NMX Sample Environment, Sample Handling, Data Analysis

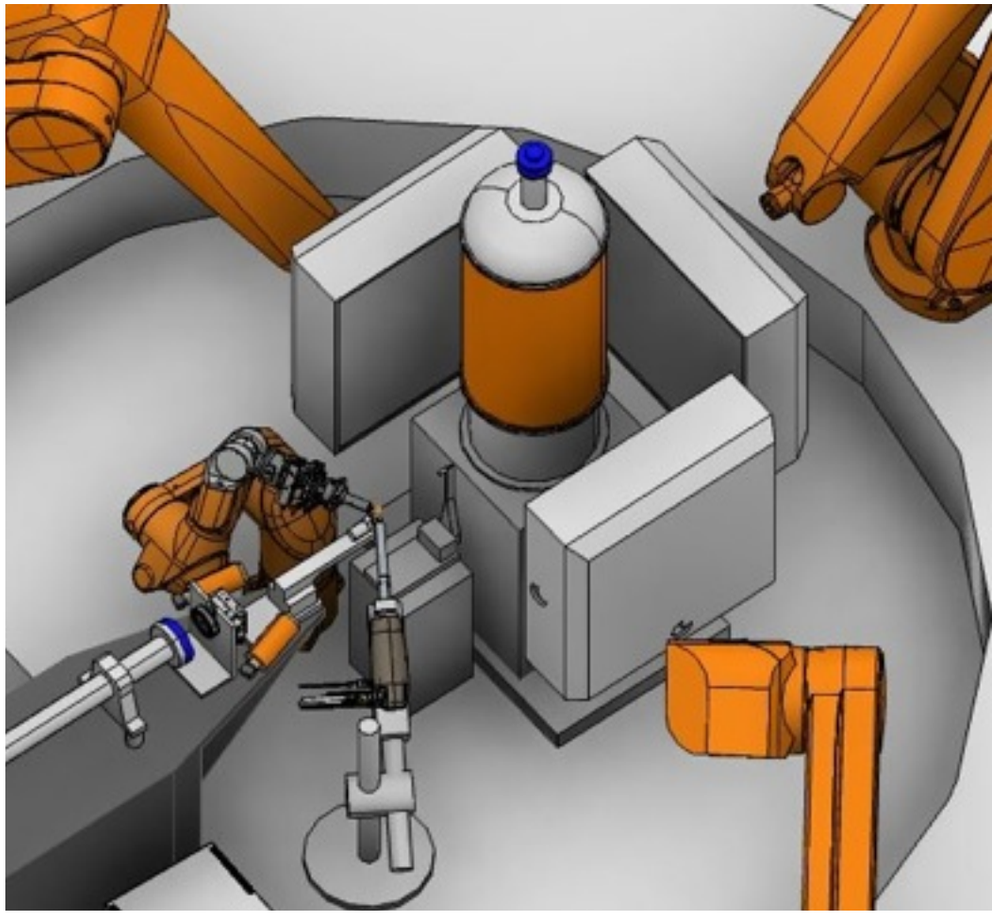
NMX Tollgate 2 Review

2014-12-11

Esko Oksanen
Instrument Scientist,
Macromolecular
Crystallography

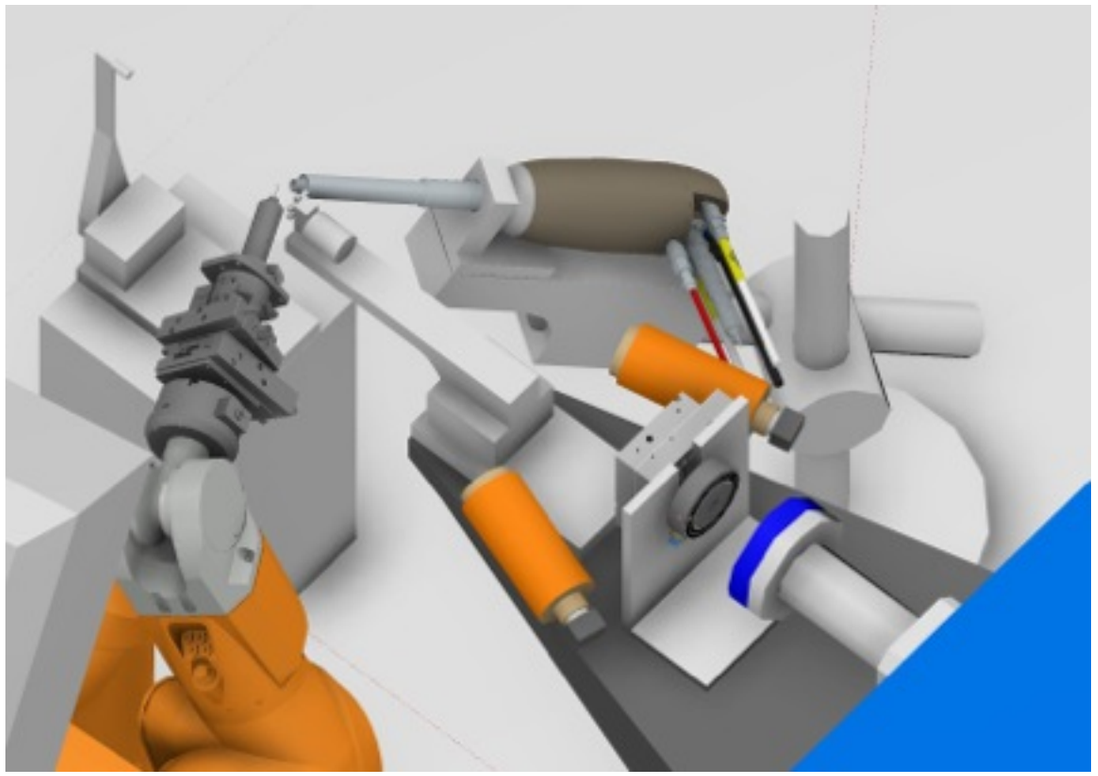
Sample environment

Materials Science



- Pressure cells can be mounted on sample positioned
- Bulky sample environments (up to 600 mm diameter) an alternative sample position is available
- Allows 4T compensated cryomagnet, 15T uncompensated (may cause issues with robots)

Macromolecular Crystallography

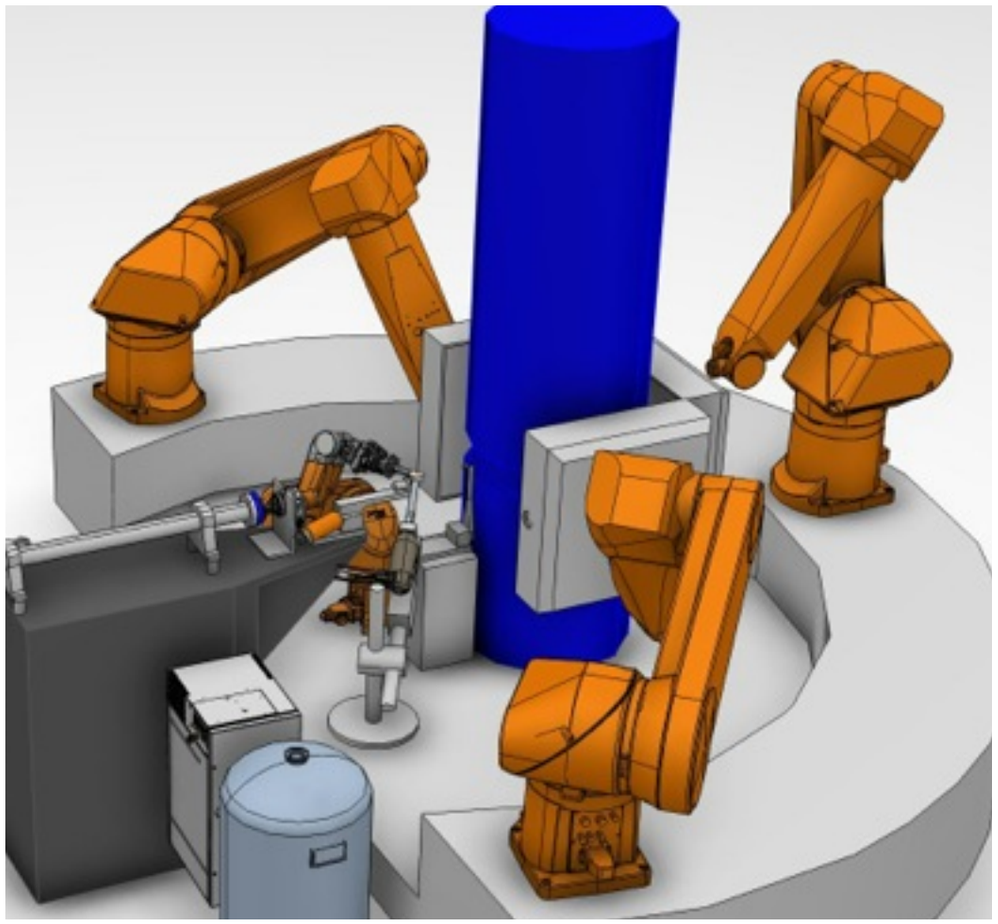


- N_2 cryostream (100K) available
- Humidity control with D_2O (e.g. HC1) foreseen

Sample environment board provides interface with SE pool equipment

Sample environment

Materials Science



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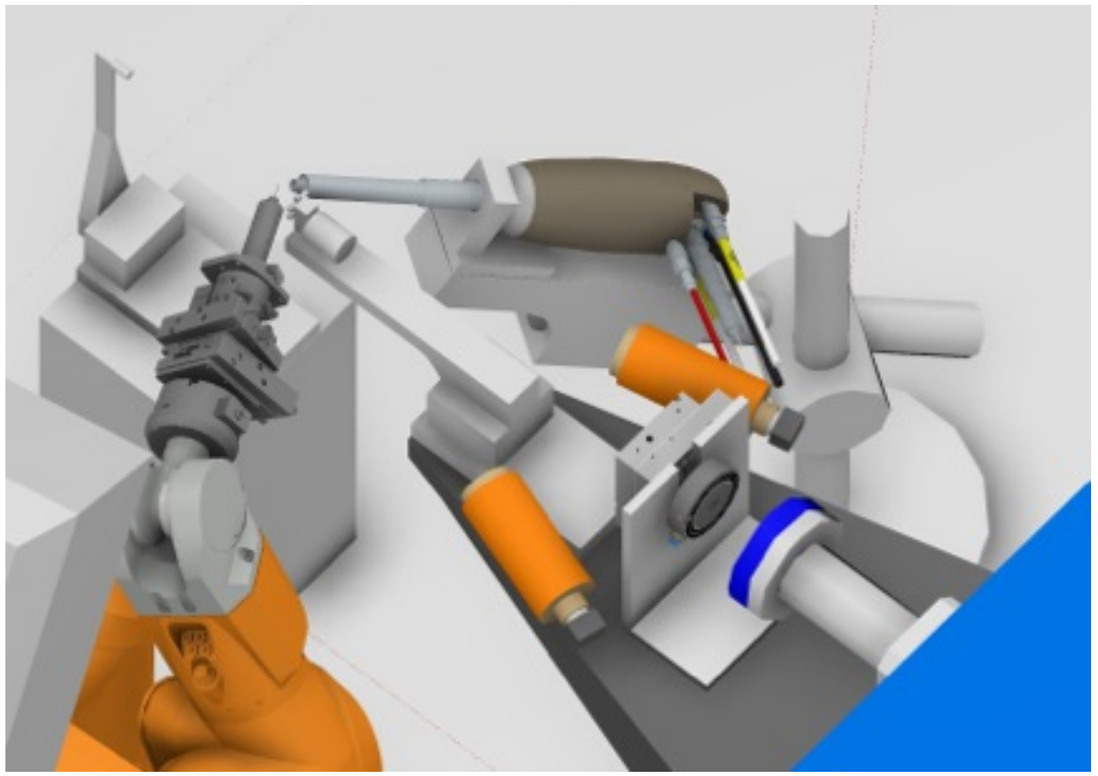
Macromolecular Crystallography



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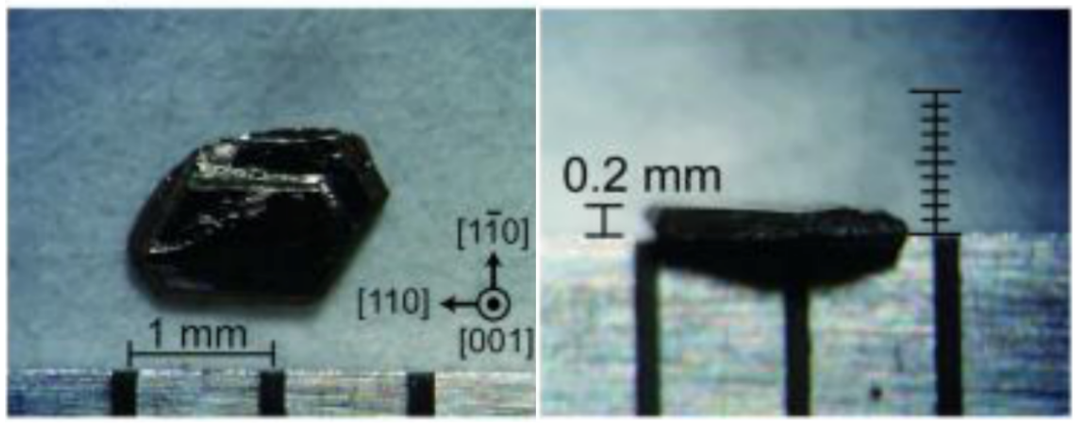
Sample handling

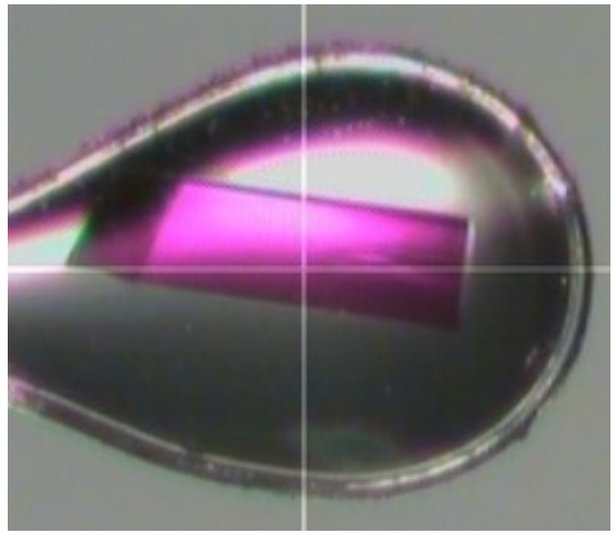
General sample workflow developed by Scientific Activities Division

Materials Science



- Crystals mounted on pins
- Inside sample environment
- Activation may be more severe; remote handling possible with robot

Macromolecular Crystallography



- Crystals mounted in capillaries or cryo-loops with mother liquor
- Consist of light elements; less activation

Sample mounting and storage available at the instrument, support laboratories on campus

Data processing workflow

Find spots

↓

Index spots

↓

Integrate spot intensities

↓

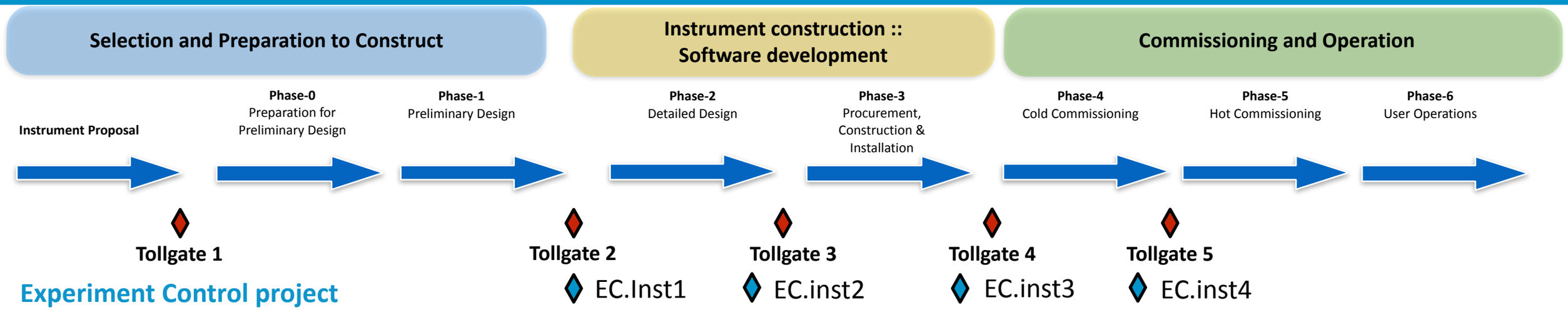
Scale intensities

Algoritms exist for all steps; need to be implemented in a pipeline

Instrument sub task project milestone descriptions against instrument tollgates
Baseline and detailed deliverables capture all aspects of instrument science case
MX and Materials science

EUROPEAN SPALLATION SOURCE

Instrument data group



Experiment Control project instrument subtask

Live reduction & Vis instrument sub task

LRV.inst1 LRV.inst2 LRV.inst3 LRV.inst4

	Description	output	Date
EC.NMX1	Baseline requirements for instrument specific aspects of experiment control	Requirements Document	TG2
EC.NMX2	Review of detailed design & deliverables for instrument specific aspects of EC system	Reviewed RD & deliverable list & costa and time —> feed to DEV team	TG3 - 3m
EC.NMX3	Instrument specific EC system ready for CC	System testing report + debug list	TG4 - 6m
EC.NMX4	Tested and debugged system ready for HC	Debugged system test + report	TG5 - 6m
LRV.NMX1	Baseline requirements for data reduction	Requirements Document	TG2
LRV.NMX2	Review of detailed design and deliverables for reduction	Reviewed RD & deliverable list & costa and time —> feed to DEV team	TG3 - 3m
LRV.NMX3	Live reduction system ready for CC	System testing report + debug list	TG4 - 6m
LRV.NMX4	Tested and debugged Live reduction system ready for HC	Debugged system test report	TG5 - 2m

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Questions?

Esko Oksanen, European Spallation Source