Understanding Rapid Cycling Temperature Logs from the Vulcan Diffractometer

Garrett E. Granroth, Peter F. Peterson, Wenduo Zhou
Spectroscopy Group, Neutron Scattering Division
Oak Ridge National Laboratory

Introduction

The Spallation Neutron Source (SNS) facility at the Oak Ridge National Laboratory is designed to generate high-intensity neutron pulses for the study of materials. In recent years, time-resolved neutron experiments are enabling a broad set of new experiments at the SNS [1]. Often an external parameter such as temperature is varied as a function of time over the course of a measurement and then the datasets are sliced up according to that parameter. Using the external parameter to define the times at which the data is sliced allows the slicing to occur close to the experiment.

Dataset

The dataset provided is a sample environment log of temperature vs. acquisition time for a measurement on the Vulcan [2] beamline. The overall purpose of the neutron measurement is to understand the changes in structure of the material as a function of temperature. To do such a measurement, the sample is rapidly heated, and then the heat source is turned off so the sample temperature can relax. After the sample reaches equilibrium, it is rapidly heated again. The neutron events are acquired over the whole experiment, but we want to associate these events within a certain temperature bin upon cooling. Furthermore, the data will be time sliced, and then events of equivalent temperature will be combined. To that end, we need to understand the time of each temperature bin that we want to combine. This data challenge involves working with this temperature vs. time data [3] to arrive at information that would later be used for event processing.

File name	Description	Size
furnace2c.csv	Columns: (log of temperature, measured value)	1.2 MB

Questions/Challenges:

1. Identify the number of heat cycles.
2. Identify the time at which each heat starts (and the previous one stops).
   Note: Heat cycles with different heights are included in the dataset. We may decide to work with heat cycles of the same height.
3. Provide a function that will find the number of cycles of each height, within a given uncertainty.
4. Extend the function to provide the start and stop time for each heat cycle with a given height.
5. Provide a function that, for a given height of heat cycle and a temperature step size, will give a list of times for each temperature that would be used for combining.
   Note: We would be interested in some diagnostics to alert the researcher if the dataset shows that heat pulses expected to be identical are not.
6. Provide a function that indicates how each identical heat cycle of a given function would be helpful for answering the Data Challenge.
7. Devise a function that provides a visualization of the variation from one cycle to the next.

Our preference is for algorithms to be implemented in Python with the use of Numpy or other widely available libraries, although other libraries are welcome.

References:

[1] Granroth, G.E., An, K., Smith, H.L., Whitfield, P., Neuefeind, J.C., Lee, J., Zhou, W., Sedov, V.N., Peterson, P.F., Parizzi, A., and Skorpenske, H., 2018. Event-based processing of neutron scattering data at the Spallation Neutron Source. *Journal of Applied Crystallography*, *51*(3).

[2] Wang, X.L., Holden, T., Stoica, A.D., An, K., Skorpenske, H.D., Jones, A.B., Rennich, G.Q., and Iverson, E.B., 2010. First results from the VULCAN diffractometer at the SNS. In *Materials Science Forum* (vol. 652, pp. 105–110). Trans Tech Publications.

[3] Niyanth. S, Noyan I.C., Seren, M.H., and An, K., Vulcan Beamline dataset. Partly supported by the US Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office program. This research used resources at the SNS, a DOE Office of Science User Facility operated by Oak Ridge National Laboratory.