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Constraining neutron guide optimizations with phase-space considerations

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ABSTRACT

We introduce a method named the Minimalist Principle that serves to reduce the parameter space for neutron guide optimization when the required beam divergence is limited. The reduced parameter space will restrict the optimization to guides with a minimal neutron intake that are still theoretically able to deliver the maximal possible performance. The geometrical constraints are derived using phase-space propagation from moderator to guide and from guide to sample, while assuming that the optimized guides will achieve perfect transport of the limited neutron intake.

Guide systems optimized using these constraints are shown to provide performance close to guides optimized without any constraints, however the divergence received at the sample is limited to the desired interval, even when the neutron transport is not limited by the supermirrors used in the guide.

As the constraints strongly limit the parameter space for the optimizer, two control parameters are introduced that can be used to adjust the selected subspace, effectively balancing between maximizing neutron transport and avoiding background from unnecessary neutrons. One parameter is needed to describe the expected focusing abilities of the guide to be optimized, going from perfectly focusing to no correlation between position and velocity. The second parameter controls neutron intake into the guide, so that one can select exactly how aggressively the background should be limited.

We show examples of guides optimized using these constraints which demonstrates the higher signal to noise than conventional optimizations. Furthermore the parameter controlling neutron intake is explored which shows that the simulated optimal neutron intake is close to the analytically predicted, when assuming that the guide is dominated by multiple scattering events.

1. Introduction

The European Spallation Source [1] will be the first neutron source to utilize a long pulse design [2], and as the time structure favours long time of flight instruments [3,4], it has spawned a renewed interest in neutron guide design [5–9]. Recent findings suggesting novel moderator geometries with limited height [10] have yet again posed new challenges in guide design. Monte Carlo ray tracing techniques have been used for decades, starting with NISP [11] and later McStas [12–15], Vitess [16,17] and ResTrax [18], but it is only in recent years that the use of numerical optimizers [19,20] has become a standard tool of the trade. The optimizer will control parameters in the guide model, and run the underlying ray tracer for each step in order to maximize a particular figure of merit (FOM), often taken to be flux on sample within a wavelength interval.

This optimization technique caused guides to reach new performance levels, and it became relevant to compare the quality of the beam with the theoretical maximum, which can be described using Liouville's theorem [21]. The so-called brilliance transfer [22] is bounded between zero and unity, and expresses the ratio of phase-space density at the moderator and sample for a given closed phase-space volume. The requirement of a closed phase-space volume meant the FOM was changed to the neutron intensity within a fixed sample area, divergence interval, and wavelength interval.

Unfortunately, guides designed using numerical optimizers in this way are only guaranteed to provide a high neutron brilliance, not a low background. A neutron source generates a large number of high energy particles that can only be suppressed by large quantities of shielding, but the typical unrestrained solution from the optimizer would have an abnormally large guide entrance near the moderator, which allows also a large amount of these particles to enter the guide system. In addition, the improved transport efficiency of these guides allows for a high number of thermal

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neutrons transported that does not contribute to the FOM, and thus becomes a secondary source of background close to the neutron instrument. In addition it was observed that running the same optimization several times would give rise to very different guide geometries with strikingly similar performance, making it prudent to optimize the same guide geometry several times in order to get a solution with reasonable background characteristics.

The long term solution to these problems is obviously to include detailed background simulations in the Monte Carlo ray tracing simulation of each guide [23,24] in the optimization procedure, but as this requires unrealistic amounts of computing power and considerable amounts of specialized code for every guide geometry, a simpler solution is highly relevant.

We here propose a principle where analytical calculations on the propagation of phase-space volumes using acceptance diagrams [25] are used to constrain the optimizer to guides with a reasonable balance between neutron intake and the ability to reach a brilliance transfer of unity. This is done by considering propagation from the moderator to the guide, and from the guide to the sample. Inside the guide, it is assumed the optimizer will find a solution that transports the entire neutron intake to the end of the guide. The balance between background reduction and performance can be tuned using two control parameters with intuitive meanings, instead of manually scanning e.g. the entrance dimensions of the guide. We show that this method will effectively reduce the parameter space of the optimizer to guides with minimal background, still potentially able to reach a brilliance transfer of unity. Hence we call the method the “Minimalist Principle” (MP).

This describes the ideas necessary for understanding the MP before deriving it, and then show examples on guides optimized under varying circumstances to highlight the benefits of this alternative method for guide optimization.

2. Reasoning behind the Minimalist Principle

It follows from Liouville's theorem that the phase-space density at the sample cannot exceed that of the phase-space density near the moderator. If one requires a neutron beam described by a closed phase-space volume, it follows that there is a maximum possible neutron flux in this phase-space volume. This limit is the foundation of the MP, as there is a point where additional neutron intake cannot possibly contribute to the brilliance transfer.

When optimizing a guide system with the FOM chosen as the number of neutrons in such a phase-space volume, there is a corresponding maximum FOM. It is of interest to find a guide which delivers a FOM close to this maximum, but it is also important to limit the potential background from the neutron source. The background can be split into high energy particles that should be absorbed by shielding, and unwanted cold and thermal neutrons are to be reflected by the neutron mirrors. The high energy background is not taken into account in this paper, but is expected to be handled by choosing a guide geometry that allows sufficient shielding between moderator and sample.

In the MP, geometrical constraints on the guide geometry are designed to minimize the background from unnecessary cold and thermal neutrons. This is done by only transporting the neutrons necessary to fully illuminate the FOM phase-space volume. In order to calculate which neutrons are necessary, the phase-space volume corresponding to the FOM is propagated from the sample back to the end of the guide by acceptance diagrams. This yields the phase-space volume the guide should be able to deliver, and as this volume has a certain spatial width, the dimensions of the end of the guide can be determined, which is the first important constraint.

As it is theoretically possible for a guide to transport a phase-space volume without increasing its size or decreasing its phase-space density, the size of the phase-space volume that enters the guide should be at least equal to the size of the phase-space volume that the guide must deliver. If the size of the incoming phase-space volume is smaller than needed, it is not possible to reach the maximum FOM. By providing the guide with a phase-space volume of the same size as the one it has to deliver, the optimal brilliance transfer should be achievable. Increasing the incoming phase-space volume at this point would only increase the background if a perfect brilliance transfer is already achieved. As the incoming phase-space volume size depends on the size of the guide entrance, the distance to the source and the source dimensions, this requirement results in a constraint on these parameters.

A guide that only delivers the exact phase-space volume needed to evenly illuminate the sample is considered truly focusing. Such guides exist, for example the Selene guide system as described in [26]. A truly focusing guide will work through single reflections per guide element, because multiple reflections will destroy the necessary perfect correlations in phase-space.

Most guide designs rely on multiple reflections. Even a perfect elliptical guide will have large amounts of the intensity from this process for anything but point sources [8]. An ideal multiple reflecting guide is assumed to have a divergence distribution that is independent of position, or at least a weaker correlation than that of a truly focusing guide. Without the focusing ability, the delivered phase-space needs to be larger than for a focusing guide in order to cover the FOM. The exact size of this larger phase-space volume is again derived using acceptance diagrams.

Guides designed using the MP constraints have a more direct control over the outgoing divergence, which will be limited to the divergence limits of the FOM in the case of a perfect guide. In practice there will be unwanted neutrons at higher divergences than requested on some parts of the sample, but very limited in comparison to a guide optimized without any constraints. In addition, the amount of neutrons entering the guide is as low as possible, under the condition that the guide is still theoretically able to achieve the maximum possible FOM. This causes lower neutron losses along the guide than traditional geometries, yielding a guide which is highly efficient in terms of neutrons delivered in relation to background generated from absorbing these neutrons either in the guide or near the sample. It will also reduce radiation damage on the supermirrors and necessary shielding along the guide.

3. Derivation of the Minimalist Principle

In this section appropriate terminology and notation is introduced, followed by a derivation of the MP using acceptance diagrams.

3.1. Phase-space terminology

A phase-space is a space spanned by canonical variable pairs, here position and velocity are used [27]. The z direction is selected to be along the beam direction, and the 5 dimensional phase-space consists of $(x, y, \eta_x, \eta_y, \lambda)$ where the wavelength is often ignored as it does not change inside a neutron guide system. For a comprehensive description see [28]. When assuming rectangular cross sections of the guides, the x and y components are independent and the phase-space is split into two subspaces, (x, η_x) and (y, η_y). A closed set in a space is referred to as a phase-space volume. The size of a phase-space volume is defined to be the volume of this