MY SCIENTIFIC JOURNEY TO EMBRACING JULIA

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SC24
Atlanta, GA | hpc creates.

Neutron & X-ray Scattering, Scientific Software

- PhD research: Inelastic x-ray scattering and electronic structure calculations
  - HPC user, Python scripting
- Postdoctoral research: Inelastic neutron scattering and spin wave modelling
  - C++11 software development
- Neutron data reduction, analysis and visualization
  - Inconvenient data sizes
  - Large (256 GB+) memory CPU workstations
  - Python & C++

Transitioning to High Performance Computing

- Research Software Engineer
  - Plasma physics (ASGarD, KORC), Materials science (QMCPACK), and Power grid (RE-INTEGRATE)
  - C++, multi-node, GPU accelerators
- Neutron scattering software and Julia
  - Incorporate instrument effects into calculations
    - Emerging Julia software stack
  - Processing raw neutron scattering data in OLCF resources
    - JACC.jl for performance portability

Current Thoughts

- User experience,
  - Learning curve, differentiation
- Developer productivity
  - Finite software engineering resources
- Language interoperability
  - Bindings? Alternative implementations? Rewrite?
- Performance portability
  - Heterogeneous computing landscape