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Optimising complex neutron optical configurations with a global search in a high dimensional space

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Modern pulsed neutron sources offer significantly higher peak brightness and a much higher time integrated neutron flux. The geometries of the moderators are more refined and optimised for beam experiments. The number and variability of readily available neutron optical components is increasing. Not surprisingly the demand from the experimentalists to develop highly sophisticated instrument concepts is growing accordingly. A consequence of this development is that the parameter space neutron beam instrumentation has to work with has more dimensions and a wider range of limits for the many of its variables. Instrument simulations with the purpose of optimising more than a few parameters are time-consuming, tedious and inefficient if done manually or with a brute force approach - even worse it is very likely that a 'local optimum' is chosen because the parameter space is too vast for a thorough exploration. We demonstrate how an efficient global search algorithm can help to find parameter vectors which are selected based on multiple, simultaneous objectives as defined by the science driving the instrument design.

Our example is the BER-SANS instrument at beamline STS-01 at the SNS.

The overall optimisation criterion is to provide as many neutrons as possible on a small sample (e.g., a few mm in diameter) with a moderate minimum q -value of 0.01\AA^{-1} . The third objective is the capability to rapidly distinguish two states of samples, e.g., two conformations of the same protein, with a given instrumental resolution. Any neutron optical concept will compromise on each of those requirements in different ways and the scientific community has the opportunity to choose their preferred option.

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