HARVARD UNIVERSITY

FAS RESEARCH COMPUTING
HARVARD UNIVERSITY
FACULTY OF ARTS & SCIENCES

Virtual Residency Intermediate/Advanced Workshop 2020:

Mapping Research Requirements to Software Tools

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Software Use in Research

- Significant software use in recently published journal papers
- Integral part of research methods
- Affect every step of scientific discovery
- Enrich research productivity and reliability
- More support for software development in research (NOT-OD-20-073)
- Increasing demand due to rise of ML/DL/AI in every research

Large Hadron Collider (Image: Anna Pantelia/CERN)

Credit: EHT collaboration

Software Use in Research

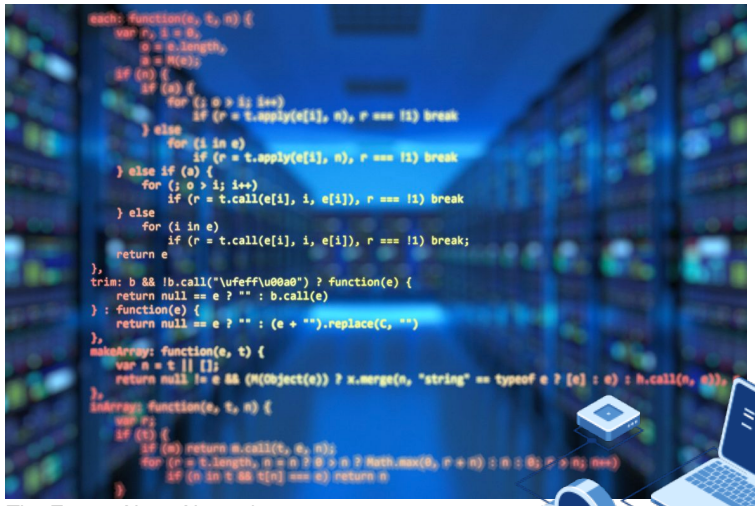
- Reproducibility in research
- Interdisciplinary collaboration
- Data-driven science vs traditional computational & simulation science
- Visualization
- Subdisciplines such as Bioinformatics

Large Hadron Collider (Image: Anna Pantelia/CERN)

Credit: EHT collaboration

Mapping Research Requirements to Software

- ❑ Survey researchers especially in data-driven research
- ❑ Survey of available commercial and open-source tools
- ❑ Cost $
- ❑ Reliability
- ❑ Sustainability
- ❑ Maintainability
- ❑ Scalability
- ❑ Training
- ❑ **Infrastructure**
- ❑ Collaboration



The Energy News Network

Veritis Group Inc

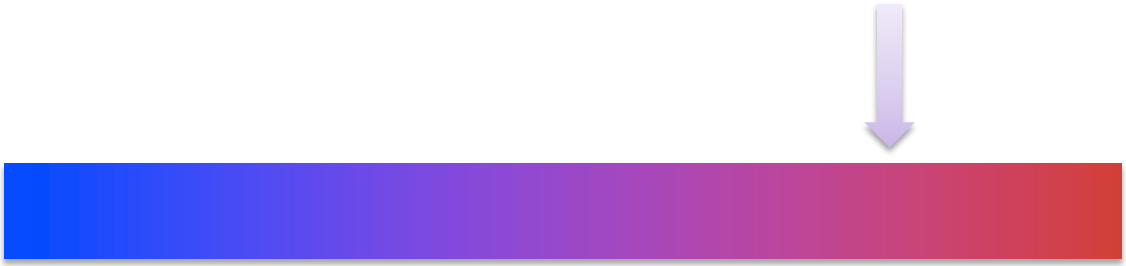
Commercial vs. Open-Source

- Commercial Software Tools (COMSOL, MATLAB, ANSYS, Abaqus)
  - Authorized license
  - Faster Solution
  - Software issue support
  - Security
  - Reliability
  - Limited collaboration
  - Limited features
  - Comfort zone!

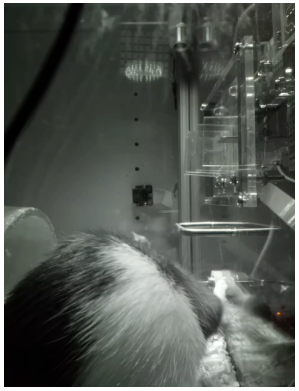
- Open-Source Software (OpenFOAM, Keras, TensorFlow)
  - Free
  - Flexibility
  - Community engagement
  - Customization

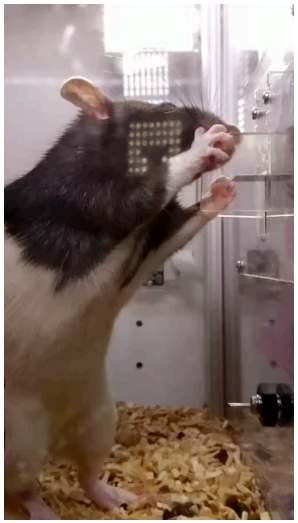
Research Software Development Challenges

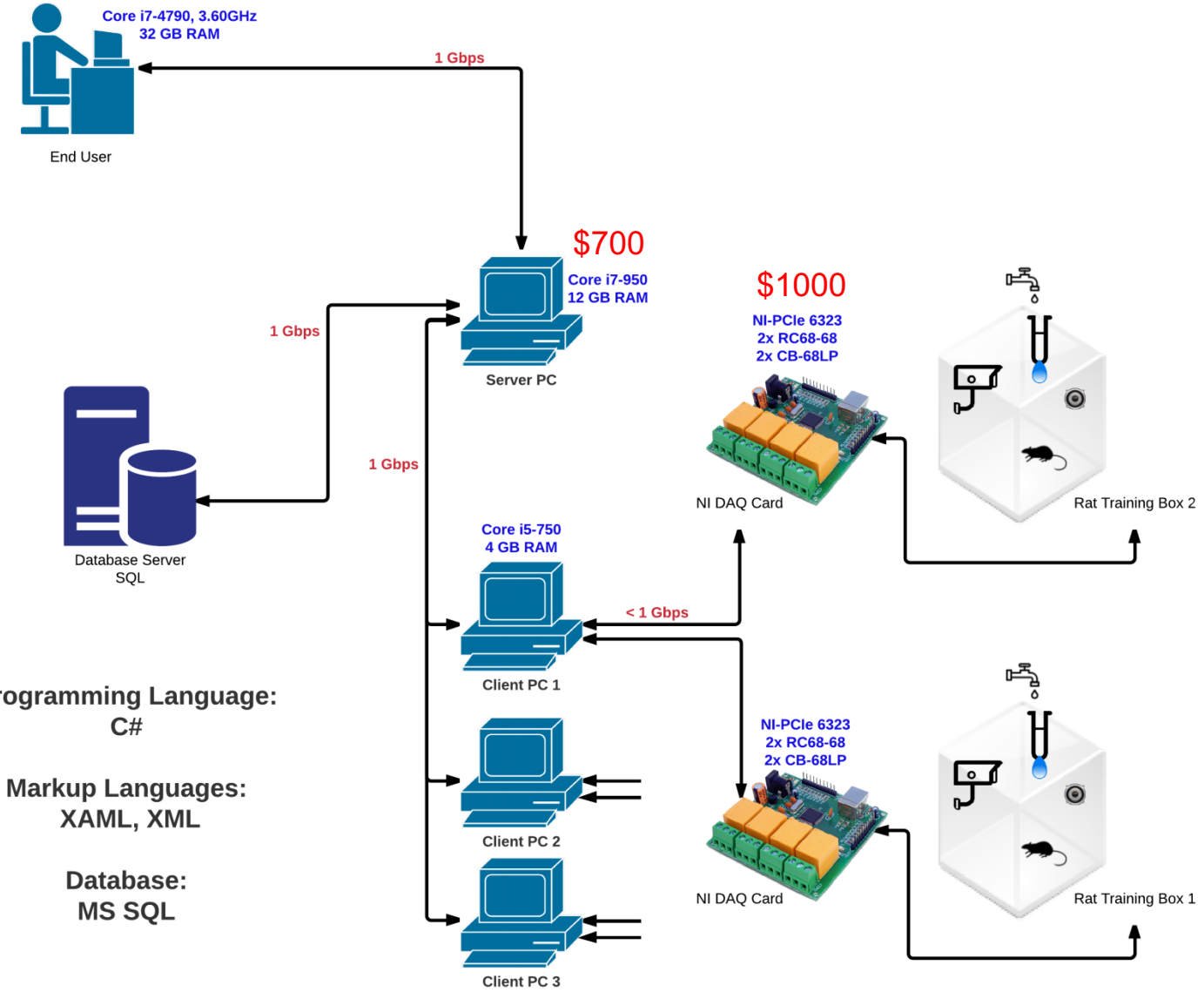
- ❑ Software engineering best practices
- ❑ Software quality
- ❑ Maintainability
- ❑ Reliability
- ❑ Robustness
- ❑ Scalability
- ❑ Sustainability
- ❑ Portability
- ❑ Software Testing
- ❑ Interoperability
- ❑ Infrastructure
- ❑ Cloud readiness



Operant Conditioning Software V1.0







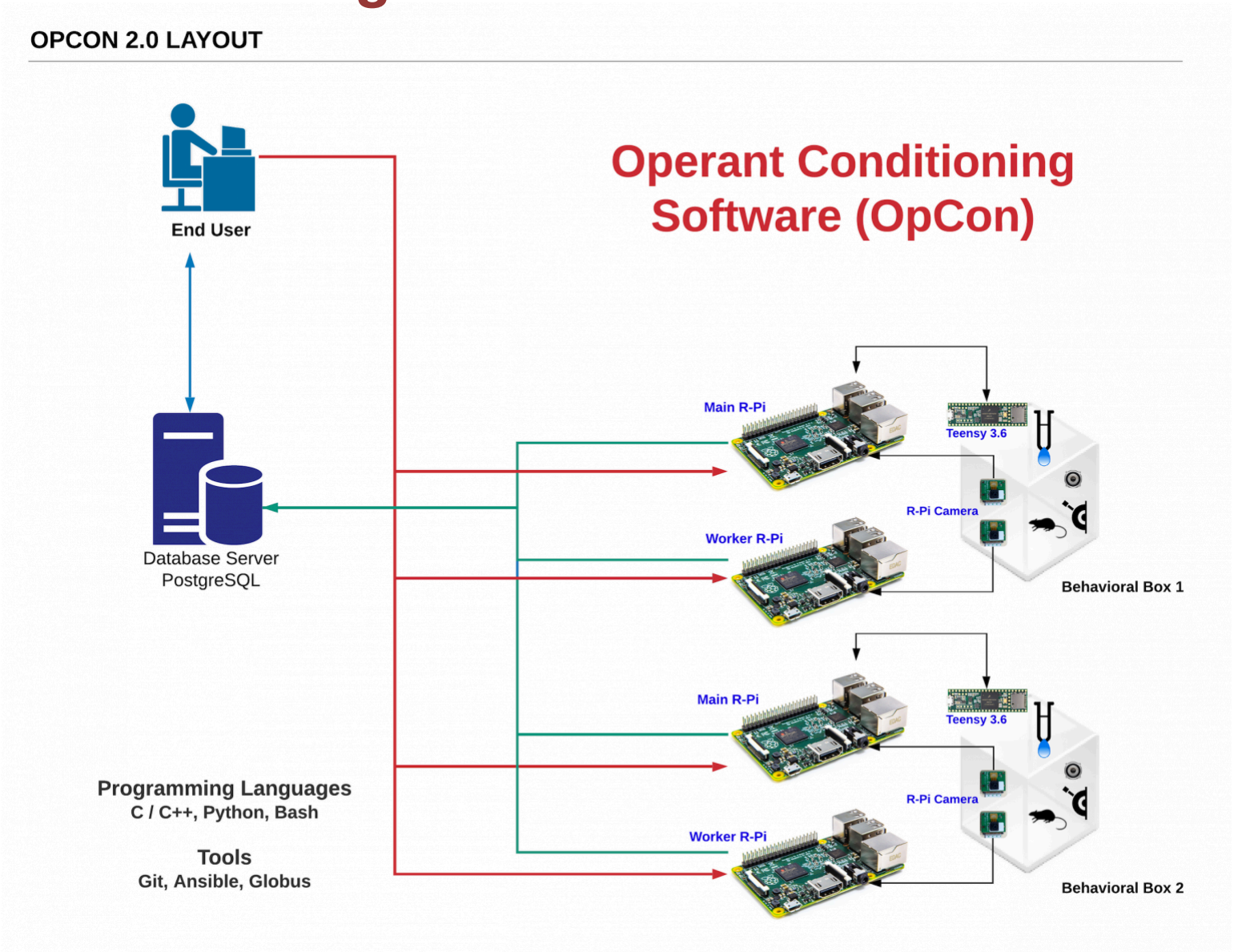
Programming Language:
C#

Markup Languages:
XAML, XML

Database:
MS SQL

Operant Conditioning Software V2.0

C Language



Research Software Engineering Team at Harvard FAS Research Computing

Front-End Developer
Node.js, Angular, React, jQuery, Bootstrap
Priority Bar >>

Visualization Expert
D3, Blender, ParaView, Tecplot

Scientific Software Developer
C++, Python, Julia, Fortran, MATLAB

HPC Expert
MPI, GPGPU

Professional Software Developer
C++, Java, Python, C#

Big Data Expert
Hadoop, Spark, MapReduce, BigQuery, NoSQL

Database Expert / Data Engineer
SQL, NoSQL

ML/DS/AI Expert
TensorFlow+Keras / PyTorch

Resources

software carpentry

Leading inclusive community teaching data and coding skills.

US RSE

US RESEARCH SOFTWARE ENGINEER ASSOCIATION

https://us-rse.org

URSSI

US Research Software Sustainability Institute

http://urssi.us

Thank You!

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