

QtiSAS | JNSE v.2021-01-05

Implementation (transfer) of J-NSE tools to QtiSAS



Compile Fitting Functions

C	10	0 f(x) 0 20	9 f(x,y,)	😭 save	delete	le
ate	egor	ries			Functions	+
ipi ipi ipi ID IIS	egral opro osor RG/ P-fu T-F	Is Test oteins me-Scatterir mes ARITA inctions IT-TESTS	ng-SMA		doubleDiffusion jumpDiffusion simpleDiffusion stretchedExp	
S	E				doubleDiffusion	
				0		
p	end	lent variable	lqt			۲
le	pen	ndent variab	le(s) t			
		Name	Initial Value [FromTo]	Vary?	Info	1
	^	q	1[0inf]		Wavevector	
	^	AO	1[0inf]		Prefactor	
	٨	A1	1[0inf]		Prefactor	
	^	DO	0[0inf]		Diffusion coefficient in units [[q]**-2/[t]]	
			1			1
	Co	de +	Included +Fortran	Info	Fit.Control Files Opt	ions 😱
	sat	sview qtikws	/qtisas fortran			
00	6 7 8	//> lqt = lqt = A0 * c lqt+= A1 * c	:f(1, {P1,}); exp(-q~q * (D0 * t + 0.5 * fab exp(-q~q * (D1 * t + 0.5 * fab	s(w0) * w0 * s(w1) * w1 *	t * t)); t * t));	



666

JNS

- In "NSE" folder few examples of NSE-related fit functions
- If not inside: download nse.zip file and un-zip it in fitFunctions folder
- Compile all functions: "compile all"

Fitting Interface

10.00

00	FITTABLE(s)	ing m		DAN
Categories	Load Fitting Session Select Function Functions	Fitting Session		
Fio Form Factors Form Structure General HF Instrumentation Integrals Test Lipoproteins Liposome-Scattering-SMA Liposomes MARGARITA	jumpDiffusion simpleDiffusion stretchedExp			FIT
NDP-functions NST-PTT-TESTS NSE Origin::Built-In Origin::User-Defined PeakFunctions PeakFunctionsEfit Pederson QENS Rei SASfit Scatt. Laws				FIT
Info :: Fun	Info :: Parameters	Options		
				SVD
		•	Select "NSE" in Categories	
				JNSE
Fit Curve(s)	v.5.2-23.12.2020	Vitaliy Pipich @ JCNS		



J-NSE interface: data import tools

N								
	Multi-Fit	ting						
				(٦
tation/J	JNSE/da	ita			1		2	
					_			í
			_					-
							ple)	
NSE	E-da	ta						
NSE	E-da	ta						
NSE	E-da	ta						
NSE le r	E-da nam	ta e (f	or	inf	ō-t	abl	le)	
NSE le r	E-da nam	ta e (f	or	inf	o-t	abl	le)	
NSE le r	E-da nam	ta e (f 	or	inf	ō-t	abl	le)	
elect path to let default tab	elect path to NSI	elect path to NSE-da	elect path to NSE-data et default table name (f	t default table name (for	t default table name (for inf	t default table name (for info-t	t default table name (for info-tab	elect path to NSE-data
NS le	se r	SE-da nam	E-data name (f	name (for	name (for inf	name (for info-t	name (for info-tab	E-data name (for info-table)



5,6,6	
DAN SANS	
FIT	
FIT	
SVD	

Path / JNSE :: Import of *.dtr files 3 Import of *.dtr files Cancel OK 4	
1: Select path to NSE-data 2: Set default table name (for info-table)	
 3: Push button to import data (*.dtr) 4: Modify if needed table name 5: Select needed file(s) 	SVD
Downloads qtikws16 qtisas18 doc doc V Folder Cancel Open	JNSE
Jülich-Neutron-Spin-Echo Tools v.3.0-23.12.2020	

J-NSE interface:: generated tables



info-table

0 0

MBP4MGndfatparameterq0.374q_var0.489q_unit_SI0.100t_unit_SI0.100temp0.000numor1213ref1213bgr1213withbartfac_bgr.tfac_bgr0.100yolinstbinstbins0.000gbinstbinsyrd_cnt511	vs t/ns 2136 6068E-01 9310E-03 0000E+11 0000E+00 67 47 92 0000E+01 0000E+01 11 14 10 04	701	File: repo	ort21367	7_7.5	.dtr
values Cau/ns 0.9724260E-01 0.1952923E+00 0.4942220E+00 0.2984534E+01 0.4976874E+01 0.6970518E+01 0.9957600E+01 0.1841491E+02 0.1841491E+02 0.2487222E+02 0.3391548E+02 0.6060624E+02 0.6060624E+02 0.6060624E+02 0.8351547E+03 #nxt MBP4MGndC1, "d-MB	S(g,1)/S(q) .8832512E+00 .9573234E+00 .9573234E+00 .9573234E+00 .9528290E+00 0.964007TE+00 0.8863831E+00 0.8863831E+00 0.8363668E+00 0.8363668E+00 0.7573565E+00 0.5847356E+00 0.5847356E+00 0.4712725E+00 P pD 7.0 in 4M vs t/ns 2136	err(sqt/sq) 0.1828554E-01 0.1282973E-01 0.1305659E-01 0.1323055E-01 0.137350E-01 0.137350E-01 0.137350E-01 0.137350E-01 0.109634E-01 0.1099634E-01 0.1518850E-01 0.9707090E-02 0.1049252E-01 0.145950E-01 0.145950E-01 0.1883388E-01 d-Guanidinium H 702	<pre>var(sgt/sg) 0.3411799E+00 0.2674864E+00 0.2257162E+00 0.2193089E+00 0.2046209E+00 0.1852137E+00 0.1833600E+00 0.183415E+00 0.1843415E+00 0.2208167E+00 0.2908167E+00 0.4217901E+00 ydrochlorid, 2m</pre>	<pre>var(tau)/ns 0.1319645E-06 0.1302189E-02 0.1366497E-02 0.1310810E-02 0.131154E-02 0.9155134E-06 0.1250521E-02 0.9891278E+00 0.1680554E+01 0.1680554E+01 0.874868E+01 0.7851879E+01 0.1128113E+02 m hellma cell,</pre>	nupdates. 96 234 234 234 234 234 234 234 234 336 192 578 610 530 664	Qeff/A**-1 0.3805328E-01 0.36809456E-01 0.3731082E-01 0.3731082E-01 0.3724017E-01 0.3724017E-01 0.3729524E-01 0.3755998E-01 0.3755998E-01 0.3738920E-01 0.376229E-01 0.3706251E-01 0.3741368E-01
parameter q 0.4%6 q_var 0.11 q_unit_SI 0.100 t_unit_SI 0.100 temp 0.000 numor1 213 ref1 13 bgr1 13	6323E-01 9059E-03 0000E+11 0000E-08 0000E+00 67 47 92 SE Headers					

	sample-code	sample-info	mode	run-numbei	q[X]	dq[xEr]	q-unit	t-unit	temp	numor	ref	bgr	with-bgr	tfac-bgr	volfrac	qbins	tbins	oor-cnt	upd-cnt	table-name
1	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136701	0.037461	0.00049	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136701-v-
2	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136702	0.049663	0.000172	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136702-v-
3	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136703	0.062617	0.000193	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136703-v-
4	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136704	0.075197	0.000767	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136704-v-
5	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136705	0.088491	0.000749	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136705-v-
6	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136706	0.10134	0.000241	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136706-v-
7	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136707	0.11413	0.000841	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136707-v-1
8	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136708	0.12679	0.00106	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136708-v-
9	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136709	0.13961	0.000246	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136709-v-
10	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136710	0.15126	0.000232	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136710-v-1
11	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-0	fqt	2136711	0.15666	0	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136711-v-1

I vs time; for different

•			repor	mreport21367_7-5-2136701-v-1 - NSE Dataset								
	tau-ns[X]	Sqt-To-Sq[Y]	d-Sqt-To-Sq[yEr]	var-Sqt-To-Sq[yEr]	var-tau-ns[xEr]	nupdates[Y]	Qeff[Y]					
1	9.724260E-02	8.832512E-01	1.828554E-02	3.411799E-01	1.319645E-07	9.600000E+01	3.805328E-02					
2	1.952923E-01	9.442981E-01	1.282973E-02	2.674864E-01	1.302189E-03	2.340000E+02	3.699456E-02					
3	4.942220E-01	9.573234E-01	1.305659E-02	2.789773E-01	1.366497E-03	2.360000E+02	3.686028E-02					
4	9.922240E-01	9.528290E-01	1.323055E-02	2.257162E-01	1.325221E-03	2.340000E+02	3.731082E-02					
5	2.984534E+00	9.746612E-01	1.381281E-02	2.193089E-01	1.310810E-03	2.340000E+02	3.746738E-02					
6	4.976874E+00	9.640077E-01	1.373500E-02	2.046209E-01	1.311154E-03	2.380000E+02	3.724017E-02					
7	6.970518E+00	8.906754E-01	2.010855E-02	1.852137E-01	9.155134E-07	9.400000E+01	3.855767E-02					
8	9.957600E+00	8.863031E-01	1.300164E-02	2.000779E-01	1.250521E-03	2.340000E+02	3.719147E-02					
9	1.404848E+01	9.054503E-01	1.339112E-02	1.833600E-01	9.891278E-01	2.340000E+02	3.729524E-02					
10	1.841491E+01	8.363668E-01	1.099634E-02	1.843415E-01	1.680554E+00	3.360000E+02	3.755998E-02					
11	2.487222E+01	7.994278E-01	1.518850E-02	1.921554E-01	1.992017E+00	1.920000E+02	3.844471E-02					
12	3.391548E+01	7.573565E-01	9:727090E-03	2.170580E-01	4.497509E+00	5.780000E+02	3.738920E-02					
13	6.060624E+01	6.604147E-01	1.049252E-02	2.508167E-01	8.374868E+00	6.100000E+02	3.706229E-02					
14	8.351547E+01	5.847356E-01	1.459630E-02	2.903003E-01	7.851879E+00	5.300000E+02	3.706951E-02					
15	1.251047E+02	4.712725E-01	1.883388E-02	4.217901E-01	1.128113E+01	6.640000E+02	3.741368E-02					

parameter	
q	0.3746068E-01
g var	0.4899310E-03
g unit SI	0.1000000E+11
t unit SI	0.100000E-08
temp	0.000000E+00
numor1	21367
ref1	21347
bar1	21392
withbor	0
tfac bor	-0,1000000E+01
volfrac	0.1000000E+01
abins	11
thins	14
por cnt	3510
und cnt	51104

-							Construction of the Construction of the Construction of the
	tau/ns	5(q,t)/5(q)	err(sqt/sq)	var(sqt/sq)	var(tau)/ns	nupdates	Qeff/A**-1
	0.9724260E-01	0.8832512E+00	0.1828554E-01	0.3411799E+00	0.1319645E-06	96	0.3805328E-01
	0.1952923E+00	8.9442981E+08	0.1282973E-01	0.2674864E+00	0.1302189E-02	234	0.3699456E-01
	0.4942220E+00	0.9573234E+00	0.1305659E-01	0.2789773E+00	0.1366497E-02	236	0.3686028E-01
	0.9922240E+00	0.9528290E+00	0.1323055E-01	0.2257162E+00	0.1325221E-02	234	0.3731082E-01
	0.2984534E+01	0.9746612E+00	0.1381281E-01	0.2193089E+00	0.1310810E-02	234	0.3746738E-01
	0.4976874E+01	0.9640077E+00	0.1373500E-01	@.2046209E+00	0.1311154E-02	238	0.3724017E-01
	0.6970518E+01	0.8906754E+00	0.2010855E-01	0.1852137E+00	0.9155134E-06	94	0.3855767E-01
	0.9957600E+01	0.8863031E+00	0.1300164E-01	0.2000779E+00	0.1250521E-02	234	0.3719147E-01
	0.1404848E+02	0.9054503E+00	0.1339112E-01	0.1833600E+00	0.9891278E+00	234	0.3729524E-01
	0.1841491E+02	0.8363668E+00	0.1099634E-01	0.1843415E+00	0.1680554E+01	336	0.3755998E-01
	0.2487222E+02	0.7994278E+00	0.1518850E-01	0.1921554E+00	0.1992017E+01	192	0.3844471E-01
	0.3391548E+02	0.7573565E+00	0.9707090E-02	0.2170580E+00	0.4497509E+01	578	0.3738920E-01
	0.6060624E+02	0.6604147E+00	0.1049252E-01	0.2508167E+00	0.8374868E+01	610	0.3706229E-01
	0.8351547E+02	0.5847356E+00	0.1459630E-01	0.2903003E+00	0.7851879E+01	530	0.3706951E-01
	0.1251047E+03	0.4712725E+00	0.1883388E-01	0.4217901E+00	0.1128113E+02	664	0.3741368E-01

MBP4MGngCl "d-MBP pD 7.0 in 4M d_Guanidinium Hydrychlorid, 2mm hollma cell, 22 d MBP4MGnd_fqt_vs_t/ns_2136702

MBP4MGndCl "d-MBP pD 7.0 in 4M <u>d-Guanidinium</u> Hydrochlorid, 2mm <u>hellma</u> cell, 22 d MBP4MGnd_fgt_vs_t/ns_2136701

parameter	
q	0.4966323E-01
g_var	0.1719059E-03
q_unit_SI	0.100000E+11
t unit_SI	0.1000008E-08
temp	0.000000E+00
numor1	21367
ref1	21347
bar1	21392

UNTITLED	Name Type	View	Created	Label
JNSE :: *.dtr files	minfo1 Table	Normal	05.01.21	23:34 NSE Headers
4	mreport21367_7-5-2136701-v-1 Table	Maximize	d 05.01.21	23:34 NSE Dataset
	report21367_7-5-2136702-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136703-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136704-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136705-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136706-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136707-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136708-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	report21367_7-5-2136709-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	mreport21367_7-5-2136710-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset
	mreport21367 7-5-2136711-v-1 Table	Hidden	05.01.21	23:34 NSE Dataset

J-NSE interface: Multi-Fitting

00	JNS			00			FITT	ABLE(s)		
Select Table of Headers	Data Import M	ulti-Fitting				5	Save Current Fit	ting Session		
1 info1				Select Fu	nction	0	Fitting Se	ssion 🕞	Generate F	Results
Select Row-range				Data	Function	n	Parameters	Global Lim	nits Fit - C	ontrol
Erem 1					Share?	?Fron	Value #1	Error #1	Vary?FromTo	Value #
2 ^{-rom: 1}			<u> </u>	q	0		0.037461			0.049663
Select Fitting Function				AO			1		. .	1
doubleDiffusion				A1	0		1	***		1
doublechildsion				D0			0			0
Init Multi-Fit				w0	0		0		· · ·	0
4				w1	0	10	0			0
1: Select nee	eded info-tal	ole								
1: Select nee 2: Select ran 3: Select Fitt 4: Push "Init	eded info-tal ige of rows in ing Functior Multi-Fit"	ole n the info-tab า	ole	Fittin	g Inte	erfa	ce is rea	ady for	global F	it
1: Select nee 2: Select ran 3: Select Fitt 4: Push "Init	eded info-tal ige of rows i ing Functior Multi-Fit"	ole n the info-tab n	ole	Fittin	g Inte	erfa s	ce is rea	ady for	global F Statistics Notes	it [after Fit]
1: Select nee 2: Select ran 3: Select Fitt 4: Push "Init	eded info-tal ige of rows i ing Functior Multi-Fit"	ole n the info-tab n	ble	Fittin Auto Simulat	g Inte	s Simul	ce is rea	ady for	global F Statistics Notes 5.87776	it [after Fit] 88116E+00]
1: Select nee 2: Select ran 3: Select Fitt 4: Push "Init	eded info-tal ige of rows i ing Functior Multi-Fit"	ole n the info-tab n	ble	Fittin Auto Simulat	g Inte	simul re Fit	ce is rea	Save Session 2/dof=	global F Statistics Notes 5.87776 3.181940 58 ms - 11	it [after Fit] 88116E+00 00380E+05 iteration(s)
1: Select nee 2: Select ran 3: Select Fitt 4: Push "Init	eded info-tal ige of rows i ing Functior Multi-Fit"	ole n the info-tab n	ble	Fittin Auto Simulat Fit CoubleDiffusion	g Inte	s Simul re Fit	ce is rea	Save Session 2/dof=	global F Statistics Notes 5.87776 3.181940 58 ms - 11	it [after Fit] = 88116E+00] 00380E+05] iteration(s)

J-NSE interface: Global-Fit

				Data Function Parameters	Global	Limits Fit - Control		
	Checks #1	Dataset #1	Checks #2	Dataset #2	Checks #3	Dataset #3	Checks #4	Dataset #4
Data Set(s)		report21367_7-5-2136701-v-1_Sqt-To-Sq		report21367_7-5-2136702-v-1_Sqt-To-Sq		report21367_7-5-2136703-v-1_Sqt-To-Sq		report21367_7-5-2136704-v-1_Sqt-To-Sq
N	N 🔁	15	N O	15	N 🖸	15	N 🖸	15
First Point		1	0	1	0	1	0	1
Last Point	0	15	0	15	0	15	0	15
Weighting	💟 on	report21367_7-5-2136701-v-1_d-Sqt-To-Sq 👩	💟 on	report21367_7-5-2136702-v-1_d-Sqt-To-Sq	🖸 on	report21367_7-5-2136703-v-1_d-Sqt-To-Sq	💟 on	report21367_7-5-2136704-v-1_d-Sqt-To-Sq

Data	Function Parameters	Global Limits	Fit - Control	
doubleDiffusi	ion			
# Parameters	s: 7 C # Indep. Variables:	1 0 # Dep.	Variables: 4	1
doubleDiffusi	ion			
Two exponer	ntial decaving functions describing diffu	sion.		
mothu l/a f	1 4 1 4 4 0 5 4 4 0 5 4 4 0 5 4 4 0 1 1 1 1	0-4(-40 (D 0)	0.000000	
math:: I(g.t	n = 0 10/1-0/2/11 11 + 11 5 1/1 1/2//2/11 +			
	1)-A_10 (-4 2 (D_11+0.5W_1 21 2))+1	4_2er(-qr2 (D_2t +	0.5W_2^2t^2)}	
	()=A_16 (-4 2 (D_1(+0.5w_1 2(2))+)	4_20'\-q''2 (D_2t +	0.5W_2^2(^2)}	
	ין=ר_ופיניע צ (ש_ווד ט.טש_ו צו צו) דו	4_20^{-q^2 (U_2t +	0.5W_2*2(*2)}	
	() IO (' ע צ (D II + 0.5wI - 2i - 2)) + 1	4_2e^{-q^2 (D_2t +	0.5W_2^2{^2}}	
q	Wavevector	4_28°{-q°2 (D_2ĭ +	0.5w_2*2(*2)}	
q A0	Wavevector Prefactor	4_28°{-q°2 (D_2ĭ +	0.5W_2"2{"2}}	
q A0 A1	Wavevector Prefactor Prefactor	4_28°{-q^2 (D_2t +	0.5w_2*2(*2)}	
q A0 A1 D0	Wavevector Prefactor Diffusion coefficient in units [[c	a_zer(-qr2 (D_2t +	0.5w_2*2(*2)}	
q A0 A1 D0 D1	Wavevector Prefactor Diffusion coefficient in units [[c Diffusion coefficient in units [[c	4_28°(-q°2 (D_2t +]]**-2/[t]]]**-2/[t]]	0.5w_2*2(*2)}	
q A0 A1 D0 D1 w0	Wavevector Prefactor Diffusion coefficient in units [[c Width of diffusion coefficient di	a_zer(-qr2 (D_2t +]**-2/[t]]]**-2/[t]] stributions in D unit	0.5w_2*2(*2)}	

1: q-values moved from info-table

				Data Funct	ion Para	meters GI	obal Limits	Fit - Control				
Gharot	Vary1110IIITo	Value #1	Citor #1	VaryThom.To	Value #2	End #2	VaryThomTo	Value #0	Enter #G	VaryThomTo	Value P4	End #4
		0.037461	***		0.049663	***		0.062617			0.075197	***
0		1		17	1		17	1		1 2	1	
	2	1		2	1		.	1		2	1	
	.	0		. .	0		. .	0			0	
0	. .	0			0		.	0		2	0	
0		0	***		0			0			0	***
0	0	0		0.4	0		—	0	****	0	0	

DAN

SANS

SVD

NSE: Global Fit

