Manual for WAND² Powder Data Reduction

July 2021 Daria Soboleva, Virtual Summer Research Intern at Oak Ridge National Laboratory Mentor: Matthias D. Frontzek



Index

I. Loading the data	3
a. IPTS and Run Numbers	3
b. Initiating ThinLinc client session	4
c. Loading the data and Vanadium	5
d. Showing the data	8
e. <u>Metadata</u>	8
II. <u>Reducing Powder Data</u>	9
a. <u>WANDPowderReduction</u>	9
b. <u>Plotting the data</u>	10
III. Saving single and multiple powder patterns	12
a. <u>Saving one file</u>	12
b. <u>Saving multiple powder patterns</u>	13
c. <u>Downloading the data</u>	15

In this manual, you will find detailed instructions on how to load, reduce, and save powder diffraction data using MantidWorkbench Nightly. Instructions on how to use MantidWorkbench Nightly can be found in the dedicated manual (same webpage).

I) Loading data:

1) Go to <u>https://oncat.ornl.gov/#/</u> to correlate scan numbers to the scan title so you know what scan ranges are relevant for the reduction, and download data for Mantid if necessary. Click "Explore" and log in to OnCAT catalog with UCAMS.



2) Search for proposal number (IPTS) through: HFIR \rightarrow HB-2C \rightarrow IPTS.

			CG1B	DEV BEAM	Instrument Development Beam Line
HFIR	High Flux Isotope Reactor	_	CG1D	IMAGING	Neutron Imaging Facility
010	Challation Neutron Course		CG2	GP-SANS	General-Purpose Small-Angle Neutron Scattering Diffractomete
SNS	Spanation Neutron Source	_	C G 3	BIO-SANS	Biological Small-Angle Neutron Scattering Instrument
			CG4C	CTAX	Cold Neutron Triple-Axis Spectrometer
			HB1	PTAX	Polarized Triple-Axis Spectrometer
			HB1A	FIE-TAX	Fixed-Incident-Energy Triple-Axis Spectrometer
			HB2A	POWDER	Neutron Powder Diffractometer
			НВ2В	HIDRA	High Intensity Diffractometer for Residual stress Analysis
			НВ2С	WAND2	Wide-Angle Neutron Diffractometer
			НВЗ	TAX	Triple-Axis Spectrometer
			НВЗА	DEMAND	Dimensional Extreme Magnetic Neutron Diffractometer

3) Hit the according IPTS and click download icon for a file with data.

			NTS II RUNS II SCANS						🔲 RUNS 🔷 D	OWNLOAD	INFO						
Experiments				IPTS, E	≡ Runs			_	Run R	ange(s), e.g.	*12-15, 17	•	a t	×	=(۵	b.
IPTS	Exp(s)	Title	PI	From	Created	Run #	Sample Name	Notes	Title	Duration	Motor S1 Mean	Sample Temp Mean			Path		
IPTS-23858		WAND ² - Vanadium	Matthias Frontzek	2016/12/3	2021/05/25 15:42:07 EDT	531821	Vanadium Single Crystal	(unset)	Vanadium cycle 492	01:58:49	0	0	/HFIR/HB2C)	IPTS-2385	8/nexus/HB	82C_53182	1.nxs.h5
IPTS-22745		WAND ² - Calibration and Standards	Matthias Frontzek	2019/10/3	2021/04/13 11:56:55 EDT	474116	Vanadium Single Crystal	(unset)	Vanadium cycle 491	02:13:54	0	0	/HFIR/HB2C)	IPTS-2385	8/nexus/HB	B2C_47411	6.nxs.h5
	exp115 exp122				2021/02/25 13:28:50 EST	425539	Vanadium Single Crystal	(unset)	Vanadium cycle 490	02:26:53	0	0	/HFIR/HB2C)	IPTS-2385	8/nexus/HB	B2C_42553	9.nxs.h5
	exp124 exp129				2021/02/25 10:25:04 EST	425532	Vanadium Single Crystal	(unset)	Vanadium 490	00:19:15	0	0	/HFIR/HB2C)	IPTS-2385	8/nexus/HB	B2C_42553	2.nxs.h5
	exp136				2020/08/21 12:41:02 EDT	376206	Vanadium Single Crystal	(unset)	Vanadium	01:21:06	0	0	/HFIR/HB2C)	IPTS-2385	8/nexus/HB	B2C_37620	6.nxs.h5



4) Note run numbers for sample and Vanadium normalization found in excel downloaded file. You will need the Vanadium IPTS and scan number to input to the powder reduction algorithm.

2021/05/25 15:42:07 EDT	531821	Vanadium Single Crystal	(unset)	Vanadium cycle 492	01:58:49
2021/04/13 11:56:55 EDT	474116	Vanadium Single Crystal	(unset)	Vanadium cycle 491	02:13:54
2021/02/25 13:28:50 EST	425539	Vanadium Single Crystal	(unset)	Vanadium cycle 490	02:26:53
2021/02/25 10:25:04 EST	425532	Vanadium Single Crystal	(unset)	Vanadium 490	00:19:15
2020/08/21 12:41:02 EDT	376206	Vanadium Single Crystal	(unset)	Vanadium	01:21:06
2020/08/18 13:47:32 EDT	368223	Vanadium Single Crystal	(unset)	Vanadium Cycle 489	01:11:20
2020/07/07 13:53:53 EDT	368221	Vanadium Single Crystal	(unset)	Vana cycle 489	02:59:02

5) Go to SNS Cluster Link at <u>https://analysis.sns.gov/</u> and log in with UCAMS username and password. You can find more information on how to access ThinLinc client session and how to use MantidWorkbench on our website.



6) Once logged in, on the left upper corner, go to Application \rightarrow Education \rightarrow Mantid Workbench Nightly.



7) When MantidWorkbench opens, there will be an option to personalize the setup and tutorial available if needed. If a personalized setup is not necessary, close the "Welcome" window. You should see the following on your screen.

Back to Index

WAND² Powder Data Reduction on Mantid Workbench Nightly

Chromium Web Browser About Mantid Workb	ench 6.1.20210608.2323 ×		Chromie	ium V	/eb Browser Mantid Workbench		-	• ×
Access the Internet		File View Interfaces Help	Acce					
		Workspaces	l∎ ×	Ed	litor	₫ ×	Messages	@ ×
MANTID version 6.1.202106	508.2323	Load V Delete Clear		+	New × 1# import mantid algorithms, numpy and matplotlib	Doptions 🔻	Welcome to Mantid 6.1.20210608 Please cite: http://dx.doi.org 10.1016/j.nima.2014.07.029 and	8.2323 g/ d this
		Situation Save			<pre>2 from mantid.simpleapi import * 3 import matplotlib.pyplot as plt</pre>		release: http://dx.doi.org/10. Software/Mantid	.5286/
Welcome	Personal Setup	Vorkspaces	-		4 import numpy as np 5 6		date	10
Release Notes	Default Facility SNS Default Instrument ARCS							
Sample Datasets	Set data directories Manage User Directories							
Tutorials	Report Usage Data Privacy Policy	Algorithms	₪ ×					
Mantid Introduction	7	Execute	•					
Introduction to Python		Arithmetic CorrectionFunctions						
Python In Mantid	OAR RIDGE National Laboratory	 Crystal DataHandling 						
Extending Mantid with Pyth		Diagnostics Idle. Deta	ails	s	atus: Idie.			
Do not show again until next release	Close	Algorithms Plots		Ĩ	Editor IPython			

8) Go to Algorithms, and Type "LoadWAND" next to 'Execute' for powder data.



9) In the LoadWAND input dialog, enter IPTS and Run Numbers manually (**recommended**) **OR** hit "Browse" to locate IPTS file under data \rightarrow HFIR \rightarrow HB2C \rightarrow According IPTS \rightarrow nexus; select nexus from IPTS and find run number used.

nd sets proton charg	e to monitor counts	J	
Filename		Browse	
IPTS	22745		٢
RunNumbers	531817, 531818		0
	ApplyMask		
Grouping	None 👻		8
OutputWorkspace			81

Separate the RunNumbers by comma to load multiple run numbers or use dash to select range.

OR

Filename				Browse	
IPTS					8
RunNumbers					8
	Appl	yMask			
Grouping	None		•		8
OutputWorkspace					81

10) Check "Apply Mask" to mask detector edge limits (see algorithm description in docs.mantidproject.org for more information). Use 4x4 grouping if many manipulations will be done with the dataset; use of 2x2 grouping is recommended for faster processing without resolution loss.

	ApplyMask	
Grouping	2x2 💌	O
OutputWorkspace		⊗★
?	Keep Open 🗌 Run	Close

11) Name Output Workspace and hit "Run".

		🖌 Apply	Mask				
Groupir	ng	2x2				•	O
Output	Works						⊗★
?	Select the box the input dialo load Vanadiur	to keep g open to n later.		Кеер Ор	en 🗌	Run	Close

- 12) To upload Vanadium standard, use Filename or IPTS and run number determined from step
- 4. Check "Apply mask", name Output Workspace, and hit run to finish setting up workspace.

	LoadWAND input dialog	×
Loads Event Nexus goniometer, and sets p	file, integrates events, sets wavelength roton charge to monitor counts	, mask, and
Filename	Brow	wse
IPTS	23858	8
RunNumbers	320259	8
	✓ ApplyMask	
Grouping	2x2 •	O
OutputWorkspace	Vanadium	•
?	Keep Open 🗌 Run	Close

13) A folder will be created, which groups all the runs into a single workspace. Click on the arrow to see all the data.

Load 💌	Delete	Clear	Click on	data ar	nd sele	ct "Ungr	oup"	is nece	essary.	Similarly	y, selec
Ungroup	Sort 💌	Save 🔻	the data	Workspaces	Grou	p" to red # ×	uce	WO OF N	nore file	es.	×
Filter Works	paces			Load 🔻	Delete	Clear		Load 👻	Delete	Clear	
Workspaces			-	Ungroup	Sort 💌	Save 🔻		Group	Sort 💌	Save	
👻 🏛 Silicon				Filter Works	paces			Filter Works	paces		
🕨 🖩 Silic	on_1			Workspaces				Workspaces	_1		
► 🏼 Silic	on_2							Silicon	_2		

14) To view the data as it was collected on the detector, right click on data file in workspace and click "Show instrument".



15) To view metadata, environmental and instrument parameters for a run, right click on data and select "Show Sample logs" to show values of slits, temperature, and allow them to be plotted to see their values over the course of the run.

Workspa	ces	
🚽 🖿 Silic	on	
	Plot I	•
	Show Data	_
Algorithms	Show History	ē :
Execut	Show Instrument	-
	Show Sample Logs	
- Arichn	Show Slice Viewer	
- Crysta	Show Detectors	
▶- Dataŀ	Show Sample Material	
▶- Diagn	Rename	
	Save NeXus	s

	Name	Type	/alue	Units
1	1K_Plate	float series	0	к
2	CollimatorSensor1	int series	(1	
3	CollimatorSensor2	int series	(6	
4	HB2C:CS:CrystalAlign:UBMatrix	string series	arr	
5	HB2C:CS:ITEMS	int series	38	
	HB2C:CS:ITEMS:CanBarcode	string series	N/	
	HB2C:CS:ITEMS:CanIndicator	string series	N	
8	HB2C:CS:ITEMS:CanMaterials	string series	N/	
9	HB2C:CS:ITEMS:CanName	string series	N/	
10	HB2C:CS:ITEMS:Comments	string series	N/	
11	HB2C:CS:ITEMS:Component	string series	AL	
12	HB2C:CS:ITEMS:Container	string series	Al	
13	HB2C:CS:ITEMS:ContainerId	string series	AL	
14	HB2C:CS:ITEMS:Density	float series	0	
15	HB2C:CS:ITEMS:DensityUnits	string series	g/	
16	HB2C:CS:ITEMS:Description	string series	Va	
17	HB2C:CS:ITEMS:Formula	string series	V	
18	HB2C:CS:ITEMS:HeightInContainer	float series	0	
19	HB2C·CS·ITEMS·HeightInContainerLInits	string series	lu	

II) Reducing Powder Data:

Now that we've loaded the data into MantidWorkbench, we will integrate it into a 1D powder pattern for use in standard powder analysis software.

1) To reduce the data into a 1D powder pattern, we will use the WANDPowderReduction algorithm. Go to Algorithms, and Type "**WANDPowderReduction**" next to 'Execute' for powder data.

In the WANDPowderReduction GUI, we will need to pick an InputWorkspace (only workspaces loaded prior to the execution of the algorithm will show up in the dropdown list,) a calibration workspace (the Vanadium run,) provide the correct wavelength (usually 1.486AA but could be different depending on your experiment,) the desired x space, bin size and normalization parameters.

WAND	PowderReduction input dialog				
Performs powder diffract	ion data reduction for WAND				
InputWorkspace	Silicon Silicon_1 Silicon_2		*	Select group or individual file for input workspace	
BackgroundWorkspace CalibrationWorkspace BackgroundScale	Vanadium 1	•	C	Choose Vanadium for calibration	
MaskWorkspace		•	!		
Wavelength	0.946		Ċ	Background and Ma	ask
Target	Theta	•	Ċ	Workspaces are op	tional - leave
XMin				it, click on the arrow	w next to the
?	Keep Open 🗌 Run		Close	text box and select appropriate works	the bace.

2) Scroll down.

WA	NDPowderReduction input dialog	
Performs powder diffra	ction data reduction for WAND	Select "Theta" for Target (wavelength not needed if Theta
Target	Theta 🗸	is used). If selecting "ElasticQ" or "ElasticDSpacing" for
XMin XMax	Theta ElasticQ ElasticDSpacing	Target, the wavelength needs to be specified, default value 1.4865 A.
NumberBins	LogBinning	Select value for Number Bins. 1200 is recommended, which does 0.1° binning since the detector covers 120°.
MaskAngle OutputWorkspace	None Time Monitor	Select " Monitor " or " Time " to Normalize by; Monitor is recommended, which counts the number of neutrons.
	✓ Sum C	
?	Keep Open 🗌 Run Close	
Workspa	ces can be reduced individual	ly or can be
summed	together by clicking on Sum (e. g. measured at
two dete	ctor positions).	

3) Name the Output Workspace and hit "Run". Using the icon on the right will copy calibration workspace name and will not copy the name of the input workspace, so it is not recommended as it can possible overwrite calibration workspace. Name workspaces independently for changes to be made later without reloading the data.

OutputWorkspace	Si_reduced	Si_reduced		
	Sum	G		
?	Кеер Оре	Run	Close	

4) After the reduction is completed, right click on the data and select "**Plot...**", then "**Spectrum with errors**" to view reduced powder data and to make comparisons between intensities at different temperatures more meaningful.



5) Scale data to make it easier for *Fullprof*. Data files have intensities around 1 because they are normalized by the Vanadium. Go to Algorithms and execute "**MultiplyRange**".

MultiplyRange input dialog ×					
An algorithm to multip	ly a range of bins in a workspace by the factor	given.			
InputWorkspace	Si_van_reduced				
OutputWorkspace	Si_van_reduced_100				
StartBin	0				
EndBin					
Factor 100					
?	Keep Open 🗌 Run	Close			

Change the factor from 1 to 100. **100** is recommended (though the specific value is not hugely important: it has to be >>1 and be used consistently for all data reduced as part of the same analysis). Hit **Run**.

III) Saving Single and Multiple Powder Patterns:

1) Export XYE file in 1 of 2 ways:

a. When saving one file, execute "SaveFocusedXYE".

			SaveFocusedXYE i	nput dialog	×	
gorithms	回 ×	Saves a focused data exclusively) into a thre	set (usually the output o ee column format contain	of a diffraction focusing routi ning X_i, Y_i, and E_i.	ine but not reduced da the Input	ta fo
Execute SaveE	-	InputWorkspace	Si_out	*	Workspace	
SaveFITS		Filename	Si_van_reduced	Browse	e *	
Arithmetic SaveFocused)	KYE		Silicon Silicon_531817			
Correction SaveFullprofR	lesolution	StartAtBankNumber	Silicon_531818		Lit Browse to or	
 Crystal 			Vanadium		data in usors SN	ave c
 DataHandling 					foldor: namo the	2
 Diagnostics 		Format	VVE	-	filo bit Savo	-
		Format	ATE	•	me, mt save	
Idle.	Details	?	Кеер	Open 🗌 Run	Close	
Chromium Web Browser Access the Internet Name Silicon			Save			
dariasoboleva			Size Modified -			
TIS Decitor			14 Jun 14 Jun			
data			14 Jun 15 Jun			
Videos Pictures			Thu Thu			
Music			Thu Thu			
Public			Thu			
Downloads			Thu			
	SaveFocusedXYE in	put dialog	×			
		-				
Saves a focused data exclusively) into a thre	set (usually the output of ee column format contain	a diffraction focusin ing X_i, Y_i, and E_i.	g routine but not			
InputWorkspace	Si_van_reduced	-	0*			
InputWorkspace	Si_van_reduced	✓ /Silicon				
InputWorkspace	Si_van_reduced /SNS/users/	✓ /Silicon E	⊘★ Browse			
InputWorkspace Filename	Si_van_reduced /SNS/users/ SplitFiles	▼ /Silicon E	⊘★ Browse			
InputWorkspace Filename StartAtBankNumber	Si_van_reduced /SNS/users/ ✓ SplitFiles 0	✓ /Silicon E	⊘★ Browse			
InputWorkspace Filename StartAtBankNumber	Si_van_reduced /SNS/users/ SplitFiles 0 Append IncludeHeader	✓ /Silicon E	⊘★ Browse			
InputWorkspace Filename StartAtBankNumber	Si_van_reduced /SNS/users/ SplitFiles 0 Append IncludeHeader	✓	⊘★ Browse			
InputWorkspace Filename StartAtBankNumber Format	Si_van_reduced /SNS/users/ ✓ SplitFiles 0 △ Append ✓ IncludeHeader XYE	▼ /Silicon E	⊘★ Browse			7
InputWorkspace Filename StartAtBankNumber Format	Si_van_reduced /SNS/users/ ✓ SplitFiles 0 △ Append ✓ IncludeHeader XYE	Vilicon E	⊘★ Browse	Hit Run. Then	check is the file]

b. When saving <u>multiple powder patterns</u>, make sure that the files are grouped. Once they are, go to **File** on the left upper corner and hit "**Open Script**" or **Ctrl+O**.

File View Interfaces Help						
Open Script	Ctrl+O					
Open Project						
Save Script	Ctrl+S					
Save Script as						
Open Recently Closed Scripts	•					
Generate Recovery Script						

i. Follow the path data \rightarrow HFIR \rightarrow HB2C \rightarrow shared \rightarrow WANDscripts and locate

"save_multiple_powder.py".

•		data	HFIR	HB2C	shared	WANDscripts	•
	writer.py					2.5 KB	/ Mar
	writer2.py					2.5 kB	7 Mar
	Old						9 Mar
	workaround_nuclear.py					1.1 kB	12 Apr
	save_multiple_powder.py					1.1 kB	19 Apr
	SCD_MDE_Vana.py					1.4 kB	29 Apr
	scd						24 May
	Filter_combined_ZYP.py					6.9 kB	25 May

ii. Before running the script, it is necessary to change the group workspace name to the one used in your reduction and then select the code snippet for how you wish to name the saved the individual files Edit file by editing the second line, group name. Type output workspace into brackets.

+	New ×	save_multiple_powder.py	×	+
	2 grp = mtd	'output_th']		
	4 # Save by	title		
	5 for ws in	grp:		

+	New ×	save_multiple_powder.py*	×
	1 from manti	id.simpleapi import *	
	2 grp = mtd	['Si_van_reduced_100']	
	3		

iii. Highlight the first two lines of the script (or hit Ctrl + Enter) and hit Execute. Running these

two lines will load into mantid a variable with the name of the workspace you want to save.

+	New ×	save_multiple_powder.py*	×	Deptions V
	1 from mant 2 grp = mtd 3	id.simpleapi import * ['Si_van_reduced_100']		

iv. Next, you will have to decide how you wish to name the saved files and select the relevant code snippet for that naming convention. The script has several options, to save by run number/title, by run number, by run title, by time averaged value, etc. Highlight the **#Save by run number and title** and all the lines below to save the file by title and run number; similarly, the file can be saved by other characteristics (**#Save by run number** the **#Save by title**, **#Save by time average value**, etc.). Once you've highlighted the relevant code snippet click run (or **Ctrl + Enter**) to execute those lines of code.



v. In order to locate the saved data, go to File, navigate to the folder where you've been saving the files, and click on Modified to organize by the latest modification.

🔩 Activities 🛛 Applications 🔫	Places 👻 📻 📄 🔚 작 Mantid Wor 👻
	Chromium Web Fileswser A cAccess and organize files
File View Interfaces Help	
Workspaces	回 × Editor

Name	Size	Modified 🔺
531817-Si standard 0.946A 2theta=35deg.xye	62.4 kB	16:37
Si standard 0.946A 2theta=35deg.xye	62.4 kB	14:08
531817.xye	62.4 kB	10:50

vi. If you want to download these files for use with Rietveld refinements on your local PC/laptop, you can either use a server storage service like Google drive or Dropbox, or download using FileZilla or WinSCP (link on the webpage)..