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Efficient simulation and AI surrogate models for real-time optimisation

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In order to aid the design and development of optical elements, such as Reflection Zone Plates, and automate the process of aligning optics in both spectrometers and beamlines, we have developed new simulation software as well as deep learning AI methods.

RAY-X, our open-source state-of-the-art physics-based ray tracing software is designed to utilise modern GPUs to reduce trace time of simulated beamlines and allow for easier multi-processing of tasks. RAY-X fundamentally restructures the architecture of the well-known RAY and RAY-UI software [1, 2] and uses the Vulkan framework [3], an industry leading graphics and computing API, to provide high efficiency, cross-platform access to modern GPUs.

The capabilities of RAY-X have afforded us the capacity to generate large datasets in order to train complex neural networks as surrogate models for both beamlines and Spectrometers. These surrogate models have inference times of milliseconds and can therefore be deployed in situ at beamlines for the purpose of automated real-time alignment of optical elements.

References:

1. F. Schäfers, "RAY - The BESSY Raytrace Program", in: Modern Developments in X-Ray and Neutron Optics, Springer Series in Modern Optical Sciences, eds A. Erko, M. Idir, Th. Krist, A.G. Michette, Vol. 137, 9–41 (2008) https://doi.org/10.1007/978-3-540-74561-7_2
2. RAY-UI: New features and extensions. AIP Conference Proceedings 2054, 060034 (2019) <https://aip.scitation.org/doi/abs/10.1063/1.50846>
3. <https://www.khronos.org/vulkan/>

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yes

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