X-ray volume scan and centring

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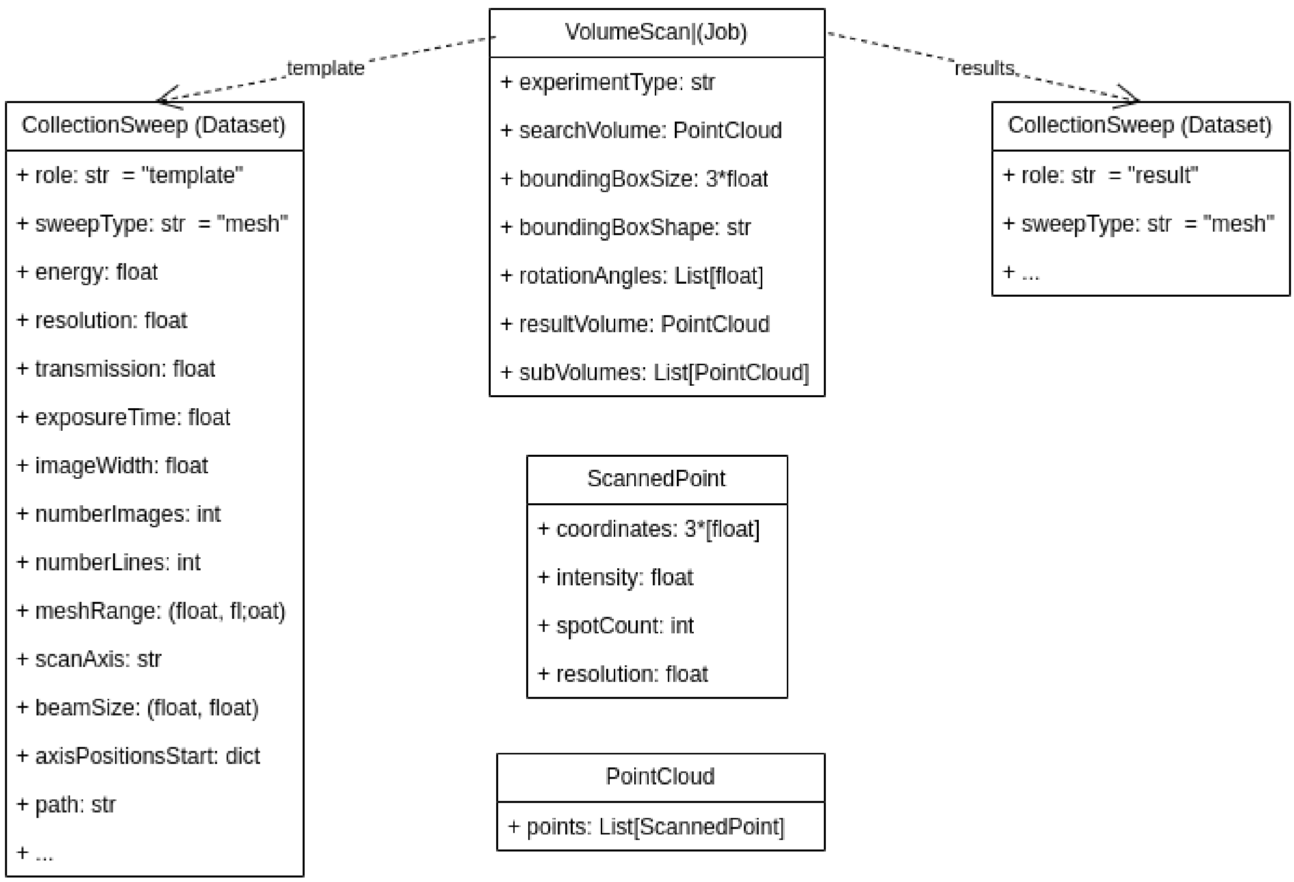
Introduction

This is a presentation of the modeling done to support X-ray centring. The VolumeScan class was generated to support X-ray centring, but we are trying to take account of other centring methods and possible uses of multiple mesh scans. With a few tweaks the same framework could be adapted for use with Tomogaraphy, optical centring, or even three-click centring if so desired.

Contents

This shows the relevant par of the model



There are three new classes:

- ScannedPoint. A Datatype containing
    - coordinates: (Tuple[float, float, float]) in goniostat coordinate system at omega==kappa==phi==0
    - intensity: (number) Measured intensity at point, in arbitrary units
    - resolution (float > 0) Resolution observed at the scanned point
    - spotCount: (positive int) Number of spots observed at the scanned point

PoinCloud:

points (List[ScannedPoint]) List of points making up the PointCloud

- VolumeScan(Job): A Volume scan (e.g. X-ray centring) experiment.

Attributes are:

- experimentType (str) E.g. ‘Xray.centring’, ‘Xray.recentring’, ‘Xray.exploration’
  String describing the type and function of the experiment – allowing you to select appropriate defaults. NB, there might at some point be other types than mesh scan, e.g. tomography,, and maybe optics(?)
- rotationAngles (List[float]) List of omega offsets from the starting omega position to use for volume scan, in degrees
- searchVolume (PointCloud) The (input) volume to search, as a list of ScannedPoint
- boundingBoxSize. (float, float, float) The size of the bounding box to use, in microscope coordinate system coordinates (horizontal, vertical, beam). The bounding box is centred on the intersection between the omega axis and the beam.
- boundingBoxShape (str) Shape of bounding box, either “Box” or “Ellipsoid”
- resultVolume (PointCloud)Volume of all active points found
- subVolumes (List[PointCloud]) List of individual compact subvolumes selected from resultVolume

In addition the VolumeScan would have a single templateData object, a CollectionSweep containing acquisition parameters to use, most importantly the starting motor positions, axisPositionsStart that determine the position and orientation of the crystal relative to the BoundingBox. The VolumeScan experiment could produce CollectionSweep objects, one for each line or mesh scan exercuted.

Doing Mesh Scans

Before we get to use cases we need to look at how mesh scans are specified and executed. The relevant parameters are all in CollectionSweep. There are all the standard ones, (energy, transmission image width, etc.) but I concentrate on those directly relevant for the mesh scan:

- sweepType 'mesh' (or 'line' determines that this is a scan)
- numberImages and numberLines determine the grid pattern
- The motor positions set in axisPositionsStart specify the orientation, and the position at the centre of the mesh (which is the one on beam at these positions).
- meshRange determines the horizontal and vertical extent of the mesh in mm
- scanAxis is set to either 'horizontal' or 'vertical' to determine which dimension is scanned fastest and how the mech is oriented.
- If necessary we could add an extra attribute to determine the zigzag scanning pattern, but that can wait till it is needed.

Setting up a mesh scan the requires setting these parameters in a Collection Sweep, and executing it with an MxExperiment job that specifies the mesh scan.

Scanning and its use cases

The VolumeScan job will work by setting up a series of Mesh scans (there may be other variants later (like tomography?) but for now we only look at this). The inputs come from the VolumeScan attributes and the template CollectionSweep attached to the VolumeScan. I can see three operation modes. For all of them the number of meshes and their orientation is determined from the VolumeScan.rotationAngles attribute, set either explicitly or by defaults selected using to the VolumeScan.experimentType.

Starting from a bounding box.

If you simply have a rough loop orientation rather than a proper point cloud, you would specify only a bounding box. This is done by first setting the axisPositionsStart in the template so that the desired volume is oriented along the horizontal/vertical/beam axes and centred on the beam position. The boundingBoxSize and bondingBoxShape then determine the relevant volume, which can be used to define the axisPositionsStart, meshRanges and other mesh control parameters that specify the individual mesh scan for each rotationAngle. Note that not all box-shaped volumes can be aligned so as to have the axes parallel with the horizontal/vertical/beam axes. If this is your case you must specify your input as a point cloud, or first convert the actual volume of interest to a larger box that can be aligned appropriately.

Starting from a point cloud

If you have your volume of interest as a point cloud, you pass that as input to the VolumeScan as the searchVolume. This can then be used to calculate the axisPositionStart and a boundingBox (in the appropriate coordinate system). Alternatively you can skip this step and have your algorithm determine the individual mesh scans directly from the point cloud.

Starting from a point – recentring

If you are simply doing ‘touch-up’ recentring all you want to do is to pass in the desired orientation and calculated motor positions for the centring. For that you need only to set the axisPostionsStart values to the orientation and centring you want, set experimentType to ‘Xray.recentring’ and then execute the VolumeScan. The bounding box will then be set to a suitable set of default parameters, and the mesh scans calculated from there.

Output

Output comes as a resultVolume, which is a pointCloud with all measured points, and a list of subVolumes, which is a filtered list of (presumably compact) point clouds found. For any practical use you would presumably need to work off the subVolumes, so you need a routine to select them, filter them, and a way to decide which one(s) to use if there is more than one. For (re)centring, particularly, you need to decide which point you are recentring, and you need to convert from the point cloud of that subvolume , first to get a single centroid point, and then to convert the goniostat coordinate system coordinates of that point (together with the axisPositionsStart of the experiment) to a set of motor positions to use. We still need to think if these operations require additions to the model.

Open Questions

In order to complete this work we need to know more about how people are going to be using the X-ray centring / volume scan, and what output they need to generate with it.

The input, mesh scans and first analysis steps should be covered in the current model. At the end you get the scanned volume described as a point cloud where each point can be associated with an intensity a spot count, and an observed resolution.

First question: Is this set of information enough to start with (we can add more later), or are there other things that are clearly needed?

Next question: what to do then? For simple centring it is a matter of selecting a point for optimal centring and generating the centring motor positions for centring it. But there are other possible actions.

- You might want to filter out low-intensity voxels and define a volume representing a crystal.
- Or maybe multiple volumes defining several crystals.
- The you might want to define multiple centring positions, either one per crystal or several, and possibly to set some kind of quality factor for each.
- Or you might want to use the crystal volume(s) to set up helical scans, or to do a RADDOSE analysis.

The model currently has slots for a single output volume for the entire scan, as well as a list of subvolumes. There is no slot to store output centring positions, however, so these would have to be calculated on-the-fly from the (sub)volumes. Depending on intended use we might need to make some changes here. Do we, for instance, need to output subvolumes at all? Do we (just?) need one or more centring positions? Once we know the use cases we can deal with these questions.