

Serial crystallography at the beamline P11, PETRA III

Monday 22 September 2025 15:10 (15 minutes)

P11 at PETRA III (DESY, Hamburg) is a high-throughput instrument for macromolecular crystallography [1]. The beamline has tuneable photon energy between 5.5 - 28 keV and beam sizes from 200 x 200 μm to 4 x 9 μm^2 can be used with a maximum photon flux of 1×10^{13} ph/s at 12 keV energy. Equipped with a fast detector Eiger2 X 16M as the stationary detector (max 133 Hz), this high flux instrument is perfect for serial synchrotron crystallography (SSX).

For SSX, the sample delivery is achieved through various types of solid supports and the TapeDrive setup, which allows time-resolved room temperature experiments by the mix-and-diffuse method [2, 3], and has been developed at P11 along with the real-time autoprocessing with CrystFEL [4, 5]. In this method, the samples are delivered on to a continuously drawn polyimide tape through a 3D-printed microfluidic nozzle with two channels ($\varnothing$ 150 μm each), one for the crystal slurry and second, for example, for mixing the crystals with a ligand or adjusting their pH. The mixing time can be modified by the speed of the tape and the distance of the nozzle from the X-ray focus point (delay times of 50 ms – 180 s).

In order to mitigate possible radiation damage, the exposure time per frame can be reduced from 7.5 ms instead of 3.5 ms with a chopper wheel. SSX experiments are currently controlled through a separate graphical user interface, and online data analysis is available for real-time evaluation and indexing via OnDA Monitor [6].

We will present the TapeDrive setup used for SSX, the real time data processing implemented as well as several scientific examples exploiting the capabilities of the setup (time-resolved, mix-and-diffuse experiments, temperature control...).

[1] Burkhardt, A., Pakendorf, T., Reime, B., Meyer, J., Fischer, P., Stübe, N., Panneerselvam, S., Lorbeer, O., Stachnik, K., Warmer, M., Rödig, P., Göries, D. & Meents, A. (2016). Eur. Phys. J. Plus 131, 56.

[2] Beyerlein, K. R., Dierksmeyer, D., Mariani, V., Kuhn, M., Sarrou, I., Ottaviano, A., Awel, S., Knoska, J., Fuglerud, S., Jönsson, O., Stern, S., Wiedorn, M. O., Yefanov, O., Adriano, L., Bean, R., Burkhardt, A., Fischer, P., Heymann, M., Horke, D. A., Jungnickel, K. E. J., Kovaleva, E., Lorbeer, O., Metz, M., Meyer, J., Morgan, A., Pande, K., Panneerselvam, S., Seuring, C., Tolstikova, A., Lieske, J., Aplin, S., Roessle, M., White, T. A., Chapman, H. N., Meents, A. & Oberthuer, D. (2017). IUCrJ 4, 769.

[3] Henkel, A., Maracke, J., Munke, A., Galchenkova, M., Rahmani Mashhour, A., Reinke, P., Dommarack, M., Fleckenstein, H., Hakanpää, J., Meyer, J., Tolstikova, A., Carnis, J., Middendorf, P., Gelisio, L., Yefanov, O., Chapman, H. N. & Oberthür, D. (2022). Acta Cryst. A78, e560.

[4] White, T. A., Mariani, V., Brehm, W., Yefanov, O., Barty, A., Beyerlein, K. R., Chervinskii, F., Galli, L., Gati, C., Nakane, T., Tolstikova, A., Yamashita, K., Yoon, C. H., Diederichs, K. & Chapman, H. N. (2016). J. Appl. Cryst. 49, 680.

[5] White, T. A., Schoof, T., Yakubov, S., Tolstikova, A., Middendorf, P., Karnevskiy, M., Mariani, V., Henkel, A., Klopprogge, B., Hannappel, J., Oberthür, D., De Gennaro Aquino, I., Egorov, D., Munke, A., Sprenger, J., Pompidor, G., Taberman, H., Gruzinov, A., Meyer, J., Hakanpää, J., & Gasthuber, G. (2025). IUCrJ 12, 97.

[6] Mariani, V., Morgan, A., Yoon, C. H., Lane, T. J., White, T. A., O'Grady, C., Kuhn, M., Aplin, S., Koglin, J., Barty, A. & Chapman, H. N. (2016). J. Appl. Cryst. 49, 1073.

Co-authors:

Alessandra Henkel, Julia Maracke, Spyridon Chatziefthymiou, Alexander Grebentsov, Andrey Gruzinov, Olga Merkulova, Philipp Middendorf, Alexandra Tolstikova, Thomas White, Dominik Oberthür, Johanna Hakanpää

Presenter: POMPIDOR, Guillaume (DESY)

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