SSX experiments with MXCuBE @ ESRF

David von Stetten

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Overview

- Serial crystallography using a viscous jet
- Jet crystallography with MXCuBE

Classical crystallography

- single crystal
- diffraction images recorded during continuous rotation, *e.g.*, $1800 \times 0.1^{\circ}$

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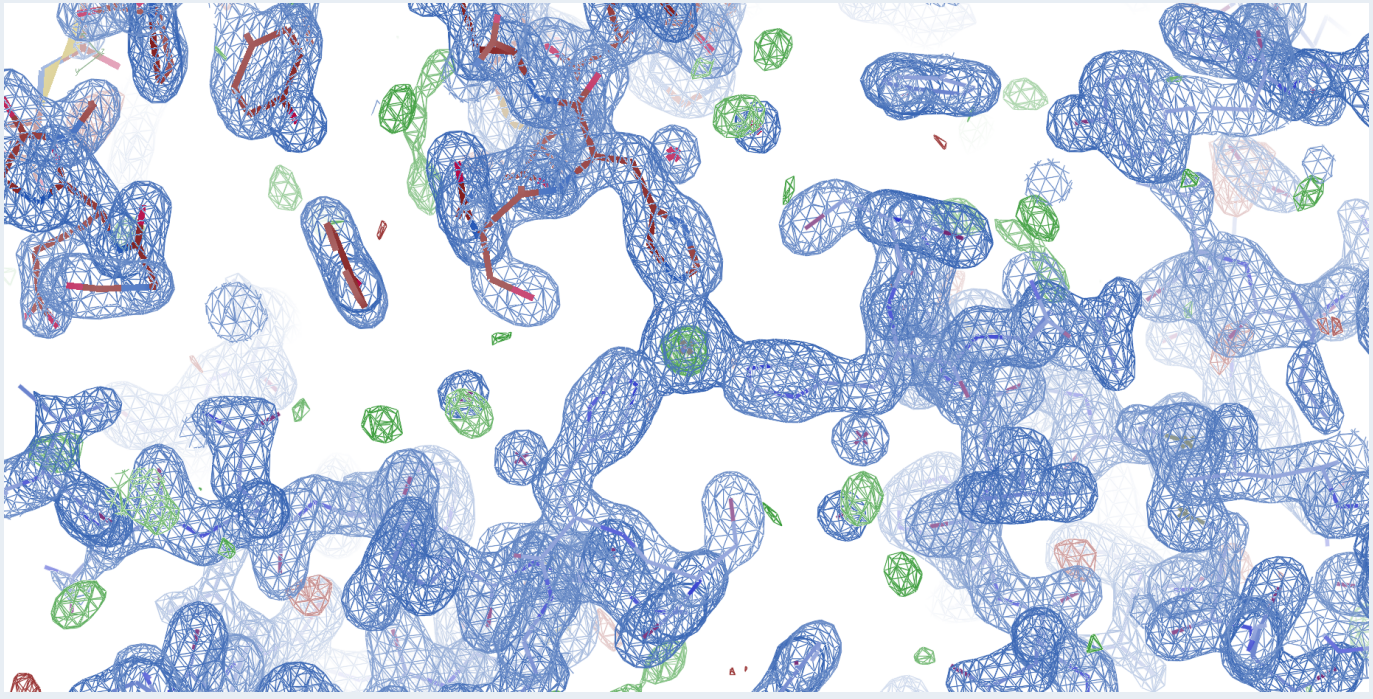
Apply some mathematics to obtain electron density map:



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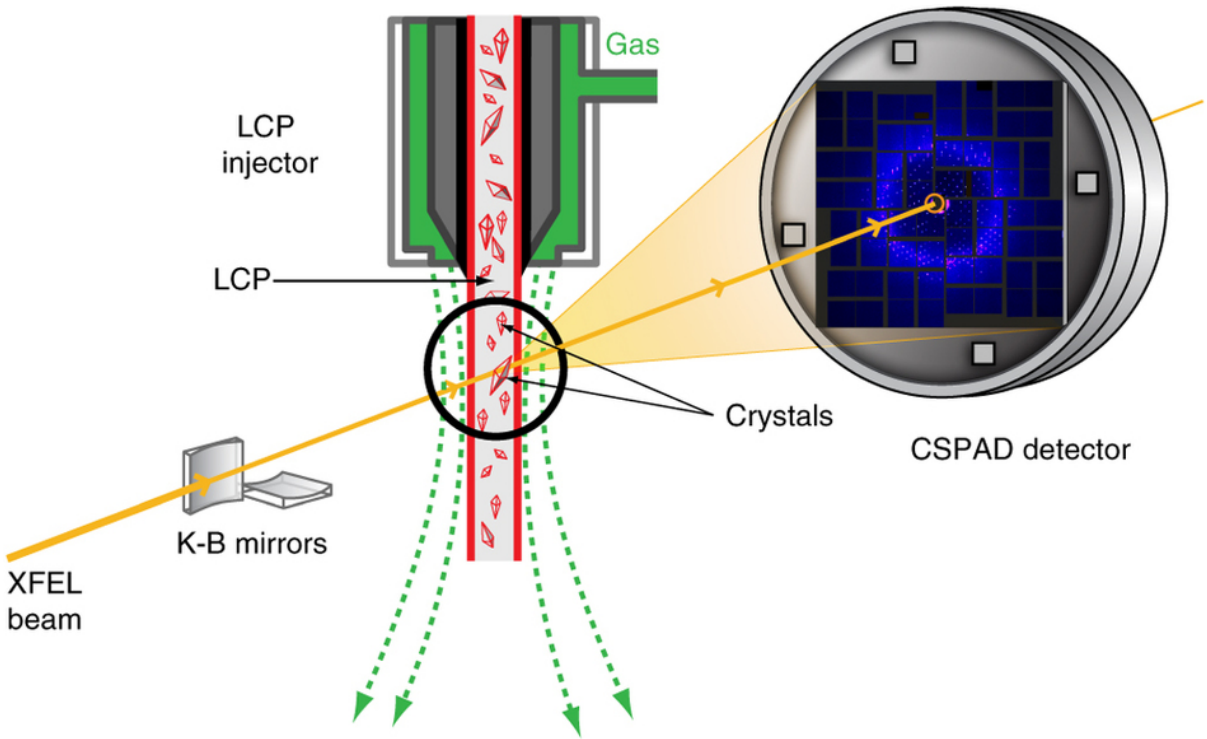
Serial crystallography with jets

- developed for XFELs because of extreme radiation damage
- only one image per crystal
- many crystals embedded in a stream of, *e.g.*, water or grease



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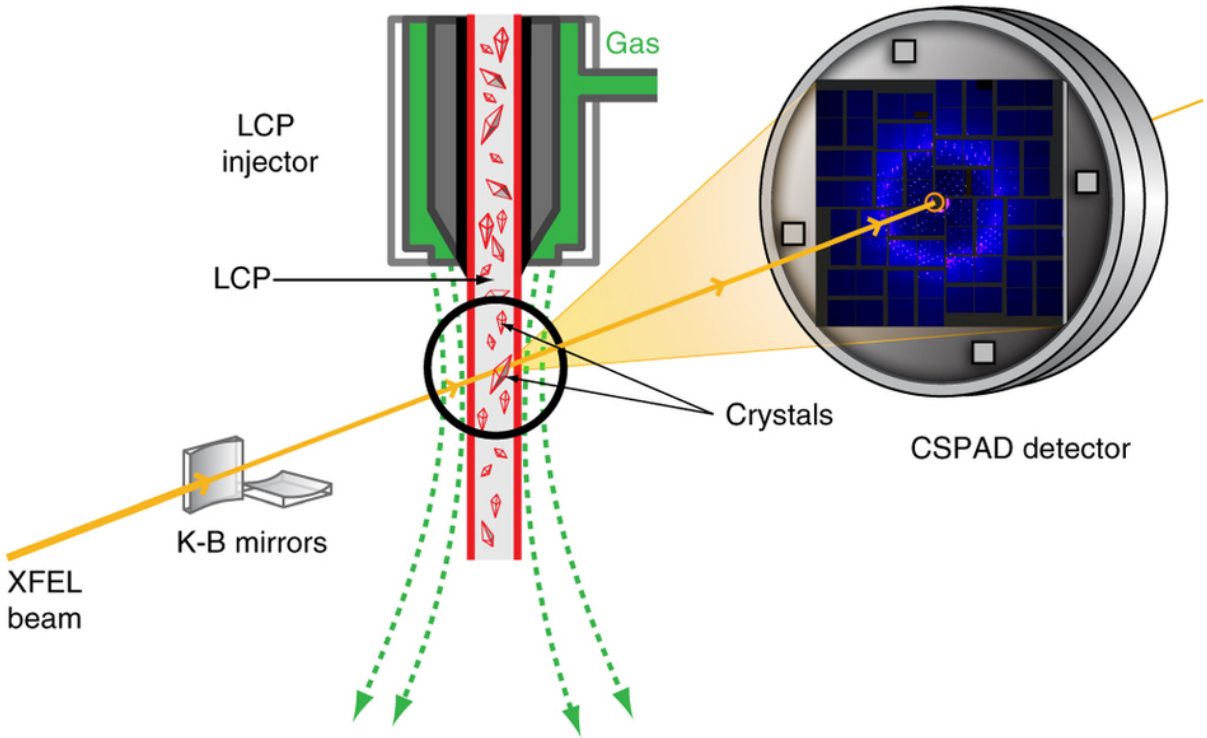
Serial crystallography with jets

- developed for XFELs because of extreme radiation damage
- only one image per crystal
- many crystals embedded in a stream of, *e.g.*, water or grease
- still images recorded at random orientations
  $\Rightarrow$ needs many more images



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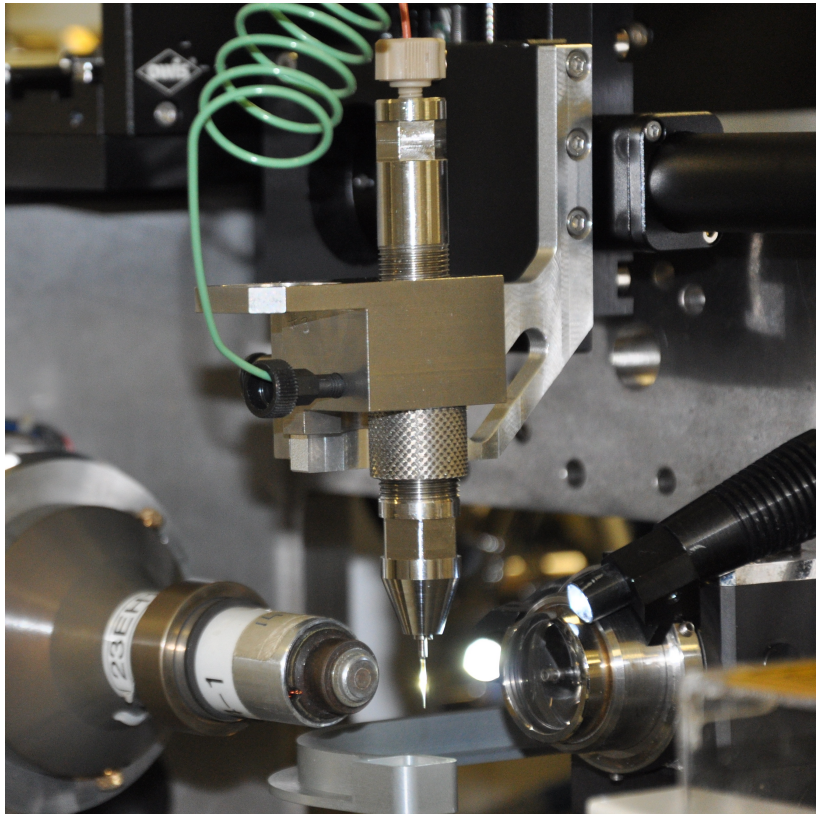
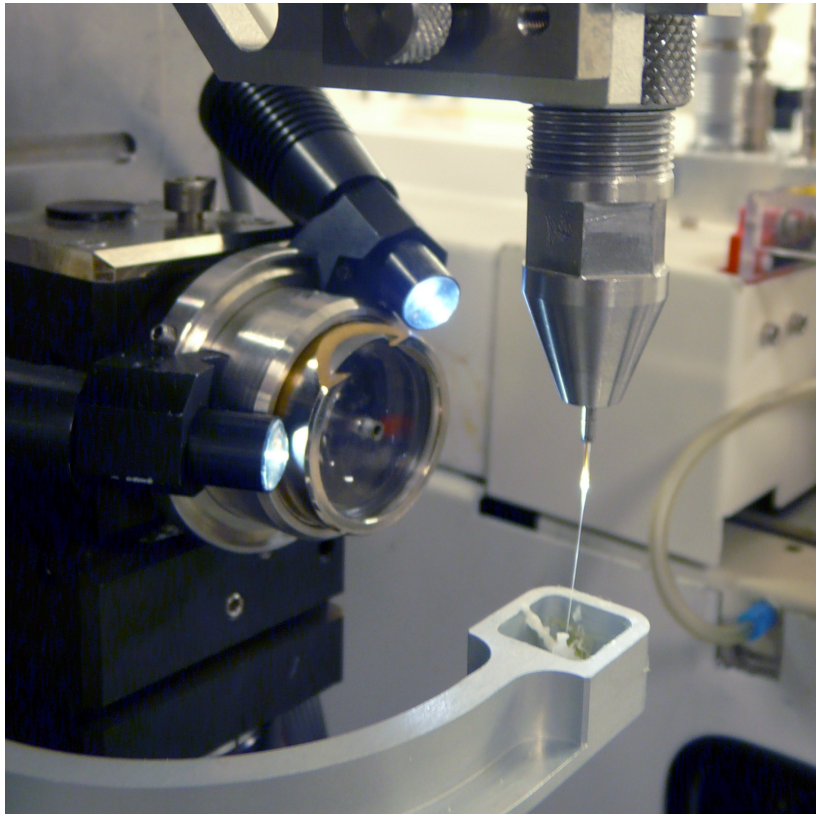
SSX on MASSIF-3





Injector filled with 30 µl grease mixed with protein crystals.

[Botha *et al.*, Acta Cryst. D**71**, 387 (2015)]

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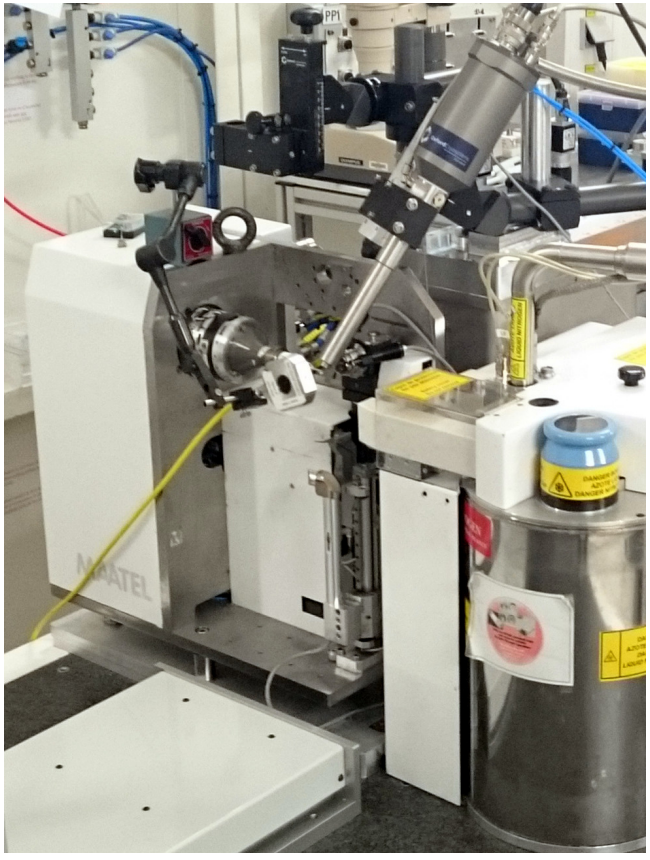
MASSIF-3 (a.k.a. ID30A-3)

MX beamline:

- beam diameter: 15 µm
- 1.5×10^{13} ph/s
- Eiger 4M: up to 750 img/s



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- 200 img/s, 100% transmission: OK
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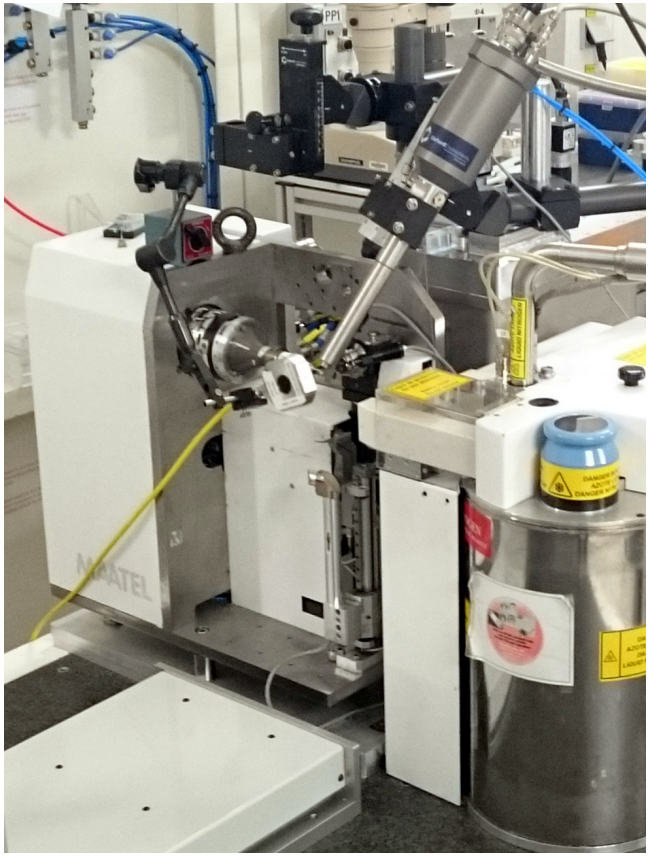
- 500 img/s, 100% transmission: stops after 220k images



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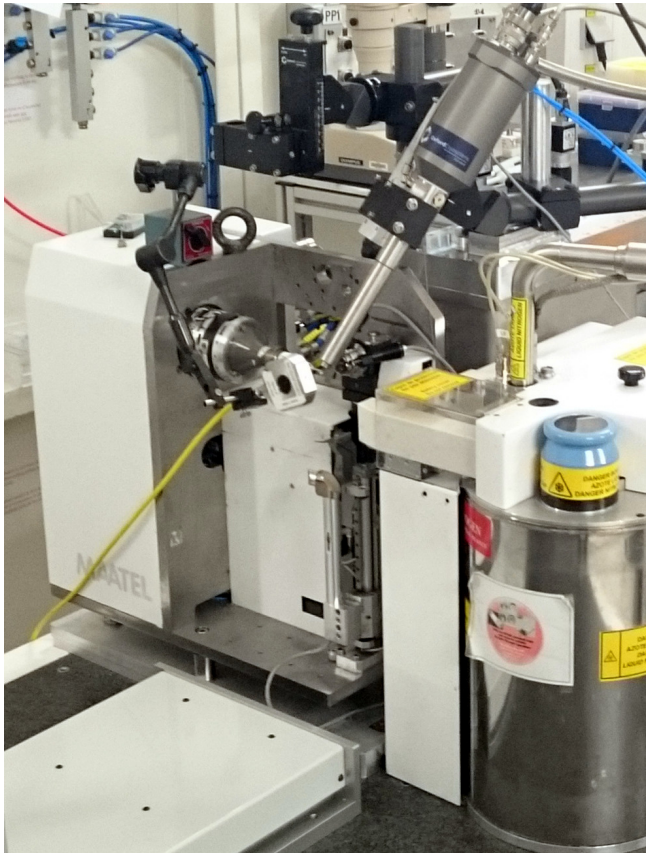
Note:

Depends on photon flux:
with higher flux, numbers will be lower!



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SSX: examples

	lysozyme	**lysozyme+Gd**	**insulin**
space group	$P4_32_12$	$P4_32_12$	$H3$
images/second	200	200	500
number of images	**539 000**	**539 000**	**1 000 000**
indexed patterns	**20 683**	**47 482**	**37 462**
resolution range [Å]	56.0–**1.8**	55.4–**1.8**	41.3–**1.6**
completeness [%]	100.0 (100.0)	100.0 (100.0)	100.0 (100.0)
redundancy (low / high)	613 / 101	1093 / 175	404 / 117
R_{split} [%]	11.9 (62.9)	9.3 (52.2)	12.5 (41.6)
CC^* [%]	99.1 (49.5)	99.5 (65.1)	99.4 (89.9)
SNR	7.2 (2.0)	8.2 (2.2)	6.2 (2.4)
R_{work} / R_{free}	17.5 / 19.8	14.7 / 19.3	14.9 / 19.9

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Classical vs. serial crystallography

	classical MX	**SSX**
number of crystals:	1	$> 1\,000$
number of images:	$\approx 1\,000$	$> 100\,000$
rotation per image:	0.1°	0°
processing:	XDS, mosflm,...	CrystFEL, cctbx.xfel,...

MXCuBE: minimal changes

manual patches to MXCuBE for each SSX experiment:

- disable confirmation dialog (file checking takes minutes)
- disable autoprocessing (takes hours to fail)
- increase number of images per HDF5 files from 100 to 1000

MXCuBE: wishlist for jet experiments

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- detector triggered by omega axis
  $\Rightarrow$ gonio spinning back 100000° takes ages
- flexible triggering schemes with MUSST for TR-SSX

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- flexible triggering schemes with MUSST for TR-SSX
- DOZOR for hit finding

Acknowledgements

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