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KDSource, an Open-Source Code for the generation of Monte Carlo particle sources using Kernel Density Estimation

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The design of neutron instruments usually is related to the calculation of radiation beams, and these simulations are normally decoupled from the source since the nuclear reactions that govern the generation of particles in the source are independent of the specific interactions that take place in the beam path. Also, radiation beams are usually transported far away from the source to reduce the background signal in the measurements and the radiation dose of the personnel. When evaluating the beam under different operating conditions, it is useful to have a source that can be re-sampled.

Different types of solutions are available to solve this problem: capture the particles that are produced in the position of the source and transport them into the beam, use track files with the particles that cross a specific surface and reuse them in a downstream simulation, or use a synthetic source, fitting an analytical distribution for each of the source variables (energy, position, direction and time) are recorded

KDSource [1] is an open-source code that uses the adaptive multivariate Kernel Density Estimation (KDE) method to estimate the source distribution at a given point in the beam trajectory, which seeks to overcome the discussed limitations of the previous approaches. This approach presents a novel methodology to optimize source modeling using adaptive multivariate kernel density estimation, which may be especially suited for radiation beam and radiation shielding simulations.

The core idea of the methodology is to use some machine learning libraries and algorithms (like scikit-learn in Python) to optimize the bandwidth selection for each source variable. With this strategy, smooth estimates of the variable distributions may be obtained from particle lists at a given point in a simulation that maintains correlations among variables. The code implements the proposed methodology in Python and C, and it consists of a module for KDE model optimization and another for sampling (i.e. generating new particles using the previously optimized model).

The objective of this work is to present to the community the theory behind kernel density estimation, and how the KDSource code works. Also, some examples of using this tool to simulate neutron time-of-flight experiments and to design the neutron imaging instruments for the High Brilliance Neutron Source project will be shown.

[1] N.S. Schmidt et al, 2022. KDSource, a tool for the generation of Monte Carlo particle sources using kernel density estimation. Ann. Nucl. Energy 177.
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GitHub URL: https://github.com/KDSource/KDSource

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