ADDIE User Manual

ADvanced DIffraction Environment

Data reduction software for NOMAD

April 4, 2017 version

Contents

Chapter 1

Introduction

1.1   What is ADDIE

The ADvanced DIffraction Environment (ADDIE) is User software for reducing and analyzing data on the Nanoscale Ordered MAterials Diffractometer (NO-MAD) instrument at the Spallation Neuron Source (SNS). Now, with a full plate of acronyms, let's begin.

ADDIE provides a graphical user interface (GUI) to interact with the underlying data reduction software. ADDIE aims to guide the workflow to go from launching the reduction of raw neutron data to provided processed individual runs, post-processing of these individual runs by applying optional corrections and summations, finally to visualization and output of the diffraction and pair distribution function data.

ADDIE in pre-installed on the Analysis cluster at the SNS (http://analysis.sns.gov). Instructions are provided for Neutron Sciences users to setup the Remote Desktop capablities to view, analyze and download your data from anywhere you go. Options are provided Windows, Mac, and Linux. Also, contact support information is provided in the case of any issues or needed troubleshooting.

ADDIE is also avaible open-source. Please contact your Local Contact from NOMAD if you would like to know more about the repository (or to contribute!)

1.2 Using ADDIE

ADDIE development has been funded by the US Department of Energy (DOE).

If you use ADDIE results in your published work, please cite the following papers:

(INSERT - ADDIE paper) (INSERT - other reduction dependencies - Mantid, GUDRUN, etc.)

For any of the following features for your published work, please cite the associated papers:

(INSERT - specific feature papers)

From the following, you can download a BibTex file with all citations.

Chapter 2

Getting Started

2.1 Background

What does ADDIE actually do during data reduction? For each run, we must have the following measurements for data reduction:

$$
\begin{aligned}
I_{sample} &= \text{sample intensity} \\
I_C &= \text{sample container intensity} \\
I_{Cb} &= \text{container background intensity} \\
I_V &= \text{vanadium intensity} \\
I_{Vb} &= \text{vanadium background intensity}
\end{aligned}
\tag{2.1}
$$

Why all these measurements for a single run? We want to measure only the coherent sample scattering (I_{sample}^{coh}). Unfortunately, we cannot suspend the sample in space inside the instrument. We must have a sample container. Thus, we measure the empty sample container intensity (I_C) in the instrument to subtract this from the sample scattering intensity (I_{sample}). Yet, we can have many different types of "containers" (i.e. sample environments such as a furnace or

cryostat, vanadium cans, quartz tubes, tubes in cans, etc.) Therefore, we must correct "from the outside in" where we subtract a completely empty instrument from the outermost containment scattering intensity, then subtract this from the next layer of containment and continue till we reach the sample subtracted (I_{sample}) from this collective background ($I_C + I_{Cb}$). Also, we do not know the exact beam profile to put the sample scattering intensity on an absolute scale. For this, we use vanadium to normalize the sample scattering intensity to extract the coherent scattering (I_{sample}^{coh}) from the incoherent scattering (I_{sample}^{inc}) on an absolute scale.

Why vanadium for normalization? We use vanadium for a few different reasons. 1) Vanadium has a small coherent scattering length but is a great incoherent scattering material. Thus, it does not contain large Bragg reflections in its profile that would have to be removed but provides a well-defined total beam profile. 2) Vanadium is a solid metal with well known density and stable without a container. 3) The large mass of vanadium atoms reduces the need to correct for inelastic scattering effects.

What else before we get our coherent sample intensity? Last, we must take into account the loss of intensity of the neutron beam as it passes through every material present in the experiment. To some degree, the sample, container, and vanadium will all attenuate the neutron beam. Ignoring the sample attenuation, we have:

$$I_{sample}^{coh} = \frac{I_{sample} - \alpha_c(I_C - I_{Cb})}{\alpha_v(I_V - I_{Vb})} \tag{2.2}$$

From the coherent scattering, we have the total scattering structure function given as:

$$
\begin{aligned}
S(Q) - 1 &= \frac{\frac{I_{sample}^{coh}}{N} - \langle b^2 \rangle}{\langle b \rangle^2} \\
&= \frac{\frac{d\sigma}{d\Omega} - \langle b^2 \rangle}{\langle b \rangle^2} \\
&=
\end{aligned}
\tag{2.3}
$$

5

where $\langle b \rangle^2$ and $\langle b^2 \rangle$ are the squared average and average squared scattering power of the sample where:

$$\langle b \rangle = \frac{\sum_i^N b_i}{N} \tag{2.4}$$

where b_i is the scattering power of atom i and N is the total number of atoms in the sample.

The pair distribution function (PDF) is obtained from the Fourier transform of $S(Q) - 1$:

$$G(r) = \frac{2}{\pi} \int_{\text{inf}}^0 Q[S(Q) - 1]\sin(Qr)dQ \tag{2.5}$$

2.2 Specifics of NOMAD data reduction

To obtain $S(Q)$ we using the following:

$$S(Q) - 1 = \frac{\frac{I_{sample}^{coh}}{N} - I_{poly}}{I_poly} \tag{2.6}$$

where

$$I_{poly} = \begin{cases} \frac{\rho\sigma d^2}{\rho_v \sigma_v d_v^2} & hyd = -1 & \text{absolute normalization} \\ & & \text{requires knowledge of sample properties} \\ & & \text{not done in autoreduction} \\ a_0 + a_1 q + ...a_n q^n & hyd = 0 & \text{least-square polynomial fit} \\ & & \text{of q-region qminpla} < Q < \text{qmaxpla} \\ xL(q_0) + (1-x)G(q_0) & hyd = 2 & \text{non-linear least square fit to pseudo-Voigt function.} \\ & & L(q) = \text{Lorenztian}, \ G(q) = \text{Gaussian} \\ & & \text{Used for samples containing hydrogen or deuterium} \end{cases}$$

Chapter 3

Workflow for Data Reduction

Just a test

3.1 Launch reduction of individual runs

3.1.1 Load input

3.2 Post-Processing of runs

3.2.1 Load Runs into Table

3.2.2 Selection of Runs

3.2.3 Selection of Post-Processing

3.2.4 Launch Post-Processing

3.3 Visualize Bragg Diffraction

3.3.1 Load Bragg data

3.3.2 Adjust Graphs

3.4 Visualize S(Q) and G(r)

3.4.1 Load S(Q) data

3.4.2 Adjust S(Q) graphs

3.4.3 Load G(r) data

3.4.4 Optimize G(r)