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pyXRSA2: A Ray-Tracing Simulation Code for X-ray Spectroscopy based on the Finite Element Discretization Method

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pyXRSA2, a ray-tracing code for X-ray spectroscopy, is recently developed from its predecessor, XRSA, which was used in the design of ITER X-Ray Crystal Spectroscopy (XRCS) systems [1]. The ray-tracing simulations can provide the system responses essential for design validation and performance assessments, thus playing a crucial role in designing complex X-ray spectrometry systems for future reactor-scale tokamaks like ITER.

PyXRSA2 utilizes a self-adaptive Finite Element (FE) method to trace the X-ray beams, for which the joint distribution functions encompassing spatial, angular, and wavelength distributions are introduced. Key components, such as dispersion crystals, are treated both as receivers and secondary sources. The code discretizes spatial and angular distributions on 3D triangular-meshed surfaces and defines these on unit spheres centered at the origin with a radius of one. Wavelength distributions are treated as 1D scalar functions, and the angular distribution functions are defined on each spatial mesh node with the wavelength functions applied on each angular mesh node.

To enhance computational efficiency, pyXRSA2 implements various innovative solutions. Firstly, it employs a self-adaptive mesh refinement technique based on the effective response areas through iterative method, aiming to adapt the issue for the X-ray diffraction processes accompanied with very narrow bandwidths. The effective response areas are typically highly anisotropic as depicted in Figure 1&2. Secondly, to address the high computational cost associated with generating angular meshes, the code generates these meshes on standard base meshes and adapitates them using transformation encoders to varied orientations based on the continuous variation across spatial domains.

Furthermore, pyXRSA2 supports extensive integration capabilities, including arbitrary geometry inputs through the GMSH module and compatibility with High Performance Computation (HPC) platforms.

The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

References

[1] Z.F. Cheng *et al*, Rev. Sci. Instrum. **93**, 073502 (2022)

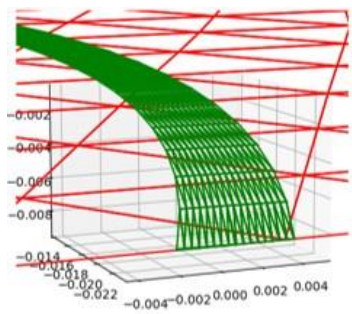

Figure 1. Updated mesh according to the effective response area with the self-adaptive method.

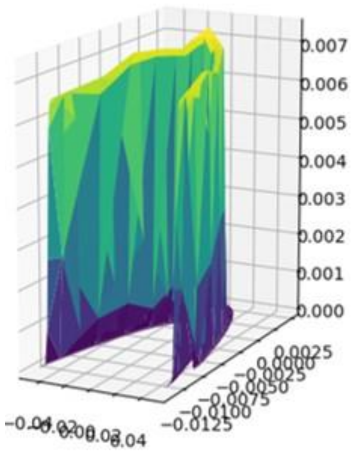

Figure 2. A response distribution function defined with the Self-Adaptive FEM in pyXRSA2.