Bug in ratpac-two Scintillation Spectrum Sampling

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ratpac-two issue

ratpac-two does not calculate the spectrum for scintillation light appropriately when given the spectrum as a function of wavelength.



Test setup

Generate a 'fake' scintillation material with the following emission spectrum:

```
SCINTILLATION_option: "wavelength",
SCINTILLATION_value1: [200.0, 800.0,],
SCINTILLATION_value2: [1.0,1.0,],
```

Run simulation many times and extract the photon energy at the beginning of each optical photon track and histogram the results

ratpac-two pdf sampling

The function ratpac uses to sample the scintillation spectrum is done with energy rather than wavelength as the random variable and when the ratdb entry is passed to this function, it calculates the transformation incorrectly



Change of coordinates with pdfs

Take some pdf q(y) and calculate the new pdf it in a more convenient coordinate system p(x) related by coordinate transformation y = g(x).

Conservation of probability over equal intervals: $P(a \le X \le b) = P(g(a) \le Y \le g(b))$

Use the Jacobian to preserve the measure. Skipping the math:

$$p(x) = q(g(x)) \left| \frac{d(g(x))}{dy} \right|$$

Simple Example: Uniform Distribution

Linear rescaling of your coordinates e.g. going from units of m to mm.

Assume we have a uniform distribution from 0 to 1 m q(y) = 1

Rescaling to mm we have y = g(x) = x/1000

Using equation from previous slide, we get the uniform distribution from 0 to 1000 we expect: p(x) = q(x/1000)/1000

Scintillation PDF: Wavelength to Energy

To convert a pdf in wavelength to a pdf in energy space we start with the user defined ratdb spectrum $q(\lambda)$ and transformation $\lambda = g(E) = \frac{hc}{E}$

Using the equation from the bottom of slide 5:

$$p(E) = q\left(\frac{hc}{E}\right) * \frac{hc}{E^2}$$

The red portion is what ratpac is missing

Revisiting the Problem

If we plot what we expect the distribution to be without the $\frac{hc}{E^2}$ scaling, we reproduce the distribution generated by ratpac in the toy model



Next steps

- Issue has been raised on Github
- Double check what scaling should be for dy_dwavelength
- Check impact on Eos simulation results
- Get everyone to update ratpac to eliminate issue from simulation data



Raw simulation output

In the previous slides I transformed ratpac output to be in wavelength to make the results less confusing since the user input was a flat spectrum. Here I histogram the 'raw' energy values from the sim and plot the expected theoretical distribution for flat scint spectrum from 200 to 800 nm in terms of energy for completeness

ratpac-two output 0.8 Theoretical PDF Normalized Photon Count 6. 7. 7. 9.0 7. 9.0 0.0 5 Photon Energy (eV)

Photon Emission Spectrum as a Function of Energy