Modeling of diffuse and inelastic magnetic scattering from quantum materials

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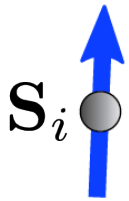
Quantum Magnetism

❑ Ground-state of an antiferromagnetic spin dimer



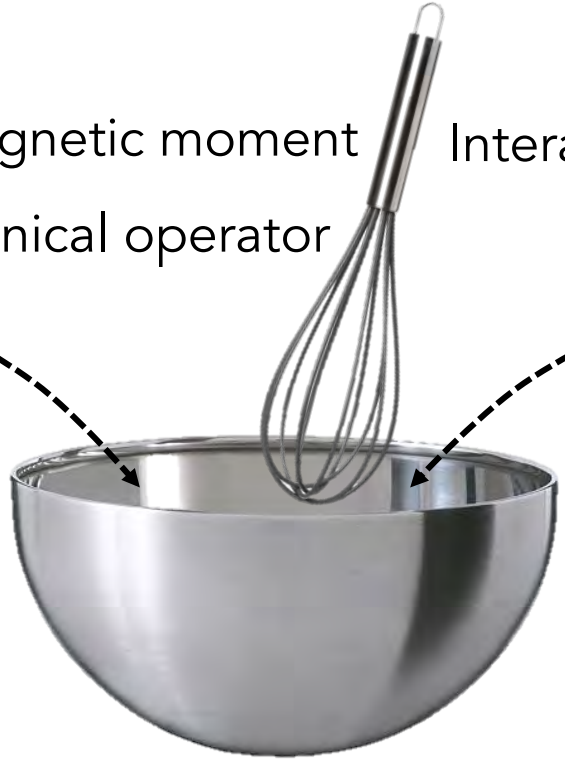
Spin ½ : atomic scale magnetic moment

quantum-mechanical operator

QM

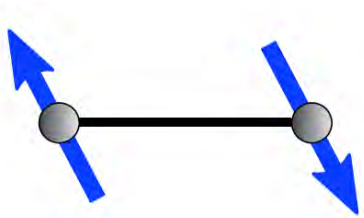
Interaction : Heisenberg exchange

$$\mathcal{H} = |J| \, \mathbf{S}_1 \cdot \mathbf{S}_2$$



Spin as classical vector

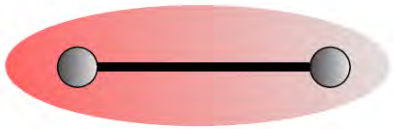
Breaks spin-rotation symmetry



Spin as quantum operator

Preserves spin-rotation symmetry

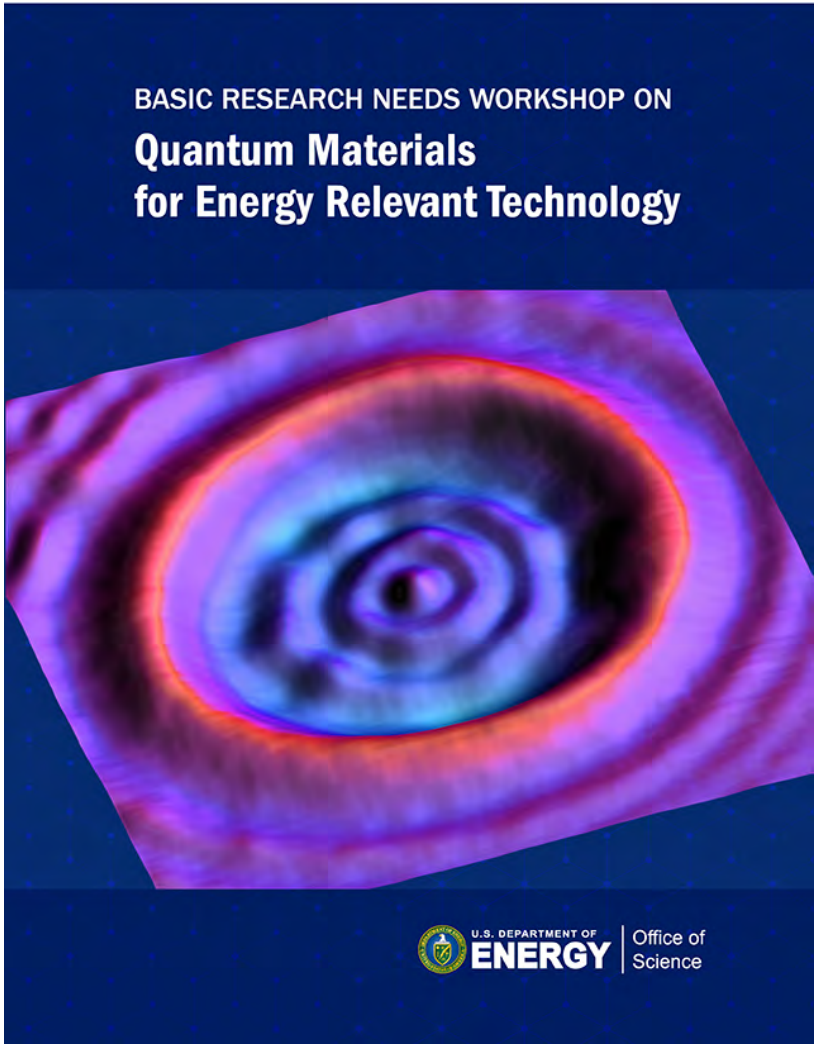
Entanglement



singlet $\frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$

Spin-Liquids in Quantum Materials

- We want this to happen in real materials with extended lattice



Spin-Liquids in Quantum Materials

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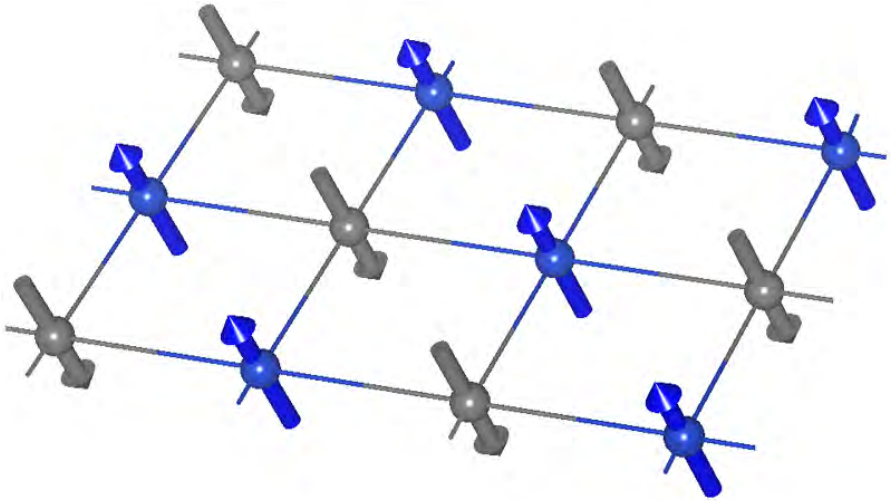
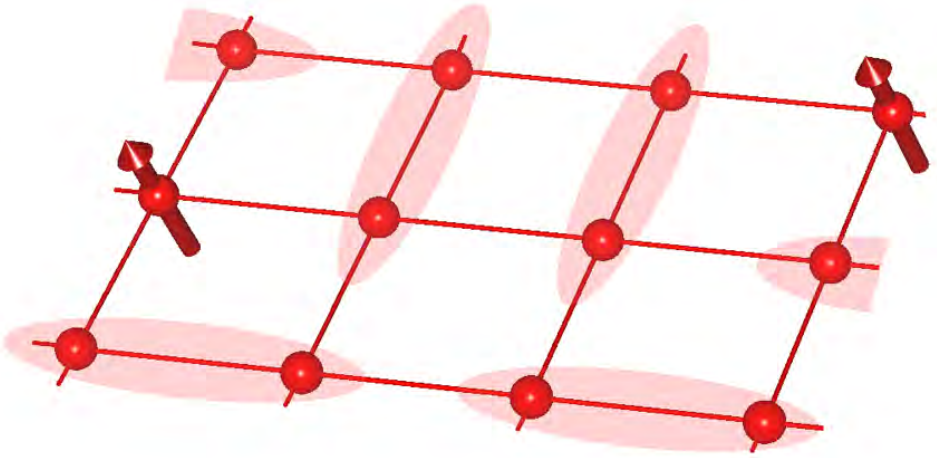


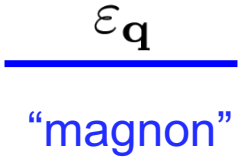


Ordered antiferromagnet

Symmetry breaking:
order parameter

No Entanglement

Spin-wave excitations

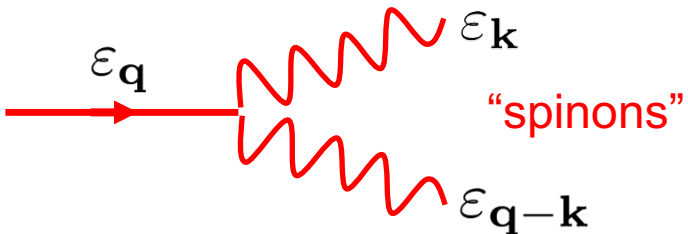


Quantum Spin Liquid

No symmetry breaking:
non-local (topological) order

Entanglement

Fractional excitations



Spin-Liquids in Quantum Materials

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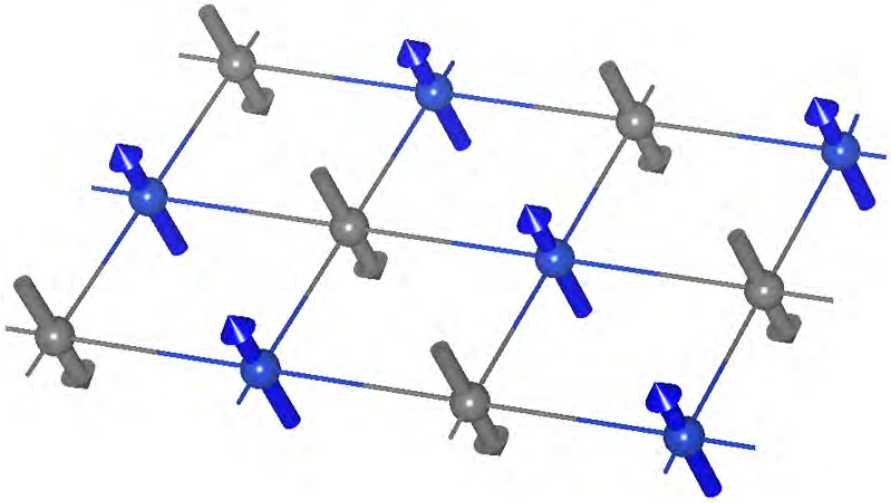
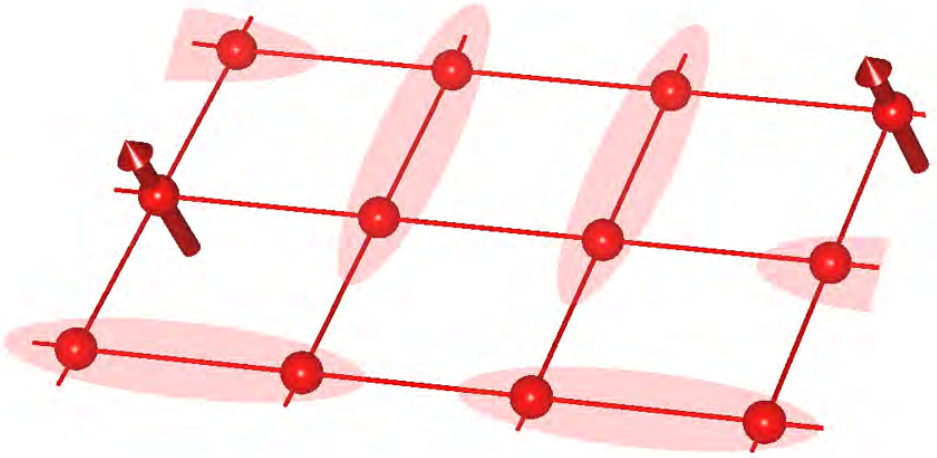
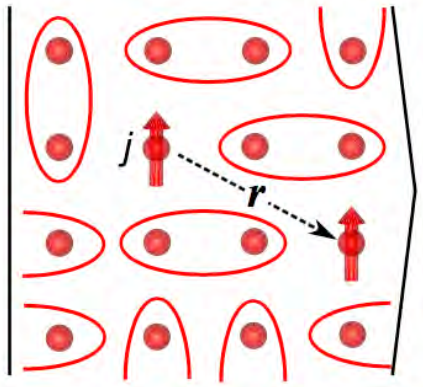


Ordered antiferromagnet



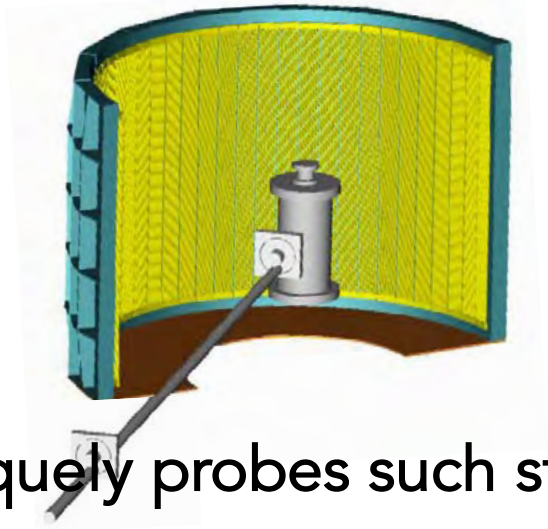
Quantum Spin Liquid



$$\chi''_{\alpha\beta}(\mathbf{q},\omega)$$

MANTID

At the forefront

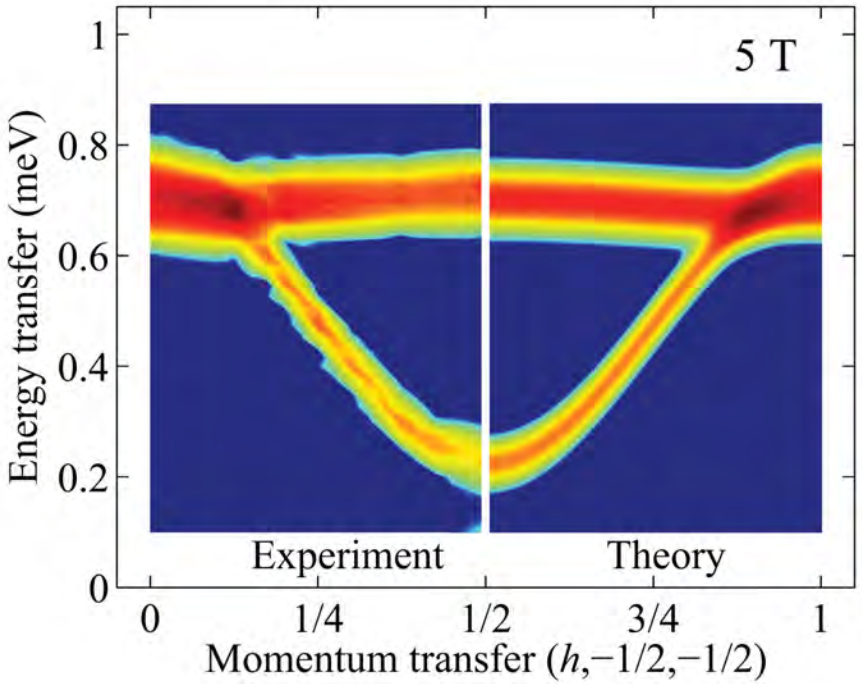


Diffuse & inelastic neutron scattering uniquely probes such states

Spin-Liquids in Quantum Materials

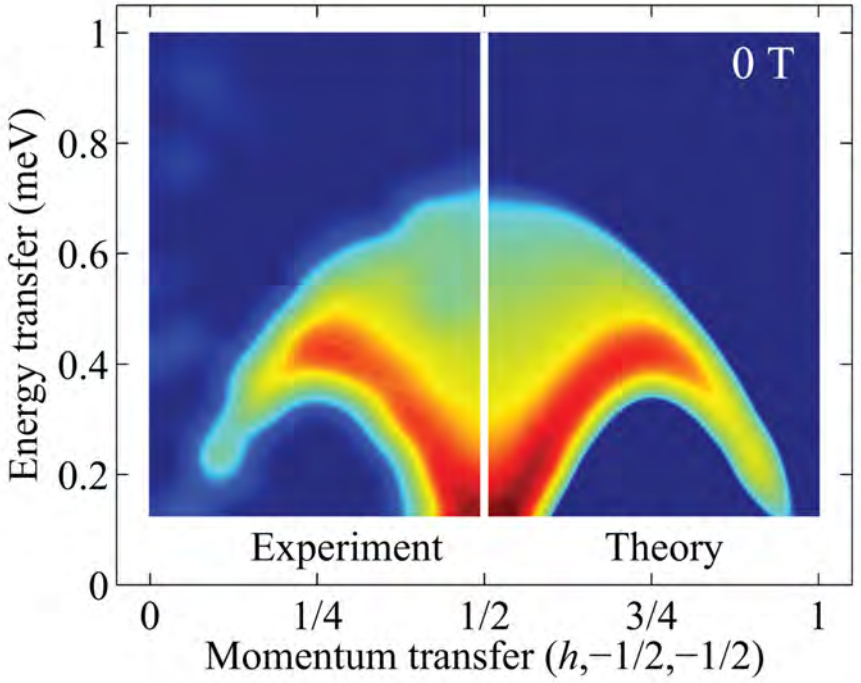
- We want this to happen in real materials with extended lattice

Ordered magnet



Sharp response in energy and momentum

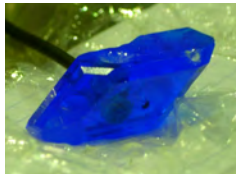
Quantum Spin Liquid



Broad response in both energy and momentum

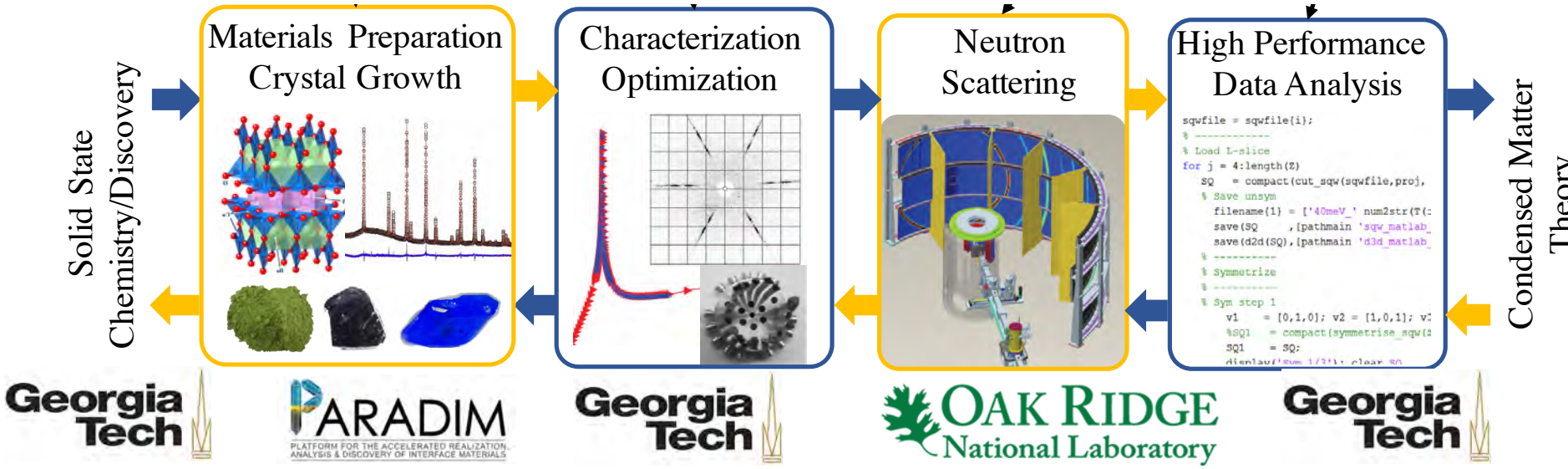
M. Mourigal *et al.*, Nature Physics **9**, 435-441 (2013)

$CuSO_4.5D2O$



University Research Groups

- My group: realize & study quantum magnets in 2D and 3D



Crucial Part of our Research
Invested 20k$ in computers

- My problem:

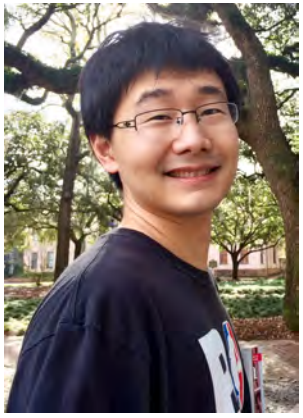
I am busy (teaching, funding, management etc). Students do the research.
But I want quality control, funding agencies/scientific integrity requires complete documentation of what has been done to the data: no black box.

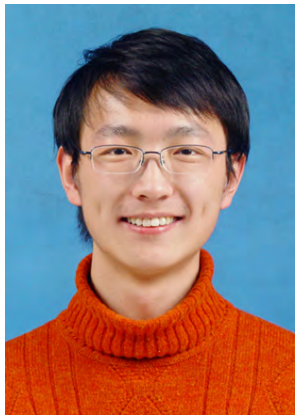
MANTID at the forefront

MANTID

University Research Groups

- My group. What do you see?



Zhiling	Darian	Marcus	Xiaojian	Hannah	Joe
Origin	Matlab	Matlab	Mathematica	Java	Fortran

- My problem:

Every student is different and masters coding differently. Likes or is trained in a different programing language. Data analysis tool requires flexibility and ability to export/import data at many different stages

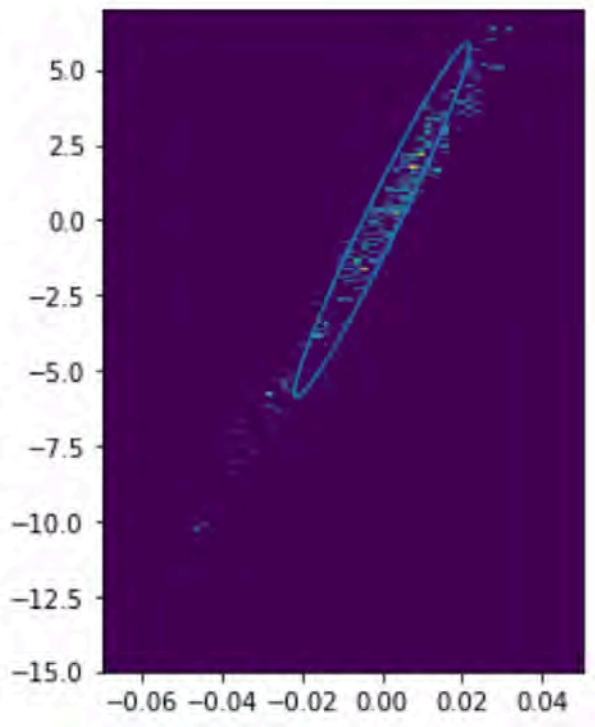
Again, MANTID at the forefront

Recent successes: ORNL Challenge Program

- Calculation of resolution function for DGS (McVine + ML)

Patrick Nave and Mike Wadell

Supervised at ORNL by Jiao Lin and Matt Stone

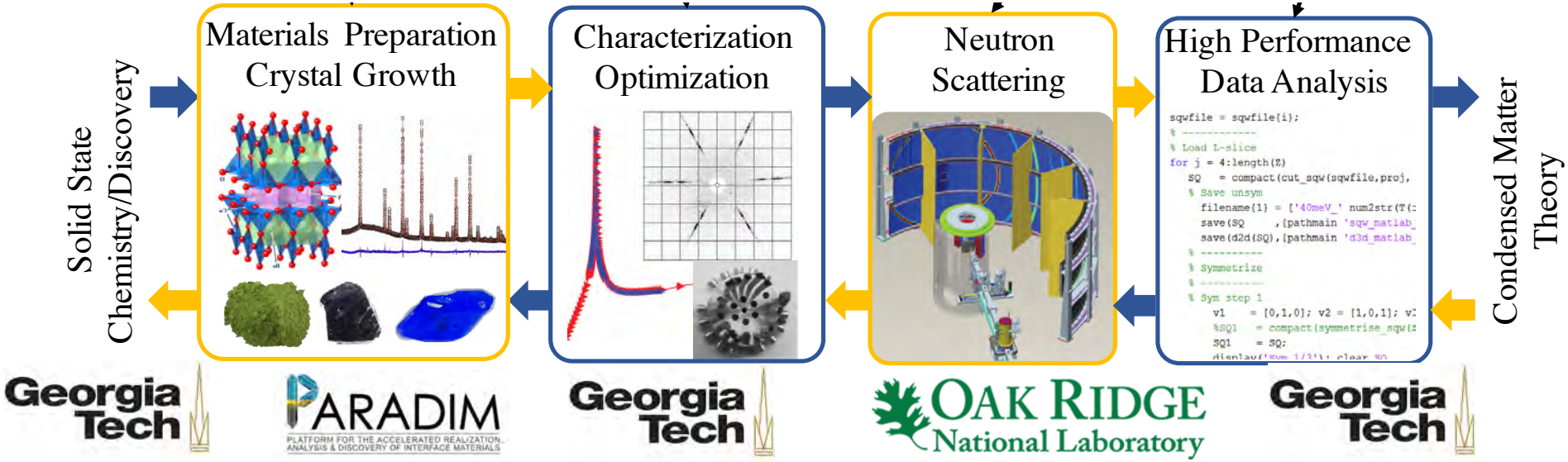


Train analytical model
on McVine Samples

Students can be absolutely awesome!

Going Forward

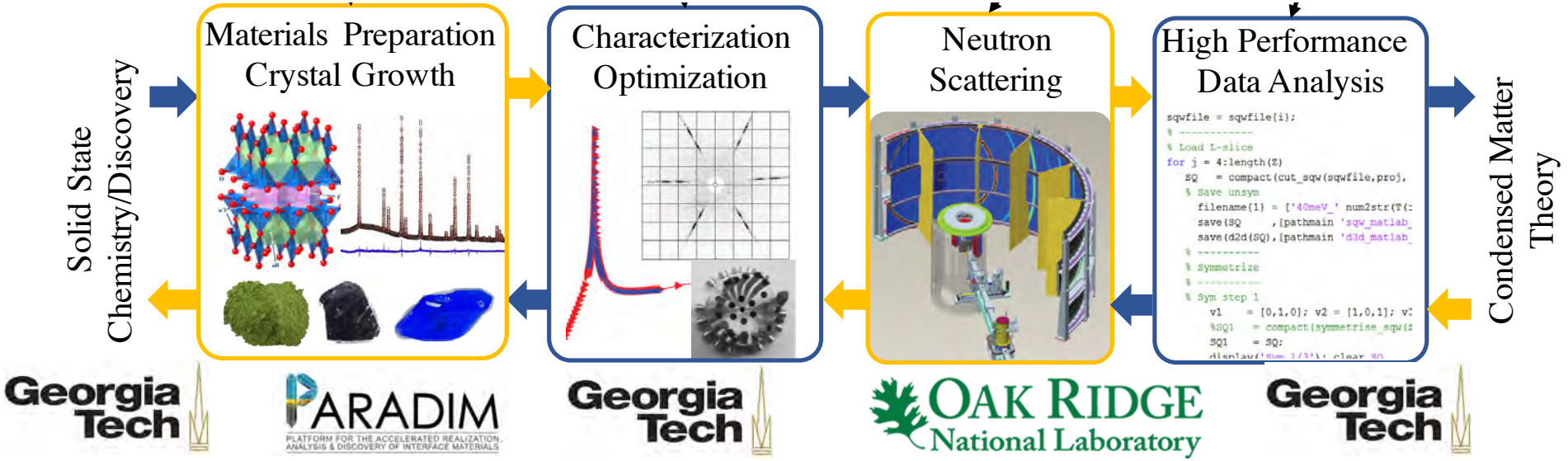
- Best results when neutron scattering integrated in program



MANTID is our gateway to $\chi''_{\alpha\beta}(\mathbf{q},\omega)$

Going Forward

- Best results when neutron scattering integrated in program



1. Data Reduction and analysis and the heart of our strategy
2. Mostly done by students (except extreme expert users)
3. Often the most important part of the neutron work
4. We want and need to know what's in the box (quality control)
5. Two levels: on-the fly analysis during experiment (GUI ok)
   post-experiment treatment (stable scripts)
6. Data will ultimately enter all sorts of analysis (flexibility I/O)