

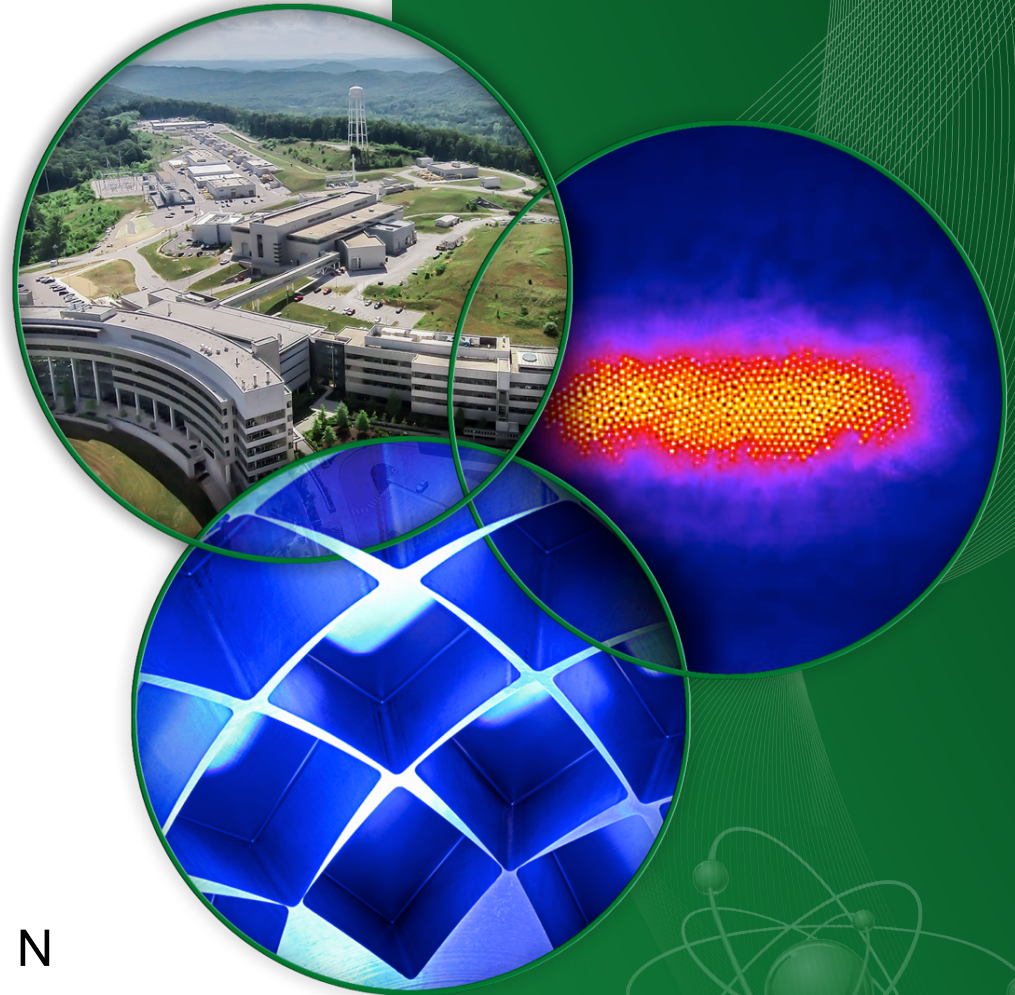
ICE-MAN and VirtuES, the Integrated Computational Environment-Modeling & Analysis for Neutrons at ORNL

Timmy Ramirez-Cuesta,

Luke Daemen, YQ Cheng, E Mamontov, N Jalarvo, Eric Novak, Naresh Osti, NScD, ORNL

Robert Smith, Jay Jay Billings
CSD, ORNL

ORNL is managed by UT-Battelle
for the US Department of Energy



VISION

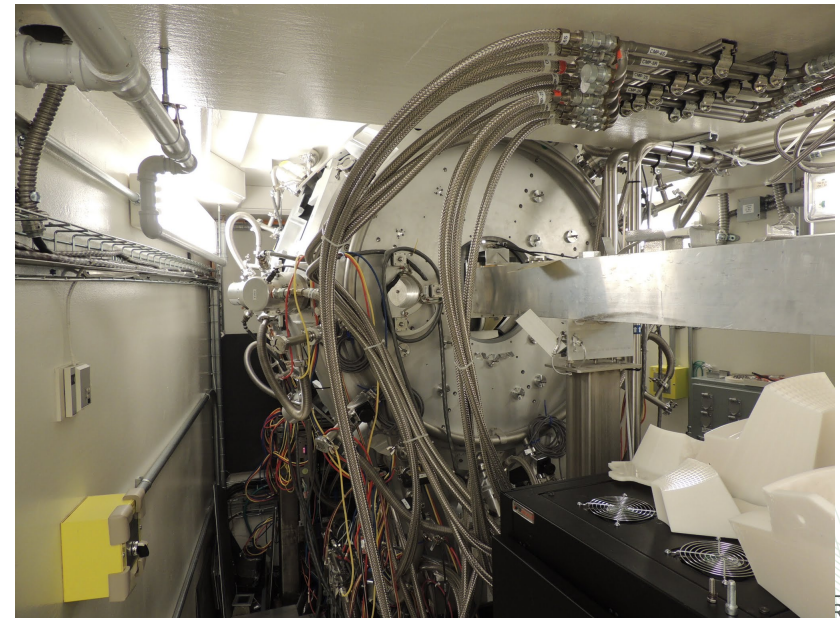
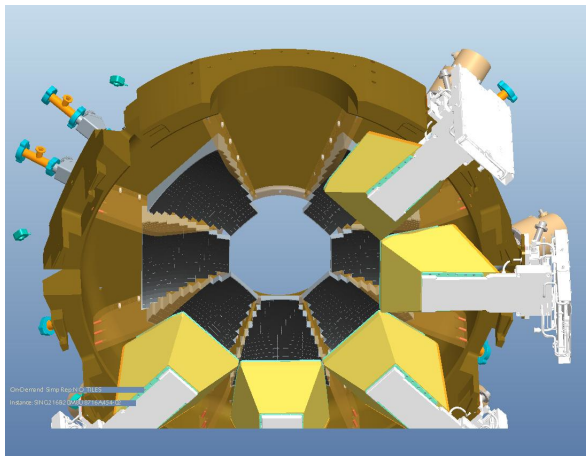
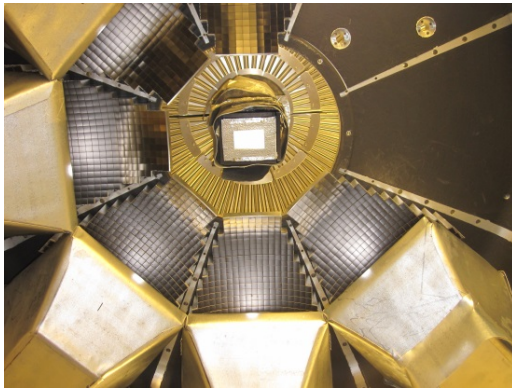
neutron beam

diffraction detectors

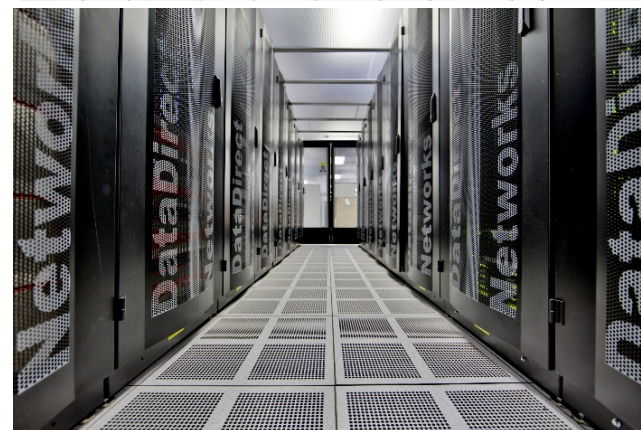
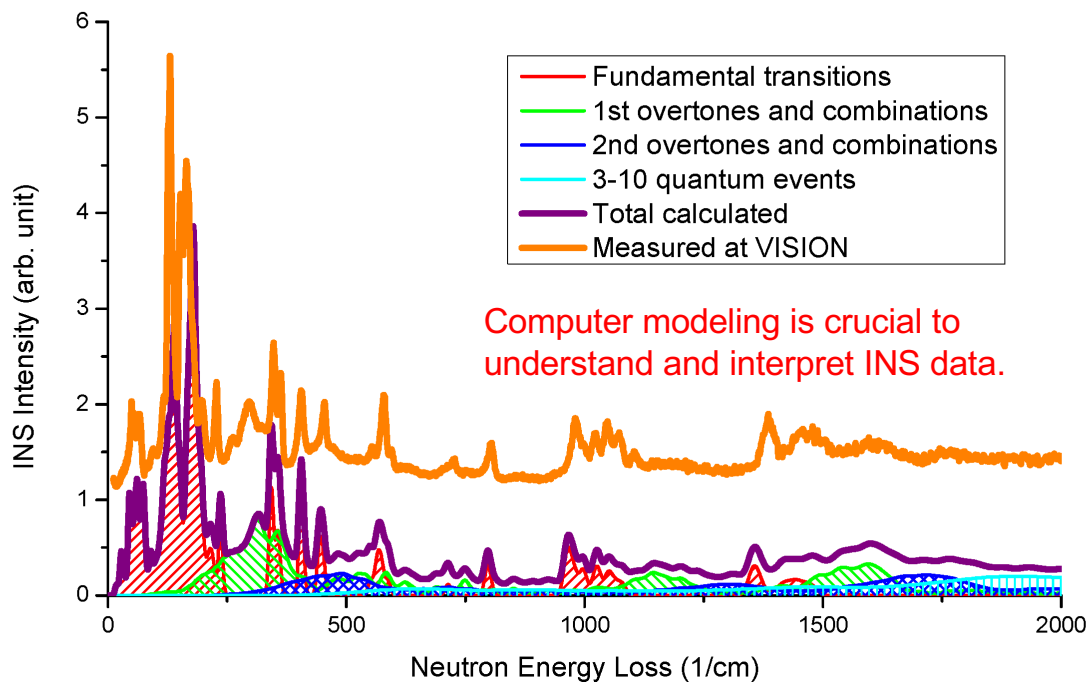
analyzers

inelastic detectors

- Indirect geometry spectrometer optimized to study chemical systems
- High flux/throughput
- Broadband (-2 to 1000 meV)
- Constant dE/E ($\sim 1.5\%$)
- Elastic line HMF ~ 150 μeV
- Simultaneous diffraction



Integrated modeling for data interpretation

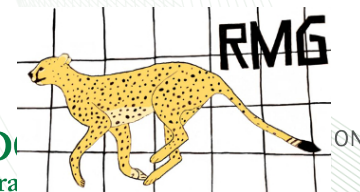


VirtuES cluster

- Dual 16 core Intel Haswell E5-2698v3 3.2 GHz Processors per node
- 50 compute nodes, 1600 (non-hyperthreaded) cores
- 128 GB memory/node, 6.4 TB Total memory
- Each node has 10Gbe and Infiniband networking for connectivity.
- Installed as part of the ORNL Compute and Data Environment for Science (CADES)



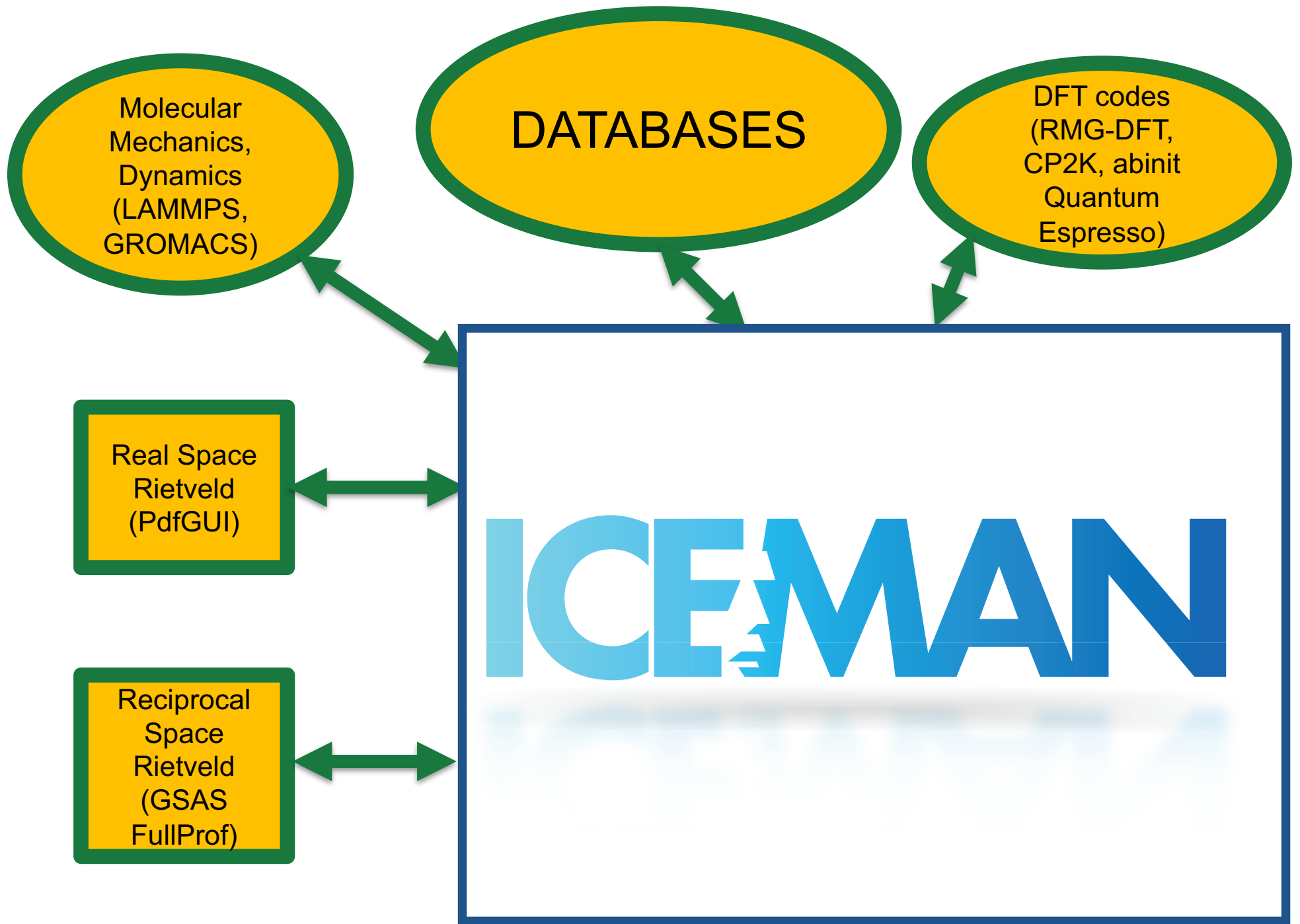
NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL
CHEMISTRY SOFTWARE



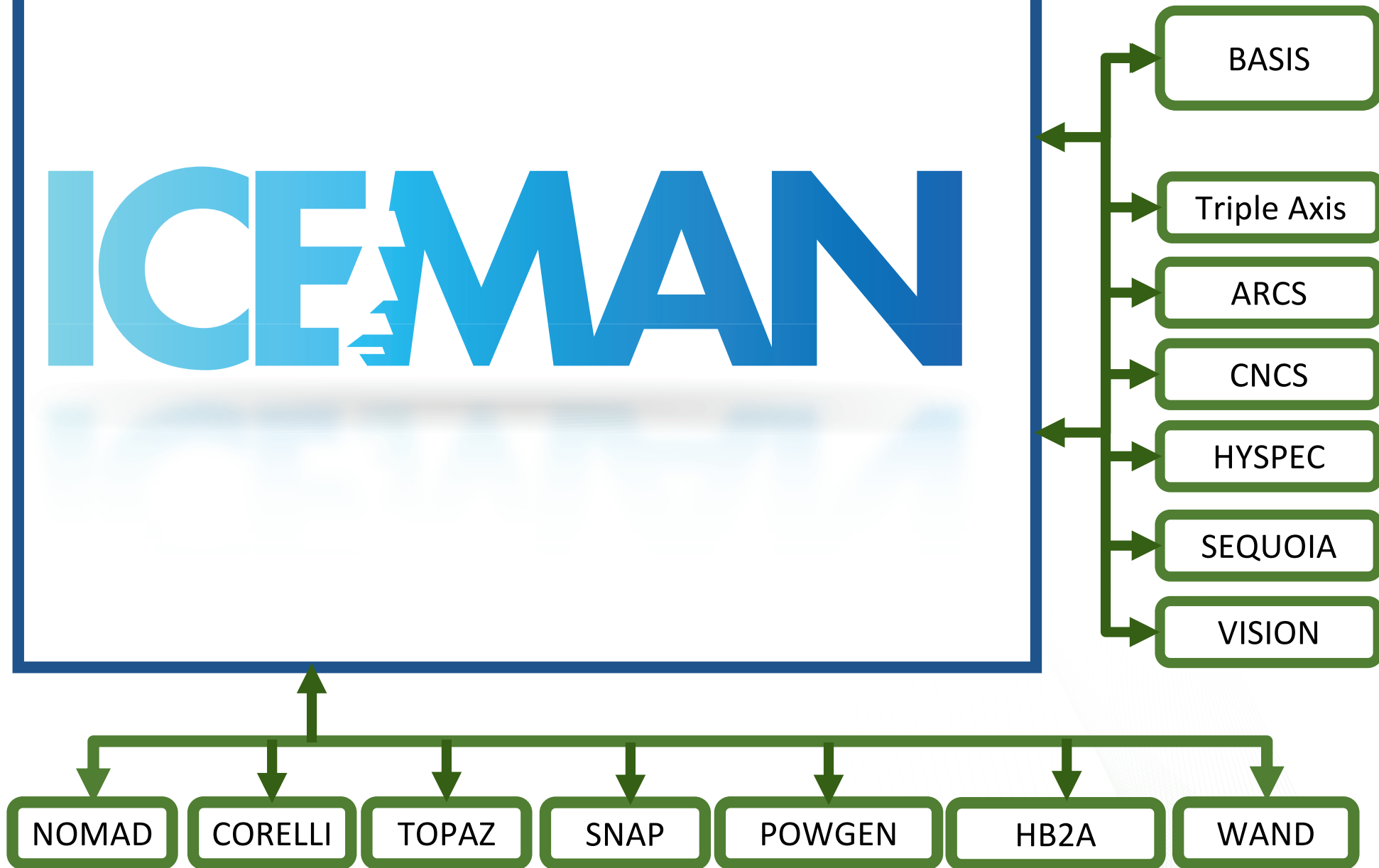
Integrated Computational Environment, for Modeling and Analysis of Neutron data

ICEMAN

Acknowledgement: Laboratory Directed Research and Development program at ORNL




ICE MAN



Why do we need simulations for NVS (or INS in general)?

- Interpret neutron data
 - assigning peaks to vibrational modes
- Obtain insight on fundamental properties
 - understanding interatomic interactions, anharmonicity, complex excitations, phase transitions, chemical reactions
- Connect theory and experiment
 - simulation is a virtual experiment and an *in silico* implementation of theory

We can measure it.  We do understand it.

What to simulate for INS?

- Double differential cross-section

$$\frac{d^2\sigma}{d\Omega dE'} = \text{(number of neutrons scattered per second into a small solid angle } d\Omega \text{ in the direction } \theta, \phi \text{ with final energy between } E' \text{ and } E' + dE') / \Phi d\Omega dE',$$

- Fermi's golden rule

$$\left(\frac{d^2\sigma}{d\Omega dE'} \right)_{\lambda \rightarrow \lambda'} = \frac{k'}{k} \left(\frac{m}{2\pi\hbar^2} \right) |\langle \mathbf{k}' \lambda' | V | \mathbf{k} \lambda \rangle|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega) \propto \frac{k'}{k} S(Q, \omega)$$

V : potential describing the interaction between neutrons and the system

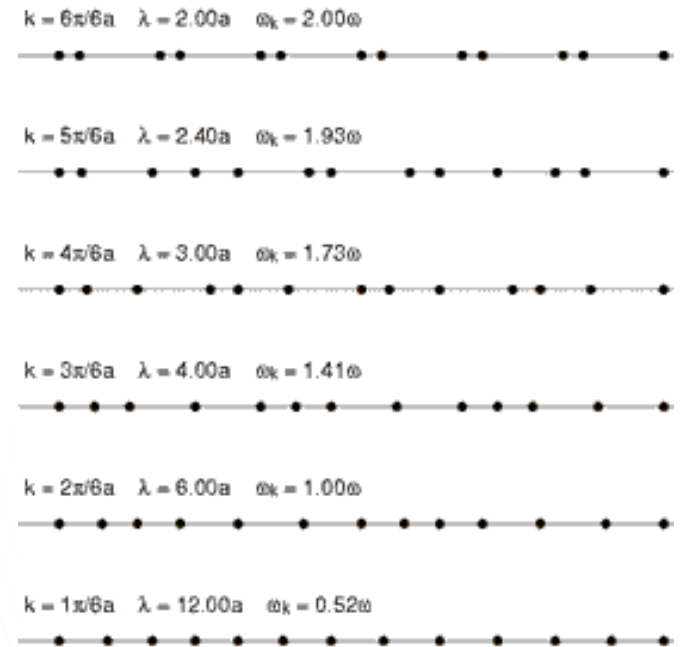
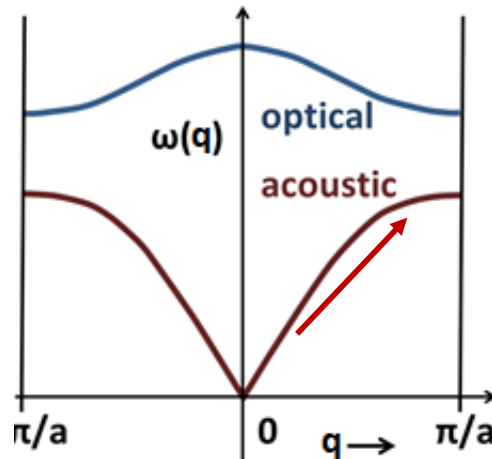
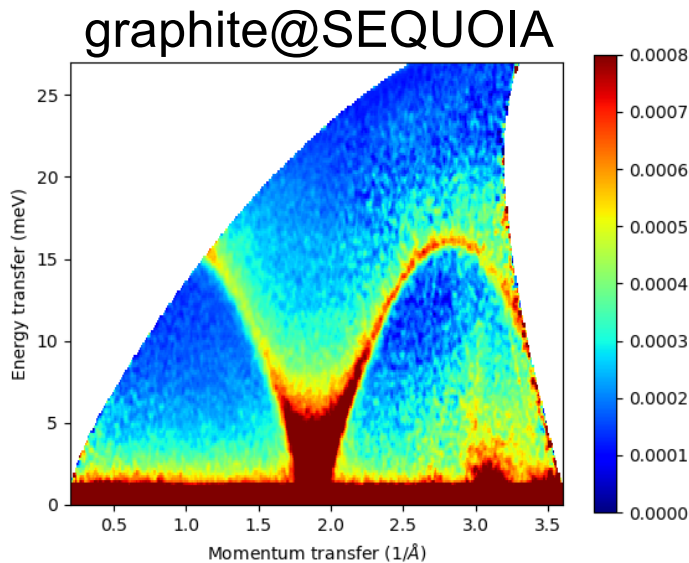
$\hbar\omega$: fundamental excitation in the system

- The goal is to formulate the interaction between neutrons and the system, so that $S(Q, \omega)$ can be expressed by the excitations of interest.

Coherent inelastic scattering

- One-phonon $S(Q, \omega)$

$$S_{coh\pm 1}(\mathbf{Q}, \omega) = \frac{1}{2N} \sum_s \sum_{\tau} \frac{1}{\omega_s} \left| \sum_d \frac{\bar{b}_d}{\sqrt{m_d}} \exp(-W_d) \exp(i\mathbf{Q} \cdot \mathbf{r}_d) (\mathbf{Q} \cdot \mathbf{e}_{ds}) \right|^2 \times \langle n_s + \frac{1}{2} \pm \frac{1}{2} \rangle \delta(\omega \mp \omega_s) \delta(\mathbf{Q} \mp \mathbf{q} - \boldsymbol{\tau})$$



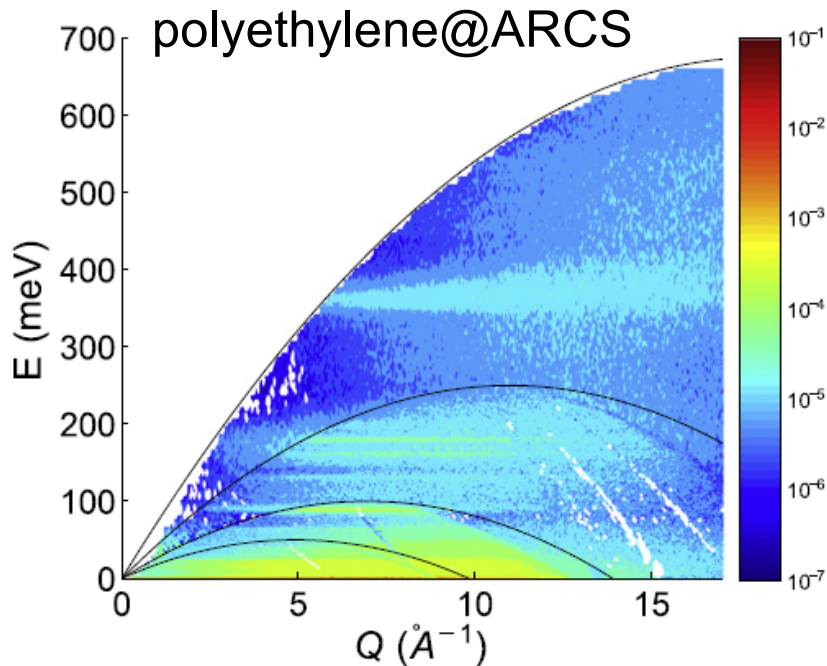
- Peak position in energy depends on Q .
- Total intensity determined by not only how each atom moves, but also their relative phase.

From: wikipedia

Incoherent inelastic scattering

- One-phonon $S(Q, \omega)$

$$S_{inc\pm 1}(\mathbf{Q}, \omega) = \sum_d \frac{1}{2m_d} \left\{ \bar{b}_d^2 - (\bar{b}_d)^2 \right\} \exp(-2W_d) \sum_s \frac{|\mathbf{Q} \cdot \mathbf{e}_{ds}|^2}{\omega_s} \left\langle n_s + \frac{1}{2} \pm \frac{1}{2} \right\rangle \delta(\omega \mp \omega_s)$$



C.M. Lavelle et al. / Nuclear Instruments and Methods in Physics Research A 711 (2013) 166–179



Coherent



Incoherent

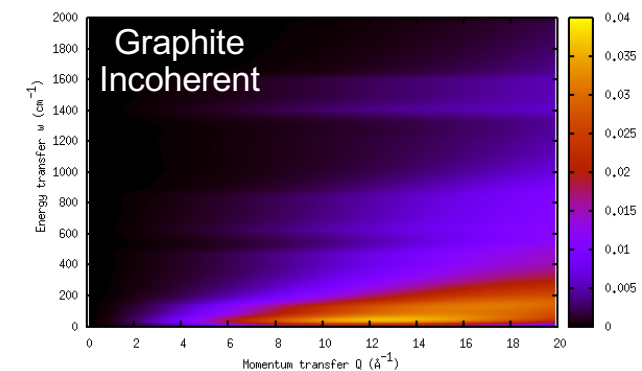
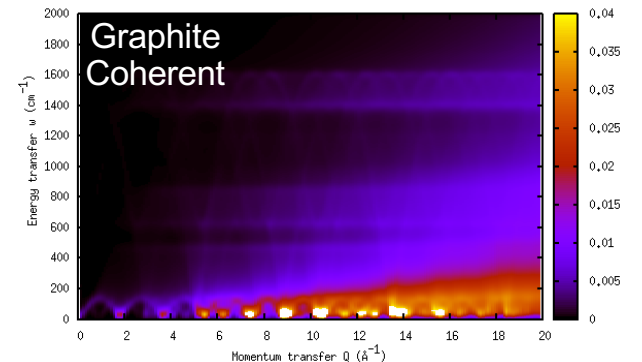
- **Peak position in energy does not depend on Q**
- **Each atom contributes to the total intensity independently.**

Incoherent approximation

- When and why

- Elements/isotopes with large incoherent scattering cross-section (e.g., hydrogen, vanadium) – **The scattering itself is intrinsically incoherent.**
- High Q or large unit cell (small Brillouin zone), e.g. in low symmetry or disordered structure – **The scattering may be coherent, but the ruler is too big for the pattern to be resolved.**

$$S_{coh\pm 1}(\mathbf{Q}, \omega) = \frac{1}{2N} \sum_s \sum_{\tau} \frac{1}{\omega_s} \left| \sum_d \frac{\bar{b}_d}{\sqrt{m_d}} \exp(-W_d) \exp(i\mathbf{Q} \cdot \mathbf{r}_d) (\mathbf{Q} \cdot \mathbf{e}_{ds}) \right|^2 \times \langle n_s + \frac{1}{2} \pm \frac{1}{2} \rangle \delta(\omega \mp \omega_s) \delta(\mathbf{Q} \mp \mathbf{q} - \boldsymbol{\tau})$$



$$S(\mathbf{Q}, n\omega_s) = \frac{(\mathbf{Q} \cdot \mathbf{U}_s)^{2n}}{n!} \exp[-(\mathbf{Q} \cdot \mathbf{U}_{total})^2]$$

$$U_s = \sqrt{\frac{\hbar}{2m\omega_s}}$$

Development of OCLIMAX

- Started 2016
- First version released 2017
- Paper published 2019
- Used to analyze data from VISION and multiple other neutron spectrometers

Features:

- ❖ Incoherent and coherent scattering
- ❖ Powders and single crystals
- ❖ Temperature effects
- ❖ Multiphonon excitations
- ❖ Arbitrary instrument geometry and resolution
- ❖ Arbitrary cuts in 4-dimensional Q-E space
- ❖ Interface with atomistic modeling tools (e.g. DFT codes)
- ❖ Interface with INS data analysis tools (e.g. DAVE and Mantid)
- ❖ User-friendly (multiple platform, easy to use, fast on PCs)

JCTC

Journal of Chemical Theory and Computation

Article

Cite This: *J. Chem. Theory Comput.* 2019, 15, 1974–1982

pubs.acs.org/JCTC

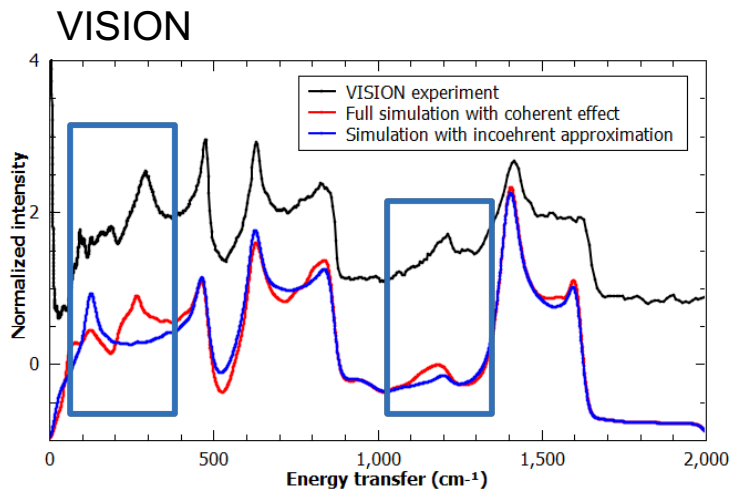
Simulation of Inelastic Neutron Scattering Spectra Using OCLIMAX

Y. Q. Cheng,^{*} L. L. Daemen, A. I. Kolesnikov,[Ⓢ] and A. J. Ramirez-Cuesta^{*}

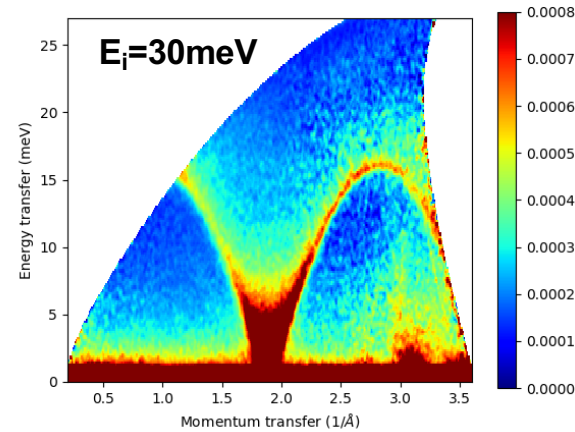
Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge Tennessee 37831, United States

OCLIMAX example: graphite

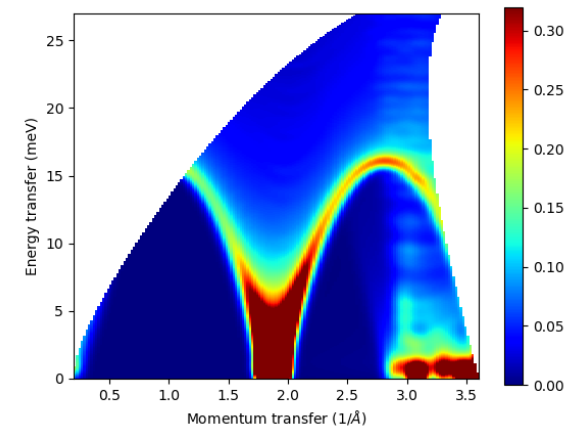
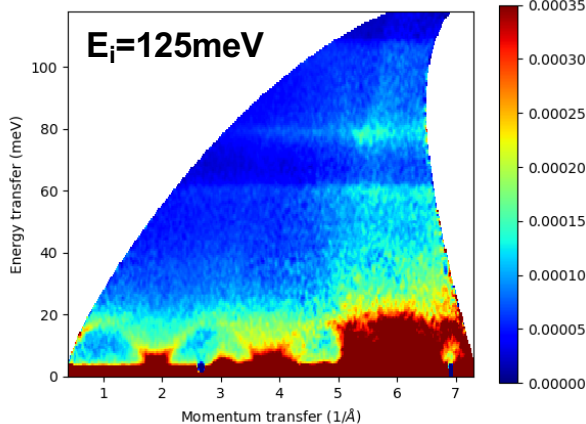
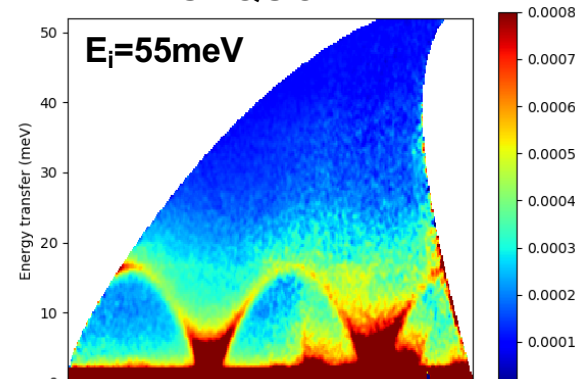
- Coherent scattering
 - Powders
 - Single crystal
- Kinematics
 - Option to generate masks in the map



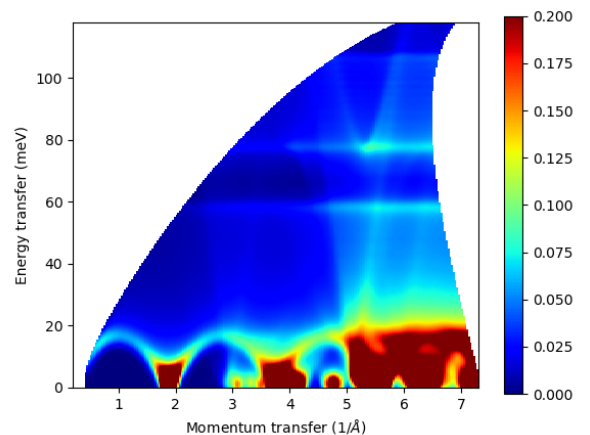
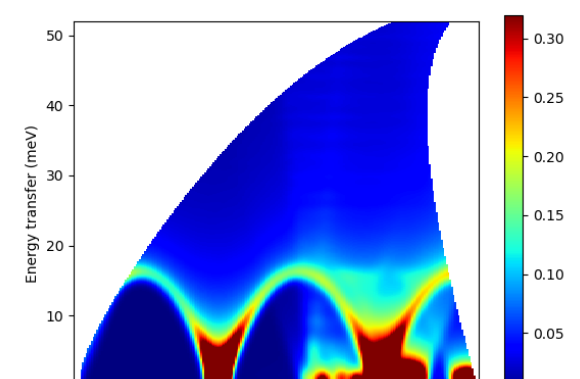
Full calculation versus incoherent approximation



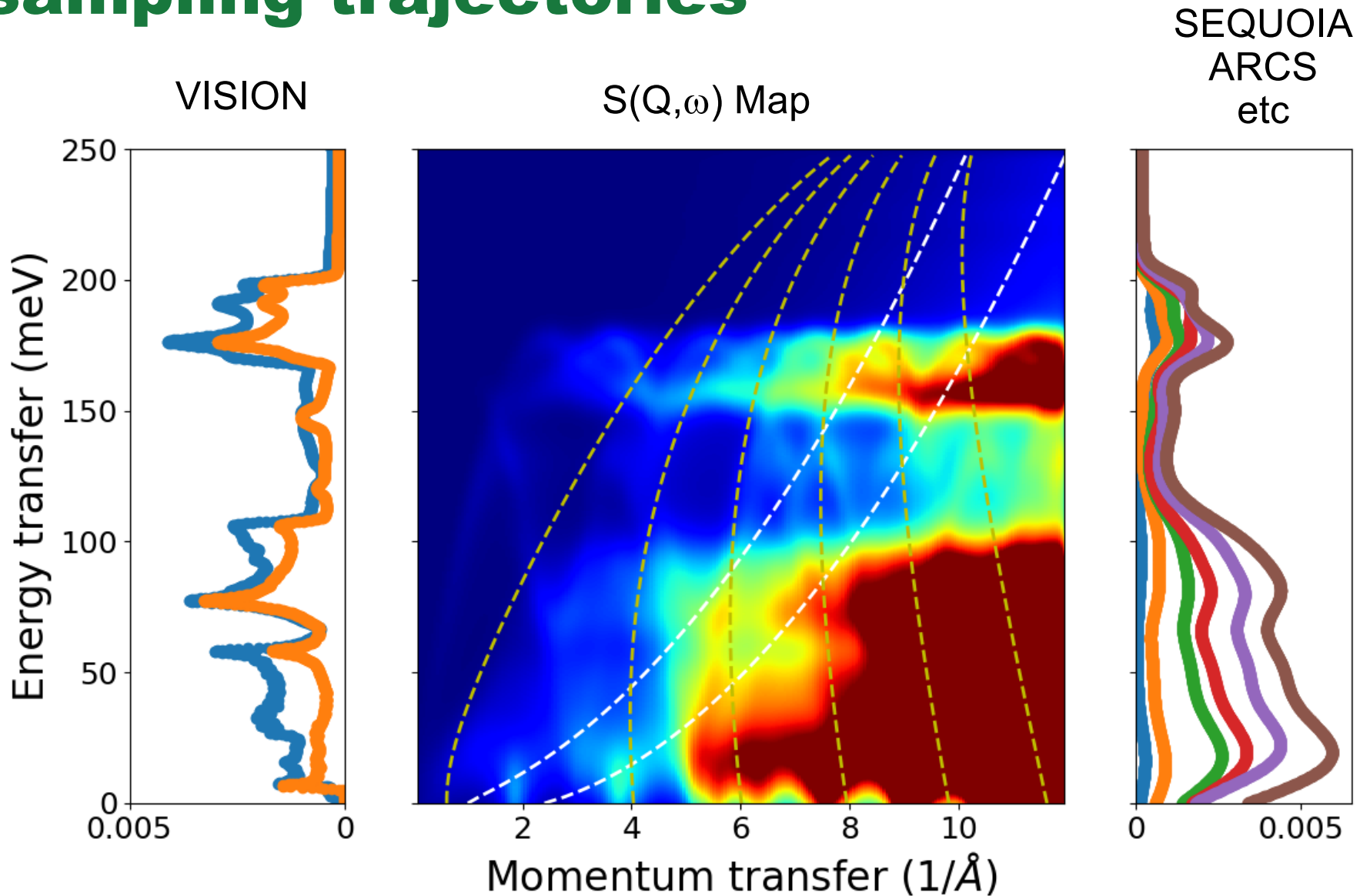
SEQUOIA



OCLIMAX

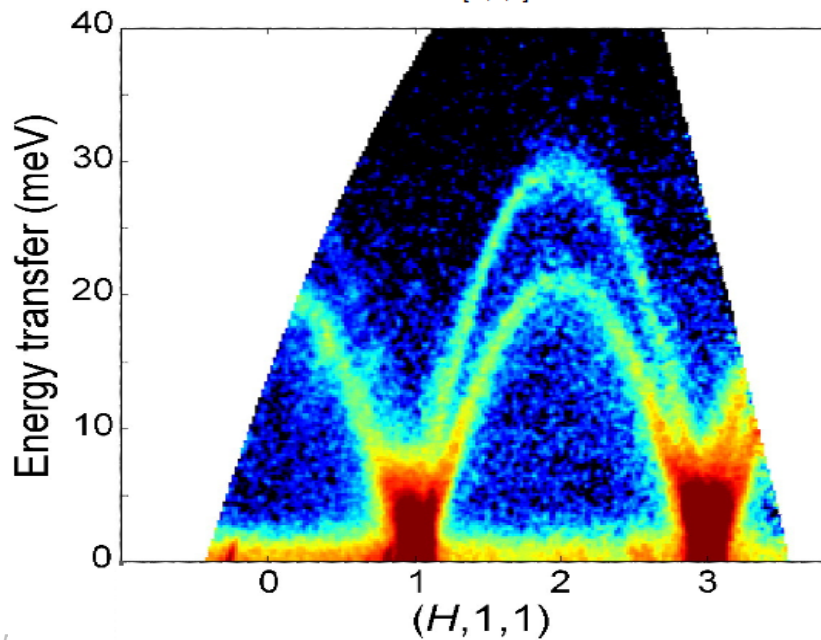
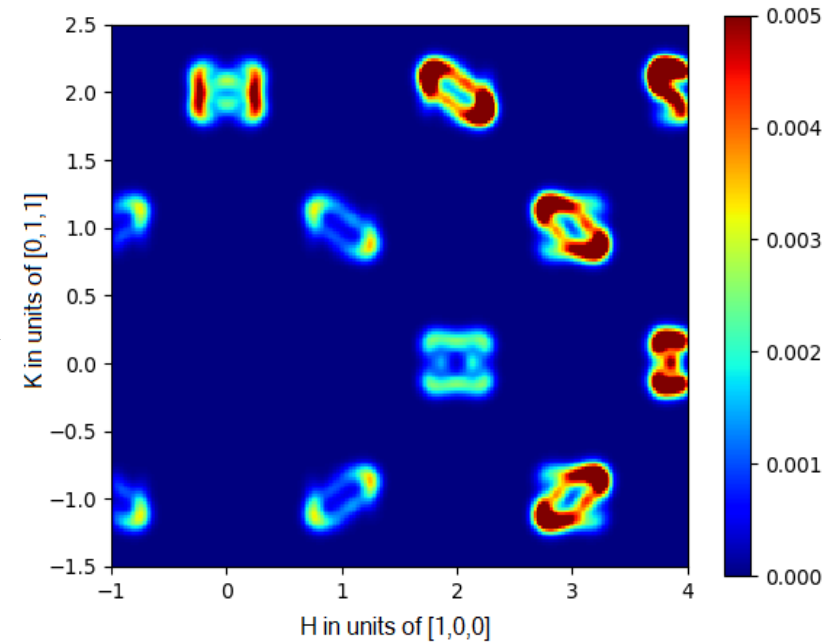
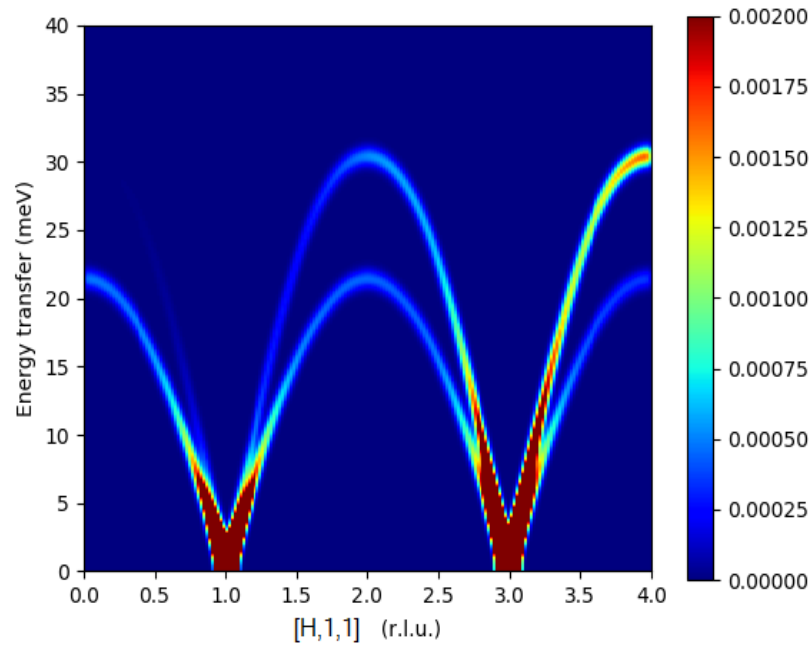


Calculated $S(Q, \omega)$ map and various sampling trajectories



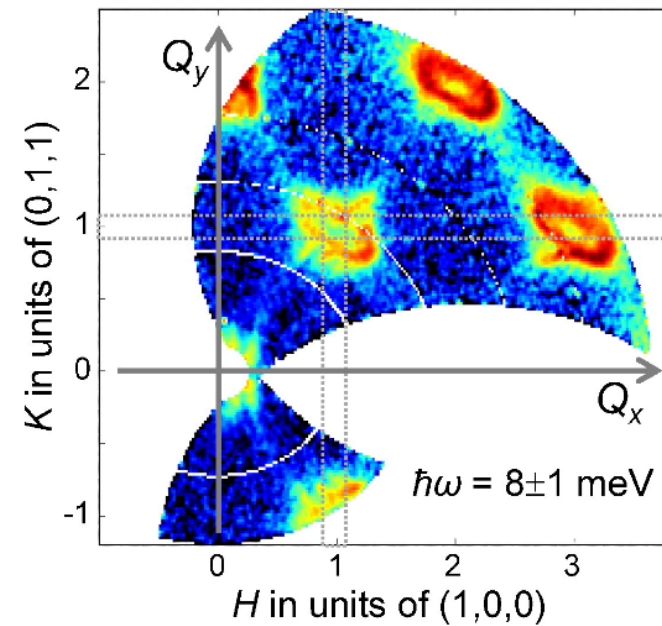
Cheng Y.Q., Daemen L.L., Kolesnikov A.I., Ramirez-Cuesta A.J., "Simulation of inelastic neutron scattering spectra using OCLIMAX", Journal of Chemical Theory and Computation, 15, 3, 1974-1982 (2019).

OCCLIMAX example: single crystal

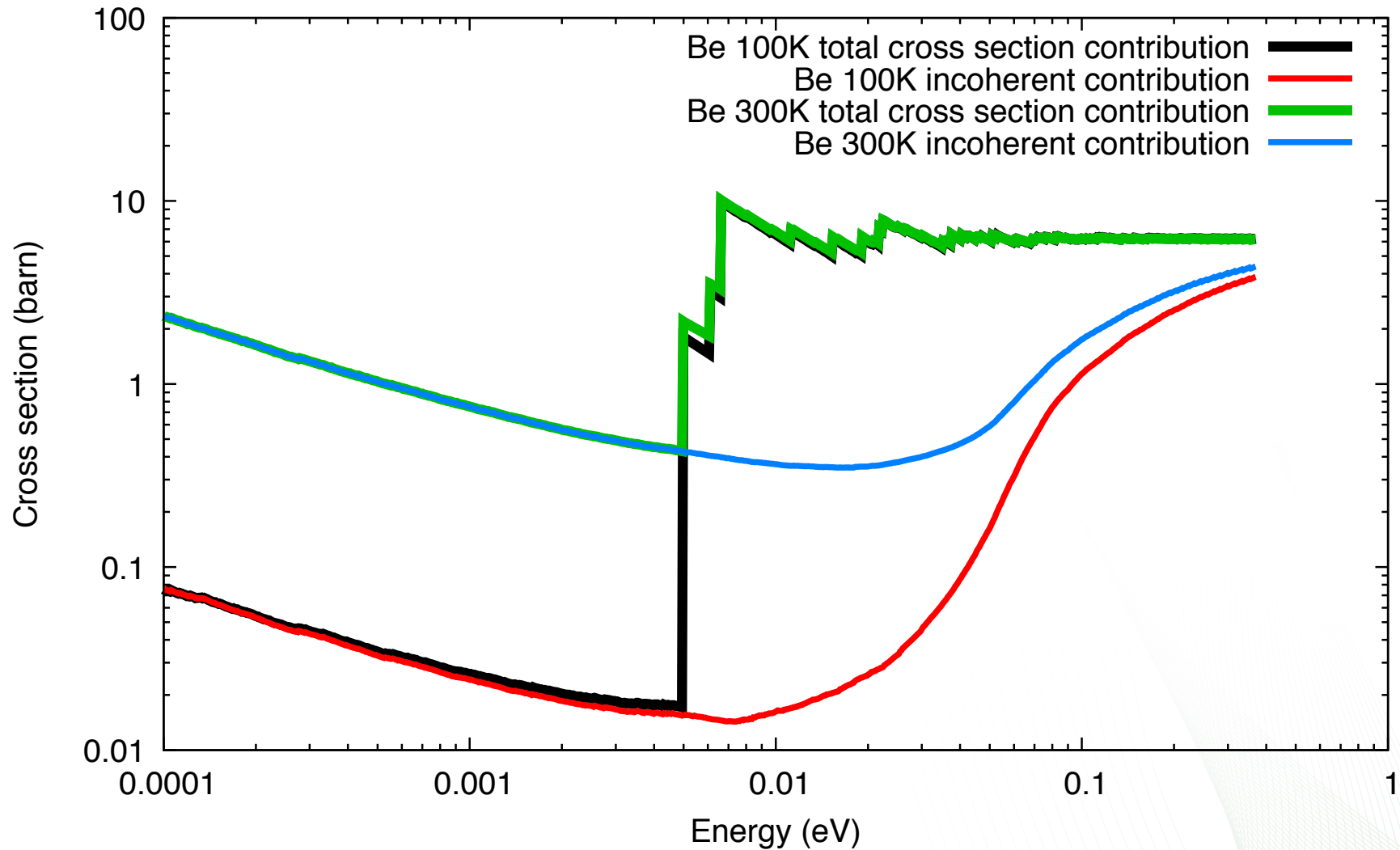


4SEASONS
@J-PARC

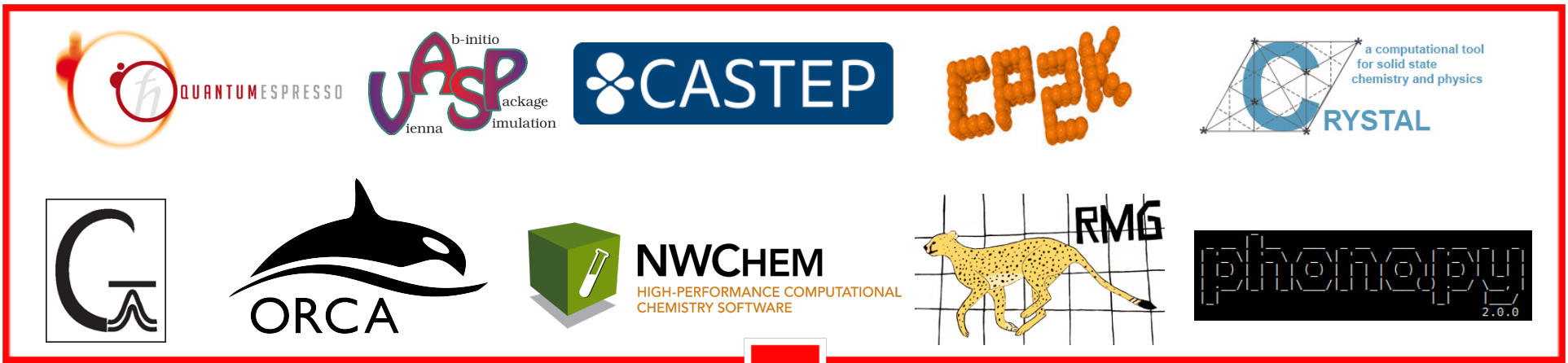
- ✓ Validating phonon frequencies, polarization vectors, and force constants
- ✓ Understanding phonon anomalies.



Total cross sections for solids from first principles calculations

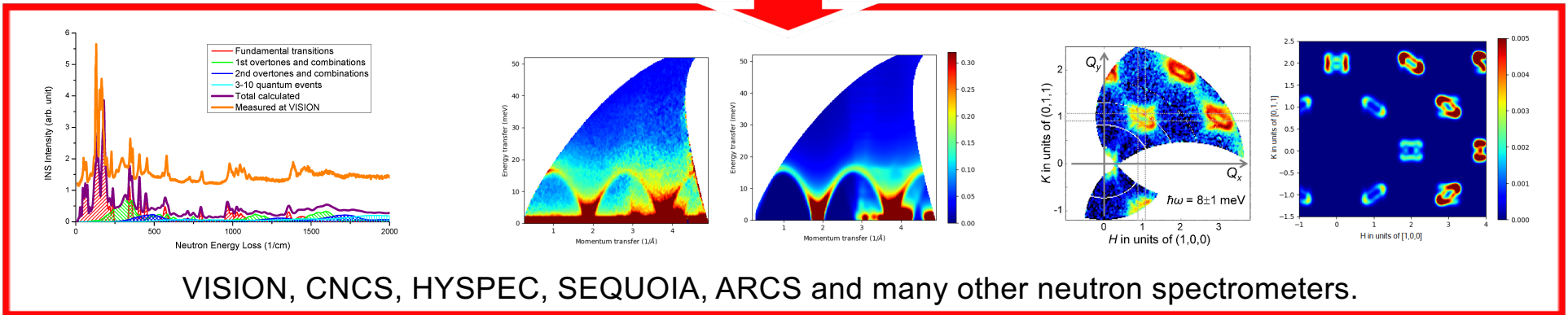


OCLIMAX bridges theory and INS experiments



OCLIMAX

ICEMAN



ICE MAN

Triple Axis

ARCS

CNCS

HYSPEC

SEQUOIA

VISION

ICE MAN

BASIS

Triple Axis

ARCS

CNCS

HYSPEC

SEQUOIA

VISION

Traditional methods

- Minimization, least squares algorithms
- Sequentially fitting QENS functions to data
- Parameters collected
- Plot parameters vs Q
- Fit parameters to functionality

- Laborious, time consuming
- Tedious, error prone method
- It is very difficult to track what's been done to the data

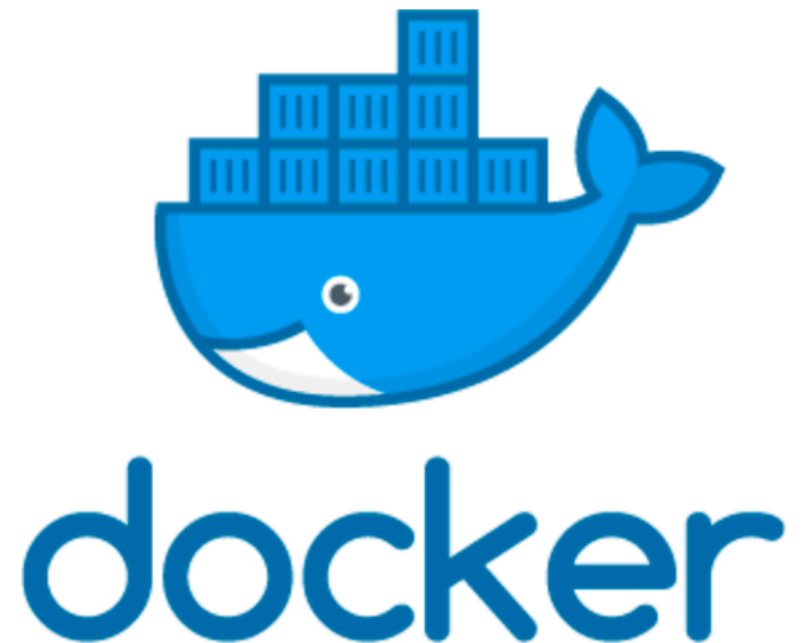
$$I(Q, E) = \left[f_{eisy}(Q) \frac{1}{\pi} \frac{\Gamma_n(Q)}{\Gamma_n(Q)^2 + E^2} + (1 - f_{eisy}(Q)) \frac{1}{\pi} \frac{\Gamma_b(Q)}{\Gamma_b(Q)^2 + E^2} \right] \\ \otimes R(Q, E) + (C_1(Q)E + C_2(Q))$$

QClimax

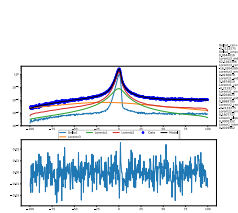
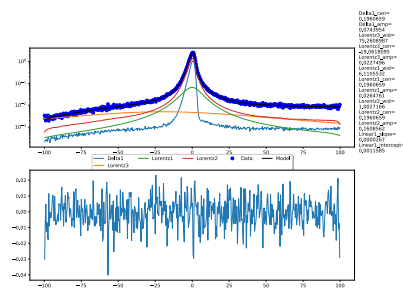
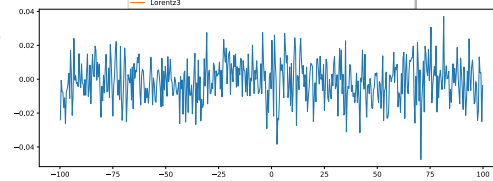
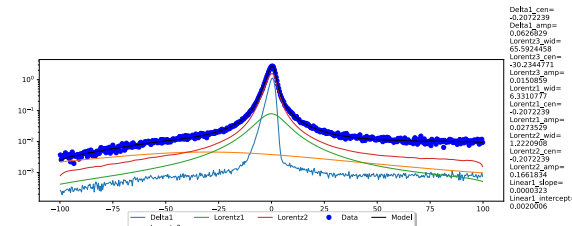
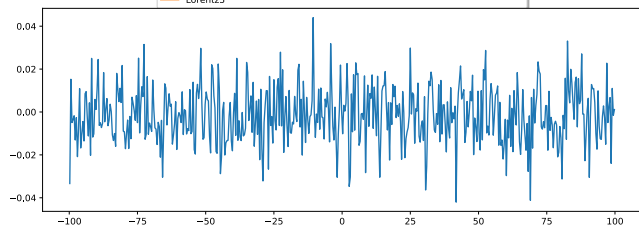
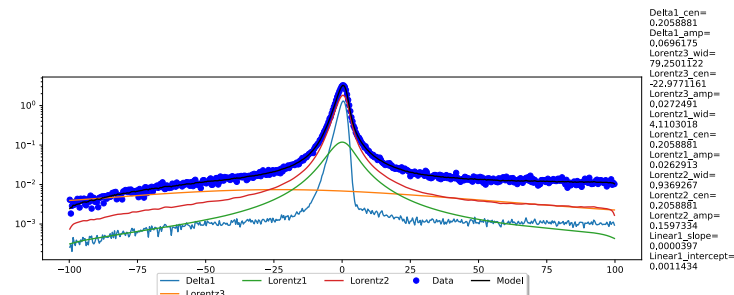
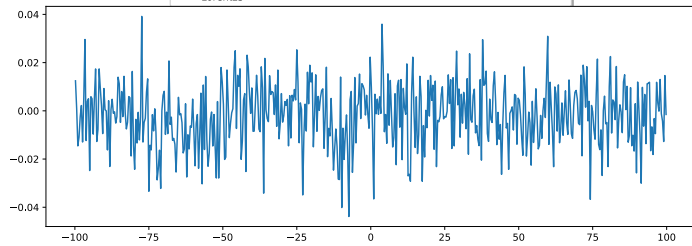
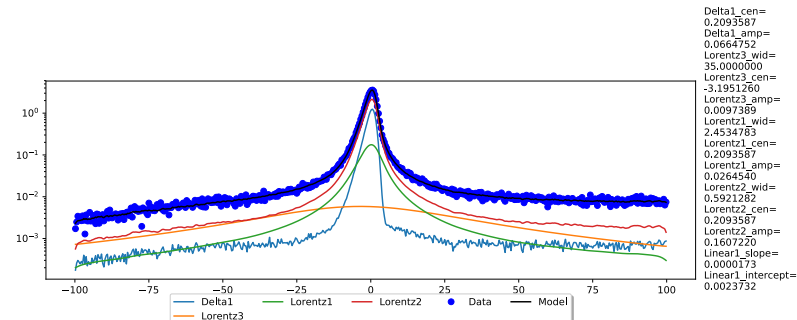
Non-Linear Least-Squares Minimization and Curve-Fitting for Python

Release 0.9.6

Matthew Newville, Till Stensitzki, and others



Qclimax



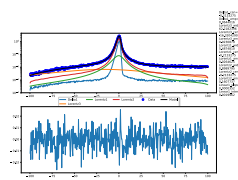
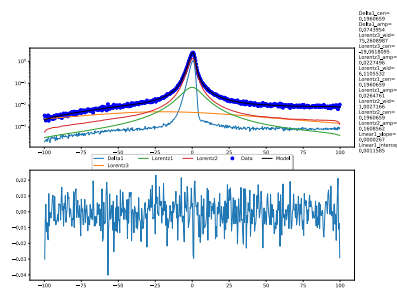
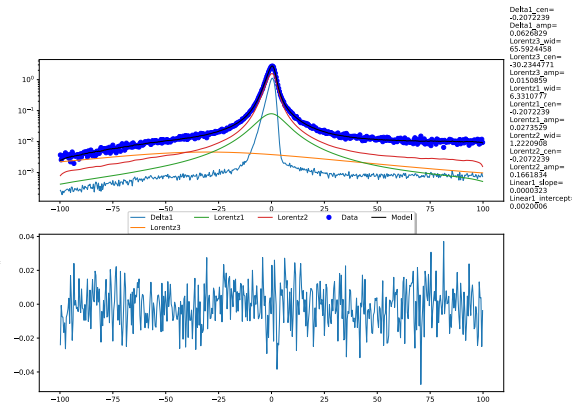
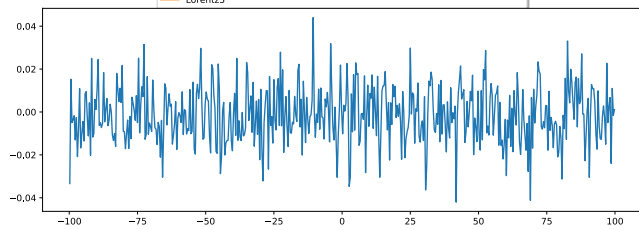
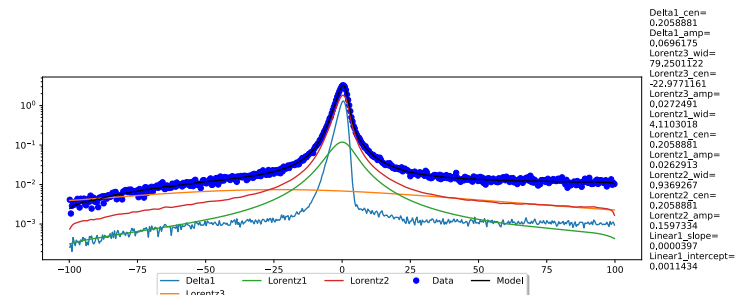
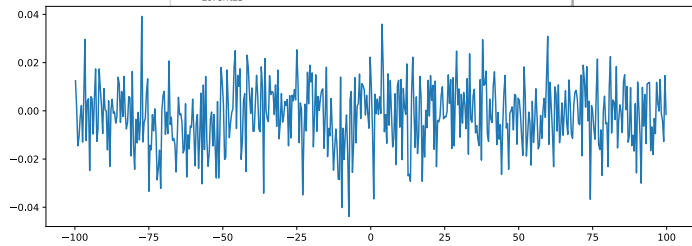
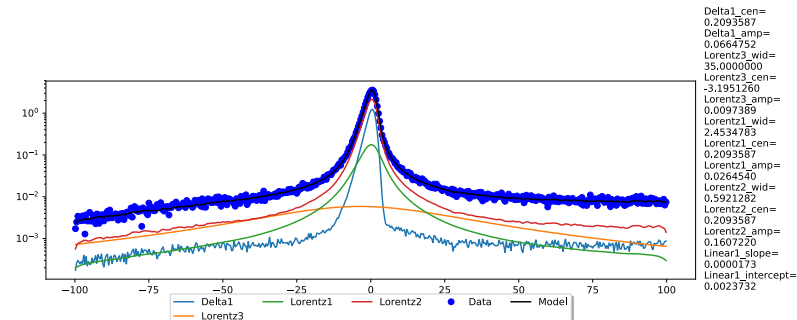
Global fitting of the data

Fitting data using parameter while imposing constraints overt this parameter:

$$FWHM = f(\alpha, \beta, \gamma, \dots, \omega, Q)$$

Returning best fit values for $\alpha, \beta, \gamma \dots$ and so forth

Qclimax



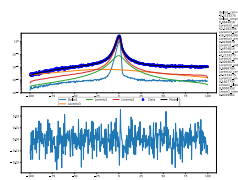
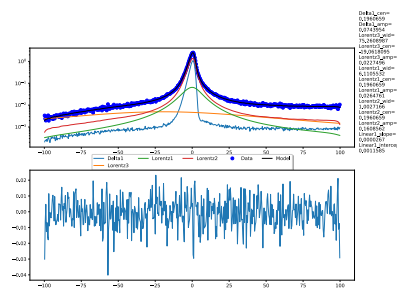
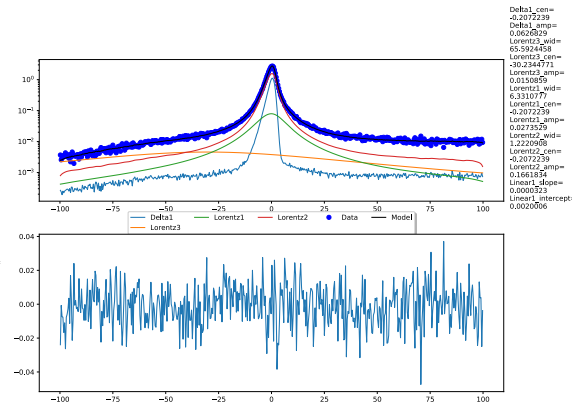
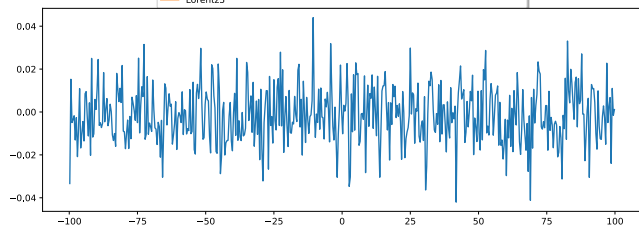
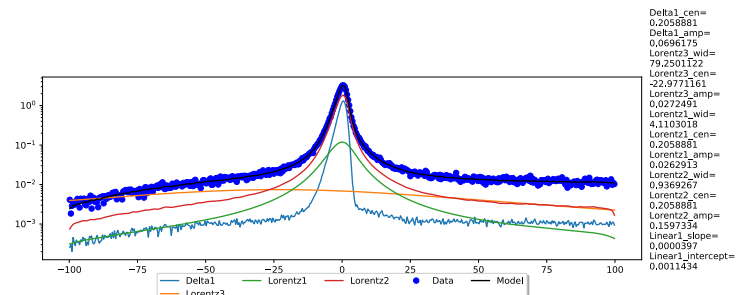
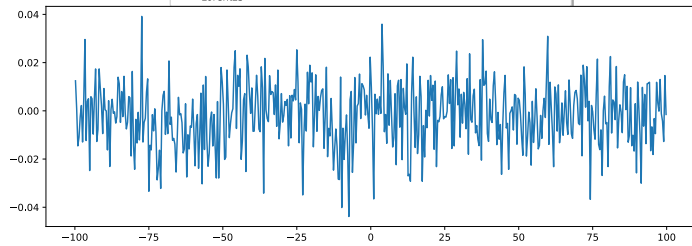
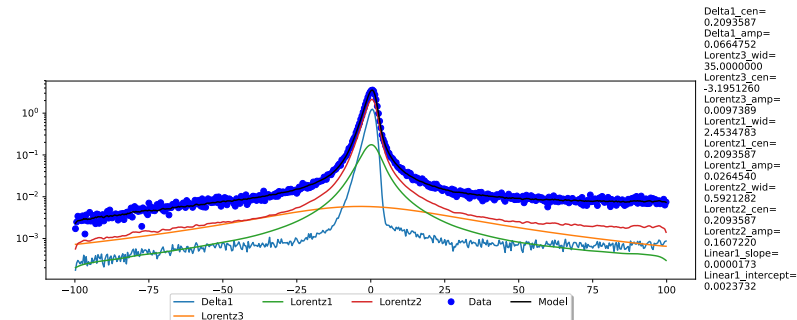
Global fitting of the data

Fitting data using parameter while imposing constraints overt this parameter:

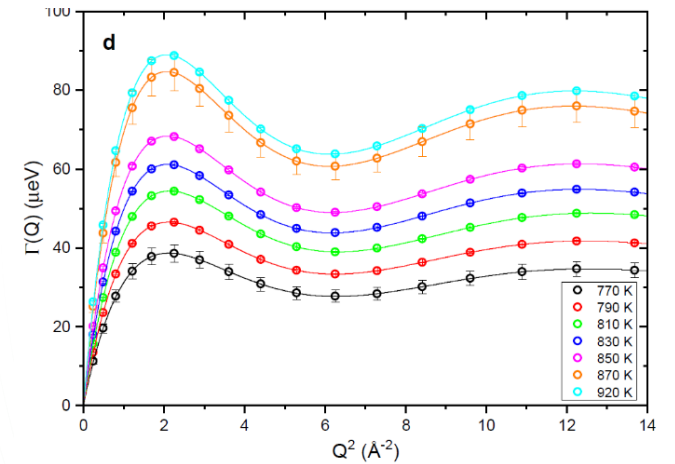
$$FWHM = f(\alpha, \beta, \gamma, \dots, \omega, Q)$$

Returning best fit values for $\alpha, \beta, \gamma \dots$ and so forth

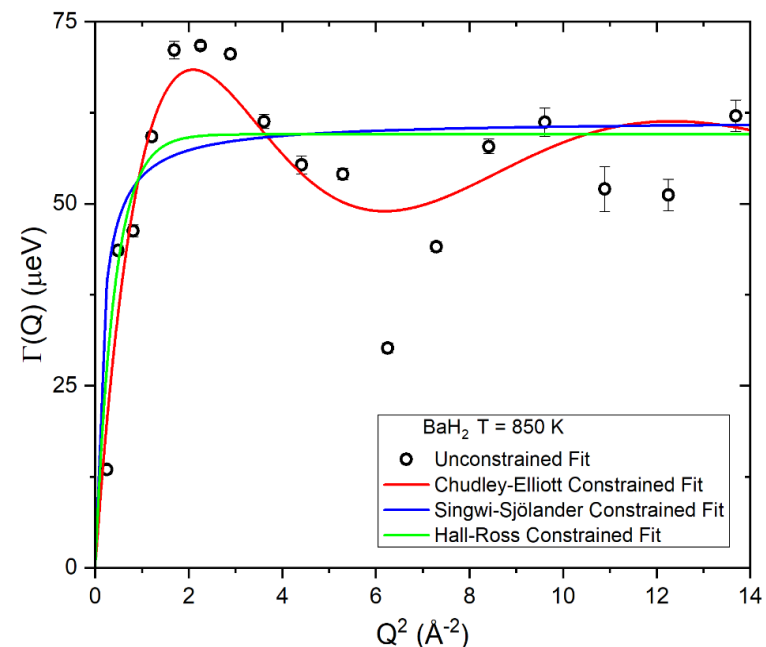
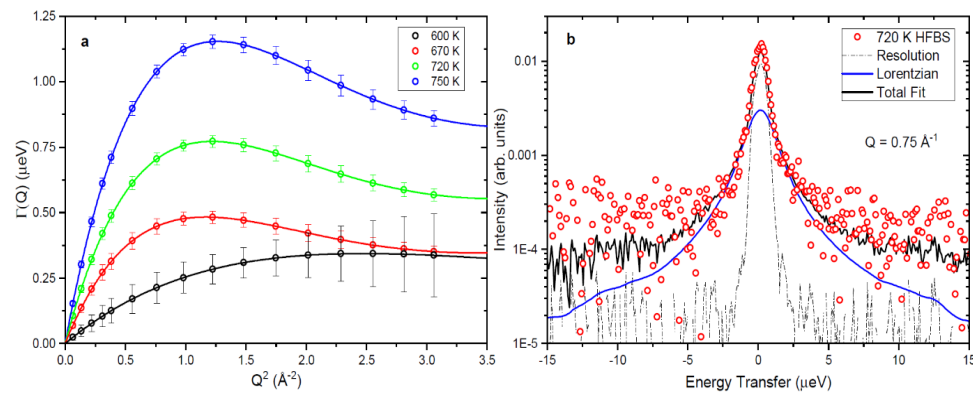
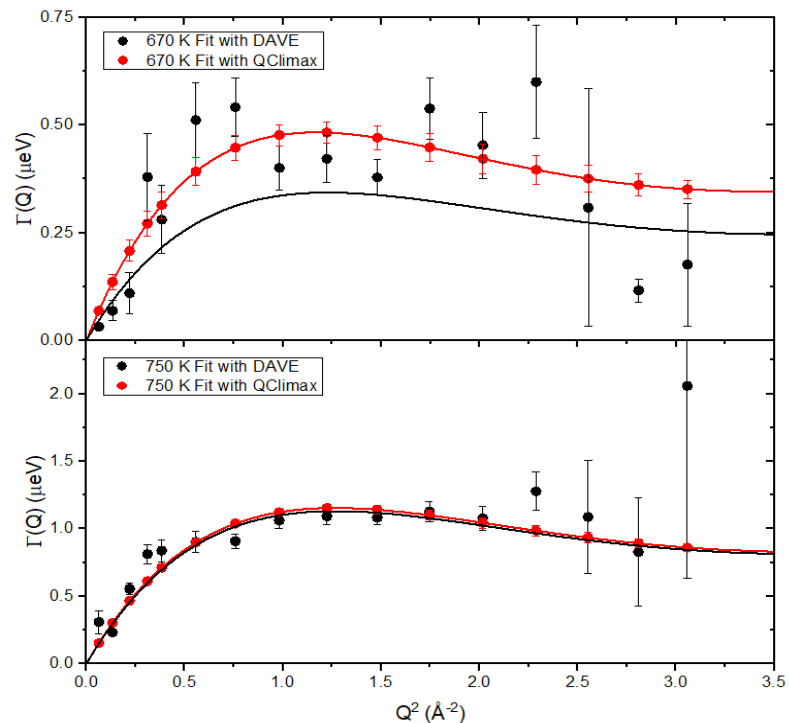
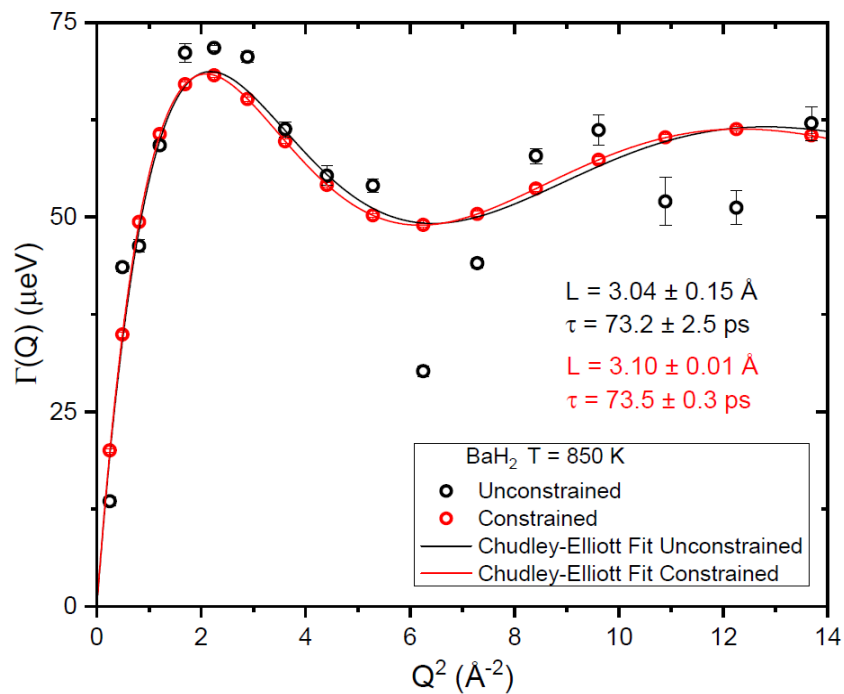
Qclimax



Example:
Chudley-Elliot fit to hydrogen in metal hydrides

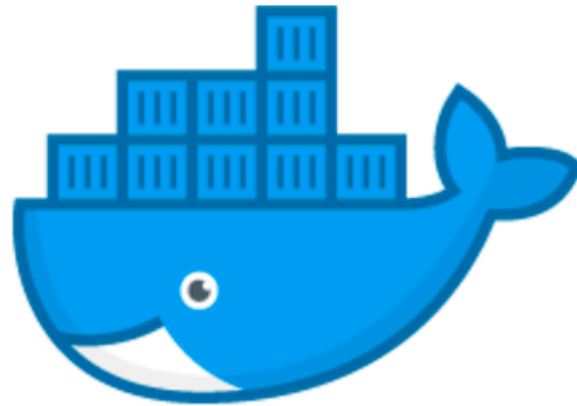


Bayesian behaviour



Many flavours

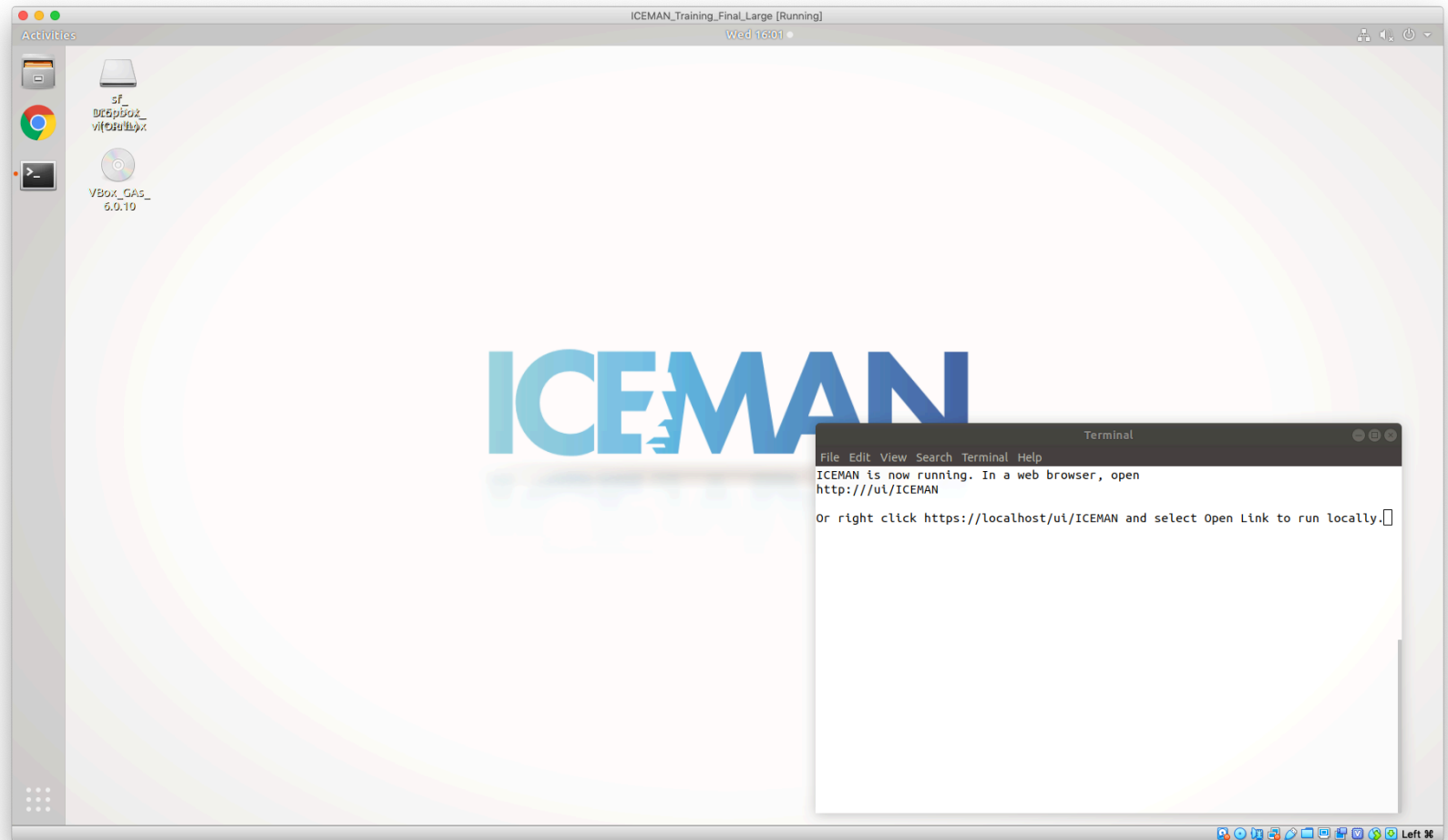
- Docker container



docker

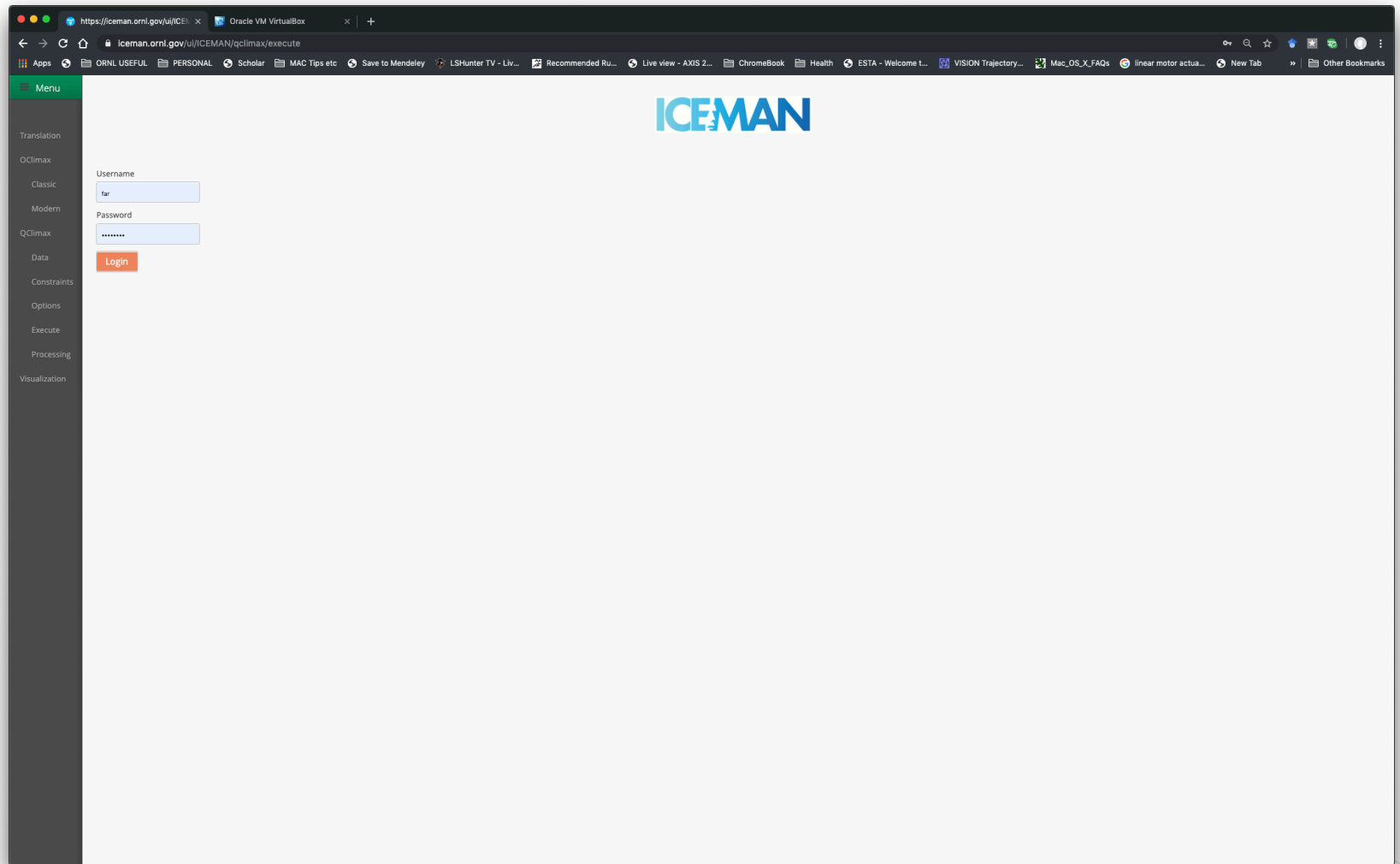
Many flavours

- Virtual machine



Many flavours

- Web access (hosted at ORNL, CADES)



Simple interface

The screenshot displays the ICEMAN web interface. The top navigation bar includes the ICEMAN logo and a user profile dropdown for 'Ramirez Cuesta, Anibal'. The left sidebar contains a 'Menu' section with options: Translation, QClimax, Classic, Modern, QClimax, Data, Constraints, Options, Execute, Processing, and Visualization. The main content area is divided into two primary sections: 'BASIS' and 'Model Functions'.

BASIS Section:

- Resolution File: BaH2_300K_111.dat. Buttons: Select File, Select Function, Graph.
- Select which Q values to use in the fitting: Q0(0.3) Q1(0.5) Q2(0.7) Q3(1.0).
- Data Files: Select Data, Specify temperatures, Graph. A list of files is shown: File, BaH2_710K_111.dat, BaH2_730K_111.dat, BaH2_750K_111.dat, BaH2_690K_111.dat.

Model Functions Section:

- Linear1 (Linear):** Graph, X. Parameters: intercept (1.0E-8), slope (1.0E-8).
- Delta1 (Delta):** Graph, X. Parameters: amp (1.0, Min 0.0), cen (0.0, Min -3900.0, Max 3900.0).
- Lorentz1 (Lorentz):** Graph, X. Parameters: amp (1.0, Min 0.0), cen (1.0E-4, Min -100.0, Max 100.0), wid (0.5, Min 0.025).
- Lorentz2 (Lorentz):** Graph, X. Parameters: amp (1.0, Min 0.0), cen (1.0E-4, Min -100.0, Max 100.0), wid (0.5, Min 0.025).
- Lorentz3 (Lorentz):** Graph, X. Parameters: amp (1.0, Min 0.0), cen (1.0E-4, Min -100.0, Max 100.0), wid (75.0, Min 5.0, Max 140.0).

Simple interface

The screenshot displays the ICEMAN web interface. The top navigation bar includes the ICEMAN logo and a user profile dropdown for 'Ramirez Cuesta, Anibal'. The left sidebar contains a 'Menu' with options: Translation, QClimax, Classic, Modern, QClimax, Data, Constraints, Options, Execute, Processing, and Visualization.

The main content area is divided into two primary sections:

- BASIS:** This section is highlighted with a blue circle. It features a 'Resolution File' section with a text input 'BaH2_300K_111.dat' and buttons for 'Select File', 'Select Function', and 'Graph'. Below this is a 'Select which Q values to use in the fitting' section with checkboxes for 'Q0(0.3)', 'Q1(0.5)', 'Q2(0.7)', and 'Q3(1.0)'. The 'Data Files' section includes a 'Select Data' button, a 'Specify temperatures' checkbox, and a list of files: 'BaH2_710K_111.dat', 'BaH2_730K_111.dat', 'BaH2_750K_111.dat', and 'BaH2_690K_111.dat'.
- Model Functions:** This section contains three function configurations, each with a 'Graph' button and a close button (X):
 - Linear1:** Linear function with parameters: intercept (1.0E-8), slope (1.0E-8).
 - Delta1:** Delta function with parameters: amp (1.0), cen (0.0), Min (-3900.0), Max (3900.0).
 - Lorentz1:** Lorentz function with parameters: amp (1.0), cen (1.0E-4), Min (-100.0), Max (100.0), wid (0.5).
 - Lorentz2:** Lorentz function with parameters: amp (1.0), cen (1.0E-4), Min (-100.0), Max (100.0), wid (0.5).
 - Lorentz3:** Lorentz function with parameters: amp (1.0), cen (1.0E-4), Min (-100.0), Max (100.0), wid (75.0).

Simple interface

The screenshot displays the ICEMAN web interface. The top navigation bar includes the ICEMAN logo and a user profile dropdown for 'Ramirez Cuesta, Anibal'. The left sidebar contains a 'Menu' section with options like Translation, QClimax, Classic, Modern, QClimax, Data, Constraints, Options, Execute, Processing, and Visualization. The main content area is divided into two primary sections: 'BASIS' and 'Model Functions'.

BASIS Section:

- Resolution File: BaH2_300K_111.dat. Buttons: Select File, Select Function, Graph.
- Select which Q values to use in the fitting: Q0(0.3), Q1(0.5), Q2(0.7), Q3(1.0).
- Data Files: Specify temperatures. Buttons: Select Data, Graph.
- File list:

File
BaH2_710K_111.dat
BaH2_730K_111.dat
BaH2_750K_111.dat
BaH2_690K_111.dat

Model Functions Section:

- Linear1: Linear. Buttons: Graph, X.
- Delta1: Delta. Buttons: Graph, X.
- Lorentz1: Lorentz. Buttons: Graph, X.
- Lorentz2: Lorentz. Buttons: Graph, X.
- Lorentz3: Lorentz. Buttons: Graph, X.

Each function section includes a table of parameters:

Name	Starting Value	Min	Max
intercept	1.0E-8		
slope	1.0E-8		

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	0.0	-3900.0	3900.0

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	1.0E-4	-100.0	100.0
wid	0.5	0.025	

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	1.0E-4	-100.0	100.0
wid	0.5	0.025	

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	1.0E-4	-100.0	100.0
wid	75.0	5.0	140.0

Simple interface

The screenshot shows the ICEMAN web interface. The main header includes the ICEMAN logo and a user profile for 'Ramirez Cuesta, Anibal'. A left sidebar contains a 'Menu' with options like Translation, QClimax, Classic, Modern, QClimax, Data, Constraints, Options, Execute, Processing, and Visualization. The main content area is divided into sections: 'BASIS' (with a search box and a list of files), 'Resolution File' (with a file selection box and 'Select File', 'Select Function', and 'Graph' buttons), and 'Data Files' (with a 'Select Data' button and a list of files). A 'Model Functions' panel is circled in blue, containing three function configurations: 'Linear1' (Linear), 'Delta1' (Delta), and two 'Lorentz' functions (Lorentz1 and Lorentz2). Each function configuration includes a name field, a 'Graph' button, and a table of parameters.

Model Functions

Linear1 Linear Graph X

Name	Starting Value	Min	Max
intercept	1.0E-8		
slope	1.0E-8		

Delta1 Delta Graph X

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	0.0	-3900.0	3900.0

Lorentz1 Lorentz Graph X

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	1.0E-4	-100.0	100.0
wid	0.5	0.025	

Lorentz2 Lorentz Graph X

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	1.0E-4	-100.0	100.0
wid	0.5	0.025	

Lorentz3 Lorentz Graph X

Name	Starting Value	Min	Max
amp	1.0	0.0	
cen	1.0E-4	-100.0	100.0
wid	75.0	5.0	140.0

Use your constraints

The screenshot shows the ICEMAN web interface. The browser address bar is <https://iceman.ornl.gov/ui/ICEMAN/qclimax/constraints>. The page title is "ICEMAN" and the user is "Ramírez Cuesta, Anibal". The interface is for configuring constraints for a simulation run named "Run1".

At the top, there are buttons for "+", "x", and "Single center". Below these, there are tabs for "Global" and "Individual Q". The "Global" tab is active.

The main area contains a table of constraints. Each row represents a constraint with its name, a formula, and several control options: "Set Constraint", "Relax constraint", "Rattle value", "Relaxation %", and "Deactivated".

Constraint Name	Formula	Set Constraint	Relax constraint	Rattle value	Relaxation %	Deactivated
Linear1_intercept		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Linear1_slope		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Delta1_amp		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Delta1_cen	P[Lorentz2_cen]	<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz1_amp		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz1_cen	P[Lorentz2_cen]	<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz1_wid	ChudleyElliott(3.6,Lorentz1widtau,Q...	<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz2_amp	P[Lorentz1_amp]*C	<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz2_cen		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz2_wid	ChudleyElliott(4.2,Lorentz2widtau,Q...	<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz3_amp		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz3_cen		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>
Lorentz3_wid		<input type="button" value="Set Constraint"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>	<input type="checkbox"/>

Constraints not there? No problem write them in python!

The screenshot shows the ICEMAN web interface. The main panel displays a list of constraints with columns for Name and Starting Value. A modal window is open for editing a constraint, showing a Python function definition. The function is named `ChudleyElliott` and takes `symsymbol`, `L`, `tau`, and `Q_VALUE` as arguments. The function body includes comments explaining the units and the calculation of `tau` based on `Q` and `L`. The modal also has buttons for 'OK', 'Cancel', and 'Download'. To the right of the modal, an 'Available Parameters' list shows various parameters like `Linear1_intercept`, `Delta1_amp`, etc.

Name	Starting Value
Lorentz1widtau	350.0
Lorentz2widtau	450.0
C	0.5

```
1 # Write a Python function here, describing the constraint you want to use.
2 # The first line consists of the function name and its parameters. Replace Constraint_Name with the name you want for your
3 # Inside the parentheses are the arguments. The first argument will always be symsymbol. This is a Python data structure so
4 # the fitting as well as the other functions, whether built in or written by you
5 def ChudleyElliott(symsymbol, L,tau,Q_VALUE):
6     """Custom constraint. Equivalent to the command argument1 + argument2 * sin(Delta1_amp) """
7     # Write your custom constraint below
8     # You can use the symsymbol to access functions or parameters by writing symsymbol[name] as seen below
9     # In order to use this function in your constraint, you must use it as you would a normal function but leaving out the
10    # For example Constraint_Name(1,2)
11    # Units are:
12    # 10E-10 m^2/sec, then 10E-10 m^2/sec * 1/Angstrom =
13    # 10E-10 m^2/sec * 1/1E-20 m^2 = 10E10 1/sec
14    # Reduced Plank's constant = 6.58211951E-16 eV*sec
15    # therefore
16    # 10E10 1/sec * 6.58211951E-16 eV*sec = 6.58211951E-06 eV = 6.58211951 micro eV
17    # in this case D = 10E-10 m^2/sec
18    # Units of tau:
19    # tau * D * Q^2 = 1
20    # tau = 1/(D * Q^2) = 1/(1E-10 m^2/sec * 1/(1E-20 m^2)) = 1E-10
21    # multiplying tau *1E2 gives tau in 1E-12 sec = 1 ps
22
23    x=Q_VALUE
```

Available Parameters:

- Linear1_intercept
- Linear1_slope
- Delta1_amp
- Delta1_cen
- Lorentz1_amp
- Lorentz1_cen
- Lorentz1_wid
- Lorentz2_cen
- Lorentz2_wid

Select methods

The screenshot shows the ICEMAN web interface. At the top, the URL is `https://iceman.ornl.gov/ui/ICEMAN/qclimax/options`. The page features the ICEMAN logo and a user dropdown menu for "Ramirez Cuesta, Anibal".

The main configuration area includes the following fields and options:

- Name:** BaH2_LT_111_3p6_4p2
- Minimization Method:** Levenberg-Marquardt
- Error Calculation Method:** Average
- # of Error Calculation Steps:** 10
- Epsilon:** (empty field)

Additional options are listed on the right:

- Force Error Calculation
- Convolve Background
- Single Q Prefit
- Center Prefit
- Linear Plot
- Plot Background

Below the main configuration, there are two sections:

- Data Ranges for Temperatures:** A table with columns for Temperature, Min, and Max. The table is currently empty.
- Saved QClimax Configurations:** A list of parameter initialization files:
 - BaH2_300K_111.ini
 - BaH2_300K_111_2L_CE.ini
 - BaH2_300K_111_3L_CE.ini
 - BaH2_LT_111_3p2_4p2.ini
 - BaH2_LT_111_3p6_4p2.iniButtons for "Upload" and "Download" are provided.

Repeat old runs

The screenshot shows the ICEMAN web interface in a browser window. The URL is <https://iceman.ornl.gov/ui/ICEMAN/qclimax/options>. The interface includes a sidebar menu with options like Translation, OClimax, and Options. The main content area features the ICEMAN logo and a user dropdown menu for 'Ramirez Cuesta, Anibal'. Below the logo, there are configuration fields for Name, Minimization Method, Error Calculation Method, # of Error Calculation Steps, and Epsilon. A list of checkboxes allows for selecting various options like Force Error Calculation, Convolve Background, etc. At the bottom, there are sections for 'Data Ranges for Temperatures' and 'Saved QClimax Configurations'. The 'Saved QClimax Configurations' section is circled in blue and contains a list of files: BaH2_300K_111.ini, BaH2_300K_111_2L_CE.ini, BaH2_300K_111_3L_CE.ini, BaH2_LT_111_3p2_4p2.ini, and BaH2_LT_111_3p6_4p2.ini. There are also 'Upload' and 'Download' buttons.

Menu

Translation

OClimax

Classic

Modern

QClimax

Data

Constraints

Options

Execute

Processing

Visualization

ICEMAN

Ramirez Cuesta, Anibal

Name: BaH2_LT_111_3p6_4p2

Minimization Method: Levenberg-Marquardt

Error Calculation Method: Average

of Error Calculation Steps: 10

Epsilon:

Force Error Calculation

Convolve Background

Single Q Prefit

Center Prefit

Linear Plot

Plot Background

Data Ranges for Temperatures

Temperature	Min	Max
-------------	-----	-----

Parameter Initialization files

Saved QClimax Configurations

- BaH2_300K_111.ini
- BaH2_300K_111_2L_CE.ini
- BaH2_300K_111_3L_CE.ini
- BaH2_LT_111_3p2_4p2.ini
- BaH2_LT_111_3p6_4p2.ini

Or select a file to upload with the file browser

Upload

Download

Modify old runs, make expert changes

The screenshot shows the ICEMAN web interface. The main area contains the following configuration options:

- Name: BaH2_LT_111_3p6_4p2
- Minimization Method: Levenberg-Marquardt
- Error Calculation Method: Average
- # of Error Calculation Steps: 10
- Epsilon: (empty field)
- Force Error Calculation:
- Convolve Background:
- Single Q Prefit:
- Center Prefit:
- Linear Plot:
- Plot Background:

Below these options is a section for "Data Ranges for Temperatures" with a table:

	Temperature	Min	Max

A modal window is open, displaying a list of command-line options for the simulation:

```
1 -error-calculation average
2 -error-calculation-steps 10
3 -select-gs 0,1,2,3,4,5,6,7,8
4 -export-params
5 -params Lorentz1widtau,value=350.0,min=100.0,max=1000.0 Lorentz2widtau,value=450.0,min=100.0,max=2000.0 C,value=0.5,min=1.0E
6 -method leastsq
7 -instrument BASIS
8 -resolution BaH2_300K_111.dat
9
10 -data BaH2_710K_111.dat,BaH2_730K_111.dat,BaH2_750K_111.dat,BaH2_690K_111.dat
11 -function Linear:intercept,value=1.0E-8:slope,value=1.0E-8
12 -function Delta:amp,value=1.0,min=0.0:cen,value=0.0,min=-3900.0,max=3900.0
13 -function Lorentz:amp,value=1.0,min=0.0:cen,value=1.0E-4,min=-100.0,max=100.0:wid,value=0.5,min=0.025
14 -function Lorentz:amp,value=1.0,min=0.0:cen,value=1.0E-4,min=-100.0,max=100.0:wid,value=0.5,min=0.025
15 -function Lorentz:amp,value=1.0,min=0.0:cen,value=1.0E-4,min=-100.0,max=100.0:wid,value=75.0,min=5.0,max=140.0
16
17 -run
18 -constraint Lorentz2_amp P[Lorentz1_amp]*C
19 -constraint Lorentz1_wid ChudleyElliott(3.1,Lorentz1widtau,Q.VALUE)
20 -constraint Lorentz2_wid ChudleyElliott(4.2,Lorentz2widtau,Q.VALUE)
21 -constraint Lorentz1_cen P[Lorentz2_cen]
22 -constraint Delta1_cen P[Lorentz2_cen]
23
24
```

A "Save" button is located below the modal window.

Run fittings

https://iceman.ornl.gov/ui/ICEI Oracle VM VirtualBox

iceman.ornl.gov/ui/ICEMAN/qclimax/execute

Menu

Translation

OClimax

Classic

Modern

QClimax

Data

Constraints

Options

Execute

Processing

Visualization

Ramirez Cuesta, Anibal

Save Configuration File Batch Execute Run Abort View output for: Current Process Refresh

```
QClimax Starting...
-error-calculation average
-error-calculation-steps 10
-select-qs 0,1,2,3,4,5,6,7,8
-export-params
-params Lorentz1widtau,value=350.0,min=1.0,max=1000.0 Lorentz2widtau,value=450.0,min=1.0,max=1000.0 C,value=0.5,min=1.0E-5,max=50.0
-method leastsq
-instrument BASIS
-resolution BaH2_300K_111.dat

-data BaH2_710K_111.dat,BaH2_730K_111.dat,BaH2_750K_111.dat,BaH2_690K_111.dat
-function Linear:intercept,value=1.0E-8:slope,value=1.0E-8
-function Delta:amp,value=1.0,min=0.0:cen,value=0.0,min=-3900.0,max=3900.0
-function Lorentz:amp,value=1.0,min=0.0:cen,value=1.0E-4,min=-100.0,max=100.0:wid,value=0.5,min=0.025
-function Lorentz:amp,value=1.0,min=0.0:cen,value=1.0E-4,min=-100.0,max=100.0:wid,value=0.5,min=0.025
-function Lorentz:amp,value=1.0,min=0.0:cen,value=1.0E-4,min=-100.0,max=100.0:wid,value=75.0,min=5.0,max=140.0

-run
-constraint Lorentz2_amp P[Lorentz1_amp]*C
-constraint Lorentz1_wid ChudleyElliott(3.6,Lorentz1widtau,Q_VALUE)
-constraint Lorentz2_wid ChudleyElliott(4.2,Lorentz2widtau,Q_VALUE)
-constraint Lorentz1_cen P[Lorentz2_cen]
-constraint Delta1_cen P[Lorentz2_cen]

#####
Data: BaH2_710K_111.dat Resolution: BaH2_300K_111.dat
```

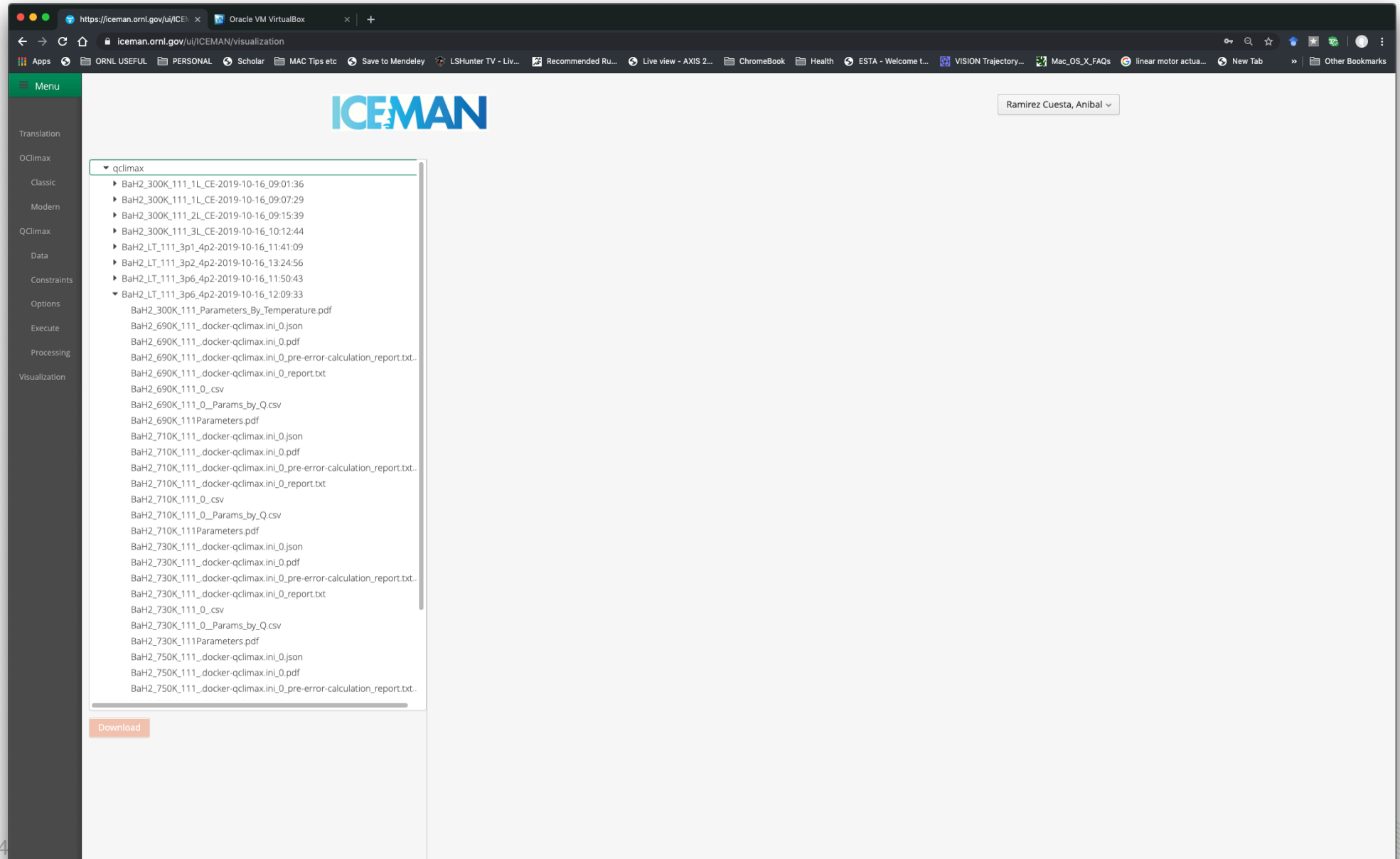
Visualize, edit results, get new starting configurations, download etc.

The screenshot shows a web browser window with the URL <https://iceman.ornl.gov/ui/ICEMAN/visualization>. The page features the ICEMAN logo at the top center and a user profile for "Ramirez Cuesta, Anibal" in the top right. On the left, a dark sidebar menu lists various options: Translation, QClimax, Classic, Modern, QClimax, Data, Constraints, Options, Execute, Processing, and Visualization. The main content area displays a dropdown menu for "qclimax" with a list of simulation configurations, each with a timestamp:

- BaH2_300K_111_1L_CE-2019-10-16_09:01:36
- BaH2_300K_111_1L_CE-2019-10-16_09:07:29
- BaH2_300K_111_2L_CE-2019-10-16_09:15:39
- BaH2_300K_111_3L_CE-2019-10-16_10:12:44
- BaH2_LT_111_3p1_4p2-2019-10-16_11:41:09
- BaH2_LT_111_3p2_4p2-2019-10-16_13:24:56
- BaH2_LT_111_3p6_4p2-2019-10-16_11:50:43
- BaH2_LT_111_3p6_4p2-2019-10-16_12:09:33

Below the list, there is a "temp" option and a "Download" button.

Visualize, edit results, get new starting configurations, download etc.



The screenshot shows a web browser window displaying the ICEMAN interface. The browser's address bar shows the URL `https://iceman.ornl.gov/ui/ICEMAN/visualization`. The page header includes the ICEMAN logo and a user profile dropdown for "Ramirez Cuesta, Anibal". A left-hand navigation menu lists various options: Translation, OClimax, Classic, Modern, QClimax, Data, Constraints, Options, Execute, Processing, and Visualization. The main content area displays a file explorer view for a folder named "qclimax". The file list includes:

- BaH2_300K_111_1L_CE-2019-10-16_09:01:36
- BaH2_300K_111_1L_CE-2019-10-16_09:07:29
- BaH2_300K_111_2L_CE-2019-10-16_09:15:39
- BaH2_300K_111_3L_CE-2019-10-16_10:12:44
- BaH2_LT_111_3p1_4p2-2019-10-16_11:41:09
- BaH2_LT_111_3p2_4p2-2019-10-16_13:24:56
- BaH2_LT_111_3p6_4p2-2019-10-16_11:50:43
- BaH2_LT_111_3p6_4p2-2019-10-16_12:09:33
 - BaH2_300K_111_Parameters_By_Temperature.pdf
 - BaH2_690K_111_docker-qclimax.ini_0.json
 - BaH2_690K_111_docker-qclimax.ini_0.pdf
 - BaH2_690K_111_docker-qclimax.ini_0_pre-error-calculation_report.txt..
 - BaH2_690K_111_docker-qclimax.ini_0_report.txt
 - BaH2_690K_111_0_csv
 - BaH2_690K_111_0_Params_by_Q.csv
 - BaH2_690K_111Parameters.pdf
 - BaH2_710K_111_docker-qclimax.ini_0.json
 - BaH2_710K_111_docker-qclimax.ini_0.pdf
 - BaH2_710K_111_docker-qclimax.ini_0_pre-error-calculation_report.txt..
 - BaH2_710K_111_docker-qclimax.ini_0_report.txt
 - BaH2_710K_111_0_csv
 - BaH2_710K_111_0_Params_by_Q.csv
 - BaH2_710K_111Parameters.pdf
 - BaH2_730K_111_docker-qclimax.ini_0.json
 - BaH2_730K_111_docker-qclimax.ini_0.pdf
 - BaH2_730K_111_docker-qclimax.ini_0_pre-error-calculation_report.txt..
 - BaH2_730K_111_docker-qclimax.ini_0_report.txt
 - BaH2_730K_111_0_csv
 - BaH2_730K_111_0_Params_by_Q.csv
 - BaH2_730K_111Parameters.pdf
 - BaH2_750K_111_docker-qclimax.ini_0.json
 - BaH2_750K_111_docker-qclimax.ini_0.pdf
 - BaH2_750K_111_docker-qclimax.ini_0_pre-error-calculation_report.txt..

At the bottom of the file list, there is a "Download" button.

Structure of heterogeneous software

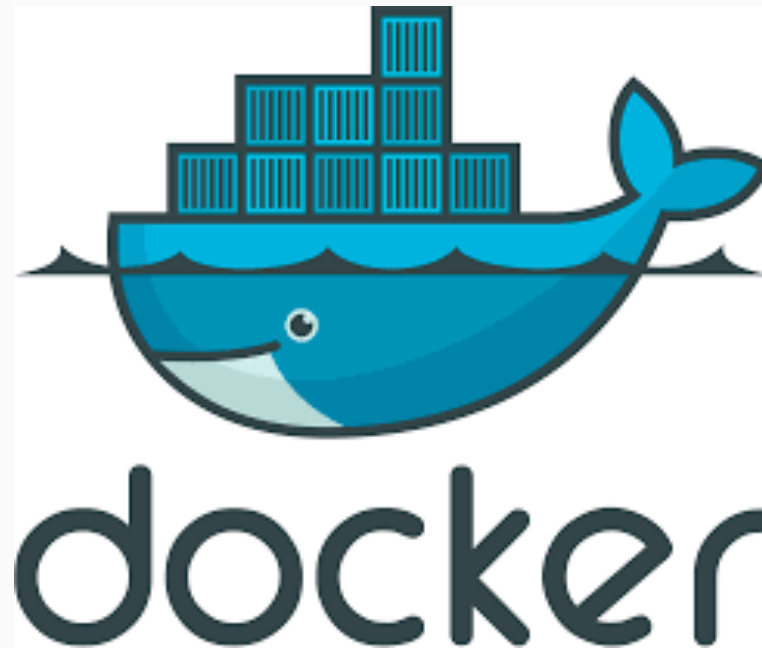


Structure of heterogeneous software



User computer Linux, mac, PC

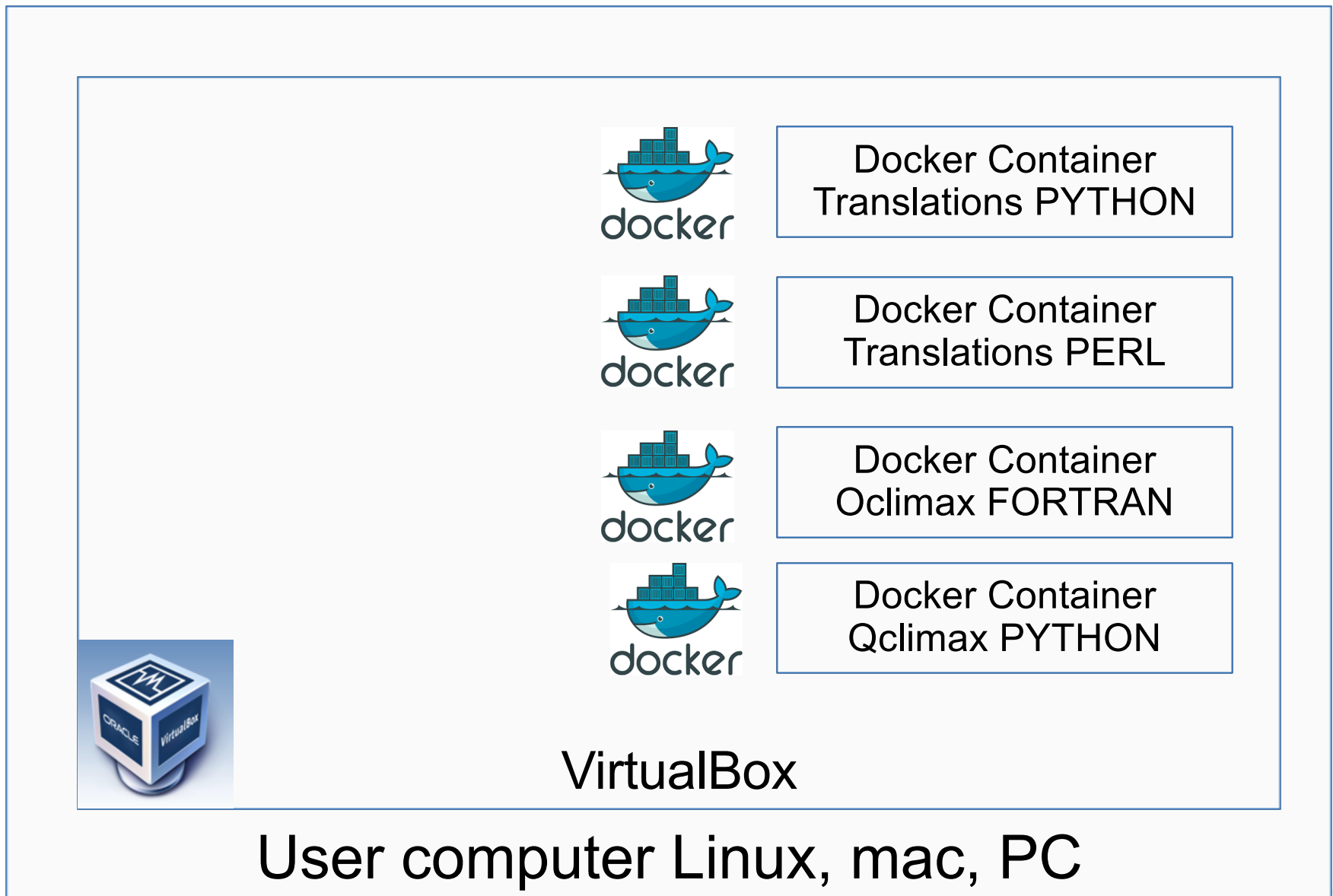
Structure of heterogeneous software



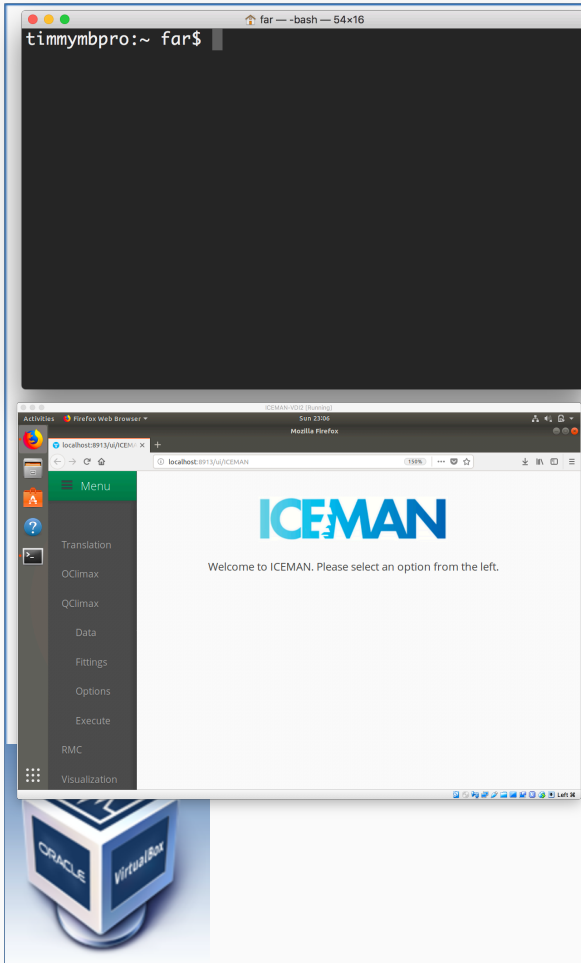
VirtualBox

User computer Linux, mac, PC

Structure of heterogeneous software



Structure of heterogeneous software



Docker Container
Translations PYTHON



Docker Container
Translations PERL



Docker Container
Oclimax FORTRAN



Docker Container
Qclimax PYTHON

VirtualBox

User computer Linux, mac, PC

Conclusion

- Instrumental needs in VISION at SNS require respectable computer resources (1600+ cores cluster today) to help interpret the data
- The VirtuES cluster is available for users to run mostly DFT
- Software to generate inelastic neutron spectra from calculations to directly compare with experimental data has been developed (Oclimax)
- Software to analyze QENS data using global fitting and easy interface and extensibility in the fitting functions and constraints is also available.
- Virtual machine technologies, VirtualBox and Docker are used to produce software that is easy to maintain, expand and that can be operated from the command line and a web interface if desired.
- Secondary objective for software is to automate processes by exchanging file formats and generate a number of input/output files for different codes
- And much more...
- These codes provide the basis for a different approach to automation and reproducibility of neutron data analysis as well as routine integration of computer modeling in neutron scattering.
- Questions?

