DCS data reduction and analysis: a quick manual

In the summer school, we are doing QENS experiments on powder samples using DCS. Here is a quick manual showing how we do data reduction and analysis. (Note that for DCS data on single crystal samples, the data reduction procedure would be significantly different.)

We use the program Mslice in the DAVE package for data reduction. (For detailed instructions on how to use Mslice, please refer to:

 \times Untitled - Data Analysis and Visualization Environment Data Input/Ouput Data Reduction **Planning Tools** File Analysis Misc Tools Help NCNR DCS Reduction (Mslice) > ଳି 📕 ରେସ PSI > FANS Reduction Data Browser Visualization Brow ISIS > **NSE Reduction**🖻 Data ILL > MACS Reduction (Mslice) HFBS > TAS > $\mathbf{1}$ \mathbf{X} Parameters:types of the BARPLOT visualization Parameters Y: IDLVECTOR Select a visualization BARPLOT ~ X: IDLVECTOR Y * VERTICES : IDLARRAY2D Х Y ERROR : IDLVECTOR, IDLARRAY2D X ERROR : IDLVECTOR, IDLARRAY2D VERTICES PALETTE : IDLPALETTE, IDLARRAY2D Y ERROR VERTEX COLORS : IDLVECTOR, IDLARR **X ERROR** < > * indicates a required parameter Visualization Task:
New Modify Add New Visualization

http://www.ncnr.nist.gov/dave/documentation/dcs_mslice.pdf)

In Mslice, we can set the Data Directory and Working Directory, just for convenience.

slice	Ms	lice for	DCS						_			\times
File	Para	meter	Back	grour	nd M	lask	Optior	ns Windov	v Help			
Driv	6 10 10	Load F Save F	Param Param	neters. neters						Ctrl+ Ctrl+	-L S	
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4101 4251 D-4(Dark		Chang Chang	e File e Em	e Com pty Ca	binati an Su	on To btrac	olerance tion To	e Value lerance Valu	ıe)ata (
Van		Set Da	ita Di	rector	y							
View		Set W	orkin	g Dire	ctory.							
u1	Q		~	Lat Q	bel							
u2	En	ergy	\sim	E					Calcula	ate Pr	rojecti	ons
Slice	C	ut De	etecto	r Traje	ctory	Calcu	ulator					
x	Q		\sim	from:	0.3		to:	1.85	step	0	.1	
у	En	ergy	\sim	from:	-1		to:	1	step	0	.01	
		intensi	ty ran	ge			to:		color	table	e	
	smoothing level 0 shading Flat V CB-Spectral V											
							Fit	Plot Slice	Oplot Sli	ce	Surf S	Slice

For the program to take care of background subtraction during data reduction, highlight the corresponding files and load them. Shown below is the "dark count" (beam closed) background subtraction.

M slice	-Mslice for	DCS				_		×
File	Parameter	Backgrou	nd Mask	Option	ns Window	v Help		
Drive	e: C:\ < C:\Users\ 0619_009.dd	Load Load Load	Empty Ca Detector Time Cha	an File(s) Backgro annel Bac	und File(s) kground Fi	 le(s)		r v
		Load	Dark Cou	unt File(s))			nit)
		Set C	verall Bac	kground	Rate			
		Clear	Backgrou	Ind				
		Load	Vanadiur	n File(s)				dd Data
		Clear	Vanadiur	n				ta
Viewir	ng Axes:	La	bel					
u1	 Q 	~ Q						
u2	Energy	~ E				Calcul	ate Pr	ojections
Slice	Cut De	etector Traje	ctory Calo	culator				
x	Q	✓ from:	0.3	to:	1.85	step	0.	.1
у	Energy	✓ from:	-1	to:	1	step	0.	.01
	intensi	ty range		to:		color	table	÷
	smooth	ning level	0	shading	Flat 🖂	CB-Spe	ctral	×.
				Fit	Plot Slice	Oplot S	lice	Surf Slice

If we have data measured for the empty can, we can do empty can background subtraction, in which case we would not need the "dark count" background subtraction (the empty can data would already include dark count fast background).

slice	Mslice for	DCS							_		×
File I	Parameter	Back	groun	d Ma	ask	Optior	าร	Window	/ Help		
Drive	e: C:\ ×		Load	Empty	/ Ca	n File(s)					
(2) (C:\Users\		Load	Detect	tor E	Backgro	un	d File(s)	•		r
2012	1113_008.d	_	Load	Time (Char	nnel Bac	:kg	round Fi	le(s)		~~
2012	1113_009.d	\checkmark	Load	Dark (Cour	nt File(s)				nit)
2012	1113_010.d		Set O	verall	Back	ground	d R	ate			
			Clear	Backg	rour	nd					
		\checkmark	Load	Vanad	lium	File(s)					dd Data
		_	Clear	Vanad	lium		_				ta
Viewir	ng Axes:		Lab	el							
ul	Q _	~~									
u2	Energy	×.	E						Calcu	late	Projections
Slice	Cut De	etecto	or Trajec	tory (Calcu	ulator					
x	 Q	\sim	from:	0.3		to:	1.8	35	step)	0.1
у	Energy	\sim	from:	-1		to:	1		step)	0.01
	intensi	y ran	ge			to:			color	ta	ble
	smooth	ing le	vel	0		shading	Fla	at 🖂	CB-Spe	ectra	×
						Fit	Ρ	lot Slice	Oplot S	lice	Surf Slice

To correct detector efficiencies, we load the vanadium files.

sice -	-Mslice for	DCS					_		×
File	Parameter	Backgr	round	Mask	Optior	ns Window	v Help		
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2012	1113_011.u	Cl	lear Ba	ckgrou	nd				
		Lo	oad Va	nadium	n File(s)				dd Data
		Cl	lear Va	nadium	1				ta
Viewii u1	ng Axes:	~ G	Label 2						
u2	Energy	×					Calcul	ate F	Projections
Slice	Cut De	etector T	rajecto	y Calc	ulator				
x	Q	× fr	om: 0.3	3	to:	1.85	step	(0.1
у	Energy	× fre	om: -1		to:	1	step	(0.01
	intensi	ty range			to:		color	tab	le
	smooth	ing level	0		shading	Flat 🖂	CB-Spe	ctral	
					Fit	Plot Slice	Oplot S	lice	Surf Slice

For QENS analysis, to omit detectors that contain Bragg peak intensity, we load the sample data first, and then "Mask Bragg Peaks".

M	Malico for	DCC								\sim	
slice	-IVISIICE TOP	DC2								\sim	
File I	Parameter	Back	grour	nd M	lask	Optior	ns Window	v Help			
Drive	: C:\ ×										
r a		wzho	J\Desk	top\G	rou	Sam	ple Type	Powder			
2013()619_015_d	e 07				E Re	bin Size	1 ~			
20130)619_016.dd	s.gz				Intens	sity Label	Intensity	ntensity (arb. unit)		
20130	0619_017.dc	cs.gz				Title L	abel 💣				
20130)620_002.do	s.gz				Lege	nd Label				
20130	0620_003.dd	cs.gz					L	Load Da	ata	Add Data	
								Select	the f	iles first or	
	A							Delece			
viewir	ig Axes:		Lat	bel							
u1	 Q	\sim	Q		7						
u2	Energy	\sim	E		1			Calcu	late F	Projections	
Slice	Cut De	tocto	r Traio	ctony		ator					
0100			i naje		Calcul	ator] .	1.05	1.	Γ	0.1	
x	IQ	~~	from:	0.3		to:	1.85	step)	0.1	
у	Energy	~~~	from:	-1		to:	1	step		0.01	
	intensit	y ran	ge			to:		color	tab	le	
	smooth	ing le	vel	0		shading	Flat 🗸 🗸	CB-Spe	ectral	\sim	
						Fit	Plot Slice	Oplot S	lice	Surf Slice	

🔝Mslice for DCS				_			\times	
File Parameter Background	Mas	k Optior	s Window	wН	elp			
Drive: C:\ ~	-	DCS Mas	k	>				
😰 🗈 C:\Users\wzhou\Desktop)	Set Mask		>	Pow	/der		
20130619_015.dcs.gz	Plot Mask			>	> By Detector N			lumber
20130619_016.dcs.gz	Read Mask File By Detector				ector A	ngle		
20130619_017.dcs.gz		Save Mas	sk File		N	lask B	Bragg F	eaks
20130620_002.dcs.gz		Clear Mas	sk		эκ			
20130020_003.dc3.gz				Loa	d Data	Add	Data	
					Clear	Data		
Viewing Axes:								
Label								
u1 Q ~ Q								
u2 Energy V E				Ca	alculate	Projec	ctions	
Slice Cut Detector Trajecto	ry Ca	lculator						
x Q × from: 0.3	3	to:	1.85		step	0.1		
y Energy \checkmark from: -1		to:	1		step	0.01		
intensity range		to:		C	olor tal	ble		
smoothing level		shading	Flat 🖂	CB-	Spectra	I	~	
		Fit	Plot Slice	Opl	ot Slice	Surf	Slice	



For QENS analysis, the symmetrized $S(Q, \omega)$ is what we want, so we change the "View Intensity As" selection accordingly.

	M slice	-Mslice for DCS		– 🗆 🗙	
	File	Parameter Background Mask	Ор	tions Window Help	
	Drive	a. C:\ ∨	_	Instrument Geometry	>
	S(0	Q,omega)		View Intensity As	>
•	 Syr 	mmetrized S(Q,omega)		Binning Method	>
	d2	!(sigma)/d(Omega)d(Ef)		Monitor Count	>
	Ch	ii(Q,omega)		Absorption Correction	>
	GE	OOS		Viewing Axis	>
	VD	OOS		Folding Type	>
	J(C	2,y)		Show Powder Line	>
	Un	adjusted by ki/kf factor		Elastic Peak Position Adjustment	>
	E-I	Integrated Intensity		Empty Can Subtraction Tolerance Method	>
	u1	Q × Q		Allow Overplotting to Other Mslice Plots	>
	u2	Energy V E		Allow Voronoi Diagram	>
	Slice	Cut Detector Trajectory Cal		Slice Plot Empty Grid Color	>
	~			Plot Window Background Color	>
	X		_	Plot Window Default Size	>
	У	Energy v from: -1	-	Plot Window Text Rendering Method	>
		intensity range	_	User Macro	
		smoothing level	-	Dark Angle Correction	
				Show Dark Angle Trajectory	
			~	E-Dependent Detector Efficiency Correction	
				Hide Error Bar	
				Allow NCNR FTP Server	
				View Spurions	>

Now we can reload the data and click "Calculate Projections".

sice -								
	-Mslice for	DCS					- 🗆	\times
File	Parameter	Back	grour	nd Mask	Option	ns Windo	w Help	
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2013	0619_016.d 0619_017.d	ics.gz lcs.gz			Inten:	sity Label	Intensity (art	0. UNIT)
2013 2013	0620_001.d 0620_002.d	cs.gz cs.gz			Leae	nd Label	T=410 K	5313#2 1-4
2013	0620_003.d	lcs.gz			Logo		Load Data	Add Data
							Clear	Data
Viewi	na Axes							
			Lat	bel				
u1	Q	×.	Q					
u2	Energy		E				Calculate	Projections
Slice	Cut De	etecto	r Traje	ctory Cal	culator			
x	Q	×	from:	0.3	to:	1.85	step	0.1
у	Energy	\sim	from:	-1	to:	1	step	0.01
	intensi	ity ranç	ge		to:		color ta	ble
	smooth	ning le	vel	0	shading	Flat ~	CB-Spectra	× –
					Fit	Plot Slice	Oplot Slice	Surf Slice
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D.	Parameter	Back	cgrou	nd Mask	c Optio	ns Windo	ow Help	
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Drive 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015 2015	e: C:\ c: USers 0619_015.d 0619_016.d 0619_017.d 0620_001.d 0620_002.d 0620_003.d ng Axes: Q Energy Cut QI Energy intensis smooth	Back	kgroun u\Desk IQI E from: from: ge vel	bel ctory Cal 0.3 -1	culator culator to: shadin	ns Windo ple Type ebin Size sity Label abel and Label 1.85 1	Pow Help Pov 1 Intensity (arl mn.dcs.pyz 3 T=410 K Load Data Clear Calculate step step color ta CB-Spectra	vder b. unit) SS13 #2 T=4 Add Data r Data Projections 0.1 0.01 bble al ~

Now we are ready to plot the data. We can use "Plot Slice" to plot the Intensity as function of both Q and E.

M slice -	-Mslice for	DCS							_			×
File	Parameter	Back	grour	nd N	/lask	Optior	ns Wir	ndov	v Help			
Drive	e: C:\ ~											
1	C:\Users	wzho	u\Desk	top\G	irou	Sam	ple Type	,	Powder			
2013	0619_015.d	cs.gz				E Re	bin Size	,	1 ~			
2013	0619_016.d	cs.gz				Intens	sity Labe	el	Intensity (ensity (arb. unit)		
2013	0620_001.d	lcs.gz				Title Label 💣 mn.dcs.pyz						2 T=4
2013	0620_002.d	cs.gz				Lege	nd Labe	el [T=410 K			
2013	0020_003.u	ics.yz						[Load Dat	a	Add	Data
									Cle	ear	Data	
Viewin u1	ng Axes: Q	×~1	Lal	bel								
u2	Energy	~	E						Calcula	te I	Projec	tions
Slice	Cut D	etecto	or Traje	ctory	Calcu	lator						
x	Q	\sim	from:	0.3		to:	1.85		step		0.1	
у	Energy	\sim	from:	-1		to:	1		step		0.01	
	intensi	ity rang	ge			to:			color	tat	ole	
	smooth	ning le	vel	0		shading	Flat	\sim	CB-Spec	tral		
						Fit	Plot S	lice	Oplot Sli	ce	Surf	Slice



The Slice data can be saved as a DAVE file (to be analyzed using the PAN program) or in some other ASCII format.

M	Mslice for	DCS					_		×	
File	Parameter	Bac	kgrour	nd Mask	Optio	ns Windo	w Help			
	File Type				>					
	File Tools				>	ple Type	Po	owc	ler	
	Save Volum	ne Da	ita As		>	bin Size	1		×.	
	Save Slice E	Data /	As		>	DAVE	File			
	Save Cut D	ata A	S		>	SPE Fi	le			
	Save Projec	tion	As		>	I,Err,X,	Y 4-Colur	nn l	File	
	Read and P	lot A	SCII D	ata File		X,Y,I,E	rr Matrix F	-ile		
	Execute Scr	ipt Fi	le			Send	to DAVE [Data	Manager	
6	Load Sessio	on								
	Save Sessio	on								
	Recent Files	5			>					
	Clear File H	istory	/				Calcula	te P	rojections	
	Exit									
x	Q		from:	0.3	to:	1.85	step	C).1	
у	Energy	\sim	from:	-1	to:	1	step	C).01	
	intensi	ty ran	ge		to:		color	tabl	е	
	smooth	ning le	vel	0	shadin	çFlat ∽	CB-Spec	tral	~	
					Fit	Plot Slice	Oplot Slid	ce	Surf Slice	

The data can also be plotted as "Cut" (e.g., Intensity vs. Q or Intensity vs. E etc.)

sice	Mslice fo	or DCS						_			\times
File F	Paramete	r Back	grour	nd M	lask	Optior	ns Windo	w Help)		
Drive	: C:\ ×										
(j) 🗈	C:\User	s\wzho	u\Desk	top\Gi	rou	Sam	ple Type		Pov	/der	
20130	0619 015	.dcs.az				E Re	bin Size	1			\sim
20130	0619_016	dcs.gz				Inten	sity Label	Intensit	y (arł	o. unit)	
20130)619_017.)620_001.	.dcs.gz .dcs.gz				Title L	abel 💣	mn.dcs.	pyz S	SS13#	‡2 T=4
20130	0620_002	.dcs.gz				Lege	nd Label	T=410 k	<		
20130	1620_003	.acs.gz						Load D)ata	Add	Data
								(Clear	Data	
Viewir u1	ng Axes: Q		Lat	bel							
u2	Energy	×.	E					Calc	ulate	Projec	tions
Slice	Cut I	Detecto	or Traje	ctory	Calcu	ulator					
along	Energy	\sim	from:	-1		to:	1	ste	р	0.01	
	 Q 	\sim	thick			to:		symt	loc	blue	×.
у	Intensity	~~	range			to:		circle	2	solid	
							Fit	Plot (Cut	Oplo	t Cut



We can compare different data sets by loading new data and using "Oplot" to plot the data.

.	Mslice fo	or DCS						- 🗆		×
File F	Parameter	r Back	grour	nd M	1ask	Option	ns Windo	w Help		
Drive	c:\ ×									
© E	C:\User	s\wzho	u\Desk	top\G	rou	Sam	ple Type	Pov	vder	
20130	618_025.	dcs.gz				E Re	bin Size	1		2
20130	618_026.	dcs.gz				Inten	sity Label	Intensity (art	o. unit)	
20130)618_028.	dcs.gz				Title L	abel 💣	mn.dcs.pyz	SS13 #	3 T=1
20130	618_029.	dcs.gz				Lege	nd Label	T=100 K		
								Load Data	Add	Data
								Clear	Data	
Viewir u1	ng Axes: Q	×.	Lat	bel						
u2	Energy	\sim	E					Calculate	Projec	tions
Slice	Cut [Detecto	r Traje	ctory	Calcu	ulator				
along	Energy	\sim	from:	-1		to:	1	step	0.01	
	Q	~	thick			to:		symbol	blue	~~~
у	Intensity	\sim	range			to:		circle 🗠	solid	, v
							Fit	Plot Cut	Oplo	t Cut



The "Cut data" can be saved as well.



We also need to reduce the Vanadium data (to be used as instrument resolution). For Vanadium (no Bragg peaks), we don't want to use masks. Other than that, the procedure is the same.

Mslice for DCS									_			Х
File	Parameter	Back	groun	d N	1ask	Optio	ns	Windov	v H	elp		
Drive: C:\ C:\ C:\Users\wzhou\Desktop				op	DCS Mask Set Mask Plot Mask Read Mask File Save Mask File				> >	Powder		
20121113_008.dcs.gz 20121113_009.dcs.gz 20121113_010.dcs.gz 20121113_011.dcs.gz				1				File File	>	sity (arb. unit)		
					C	lear Ma	isk			эκ		
				-					Load	d Data	Add I	Data
										Clear	Data	
Viewing Axes:												
u1	Q	25	Q									
u2	Energy	\sim	E						Ca	alculate	Project	tions
Slice	Cut D	etecto	r Trajec	tory	Calc	ulator						
along	Energy	\sim	from:	1		to:	1			step	0.01	
	Q	\sim	thick			to:			sy	mbol	black	\sim
у	Intensity	\sim	range			to:			circl	e ×	solid	\sim
								Fit	Plo	ot Cut	Oplot	t Cut

Intitled - Data Analysis and Visualization Enviro	onment — 🗆 🗙
File Data Input/Ouput Data Reduction	Analysis Planning Tools
Misc Tools Help	Data Transform 1
· · · · · · · · · · · · · · · · · · ·	Data Transform 2 >
Data Browser Visualization Browser	Peak Fitting - 1D and 2D (PAN)
Data	Peak Fitting (RAINS)
	Honevcomb Diffusion Fitting
	Mslice - TOF/TAS Analysis
	Fourier Transform Toolkit
	MagProp: Workup and Analysis of Magnetic Data
	Operations Preferences
Parameters	meters:types of the BARPLOT visualization
Select a visualization BARPLOT	
Y* VERI	FICES : IDLARRAY2D
X YER VEDTIOES XEB	ROR : IDLVECTOR, IDLARRAY2D ROR : IDLVECTOR IDLARRAY2D
Y ERPOR PALE	TTE : IDLPALETTE, IDLARRAY2D
X FRBOR	TEX_COLORS : IDLVECTOR, IDLARRA
* indicates a required parameter	
New Modify	Add New Visualization
DCS	

We use the PAN program for data analysis.

We first load the DAVE file of the sample.

💹 PAN: Peak Analysis -		- 🗆 X		
File Data Resolution Plot_Options Hot_Keys Print Help				
Load DAVE file		^		
Load ASCII Data File >				
Load test data				
Load 2nd test data				
Display current file information				
Rebin data				
Crop data				
Edit Pan Mask				
Restore Original data	<	>		
Save data and fits to text file	HTML Log Controls			
F Save data, fits, and selected curve to text file	Create new HTML log file	Open existing HTML log file		
Save data and fits to EXCEL-readable ASCI	Entor commont	Add plot to log		
Save fits only to FXCEL-readable ASCI	Enter comment Add plot to log			
Fluch and close all open files	Close HTML log file			
	Log file status:	Log file name		
Fit all groups	closed			
Interrupt fit		erential Evolution Algorit		
Groups to fit	Enable DE Algorithm?	No		
	Method of Evaluating ChiSq	Mean square error (MSE		
Fitting status	Population factor (x nos para	ms) 10		
Resting	Max function evaluations	10000		
	Param Error: ChiSq Threshol	d (%) P		
View CORR matrix	Terminating ChiSq Tolerance	0		
Refresh Fit Results	Generation Count	0		
Analyze Fit Parameters	Current ChiSq	0		
Plot EISF	1			
# of MC data sets				
100				
Monte-Carlo error estimate	X: -53.9 Y: 8.90E+03			

We then load the DAVE file of Vanadium (or the data file of the sample measured at very low T if it).





Now we can fit the data. In this case, we use a linear background, a Delta function and a Lorentzian function.



Once the data fitting is done, we can "Analyze Fit Parameters" and "Plot EISF"





We can further save the EISF data as an ASCII file, and fit the data to investigate its Q dependence etc.