM, 10-ID,12-BM)
  - General Diffraction
- Don’t list only one week that you can come. Holidays?
- Special sample environment / detectors will place more constraints on schedule.
  - GE amorphous Si detector
  - Magnet
  - ….

Ratings for APS Proposals

Table 1. Definition of Ratings Used in Reviewing General User Proposals	
1 - Extraordinary	The proposal involves highly innovative research of great scientific importance. Proposed research will significantly advance knowledge in a specific field or scientific discipline. Considerable societal relevance is demonstrated. The radiation characteristics of the APS are highly desirable for the success of the proposed work.
2 - Excellent	The proposed research is of high quality and has potential for making an important contribution to a specific field or scientific discipline. The work is cutting edge and is likely to be published in a leading scientific journal. The radiation characteristics of the APS are important to the success of the proposed work.
3 - Good	The proposed research is near cutting-edge and likely to produce publishable results. Impact on a specific field or scientific discipline is likely. Synchrotron radiation is essential to accomplish the intended goals of the research. The proposed work will greatly benefit from access to the APS.
4 - Fair	The proposed research is interesting but may not significantly impact a specific field or scientific discipline. Publication may or may not result from this research. Synchrotron radiation is required, but the proposed work could be performed at other facilities.
5 - Poor	The proposed research is not well planned or is not feasible. Results would not make important contributions to fundamental or applied understanding, and work is not likely to result in publication. The need for synchrotron radiation is not clear.

APS proposals are rated on a scale from 1 to 5
Cut off score for receiving beam time varies by beamline (<1.5 to 2.2)

Proposal "**ageing**" (score improves by 0.2 each cycle it does not receive time). This is needed for getting time at some oversubscribed beamlines, so long-term planning is needed. But you have to remember to request beamtime again for every cycle.

Pick appropriate panel - Important!

Current Panels

High Pressure
Instrumentation
Imaging/Microbeam
Macromolecular Crystallography
Scattering - Condensed Matter
Scattering - Applied Materials
Scattering – Chem / Bio / Environment
Small Angle Scattering (SAXS)
Spectroscopy
Structural Science
Inelastic X-ray scattering
Pump Probe
Dynamic Compression

If multiple possibilities - Look at members & Ask staff

https://www1.aps.anl.gov/About/Committees/Proposal-Review-Panels

Proposal Review Panels

Proposal Review Panels

Real-time PRP Score Tracking Application

Archived PRP Scores Application

High Pressure

Barbara Lavina, *Chair*

- June Wicks
- Camelia Stan
- Christine Beavers
- Arianna Gleason
- Antonio Moreira dos Santos
- Shanti Deemyad
- Sang-Heon (Dan) Shim
- Maik Lang
- Thomas Fitzgibbons
- Wenli Bi
- Jason Jeffries
- Jennifer Girard
- Ross Hrubiak
- Dongzhou Zhang
- Shanti Deemyad

Instrumentation

Robert Henning, *Chair*

- Gary Navrotski
- Yu-Sheng Chen

Imaging/Microbeam

Garth Williams, *Chair*

- Bhoopesh Mishra
- Ryan Tappero
- Claire Weekley
- Dula Parkinson
- Balaji Raghothamachar
- Mingyuan Ge
- Trevor Willey

Macromolecular Crystallography

John Rose, *Chair*

- Arnon Lavie
- Anne Mulichak

Scattering—Condensed Matter

Divine Kumah, *Chair*

- Nouamane Laanait
- Phil Ryan
- Stephen Wilson
- Hua Zhou
- Sara Haravifard
- Mingda Li
- Jacob Ruff

Scattering—Applied Materials

Marcus Young, *Chair*

- Darren Pagan
- Stephan Hruszkewycz
- Tao Li
- Laura Schelhas
- Sumit Kewalramani

Scattering—Chem/Bio/Enviro

Greeshma Gadikota, *Chair*

- Ivan Kuzmenko
- Connie Lu
- Shao-Liang Zheng
- Derk Joester
- Millicent Firestone

Small-angle X-ray Scattering (SAXS)

Joe Strzalka, *Chair*

- Maria Bewley
- Andy Herring
- Samanvaya Srivastava
- David Lambright
- Joshua Hammons

Spectroscopy

George Sterbinsky, *Chair*

- Eli Stavitski
- Yulia Pushkar
- Yuji Arai
- Azzam Mansour
- Kyler Carroll
- Conan Weiland
- Padraic Shafer
- Evert Elzinga
- Xiafeng Guo
- Giuseppina Conti
- Riccardo Comin
- Tianpin Wu
- Jier Huang

Structural Science

James Kaduk, *Chair*

- Ryan Ott
- Peter Khalifah
- Craig Bridges
- Kevin Stone
- Michelle Dolgos
- Jamie Neilson
- Valeri Petkov
- Andrew Payzant
- Peter Stephens
- Scott Misture
- Craig Brown
- David Billing
- Jennifer Niedziela
- Cora Lind-Kovacs
- Zhenzhen Yu

Inelastic X-ray Scattering

Stuart Calder, *Chair*

- Raphael Hermann
- Yong Cai
- Ignace Jarrige
- Yue Cao

Pump Probe

Eric Landahl, Chair

- Anne Marie March
- Matthew DeCamp
- Marius Schmidt
- Xiaoyi Zhang

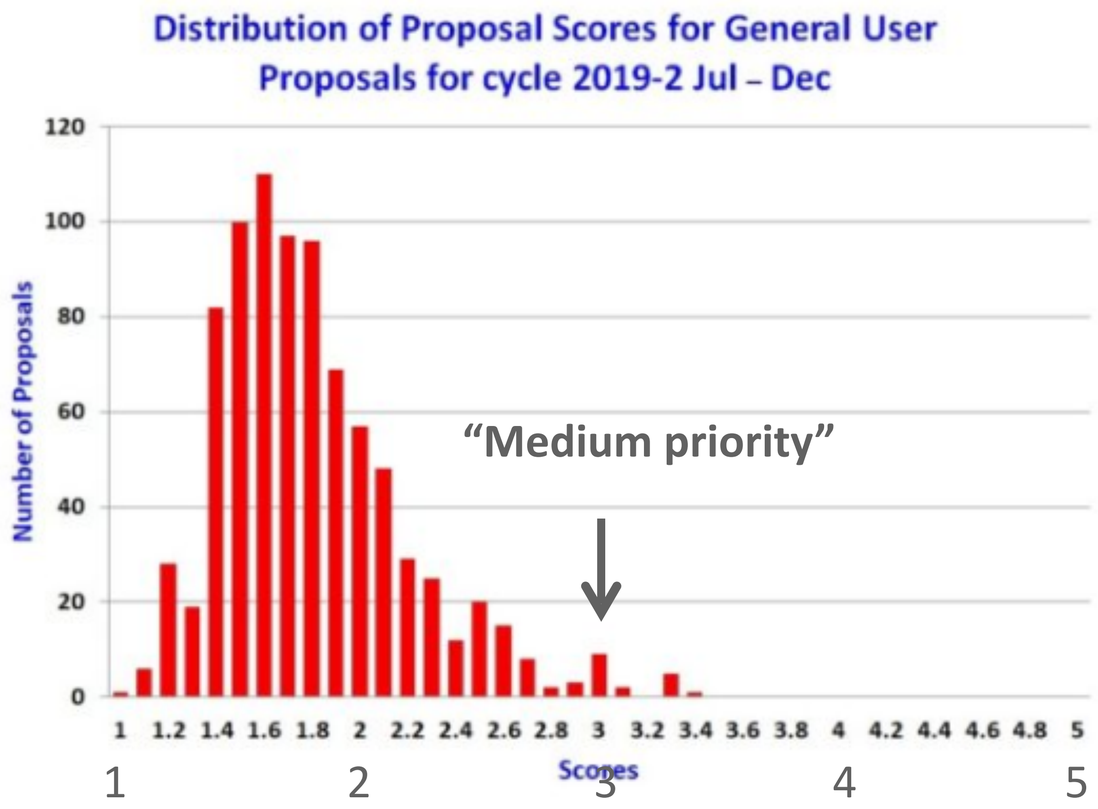
Dynamic Compression

Robert Cauble, Chair

- Justin Brown
- Tim Germann
- Thomas Gog

ALS provides cutoff scores - Helps you know what to expect

https://als.lbl.gov/general-user-proposal-score-statistics/



Beamline	% Beam Time Allocated / Requested		Cutoff Score	
1.4 (IR)	76	easier	2.84	←
2.4 (SINS)	54		2.08	
4.0.2 (Magnetic Spectroscopy/Scattering)	18		1.63	
4.0.3 (MERLIN)	22		1.68	
5.3.2.2 (Polymer STXM)	71		1.73	
5.4 (IR)	79	easier	2.40	←
6.1.2 (Soft X-Ray Microscopy)	51		1.73	
6.3.1.1 (Magnetic Spectroscopy)	25		1.80	
6.3.2 (Calibration, Optics Testing, Spectroscopy)	68		2.36	
7.0.1.2 (COSMIC)	28		1.50	
7.0.2 (Surface & Materials Science (MAESTRO))	20		1.44	
7.3.1 (ISAAC)	36		1.80	
7.3.3 (SAXS)	46		1.58	
8.0.1 (SXF)	19		1.68	
8.3.2 (Tomography)	48		1.87	
9.0 (Chemical Dynamics, Coherent Imaging)	68		2.03	
9.3.1 (Tender APXPS)	14	harder	1.20	←
9.3.2 (APXPS)	29		1.48	
10.0.1 (HERS/AMO)	24		1.76	
10.3.2 (Micro XAFS)	50		1.73	
11.0.1 (PEEM3, Soft X-Ray Scattering)	20		1.55	
11.0.2 (Molecular Environmental Sciences, STXM, ambient pressure XPS)	22	harder	1.24	←
12.2.1 (Small Molecule Crystallography)	53		1.60	
12.2.2 (High Pressure)	25		1.55	
12.3.2 (Microdiffraction)	38		1.70	

SNS/HFIR does not tell you a score or panel members. You can try asking user office or beamline.

Tips (see also: https://neutrons.ornl.gov/users/tips)

- Pick a good science question
- Give a concise explanation, with a good bit of background for non-specialist
- Provide background on importance
  - what is the bigger picture
  - what is known, what is not known
- State a clear hypothesis
  - what are you going to measure
  - how is it related to your big science question
- Include relevant details regarding the experiment, but do not get too verbose
  - Reviewer needs to judge feasibility of the experiment, choice of instrument

Tips (see also: https://neutrons.ornl.gov/users/tips)

- Talk to the local contact / instrument scientist (in particular if first time user)
  - Find out about details of the instrument, typical measuring times…
  - Over-subscription rate? Can a less popular instrument do the same measurements?
  - Send them the proposal ahead of time and ask for advice. Collaborate?
- If you have previous results from other experiments include them!
  - Home, other institution, previous experiment.
  - Sample characterization.
- Take advantage of proposal ageing. Plan ahead!
- Do not submit a bad proposal in a rush.

Several common pitfalls

- Proposer assumes committee is familiar with their specialty. Explain impact.
- Proposer writes large general vague proposal asking for multiple weeks of time. Better to write a shorter proposal with a well defined objective. Be realistic with beam time request.
- Proposer submits 2 (or more) similar proposals for related materials thinking that multiple proposals increases chances.
- Proposal deadline (for next cycle) is before scheduled beam time this cycle.

Common Reviewer comments:

- *“The score could be improved by including more experimental details, attaching previous results and expanding on the purpose and importance of the research.”*
- *“Hasn't the proposed research been published previously?”*
- *“We do not feel that granting 20 shifts/cycle for 2 years is consistent with the history of publication of this work.”*
- *“Proposer should perform initial characterization with lab sources or TEM.”*
- *“Will the signal be strong enough compared to background?”*

After submission

- Allow time for review and revisions
- Expect feedback several weeks from the call close
- Be ready to schedule experiment if approved
  - Identify participating team members
  - Respond to facility access approval information
  - Facilitate execution of user agreements
  - Complete required training
  - Confirm sample availability and description and laboratory needs
- Consider reviewer comments if not approved and plan to resubmit this proposal or a new proposal in the next call. Opportunities (# of facilities and beamlines/ facility) continue to grow.

Scientific and Funding Opportunities

As a student

- Attend neutron & x-ray schools, workshops & user meetings. Knowledge and connections have long-term impact. Collaborations are essential.
- Join SNS HFIR User Group (SHUG) and other facility user organizations
  Advocacy group, learn about and influence new developments
- Explore DOE and NSF internships, fellowships, and research programs

  SCGSR; ORISE/ORAU (HERE, GO!). Local contacts help (a lot).

  https://science.energy.gov/wdts/scgsr/how-to-apply/priority-sc-research-areas/
- Invite scientists from national labs to your campus, e.g. for seminar

As a young professional

- Continue to use “free” user facilities

  New faculty and industrial users can be favored in reviews
- Volunteer to be a reviewer on proposal panels
- Consider EPSCoR programs if located in an a participating state
- Apply for Early Career award – great for tenure application

LIST OF FACILITIES WEBPAGES

ALS	https://als.lbl.gov/
APS	https://www.aps.anl.gov
CHESS	https://chess.cornell.edu
LCLS	https://lcls.slac.stanford.edu
SSRL	https://www-ssrl.slac.stanford.edu
NSLS-II	https://www.bnl.gov/ps/
SNS/HFIR	https://neutrons.ornl.gov
NIST	https://www.nist.gov/ncnr
Worldwide resources:	https://lightsources.org/
	https://neutronsources.org/

THANKS TO

- Jonathan Lang
- John Budai
- Suzanne te Velthuis