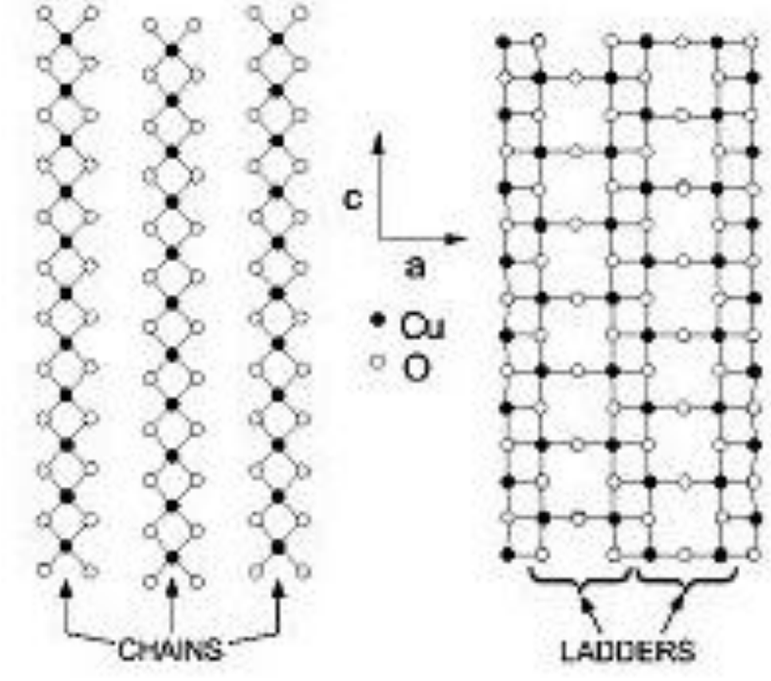
TOPAZ experience: single crystal data

Diffraction DMSC meeting

Test experiment

$Sr_{14}Cu_{24}O_{41}$: telephone number
Non magnetic



c_{chain} = 0.7 x c_{ladder}
Non integer peaks
Diffuse scattering

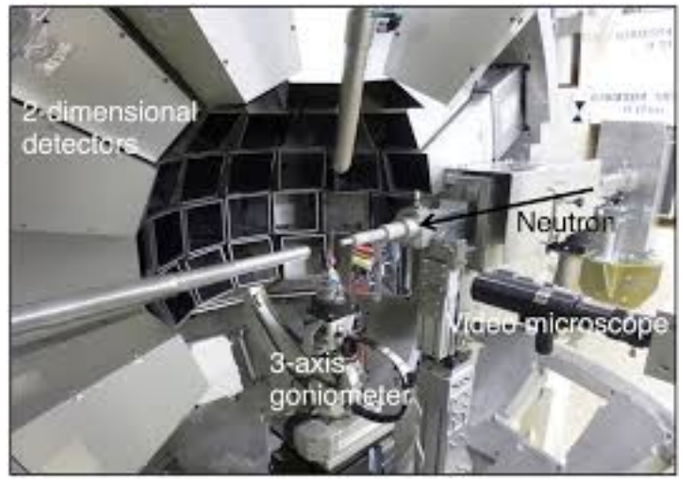
= magnetic experiment

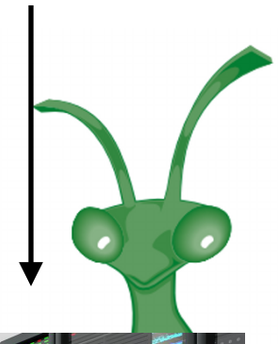
Layout

Planning of the experiment

Actual control

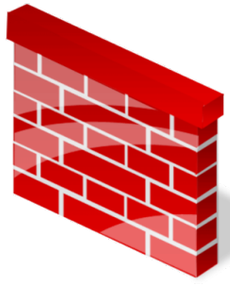
Instrument





Cluster

Terminal for reduction



Instrument controls

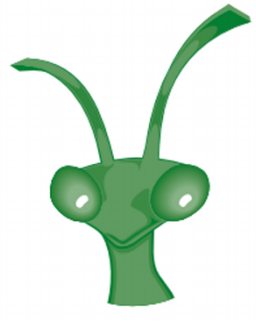
- Planning:
  - First run: orientation matrix+sample size
  - CrystalPlan: optimize Q-space coverage
  - Output: excel file with motors positions
  - Transferred to the instrument control computer

- Instrument control
  - Convert the excel file to a suitable format
  - Adjust parameters (temperature, counting time)
  - Launch acquisition

Instrument controls

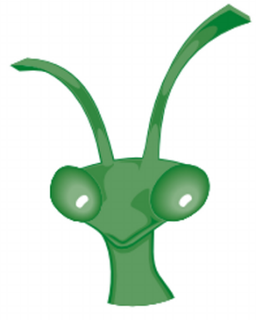
- What is missing ?
  - No command line possibility => every action is done by modifying an excel file
  - No loops => 20 steps scans at 10 temperatures
    - Mistakes !!
- What should be improved
  - Counting time is expressed in accelerator charge ($1.1x10^{11}$ means nothing to the end user)
  - One station for every action (no network or mail transfer)
  - No feedback from data reduction !

Data reduction for diffraction



- Mantid on the ORNL cluster
  - Import events mode:
    - Convert to Q-space
    - Apply Lorentz, efficiency, incident spectrum corrections
    - Clustering and sorting by density
- FindPeaks using sorted cluster list
- Refine the orientation matrix
- Search for weak peaks at predicted positions
- Integration => (hkl),I,dI,angles,crystal parameters

Data reduction for diffuse scattering (and nice pictures)



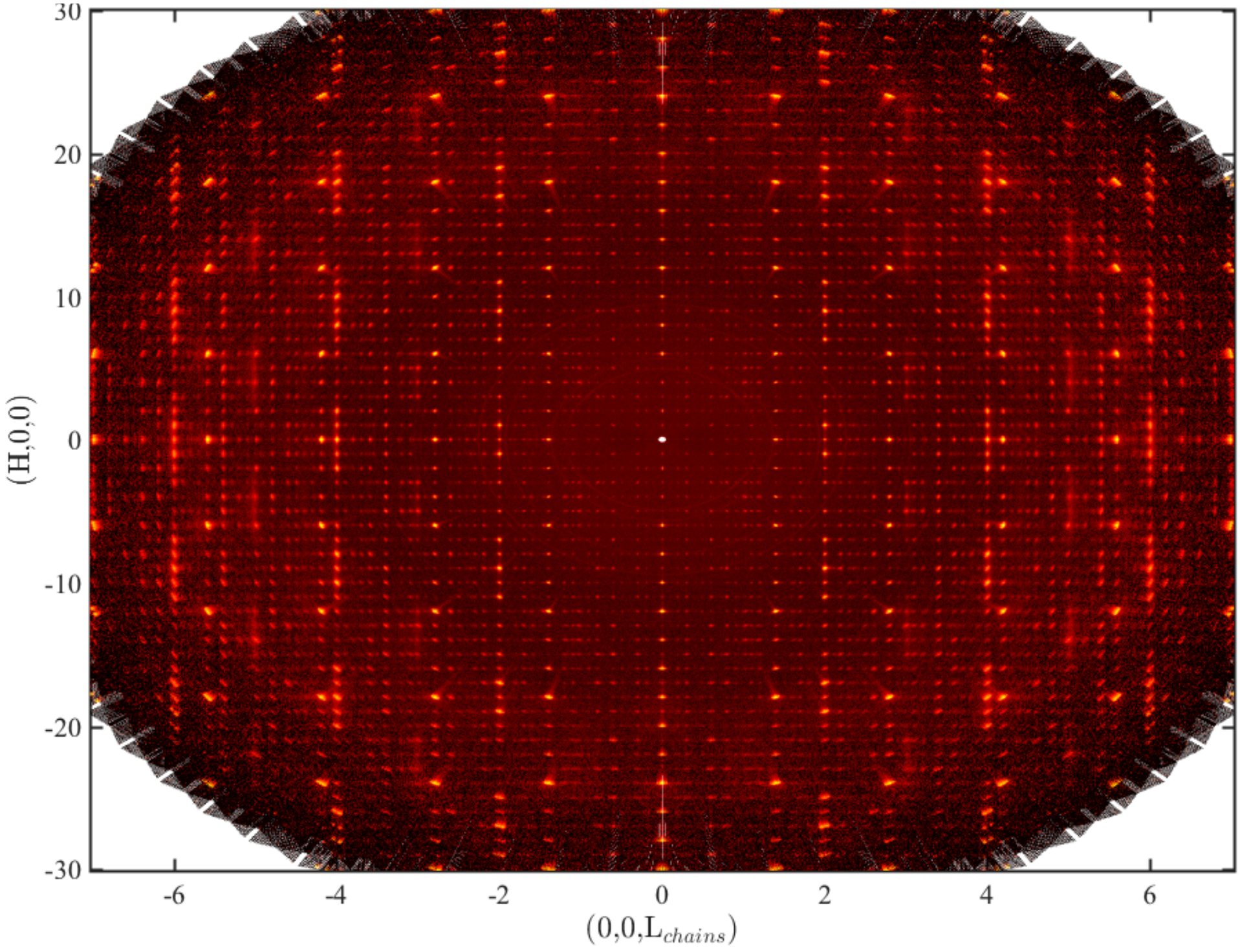
- Mantid on the ORNL cluster
  - Import events mode:
    - Convert to Q-space
    - Apply Lorentz, efficiency, incident spectrum corrections
    - Clustering and sorting by density
- FindPeaks using sorted cluster list
- Refine the orientation matrix
- Binning into Q-space + export

Our particular case

- It works … for crystallography
- 10 GB / temperature (20 nxs file/temperature)
- Long process:
  - Export to hkl: 1hr experiment = 30 mn reduction
  - Export to 3D space: 1 hr experiment = 4 hrs reduction (with 18 parallel jobs running …)

- No real support for incommensurate structure
- No parallel peak integration (1 at a time … x 20 000)

Data reduction



Data reduction on MAGiC

- Neutron flux 10 times higher than on TOPAZ
- Expected: 10^7 counts/second (10^8 in worst case)

- Polarization:
  - incident polarization: up/down
  - polarization axis: XYZ
  - on the fly change during a scan => 6 more channels to store

- 1 or 2 order of magnitude improvement mandatory !
- Current state: 1 day experiment => 1 month reduction to 3D space :/

Conclusion

- Data reduction
  - (Almost) everything is implemented in Mantid !
  - It works well … but it is slow !
  - Needs to be adapted to magnetism

- Instrument control:
  - best way to contribute is to play with it
  - is there a dummy/virtual diffractometer with current instrument control available ?