Understanding emergent properties in nanoscale systems:

anticipating the role of petascale computing and data analysis

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Thanks to Doug Abernathy & Mark Hagen (Spallation Neutron Source @ ORNL)

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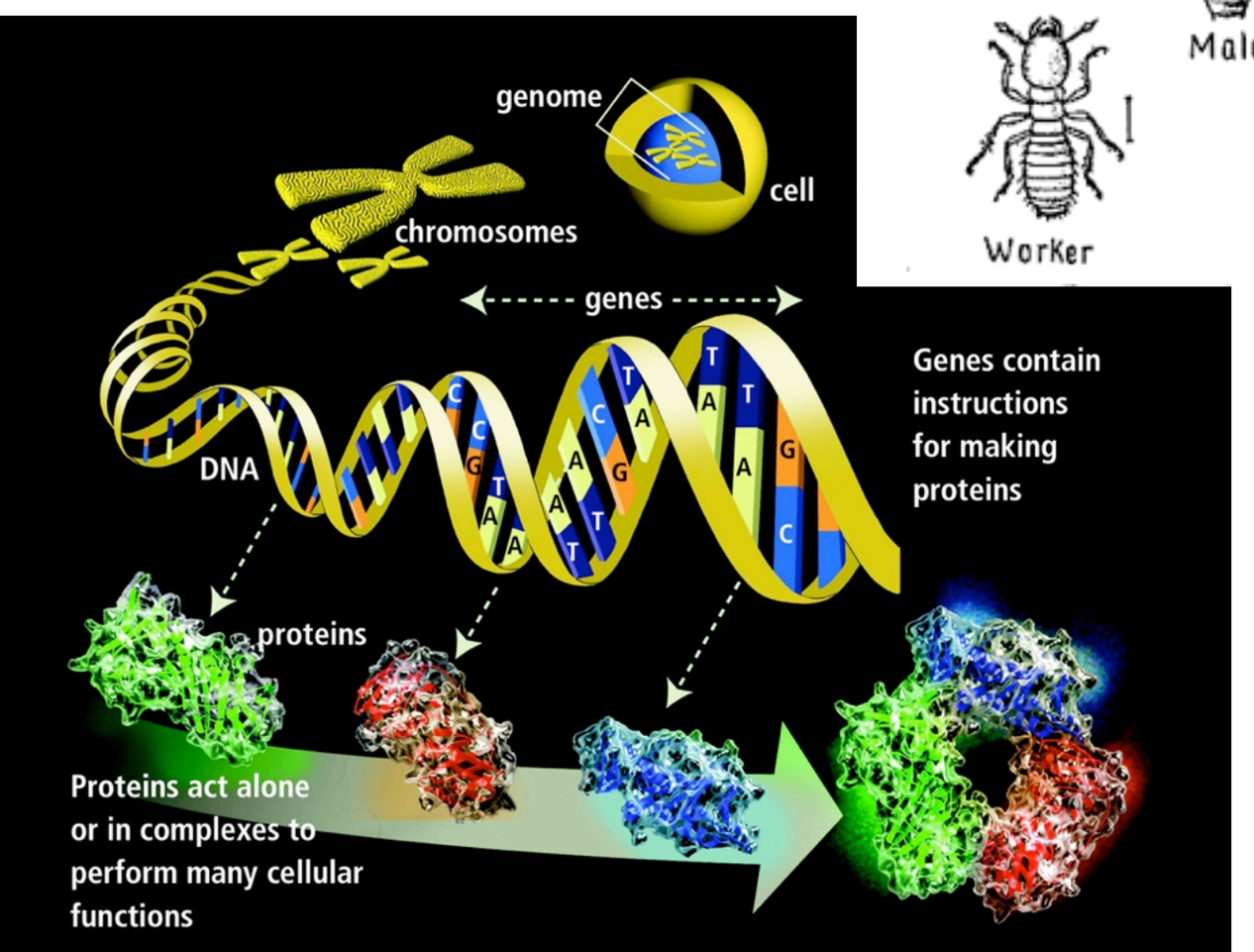
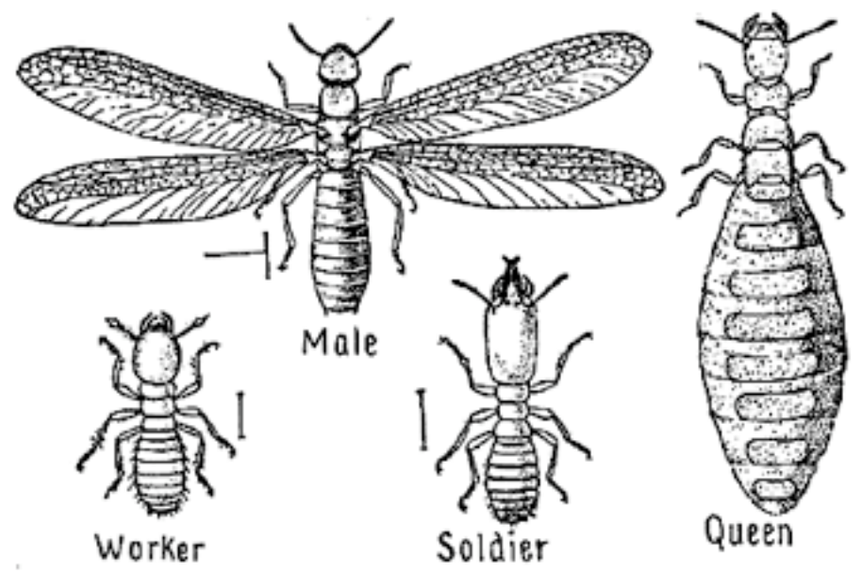
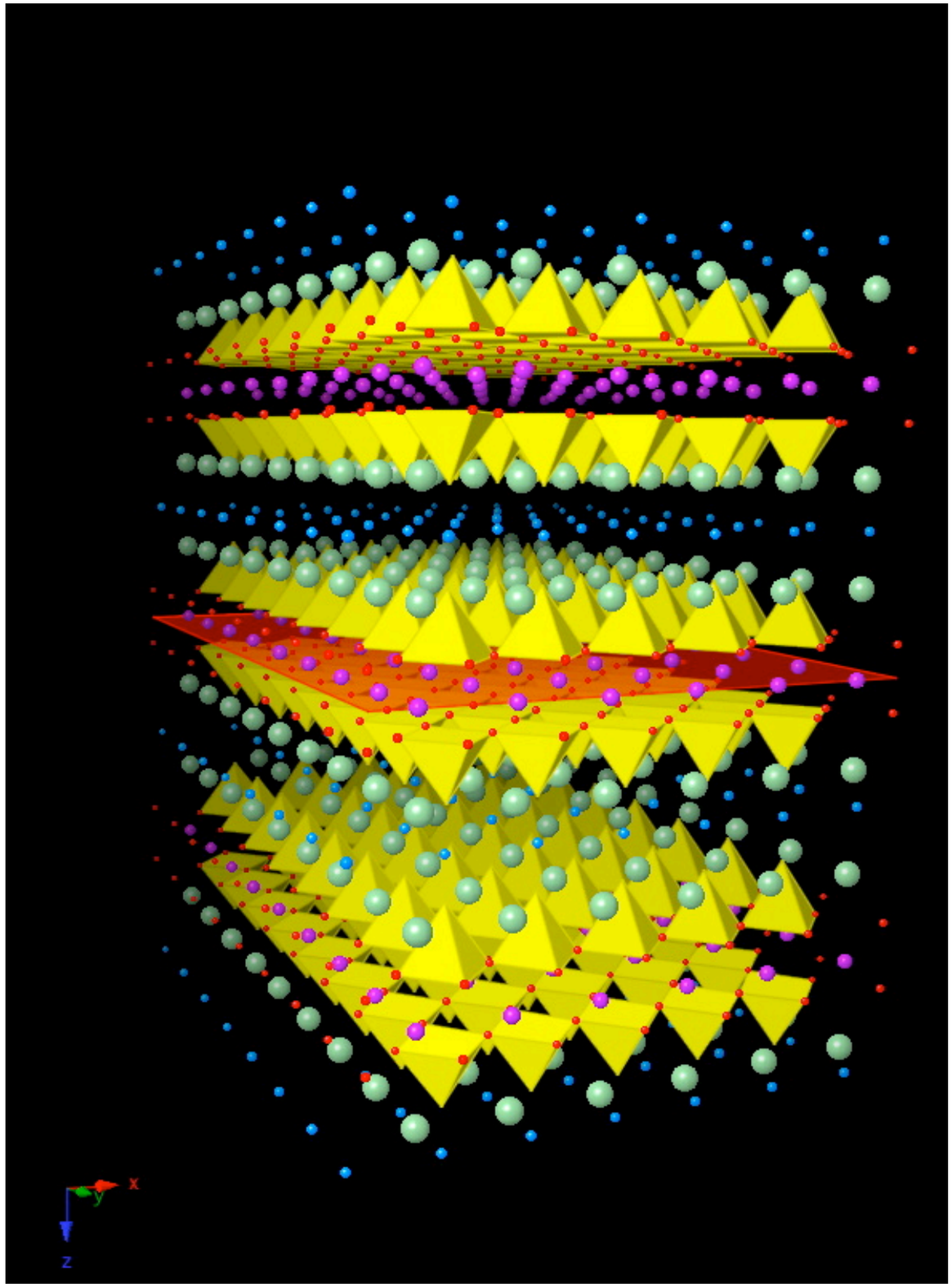
Examples of emergent behavior: biology





Examples of emergent behavior: materials



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Descriptions of emergent behavior

In philosophy, systems theory and the sciences, emergence refers to the way complex systems and patterns arise out of a multiplicity of relatively simple interactions. Emergence is central to the theory of complex systems. reference: emergence on http://en.wikipedia.org

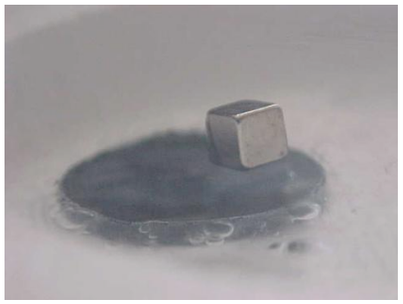
Why study the nanoscale: e.g. cuprates

Macro-scale

Nano-scale

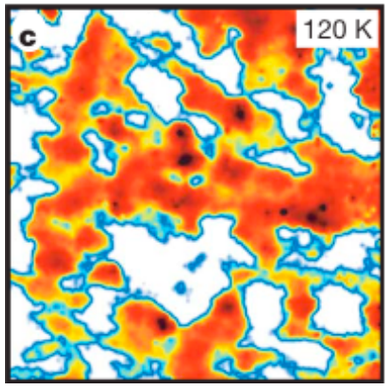
Atomic scale

Marcroscopic quantum effect



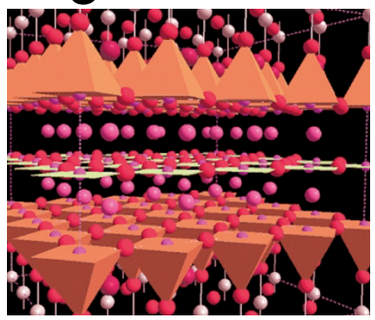
$\approx \mu\mathrm{m}$

Pairing / Inohomo-geneities



$\approx \mathrm{nm}$

Atomic scale quantum models& strong electron correlations



Thermodynamic limit

Vortex pinning

Nanoscale inhomogeneities

Formation of Cooper pairs

Strong electron correlation / competing interactions

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Nanoscience: inherently difficult but interesting

Macro-scale

Thermodynamics

Limit of large numbers

Mean field

Continuum description

$\approx \mu\mathrm{m}$

Nano-scale

Importance of temporal and compositional fluctuations

no canonical "language"

Crossover from strong to weak correlations

$\approx \mathrm{nm}$

Atomic scale

Quantum behavior and strong quantum correlaitons

Atomistic description

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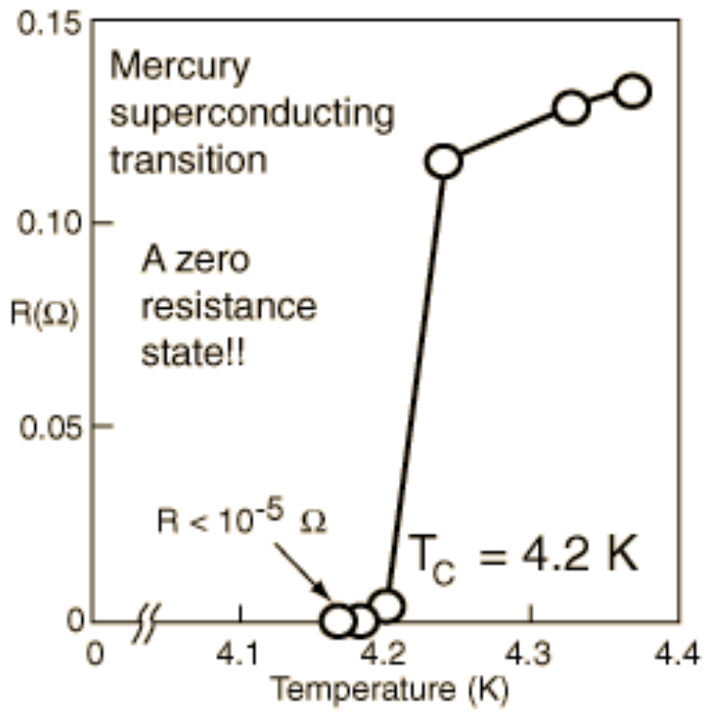
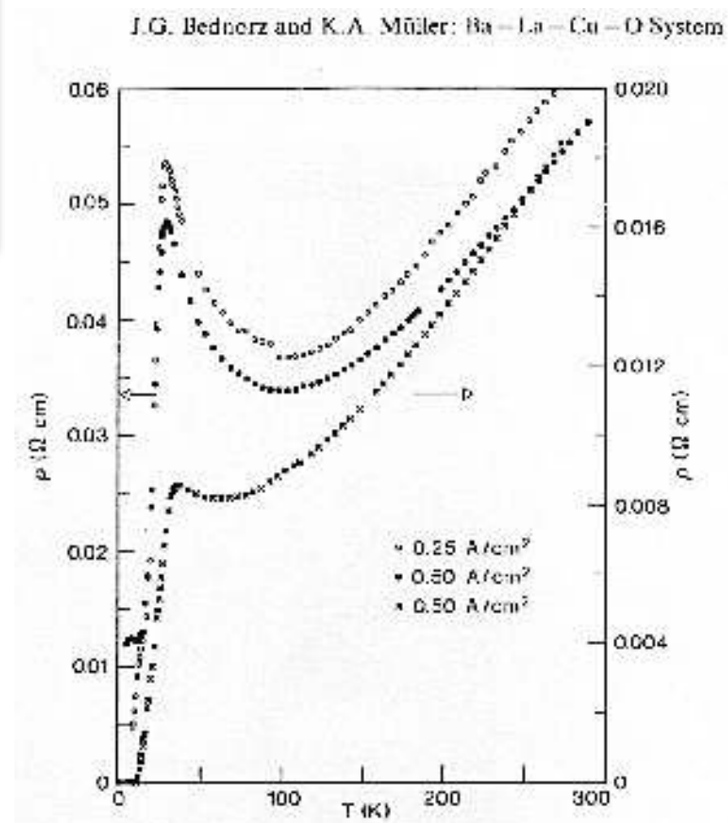
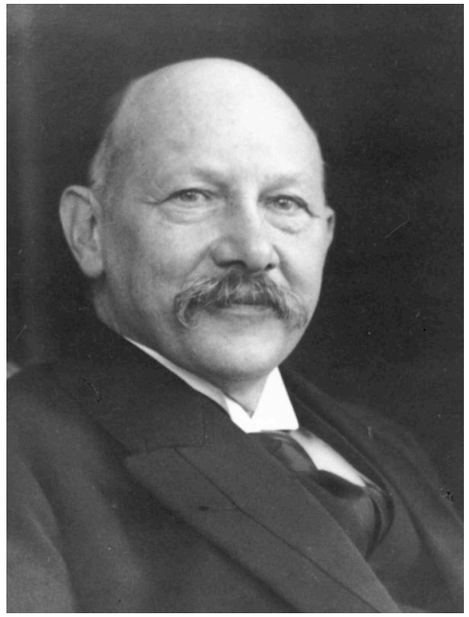
Experiment, experiment, experiment







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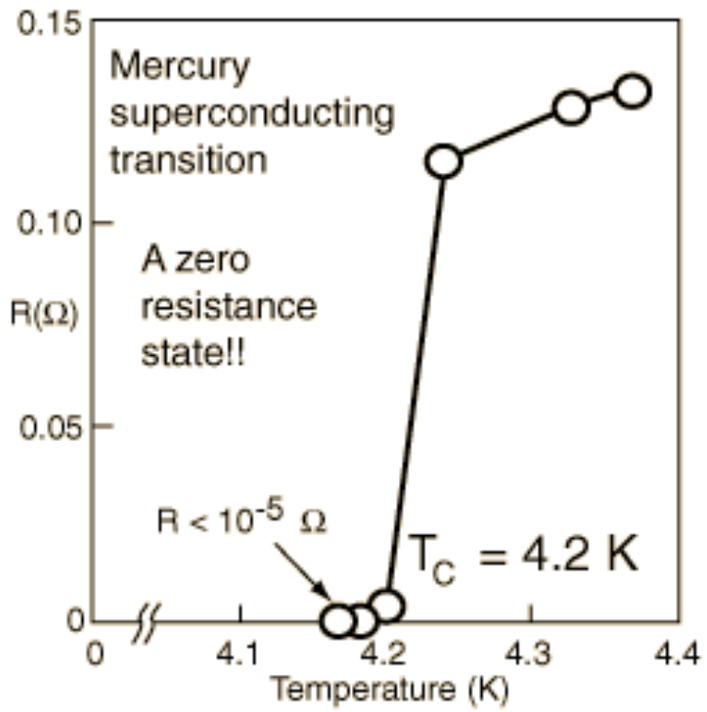
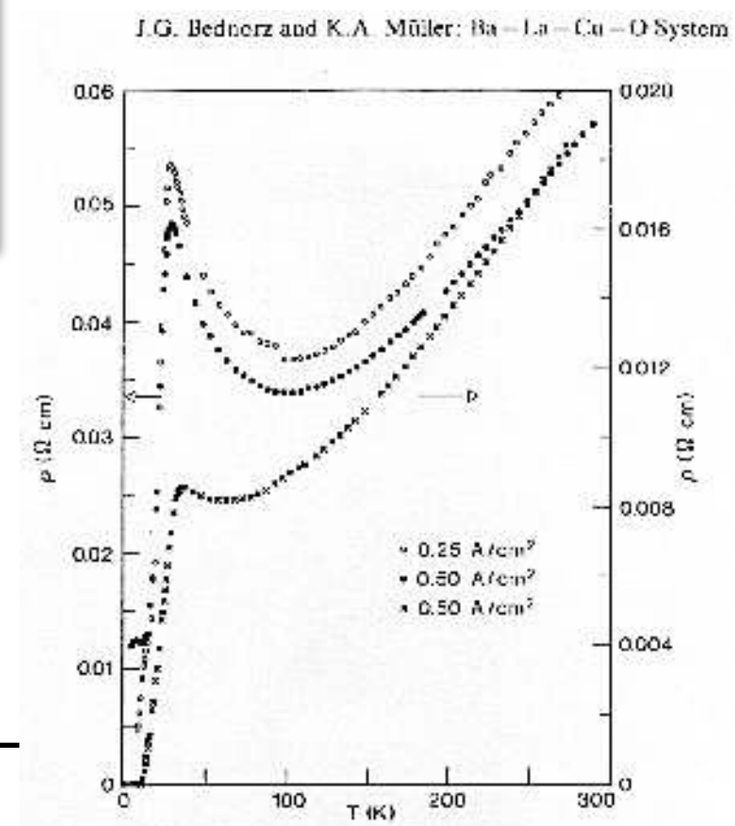
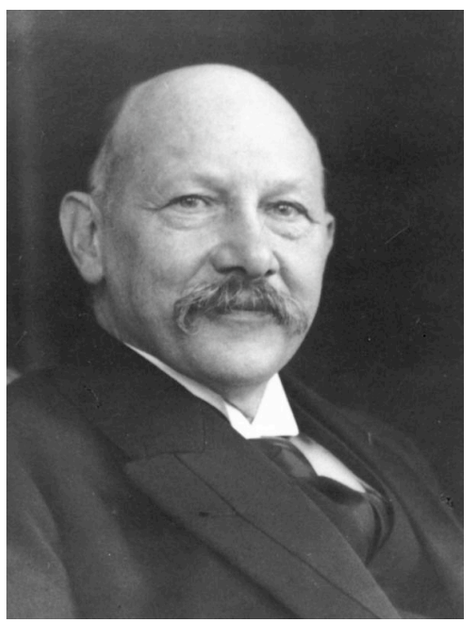
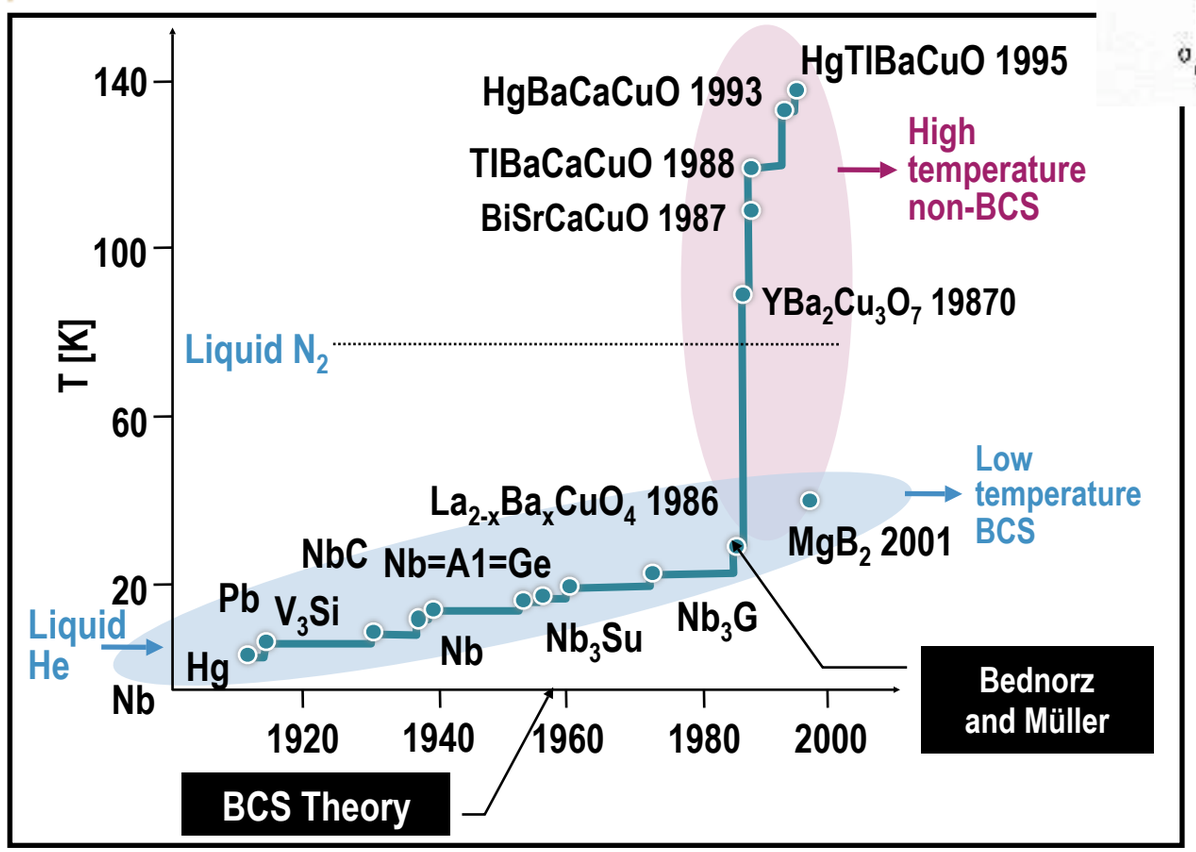




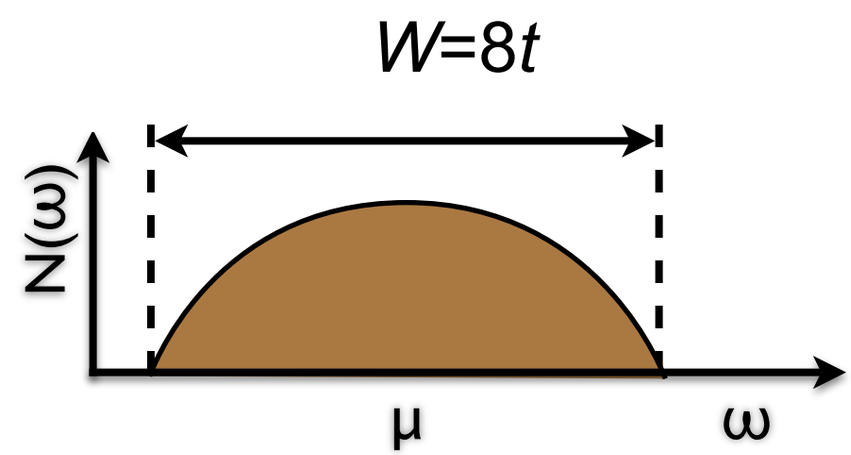




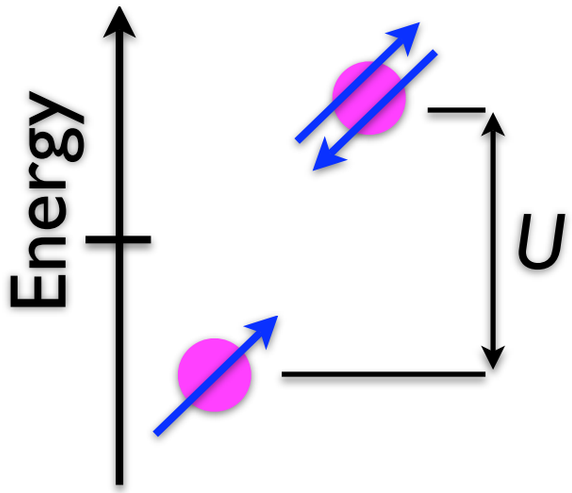
Traditional role of theory

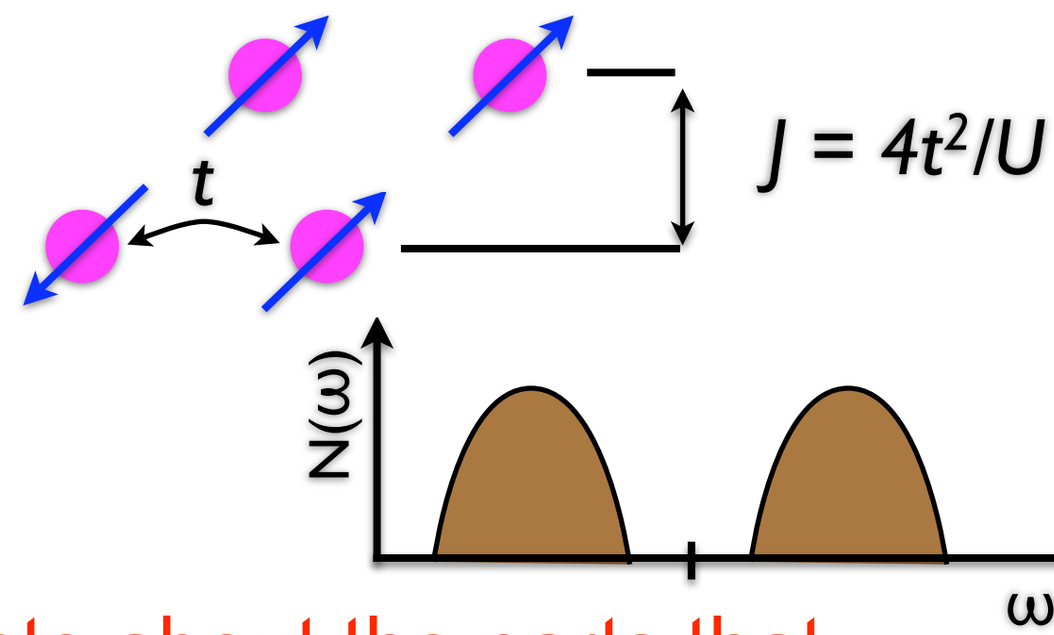
1. Write down (choose) a model

$$H = -t \sum_{<ij>,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



2. Analyze its properties





3. Discuss the physics - speculate about the parts that cannot be solved
(eg. superconductivity in the Hubbard model)

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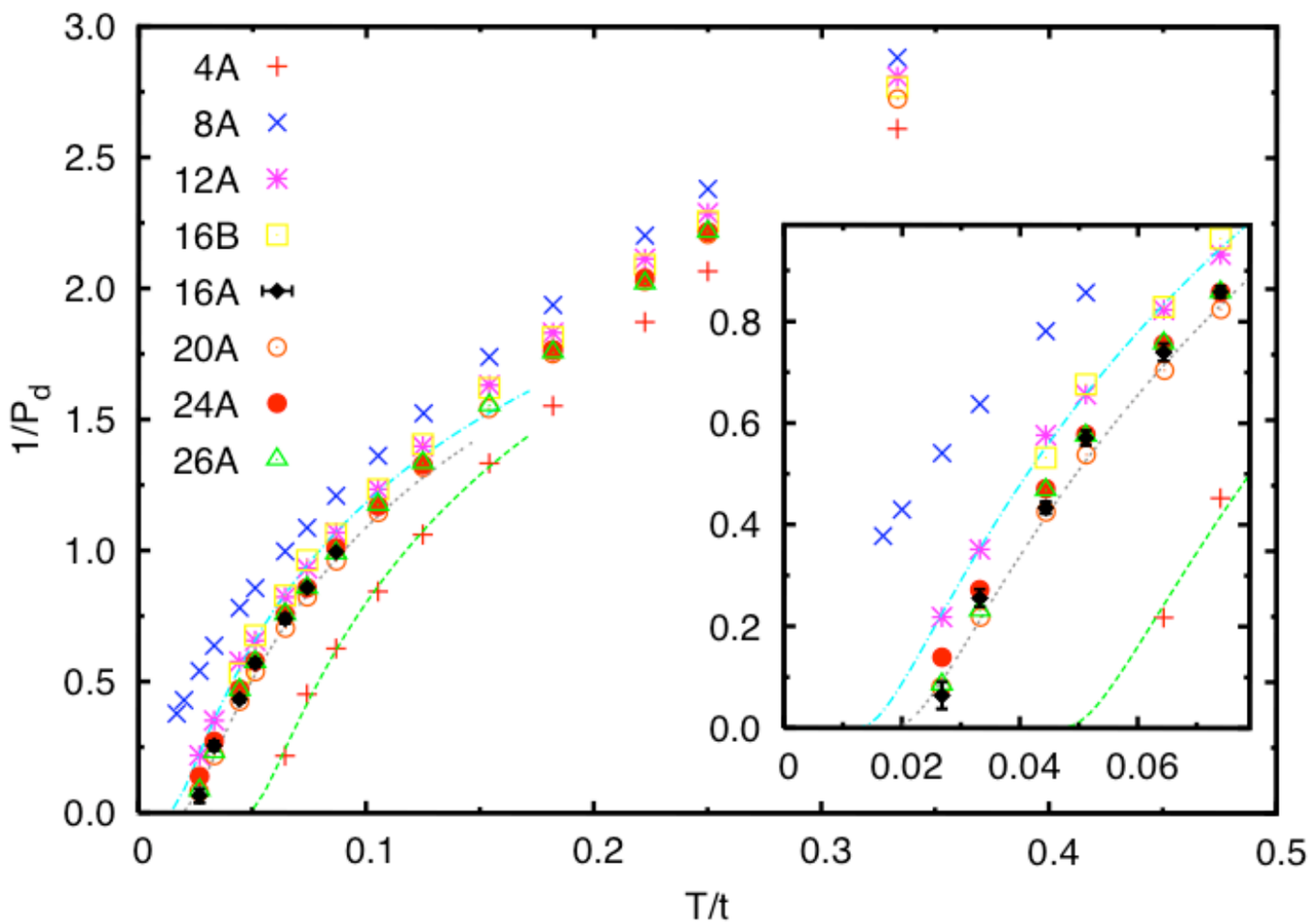
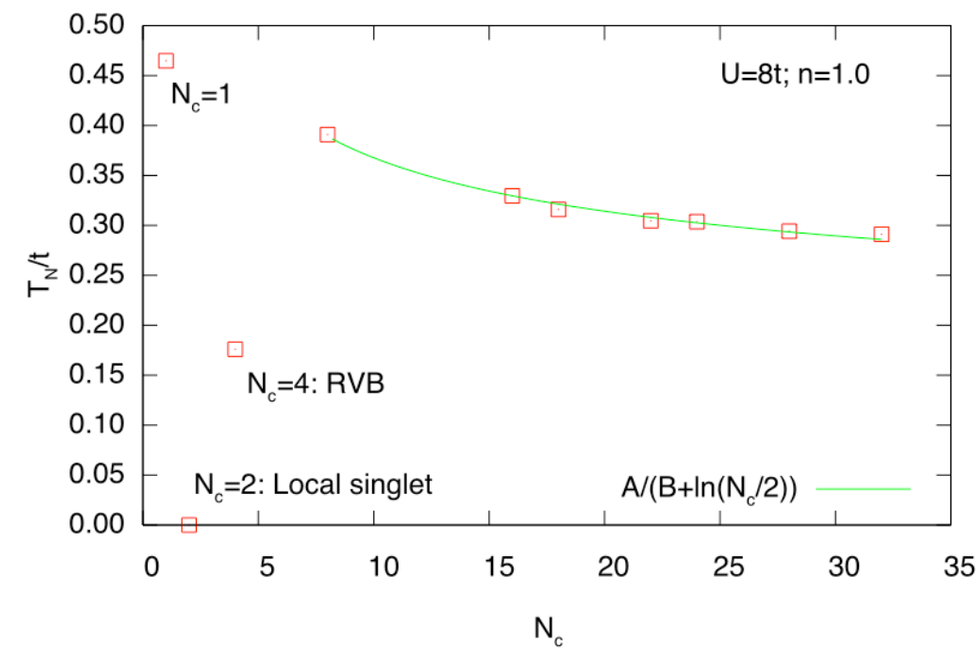
New methods + powerful computers

Cray X1/X1E @ NCCS

Systematic numerical solutions demonstrate that Hubbard model indeed describe *d*-wave pairing and superconductivity





Maier, Jarrell, Schulthess, Kent, and White, Phys. Rev. Lett. **95**, 237001 (2005)

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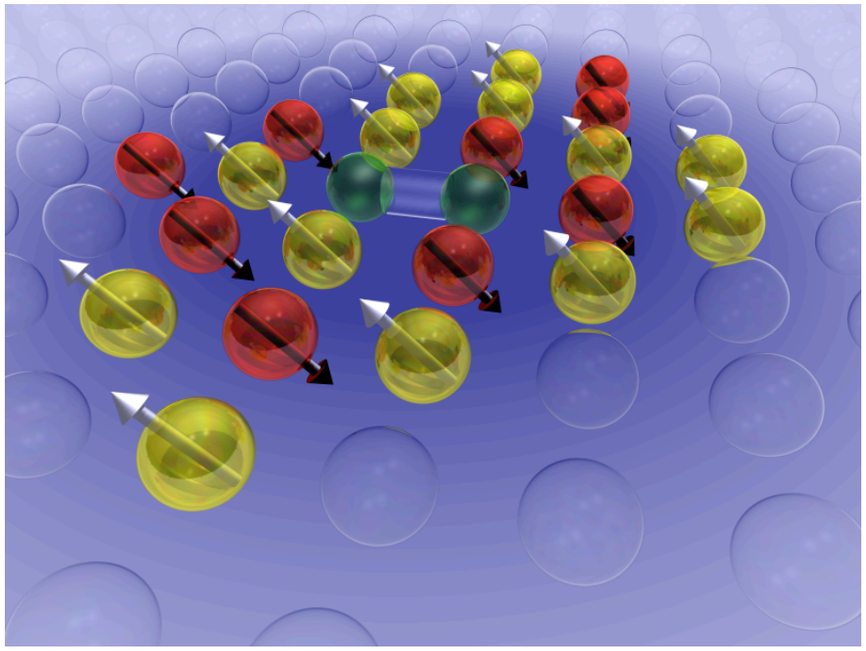
Now that the 2D Hubbard model can be solved ...

- Study the mechanism responsible for pairing in the model
  - Analyze the particle-particle vertex
  - Pairing is mediated by spin fluctuations
    Maier, Jarrell, and Scalapino,
    Phys. Rev. Lett. **96** 47005 (2006)

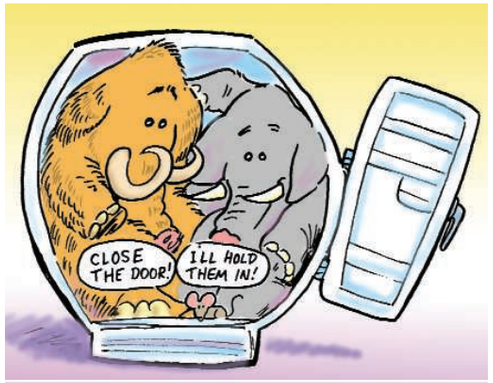


- Spin susceptibility representation of pairing interactions $3/2\bar{U}^2\chi(q,\omega)$

  Spin fluctuation "Glue"
  - test this for of pairing interaction with neutron scattering and ARPES measurments
  - Maier et al., Phys. Rev. B **75**, 134519 (2007); *ibid* **75**, 144516 (2007)
- Relative importance of spin-fluctuations and resonant valence bond mechanism
  - Maier et al., Phys. Rev. Lett. in press, arXiv:0801.4506

P.W. Anderson, Science **316**, 1705 (2007):
"We have a mammoth (U) and an elephant (J) in our refrigerator - do we care much if there is also a mouse?"

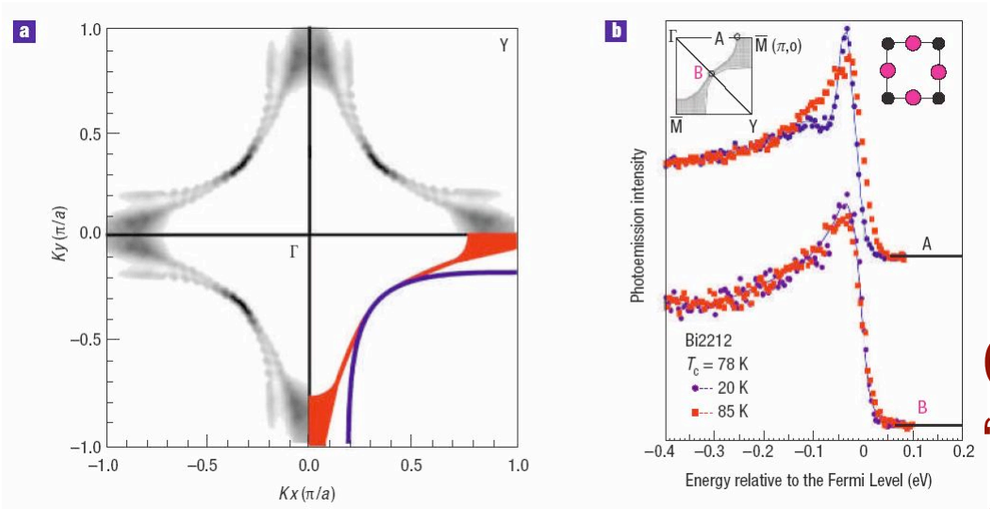
see also http://www.sciencemag.org/cgi/eletters/316/5832/1705
"Scalapino is not a glue-sniffer"



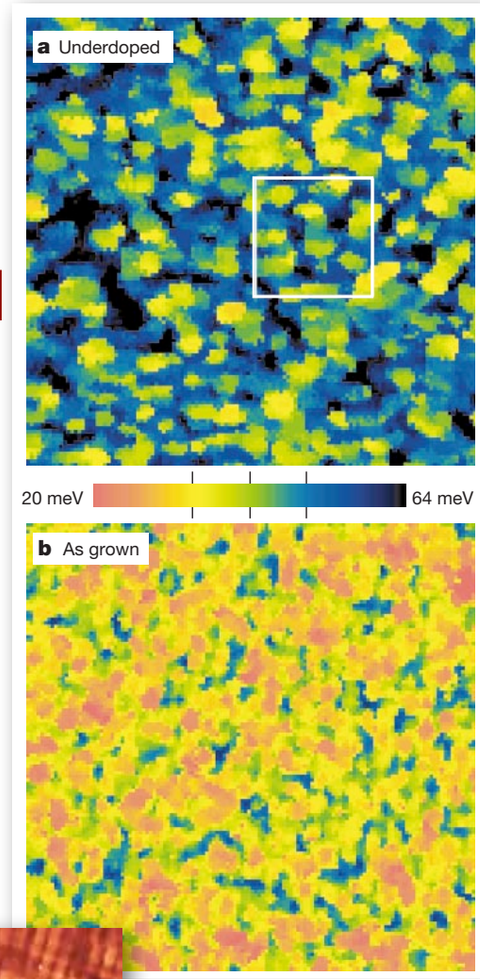
Staggering new experimental capabilities

- Neutron scattering (later in this talk)
- Synchrotron (eg. ARPES)

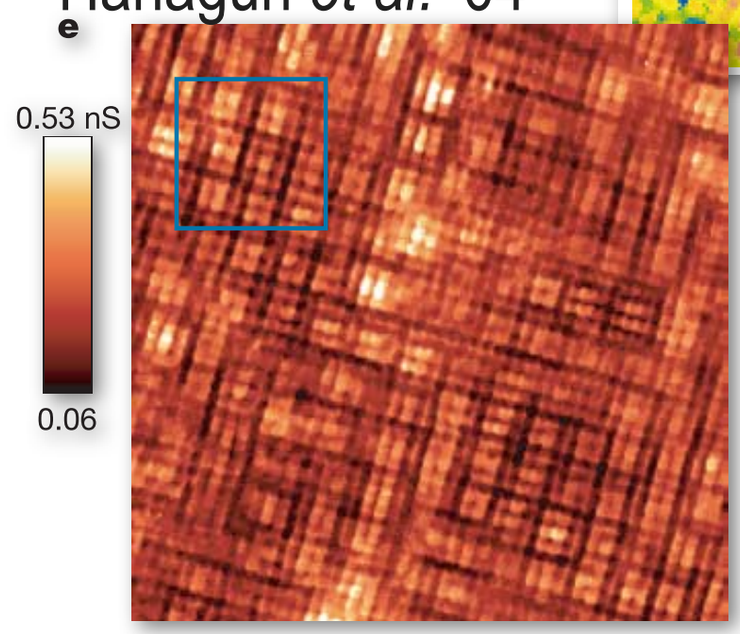
Fermi surface (BSCCO):
Bonn '06



Random SC gap modulations in STM (BSCCO):
Lang *et al.* '02

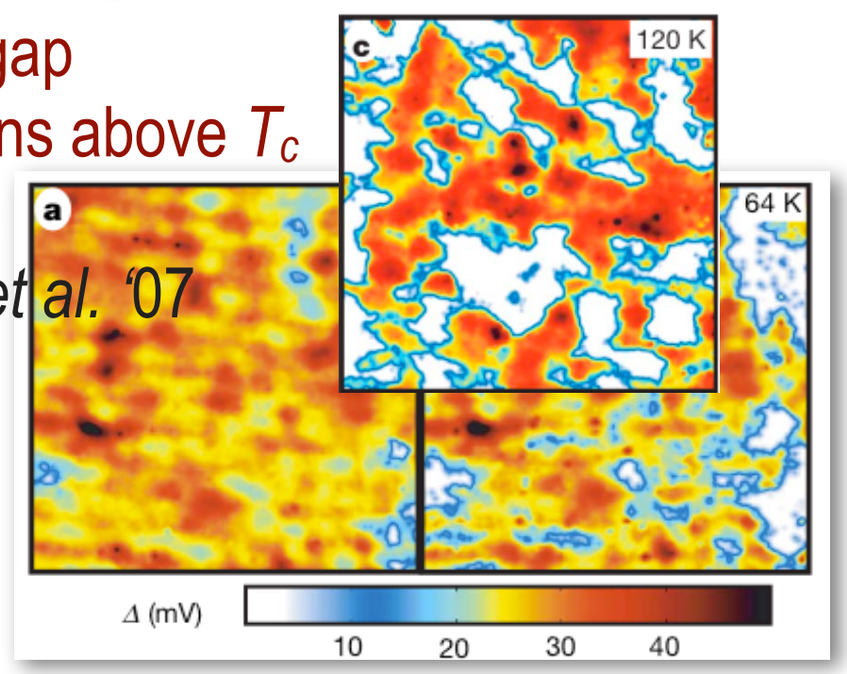


Charge ordered "checkerboard" state (Na doped cuprates):
Hanaguri *et al.* '04



- Scanning probes

Random gap modulations above T_c (BSCCO):
Gomes *et al.* '07



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Example: Spallation Neutron Source (SNS)

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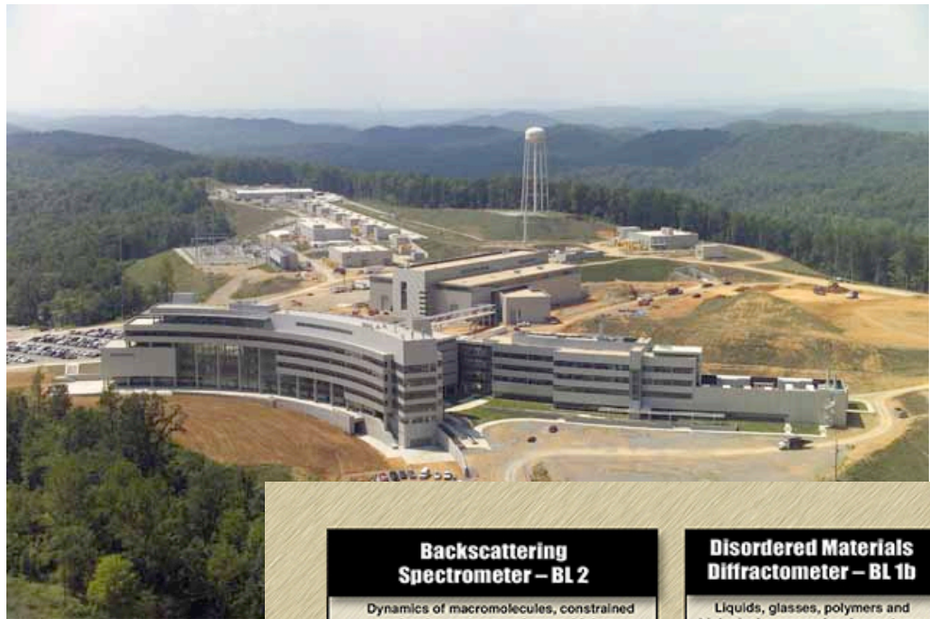

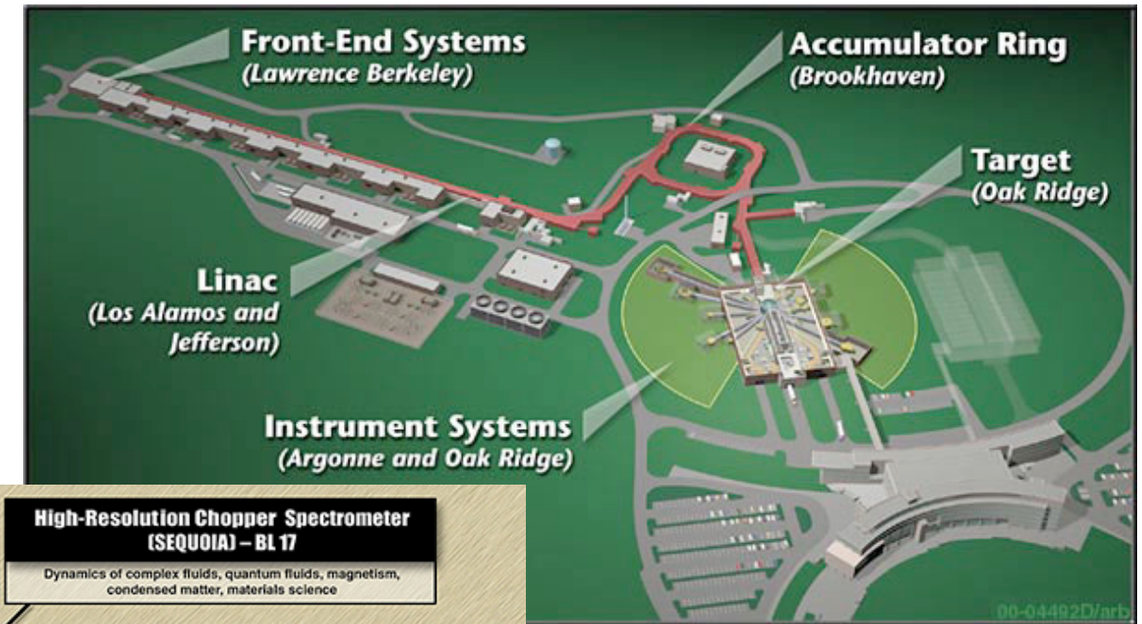

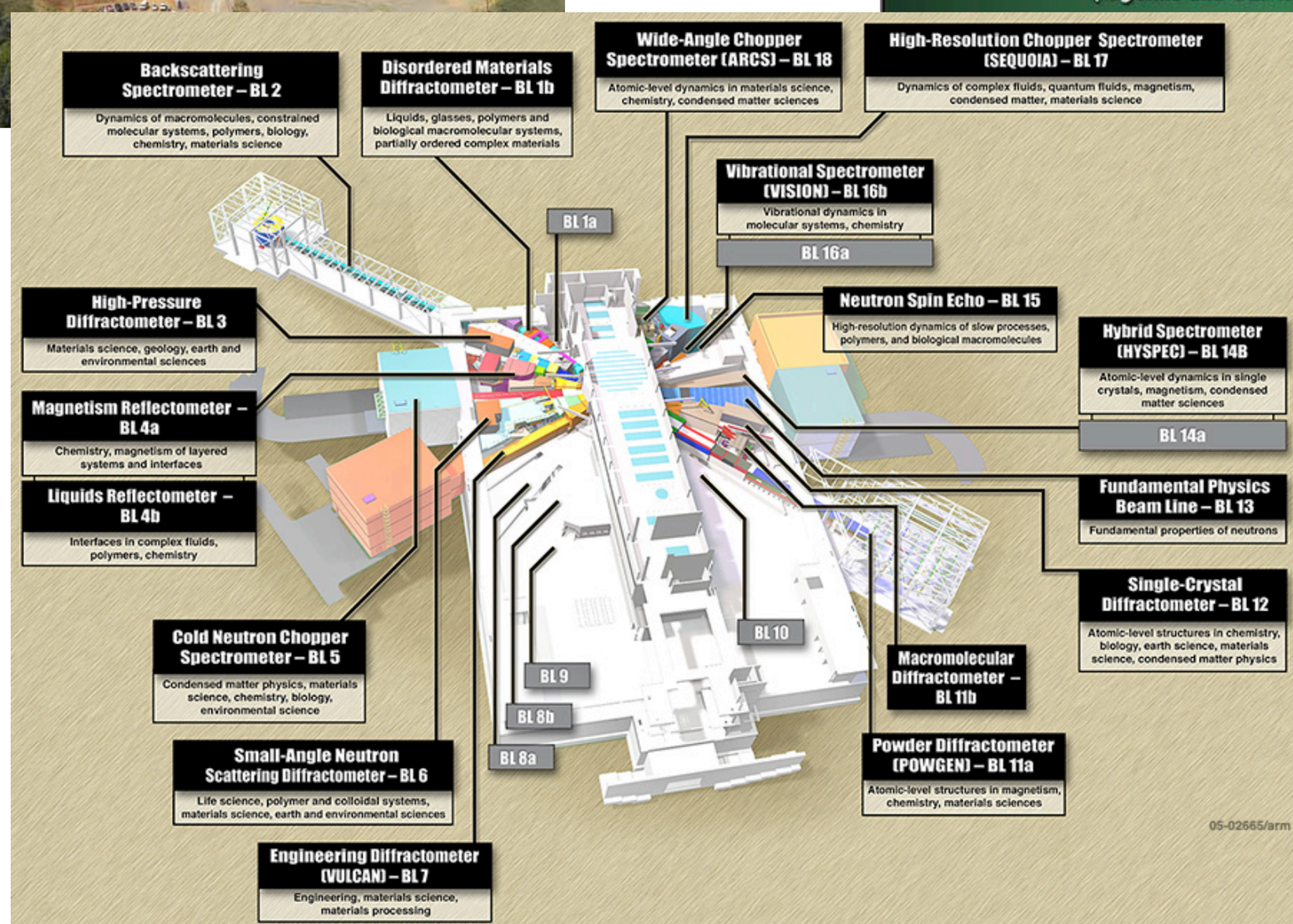

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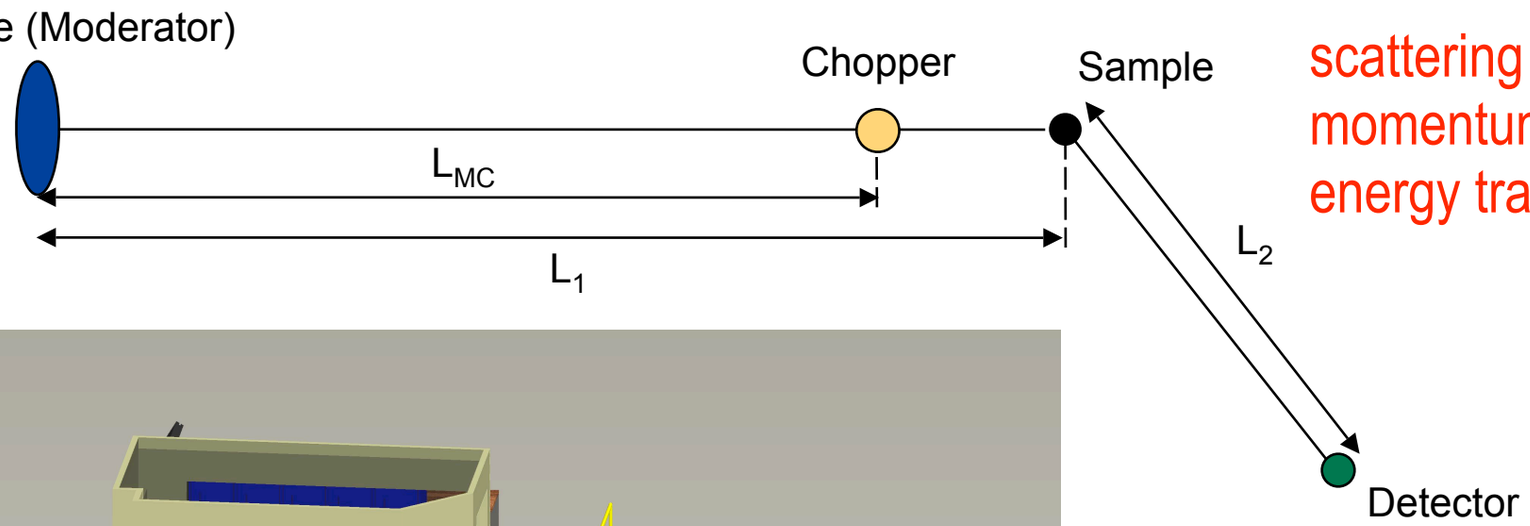
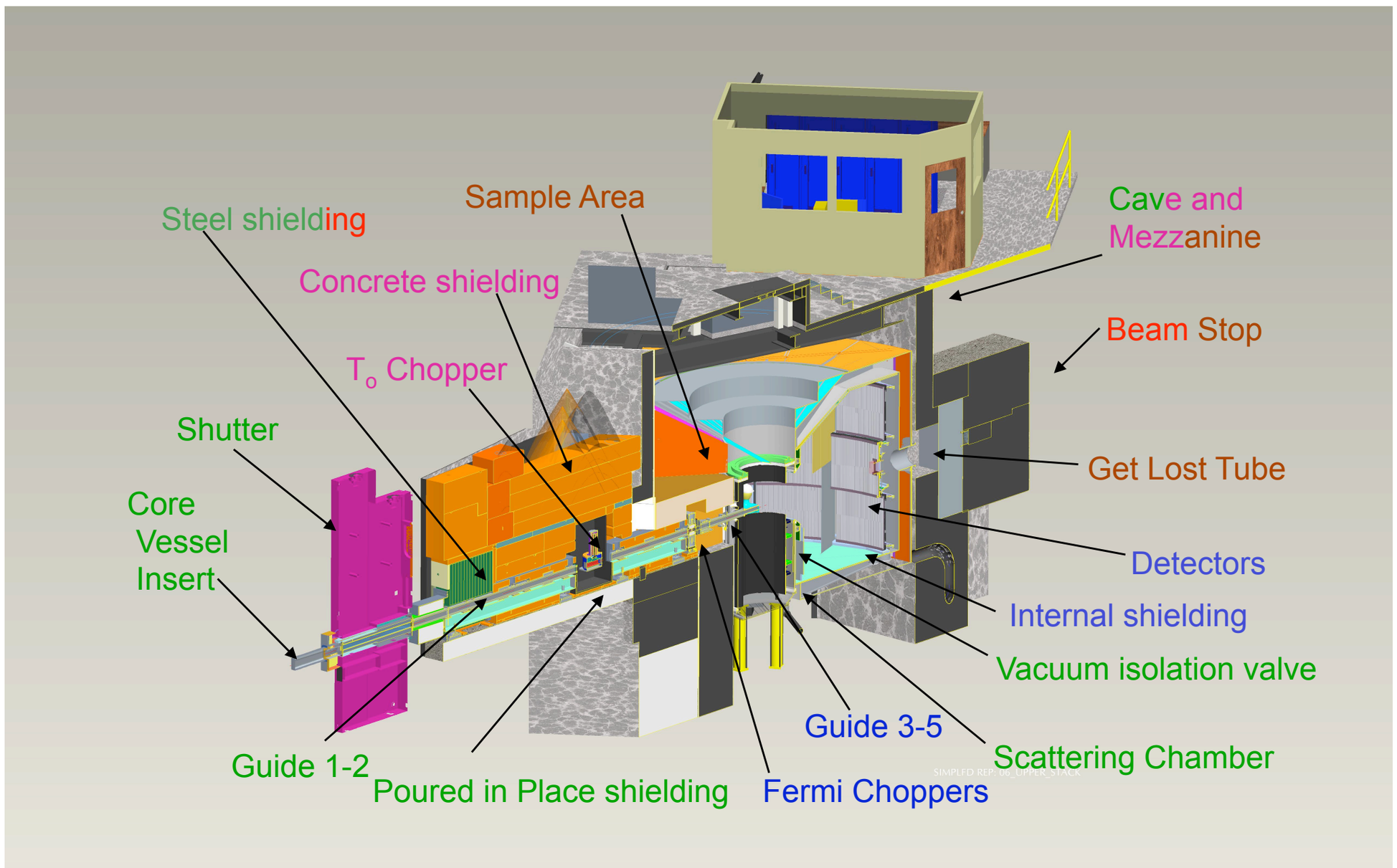
Intelastic neutron scattering experiments at SNS

Source + chopper = neutrons pulse with specific energy (velocity)

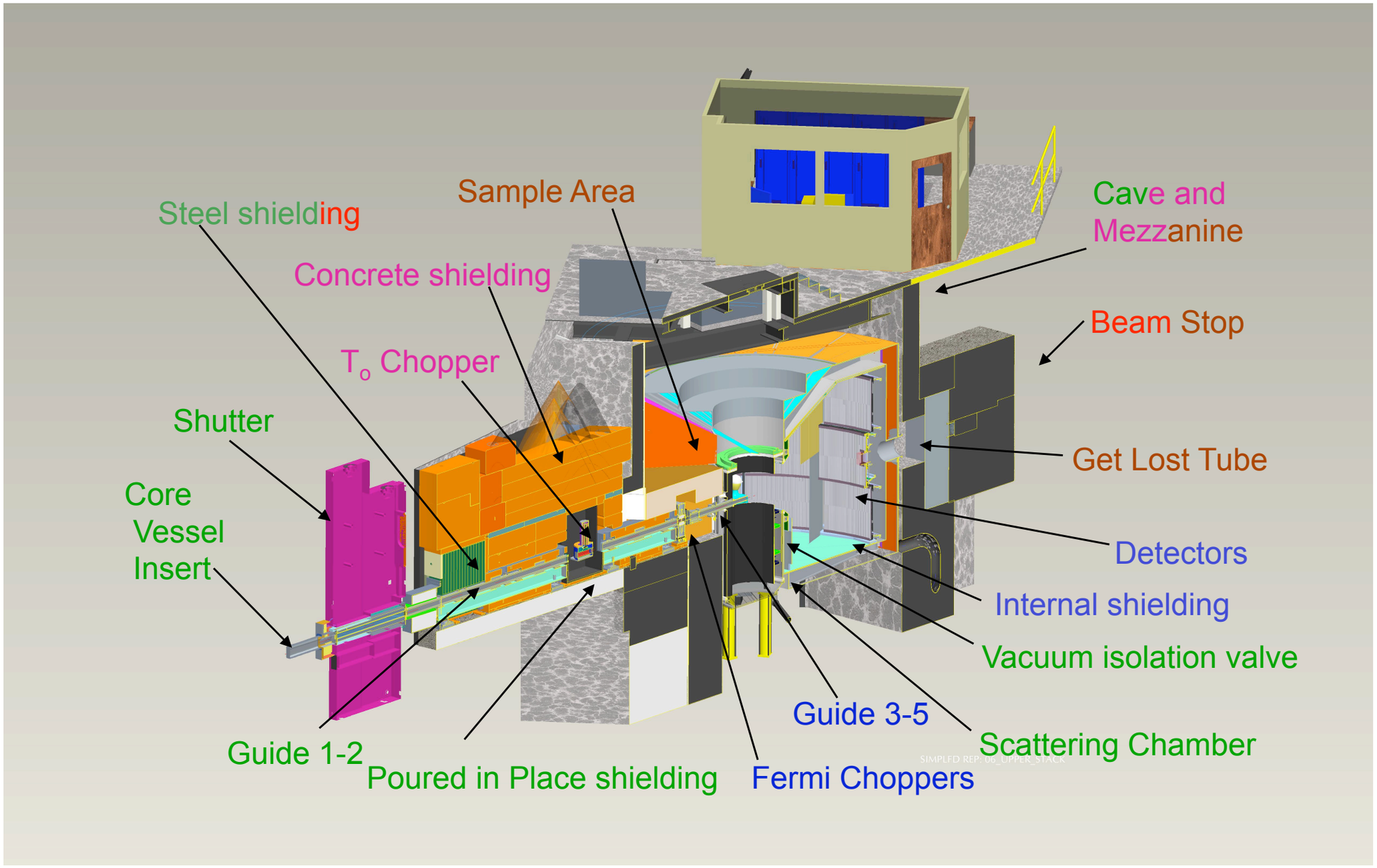


scattering = momentum & energy transfer

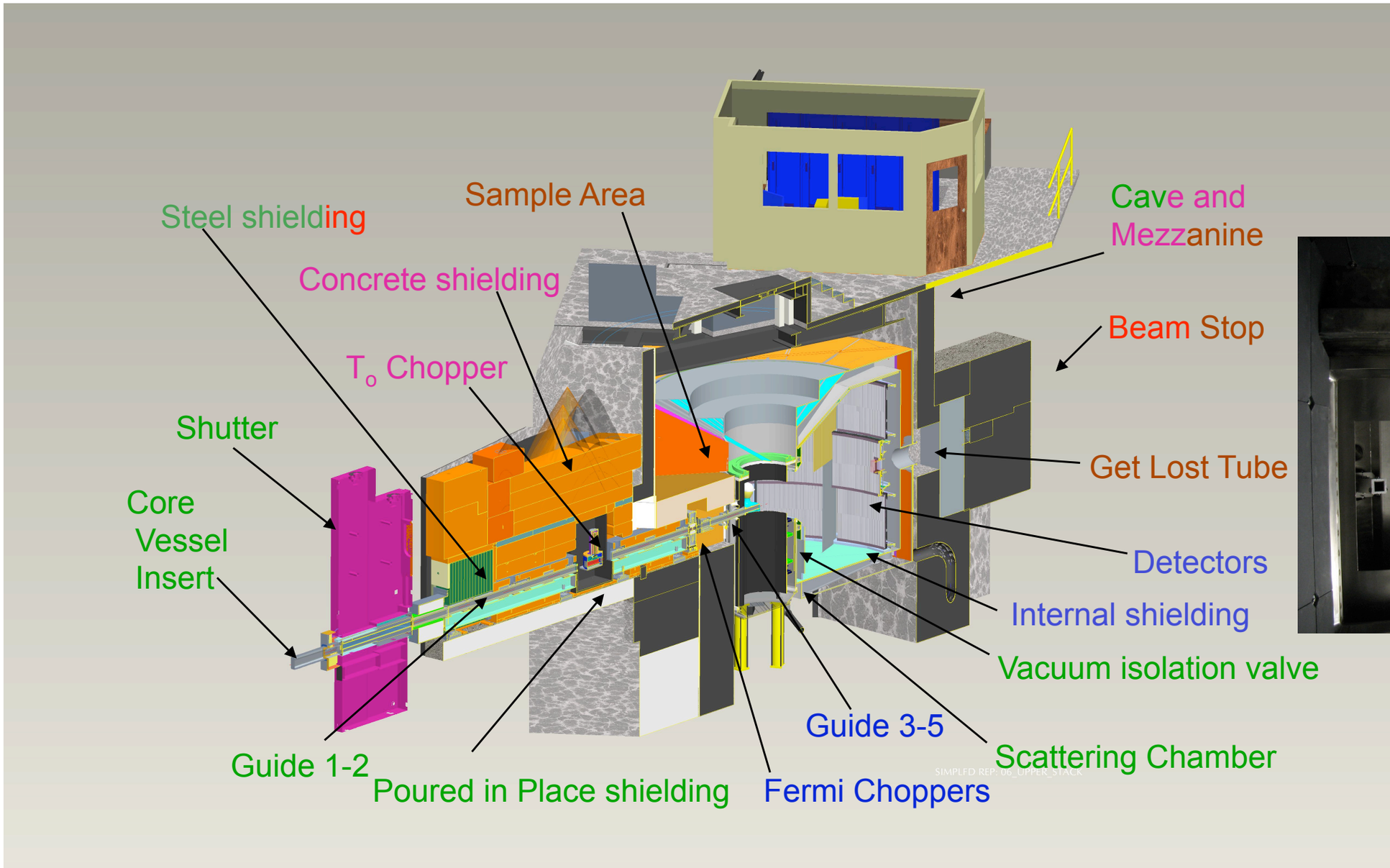


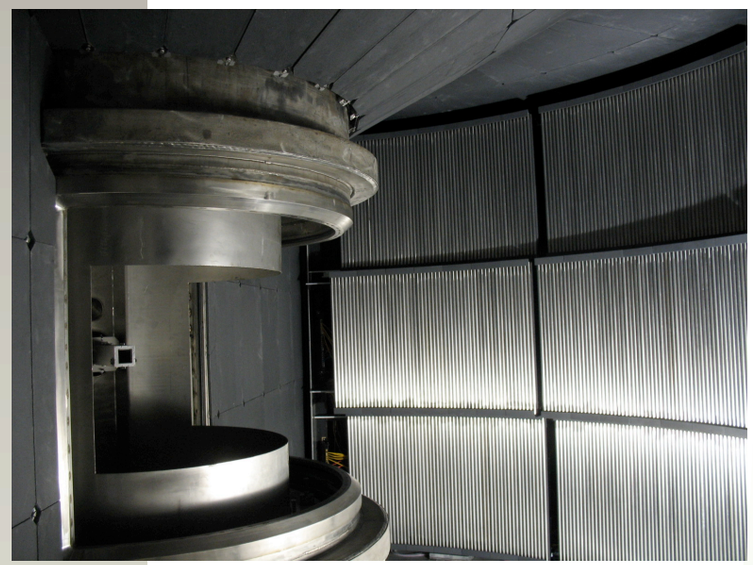
measurement at certain scattering angle and after given time of flight (final velocity)

ARCS - wide angle chopper spectrometer



ARCS - wide angle chopper spectrometer





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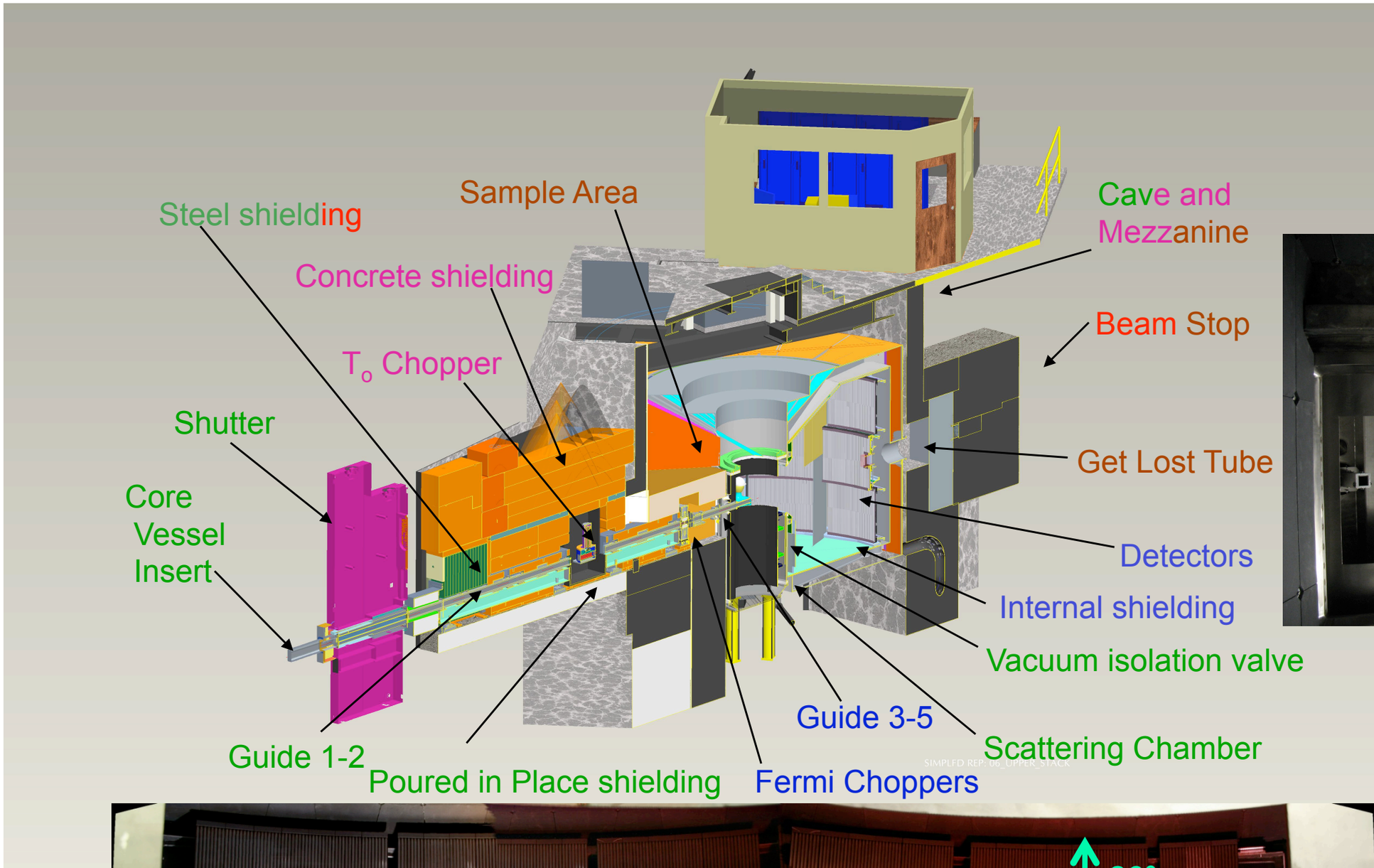
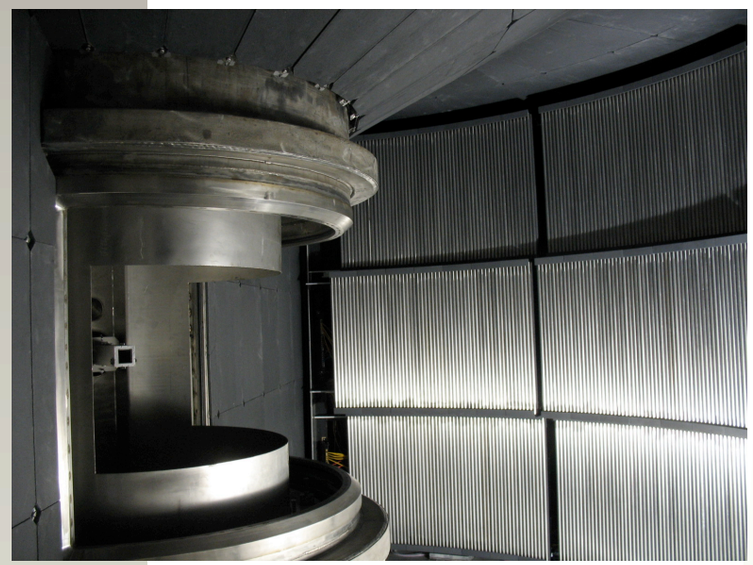
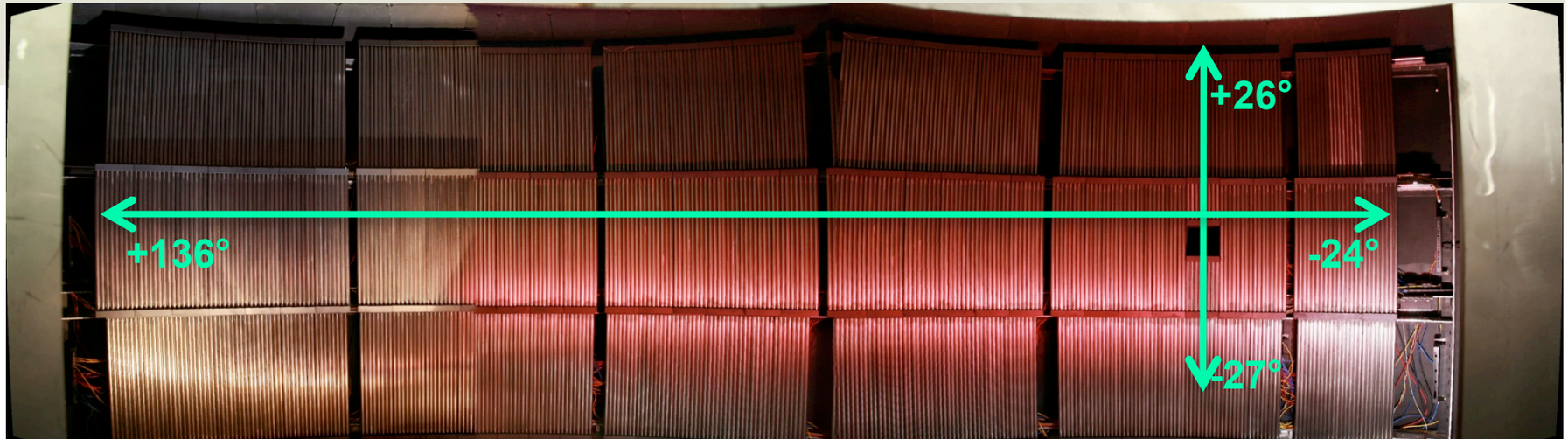
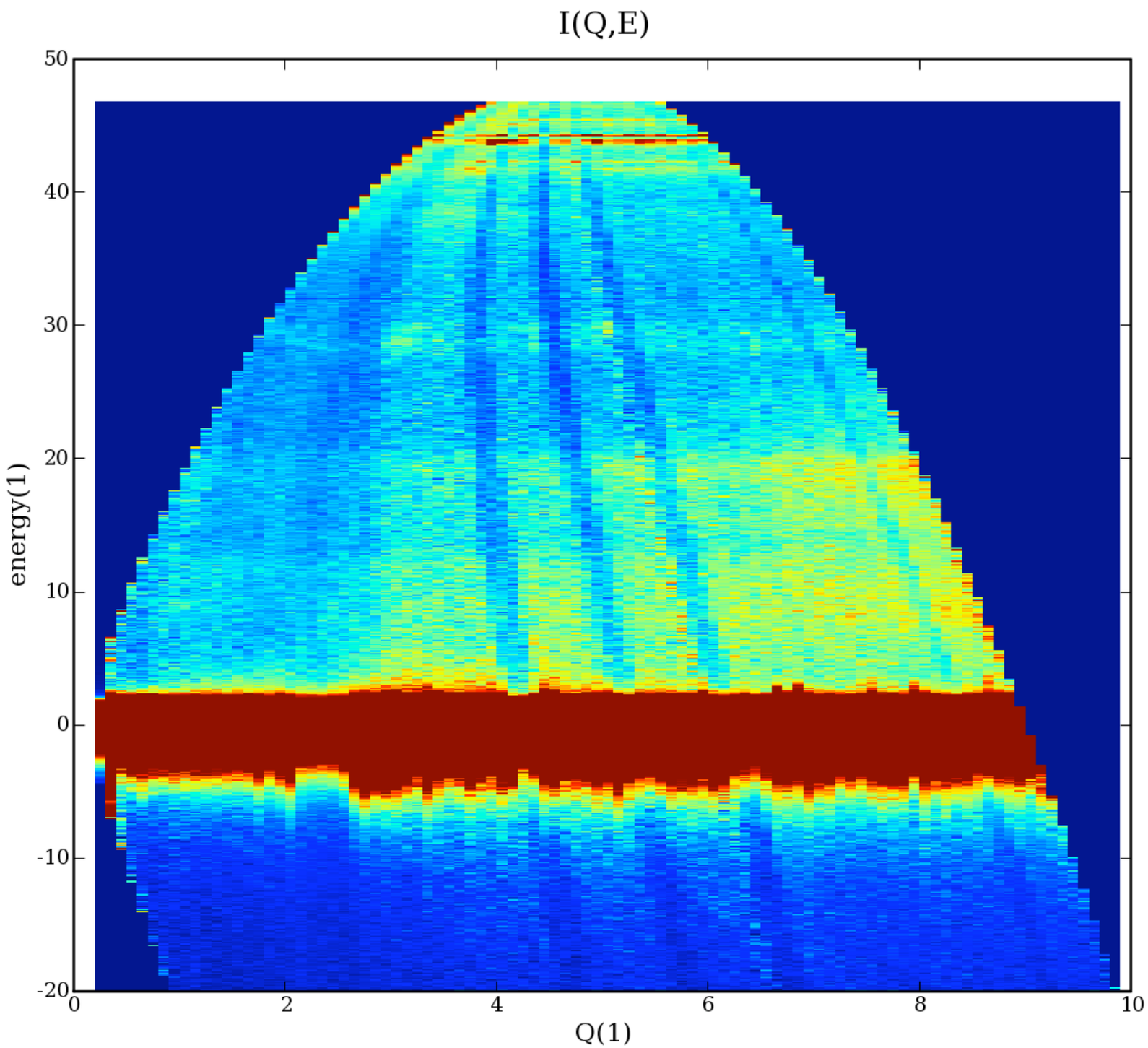






Measured intensity as function of momentum transfer (Q) and energy transfer (E)



Sufficient flux and sensitivity to take cone spectrum per hour

~ 1GB event data

~ 10GB histo-gram

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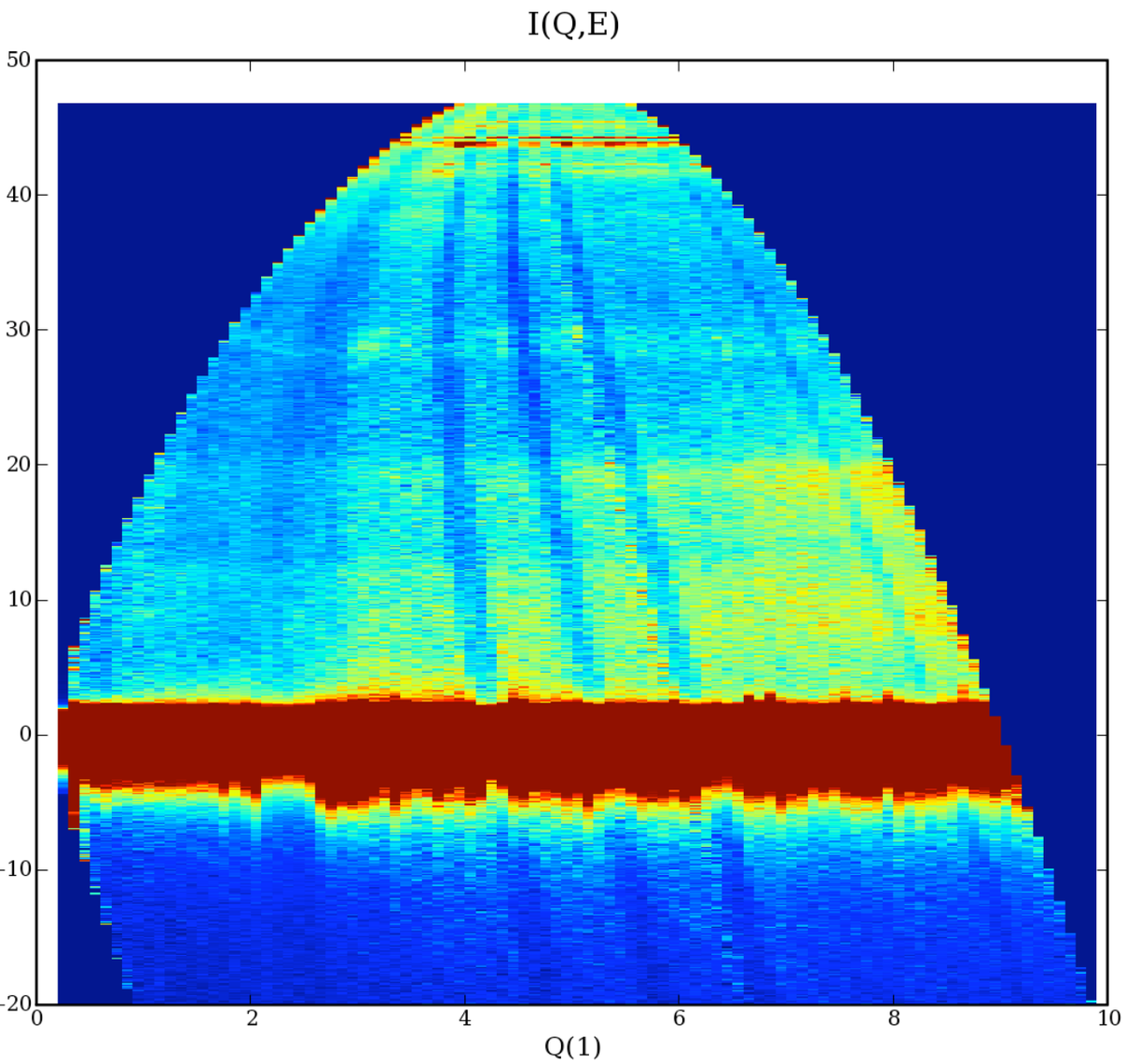
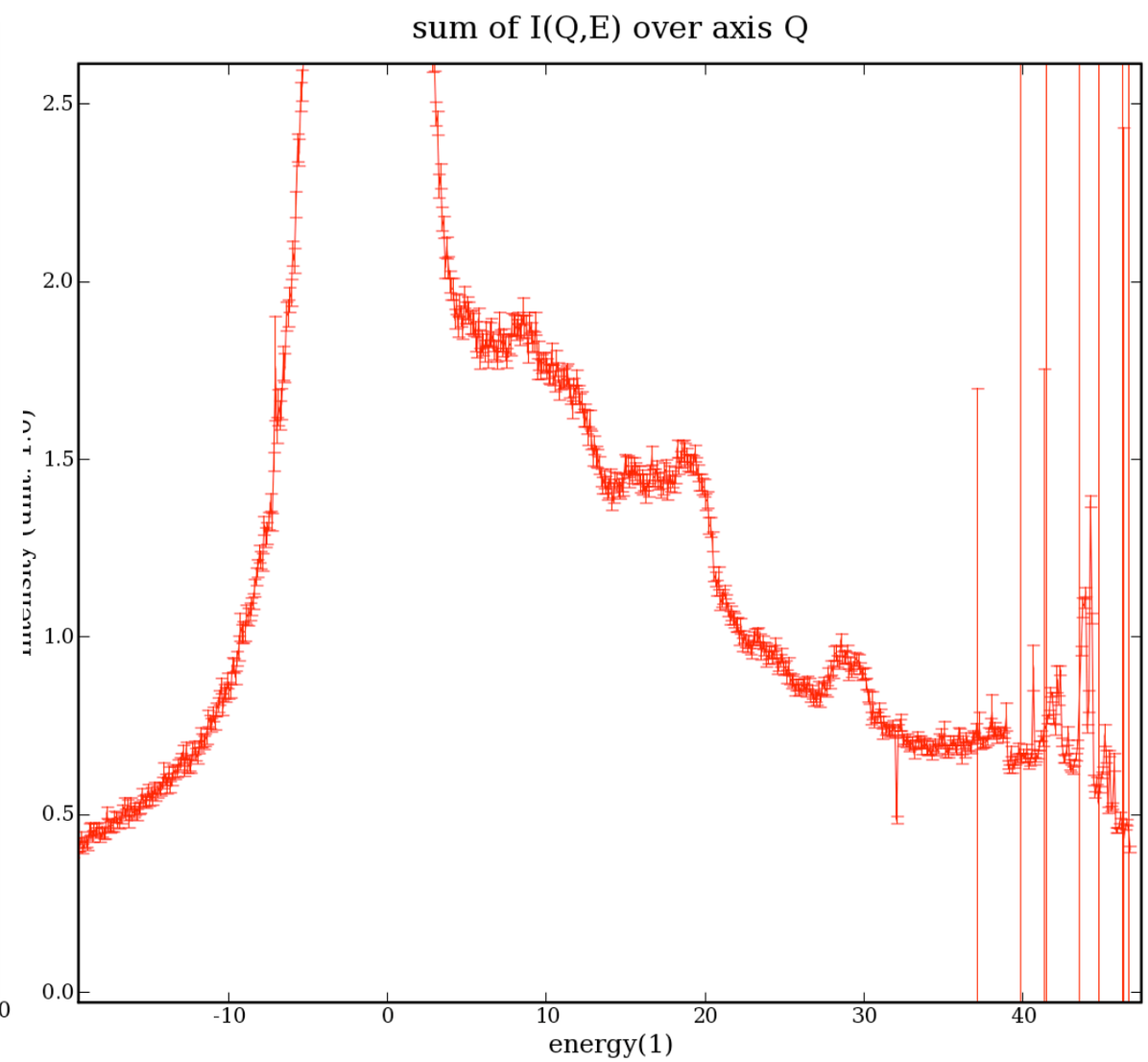
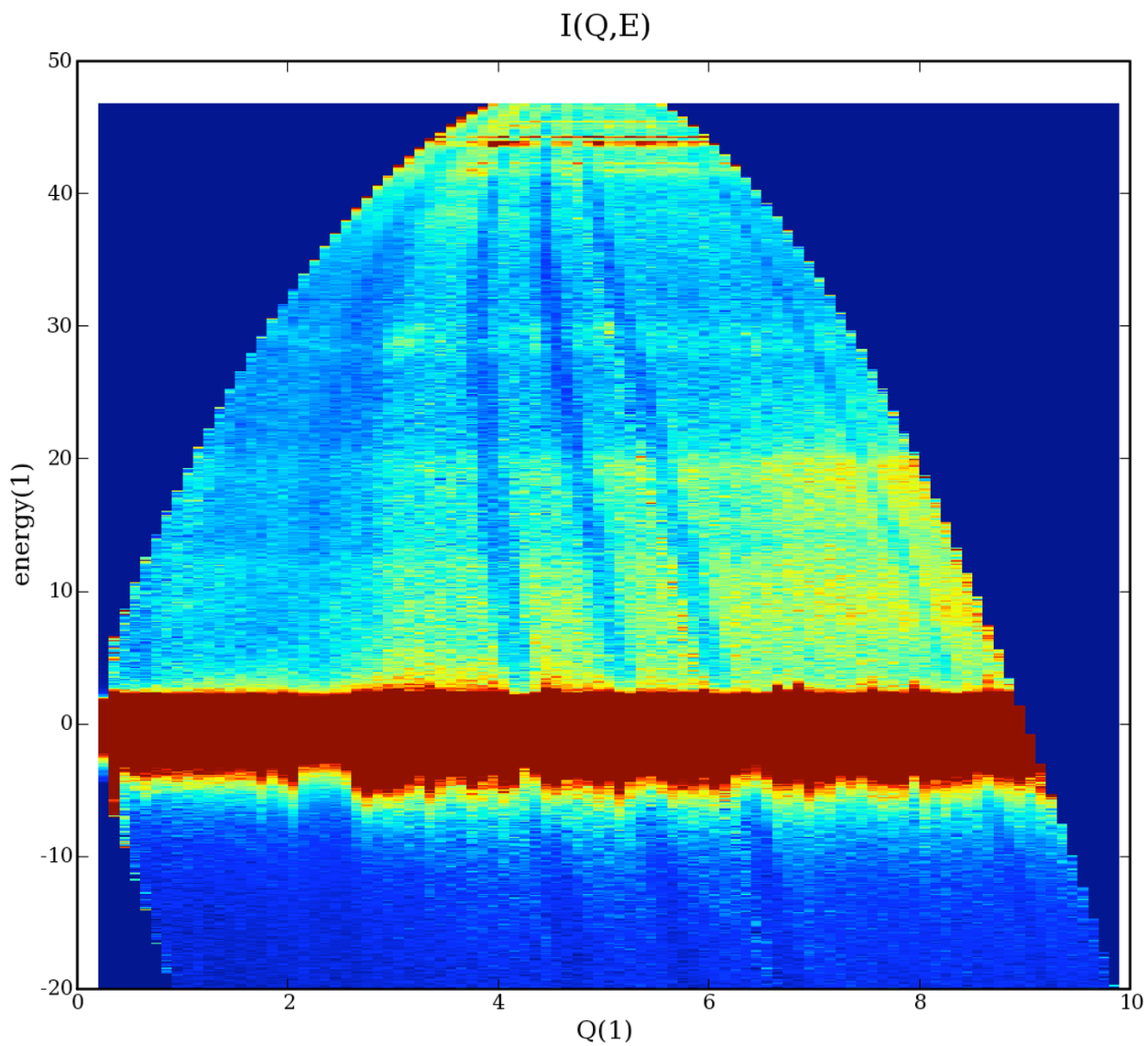
Cobaltate ($Ca_3Co_4O_9$) on ARCS: E_i = 48 meV





Elastic and inelastic scattering



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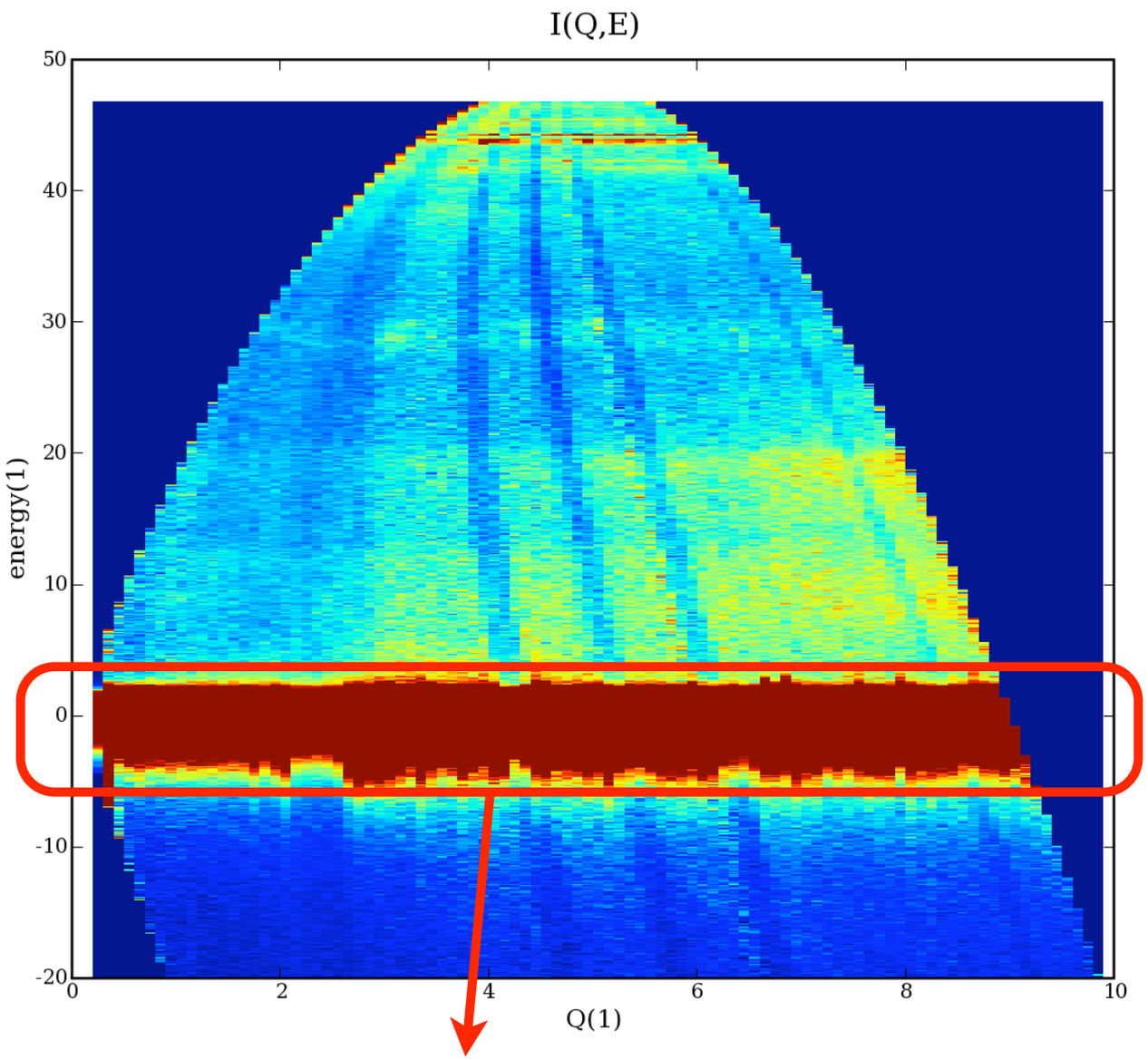

Elastic scattering/diffraction

- Usually probe structure
- Interpretation straightforward

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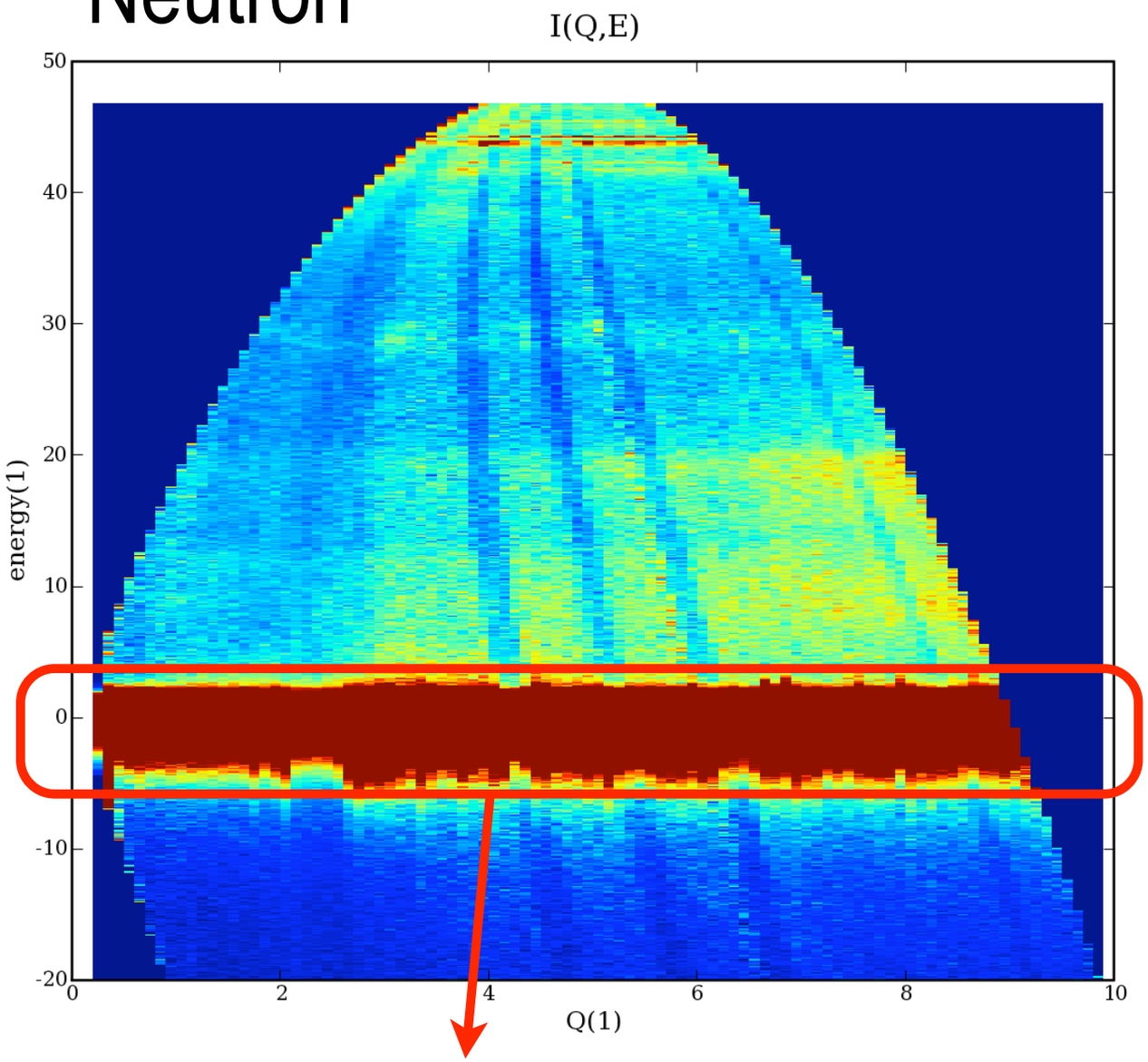
Elastic and inelastic scattering

Neutron



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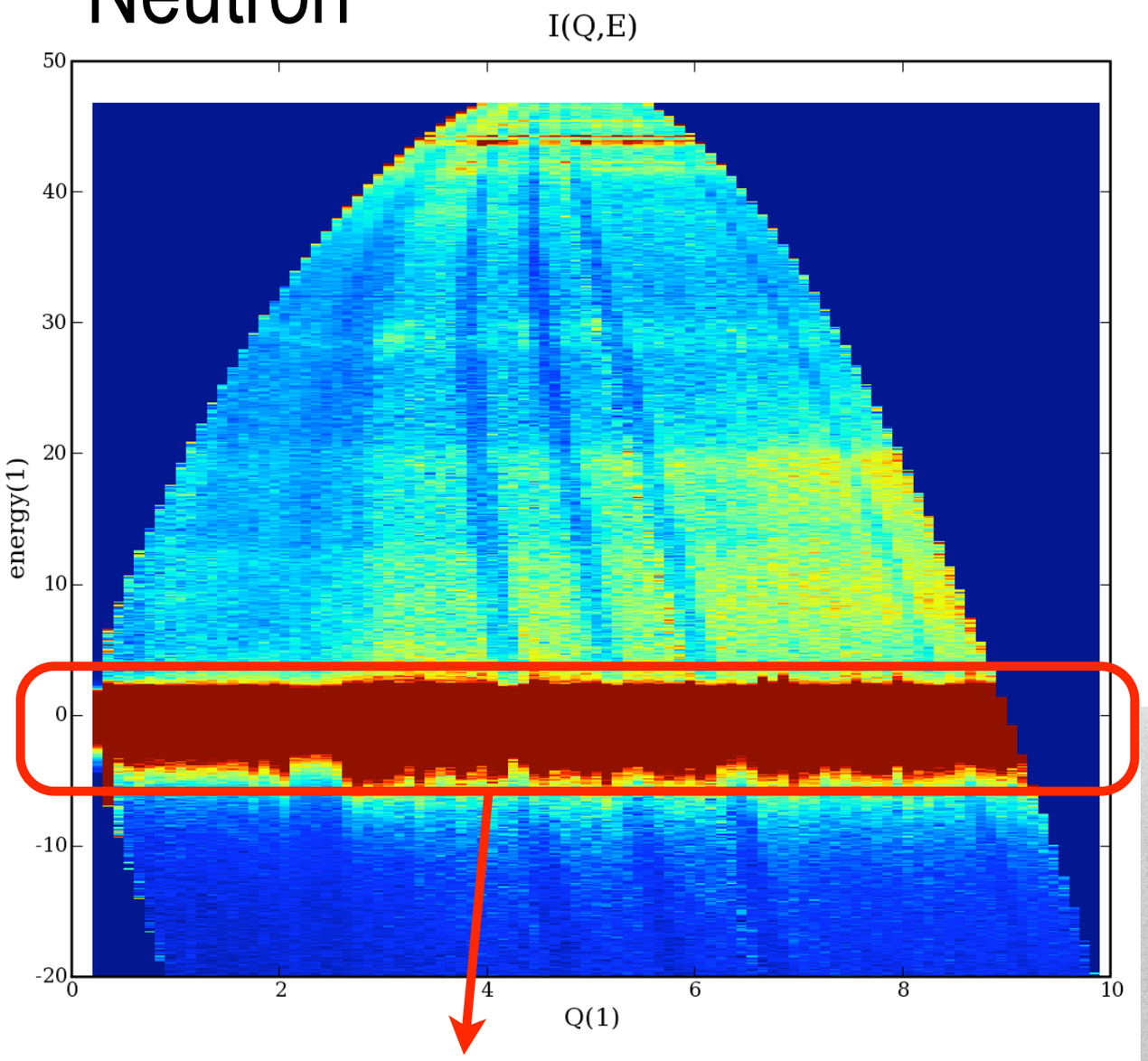
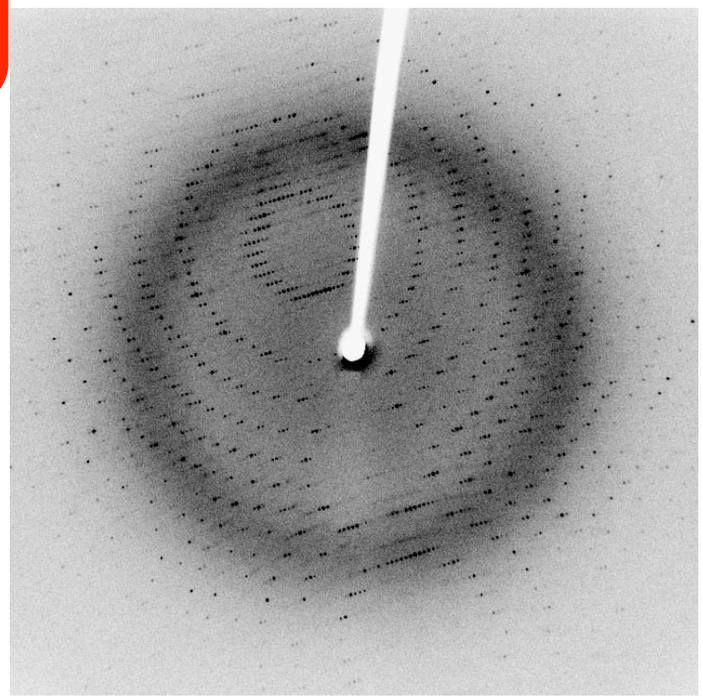


X-Ray



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Elastic and inelastic scattering

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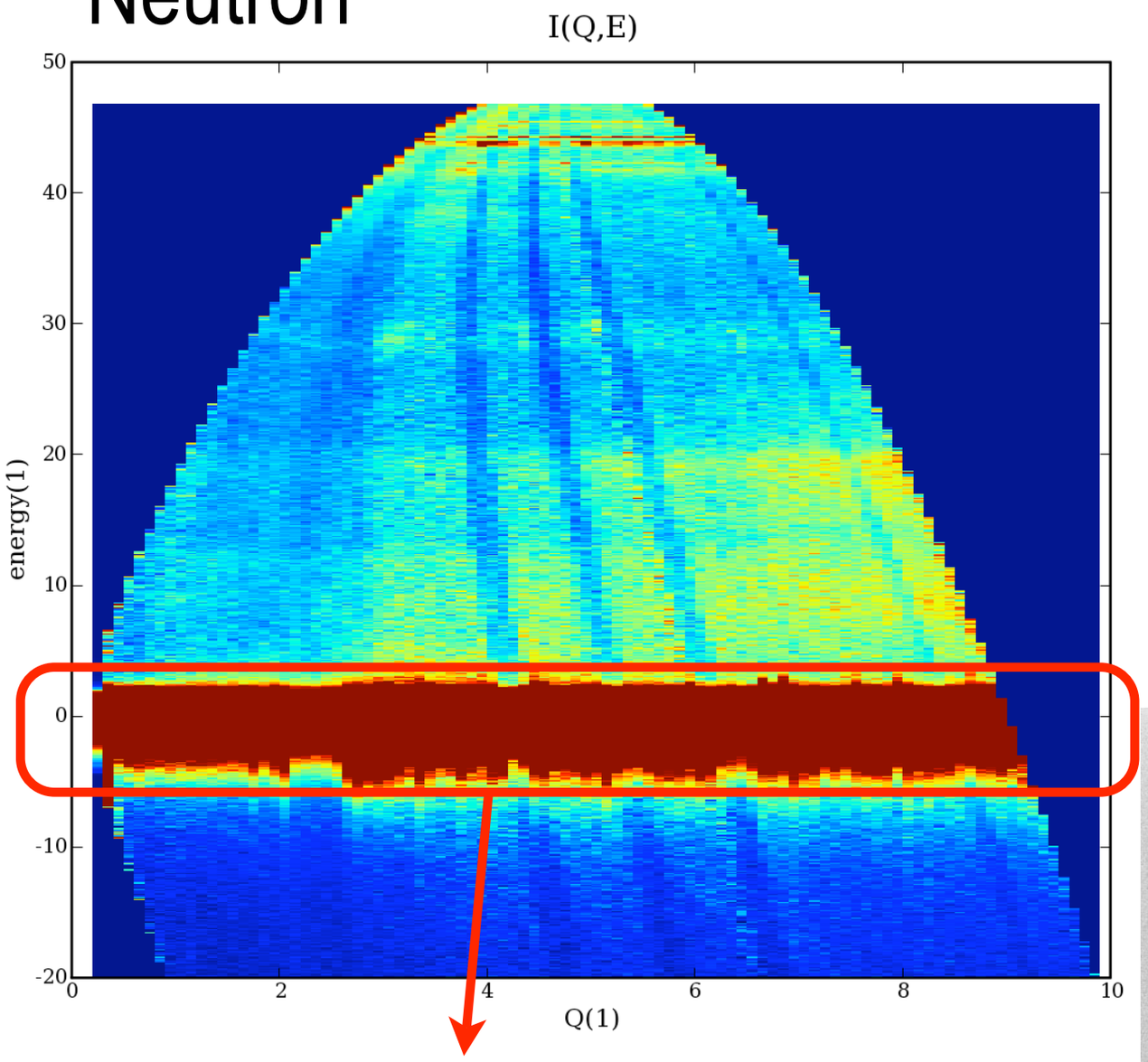

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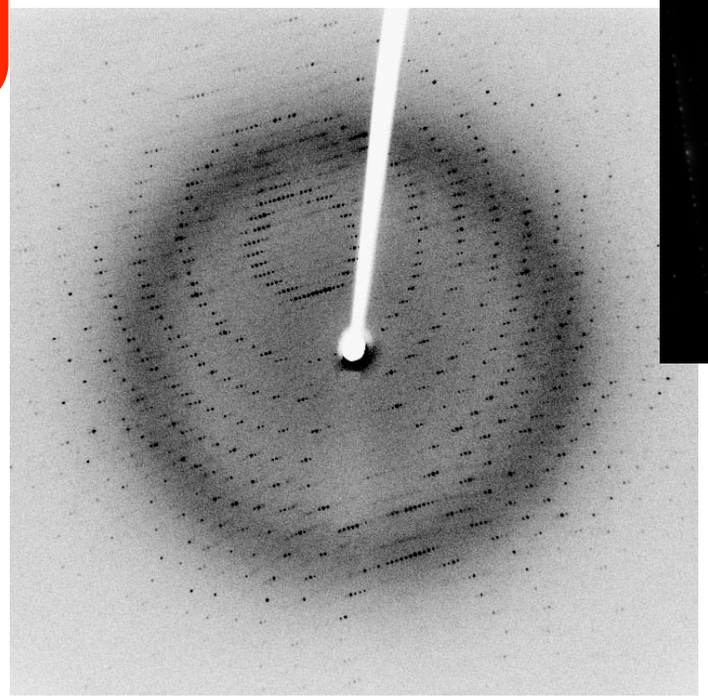

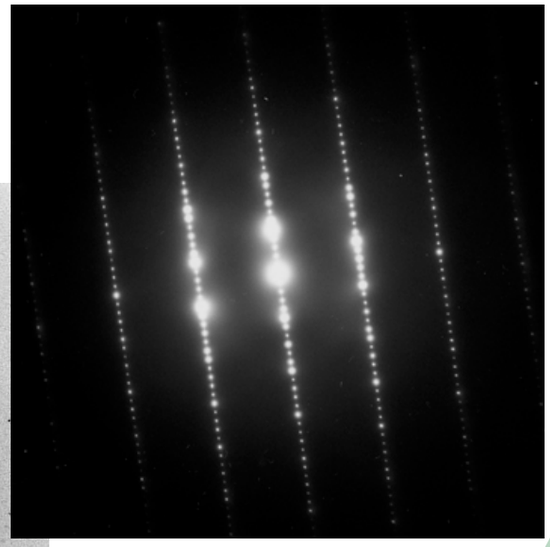

Electron

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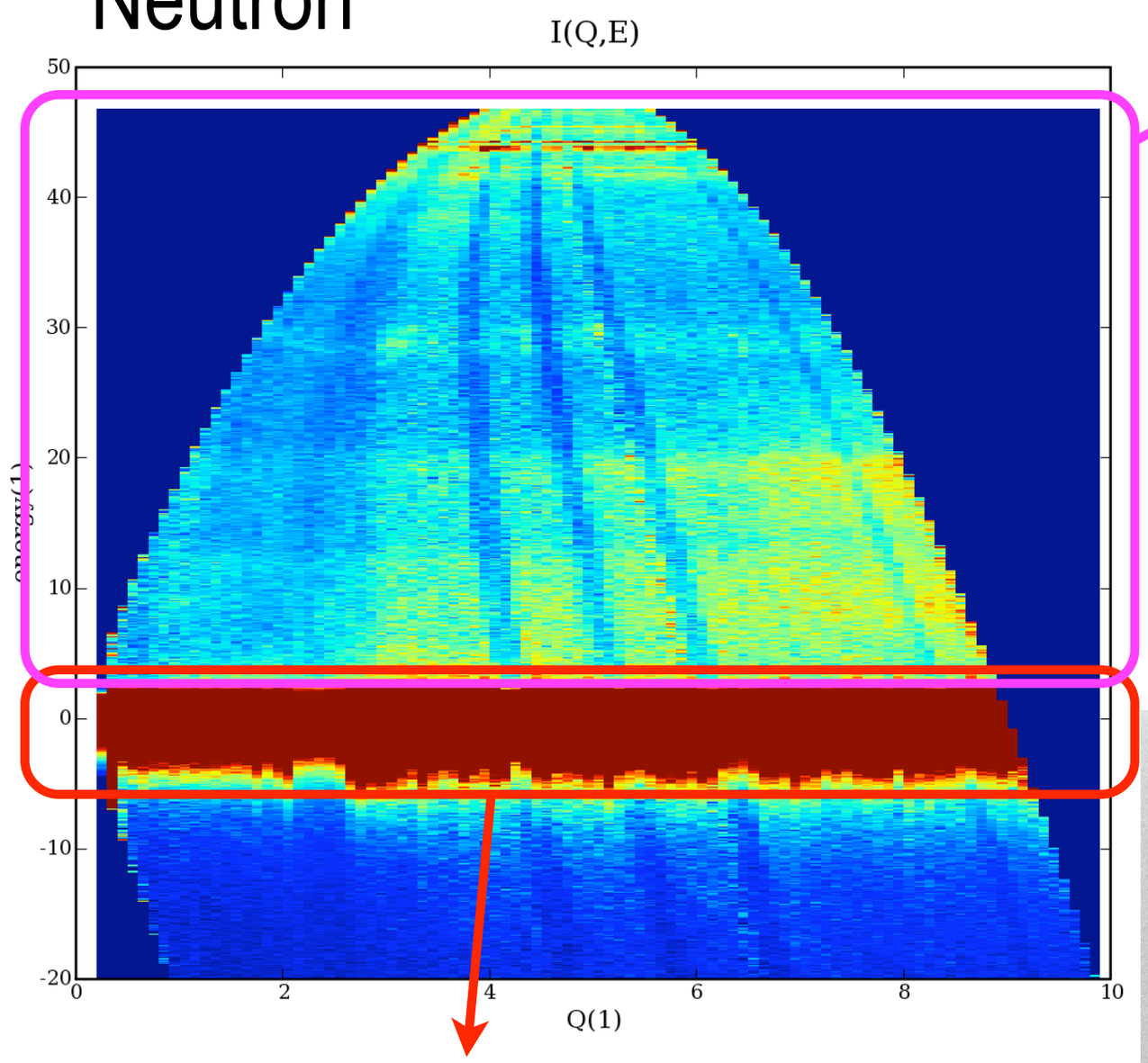
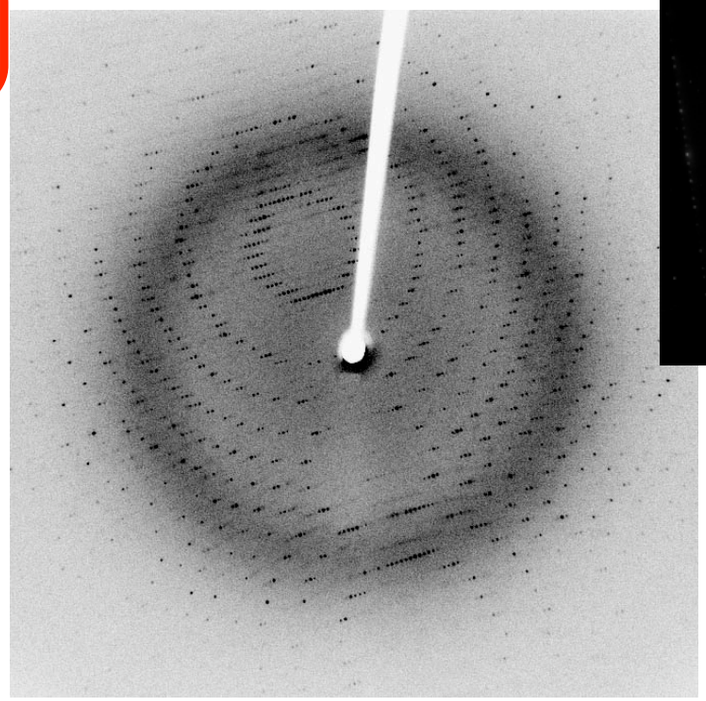
Elastic and inelastic scattering

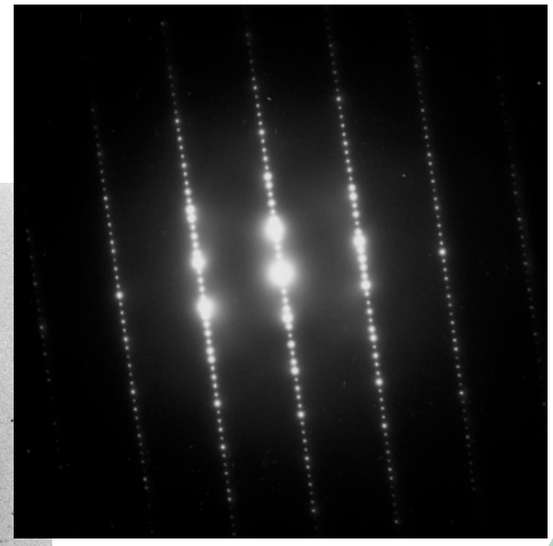
Neutron



Inelastic scattering
- Probe dynamic response / properties / functionality
- Interpretation highly nontrivial requiring heavy theory / modeling / simulations

X-Ray





Electron

Elastic scattering/diffraction
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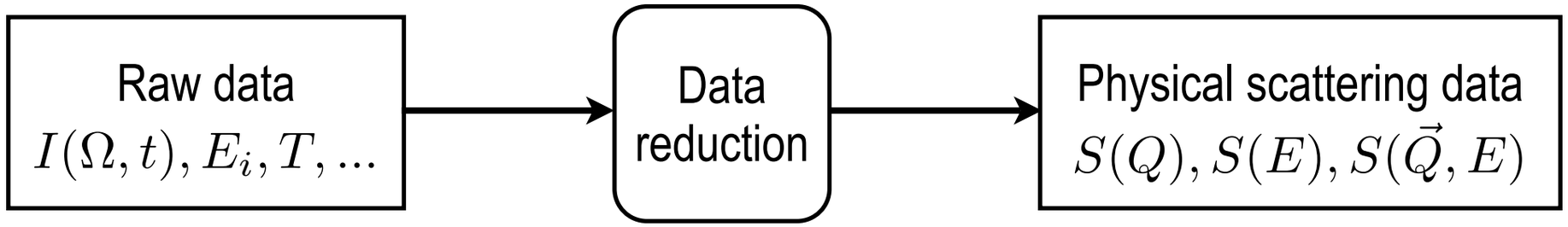
Overview of data processing/analysis



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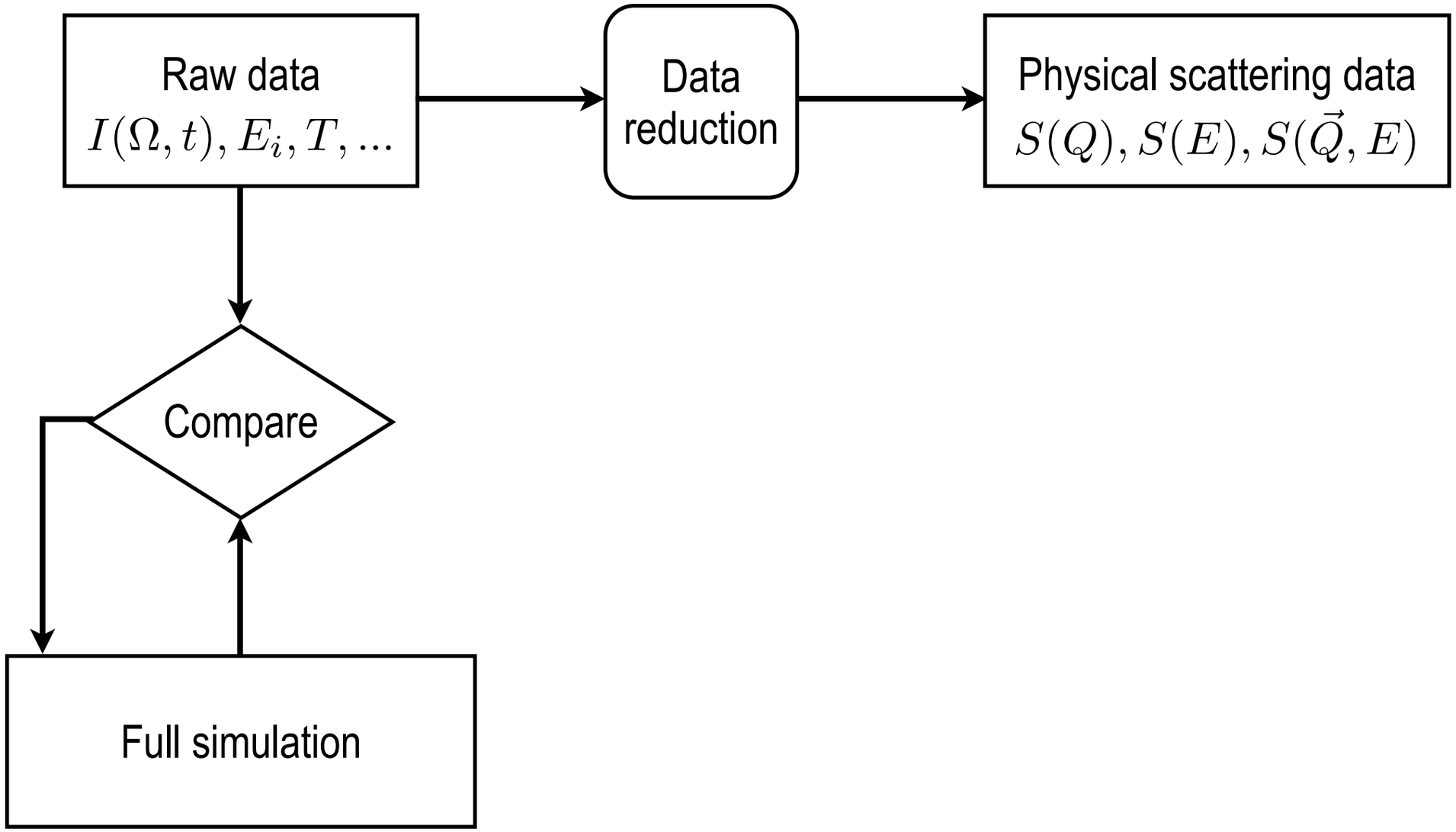
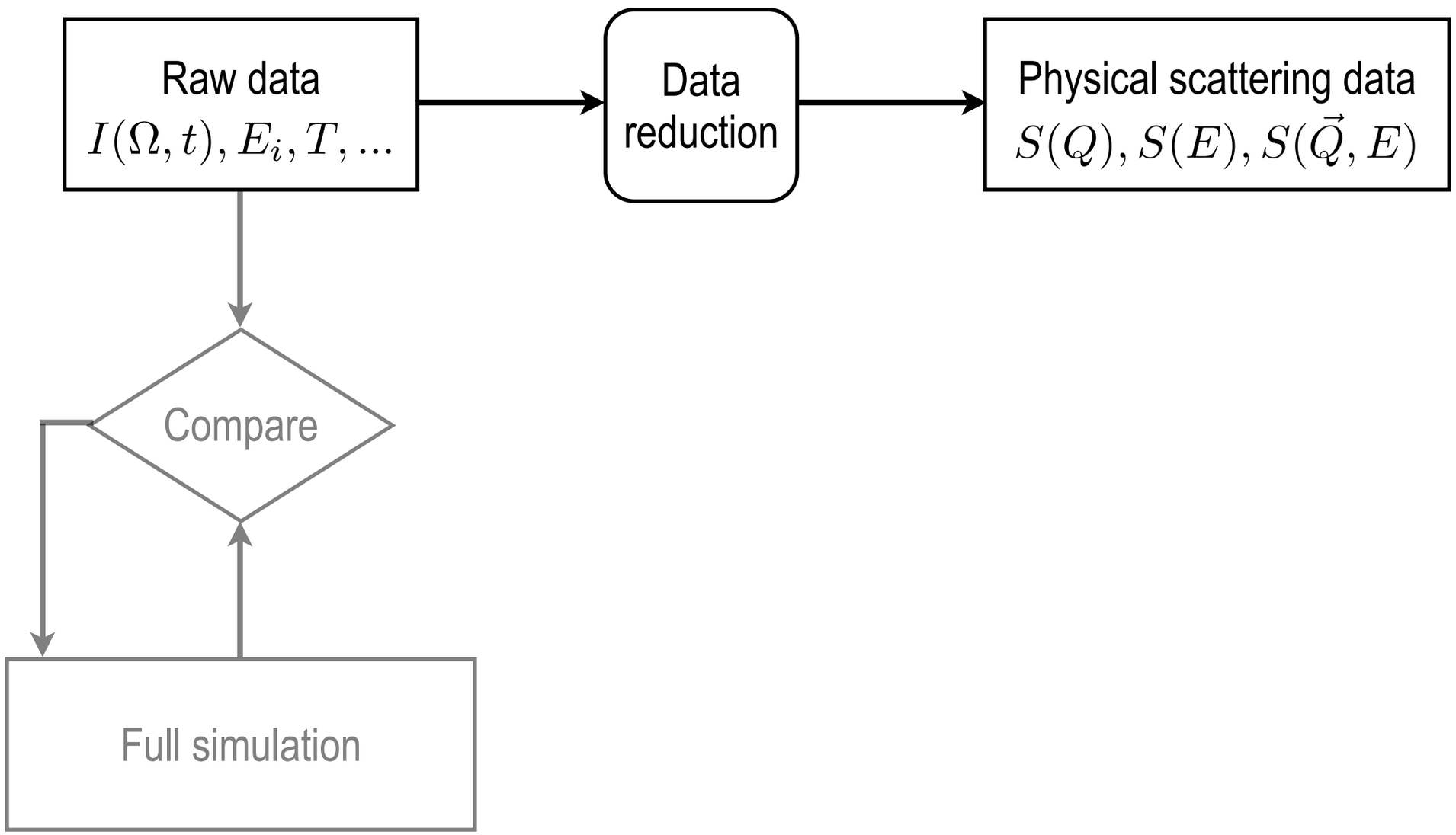
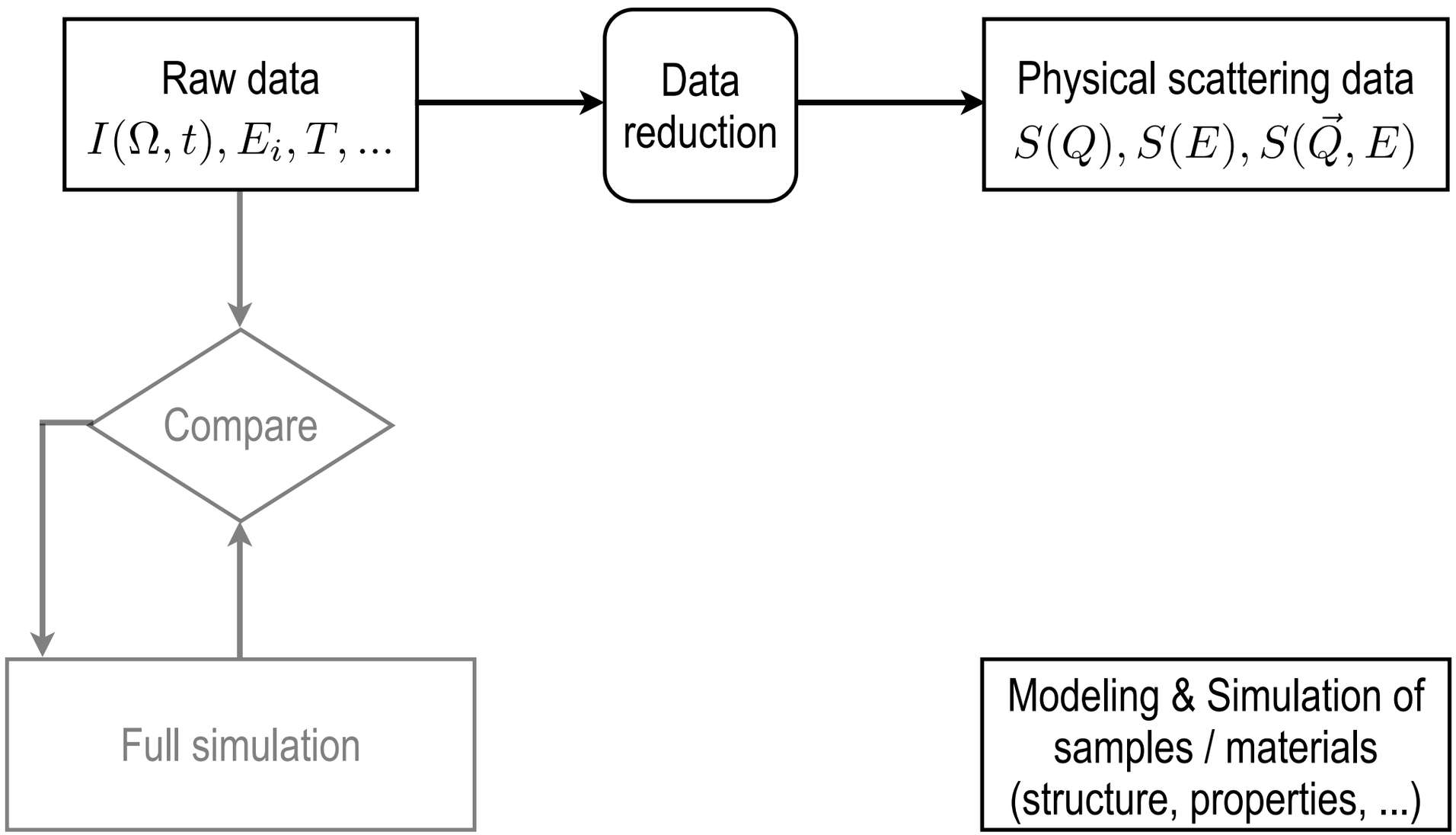


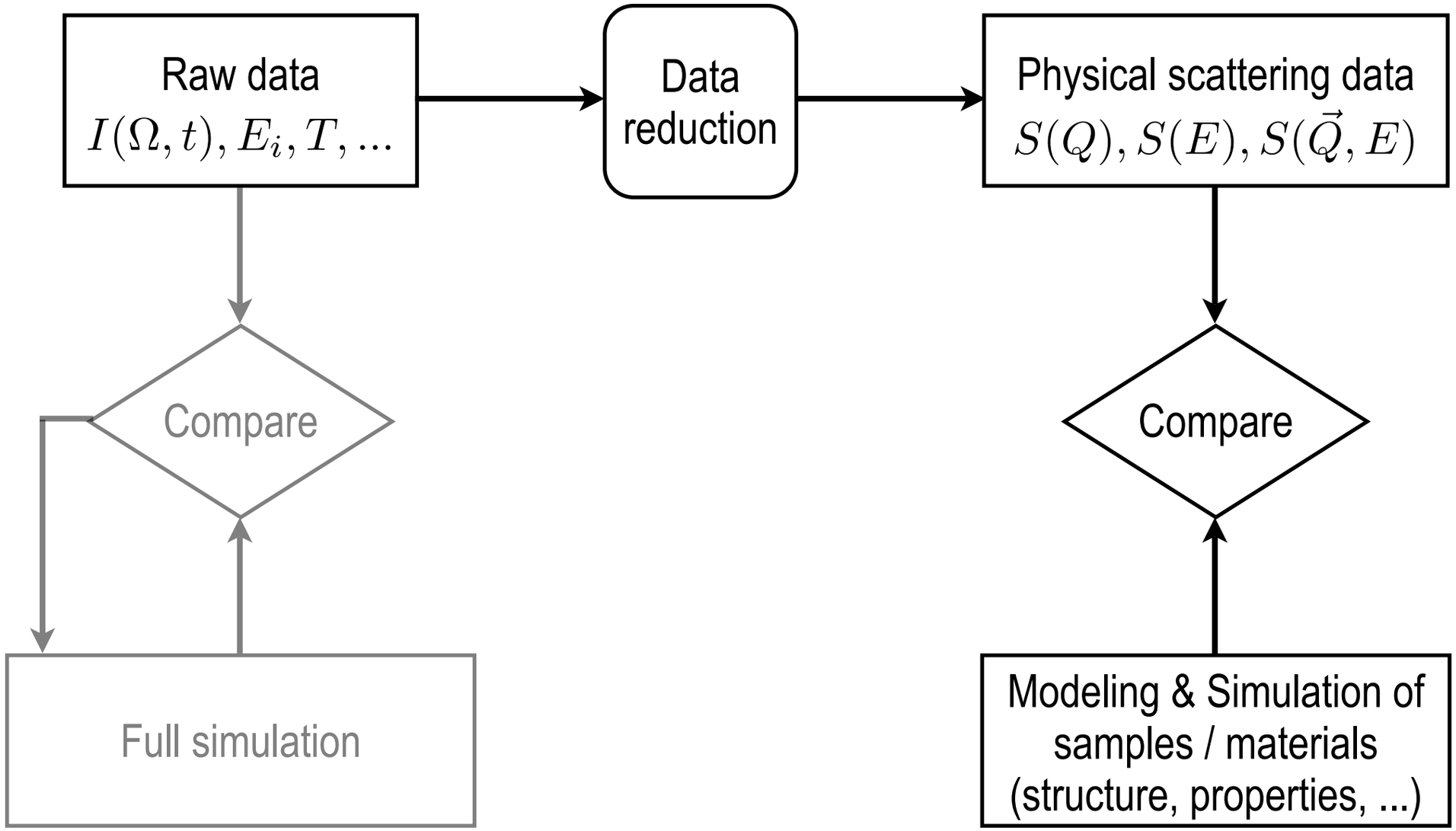
Overview of data processing/analysis



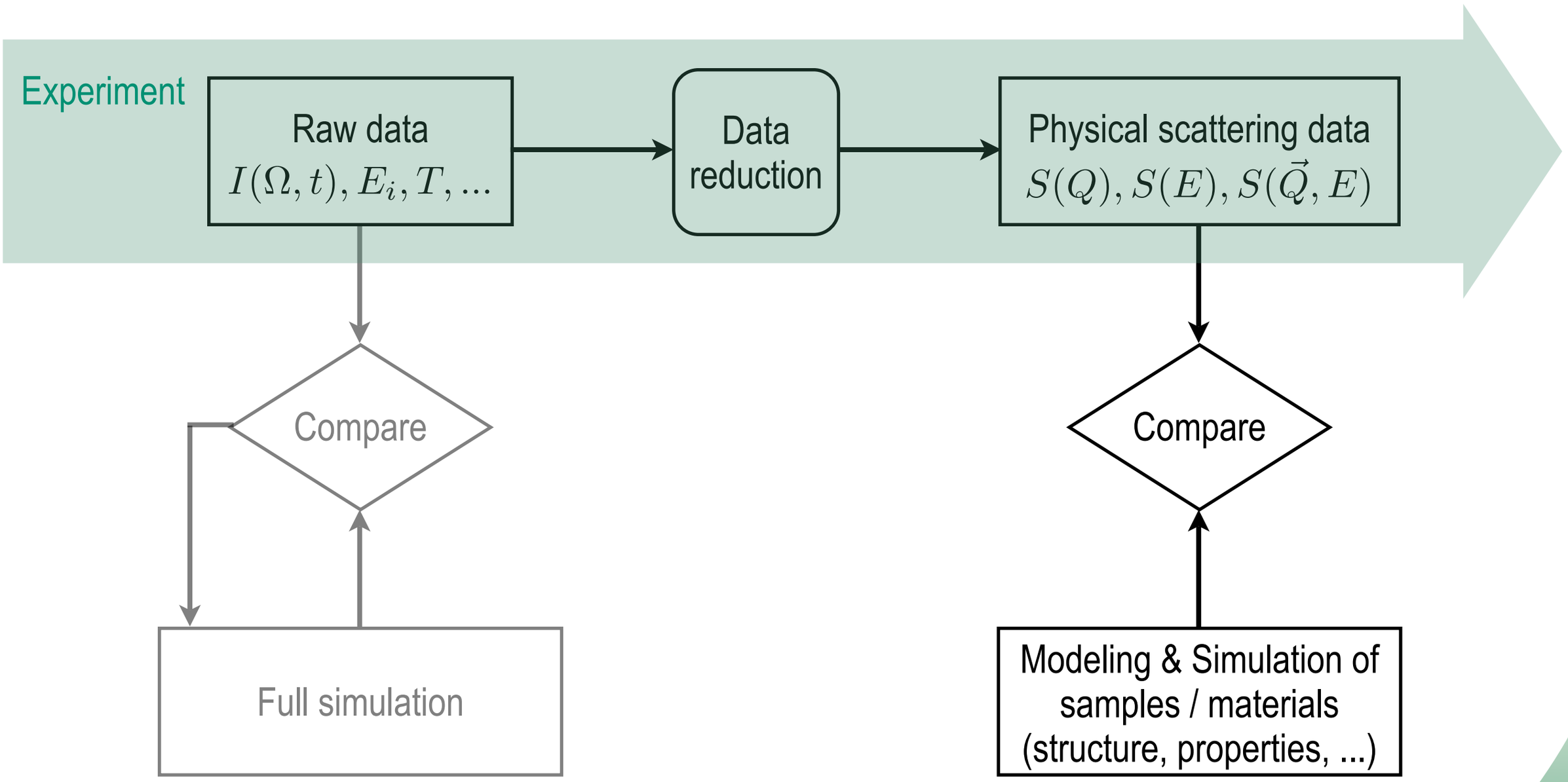
Overview of data processing/analysis



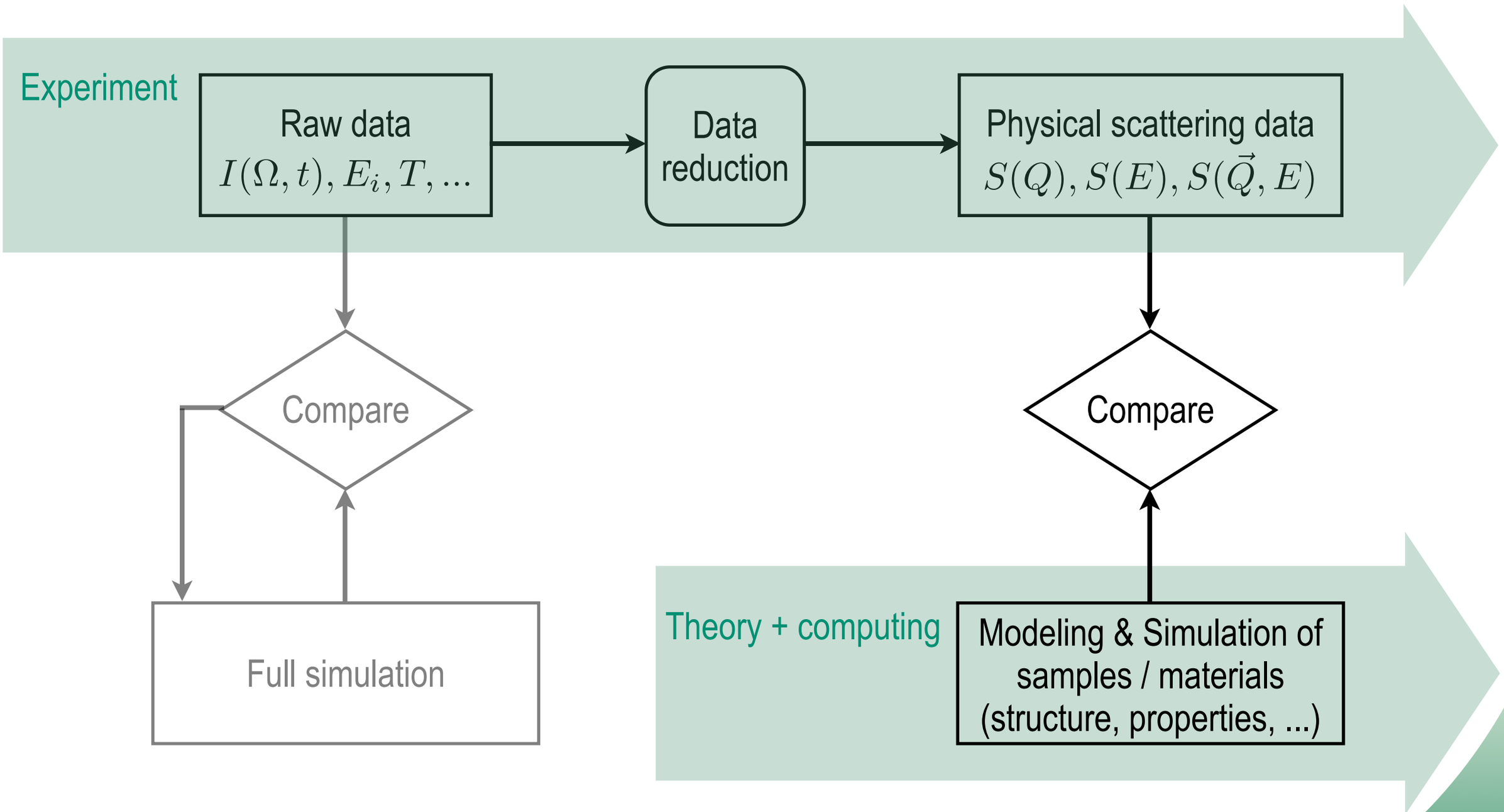
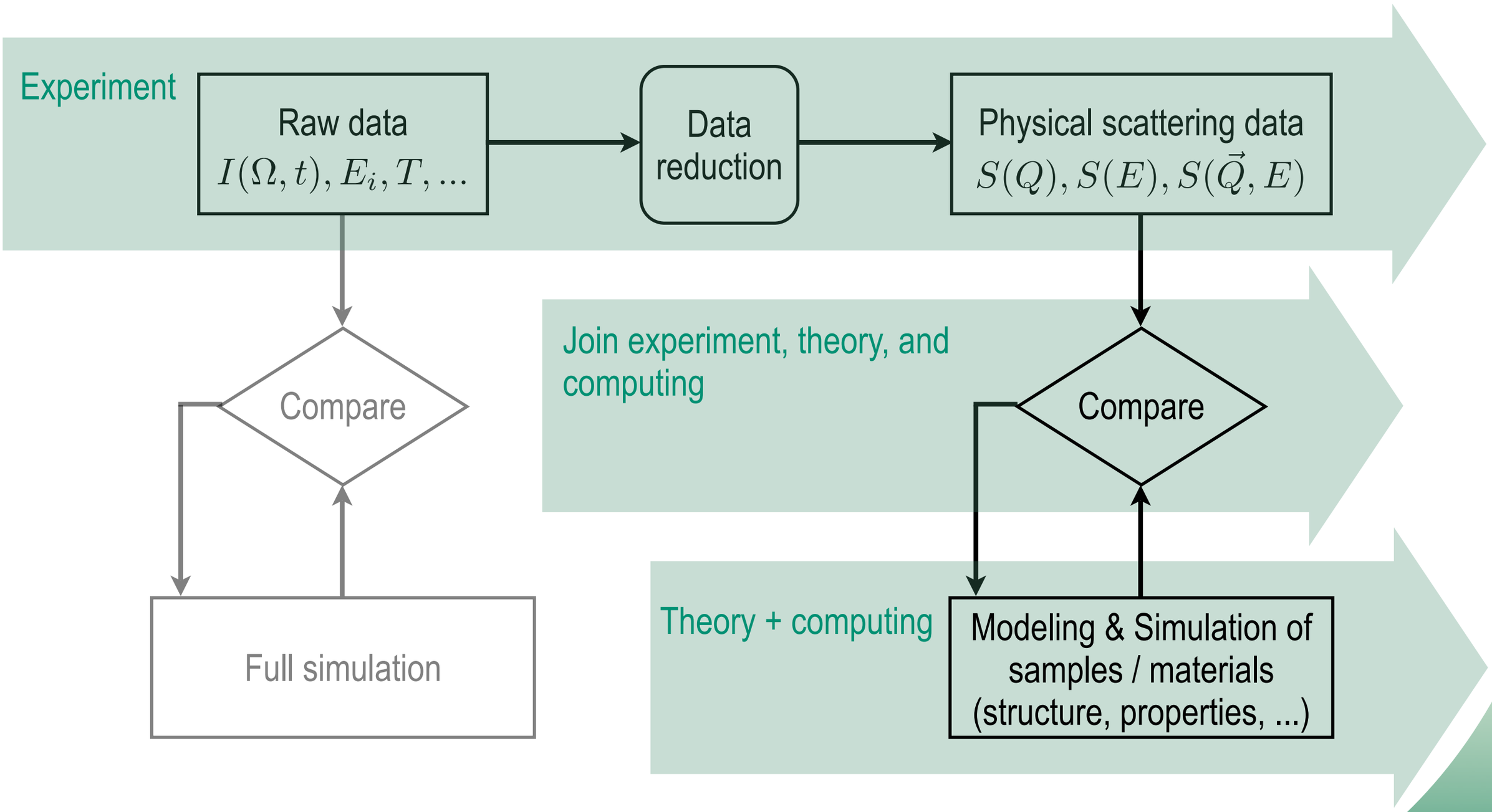
Overview of data processing/analysis



Overview of data processing/analysis



Overview of data processing/analysis



Overview of data processing/analysis