Optimization of multi-channel neutron focusing guides for extreme sample environments

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Abstract. In this work, we present and discuss simulation results for the design of multi-channel neutron focusing guides for extreme sample environments. A single focusing guide consists of any number of supermirror-coated curved outer channels surrounding a central channel. Furthermore, a guide is separated into two sections in order to allow for extension into a sample environment. The performance of a guide is evaluated through a Monte-Carlo ray tracing simulation which is further coupled to an optimization algorithm in order to find the best possible guide for a given situation. A number of population-based algorithms have been investigated for this purpose. These include particle-swarm optimization, artificial bee colony, and differential evolution. The performance of each algorithm and preliminary results of the design of a multi-channel neutron focusing guide using these methods are described. We found that a three-channel focusing guide offered the best performance, with a gain factor of 2.4 compared to no focusing guide, for the design scenario investigated in this work.

1. Introduction

The focusing of neutrons is an important technique for many neutron scattering studies. It is particularly true when investigations are to be performed on samples limited to small volumes. In this case, neutron focusing guides play a critical role in determining the feasibility of such an experiment. A number of previous studies have reported on the development of multi-channel supermirror-coated neutron guides for focusing purposes \cite{1, 2}. To benefit the most from the intensity gains of these types of guides, the focusing lens should extend close to the sample position. This is however at odds with the requirements of specific sample environments used in neutron scattering studies. Of particular interest for the current study is the use of cryomagnets to expose a sample to low temperatures and high magnetic fields. One possible solution is to extend the focusing guide into the cryomagnet itself. At the Institut Laue-Langevin (ILL), preliminary tests have been carried out which showed that some supermirrors tolerate both low temperatures and high magnetic field variations. A series of tests at the Paul Scherrer Institute (PSI) have also reported similar results at low temperatures for Ni/Ti supermirrors \cite{3}. These combined results suggest that it is feasible to install a focusing guide into a cryomagnetic sample environment.

We have begun a project to design and build a split, multi-channel neutron focusing guide that begins focusing outside a cryomagnet and completes the focusing optic within the extreme
Figure 1. The parameters describing a three-channel guide. The guide is symmetric across its central horizontal axis and thus only the bottom half of the guide is shown. The dashed regions are supermirror-coated mountings. The parameter $L$ corresponds to the length of the central channel, $L_t$ is the length of the top face of the outer channel, and $L_b$ is the length of the bottom face of the outer channel. These lengths can take on different values in the simulations, as described in the text.

sample environment apparatus. This requires optimizing two physically separate multi-channel optics with a gap for the cryomagnet beam window. This work extends the application of the software described in Ref. [4]. The software consists of a Monte-Carlo ray tracing simulation of the multi-channel guide which is coupled to an optimization code in order to find the best guide for a given scenario. We have selected the design of a multi-channel focusing guide for the IN5 instrument [5] at ILL as a test case for the software. The IN5 instrument is a possible candidate for the installation of a Cryogenic Limited [6] cryomagnet, which has already been designed to accept a focusing guide. A similar guide shall also be implemented for a 10T cryomagnet to boost further the performance of the new ThALES cold-neutron three-axis spectrometer [7]. We therefore present an initial optimization study of this double-optic system, resulting in a candidate design that is capable of extreme vertical focusing elements crossing into a sample environment system. At the same time, we will also benchmark the particle-swarm optimization software used previously [4] against some alternative metaheuristic algorithms that have recently been receiving attention.

2. Multi-channel neutron guides
The geometry of the type of focusing guide that is being investigated is shown in Fig 1. The bottom half of the guide is illustrated as it is symmetric across its central horizontal axis. It can be mentioned that all simulations reported here are carried out in two spatial dimensions. There are no inclined faces in the guide and thus the vertical and horizontal focusing are decoupled. The guide comprises two separate sections, divided by a gap of width $\Delta w$ centered at position $w$. This makes it possible to independently design both the section of the guide installed into the sample environment and the section installed outside. The central channel sections follow two separate parabolas, described by the parameters $h_{11}, h_{12}, h_{13}$ and $h_{14}$, which are the heights at points along the length $L$ of the channel. The outer channel pairs begin with a straight section of length $L_s$ and tilt $\phi_s$ with respect to the central axis. They then follow circular arcs, starting with the angles $\phi_{11}$ and $\phi_{21}$ with respect to the axis of the beam, up to the break in
the optics. Likewise, the parameters $\phi_{12}$ and $\phi_{22}$ describe the starting angles of the arcs for the second section. The entrance and exit heights $h_{21}, h_{22}, h_{23}$ and $h_{24}$ of the outer channel for the two sections are also adjustable parameters. The channel height at the transition from the straight section to the curved section of a channel is linearly interpolated between the values $h_{21}$ and $h_{22}$. The vertical offsets of the channel entrances for both sections of the guide along with the offsets of the channel exits of the first section, with respect to the previous channel, are described by the parameters $g_1, g_2$ and $g_3$. The vertical offset of the channel exit of the second section is constrained to the value $d_s = 0.45$ mm. This is equal to the thickness of two 0.2 mm pieces of glass separated by a gap of 0.05 mm. The distance $d$ of the end of the guide to the sample position is also an adjustable parameter. Each channel edge, with respect to the previous channel edge closer to the center of the guide, is allowed to extend closer to the sample with the central channel being the furthest from the sample position. In addition, any number of curved outer channel pairs can be defined in the simulation.

3. Population-based optimization algorithms

Population-based algorithms, such as Genetic algorithms (GA) \cite{8} and particle-swarm optimization (PSO) \cite{9}, have been shown to be well suited for neutron instrumentation optimization problems \cite{4, 10, 11, 12}. These types of algorithms work with a large number of candidate solutions which evolve over time towards a best solution in a particular parameter space. The evolution is guided by an appropriately selected figure of merit (FOM). In this work, the FOM is the number of neutrons impinging on a sample at the end of the focusing guide. Additional constraints to guide the simulations, such as penalty functions for the divergence at the sample position or beam missing the sample can be included in the simulation if desired.

The above described algorithms are inspired by nature. For example, GA was inspired by the self optimization of biological systems \cite{13} while PSO has its roots in the swarm behavior of social animals, such as the flocking of birds or schooling of fish \cite{9}. Neutronic optimization problems can be difficult to solve using other simple traditional optimization algorithms. This was highlighted in Ref. \cite{14} where a least-squares algorithm, based on partial derivatives, was used to optimize the design of a converging guide exit. In a multi-dimensional search the algorithm was unable to locate the global minimum. In a more recent study, a number of other optimization routines have been proposed for the optimization of neutron scattering instruments \cite{15}.

The advantages of population-based algorithms, compared to traditional approaches, are that they have a tendency to avoid local optima, thoroughly sample the parameter space, and are simple to implement partly because they require no partial derivatives. Additionally, these types of methods are less sensitive to random noise, which is important when using the Monte-Carlo method, as discussed in Ref. \cite{15}. In particular, PSO has been shown to have excellent performance for the design of multi-channel focusing guides \cite{4}. To complement these previous investigations with PSO, we have explored several other popular optimization algorithms for the design of focusing guides. These include artificial bee colony (ABC) \cite{16} and differential evolution (DE) \cite{17}, both of which have been compared to PSO in literature; see e.g. Refs. \cite{18, 19, 20}. The PSO method, applied to multi-channel focusing guides, has been described in detail in Ref. \cite{4}. The same algorithm was applied in the current work and is not described here. In the following, the ABC and DE methods will however be briefly outlined.

3.1. Artificial Bee Colony (ABC)

ABC \cite{16} is a population-based algorithm inspired by the intelligent behavior of honeybees in nature. In the algorithm, an artificial bee colony is made up of employed bees, onlooker bees, and scout bees, denoted as $n_e, n_o$ and $n_s$, respectively. Food sources represent candidate solutions, each characterized by their nectar amounts. The number of food sources is always equal to
the number of employed bees. In the first step, a population consisting of a number of food sources is initialized randomly, represented by the quantity $SN$. Each employed bee will visit an individual food source and determine a new food source based on a comparison with other surrounding sources. A parameter in the new source, represented by $v_{ij}$ where $j$ is a parameter index for the $i^{th}$ source, is produced by the following mutation of the original parameter $x_{ij}$,

$$v_{ij} = x_{ij} + \phi_{ij}(x_{ij} - x_{kj}),$$

where $k$ represents a randomly selected neighbor source and $\phi_{ij}$ is a random number between -1 and 1. The employed bee will then evaluate the nectar amount of the new source and memorize the source if it produces more nectar than the old one. Otherwise, the bee remembers the old source. After all the employed bees have visited their food sources they return to the hive and share their information with the onlooker bees. In the next step, the onlooker bees select a particular food source to visit based on the probability $p_i$, given by

$$p_i = \frac{F_i}{\sum_{n=1}^{SN} F_n},$$

where $F_i$ is the nectar amount for the $i^{th}$ source. Sources which produce more nectar are thus more likely to be visited by the onlooker bees. Once an onlooker bee arrives at a particular food source, it searches in the nearby area for a new food source and evaluates the nectar amount of the source, as given by Eq. 1. The onlooker bee memorizes the new source if it produces more nectar otherwise it remembers the old one. If a particular food source cannot be improved after a certain number of iterations, represented by the parameter $limit$, then that food source is forgotten and a scout randomly searches for a new food source. The algorithm is then repeated with the employed bees visiting their food sources and continues for a given number of iterations.

3.2. Differential Evolution (DE)

DE [17] is a type of evolutionary algorithm which operates in continuous parameter spaces. After the population of solutions is initialized and evaluated, each individual solution of the current generation, referred to as a target vector, undergoes mutation. For each $i^{th}$ target vector, a donor vector is generated by the following,

$$v_i = x_{r1} + F(x_{r2} - x_{r3}),$$

where $v_i$ represents the donor vector, $x_{r1}, x_{r2}$ and $x_{r3}$ are three different randomly selected solution vectors of the current population and $F$ is a scaling factor. The population diversity is then enhanced through a crossover operation where the donor vector exchanges a number of components with the target vector to create a trial vector. The operation is controlled by a parameter $CR$, called the crossover constant. For each parameter, crossover is performed if a randomly selected number between 0 and 1 is less than or equal to $CR$. If the trial vector performs better than or the same as the target vector, it replaces the target vector in the next iteration. In this way, the population of solutions never gets worse but can only get better or stay the same. The algorithm continues for a given number of iterations.

3.3. Comparison of the optimization methods

Two separate tests have been carried out in order to compare the three different optimization methods. These include the design of a single-channel and a three-channel guide based on the IN5 instrument at ILL [5]. The geometry is described in detail below. Single- and three-channel guides were selected for the initial tests. Our preliminary simulations suggest that a
The parameter values used in the different optimization methods. The values are taken from the indicated references. See text for the definition of the parameters for ABC and DE. For the PSO parameters, see Ref. [4].

|       | PSO [4] | ABC [19] | DE [18] |
|-------|---------|----------|---------|
| pop. size | 50      | 100      | 50      |
| d     | 0.95    | ne       | 0.8     |
| cl    | 1       | no       | F       |
| cg    | 1       | ns       | 0.5     |
|       | limit   | ne × D   |         |

The five-channel guide does not provide additional improvement over a three-channel guide for the scenario described below.

The parameters used for the optimization algorithms are given in Table 1. For PSO, the parameters and software previously implemented for the optimization of multi-channel neutron guides were used, as described in Ref. [4]. The population size was set to 50, the damping parameter d to 0.95 and both the control parameters cl and cg were set to unity. The parameters for the other two methods were adopted from literature values [18, 19]. For ABC, the colony size was 100 with ne and no both set to 50, the number of scouts ns was set to 1 and the limit parameter was given by ne × D, where D is the dimension of the problem. In DE, the population size was 50, the crossover constant CR was set to 0.8 and the scaling factor F was equal to 0.5. The optimization software was taken from Ref. [21] for ABC and Ref. [22] for DE. Both are freely available on the internet. The data resulting from each optimization run was analyzed using ROOT [23] based software.

The first test problem was the optimization of a single-channel parabolic neutron guide described by the guide length L and the entrance and exit heights h11 and h14. The parameters h12 and h13 were not adjusted individually during the runs. The entrance to sample position length was fixed to ~856 mm with a 30 mm gap between the inner and outer sections of the focusing guide centered around 591 mm. A rectangular divergence profile, filling the divergence up to m = 3, was used as input for the focusing guide. The m-value for the channels of the focusing guide itself was set to m = 4. The sample height was selected to be 10 mm. Following discussions with the IN5 instrument team, we have selected to optimize the performance of the multi-channel guide in the wavelength region of $6 - 6.5 \, \text{Å}$, i.e. where the flux starts decreasing and the resolution gets better [24]. In the current work, the wavelength of the neutrons was fixed to $\lambda = 6 \, \text{Å}$.

After setting the parameter boundary conditions, each optimization was carried out 30 separate times and the average best FOM values as a function of the number of guides evaluated were tabulated. The results are indicated in Fig 2. The FOM value represents the number of neutrons, divided by $10^5$, impinging on the target position for $10^6$ neutrons entering the guide. All three optimization methods converged to the same value. PSO reached a plateau the fastest followed closely by DE. The ABC method however required more guide evaluations to reach the same performance as the other two methods.

The second test problem was the optimization of a three-channel guide for the scenario described above and involved 20 free parameters. The 20 parameters included the heights h11, h12, h13, h14 and the length L describing the central channel, the vertical offsets g1, g2, g3 and heights h21, h22, h23, h24 of the outer channels, the angles φ12, φ22, φ23, φ24, the tilt angle φs, and the lengths Ls, Lt and Lb. In a similar fashion as above, after setting the boundary conditions...
Figure 2. Average best FOM values as a function of the number of single-channel guides evaluated. The three different optimization methods, as discussed in the text, are indicated by the different color lines.

A total of 30 independent optimization runs were carried out for each method. The average best FOM values are shown as a function of the number of guide evaluations in Fig 3. For the ABC method, the FOM value is given as a function of the average number of guides evaluated. The number of guide evaluations per iteration may be different between two independent optimization runs due to the restriction imposed by the limit parameter, as discussed in section 3.1. This number however only deviated by a maximum of 14 evaluations for a given iteration in all cases examined here. Interestingly, each of the three optimization methods approached different FOM values. ABC on average found guides with the highest performance followed closely by DE. Furthermore, the results suggest that additional improvements in performance could be reached with more ABC evaluations than indicated in the figure. DE was however able to reach its optimum on average much faster than ABC. PSO on the other hand had a tendency to find single-channel guides, and was unable to escape from the local optimum. While each method on average found different optima, the final FOM values in Fig. 3 differ by no more than 5% between the different methods.

An example of a guide optimized using the DE method is shown in Fig. 4. The left hand panel shows the final geometry settled on by the optimization algorithm and the right hand side shows the divergence of the focused beam averaged over the sample height with and without the focusing guide. The total gain in the number of neutrons at the sample position is a factor of 2.4. The gain in intensity is also accompanied with an increased divergence as indicated in the figure. The FOM used in the simulations purely maximizes the number of neutrons at the sample without considering the shape of the divergence profile. A penalty function taking into account the shape of the divergence profile or the beam missing the sample can also be introduced in the future in the software if desired. It can also be noted that the lateral shift in the position of the mirrors after the break in the optics in Fig. 4 fills out the region of phase space which would otherwise be unfilled due to the gap between the mirrors. Lastly, the three-channel guide shown in Fig. 4 outperforms the single-channel guide with ∼10% more neutrons.
arriving at the sample position. It can however be mentioned that a more detailed investigation of multi-channel guides, including wavelength dependence, number of channels and sample size, just to name a few, is the aim of future work.

4. Conclusion
To summarize, we have developed software for the optimization of multi-channel focusing guides for extreme sample environments. The software includes a Monte-Carlo calculation of the guide coupled to a number of different population-based optimization algorithms. In this work, we investigated the use of PSO, ABC and DE for this purpose. The optimization methods were compared against each other for two different guide designs. For a single-channel guide, it was found that PSO and DE on average performed the best while ABC required many more guide evaluations to reach the same performance. For a three-channel guide, it was however shown that ABC and DE on average found the best guide designs. PSO had a tendency to get stuck in the single-channel local optima. We found that the three-channel focusing guide offered the best performance, with a gain factor of 2.4 compared to no focusing guide, for the test case investigated in this work. These results also highlight the potential benefit of investigating several different optimization routines when designing focusing guides.

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Figure 4. The a) geometry for an example focusing guide and b) the divergence averaged over the sample height for the (solid line) focusing guide and (dashed line) without the focusing guide. The guide design was optimized using the DE method. The shaded regions shown in panel a) are supermirror-coated mountings. The solid vertical line represents the height of the 10 mm sample.