nMOLDYN

Computation and decomposition of **N**eutron scattering spectra from **MOL**ecular **DYN**amics simulations

nMOLDYN 1 : a bit of history

ELSEVIER

Computer Physics Communications 91 (1995) 191–214

Computer Physics Communications

*n*MOLDYN: A program package for a neutron scattering oriented analysis of Molecular Dynamics simulations

Gerald R. Kneller [a,b,1], Volker Keiner [c,2], Meinhard Kneller [c,3], Matthias Schiller [c,4]

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[b] *DBCM SBPM, CEA, CE Saclay, F-91191 Gif-sur-Yvette, France*

[c] *Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn, Germany*

Received 18 November 1994

Original Fortan 77 version

nMOLDYN 2 : a bit of history

NEUTRONS FOR SCIENCE

Software News and Updates

*n*Moldyn: A Program Package for a Neutron Scattering Oriented Analysis of Molecular Dynamics Simulations

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[1]*Departament of Biophysics, Institute of Molecular Biology, Jagiellonian University, ul. Gronostajowa 7, 30-387 Kraków, Poland*
[2]*Centre de Biophysique Moléculaire (UPR 4301 CNRS), Rue Charles Sadron, 45071 Orléans Cedex 2, France*

Received 30 July 2002; Accepted 1 November 2002

Version 2:
Fortran → Python
Inclusion of MMTK library (Hinsen)
J Comp Chem 24: 657–667, 2003

nMOLDYN 3 : a bit of history

Journal of COMPUTATIONAL CHEMISTRY WWW.C-CHEM.ORG SOFTWARE NEWS AND UPDATES

*n*Moldyn 3: Using Task Farming for a Parallel Spectroscopy-Oriented Analysis of Molecular Dynamics Simulations

Konrad Hinsen,[a,b] Eric Pellegrini,[c] Sławomir Stachura,[a,b] and Gerald R. Kneller*[a,b,d]

Version 3:
ILL involvement – Eric Pellegrini
Major code upgrade
Task-farming parallelisation (Pyro)
J of Comp Chem 2012, 33, 2043–2048

nMOLDYN @ ILL (Eric Pellgrini)

Version 3:
Agence National pour la Recherche (ANR) project – THALER (2008 – 2010 inc)
Post-doc: Eric Pellegrini

Version 4 (MDANSE):
ANR project – SPUTNIK (2011 – 2013 inc)
Post-docs: Bachir Aoun (2 yrs), Gael Goret (1 yr)
Build server/CI: Jenkins with Yannick Raoul, GitLab with Jamie Hall & Fabien Pinet (ILL/IT)
Scientific support: with Miguel Gonzalez
All supervised by Eric Pellegrini

nMOLDYN 3

NEUTRONS FOR SCIENCE

THALER Objectives:

- Improving portability → easier installation ...
- Reorganization of the code
- New scientific features
- New Graphical User Interface
- Improving readability → developer/user
- Improving ergonomy
- Improving performance → parallelization

nMOLDYN 3 – new scientific features

SCATTERING:

DYNAMICS:

STRUCTURE:

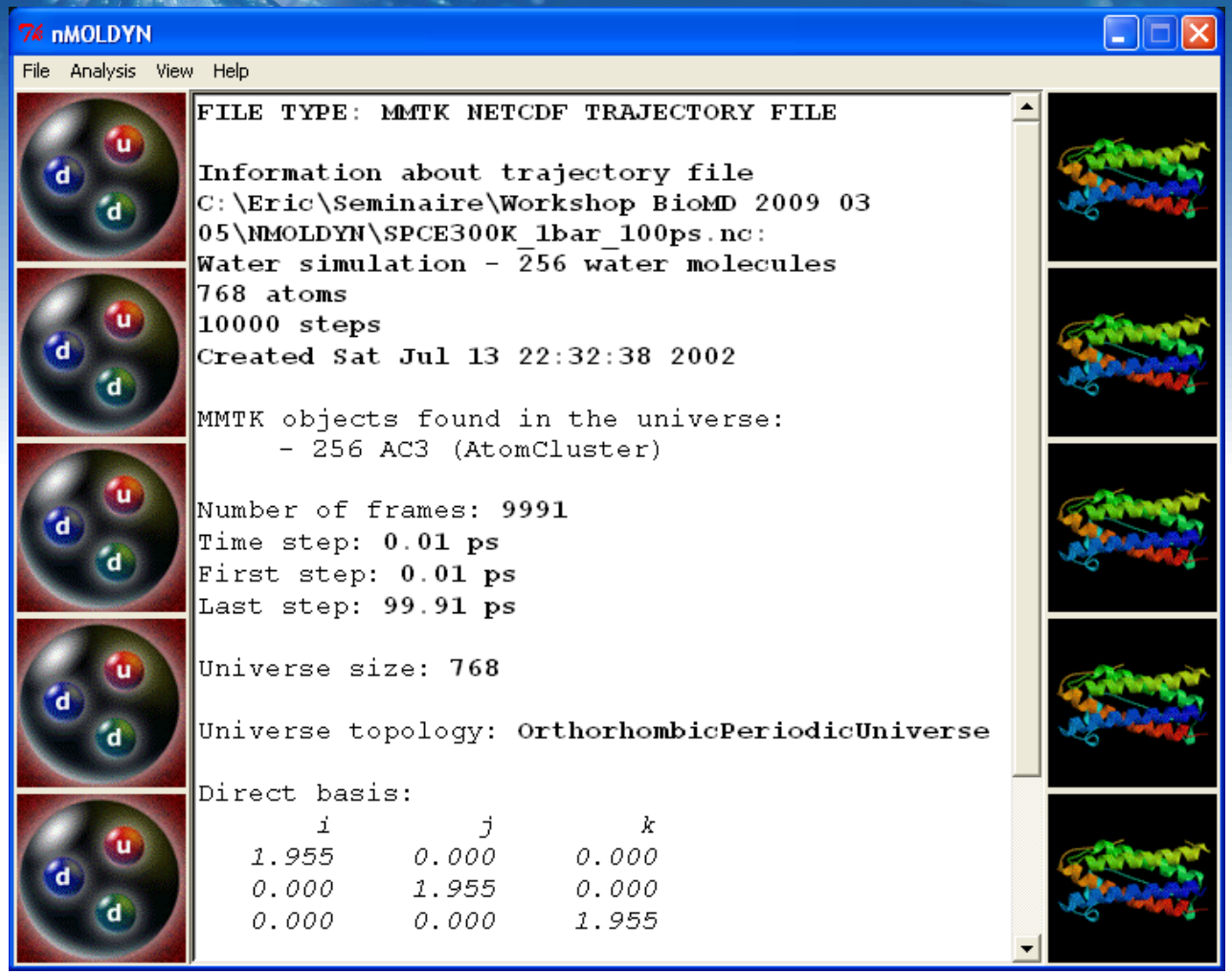
NMR:

TRAJECTORY:

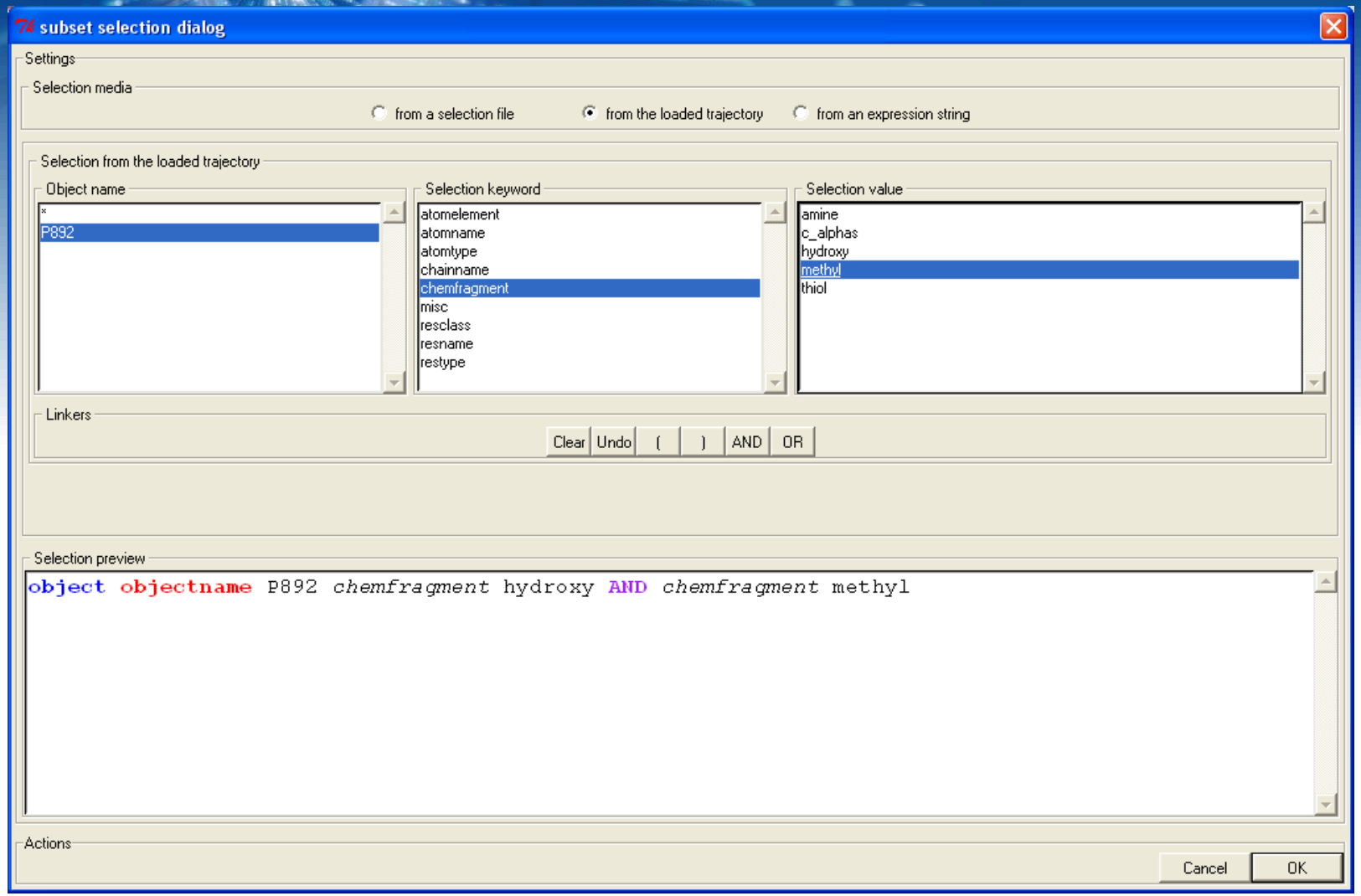
- Center Of Mass Reduced Trajectory
- Global Motion Filtered Trajectory
- Quasi Harmonic Analysis
- ScrewFit Analysis (Paolo)
- Reduced Trajectory

Read trajectories from many MD codes (classic & DFT): CHARMM, NAMD, LAMMPS, DL_POLY, (AMBER, GROMACS ?) VASP, Materials Studio (DISCOVER, FORCITE, CASTEP, DMOL, DFTB)

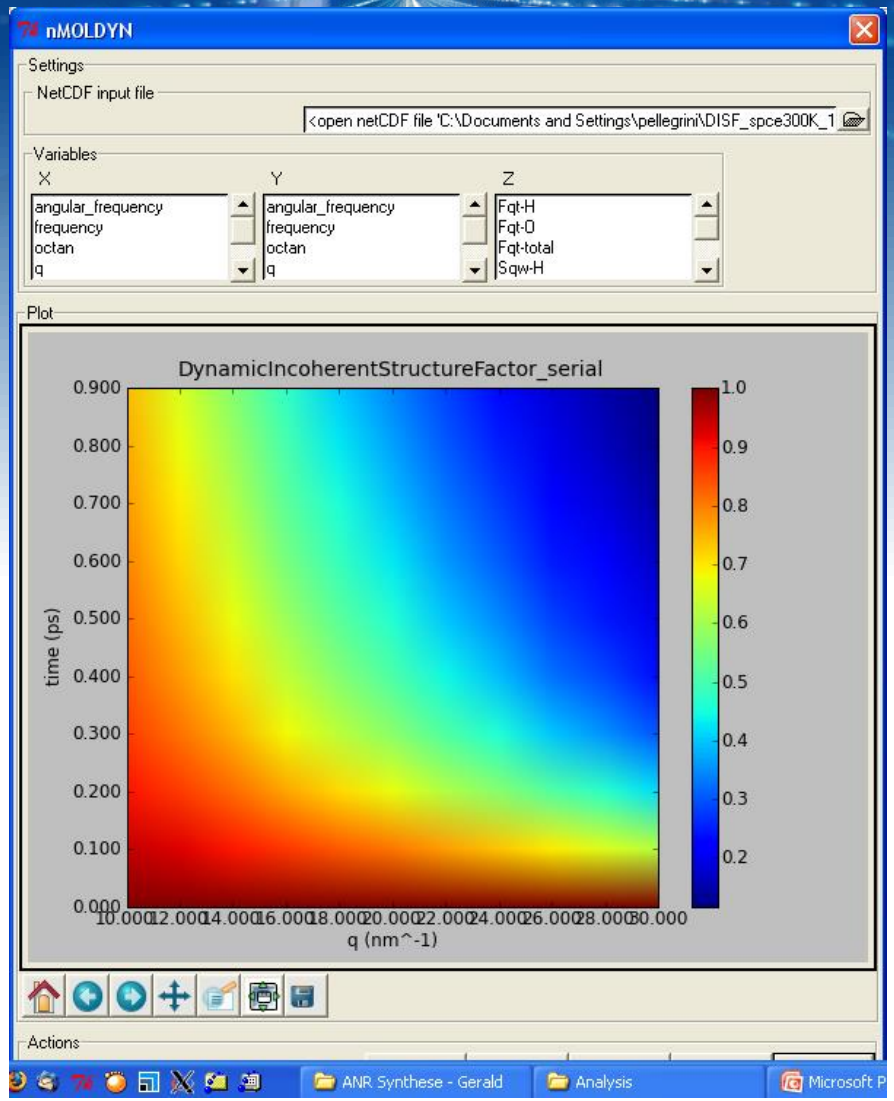
nMOLDYN 3 – new GUI

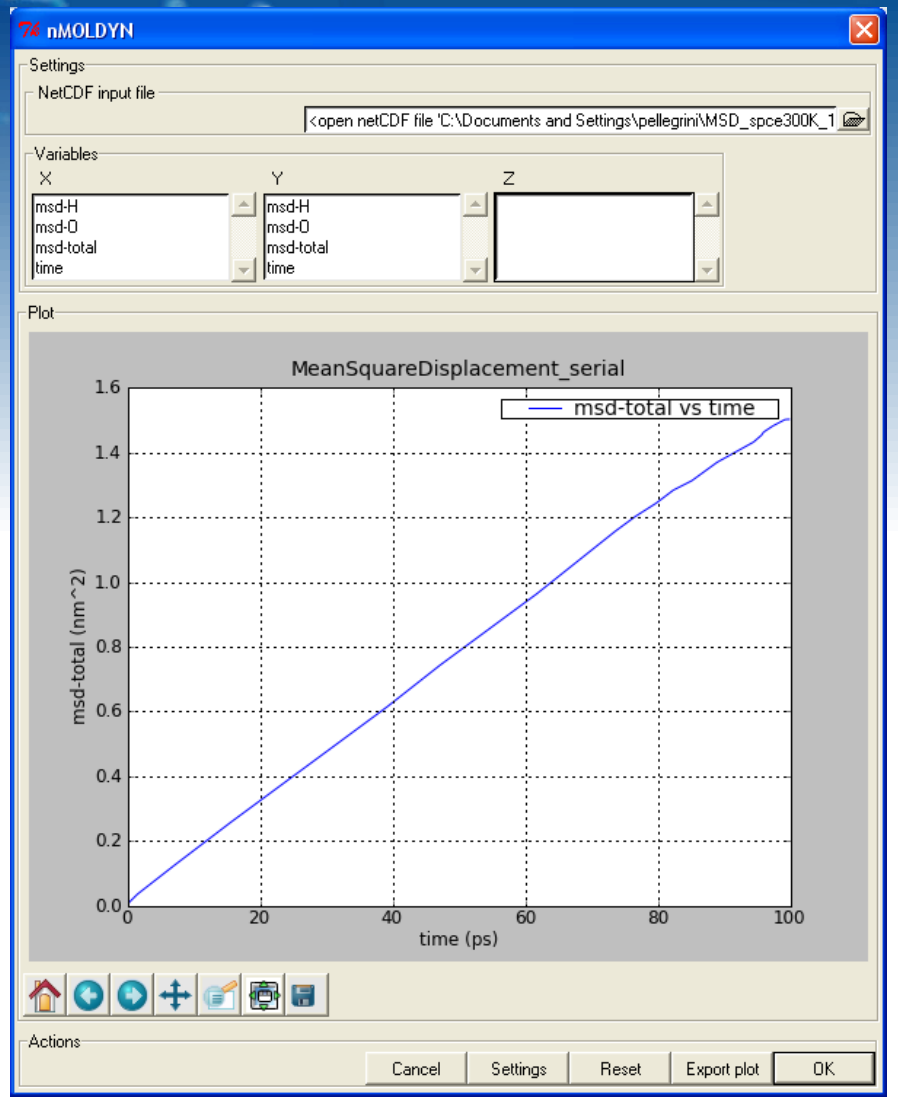


nMOLDYN 3 - new GUI

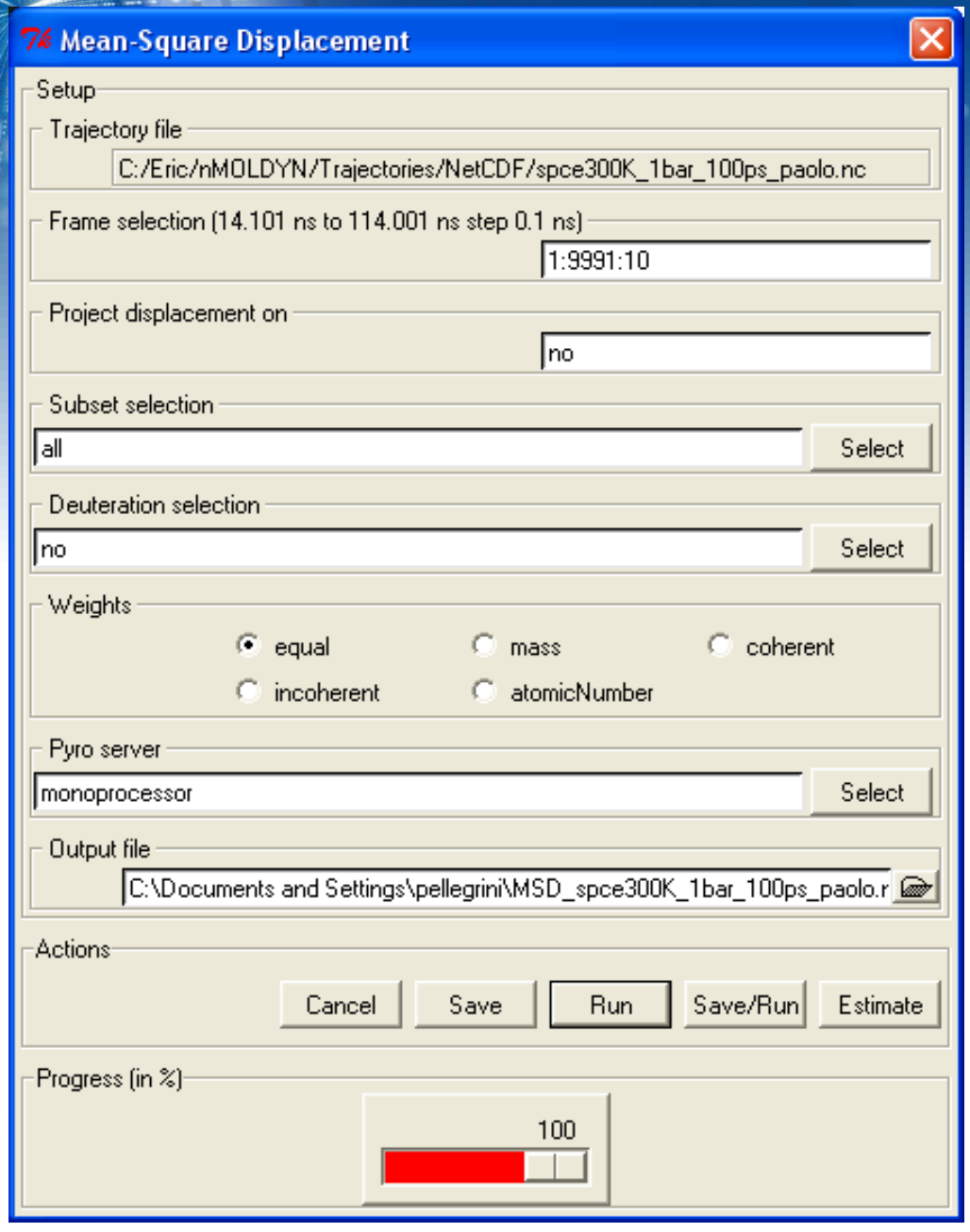


nMOLDYN 3 – new GUI





nMOLDYN 3 – new GUI



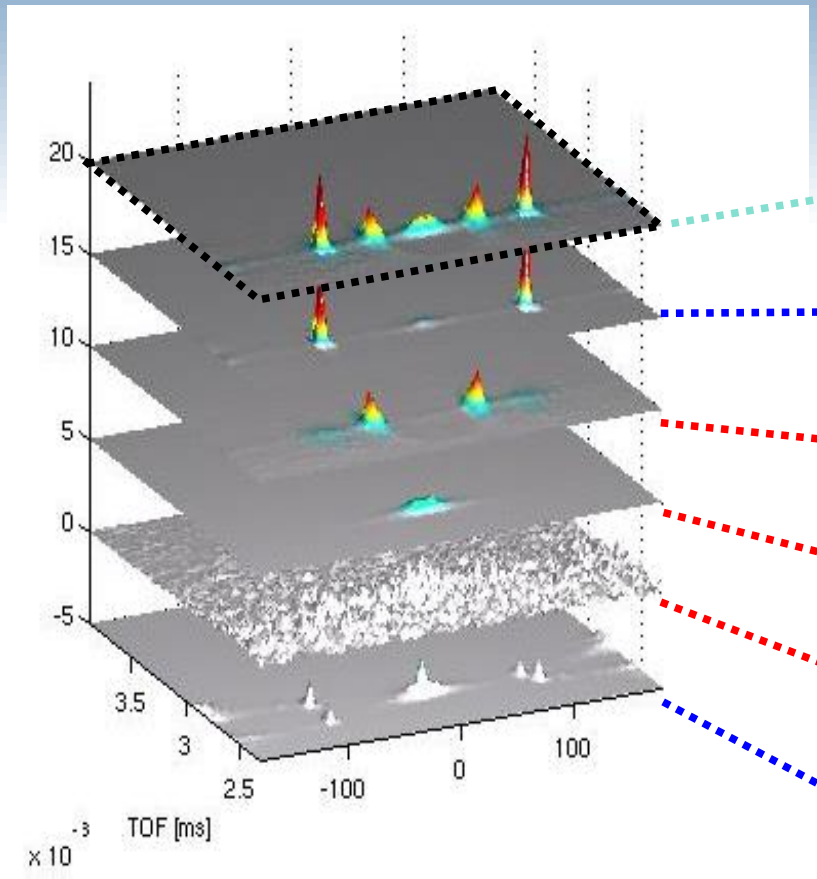
nMOLDYN 4

SPUTNIK Objectives:

- Integrating experiment related effects – neutron flight simulator
- « Combining » nMoldyn and McStas
  - Simple interface between the codes
  - Web service
- Integrating simple ray-tracing simulations in nMoldyn
- and/or analytical solutions
- On-going upgrade of nMoldyn (e.g. Linux/Mac install, 64-bit code, parallelisation/cluster optimisation, complete separation of front (GUI) and back end,…)

Instrument simulations and virtual experiments

Instrument simulations and virtual experiments



Total signal

Container (Nb)

Coherent (I-Rb)

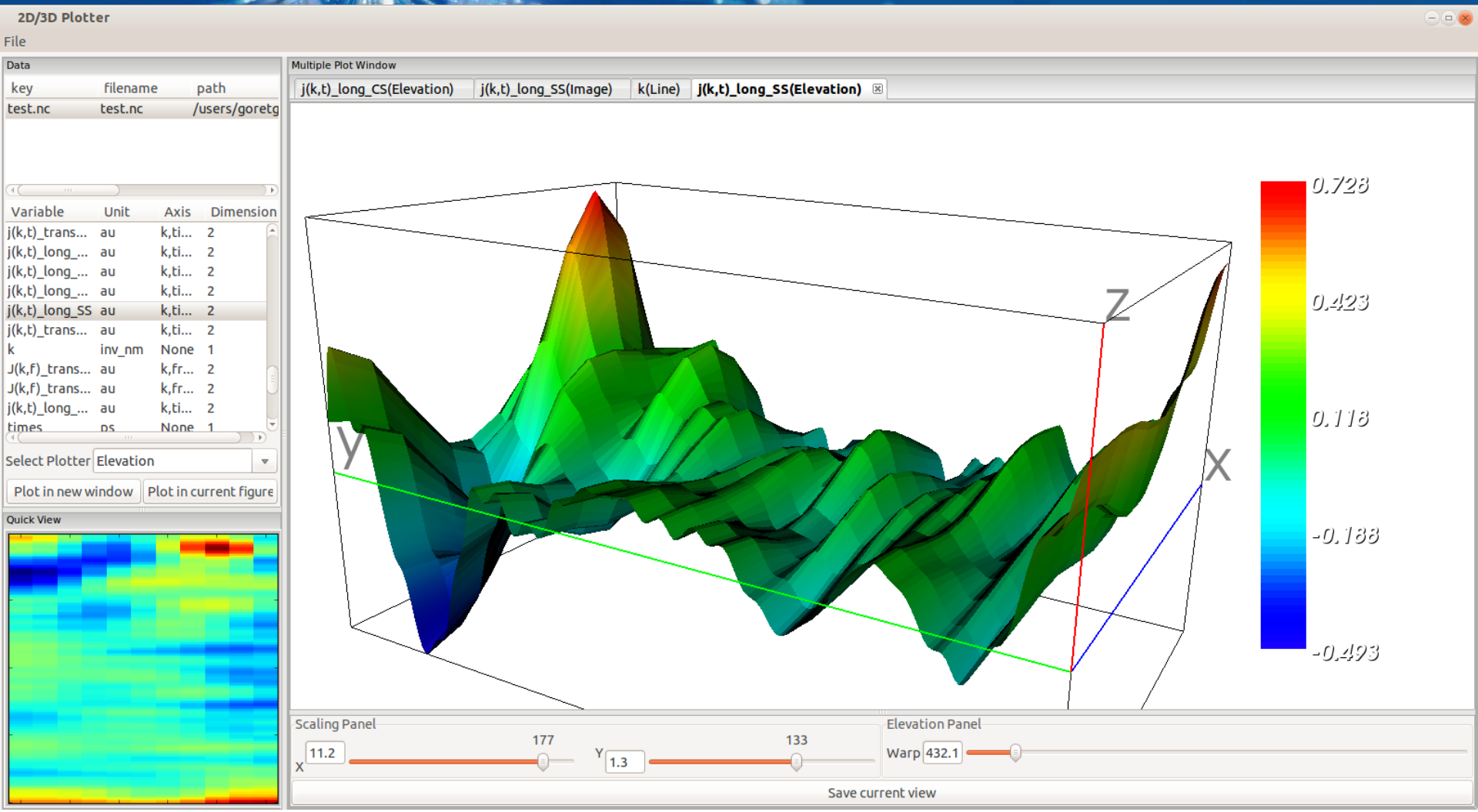
Incoherent (I-Rb)

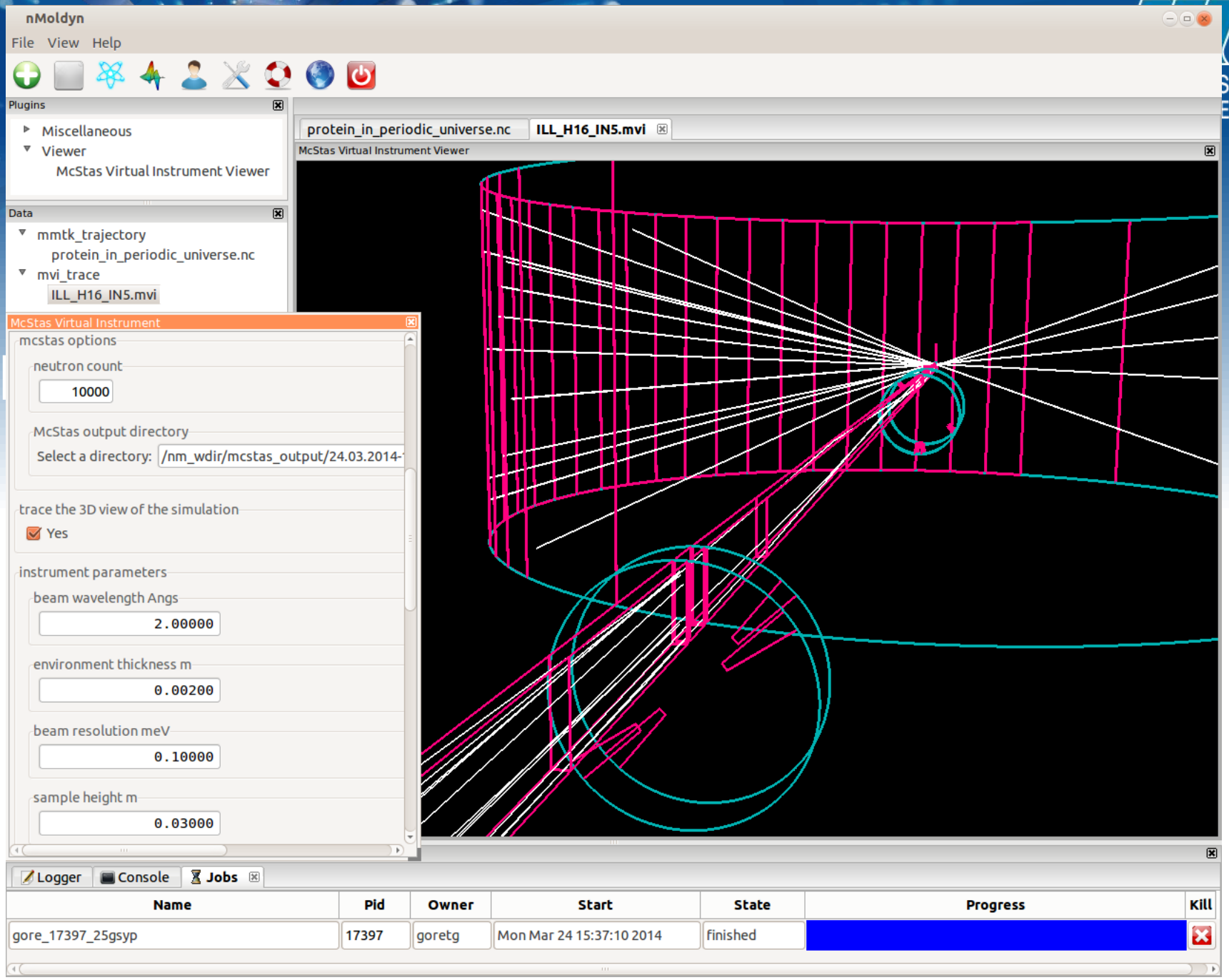
Multi. Scatt. *100

Cryo-furnace (Al) *10

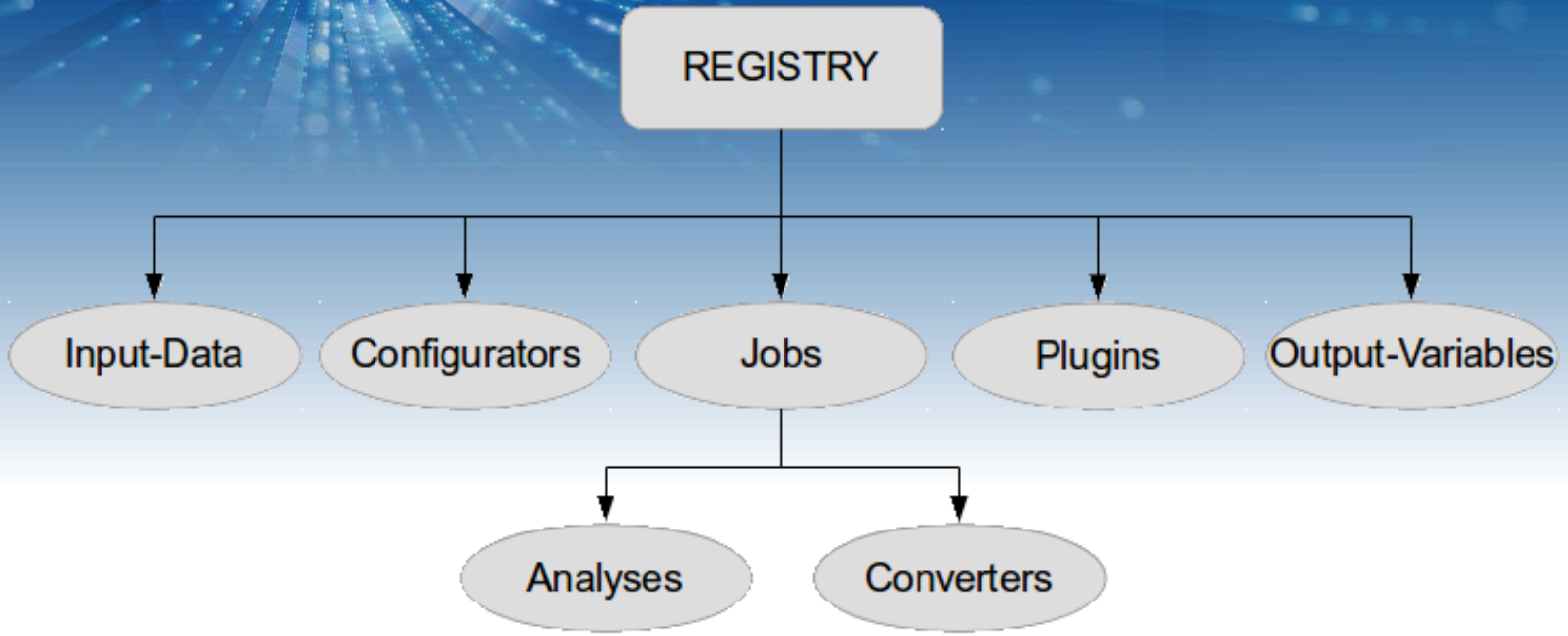

4
nMoldyn
File View Help
Plugins
Miscellaneous
K vectors
Viewer
Molecular Viewer
Analysis
Trajectory
Thermodynamics
Virtual Instruments
Dynamics
Scattering
Dynamic Coherent Structu
Elastic Incoherent Structur
Current Correlation Functi
Gaussian Dynamic Incoher
Dynamic Incoherent Struct
Structure
Static Structure Factor
Eccentricity
Coordination Number
Root Mean Square Deviati
Voronoi
Root Mean Square Fluctua
Molecular Trace
Solvent Accessible Surface
Pair Distribution Function
Radius of Gyration
Density Profile
Spatial Distribution
3
Data
mmtk_trajectory
single_wall_nanotube.n
waterbox_in_periodic_
protein_in_periodic_universe.nc
2
single_wall_nanotube.nc
protein_in_periodic_universe.nc
Molecular Viewer
1
Animation
30
95
Logger
Console
Jobs
NAME
PID
START
ELAPSED
STATE
PROGRESS
ETA
KILL
5223_3wkz
5223
04-06-2014 09:57:32
finished
N/A
5249_drds
5249
04-06-2014 09:59:03
finished
N/A
5412_1qd2
5412
04-06-2014 10:09:15
00d:00h:00m:54s
running
00d:00h:00m:06s
4

nMOLDYN 4


2D/3D Plotter
File
Data
key filename path
test.nc test.nc /users/goretg
Variable Unit Axis Dimension
j(k,t)_trans... au k,ti... 2
j(k,t)_long_... au k,ti... 2
j(k,t)_long_... au k,ti... 2
j(k,t)_long_... au k,ti... 2
j(k,t)_long_SS au k,ti... 2
j(k,t)_trans... au k,ti... 2
k inv_nm None 1
J(k,f)_trans... au k,fr... 2
J(k,f)_trans... au k,fr... 2
j(k,t)_long_... au k,ti... 2
times ps None 1
Select Plotter Elevation
Plot in new window
Plot in current figure
Quick View
Multiple Plot Window
j(k,t)_long_CS(Elevation)
j(k,t)_long_SS(Image)
k(Line)
j(k,t)_long_SS(Elevation)
Z
Y
X
0.728
0.423
0.118
-0.188
-0.493
Scaling Panel
X 11.2 177
Y 1.3 133
Elevation Panel
Warp 432.1
Save current view


nMoldyn
File View Help
Plugins
Miscellaneous
Viewer
McStas Virtual Instrument Viewer
Data
mmtk_trajectory
protein_in_periodic_universe.nc
mvi_trace
ILL_H16_IN5.mvi
McStas Virtual Instrument
mcstas options
neutron count
10000
McStas output directory
Select a directory:
/nm_wdir/mcstas_output/24.03.2014-
trace the 3D view of the simulation
Yes
instrument parameters
beam wavelength Angs
2.00000
environment thickness m
0.00200
beam resolution meV
0.10000
sample height m
0.03000
protein_in_periodic_universe.nc
ILL_H16_IN5.mvi
McStas Virtual Instrument Viewer
Logger
Console
Jobs
Name
Pid
Owner
Start
State
Progress
Kill
gore_17397_25gsyp
17397
goretg
Mon Mar 24 15:37:10 2014
finished

nMOLDYN 4 – technical



Based on Python, Cython, WxWidget, Matplotlib, VTK,…
Automated GUI generation and menu update for new analyses

nMOLDYN 4 → MDANSE

MDANSE – Molecular Dynamics to Analyse Neutron Scattering Experiments

nMoldyn

MMTK

MDANSE 4 in SINE2020 ?

SINE2020 Objectives: Idea…

- 1 person year of effort to include Lattice Dynamics in MDANSE

- Read vibration frequencies and displacement vectors (as a function of wavevector) from as many codes as possible
  - mainly DFT: VASP, CASTEP, DMOL, ABINIT, QUANTUM EXPRESSO, etc
  - or output from PHONOPY
  - alternative to PHONON from Krzysztof Parlinski, coupled to VASP, SIESTA, WIEN2K, widely used at ILL

- Analyse Lattice Dynamics
  - Calculate NS spectra for powders & single crystals on TAS (including TOSCA/Lagrange-like) and TOF
  - Provide additional analyses: thermodynamic quantities (enthalpy, entropy, free energy, heat capacity, MSD), participation ratio, Gruneisen parameters,…

SINE2020 @ ILL

Nominally

- 2 person years of effort for MANTID @ ILL in addition to ILL Bastille/Endurance funding
  - ILL has recruited 3 programmers for 3 years starting May 2 2016
  - ILL has negotiated 1 year of consulting with Tessella (Ian Bush) starting April 18 2016)

- 1 person year of effort for QENS

- 1 person year of effort for Lattice Dynamics

- Not ready to start QENS and Lattice Dynamics because of MANTID activity

- ISIS/STFC (e-Science) starting a similar Lattice Dynamics project –combine resources, decide on most appropriate, collaborative solution