OAK RIDGE National Laboratory

STS Instrument Software Needs

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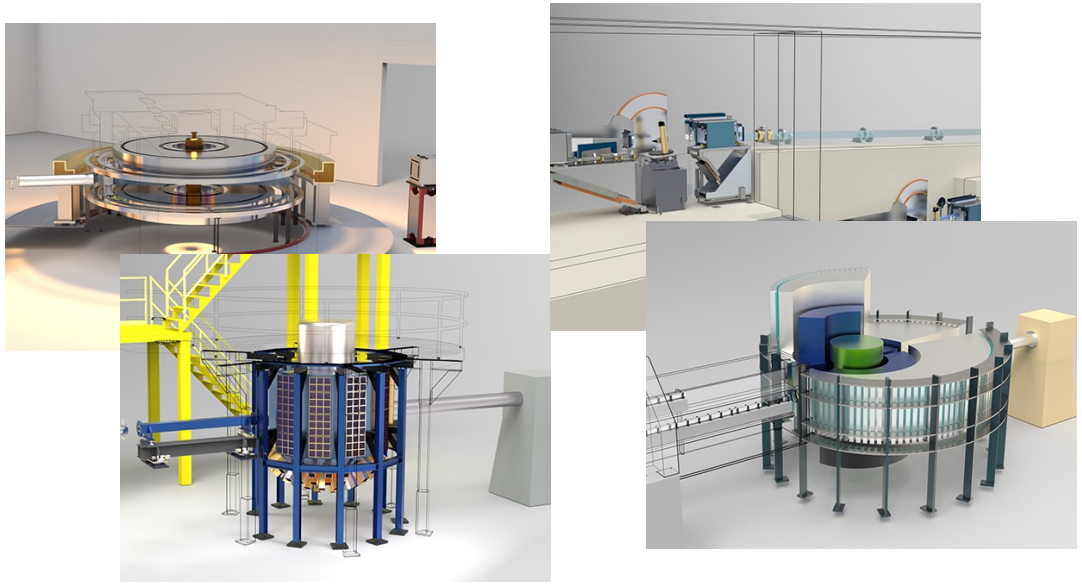
For STS/CSMD workshop 2022

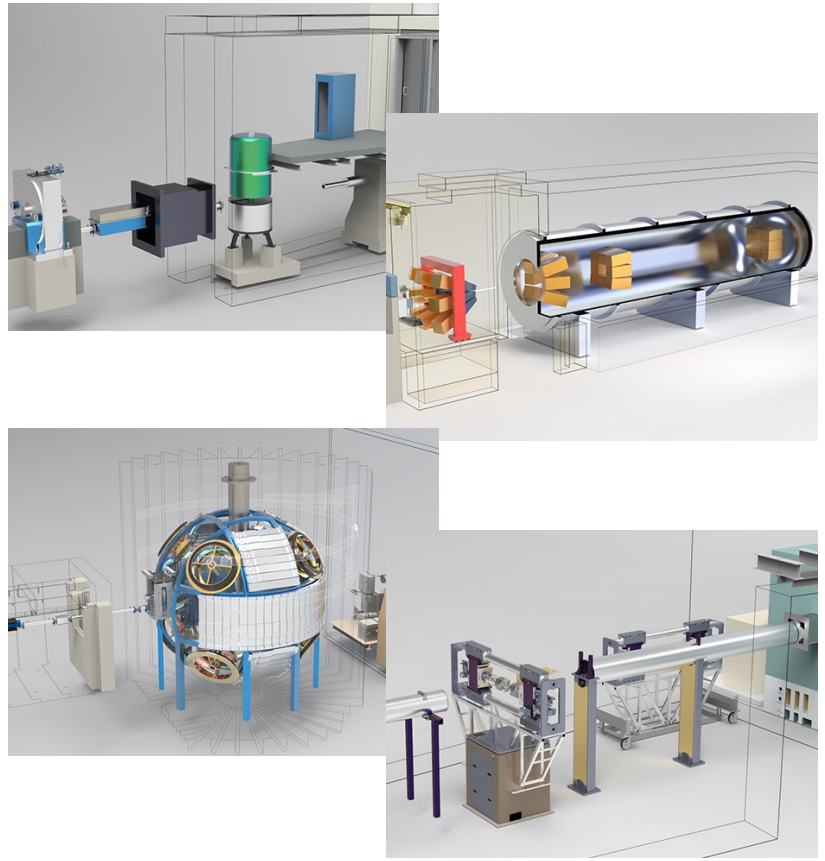
ORNL is managed by UT-Battelle LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

Overall challenges faced by STS instruments (just a few examples)

- Time-resolved measurements of kinetic processes and beyond-equilibrium matter (***higher data rate***)
- Simultaneous measurements of hierarchical architectures from the atomic scale to microns and beyond (***novel data***)
- Measuring small samples of newly discovered or synthesized materials (***higher throughput, better alignment control…***)
- Examining new frontiers in materials at extreme conditions (***complex metadata***)





A much broader user community!

BWAVES (Time-of-Flight Broadband Spectrometer)

- Typical data reduction and data size are relatively small.
- Straightforward rudimentary data analysis (e.g., peak position, width)
- New data analysis challenges:
  - combination of relaxation and excitation data
  - Data Modeling for this unique instrument
  - Simulation for data interpretation

CENTAUR (SANS / WANS Diffractometer & Spectrometer)

- Remote high-throughput experiment (est. 20-30% of beam time): a more efficient control/data workflow is needed
- Automatic data reduction & rudimentary data analysis (for some 'standardized' experiments)
  - Control and interface for different user levels or different complexity of experiment
- New capabilities:
  - Simultaneously rudimentary data fitting SANS/WANS
  - (Near) real-time data visualization/reduction/fitting
  - Open hardware/software protocol for user development
  - Autonomous experiment coupled with instrument config., sample environment, etc.

CHESS (Polarized Direct-Geometry Chopper Spectrometer)

- Using event data, with Repetition Rate Multiplication & polarization
- Efficiently retrieve/extract selective metadata with neutron data
- Tailorable software for data visualization, reduction, analysis
- Compatibility and integrable as part of pipelines
  - with VASP, SpinW, CASTEP, etc.
  - With other facilities
  - With simulation software such as MCViNE, OCLIMAX

CUPI^{2}D (High-flux, broadband, cold neutron imaging instrument)

- DAQ: event data, short-term and long-term storage, can be as high as ~10GB/s or ~1PB/day,
- Data reduction: many exist but need be adapted and further development, scripting & GUI, data vis. for raw/intermediate/ reduced data, etc.
- Data analysis
  - Commercial software exist but advanced tools are needed, e.g., strain tensor tomography
  - A framework is needed to integrate analysis tools into the whole data reduction-analysis pipeline
  - Modeling/simulation tools are under development, e.g., simulating transmission/Bragg-edge measurements, effect of grating interferometry systems

PIONEER (Single-crystal diffractometer with polarization option)

- Automatic experimental planning (with one or a few short runs)
- Data reduction (Faster, automatic, real-time & post experiment, including instrument specific info such as Q-resolution) – less user inputs, burden less instrument scientist
- New capabilities that will be more regular at STS
  - Time-resolved, pump-probe: fast data collection, new data reduction
  - Complex hybrid systems such as inter-growth multiple-component crystals, thin films: new data reduction
  - Small samples in complex sample environment: high alignment accuracy <50 μm (can AI help?)
  - Weak feature extraction, background subtraction with AI

QIKR (Quite Intense Kinetics Reflectometer)

- Provide conventional automated collection and reduction à la FTS Liquids Reflectometer
- Develop post-experiment event-mode analysis code to
  - Divide a time-dependent data set into multiple data sets by time, counts, or external state variables (metadata)
  - Statistically analyze time-slice series for changes to identify abrupt transitions
  - Auto-fit time-slice series based on templated models to track "smooth" structural changes between abrupt transitions
- Apply post-experiment code to analysis of data from a running experiment "on the fly" to provide user real-time feedback

Summary from STS Instrument Systems Workgroup Meetings Nov 2021 to Feb 2022

- **Participants:**

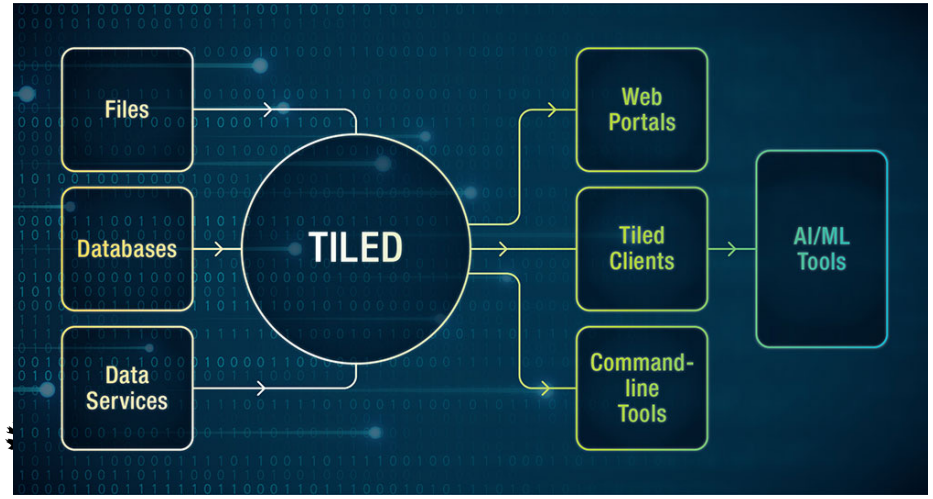
Stuart Campbell (BNL)

Alex Hexemer (LBNL)

Thomas Proffen (ORNL NScD)

Shuo Qian, Leighton Coates, Jiao Lin, Gabriele Sala, Matthew Pearson, Kay Kasemir, Ken Herwig (ORNL STS)

The draft summary can be found in the Dropbox

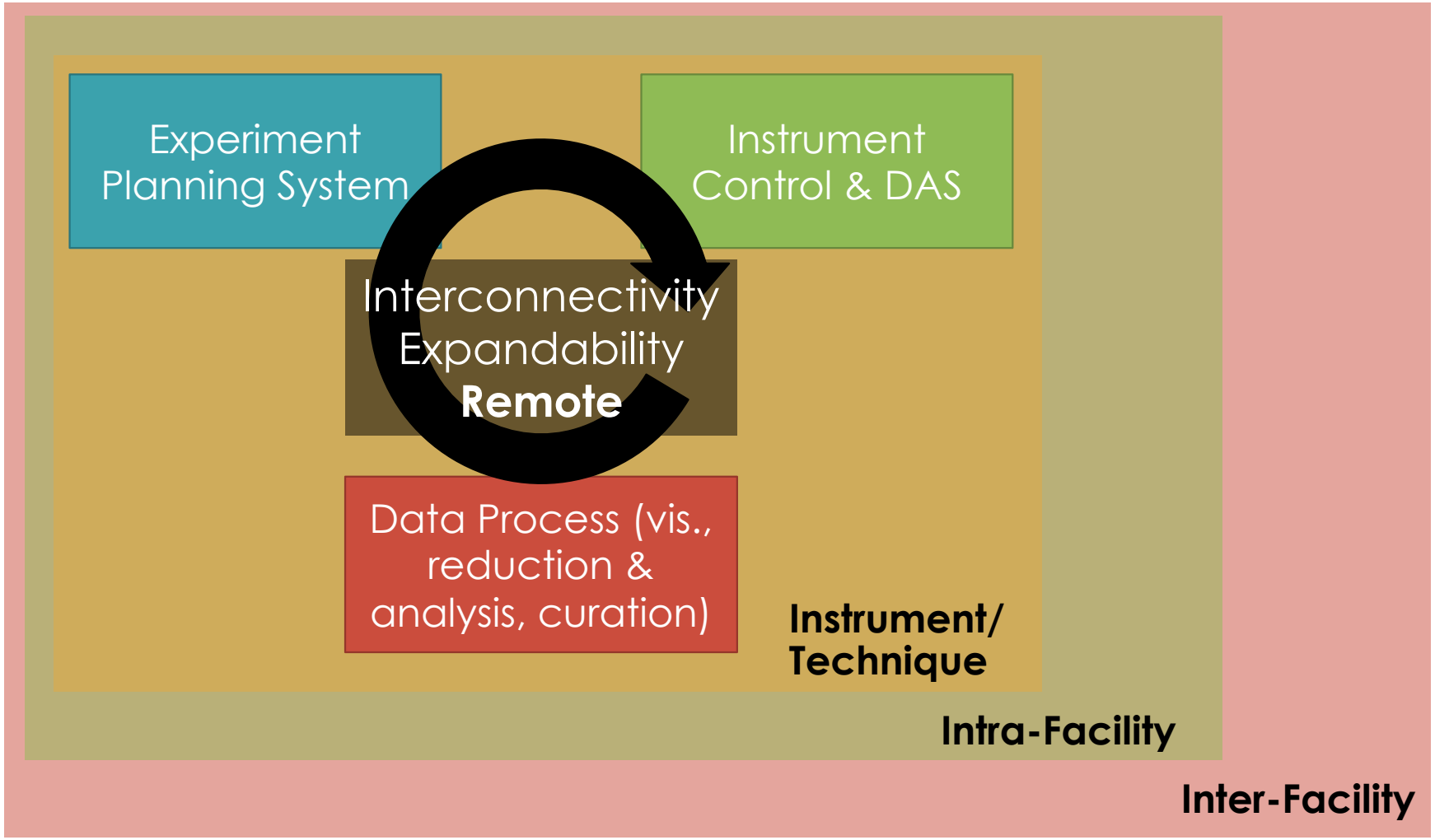


MLExchange is software infrastructure that deploys machine learning models to beamline scientists

Recommendations from the workgroup

- STS Instrument Systems (IS) works closely with NScD for a path that all neutron scattering facilities can be merged down the road, with STS IS needs fully addressed and adaptability to the existing SNS/HFIR facilities.
- Early requirements for different software will be useful. Evolvement expected.
- Data management plan, standard, etc. to be devised early and be coordinated with NScD
- STS IS needs to participate and involve in collaborations among other facilities

How can we achieve better interconnectivity, expandability and remote capability?



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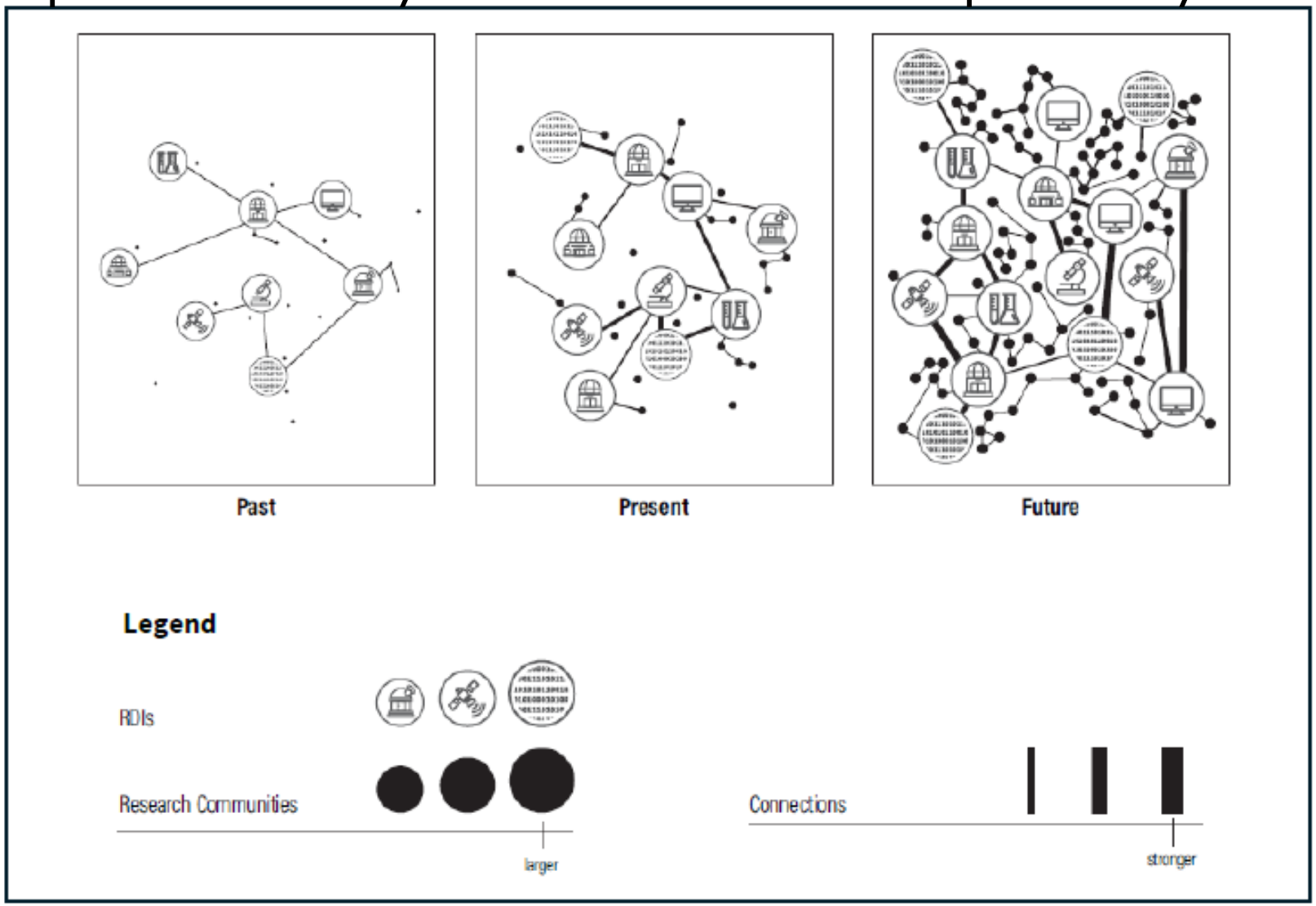


Figure 1. Evolving Interconnectedness and Interdependencies of RDIs and Research Communities

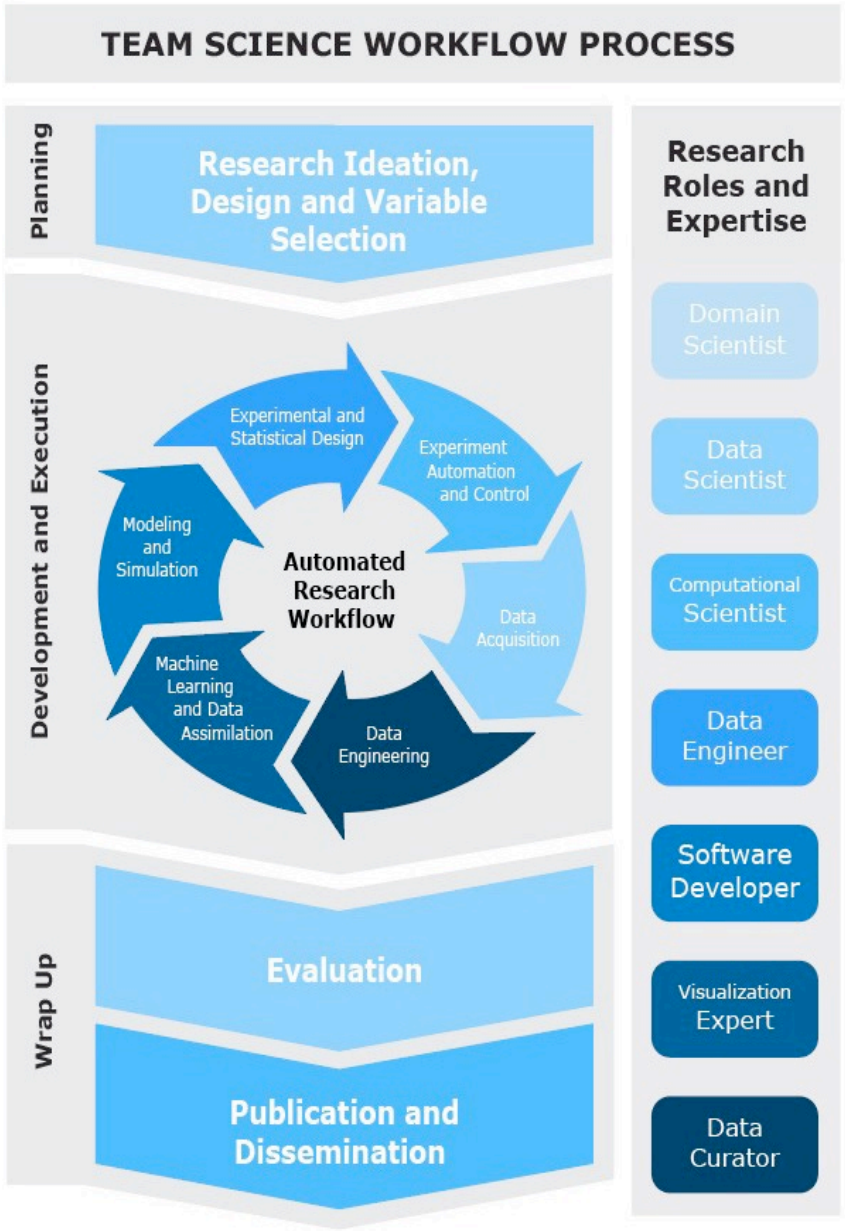
NATIONAL STRATEGIC OVERVIEW FOR RESEARCH AND DEVELOPMENT INFRASTRUCTURE

A Report by the
SUBCOMMITTEE ON RESEARCH AND DEVELOPMENT INFRASTRUCTURE
COMMITTEE ON SCIENCE AND TECHNOLOGY ENTERPRISE

of the
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

October 2021

We need to team up!



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