Optimization of virtual source parameters in neutron scattering instrumentation

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Abstract. We report on phase-space optimizations for neutron scattering instruments employing horizontal focussing crystal optics. Defining a figure of merit for a generic virtual source configuration we identify a set of optimum instrumental parameters. In order to assess the quality of the instrumental configuration we combine an evolutionary optimization algorithm with the analytical Popovici description using multidimensional Gaussian distributions. The optimum phase-space element which needs to be delivered to the virtual source by preceding neutron optics may be obtained using the same algorithm which is of general interest in instrument design.

1. Introduction
Inelastic neutron scattering provides a versatile method for investigations of single crystal excitations. To overcome the intensity limits of the technique focusing by either supermirror neutron optics, crystal optics or a combination of both is applied in state-of-the-art neutron scattering instrumentation. The latest generation three-axis spectrometers (TAS) consequently seeks to employ monochromators which do not only focus in the vertical direction but also horizontally [1-4]. The basic idea is to increase intensity per area and per unit energy by imaging a well defined aperture onto the sample, known as the virtual source concept. Although the principle is quite general and can be used in either diffractometers or spectrometers, here we consider the situation in the particular context of TAS where energy resolution is crucial.

Since beam monochromaticity, wave-vector resolution and intensity depend on a sizable number of parameters, namely on the absolute wave vector as well as on the virtual-source size, the horizontal curvature, the crystal mosaic, the geometrical dimensions of the monochromator setup and the sample size, it is advantageous to have an optimization routine at hand suggesting best performance to the experimenter. Here we report on the implementation of an evolutionary algorithm applied to a generic virtual source setup and present selected optimization results.

In particular we consider three different optimization tasks: (1) Given a built TAS with a limited number of variable parameters, what is the optimum choice of instrument parameters for given constraints on energy or wave-vector resolution? (section 4), (2) Given a defined divergence at the virtual source, fixed sample size and given wave vector, what is an optimum set of parameters for instrument design? (section 5) and (3) Given a typical sample size and fixed wave vector, what is the optimum phase-space element which needs to be delivered to the virtual-source setup? (section 6).
2. Virtual source model

We reduce the primary spectrometer part of a TAS to a generic virtual source setup consisting only of: a slit, a focussing PG(002) monochromator and a sample. As a major simplification we consider the horizontal dimension only. This is legitimate since vertical and horizontal resolution entirely decouple for practical means.

Strict monochromatic and simultaneously spatial focusing using a crystal monochromator can only be achieved for either a divergent neutron beam emerging from a point-like source or a non-divergent beam emerging from a spatially extended source. The virtual-source concept is closest to the case where a point source is imaged onto a point-like sample although in practice finite spatial dimensions apply to the source and sample. The geometry of the virtual-source setup and the ideal radii of curvature are introduced in figure 1 for the symmetric Rowland geometry. More details on this model can be found in [5].

![Figure 1. Numerically calculated neutron trajectories for the symmetric Rowland geometry. Parameters are k_I = 1.55 Å⁻¹ and L₀ = 1.75 m. The red circle corresponds to the curvature of the lattice planes with R_C = 2.897 m. The green circle is the Rowland circle with radius R_G = R_C/2 which defines the ideal loci of reflection for the individual monochromator crystallites. Black lines are neutron trajectories incident on the PG(002) monochromator while blue lines are neutron trajectories Bragg reflected by the monochromator. Red lines are normal to the reflecting lattice planes of the local crystallites. The angular range covered is ±5°.]

Stoica [6] and Popovici [7] have given the normal approximation of the resolution function for a conventional TAS in a covariance matrix formalism as derived earlier by Cooper and Nathans [8]. By comparing to Monte Carlo simulations we have shown that the Popovici model is completely adequate to investigate the virtual source problem. This allows looking into optimization issues using the much faster analytical path which reduces computational time compared to Monte Carlo simulation.

To prove the adequacy of the Gaussian model of a virtual source primary spectrometer we have cross-checked intensity, spatial beam width, width in incident energy, width in transverse incident wave vector and correlation in wavelength and divergence as a function of horizontal curvature and incident wave vector k_I with the Monte Carlo simulation package McStas [9]. There are of course differences between the McStas model and the Popovici description, e.g. the Monte Carlo model is
more accurate since it does not rely on the Gaussian approximation except for the monochromator mosaicity. Slits have rectangular openings. Spatial monochromator parameters have rectangular dimensions with a sharp cutoff rather than Gaussian shapes. Also the McStas model is three-dimensional but we do not consider the vertical dimensions and effectively integrate over the vertical components. In the McStas component the thin crystal approximation is used while the Popovici description adopted allows for finite monochromator thickness. For both parameterizations of the monochromator the crystal surface is parallel to the lattice planes.

Figure 2. The intensity at the sample position as a function of the curvature parameter $\rho_{ML}$ for different virtual source width $w_0$ and sample width $w_S$. Red: $w_0 = 2$ cm, $w_S = 2$ cm; blue: $w_0 = 1$ cm, $w_S = 2$ cm; black: $w_0 = 1$ cm, $w_S = 1$ cm. Note that the intensity is not normalized to area! The lines are results of the numerical evaluation of the analytical Popovici expression.

Figure 3. Wavelength-divergence correlation plots for flat (left) and horizontally focussed monochromator (right) integrated over a sample width $w_S = 2$ cm. The color map data are simulation results using McStas. The black ellipses are derived from the Popovici model and are lines of constant probability 50%.
Despite the differences in the models, there is in general an excellent agreement between the simulated and the calculated results. An example for the intensity as a function of monochromator curvature is shown in figure 2. The agreement between the second moments of distributions obtained from the Monte Carlo model and the same quantities obtained from the Popovici description is found to be excellent. Naturally deviations from the Gaussian distributions are not covered by the Popovici description as is seen from the phase space elements shown in figure 3.

3. Evolutionary algorithm

Here we apply an evolutionary optimization routine, known as genetic algorithm [10, 11] which is sufficiently efficient for the 10-dimensional parameter space considered. We calculate the intensity at the sample position \( I_S \), the energy width \( \Delta E_S \) and the transverse wave vector width \( \Delta k_\perp \) perpendicular to \( k_I \) with Popovici’s approach. All optimization runs discussed here use genetic evolution parameters: 95% cross-over (the percentage of reproduction events), 2% mutation (the percentage of genes in next-generation instruments that mutate) and exclusivity 1 which is the number of best instruments kept unchanged for the next generation. These parameters are explained in detail in reference [11]. We run 20 generations with a population of 30 instrument configurations per generation which samples only about \( 10^{-4} \) of the total number of possible instrument configurations. The best instrument is chosen on the basis of best fitness, i.e. the maximum figure of merit.

4. Experiment parameter optimization

For practical TAS applications the simplest optimization task is met at a given spectrometer with only a reduced number of variable parameters. We ask for the optimum virtual source width and monochromator curvature giving maximum intensity under the boundary condition of a defined energy width or a defined wave-vector width. We assume that \( k_I \) is given by other boundary conditions e.g. the total energy transfer and the accessibility of the total wave-vector transfer \( Q \).

As an example we consider \( k_I = 1.55 \, \text{Å}^{-1} \) and a set of neutron optical components which effectively provides \( m = 5 \) divergence at the entrance of a virtual source slit which can be varied in the range \( 0.1 \, \text{cm} \leq w_0 \leq 3 \, \text{cm} \) (in steps of 0.1 cm). The monochromator width is \( w_M = 30 \, \text{cm} \), monochromator mosaic is \( \eta_M = 45' \). The distances from the virtual source to the monochromator \( L_0 =1.75 \, \text{m} \) and from the monochromator to the sample \( L_1 =1.75 \, \text{m} \) are chosen to be equal for the symmetric Rowland configuration. A standard sample size \( w_S = 2 \, \text{cm} \) is considered. Limiting the energy or wave-vector width to defined values is achieved by setting the figure of merit to zero for those instrument configurations which give unacceptable resolution. We grade instrument configurations with the figure of merit

\[
 f_I = \begin{cases} 
 0 & \text{if} \quad \Delta E_S, \Delta k_\perp > \Delta E_\text{limit}, \Delta k_\perp \text{limit} \\
 10^{10} \times I_S & \text{else} 
\end{cases}
\]  

thus maximizing intensity.

Table 1 and figure 4 (left) show the results of the optimization when imposing a limit on the energy width. While the curvature stays at its optimum value for a divergent point source, the virtual source width is reduced to meet the energy width required. The worst energy width achievable with the virtual source width limited to 3 cm is 0.091 meV. Energy widths below 0.055 meV cannot be reached and thus the optimization breaks down if \( \Delta E_\text{limit} \leq 0.055 \, \text{meV} \). The result of our series of optimization runs is that the energy resolution may be improved by a factor of 1.7 just by adapting the virtual source width while the intensity is reduced by a factor of 4.3. We note that with a flat monochromator \( \rho_M = 0 \) and fully open virtual source width \( w_0 = 3 \, \text{cm} \) the intensity is \( I_S = 11.23 \times 10^{-10} \) giving an energy width \( \Delta E_S = 0.091 \, \text{meV} \). This energy width cannot be further increased since it is essentially limited by the mosaic of the monochromator crystals and \( w_0 \).
Table 2 and figure 4 (right) give optimized parameters $w_0$ and $\rho_{MH}$ for a given limit on the transverse wave-vector width $\Delta k_3$. Clearly the virtual source width stays always at the maximum constraint while the curvature changes to adapt for the wave-vector width requested. Indeed, for $\Delta k_{3\text{limit}} = 0.060 \ \text{Å}^{-1}$ and $0.055 \ \text{Å}^{-1}$ the monochromator is overfocused. The worst wave-vector width achievable with the optimum focusing $\rho_{MH} = 0.34 \ \text{m}^{-1}$ is $0.1 \ \text{Å}^{-1}$. For wave-vector widths below $0.055 \ \text{Å}^{-1}$ the optimization breaks down. As a result of our optimization the wave-vector resolution may be improved by a factor of 1.83 just by adapting the monochromator curvature $\rho_{MH}$ while the intensity is reduced by a factor of 2.

### Table 1. Results of the instrument parameter optimization maximizing intensity given an energy resolution limit, $k_I = 1.55^\circ \ \text{Å}^{-1}$, $m=5$, $w_M = 30$ cm, $\eta_M = 45^\prime$, $w_S = 2$ cm.

| $\Delta E_{\text{limit}}$ (meV) | $w_0$ (cm) | $\rho_{MH}$ (m$^{-1}$) | $I_\sigma \times 10^{10}$ | $\Delta E_S$ (meV) | $\Delta k_3$ (Å$^{-1}$) |
|---------------------------------|-------------|------------------------|---------------------------|-------------------|------------------------|
| 0.100                           | 3.0         | 0.34                   | 17.9                      | 0.091             | 0.090                  |
| 0.080                           | 2.3         | 0.32                   | 13.8                      | 0.078             | 0.098                  |
| 0.060                           | 1.2         | 0.34                   | 7.3                       | 0.060             | 0.097                  |
| 0.055                           | 0.7         | 0.30                   | 4.2                       | 0.055             | 0.095                  |

### Table 2. Results of the instrument parameter optimization maximizing intensity given a transverse wave vector resolution limit $\Delta k_3$, $k_I = 1.55^\circ \ \text{Å}^{-1}$, $m=5$, $w_M = 30$ cm, $\eta_M = 45^\prime$, $w_S = 2$ cm.

| $\Delta k_{3\text{limit}}$ (Å$^{-1}$) | $w_0$ (cm) | $\rho_{MH}$ (m$^{-1}$) | $I_\sigma \times 10^{10}$ (a.u.) | $\Delta E_S$ (meV) | $\Delta k_3$ (Å$^{-1}$) |
|--------------------------------------|-------------|------------------------|----------------------------------|-------------------|------------------------|
| 0.120                                | 3.0         | 0.34                   | 17.9                            | 0.091             | 0.099                  |
| 0.080                                | 3.0         | 0.14                   | 14.5                            | 0.091             | 0.079                  |
| 0.060                                | 3.0         | 0.73                   | 10.1                            | 0.090             | 0.059                  |
| 0.055                                | 3.0         | 0.80                   | 9.0                             | 0.090             | 0.054                  |

5. Instrument design parameter optimization

We have also investigated the situation where the available phase space before the virtual source is known and consider instrument design optimization with fixed parameters: $k_I = 1.00 \ \text{Å}^{-1}$, $1.55 \ \text{Å}^{-1}$, $3.70 \ \text{Å}^{-1}$, $L_0 = L_1 = 1.75 \ \text{m}$, $w_S = 2 \ \text{cm}$, monochromator crystal thickness $t_M = 2 \ \text{mm}$ and variables to be optimized: virtual source width $w_0$, monochromator width $w_M$, crystal mosaic $\eta_M$ and curvature $\rho_{MH}$. Each variable can take discrete values with $0.1 \ \text{cm} \leq w_0 \leq 3 \ \text{cm}$ (in steps of 0.1 cm), $1 \ \text{cm} \leq w_M \leq 50 \ \text{cm}$ (in steps of 1 cm), $5^\prime \leq \eta_M \leq 60^\prime$ (in steps of 1'), $0 \ \text{m}^{-1} \leq \rho_{MH} \leq 1.0 \ \text{m}^{-1}$ (in steps of 0.01 m$^{-1}$). Thus the parameter space consists of $8.5 \times 10^6$ instrument configurations. We have considered four different cases for the divergence in front of the virtual source slit: small divergence ($^{60}$Ni neutron guide), medium ($m=3$ neutron guide) or larger $m=5$, $m=7$ (as is the case for e.g. elliptically tapered guide sections).
We wish to maximize the intensity at the sample position $I_S$ and minimize the energy width $\Delta E_S$ of the neutron beam at the sample and define the dimensionless figure of merit

$$f_S = 10^{10} \times I_S + \frac{1}{100} \times \frac{\text{meV}}{\Delta E_S}. \quad (2)$$

Since $I_S$ is on the order of $10^{-10} - 10^{-9}$ and $\Delta E_S$ is on the order of 0.01 meV (at $k_I = 1.0 \text{ Å}^{-1}$) this choice of prefactors ensures that the individual terms are roughly the same order of magnitude. Results are summarized in Table 3.

The optimum mosaic $\eta_M$ ranges between 51 and 60 arcmin throughout the whole wave-vector range considered indicating little sensitivity to this parameter in agreement with our analytical results on the intensity as a function of $\eta_M$. The optimum mosaic value is also in agreement with extended Monte Carlo simulations performed for the upgrade of the cold triple axis spectrometer FLEX [4]. The optimized monochromator curvature is found to be close to the theoretical curvature appropriate for a divergent point-source $\rho_{\text{MH}} = 0.53 \text{ m}^{-1}, 0.35 \text{ m}^{-1}, 0.14 \text{ m}^{-1}$ for $k_I = 1.00 \text{ Å}^{-1}, 1.55 \text{ Å}^{-1}, 3.70 \text{ Å}^{-1}$ respectively. Interestingly for the smallest divergences incident on the virtual source the optimum monochromator curvature is found slightly smaller. This is expected as the optimum monochromator curvature $\rho_{\text{MH}}$ depends on the divergence and is reduced by a factor 2 in the limit of a non-divergent beam as can be derived easily from geometrical optics.

For all wave vectors and independent of the incident divergence the virtual source width $w_0$ is found to be the maximum allowed (constrained to 3 cm). The monochromator width $w_M$ is also found to be the maximum allowed (constrained to 50 cm). One cannot expect the optimization to find balanced values for monotonic parameters where the maximum figure of merit is at the end of the allowed parameter range. For such parameters we suggest to "optimize" by defining an acceptance level for the figure of merit.

The intensity at the sample varies within a factor of 50 ($I_S = 1.5 \times 10^{-10} \ldots 7.6 \times 10^{-9}$) while the energy width at the sample varies by a factor of $\sim 150$ ($\Delta E_S = 10 \mu\text{eV} \ldots 1.5 \text{ meV}$). As a result of the optimization the energy resolution is essentially independent of the incident divergence while the intensity scales linearly with the incident divergence at the expense of transverse wave vector resolution $\Delta k_L$.
Table 3. Results of the instrument design optimization based on the figure of merit $f_2$. Incident divergence and $k_l$ are fixed input parameters, while $\eta_M$ and $\rho_{MH}$ are optimized parameters.

| Incident divergence | $k_l$ ($\text{Å}^{-1}$) | $\eta_M$ (arcmin) | $\rho_{MH}$ (m$^{-1}$) | $I_s \times 10^{10}$ (a.u.) | $\Delta E_S$ (meV) | $\Delta k_0$ ($\text{Å}^{-1}$) | $f_2$ |
|---------------------|-------------------------|-------------------|------------------------|--------------------------|------------------|-----------------------------|------|
| $^{58}\text{Ni}$   | 1.0                     | 60                | 0.42                   | 1.47                     | 0.011            | 0.022                       | 2.4  |
| m=3                | 1.0                     | 56                | 0.47                   | 3.62                     | 0.011            | 0.045                       | 4.5  |
| m=5                | 1.0                     | 53                | 0.53                   | 5.76                     | 0.011            | 0.070                       | 6.7  |
| m=7                | 1.0                     | 57                | 0.51                   | 7.53                     | 0.011            | 0.090                       | 8.5  |
| $^{58}\text{Ni}$   | 1.55                    | 60                | 0.26                   | 5.19                     | 0.092            | 0.043                       | 5.3  |
| m=3                | 1.55                    | 60                | 0.33                   | 12.83                    | 0.092            | 0.074                       | 12.9 |
| m=5                | 1.55                    | 51                | 0.34                   | 20.25                    | 0.092            | 0.111                       | 20.4 |
| m=7                | 1.55                    | 60                | 0.34                   | 26.72                    | 0.092            | 0.142                       | 26.8 |
| $^{58}\text{Ni}$   | 3.70                    | 55                | 0.08                   | 14.75                    | 1.500            | 0.198                       | 14.8 |
| m=3                | 3.70                    | 54                | 0.13                   | 36.41                    | 1.500            | 0.242                       | 36.4 |
| m=5                | 3.70                    | 52                | 0.16                   | 57.33                    | 1.500            | 0.305                       | 57.3 |
| m=7                | 3.70                    | 59                | 0.16                   | 75.84                    | 1.500            | 0.368                       | 75.8 |

6. Optimum phase space tailoring

For instrument design the most important question is: what is the optimum phase-space element which needs to be delivered to the virtual source? Modern neutron optics provides an elegant solution to manipulate the phase-space area at the virtual-source section while increasing intensity in the center of the slit. Combining a neutron guide with a converging section in the horizontal dimension allows spatial compression at the expense of increase in divergence, e.g. elliptical or parabolic compression [12,13]. The basic idea here is to ensure that the phase space element transported through the neutron guide system can actually be used at the sample position. We define an extended figure of merit

$$f_3 = 10^{10} \times I_s + \frac{1}{100} \times \frac{\text{meV}}{\Delta E_S} + \frac{1}{100} \times \frac{\text{rad}}{\gamma_0}$$

aimed at maximizing the intensity at the sample $I_s$, minimizing the width of the energy spectrum at the sample $\Delta E_S$ and keeping the divergence $\gamma_0$ before the virtual source as minimal as possible. In addition $\Delta k_0$ can be minimized by using a velocity selector which pre-limits the width of the spectrum incident on the virtual source to reduce background.

We assume that the area of the phase space element $k_l \gamma_0 w_0$ before the converging section is constant and is equal to the area equivalent to an $m = 2.5$ guide with width $w_0 = 6$ cm. Thus, assuming a square distribution the divergence has a variance

$$\gamma_0 = \frac{1.1296 \times 10^{-3}}{w_0 [m] k_l [\text{Å}^{-1}]}$$

Any decrease in spatial width requires an increase in divergence due to Liouville’s theorem. We have allowed the virtual source width to vary in the range of 0.1 cm $\leq w_0 \leq$ 12 cm (in steps of 0.1 cm). Note that a source width above 6 cm would actually mean a spatially expanding beam with reduced divergence relative to m=2.5. The monochromator mosaic and curvature are allowed to vary within 5’ $\leq \eta_M \leq$ 60’ (in steps of 1’) and 0 m$^{-1}$ $\leq \rho_{MH} \leq$ 1.0 m$^{-1}$ (in steps of 0.01 m$^{-1}$). The monochromator width is kept fixed at $w_M = 30$ cm. Under these conditions we find a virtual source width which is 4 cm at
the highest wave vector considered \((k_I = 3.70 \text{ Å}^{-1})\), i.e. moderate beam compression is required corresponding to \(m = 3.75\) after the converging neutron optical section.

Our optimizations find the minimum virtual source width allowed \((w_0 = 1 \text{ mm})\) to be optimal at small wave vector and small sample size, however leading to a large, technically not achievable effective supermirror \(m\). The explanation can be found when considering the figure of merit as a function of virtual source width. At the smallest virtual source width the figure of merit has a global maximum since it is dominated by the \(1/\Delta E_S\)-term. We emphasize that great care is needed in defining the figure of merit. We note that a threshold on intensity or a limit on the effective \(m\)-coating gives the solution \(w_0 = 4 \text{ cm}\) for all wave vectors suggesting rather modest beam compression to be optimal.

7. Conclusions

We have investigated optimization of instrument parameters for a generic virtual source setup employing an evolutionary algorithm. As the combination of virtual source width and monochromator curvature gives additional flexibility to tune the energy and wave-vector resolution in order to match the instrument properties to a particular experiment it is desirable to have an optimization routine at hand suggesting best performance.

We have adopted Popovici’s analytical approach for a fast evaluation of the quantities of interest: intensity and resolution. Comparison to Monte Carlo simulation proves adequate accuracy. Most useful for the experimenter is the routine to identify instrument parameters required to achieve a particular resolution either in energy or in wave vector.

We have also applied the optimization routine to instrument design tasks. Independent of incident wave length we find the optimum PG002 mosaic at values which are conventionally in practical use for horizontally flat monochromators. In addition we have applied the algorithm to identify the optimum phase-space element to be delivered to the virtual source and found moderate compression ratios of 1.5 optimal for medium size samples. Smaller sample sizes and higher neutron energies require higher compression ratios.

Our study of the optimization problem has drawn our attention to a few general insights applicable to any optimization problem. The genetic algorithm works best on parameters which show a maximum within the parameter range as is seen with the monochromator curvature in our case. One cannot expect the optimization to find balanced values for monotonic parameters where the maximum figure of merit is at the end of the allowed parameter range. For such parameters it is best to “optimize” by defining an acceptance level for the figure of merit. In general, the definition of the figure of merit is crucial and the optimum parameters depend sensitively on the weight that a particular instrument property is given.

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