

ex5-coordinate-systems

June 2, 2021

1 Example 5: Coordinate systems

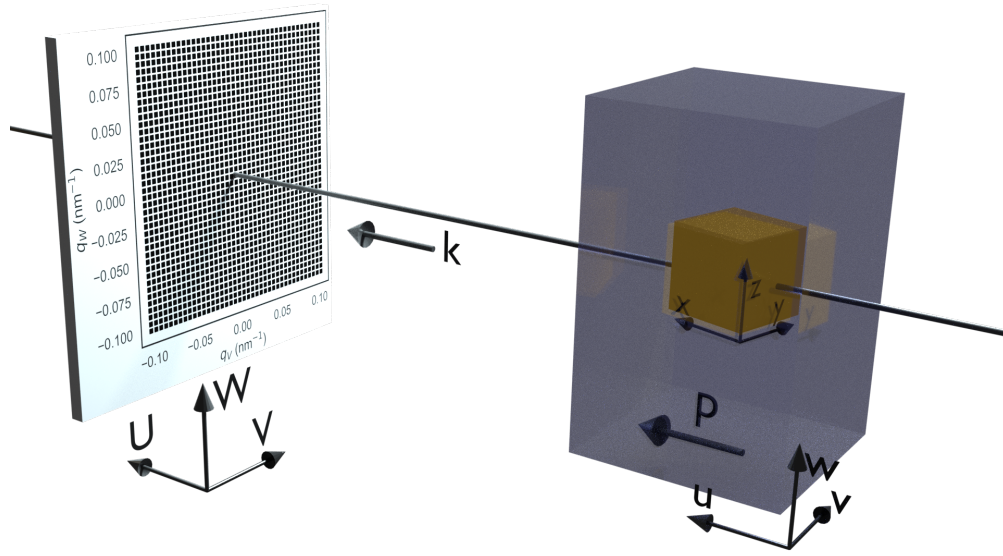


Image showing relative orientation of three coordinate systems

1.1 Overview of three coordinate systems

To describe a general SANS experiment, one needs to consider *three* coordinate systems, as shown in the figure above. These coordinate systems are:

- The *beamline coordinates*, denoted with capital letters U, V, W . The (longitudinal) direction U is parallel to the neutron beam (\vec{k}) passing through the sample. The detector plane is aligned with the transverse directions V (horizontal) and W (vertical).
- The sample is placed in a sample environment (e.g. a cryostat), which defines the *sample environment coordinates*, which are denoted with lower-case letters u, v, w . Within the code it is implicitly assumed that the neutron polarisation is defined by a field set in the sample environment.
- The *sample coordinates* x, y, z are used to specify positions \vec{R}_i and moments \vec{M}_i of the individual scatterers, e.g. which are the result of micromagnetic simulations.

If no relative rotations between the (right-handed) coordinate systems are considered, the relative alignment of the principal axes is as follows:

- $U \parallel u \parallel x$, parallel to beam direction
- $V \parallel v \parallel y$, horizontal direction in detector plane
- $W \parallel w \parallel z$, vertical direction in detector plane

Ideally, the micromagnetic simulations are done in a geometry that is largely aligned with the scattering geometry under investigation. For this it might be necessary to swap axes, e.g. for a thin film, typically one chooses a z' coordinate to be parallel to the surface normal, which would need to be swapped to the x coordinate to be parallel to the beam direction.

1.2 Specifying rotations

Rotations of the sample and the sample environment can be defined with the `mm2SANS.Probe.sample_rotations` and `mm2SANS.Probe.sample_environment_rotations`, respectively. The rotations are specified as a list of rotations around the principal axes of the sample, respectively the sample environment, which initially is collinear with the beamline coordinate system.

Rotations are specified as a combination `[rotation_type, rotation_angle]`, where the first is a string which can be "roll", "pitch" or "yaw", and the latter is the rotation angle ϕ in degrees. The types encode the following rotations:

- `roll`: Rotation around axis parallel to the neutron beam x , respectively u . Positive angles ϕ correspond to counter-clockwise rotations when viewed in the beam direction.
- `pitch`: Rotation around the horizontal axis y , respectively v . Positive angles ϕ tilt the sample/cryostat towards the detector.
- `yaw`: Rotation around the vertical axis z , respectively w . Positive angles ϕ rotate the sample/cryostat to the positive U direction.

1.3 Neutron polarisation

It is implicitly assumed that the neutron polarisation \vec{P} is defined by the magnetic field at the sample position within the sample environment. When an `mm2SANS.Experiment` object is initiated, thus the vector \vec{P} is transformed according to the rotations specified in `probe.Beamline.sample_environment_rotations`. If the neutron polarisation is set in the beamline coordinate system U, V, W , its value stored in the field `Experiment.Probe.Beamline.neutron_polarisation` needs to be reset explicitly.