



# ***ADVANCES IN NEUTRON INSTRUMENT SIMULATIONS WITH VITESS***

**Release of versions 3.7 and 3.8**

**13.04.2026 | NICOLÒ VIOLINI**

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# KEY LEARNINGS FROM USER EXPERIENCE

From an instrument design tool to a platform to support virtual experiments



## **Need to connect:**

moderator simulations, beamline optics, sample & detector



## **Emerging trend:**

virtual experiments, digital twins

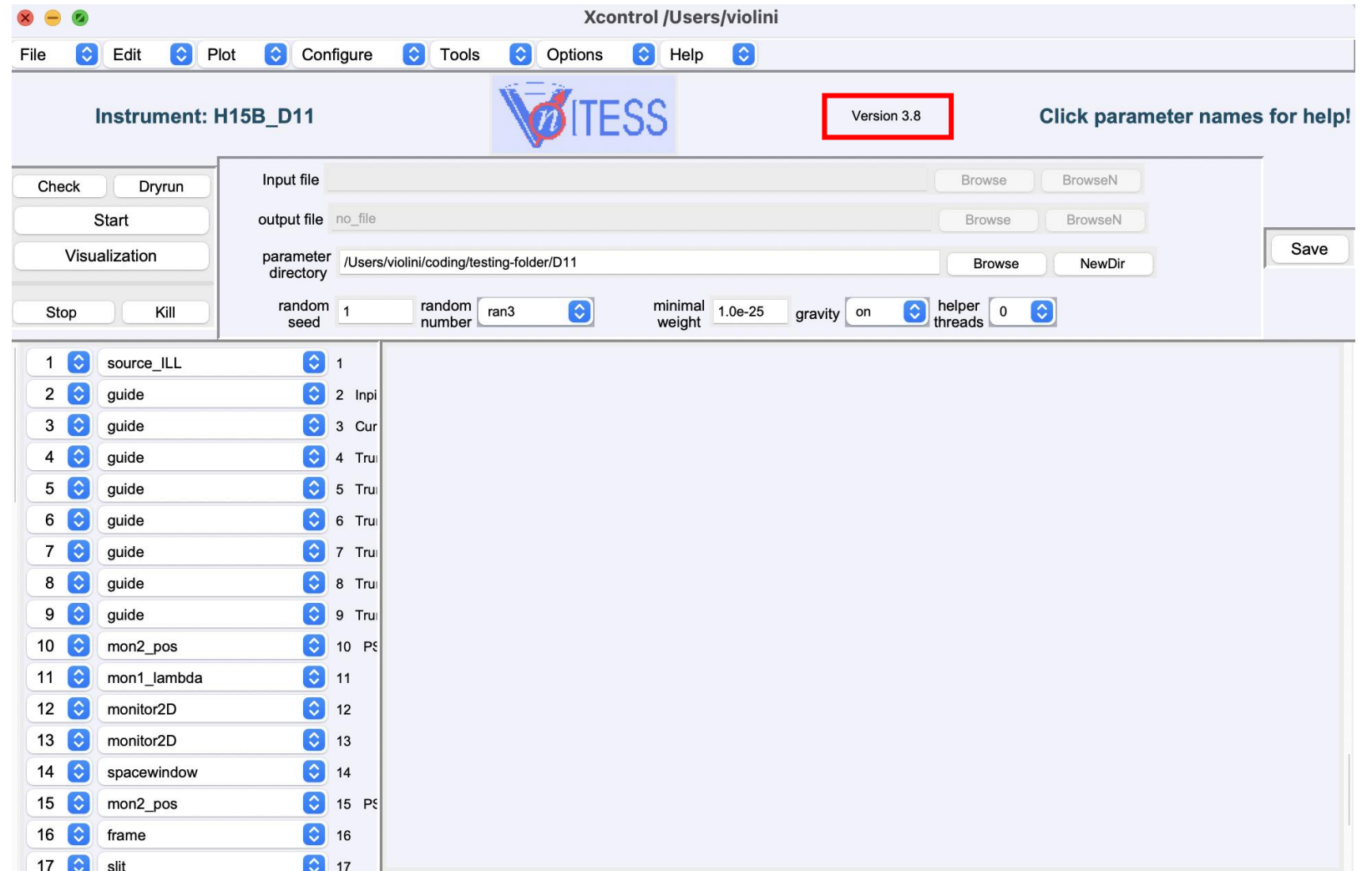


**Instrument design at modern sources is increasingly complex**

# WHAT IS VITESS

Latest released version is 3.8

- Monte Carlo neutron transport
- Modular instrument simulation
- Used for design & optimisation



# VITESS

## Release Roadmap

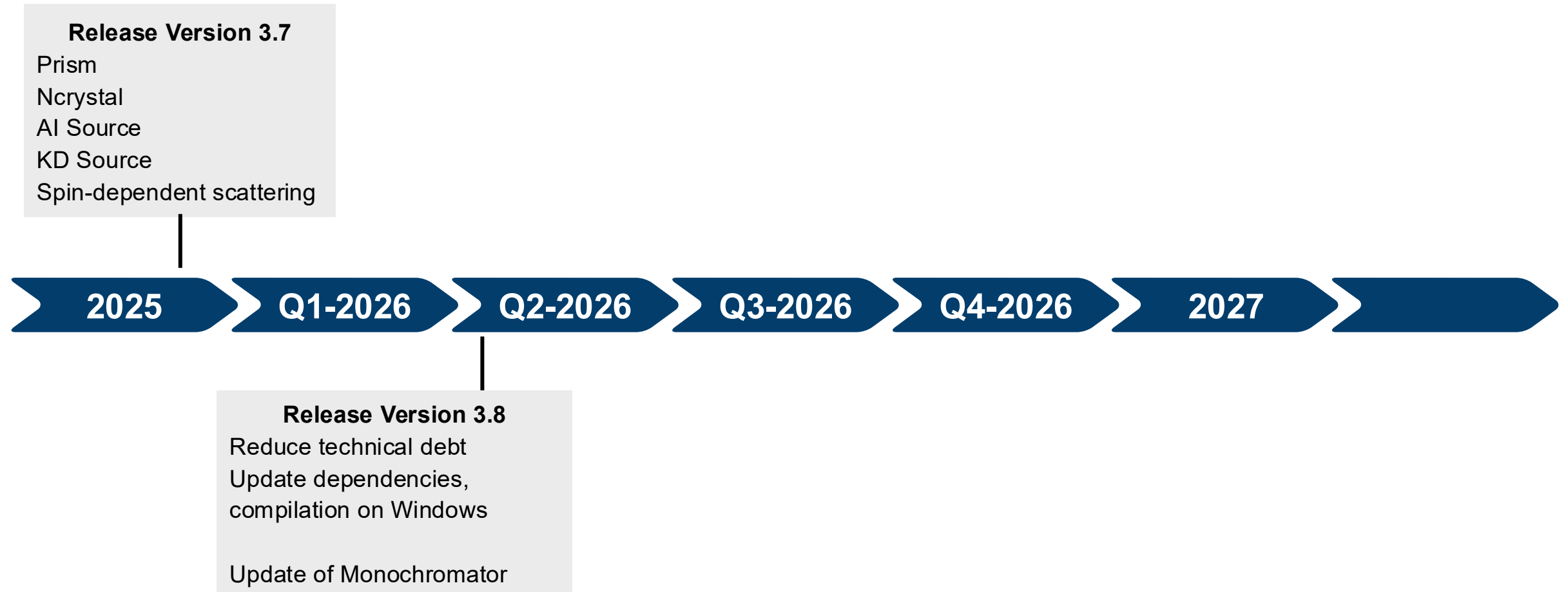
### Release Version 3.7

Prism  
Ncrystal  
AI Source  
KD Source  
Spin-dependent scattering



# VITESS

## Release Roadmap



# VITESS

## Release Roadmap

### Release Version 3.7

Prism  
Ncrystal  
AI Source  
KD Source  
Spin-dependent scattering

2025

Q1-2026

Q2-2026

### Release Version 3.8

Reduce technical debt  
Update dependencies,  
compilation on Windows

Update of Monochromator

computer programs

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Keywords: Monte Carlo simulation; neutron ray tracing; neutron scattering; computer programs.

## Vitess 3.8: a modernized framework for Monte Carlo neutron tracing simulations

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*VITESS* is a modular Monte Carlo simulation package for modeling and optimizing neutron scattering instruments through ray tracing of neutrons. The latest release, *VITESS 3.8*, introduces major advances in functionality and software infrastructure. They include new source modules for integrating external moderator simulations and artificial-intelligence-based flux modeling, as well as *prism* for beam deflection and crystalline material simulations via *NCrystal*. Existing modules have been extended to support spin-dependent scattering, advanced monochromator motions and improved polarization handling. The update also includes a Git-based continuous integration system ensuring reproducibility.

### 1. Introduction

*VITESS* (virtual instrumentation tool for the ESS) is a modular Monte Carlo simulation package designed for the modeling, optimization and performance analysis of neutron scattering instruments and virtual experiments (Zsigmond *et al.*, 2002; Zandler *et al.*, 2014; <https://vitess.fz-juelich.de>). Developed originally to support the design of instruments for the European Spallation Source (ESS), *VITESS* has evolved into a versatile and widely used framework for simulating neutron propagation through complex instrument geometries.

The software implements a ray-tracing approach, in which neutrons (particles characterized by their position, direction, wavelength and polarization) are described by rays. Each ray corresponds to a discrete number of physical neutrons. These virtual neutron rays are propagated through a sequence of instrument components—such as guides, choppers, monochromators and detectors—each represented by a dedicated simulation module, with which they are allowed to interact. Every neutron ray carries a weight (or probability) that can be decreased after each interaction, describing how many neutrons are still left in the instrument at a given point. *VITESS*'s modular structure allows researchers to flexibly assemble and modify virtual instruments, facilitating systematic studies of instrument performance and design trade-offs as well as virtual experiments.

One of the key strengths of *VITESS* lies in its balance between physical accuracy and computational efficiency. The tool accounts for the essential physics of neutron interactions with instrument components while remaining sufficiently fast for extensive parameter studies. It supports both continuous sources and pulsed source time structures, enabling the realistic simulation of modern neutron facilities. The software's ability to interface with data formats such as Monte Carlo Particle Lists (MCPL) (Kittelmann *et al.*, 2017) further



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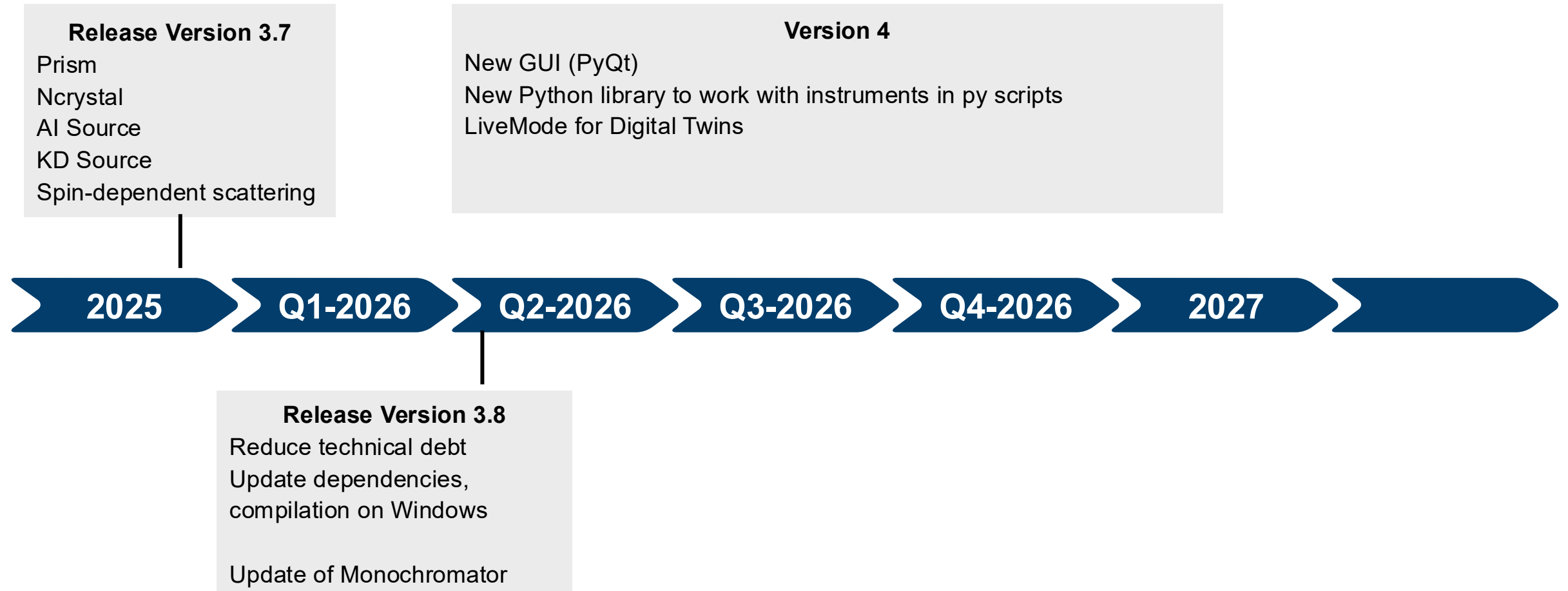
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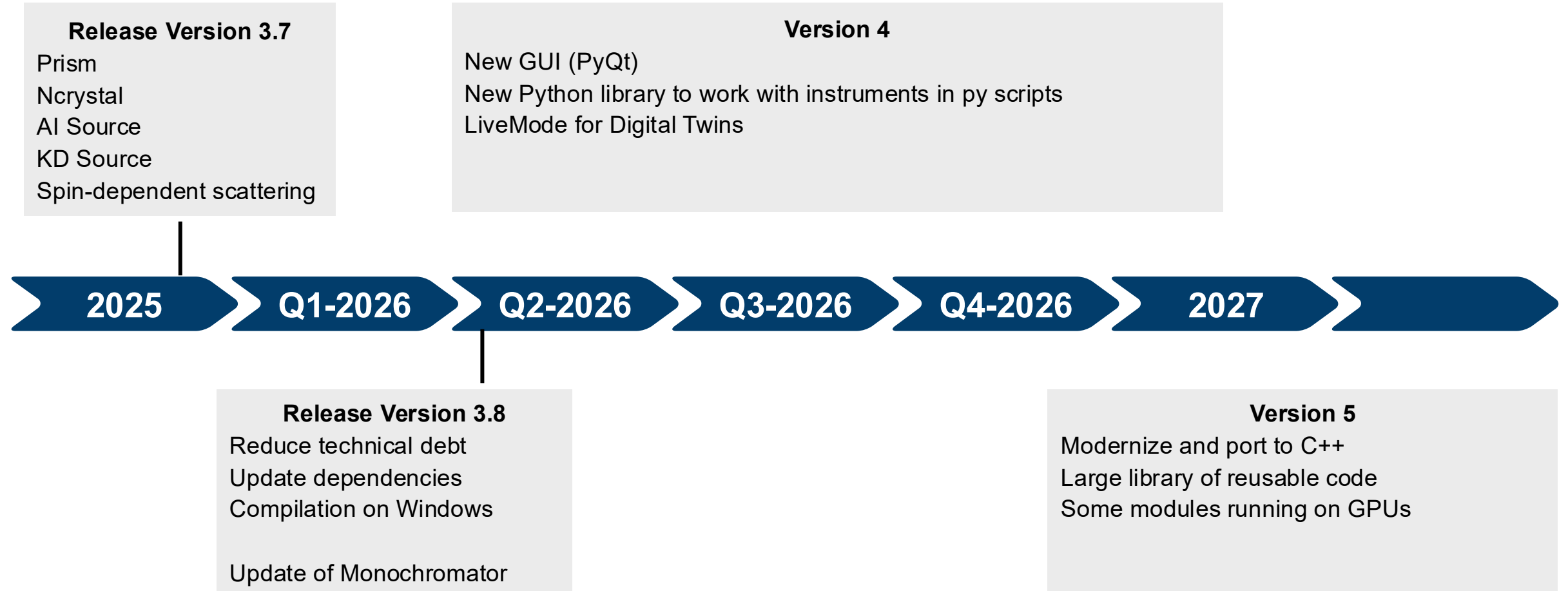
# VITESS

## Release Roadmap



# VITESS

## Release Roadmap



# VITESS 3.7

## Overview

AI-Source  
KD-Source



Improved coupling between moderator simulations and instrument modelling, use of MCPL based input

Ncrystal integration  
Spin-dependent scattering



New physics capabilities  
Extended ability to work with neutron spin

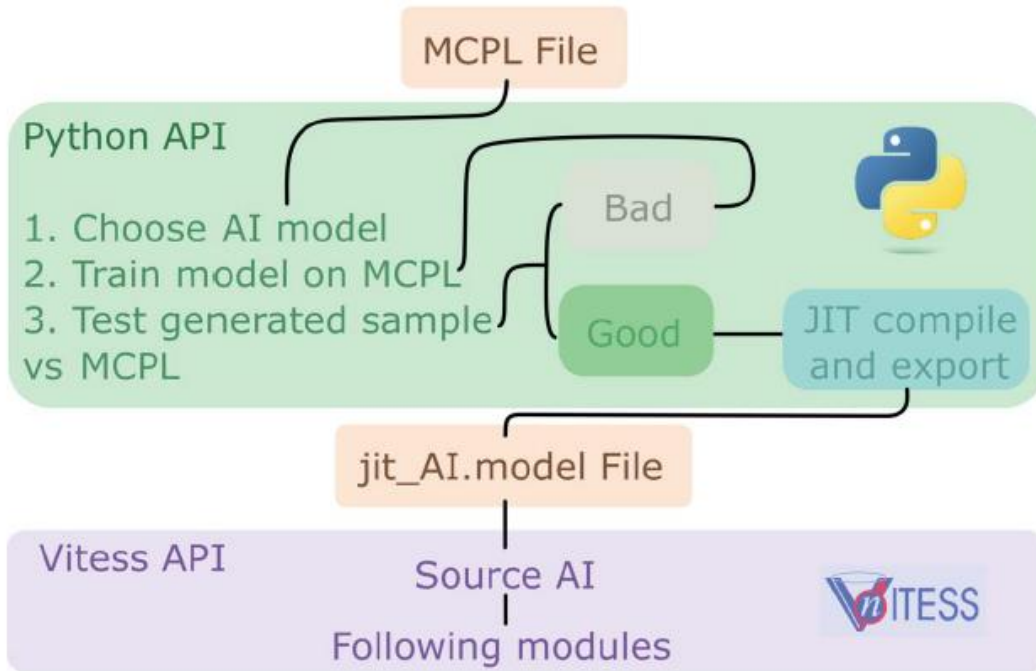
Prism  
Moving monochromator



Neutron refraction  
Ability to simulate more complex cases such as Doppler, rotating crystals, Phase Space Transformer

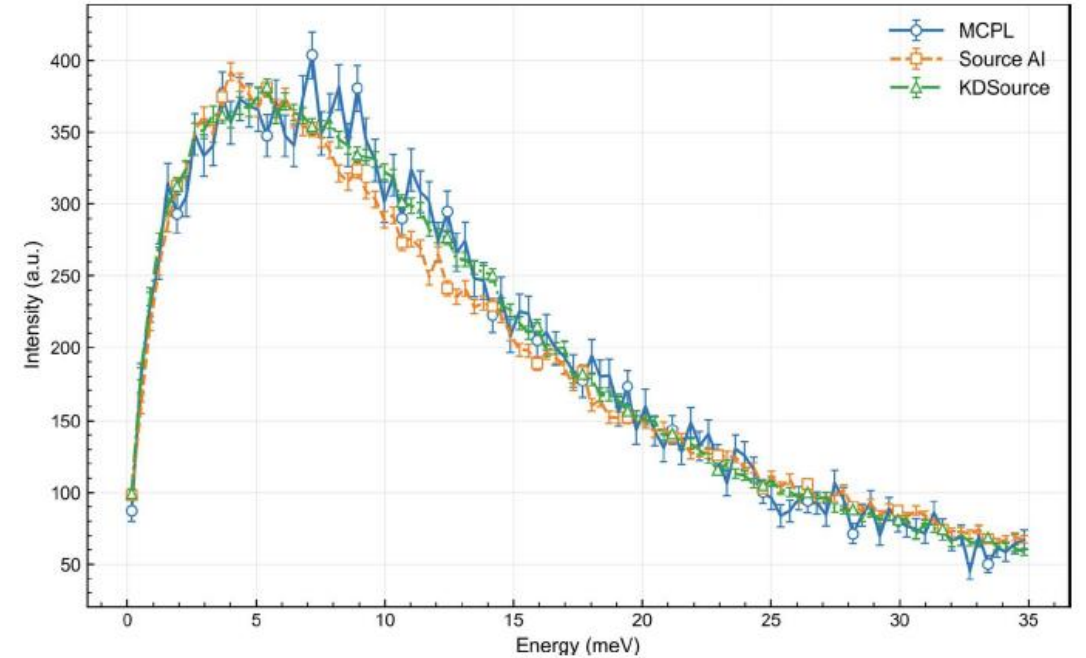
# VITESS 3.7

## KD Source (trajectory module) & Source AI (source module)



**Figure 3**

Workflow for using the `source_AI` module. Models must be trained in Python and need to be JIT compiled to be used by the `VITESS` module.



**Figure 4**

Comparison between different sampling schemes: reading in the MCPL file, sampling with a trained AI model such as a normalizing flow, or sampling with `KDSOURCE`.

# VITESS 3.7

## Ncrystal integration

Module 23 sample\_ncrystal  
NCrystal Config string definition

material file: LiquidWaterH2O\_T293.6K.ncmat [Browse] [BrowseN]

Temperature [K]: 10

Solid sample: [dropdown]

Crystal parameters  
d-cutoff [Ang]: 0.5 crystal mosaicity: 0.2 Axis 2 dir tolerance [deg]: 0.0057

Crystal directions  
Axis 1 h: 1 Axis 1 k: 1 Axis 1 l: 0  
Axis 1 dir x: 1 Axis 1 dir y: 0 Axis 1 dir z: 0  
Axis 2 h: 0 Axis 2 dir h: 1 Axis 2 l: 1  
Axis 2 dir x: 0.5 Axis 2 dir y: 0.866 Axis 2 dir z: 0

Repetitions of the same neutron event  
repetition: 1

Sample shape  
sample geometry: [dropdown]

Sample position and size  
X [cm]: 50 Y [cm]: 0 Z [cm]: 0  
thickness or diameter [cm]: 3 height [cm]: 3 inner diameter or width [cm]: 2.8  
offset angle horiz. [deg]: 0 offset angle vert. [deg]: 0

Incident neutron parameters  
incident lambda: 1.8

Output frame  
X' [cm]: 50 Y' [cm]: 0 Z' [cm]: 0  
horiz. angle [deg]: 0 vert. angle [deg]: 0

## REQUIRED INPUT

Material file

T

Solid sample: y/n

Crystal parameters: d-cutoff, mosaic, axis2 tolerance

Crystal axes directions (h,k,l) (x,y,z)

Sample shape: hollow-cyl, cyl, sphere, cuboid

Sample pos and size

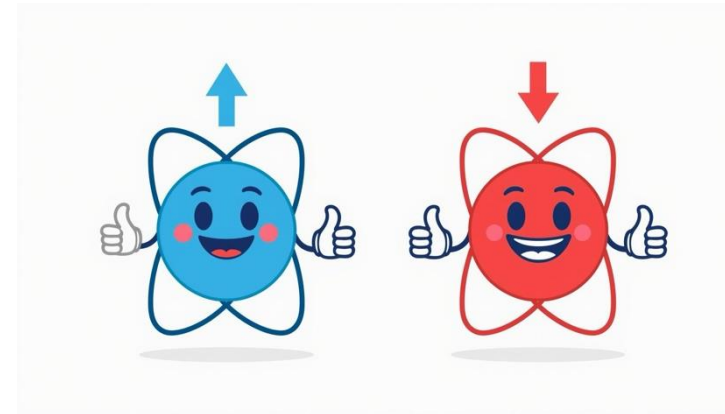
Incident neutron wavelength

Output frame

# VITESS 3.7

## Spin dependent scattering

- Spin manipulation was found faulty and fixed in the following modules:
  - polariser\_he3
  - polariser\_sm
  - pol\_mirror
  - flipper\_coil



Recommendation to our users:  
Please download the latest VITESS version and check any polarisation device

# VITESS 3.7

## Spin dependent scattering

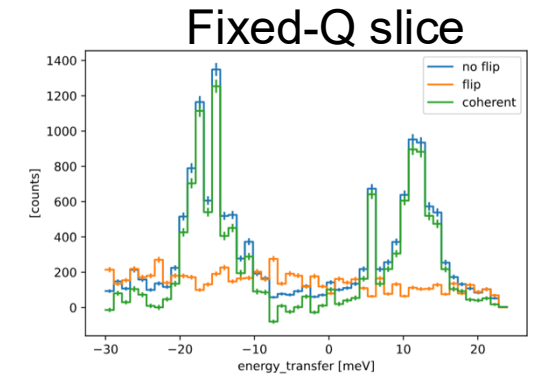
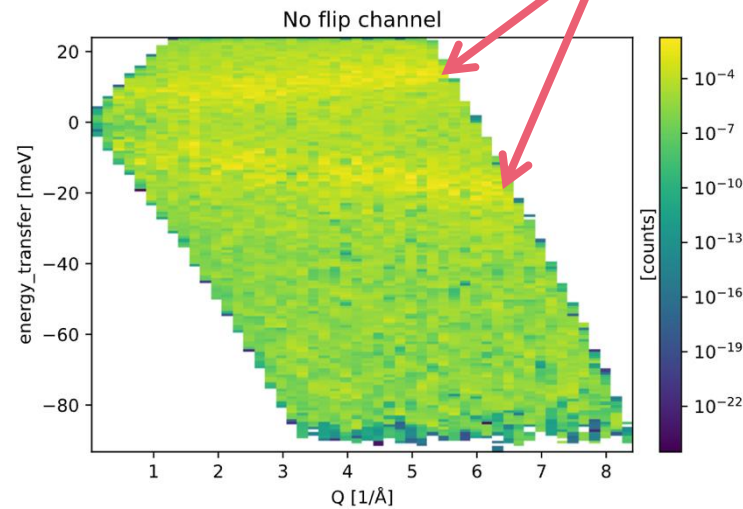
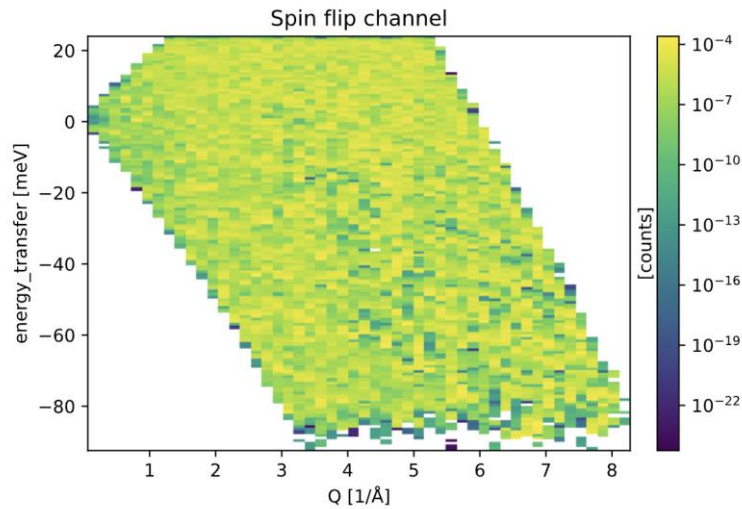
- Spin-dependent inelastic scattering: the spin option added to the following modules:

- sample\_inelast
- eval\_inelast
- detector

$$S(\mathbf{q}, \omega) = \sigma_{\text{coh}} S_{\text{coh}}(\mathbf{q}, \omega) + \sigma_{\text{incoh}} S_{\text{incoh}}(\mathbf{q}, \omega)$$

$$\mathbf{S}_f = \begin{cases} -\mathbf{S}_i, & \text{with probability } \frac{2}{3} \\ \mathbf{S}_i, & \text{with probability } \frac{1}{3} \end{cases}$$

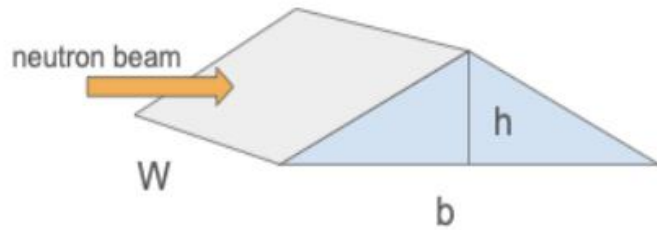
$$\omega(\mathbf{q}) = P_0 + D_x q_x + D_y q_y + D_z q_z$$



# VITESS 3.7

Prism – developed from the original contribution by T. Krist (NOB)

- Simulates neutron refraction by a prism or a stack of prisms



Gravitation corrector  
Energy analyser

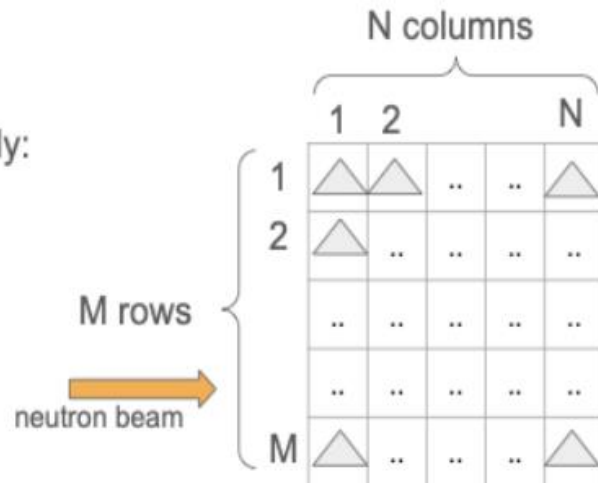
$$n = 1 - \frac{\lambda^2}{2\pi} \rho$$

Dimensions of the assembly:

Width = W  
Depth = N x b  
Height = M x h

Example:

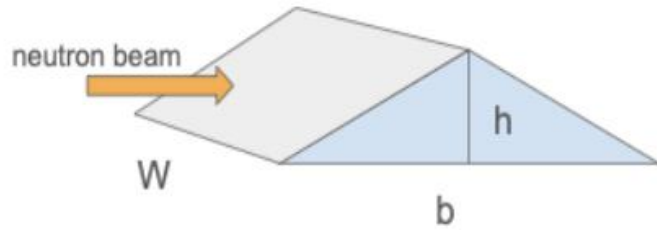
N = 16  
M = 120  
b = 0.35 mm  
h = 0.25 mm



# VITESS 3.7

## Prism

- Simulates neutron refraction by a prism or a stack of prisms



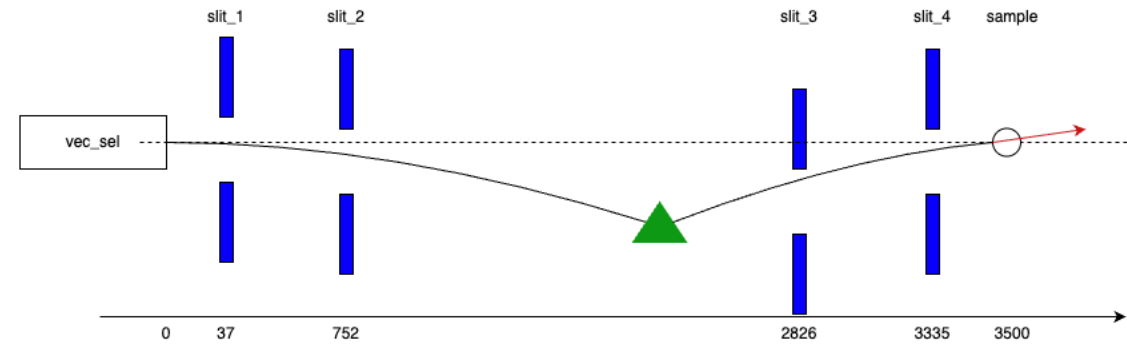
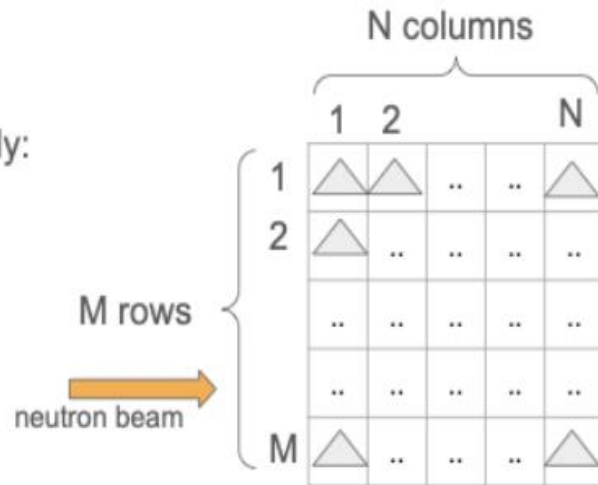
Gravitation corrector  
Energy analyser

Dimensions of the assembly:

Width = W  
Depth =  $N \times b$   
Height =  $M \times h$

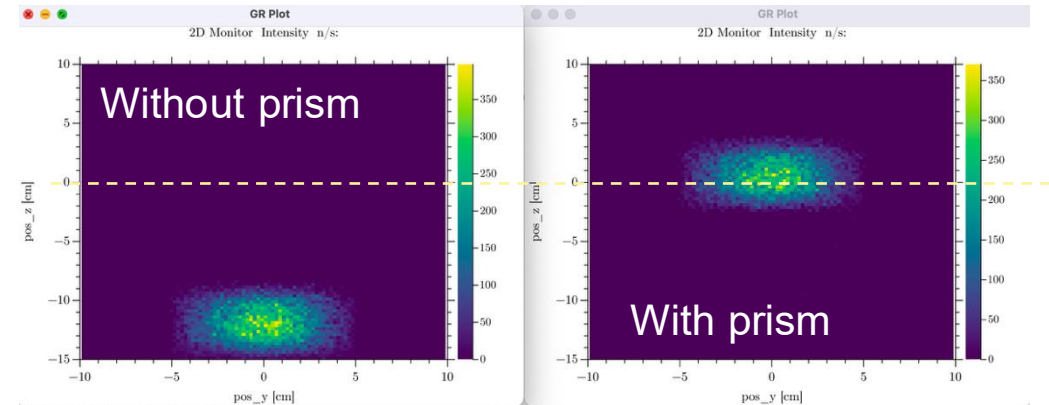
Example:

$N = 16$   
 $M = 120$   
 $b = 0.35 \text{ mm}$   
 $h = 0.25 \text{ mm}$



Example: D11 @ ILL

Neutron wavelength:  $20 \text{ \AA}$   
prism-sample distance: 17.5m

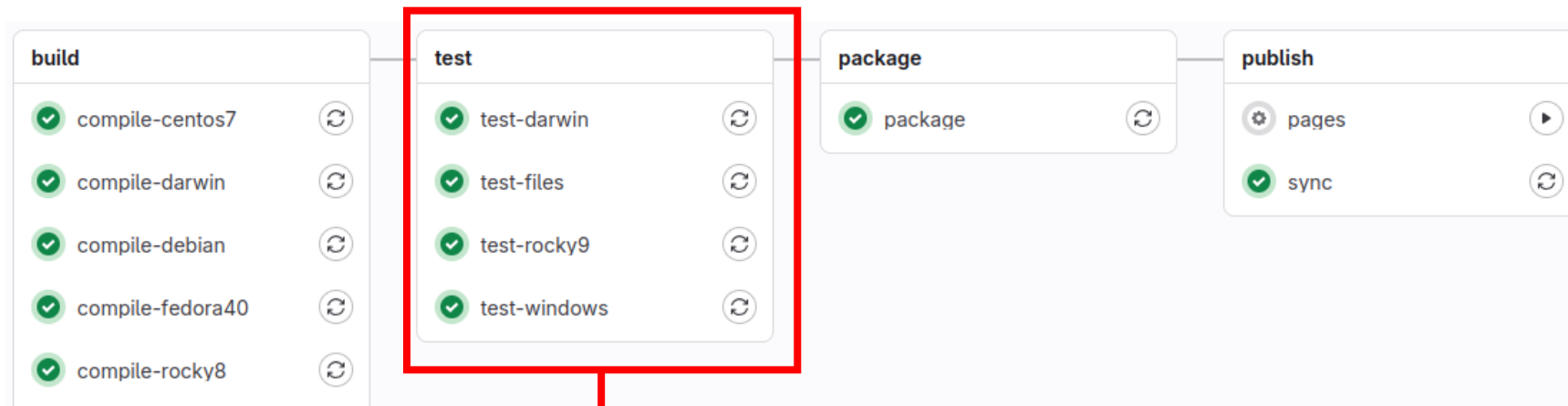


2D pos monitor at sample

# VITESS 3.8

## Overview

- automated module testing for regression, memory leaks, and undefined behaviour

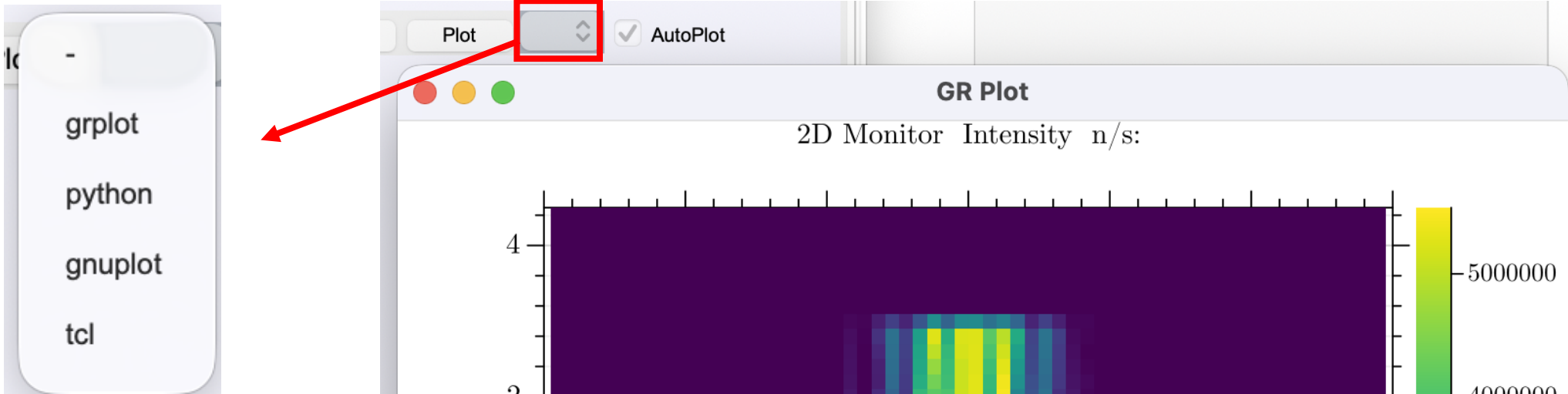


230 automated tests

# VITESS 3.8

## Overview

- automated module testing for regression, memory leaks, and undefined behaviour,
- improvements in the graphical interface and plotting tools



# VITESS 3.8

## Overview

- automated module testing for regression, memory leaks, and undefined behaviour,
- improvements in the graphical interface and plotting tools,
- better cross-platform support (ex. KDSource on Windows and Source\_AI on MacOS)
- various fixes in modules such as monochromators and monitors.

# VITESS

## Outlook – upcoming versions

- Qt will be used for the next graphical interface
- Instrument files will be written in .yaml format
- Python library to enable programmatic instrument definition and integration with python-based workflows
- Port the code to C++ and GPUs

from a

design tool

towards

a platform for comprehensive  
neutron experiment simulation

# VITESS

## Conclusions

- VITESS 3.7 introduces significant advances in source modelling and physics capabilities, enabling improved coupling between moderator simulations and instrument modelling
- VITESS 3.8 focuses on robustness and usability
- VITESS 4 and 5 will enable more comprehensive virtual experiments and digital twins

Scan the QR-code  
and  
download the latest version!



<https://iffgit.fz-juelich.de/vitess/vitess>

- Visit the website <https://vitess.fz-juelich.de>

# Thank you for your attention!

*We thank the VITESS user community for their contributions, feature requests and feedback, which directly drive the development of the code.*