Neutron transport in the tSPECT's beamline

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The goal of this simulation is to track ultracold neutron (UCN) through a beamline to see how the gravity and the particular shape influence the spectrum of energy of the ultracold neutron. The framework used to track the particles in the beamline is *Kassiopeia*[1]. It provides geometry tools and UCN interactions with surfaces and spaces.

Geometry

Variables

The XML file used for the simulation provides at the beginning of the geometry section a few inputs variables to make the structure of the beamline more adaptable for further modifications. According to a sketch provided, the useful parameters are summarized in the following table.

Name	Default Value	Description
inner_diameter	66.e-3 = 66 mm	Inner diameter of the tubes
outer_diameter	70.e-3 = 70 mm	Outer diameter of the tubes
bend1_radii	25.e-2 = 25 cm	Bend radii of the bend1 shape
bend2_radii	40.e-2 = 40 cm	Bend radii of the bend2 shape
bend3_radii	8.e-2 = 8 cm	Bend radii of the bend3 shape
bend1_angle	45°	Bend angle of the bend1 shape
bend2_angle	45°	Bend angle of the bend2 shape
bend3_angle	90°	Bend angle of the bend3 shape
tube1_length	70.e-2 = 70 cm	Length of the tube1 cylinder
tube2_length	28.e-2 = 28 cm	Length of the tube2 cylinder
tube3_length	44.e-2 = 44 cm	Length of the tube3 cylinder
tube4_length	32.e-2 = 32 cm	Length of the tube4 cylinder

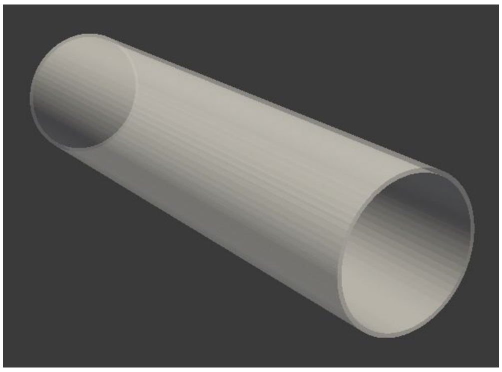
Table 1: Summary of the variable's name use to generate the geometry of the beamline

Shapes

The beamline is a simple cylindrical tube which is bent at a few part to link the neutron source to the experiment. Thus, the geometry needs to have two different basic shapes: a cylinder tube part and a cylinder bend part.

Cylinder tube space

The *KGeoBag* package included in the Kassiopeia framework provides a geometry part called *cylinder_tube_space* which can be seen as a pipe object with a width. An example of geometry is provided on the figure 1.

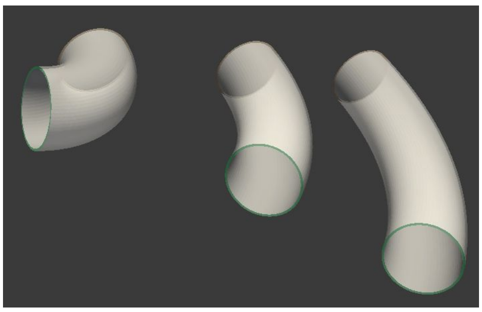


<u>Figure 1:</u> Picture of a cylinder tube part

A simpler solution would be to use a *cylinder_surface* instead. This will forbid any multiple reflection inside the material of the beamline.

Cylinder bend space

The *KGeoBag* package didn't provide a specific volume to represent a bend cylinder. To counter this lack, the XML file provides a construct space called *bend#_space_assembly* (the # is the id assembly). It is composed of two shell circle surface and two annulus surface. For proper assembly, this part has color on the annulus ring, orange for the entry and green for the exit. These color are optional. The final result can be seen on the figure 2.



<u>Figure 2:</u> Picture of a cylinder bend part

Here also, the inner shell of the bend part can be used alone to reduce the geometry and avoid any multiple reflection inside the material.

Construction

The two basic shapes can be assembled and parameterized to reproduce the structure of the beamline. The two following pictures provides an overview of the beamline's structure. It includes the name of the variables used to set the beamline and referenced in the table 1 above.

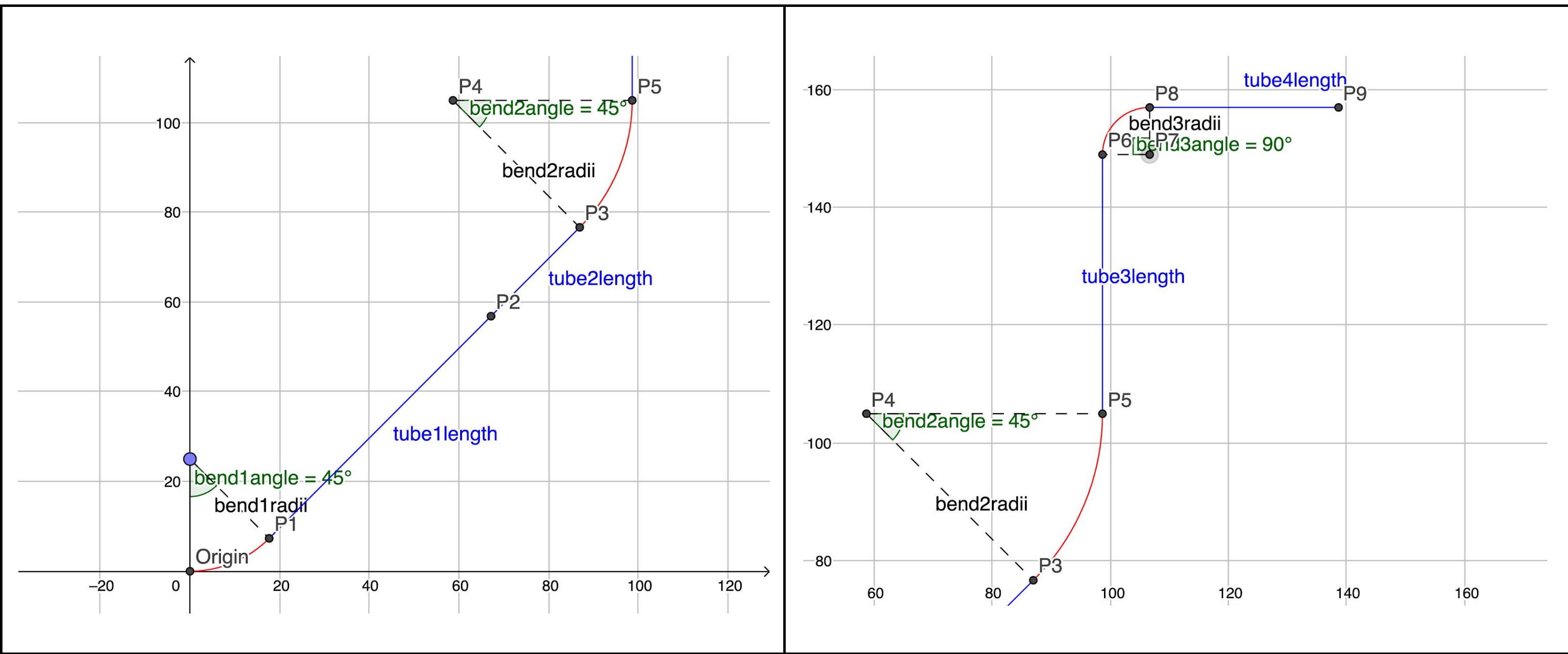


Figure 3: Drawing of the beamline with variable's name. The red lines represent the bend parts and the blue lines represent the cylinder tube part.

In the end, the final geometry in Kassiopeia can be view on the following figure.

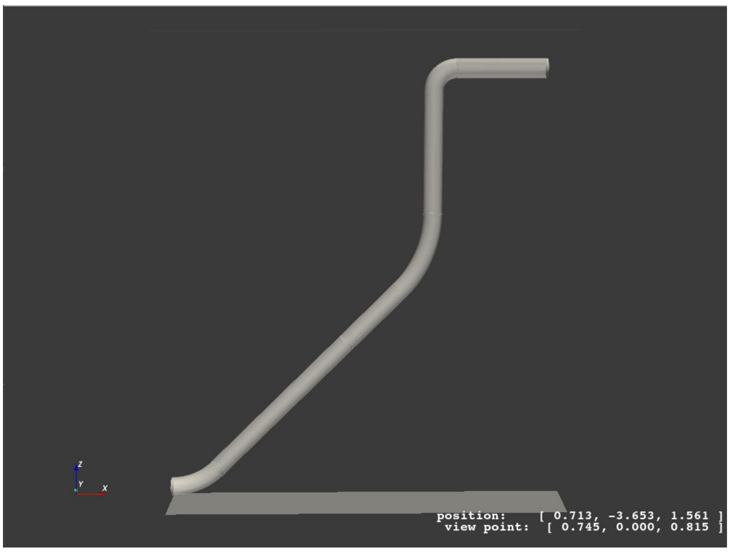


Figure 4: View of the final geometry of the beamline in Kassiopeia

Simulation

Reflection of UCN on surfaces

To contain the UCN inside the beamline, the simulation uses a special line provided by Kassiopeia[3]:

```
<ksint_surface_UCN name="int_surface_UCN" eta="2.e-4"
alpha="5.e-6" real_optical_potential="2.08e-7"
correlation_length="20.e-9"/>
```

The values of the different parameters are chosen to represent the reflection of UCN on stainless steel[4]. The eta parameter is the loss per bounce which is in the order of 10^{-4} . In this test phase, the value of eta will be tested to see if its value have an influence on the result. The value tested are 2.10^{-4} and 5.10^{-4} The alpha parameter is the spin depolarization. In the context of this paper, its value can be arbitrary. The real optical value is the fermi potential in eV. For the stainless steel, the value is 208 neV for the experiment. Finally, the correlation length is the roughness of the surface which is sometimes noted “w”. Its value here is 20 nm.

Generator source

The source can be placed at the origin coordinate of the simulation. The direction of the UCN is along the x-axis to enter in the beamline.

The particles have an initial energy given by a Boltzmann distribution. The typical temperature of UCN is a few microkelvins[2] which are nearly ~200 neV of kinetic energy. For the simulation, the temperature chosen is 3 mK.

The direction of the particles will be inside a cone of 90° of aperture. The initial position will be on an x fix with the value of 1 cm. The y and z coordinates will be given by a gaussian distribution with a mean value of 0 cm and sigma value of 5 cm.

An upper and lower boundary can be set on the initial kinetic energy, due to the gravity, the particles must have a minimum required energy to reach the top. This minimum energy is after simple calculation nearly 147 neV for the beamline. Also, the neutron can cross the beamline if the energy is higher than the fermi potential of the stainless steel. So this boundary can be set with wider energy to keep track the neutrons of interest and have a good statistics. The interval chosen is between 130 neV and 300 neV.

Trajectories

Before a great and heavy simulation, some constraints have to be managed such as time and computational resources. This section will pointed out two main factors to accelerate the simulation while keeping a good accuracy on the result.

A few parameters can be adjusted to accelerate or increase the accuracy of the simulation. These are the integrator which embedded at different order a Runge-Kutta integrator and the control time which manages the accuracy of the whole simulation. The test will be on five integrators: rk54, rk65, rk86, rk87, rk8 (the number after the name represents the order of integration) and the control time will be from 10 ns to 1 ms.

To prevent any earlier exit of the unique test particle by the entry of the beamline, a cylinder is placed at the entry. The neutron can bounce on it, like on the border of the beamline. This allows to keep the particle inside the beamline and see how far and how high can go the neutron.

Each test will have the same initial parameters. Each simulation will track one neutron with an energy of 180 neV along the x-axis which is above the minimum kinetic energy to reach the top of the beamline. The simulation stop until the neutron is at the end of the beamline or exit the beamline or reach the 10^8th step. The output saves every 100 steps the position and the kinetic energy of the particle.

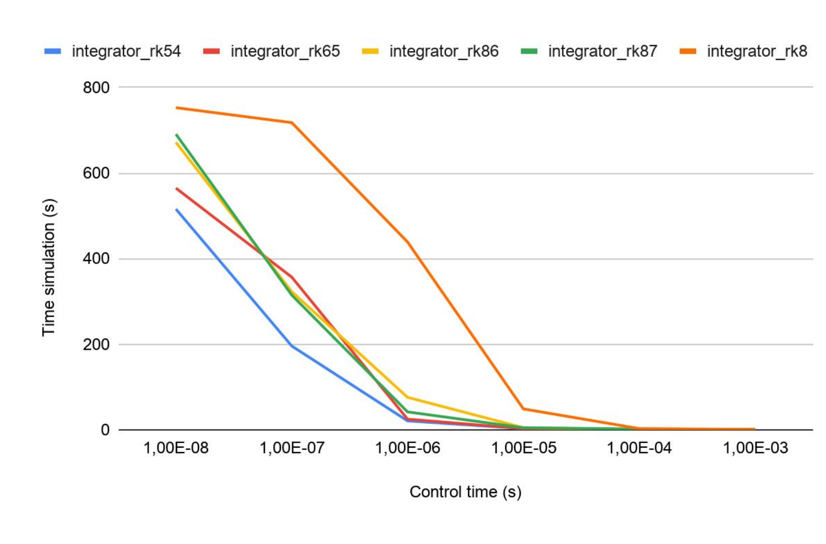
The main factors to compare the simulations are the time of a simulation, the number of steps to track the particle, the size of the output, the maximum altitude of the particle and the accuracy. Some factors will eliminate some option such as if the particle cross the beamline or if the output file is over 1Gb at the end.

After the simulations with the parameters presented above, the results can be summarized with the three following graphs.

First of all, the parameter eta for the surface interaction of UCN doesn’t influence the result of the simulation. So for the rest of the simulation, the parameter eta is fixed to 2.10^{-4} .

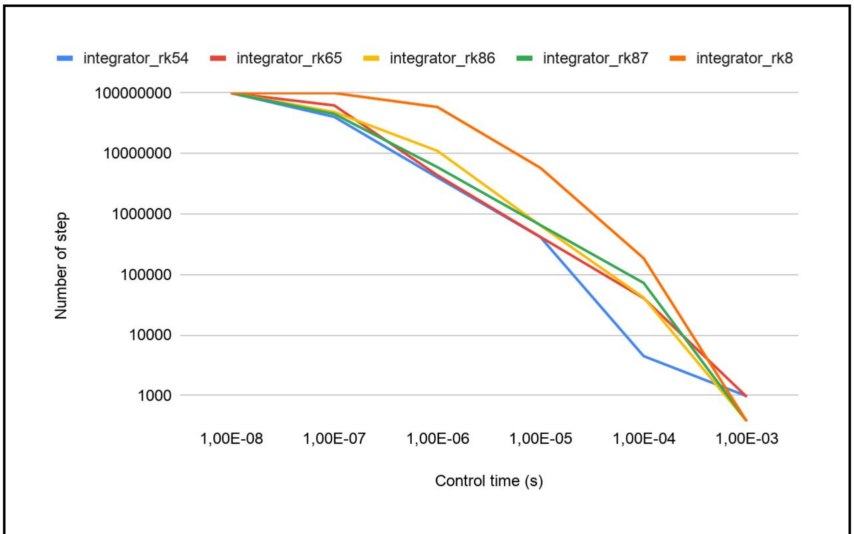
Secondly, a few simulations that have a high control time value exit the neutron of the beamline even if the energy was below the fermi potential of the stainless steel. However, some simulations pointed out an error which come from the GSL library. This error deals with finding roots of a polynomial equation. This can occur and stop the event of a particle or it can track the particle outside the beamline. Thankfully, this behavior seems to disappear when the control time value decreases.

Notice that these tests are just for one particle with the same initial condition. Other neutrons don’t produce GSL errors but it is still possible. The time of simulations changes a bit but the tests give a good overview of the impact of the different factors on the performance. A good indicator is the control time value set at 10 ns which has not produced a GSL error during the tests.



<u>Chart 1:</u> Evolution of the time of simulation against control time for different integrator

The chart 1 above show that when the control time decrease, the time of the simulation increase nearly exponentially. This trend is due to the accuracy of each integrator which are link with the control time. Of course, the lower the control time, the more accurate the results are. However this have a cost on the time of the simulation.



<u>Chart 2:</u> Evolution of the number of step against control time for different integrator

According to the chart 2, when the control time decreases, the number of step computed increase exponentially. This chart is analog with the output's size of the simulation. The more precise the run is, the heavier the output are.

To finally compare the control time values and the integrators, the following chart is constructed by divided the values of the chart 2 with the chart 1 to have number of step per second of simulation.

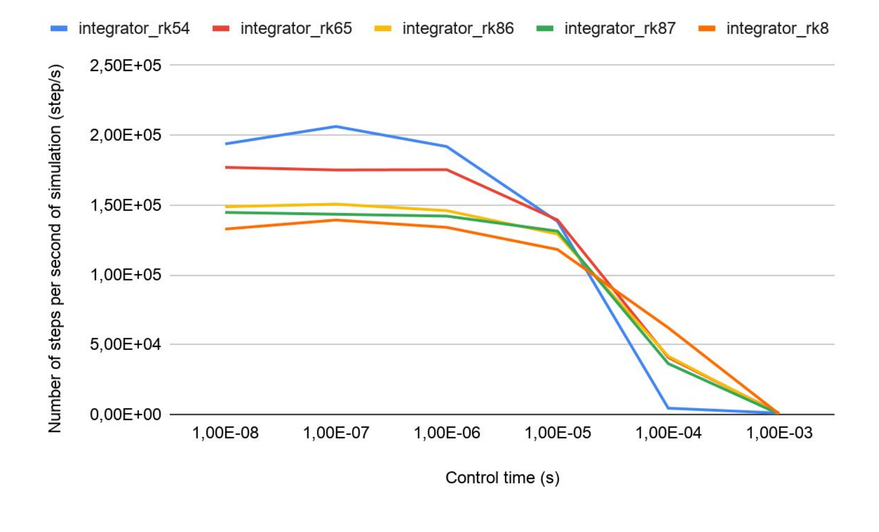


Chart 3: Evolution of the number of step per second of simulation

As the chart 3 shows, the trend seems to stabilize between 10ns and 10µs. Also the higher the value is on this chart, the more performant the simulation is. As pointed out by the two previous charts, the integrator_rk8 can't be used because it is to slow and the integrator_rk54 is the less precise.

To have faster simulation, a good compromise seems to use a control value of 10µs with the integrator_rk86 to keep a good precision with a high performance.

Another solution is to use the integrator_rk65 with a control time value of 1µs. This integrator is very fast and with a low control time the simulation keeps a good precision on the particle tracking.

Final parameters

The goal of this simulation is to interpret the effect of gravity on the spectrum of energy on the neutron at the entry and at the end of the beamline. So the output of this simulation must contain the spectrum at the initial time and at the end of each track. Adding to this the total number of steps and the terminator name to calculate the proportion which have succeeded to reach the end of the beamline. These will lighter the output file.

The geometry is composed of the beamline with the inner surface to lighter the structure and avoid neutrons inside the material. Two additional shapes are adding to this geometry. A disk places at the entry of the beamline to stop the neutrons when they exit too earlier. A cylinder places at the end to stop the neutrons and save the track into the output file, this shape can be seen as a detector. An additional structure is added to prevent an exit and reentry of the neutrons around the the detector.

The simulation must be run with a high number of neutrons inside the beamline. A test pointed out that one neutron reach the top per 10000 neutrons. To have a correct statistical results, the number of neutrons must be around 10^8 or more.

The simulations have been run with different seed and store in different outfile files. A Shell script provides an automatic run of the simulations. Another one can merge the output files to create a unique histogram to analyze.

Analysis

After nearly 83 hours of simulation and 374 entries, a trend seems to appear. Indeed, according to the two following histograms (chart 4), the UCN must have a minimum and maximum initial kinetic energy to reach the top of the beamline. In this simulation, the initial kinetic energy is in the interval [160; 280] neV. If the initial kinetic energy is too low, the neutron can't reach the top of the beamline because it can't fight the gravity. If the kinetic energy is too high, the neutrons cross the wall of the beamline.

In addition, the kinetic energy of these neutrons has decreased due to the gravity and the difference of altitude between the entry and the exit of the beamline. There is a shift of the spectrum to lower kinetic energy and now the maximum of kinetic energy is under 130 neV.

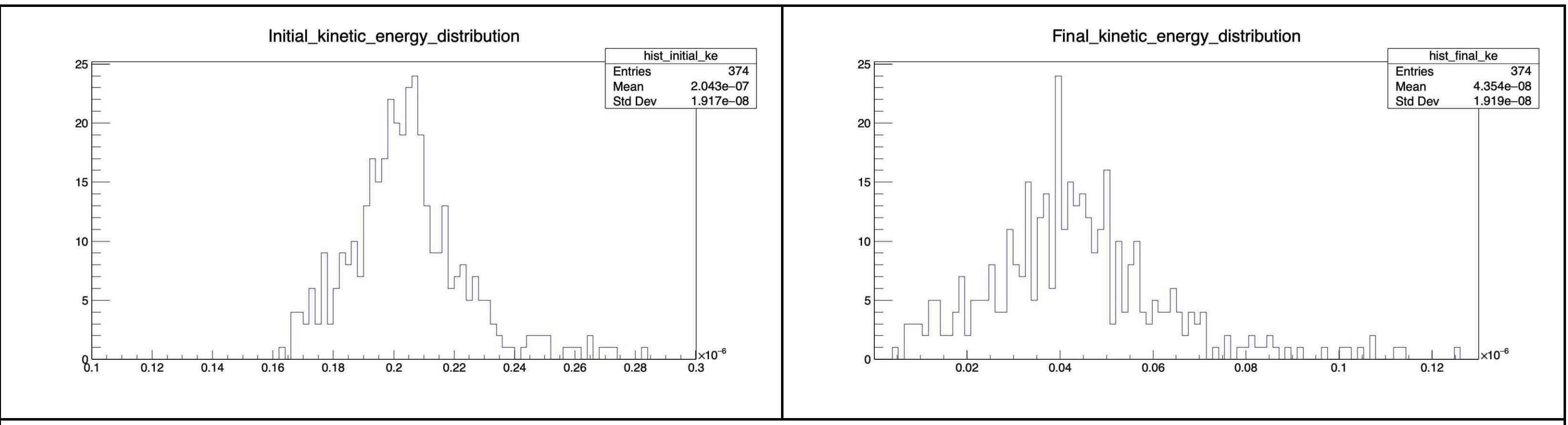


Chart 4: Histograms of the initial (left) and final (right) kinetic energy of UCN inside the beamline

The histograms have a shape that can be approached with a Boltzmann distribution. However, there is not enough data to fit a graph on the histograms.

In the end, the beamline acts like a high-pass filter for ultracold neutrons. It can provide to the experiment placed at the end a good source of ultracold neutron.

Bibliography

[1] Daniel Furse et al 2017 *New J. Phys.* 19 053012

[2] I. Altarev et al. Neutron velocity distribution from a superthermal solid 2H2 ultracold neutron source. *The European Physical Journal A*, 37: 9-14 July 2008.

[3] Z. Bogorad Ultracold Neutron Storage Simulation Using the Kassiopeia Software Package. *Massachusetts Institute of Technology 2019*, June 2019.

[4] F. Atchison et al. Diffuse reflection of ultracold neutrons from low-roughness surfaces. The European Physical Journal A, 44(1):23–29, Apr 2010.