

# Neutron-Use Optimization with Virtual Experiments to Facilitate Research-Reactor Conversion to Low-Enriched Fuel

Alexander Glaser<sup>1</sup> and Uwe Filges<sup>2</sup>

<sup>1</sup>Program on Science and Global Security, Princeton University, Princeton, NJ, USA

<sup>2</sup>Laboratory for Developments and Methods, Paul Scherrer Institute, Villigen, Switzerland

Converting research reactors from highly enriched uranium (HEU) fuel to more proliferation-resistant low-enriched fuel is critical for achieving the objective of ending the use of directly weapon-usable materials in the civilian nuclear fuel cycle. The most challenging type of reactors to convert are high-flux research reactors, which, along with upcoming strong spallation sources, are the most important neutron sources for sophisticated neutron scattering experiments. Advanced Monte-Carlo computer codes are now available that make it possible to track neutrons from the neutron source, through neutron guides, to the detector of a neutronic experimental setup, including realistic samples. These “virtual experiments” allow optimizing the performance of complete beamlines, where in many cases a large unused potential exists for increasing the neutron flux at the sample or detector position. The Monte-Carlo codes VITESS and McStas are used to compare results for typical neutron scattering setups using typical versus state-of-the-art technologies. The analysis shows that performance gains due to instrument upgrades or neutron guide renewals can dwarf potential neutron flux losses due to conversion to low-enriched fuel. Combined convert-and-upgrade strategies therefore offer unique opportunities for reactor operators and neutron scientists to significantly improve the overall performance of research facilities, and turn them into centers of excellence, while supporting the objective of phasing out the use of highly enriched uranium in the civilian nuclear fuel cycle as soon as possible.

---

Received 28 February 2012; accepted 29 June 2012.

Alexander Glaser would like to thank Franz Fujara, Darmstadt University of Technology, who first mentioned the possibility of instrument upgrades, which would more than compensate for any loss in neutron flux resulting from a conversion of a research reactor to low-enriched fuel.

Address Correspondence to Alexander Glaser, 221 Nassau St., Fl. 2, Princeton, NJ 08542, USA. E-mail: aglaser@princeton.edu

## BACKGROUND

International efforts to convert research reactors that are fueled with weapon-grade highly enriched uranium (HEU) to non-weapon-usable low-enriched uranium (LEU, less than 20 percent uranium-235) fuel have been pursued since the late 1970s,<sup>1</sup> but intensified significantly since 2002. Also, following the proposition of U.S. President Obama to “secure all vulnerable nuclear material around the world within four years,”<sup>2</sup> a series of high-level nuclear security summits has been convened since 2010. One central area of attention of these summits is to track progress toward the goal of converting HEU-fueled research reactors to low-enriched fuel.<sup>3</sup> Overall, twenty-one countries have been cleaned out of HEU as of 2011, that is, all local research reactors converted to low-enriched fuel and the associated fresh and spent fuel returned to the original supplier country.<sup>4</sup> The accomplishments so far could be neutralized, however, with the startup of only a few new high-power HEU-fueled research reactors, which would offset prior demand reductions for HEU significantly.<sup>5</sup>

As part of the international conversion efforts, new high-density low-enriched fuels are now under development and could be qualified within the next few years. These fuels will offer an unprecedented opportunity to end the use of HEU in the civilian nuclear fuel cycle entirely. Even the remaining HEU-fueled high-flux reactors, which are the main facilities used for neutron-scattering science today and account for about half of the total civilian HEU demand worldwide, could then use low-enriched fuel.<sup>6</sup> These reactors are difficult to convert because they have very compact cores with a high surface-to-volume ratio, which maximizes neutron leakage from the core and therefore makes these neutrons available for experiments, but also requires a high uranium-235 content to achieve criticality.

When transitioning from HEU to LEU, however, reductions of the neutron flux on the order of 10–15 percent are sometimes inevitable—especially if the original reactor was designed for HEU, and modifications of the core design are limited.<sup>7</sup> The criteria proposed by the International Nuclear Fuel Cycle Evaluation (INFCE) in 1980 emphasized that “*neither any loss in the overall reactor performance (e.g., flux per unit power) nor any increase in operation costs should be more than marginal.*”<sup>8</sup> Predictably, arguments in favor or against conversion of a particular facility often revolve around what constitutes an acceptable “marginal” loss of scientific usability of a reactor.

The maximum neutron flux near the reactor core, however, is only one quantity to characterize facility performance. What ultimately matters to neutron scientists is the effective neutron intensities at the sample and the detector positions. Optimizing these values is a complex process because the multi-parameter space of a full beamline characterization cannot be solved by analytic calculations. So-called “virtual experiments” are a vital new tool to guide this process.<sup>9</sup> In this article, we argue that virtual experiments can—and

should—also play an important role in evaluating convert-and-upgrade strategies for research reactors that can support an optimal allocation of the unused neutronic potential of a facility when transitioning to a new fuel.

## Virtual Experiments with Monte Carlo Ray-Tracing Codes

Virtual experiments model the path of the neutrons starting from a source, for example the surface of the cold neutron source near the core of a research reactor, through a neutron guide to the detector system of a neutron scattering instrument including realistic samples.<sup>10</sup> These virtual experiments play an increasingly important role in designing and optimizing modern neutron-scattering instruments.<sup>11</sup>

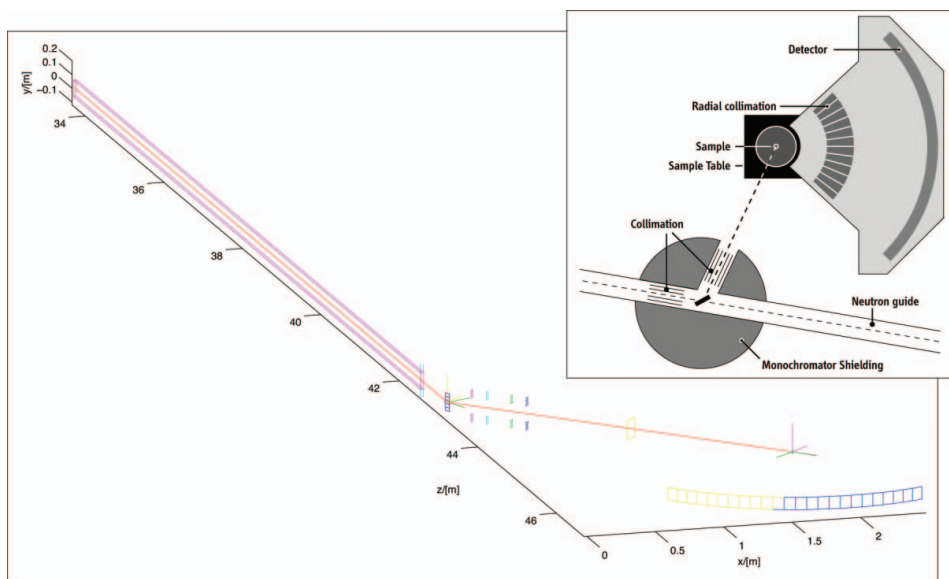
The results presented below are based on simulations with McStas (Monte Carlo Simulations of Triple Axis Spectrometer) and VITESS (Virtual Instrumentation Tool for the ESS), which are both Monte Carlo neutron ray-tracing codes for neutron scattering instruments at pulsed and continuous neutron sources.<sup>12</sup>

The software package McStas is a complex software tool for simulating various types of neutron scattering instruments. The package is being developed by a core developer team at DTU Physics (formerly RISØ National Laboratory), University of Copenhagen, Paul Scherrer Institute, and *Institut Laue-Langevin*.<sup>13</sup> Recent versions of McStas offer on the order of one hundred predefined components, which can be updated and extended by the user. The package is based on a meta-language, which has been specially written for neutron simulations and is automatically translated into ANSI-C code. McStas is available for all major operating systems and widely accepted by the neutron scattering community, as evidenced by calculated results reported in a long list of publications.

The VITESS Monte Carlo package is maintained at the *Helmholtz Zentrum Berlin* in the framework of the ESS Spallation Sources project.<sup>14</sup> VITESS has the same functionality as McStas and features a fully modular structure. Each module works as an executable individual program, reading output data from the preceding module and writing the neutron trajectories into a pipe for the following module. As with McStas, VITESS is available for all major operating systems and has been used for Monte Carlo simulations of all classes of instruments, including different beam extraction/guide systems.

## Benchmarking a Virtual Experiment

As an example of a full virtual experiment, and how it compares to experimental data, we have analyzed the cold neutron powder diffractometer DMC at the spallation source SINQ using the complex powder sample  $\text{CeRh}_2\text{Ge}_2$ .<sup>15</sup>



**Figure 1:** Basic design of DMC and the McStas model (color figure available online).

The DMC is a flexible instrument with 400 sensitive boron trifluoride ( $\text{BF}_3$ ) detectors, with an angular separation of  $0.2^\circ$ , allowing for simultaneous measurements within a scattering angle range of  $80^\circ$ . The wavelength range is  $2.3 \text{ \AA}$  to  $6.5 \text{ \AA}$ . Figure 1 shows the basic design of the DMC and the corresponding McStas model, which tracks neutrons from the cold neutron source through a 42.5-meter long neutron guide and through all other components of the instrument to the detector.

Using this model, a real measurement on DMC has been compared with a McStas Monte Carlo simulation. The results are in excellent agreement and shown in Figure 2. The comparison has been done for nine Bragg reflection peaks, including symmetrically equivalent reflections. The used wavelength was  $2.457 \text{ \AA}$ . The simulated values are normalized to the maximum count-rate of the measurement, which is observed for the Bragg peak at  $72.65^\circ$ . The comparison shows that peak position, relative peak height, and peak resolution all agree extremely well. It should be mentioned that several Bragg peaks overlap. The peak at  $79.15^\circ$ , for example, contains two Bragg reflections. This overlapping was also correctly reproduced in the simulation.

In summary, this comparison between the simulation and the experimental data demonstrates how powerful and accurate virtual experiments are today. They have become a valuable tool for designing and optimizing new neutron instruments and beamlines—and are also the starting point for upgrade investigations of instrument components.

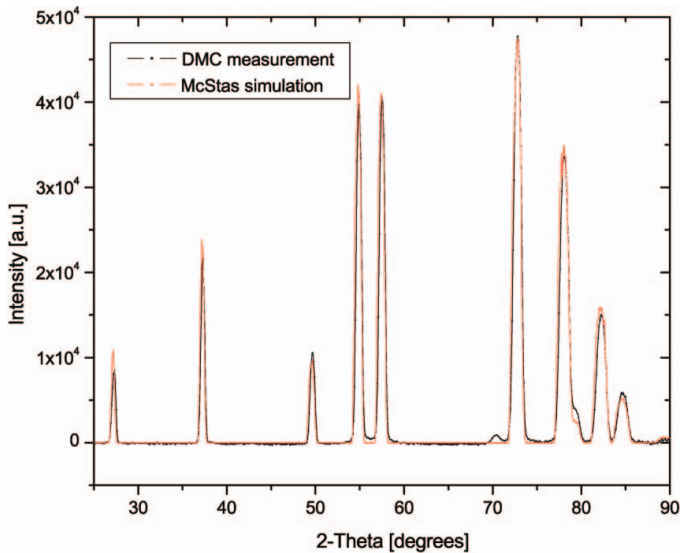


Figure 2: Comparison of simulated and measured data (color figure available online).

## Neutron Guide Investigations

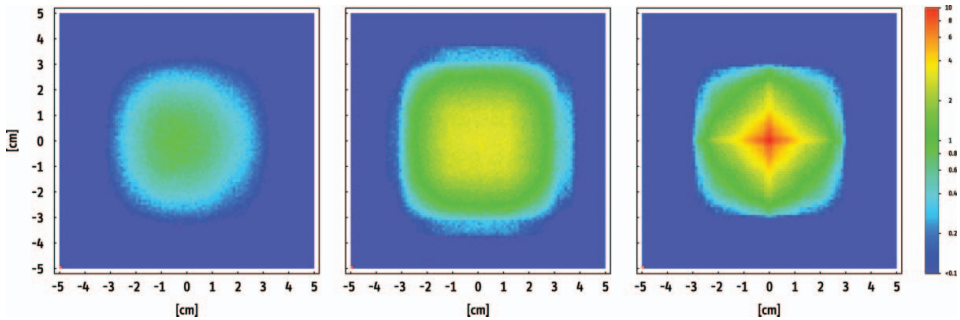
The simulation of generic and rather simple VITESS/McStas setups is sufficient to demonstrate the potential of guide upgrading because only the effectiveness of propagating neutrons through the guide is of interest here.

As the reference source for these simulations, we use the wavelength spectrum at the outer surface of the cold neutron source H5 of the High-Flux Reactor at ILL.<sup>16</sup> The neutrons enter the guide at a distance of 200 cm from the source. The guide-module then simulates the neutron flight-path through the mirrored guide, calculating the intensity loss for each reflection as a function of the neutron wavelength, reflectivity behavior of the supermirror guide, and incident angle.

We explore two basic options to optimize cold-neutron propagation through the guide: standard ballistic supermirrors and innovative (elliptic) neutron-guide geometries.<sup>17</sup> Simulation parameters and conditions at the front-end of the setup, that is, from the source to the guide entrance, remain unchanged in all cases. The neutron wavelength and spatial intensity distribution of the neutron beam (as illustrated in Figure 3) are then monitored at several distances from the exit of the guide.

### *Standard Ballistic Supermirrors Guides*

To improve propagation of neutrons through a guide, the critical angle for total reflection has to be as large as possible. In general, this angle is given by:



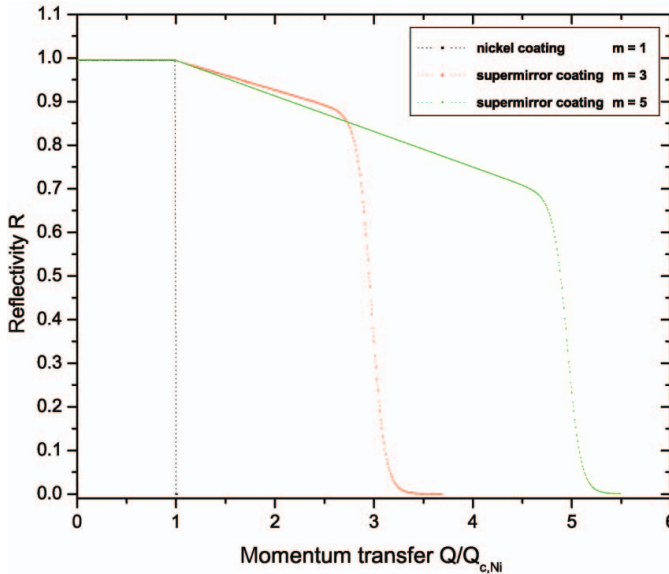
**Figure 3:** Spatial intensity distributions for selected supermirror coatings and guide geometries. These illustrative results are for a standard guide with  $m = 1$  (left), for a standard guide with  $m = 3$  (center), and for an elliptical guide with  $m = 3$  (right). The maximum intensities in arbitrary units are 0.9, 3.2, and 10.0, respectively. Shown are the planes of best focus behind the exit of a reference guide with a total length of 35 m (color figure available online).

$$\theta_c(\lambda) = \sqrt{\frac{Nb}{\pi}} \lambda.$$

Here,  $N$  is the number density and  $b$  the scattering length of the isotope. For natural nickel, the element with highest value for  $Nb$ ,  $\theta_c(\lambda) \approx 0.099^\circ \lambda(\text{\AA})/\text{\AA}$ . Supermirrors increase the effective critical angle through a large number of thin, depth-graded bilayers of two materials with high scattering contrast, for example nickel and titanium.<sup>18</sup> The performance of a supermirror is usually characterized by its  $m$ -value, which specifies the resulting critical angle compared to natural nickel, expressed as the ratio of respective momentum transfers ( $m = Q/Q_{\text{crit}(\text{Ni})}$ ). For a complete description, the reflectivity as a function of incident angle or momentum transfer has to be known. Some reflectivity files used for the simulations are shown in Figure 4.<sup>19</sup>

To demonstrate the impact of supermirror technology, we model a standard guide with a square cross-section of  $10 \times 10 \text{ cm}^2$  and a length of 30 m,<sup>20</sup> followed by a linearly tapered focusing guide of 5-meter length and an exit-window of  $5 \times 5 \text{ cm}^2$ . The 30-meter guide has a slight horizontal curvature with a radius of 2500 m to avoid a direct view on the source, which reduces the fast-neutron background at the exit and sample position.

The main results for this guide are shown in Figure 5. As expected, relative neutron intensities increase across all relevant wavelengths with increasing  $m$ -values. Compared to the standard nickel coating, the most significant improvement is observed for  $m = 2$ . Higher  $m$ -values further improve the performance of the guide, but the intensity gain is stronger for short wavelengths. For example, at 2  $\text{\AA}$ , the guide with  $m = 3$  yields a more than 3.5-fold increase in neutron intensity compared to  $m = 2$ . For wavelengths above 4  $\text{\AA}$ , neutrons are still propagated with a gain of about 50 percent. In



**Figure 4:** Reflectivity curves used for VITESS/McStas simulations: natural nickel coating and supermirror coatings with  $m = 3$  and  $m = 5$ . Coatings up to  $m = 7$  are currently under development. Theoretical reflectivity curves (as shown and used here) and experimental data are generally in excellent agreement (color figure available online).<sup>19</sup>

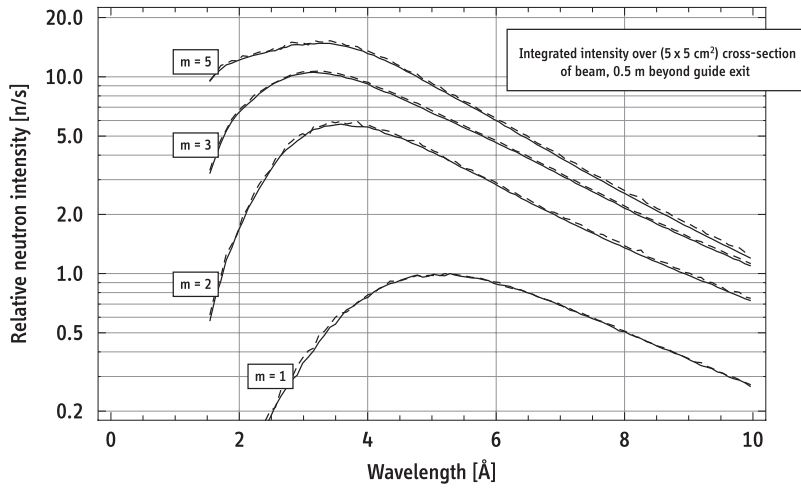
addition, Figure 5 also shows the intercomparison between VITESS and McStas. The nearly perfect agreement of the data demonstrates that both packages are suitable tools for neutron-guide evaluations.

### *Innovative Guide Geometry*

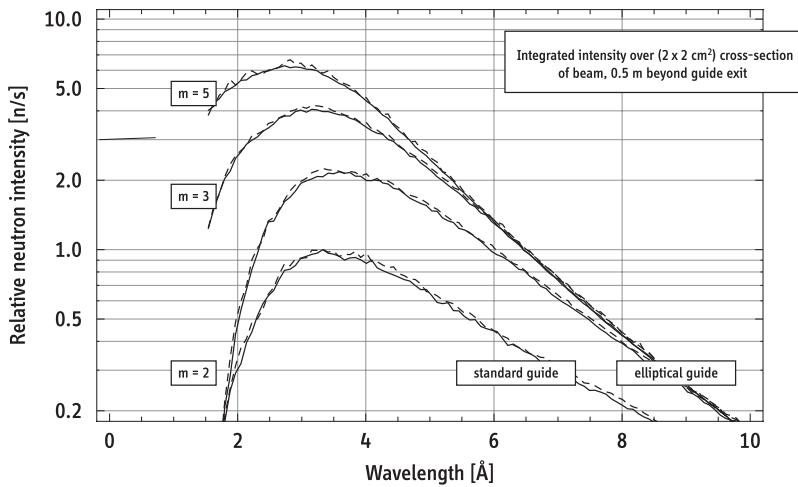
Traditional neutron guides are characterized by a rectangular shape. The concept of the so-called ballistic guide was first introduced in the 1990s and recently has been developed further with elliptical/parabolical guide geometries, which minimize the total number of neutron-reflections along the flight path.<sup>21</sup> Here, we use an elliptical guide with entrance and exit dimensions of  $10 \times 10 \text{ cm}^2$  and  $5 \times 5 \text{ cm}^2$ , respectively. The focal points are about 200 cm in front of the entrance, that is, very close to the neutron source, and 50 cm beyond the exit. The overall length of the guide is 35 m, its maximum width about 21.8 cm.

As shown in Figure 3, one distinctive feature of the elliptical guide is the strong focusing of the neutrons compared to standard guides—generally an important advantage for typical sample sizes. To account for this effect, the neutron intensity is not averaged over the entire cross-section of the beam, as done previously, but integrated over the central region of the beam only.

Figure 6 shows the relative neutron intensity as a function of neutron wavelength and again an intercomparison of VITESS and McStas simulations. It compares a traditional neutron guide with  $m = 2$  and fixed cross-section,



**Figure 5:** Comparison for the standard guide and various supermirror coatings ( $m = 2-5$ ) relative to ordinary nickel coating using VITeSS (- -) and McStas (—).



**Figure 6:** Comparison of relative neutron intensities for standard and elliptical guide geometries. Intensity is integrated over  $A^* = 2 \times 2 \text{ cm}^2$  in the center of the beam and taken at 0.5 m after the guide exit. For comparison, results obtained with VITeSS (- -) and McStas (—) are shown.



which is the standard today at modern facilities, with an elliptical guide using several advanced supermirror coatings.

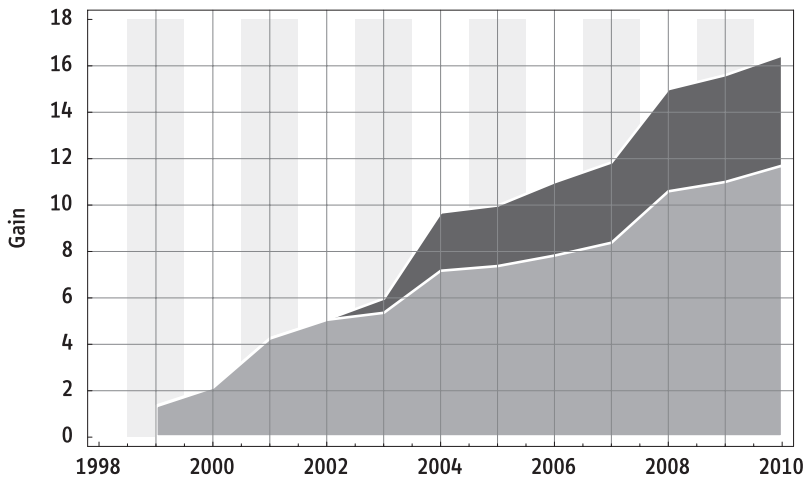
Most significantly, the elliptical guide configuration with  $m = 2$  delivers a gain factor of two for all wavelengths above  $3 \text{ \AA}$  against the standard guide, which is primarily due to the superior focusing characteristics of the guide. Comparing the elliptical guide with  $m = 3$  coating to the standard guide, the gain is significant over the full energy spectrum, but increases strongly for shorter wavelengths as a result of the higher  $m$ -value.

An important aspect of building high-performance but affordable elliptical guides is the possibility of using the highest  $m$ -material only near the entrance and the exit, where the curvature is strongest and most of the reflections occur. The  $m$ -value of the coating in the middle section of the guide is far less relevant than in the case of standard guides. The performance of an elliptical guide for wavelengths below  $5 \text{ \AA}$  can therefore be further increased, without significant additional cost. Specifically, using an advanced coating with  $m = 5$  in an elliptical guide yields a five- to six-fold increase in neutron intensity between  $3 \text{ \AA}$  and  $4 \text{ \AA}$ , and a thirty-fold increase at  $2 \text{ \AA}$  compared to the standard guide with  $m = 2$ . In practice, this gain in the shorter wavelength-range is particularly important because cold neutron scattering instruments are mainly used between  $2 \text{ \AA}$  and  $6 \text{ \AA}$ . This phenomenon opens up entirely new possibilities for neutron experiments in this wavelength range.

It must be noted, however, that the elliptical/parabolic guide cannot be used for all classes of neutron scattering instruments. Especially for Small Angle Neutron Scattering (SANS) instruments, the increase in beam divergency, which comes with focusing, is unacceptable. A further difference between a curved standard and a straight elliptical/parabolic guide is the existence of fast neutrons at the instrument position. For the elliptical/parabolic guide-geometry, several special solutions are already under discussion, for example, installing a steel kernel in the center of the guide.

## Experience with Previous and Potential for Future Facility Upgrades

Virtually all elements of the experimental setup—from the cold neutron source, neutron guide, sample environment, and detector technology—may offer potential for improvement.<sup>22</sup> Additional strategies for neutron-use optimization include renewal or upgrade of components and instruments. For example, in the case of the NBSR at the National Institute of Standards and Technology (NIST), a two-fold increase in available neutron flux has been reported after replacement of the reactor's cold neutron source in 2002. A similar performance gain has been achieved again in early 2012 after a second replacement of the source.<sup>23</sup>



**Figure 7:** Performance gain of the High-Flux Reactor (HFR) at ILL. Contributions are due to instrument upgrades (light-shaded area) and post-2002 guide renewals (dark-shaded area).<sup>24</sup> Actual results were even more favorable than anticipated: a 19-fold increase in performance has been achieved with the completion of the first project phase.

The most comprehensive effort at upgrading performance is underway at the High-Flux Reactor (HFR) at ILL. Initiated in the year 2000, this so-called “Millennium Programme” envisions systematic modernization of the reactor’s instruments and infrastructure. As illustrated in Figure 7, a 16-fold increase in overall performance of the facility was originally expected as a result of this ambitious long-term initiative.<sup>24</sup> As shown, a significant fraction of this gain is due to neutron-guide upgrades. The first phase of this program (“M-0”) has now ended and resulted in a higher-than-expected improvement of average detection rate of neutrons for all instruments by 19 times.<sup>25</sup> A second phase (“M-1”) is now underway and expected to be completed by 2014.<sup>26</sup> As part of the Millennium Programm, the institute also pursues the “ILL 20/20 Upgrade Project,” which seeks to “boost the overall efficiency of ILL’s instrument suite by a factor of thirty by 2011.”<sup>27</sup>

In general, the greatest performance gains can be expected for facilities where upgrades are most overdue. Some neutron research facilities don’t use supermirror coatings at all, very few facilities worldwide use coatings with  $m > 2$  on their neutron guides, and elliptical guides remain an exception.<sup>28</sup> For example, the cold-neutron guides of the FRM-II, which began routine operation only in 2005 at Munich University of Technology (TUM) and are currently HEU-fueled, typically use a coating of  $m = 2$ .<sup>29</sup> Thus, even the most modern facilities may be able to benefit from more advanced neutron optics.

Funding has to be available to carry out such upgrades. For example, the costs of an advanced neutron guide similar to the reference guide discussed in this article may be on the order of \$300,000–600,000<sup>30</sup>; additional installation

and infrastructure costs, could bring the total cost for replacement or installation of a new neutron guide to \$1 million. This is a significant investment, but it has to be compared to the operating costs of a modern research reactor, which can be on the order of tens of millions of dollars per year. Investments in instrument-performance are therefore quickly recovered.<sup>31</sup>

One example for a candidate facility that could benefit significantly from a convert-and-upgrade strategy is the Russian PIK reactor, which has been under construction at the Saint Petersburg Institute of Nuclear Physics since 1976. The reactor, which is designed for a power level of 100 MWt and might require on the order of 100 kg of HEU per year, was recently completed, but its startup delayed until late 2012.<sup>32</sup> According to Russian press reports, the operator apparently has insufficient funding to complete construction of several support facilities. The PIK reactor has 50 positions for neutron instruments, but a large fraction of them would currently remain unused.<sup>33</sup> Preliminary conversion analyses for the reactor were carried out in the early 2000s and, even then, a reduced enrichment of 36 percent was considered feasible.<sup>34</sup> Using advanced fuels that are available today, combined with modern neutron guides as discussed in this article, it may be possible to redesign the reactor for low-enriched fuel, while turning it into a state-of-the-art center-of-excellence for neutron research.

## CONCLUSION AND OUTLOOK

In this article, we have assessed the large potential of using supermirror coatings and elliptical guide geometries to optimize the neutron flux available for experiments at research facilities. The results of our simulations show that a *several-fold* increase in neutron intensity for short wavelengths can generally be expected through upgrades to the neutron guides alone. The discussion also highlights the importance and pivotal role of modern Monte-Carlo computer codes to optimize the overall performance of high-flux reactors and their connected instruments used for neutron research.

The performance gain from using a combination of innovative neutron-guide technologies has important implications for international efforts to end the use of highly enriched uranium fuel in research reactors. Converting these reactors to use low-enriched fuel often brings small losses in neutron flux, but in this case the win-loss relation is extremely favorable. Our analysis demonstrates that the potential flux penalties due to conversion from HEU to LEU fuel become effectively irrelevant if a facility also upgrades its neutron guides.

Funding a program to simultaneously convert a research reactor to low-enriched fuel *and* upgrade its neutron guides need not be a significant constraint. The typical costs of conversion, operating costs, and the costs for upgrading neutron guides or instruments are generally comparable.

Investments in instrument-performance are therefore quickly recovered. Given that there is now broad international acceptance of the need to end the use of highly enriched uranium in the civilian nuclear fuel cycle, and also to establish regional “centers of excellence” for neutron research, it appears that the next few years may present research reactor operators and neutron instrument groups with a unique opportunity to coordinate a combined convert-and-upgrade strategy and achieve significantly improved overall performance.

## NOTES AND REFERENCES

1. These activities are supported and coordinated by the *Reduced Enrichment for Research and Test Reactors* (RERTR) program, [www.rertr.anl.gov](http://www.rertr.anl.gov). In the United States, efforts have been consolidated since 2004 under the Global Threat Reduction Initiative (GTRI).

2. Remarks by President Barack Obama, Hradčany Square, Prague, Czech Republic, 5 April 2009, <[www.whitehouse.gov/the\\_press\\_office/Remarks-By-President-Barack-Obama-In-Prague-As-Delivered](http://www.whitehouse.gov/the_press_office/Remarks-By-President-Barack-Obama-In-Prague-As-Delivered)>.

3. The final communiqué of the 2010 Summit in Washington, DC, recognized that “highly enriched uranium and separated plutonium require special precautions and [we] agree to promote measures to secure, account for, and consolidate these materials, as appropriate; and encourage the conversion of reactors from highly enriched to low enriched uranium fuel and minimization of use of highly enriched uranium, where technically and economically feasible,” *Communiqué of the Washington Nuclear Security Summit*, 13 April 2010, <[www.whitehouse.gov/the-press-office/communiqu-washington-nuclear-security-summit](http://www.whitehouse.gov/the-press-office/communiqu-washington-nuclear-security-summit)>.

4. International Panel on Fissile Materials, *Global Fissile Material Report 2011: Nuclear Weapon and Fissile Material Stockpiles and Production*, Princeton, NJ, January 2012, pp. 11–13, <[www.ipfmlibrary.org/gfmr11.pdf](http://www.ipfmlibrary.org/gfmr11.pdf)>.

5. In addition to the well-documented case of the FRM-II in Germany, both China and Russia have recently completed large HEU-fueled research reactors. For short discussions of these cases, see International Panel on Fissile Materials, *Global Fissile Material Report 2010: Balancing the Books: Production and Stocks*, Princeton, NJ, January 2012, Chapter 1, <[www.ipfmlibrary.org/gfmr10.pdf](http://www.ipfmlibrary.org/gfmr10.pdf)>.

6. As of 2012, the IAEA lists 50 neutron scattering facilities worldwide, 11 of which are fueled with weapon-grade HEU, including many high-performance facilities, <[nucleus.iaea.org/RRDB/Content/Util/NeutronScattering.aspx](http://nucleus.iaea.org/RRDB/Content/Util/NeutronScattering.aspx)>. Important HEU-fueled high-flux reactors used for neutron scattering are: FRM-II (Germany, 20 MW), NBSR (USA, 20 MW), HFR (France, 58 MW), EWG-1 (Kazakhstan, 60 MW), and HFIR (USA, 85 MW). Major neutron scattering facilities in Russia include IVV-2M (15 MW), WWR-M (18 MW), and the new PIK reactor (100-MW), which is discussed further below.

7. A reduction of maximum neutron flux on the order of 10–15 percent is a typical value, also because operators have generally refrained from converting reactors to low-enriched fuel when they expected more significant losses. In many cases, performance of medium-power reactors even increased after conversion because new high-density fuels permitted more compact core configurations. The archived proceedings of past RERTR meetings can be consulted for numerous examples of theoretical conversion studies and post-conversion status reports. These proceedings are available online at [www.rertr.anl.gov/meetings.html](http://www.rertr.anl.gov/meetings.html).

8. United Nations International Nuclear Fuel Cycle Evaluation (INFCE), *Report of INFCE Working Group 8: Advanced Fuel Cycle and Reactor Concepts*, Vienna 1980, pp. 17–19, 42–46, and 137–172.

9. See, for example, K. Lefmann, and K. Nielsen, “McStas, A General Software Package for Neutron Ray-tracing Simulations,” *Neutron News* 10(1999): 3, 20–23.; V. Hugouvioux, E. Farhi, M. R. Johnson, W. Kob, “Virtual Neutron Scattering Experiments,” *Physica B* 350(2004): 1–3, 151–154; and P. Willendrup, U. Filges, L. Keller, E. Farhi, and K. Lefmann, “Validation of a Realistic Powder Sample Using Data from DMC at PSI,” *Physica B* 385–386(2006): 1032–1034.

10. Low-energy or cold neutrons are valuable for the study of condensed matter because they have a wavelength that corresponds to typical interatomic distances or molecular dimensions (1–4 Å or 5–80 meV). Neutrons generated in nuclear fission, however, have energies in the MeV-range and have to be slowed down (thermalized) using a moderator before they can be used for neutron diffraction or spectroscopy experiments. Cold neutrons are obtained by thermalizing them in liquid deuterium (typically at about 20 K) soon after they escape from the reactor core. These neutrons can then be propagated through neutron guides to experiments tens of meters away.

11. There is a series of international conferences on neutron optics and instrument design using computer modeling. Among the more recent events are: the *European Workshop on Neutron Optics (NOP 2007)*, 5–7 March 2007, Paul Scherrer Institute (PSI), Switzerland, <kur.web.psi.ch>; and the *International Workshop on Applications of Advanced Monte Carlo Simulations in Neutron Scattering*, 2–4 October 2006, PSI, Switzerland, <lns00.psi.ch/mcworkshop>.

12. For the presented simulations VITESS Release 2.6 and McStas version 1.10 have been used. Besides VITESS and McStas, which are two of the most commonly used simulation packages in different neutron scattering laboratories worldwide, several other dedicated Monte Carlo computer codes simulate propagation of neutrons through complex instrument architectures, for example, NISP and RESTRAX.

13. McStas, <www.mcstas.org>.

14. VITESS, <www.helmholtz-berlin.de/forschung/grossgeraete/neutronenstreuung/projekte/vitess>.

15. W. E. Fischer, “SINQ: The Spallation Neutron Source, A New Research Facility at PSI,” *Physica B* 234–236(1997): 1202–1208.

16. This wavelength spectrum is provided as a default source for VITESS.

17. On standard ballistic supermirror neutron guides, see F. Mezei, “Novel Polarized Neutron Devices: Supermirror and Spin Component Amplifier,” *Communications on Physics* 1(1976): 81–85; on innovative neutron-guide geometries, see C. Schanzer, P. Böni, U. Filges, and T. Hils, “Advanced Geometries for Ballistic Neutron Guides,” *Nuclear Instruments and Methods in Physics Research, Section A*, 529(2004): 63–68; and D. M. Rodriguez, S. J. Kennedy, and P. M. Bentley, “Properties of Elliptical Guides for Neutron Beam Transport and Applications for New Instrumentation Concepts,” *Journal of Applied Crystallography* 44(2011): 727–737.

18. H. Maier-Leibnitz, and T. Springer, “The Use of Neutron Optical Devices on Beam-hole Experiments,” *Journal of Nuclear Energy, Parts A/B, Reactor Science and Technology* 17(1963): 217–225; and V. F. Turchin, and V. A. Tarasov, “Asymptotic Formulas for Scattering of Slow Neutrons on Bound Atoms,” *Atomic Energy* 18(1965): 2, 146–150.

19. Shown reflectivity files are based on experimental data provided by *SwissNeutronics*, personal communication, May 2007. See [www.swissneutronics.ch](http://www.swissneutronics.ch) for updates.

20. This consideration is very conservative because in practice guides can be more than 100 m long.

21. For details, see C. Schanzer, P. Böni, U. Filges, and T. Hils 2004, *op. cit.*
22. The potential of innovative neutron-guide technology is of primary interest here but complementary strategies include “quantitative” upgrades, in which the total number of instruments at a facility is increased. For example, between 1998 and 2006, six new scattering instruments at the High Flux Isotope Reactor (HFIR) in Oak Ridge have been added, bringing the total from 9 to 15 instruments with a corresponding increase in facility performance. Information on HFIR instrument systems is available at [neutrons.ornl.gov](http://neutrons.ornl.gov).
23. See NIST Center for Neutron Research, National Institute of Standards and Technology, *Annual Report 2002*, pp. 6–7 and *Annual Report 2011*, p. 52. For more information, see [www.ncnr.nist.gov](http://www.ncnr.nist.gov).
24. Data for expected performance gain taken from D. Dubbers, “The Institute Laue-Langevin and its Role in Neutron Science,” Presentation at the ILL Millennium Symposium and European User Meeting, Grenoble, 27–29 April 2006, Slide 19. For more details on this initiative, see R. Wagner, “ILL Millennium Programme: Achievements for the Benefit of ILL’s User Community,” presentation at the same meeting.
25. Institut Laue-Langevin, *Renaissance: The ILL Millennium Programm 2001–2009*, July 2010, p. 8. The first phase of the project included 14 upgraded or new instruments and required an investment of €42 million.
26. For project updates, see [www.ill.eu/html/about/future-planning/the-millennium-programme-phases](http://www.ill.eu/html/about/future-planning/the-millennium-programme-phases).
27. Institut Laue-Langevin, [www.ill.eu/html/about/future-planning/the-ill2020-upgrade-projects](http://www.ill.eu/html/about/future-planning/the-ill2020-upgrade-projects).
28. A 1:10 scale model of an elliptical guide was studied at the spallation neutron source SINQ at PSI in Switzerland. Based on the result, a first prototype was installed in 2010 on the reflectometer AMOR at SINQ. The first instrument with a full-scale elliptical-guide is the high-resolution powder diffractometer HRPT at ISIS in the United Kingdom.
29. K. Zeitelhack, C. Schanzer, et al. “Measurement of Neutron Flux and Beam Divergence at the Cold Neutron Guide System of the New Munich Research Reactor FRM-II,” *Nuclear Instruments and Methods in Physics Research A*, 560(2006): 2, 444–453.
30. This cost estimate is based on a combined cost for material and coating of \$20,000–\$40,000 per square meter; see C. Rehm, M. Agamalian, and F. Klose, Neutron Supermirrors: Design and Application, Report of the Optical Components Team, Spallation Neutron Source Project, Oak Ridge National Laboratory, May 2002.
31. For example, the IAEA research reactor database quotes an annual cost of \$34 million for FRM-II and \$57 million for HFIR. If we assume, for a very rough estimate, that the annual operating cost of a neutron scattering facility is \$25 million and that the installation of a 1-million neutron guide results in a 2 percent increase of overall performance and revenue, the upgrade would be recovered in two years ( $25 \times 0.02 \times 2 = 1$ ).
32. International Panel on Fissile Materials, [www.fissilematerials.org/blog/2011/08/more\\_delays\\_for\\_pik\\_react.html](http://www.fissilematerials.org/blog/2011/08/more_delays_for_pik_react.html).
33. *PNPI RAS: Current Status and Plans for Development*, (2010), [www.ip.leontief-centre.ru/UserFiles/Files/PNPI\\_north\\_europe.pdf](http://www.ip.leontief-centre.ru/UserFiles/Files/PNPI_north_europe.pdf). See also [nrd.pnpi.spb.ru/facilities/menu\\_pik.html](http://nrd.pnpi.spb.ru/facilities/menu_pik.html).
34. Y. V. Petrov, A. N. Erykalov and M. S. Onegin, “The Fuel Cycle of Reactor PIK,” *24th International Meeting on Reduced Enrichment for Research and Test Reactors*, 3–8 November 2002, Bariloche, Argentina.