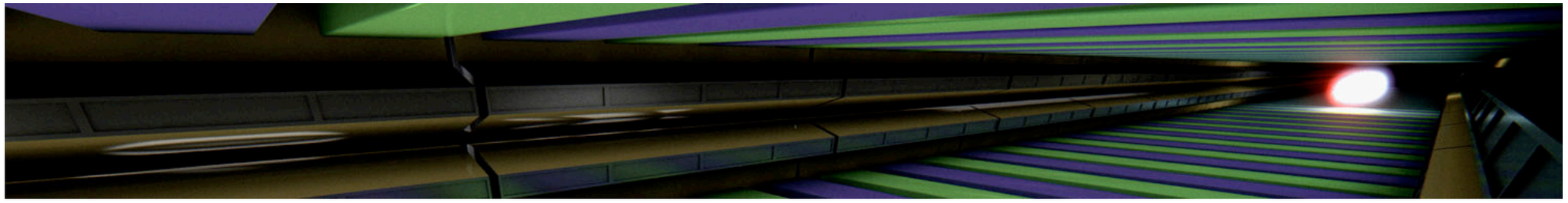


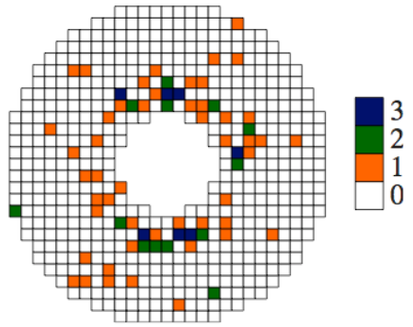
PPR-1
WP-84: SPB Instrument

Adrian Mancuso for the SPB team

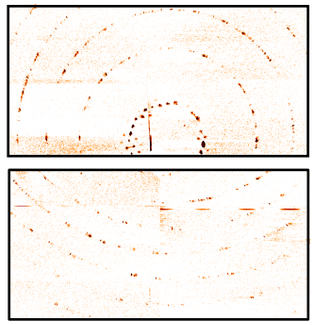
Single Particles, clusters and Biomolecules Instrument

Specifically, the SPB instrument will be designed to image single particles, which explicitly includes:

- Isolated, non-crystalline biomolecules
- Nanocrystals of biomolecules
- Atomic clusters
- Other isolated, single particles, in particular those of a “reproducible” nature



N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)



Measured diffraction pattern produced from a nanocrystal (CFEL)

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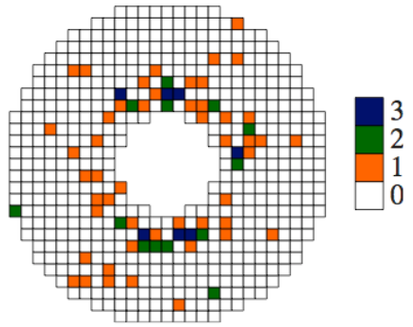

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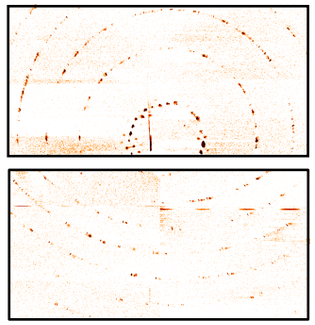

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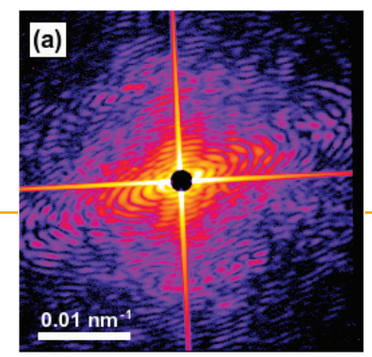

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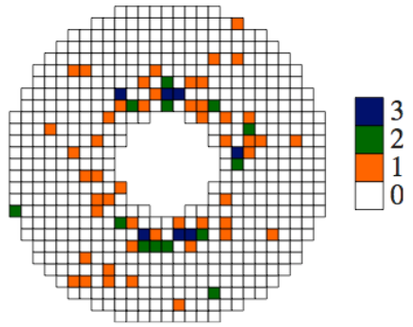

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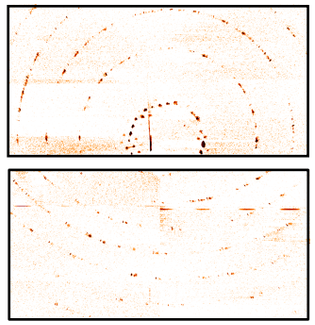

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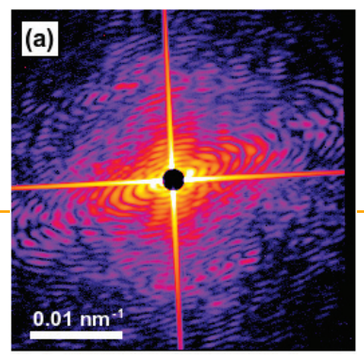

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Deliver instrumentation to perform this science

European XFEL

What has been achieved since the last PPR?

- Publication of the SPB CDR at doi:10.3204/XFEL.EU/TR-2011-007
- Calculation of required thermal stability for SPB hutch
- Creation of a first comprehensive list of required SPB controls, including axes of motion, required pumps and pumping locations, numbers and types of racks required, etc (useful start for all instruments)
- Calculation of required power to drive said motors, pumps, etc
- Calculation of the cooling required in the hutch given these sources of heat

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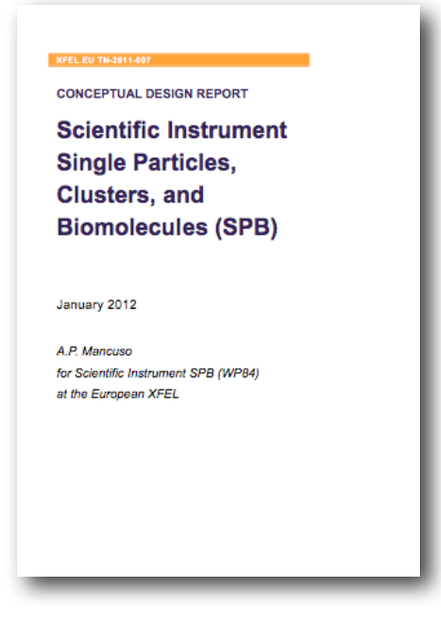
XFEL.EU TN-2011-007

CONCEPTUAL DESIGN REPORT

Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB)

January 2012

A.P. Mancuso
for Scientific Instrument SPB (WP84)
at the European XFEL

European XFEL

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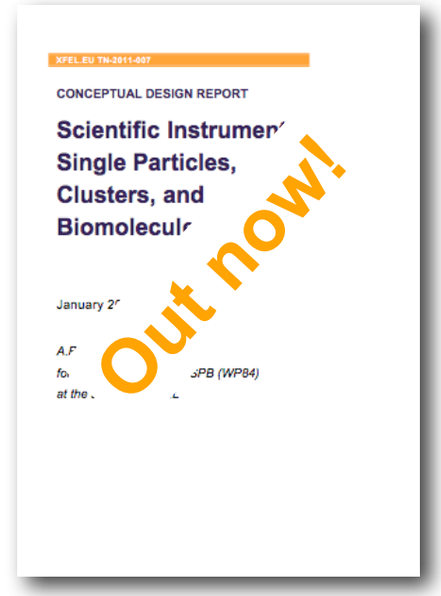


European XFEL

What has been achieved since the last PPR?

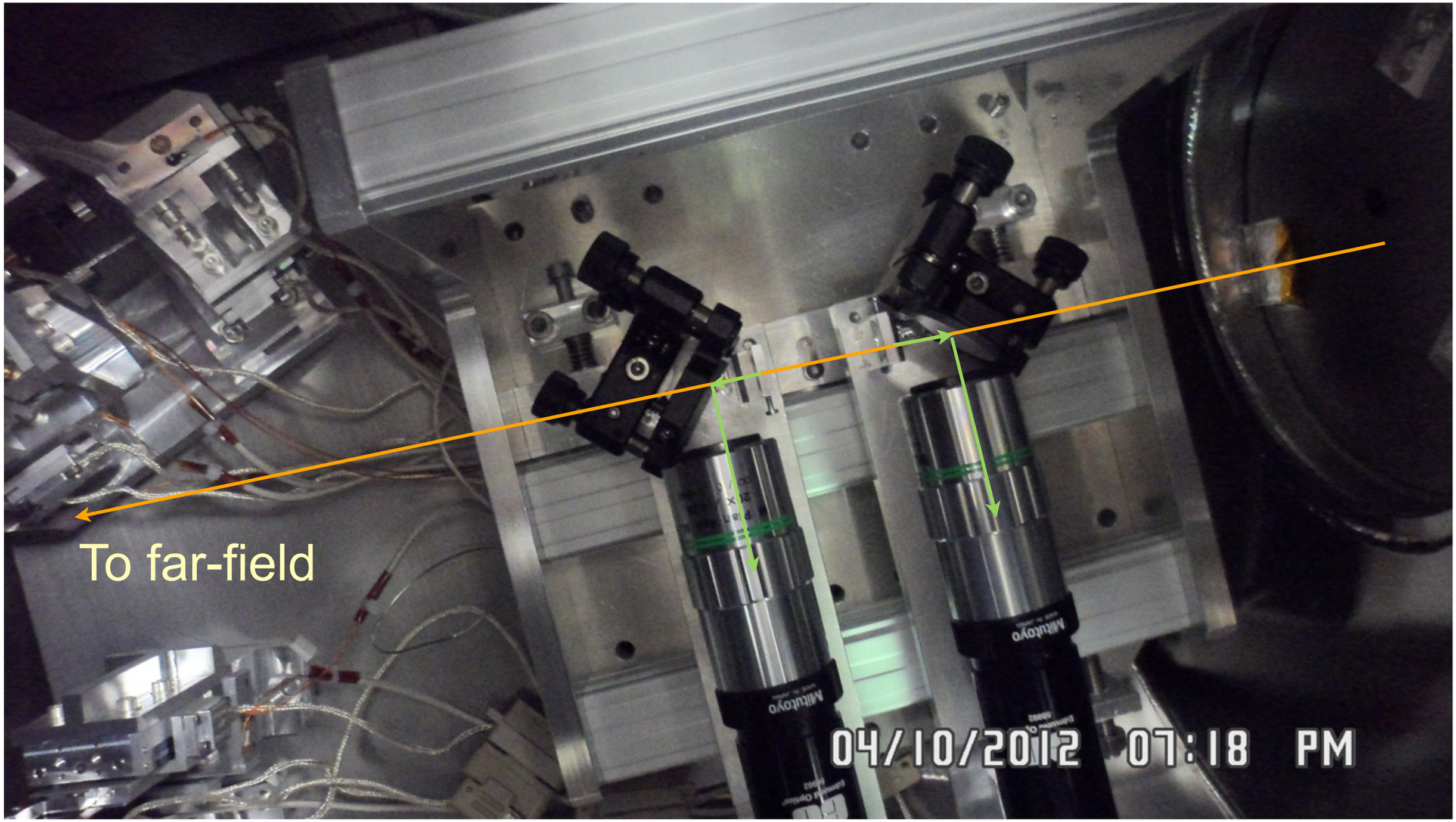
- Started a more detailed investigation of post-interaction region diagnostics (so-called ‘intelligent’ beamstop)
- Performed a review of grating based interferometry methods for beam characterisation
- First draft of focusing optics specification in preparation (concept already developed, details being refined)
- Elements of CrystFEL code implemented in XFEL software framework
- Continued modeling work in S2E simulations

European XFEL

What has been achieved since the last PPR?

- Investigated biological sample handling at comparable facilities (Diamond, LCLS)
- Performed initial comparison to existing, comparable instrument (CXI at LCLS).
- Feedback & discussion of UC proposals relevant to SPB
- Input to requirements on mechanical design of detectors (e.g. required size of hole in detectors, required pixel alignment)
- Experimental campaigns at LCLS and the APS.
  - Data analysis in progress

Multiple plane measurement experiment @ CXI, LCLS



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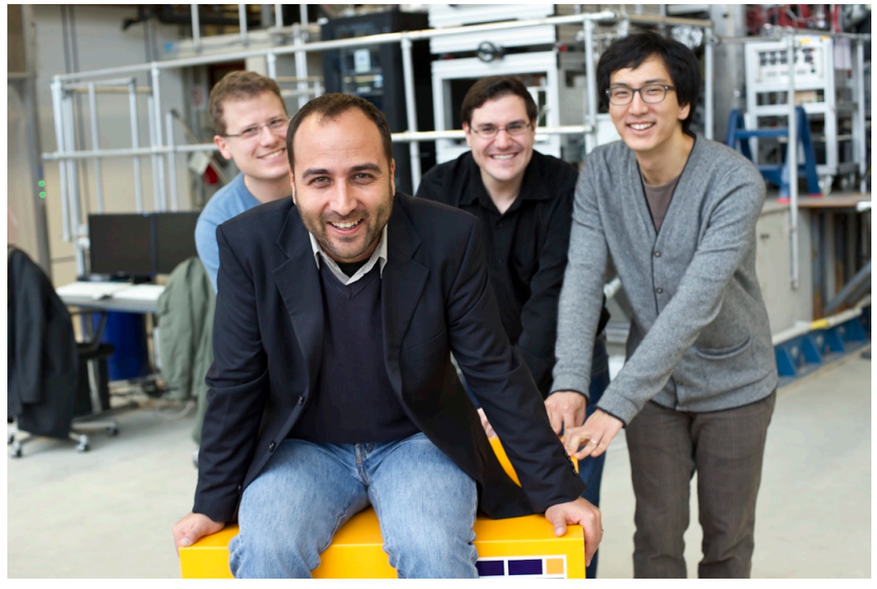
What has been achieved since the last PPR?

- Successful hiring of Nadja Reimers (experienced synchrotron beamline engineer), who joined the Central Instrumentation Engineering (CIE), assigned to SPB
- Start of Chuck Yoon (employed between CFEL & XFEL) to work on the implementation of nanocrystallographic software (developed at CFEL) in the XFEL software framework

Nadja Reimers



European XFEL

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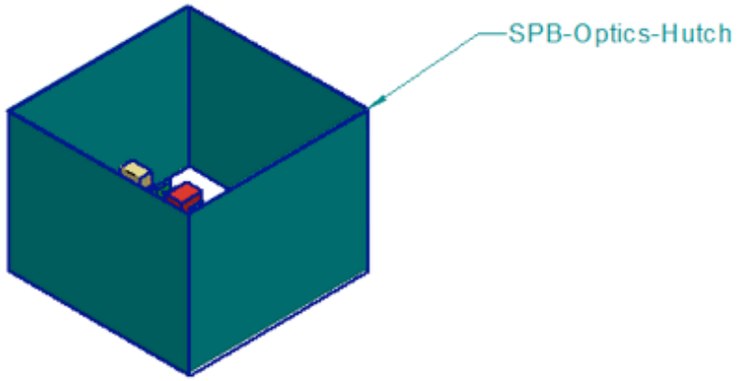

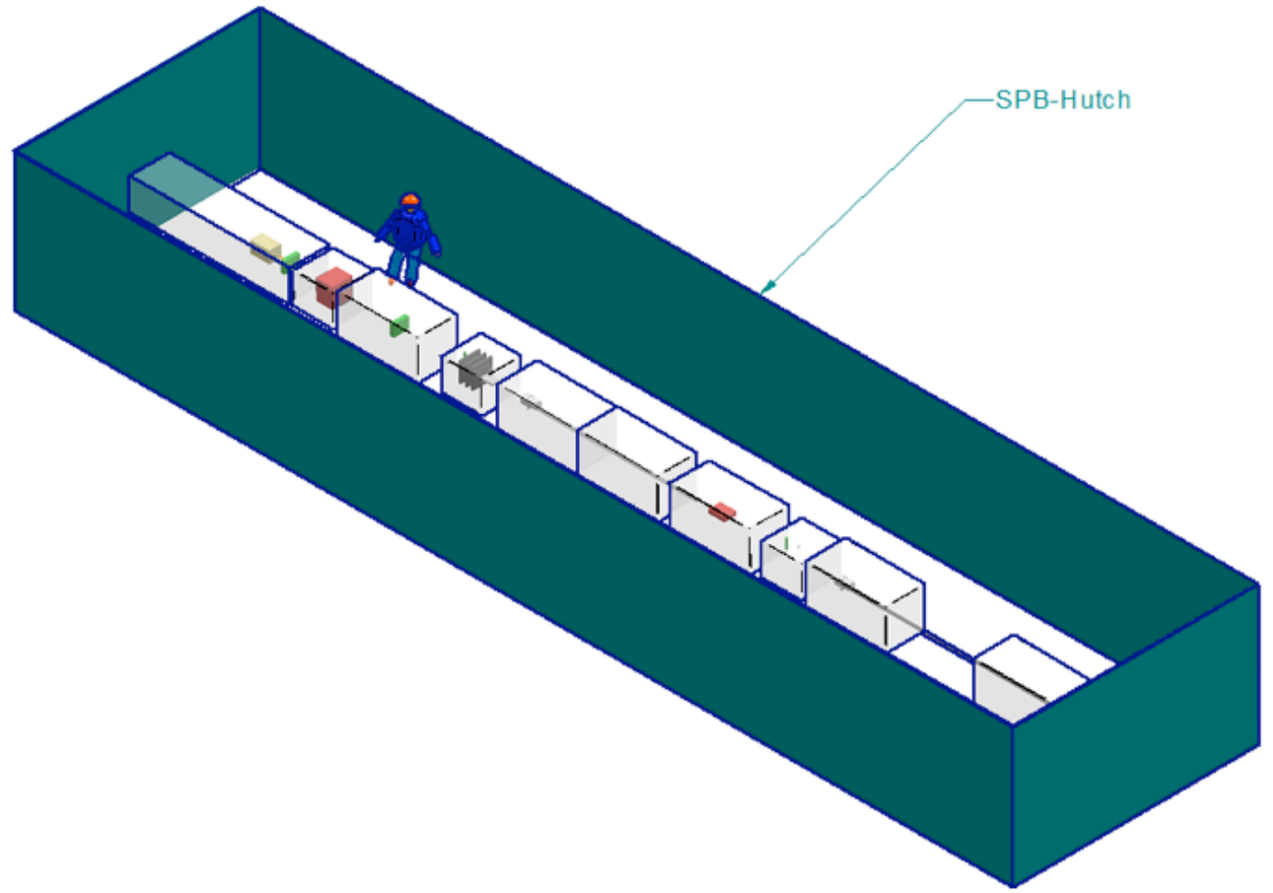

First sketch of SPB, including optics hutch

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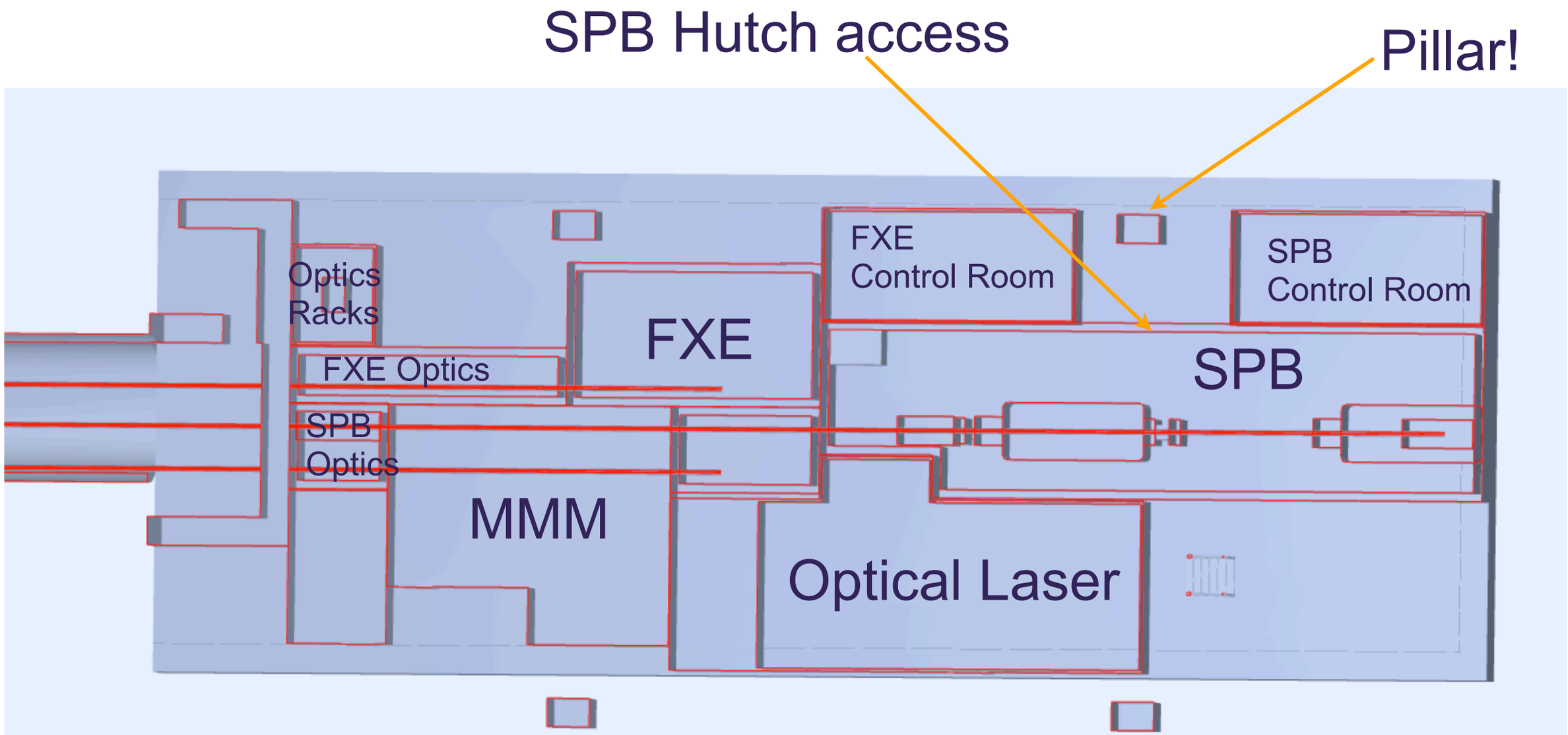
Revised SASE1 floor plan (in progress)



SASE1 floor plan yet to be finalised in light of recent changes

European XFEL

What are the next plans for WP-84?

- Finalise focusing optics specifications, including simulations of performance
- Further detail post-interaction region diagnostics–the so-called ‘intelligent’ beamstop
- Further detail the components and layout inside the SPB hutch
- Perform further FEL and synchrotron experiments to elucidate requirements at SPB (e.g. wavefront measurements, imaging experiments, optics characterisation, etc)
- Use all this knowledge to work towards TDR

European XFEL

What are the next plans for WP-84?

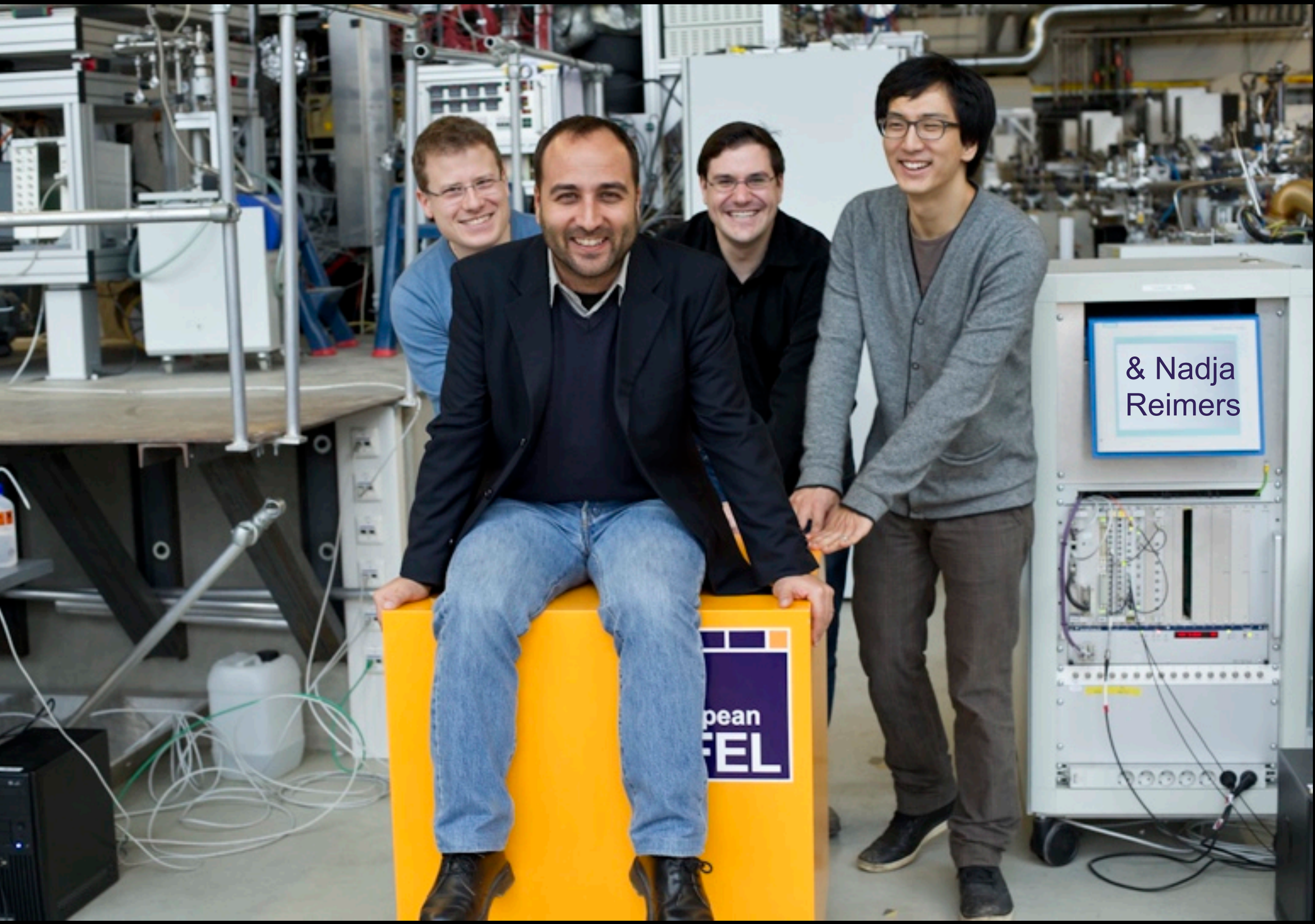
- Deliver first S2E model for simple scenario
  - For two cases: ‘ideal’ (ie Gaussian) and ‘realistic’ (SASE) beam conditions
  - 8.8 keV, 200 nm beam, 9 fs pulse, 0.5 mJ ($3x10^{11}$ ph)
  - For a small biomolecule (initially minimise computational complexity)
  - For a simplified model of radiation damage
  - Simplified model of detector
  - EMC type 3D intensity reconstruction and inversion

In collaboration with:
Beata Ziaja, Zoltan Jurek, Liuba Samoylova, Julian Becker, Duane Loh and more

European XFEL

What concerns are there for WP-84?

- Probability of hiring further qualified engineers
- Time scale for finalising and exploring procurement options for long KB mirrors
- Incorporating knowledge gained today in an ongoing project
  - We’re learning more and more about how to do these experiments each day now, and we want SPB to be as up-to-date as possible, but this has ramifications for project management
- Additional workload due to UC proposals for SPB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