How does a shot RI get help?

NIF User Forum

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How does a shot RI get help?

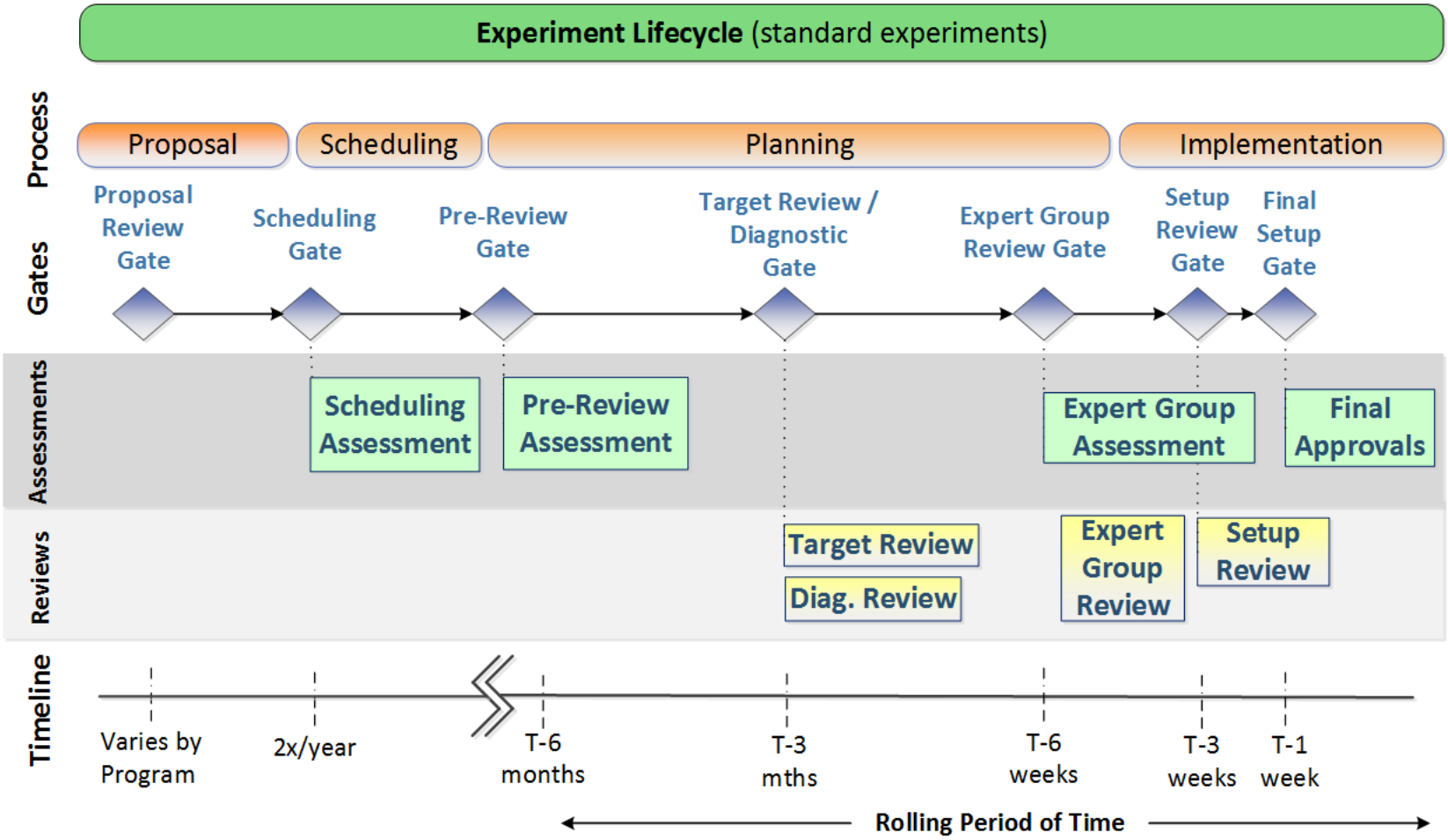
- The answer is coupled to roles and responsibilities
  - Shot RI roles and responsibilities
  - The shot lifecycle
  - Resources
  - Expectations

- This is a work-in-progress
  - As more complex and varied experiments are planned we discover additional information that is needed

The shot lifecycle has a number of steps to navigate

- Proposal
- Award
- Submission into shot planner
- Scheduling
- 6-month pre-review
- Target/diagnostics reviews as applicable
- 6-week submission for EG assessment
- 3-week setup review
- App-man sign-off
- Shot brief
- Execution
- Shot survey/feedback

The shot lifecycle has a number of steps to navigate



The shot RI is responsible for the success of the experiment

- Defining the target, laser, and target diagnostics
  - Target requirements and experiment configuration
  - Beam selection, pointing, and laser setup
  - Diagnostic use and settings
- Ensuring all aspects of the experiment meet facility requirements
  - Materials use, laser energy and optics damage, debris and shrapnel
  - Alignment sequence, TAS interference, 3w and 1w light interactions
- Ensuring reviews are completed, negotating rules of engagement
- Reviewing target and diagnostic metrology and alignment data
- Verifying alignment and diagnostic dry runs
- Providing feedback

Some of the resources that are available to the shot RI

- Organizational resources
  - Program management
  - Campaign PI
  - Project engineer
  - User Office
  - Expert groups
  - TF engineer
  - TD RS/RI
  - NIF Operations
- Information repositories
  - User Office web site
  - Contact list
  - User guide
  - Shot RI training program

The NIF User Office is publishing resource information

- NIF User Forum presentations (sharepoint)
- Shot lifecycle and review process (April Forum charts)
- Point of contact list
- User guide (update planned early 2016)
- Other useful information
  - Beam angles
  - Pointing limits
  - Shot RI tips

https://lasers.llnl.gov/content/assets/docs/for-users/nif_poc.pdf

lasers.llnl.gov

NIF Contact List

Area	Primary	Phone (925)	email	Backup	Phone (925)	email
General User Support	NIF User Office	422-2179	nifuseroffice@llnl.gov			
Tools On Call Support	nif-sds-pager@lists.llnl.gov					
CMT Suite	Doug Speck	423-4208	speck2@llnl.gov	Allan Casey	422-8276	casey20@llnl.gov
Shot Planner	Scott Reisdorf	423-7807	reisdorf1@llnl.gov	Matt Hutton	422-4232	hutton1@llnl.gov
PORT	Raelyn Clark	424-6177	clark94@llnl.gov	Allan Casey	422-8276	casey20@llnl.gov
LOCOS	Darwin Dobson	424-5979	dobson5@llnl.gov	Allan Casey	422-8276	casey20@llnl.gov
LPOM	Mike Shaw	423-8304	shaw7@llnl.gov	Ron House	422-7993	house6@llnl.gov
Archive viewer	Matt Hutton	422-4232	hutton1@llnl.gov	Allan Casey	422-8276	casey20@llnl.gov
Laser setup	Sham Dixit	423-7321	dixit1@llnl.gov	Clay Widmayer	422-9365	widmayer1@llnl.gov
Pulse shaping and Timing	Mark Bowers	423-0901	bowers5@llnl.gov	Clay Widmayer, Brad Golick	422-9365 423-3520	widmayer1@llnl.gov, golick1@llnl.gov
Power limits	Brian MacGowan	422-2250	macgowan1@llnl.gov	Kai Lafortune	423-4060	lafortune1@llnl.gov
BLIP and power balance	Kai Lafortune	423-4060	lafortune1@llnl.gov	Brian MacGowan	422-2250	macgowan1@llnl.gov
NOL	Pam Whitman	424-3583	whitman2@llnl.gov	Brian MacGowan	422-2250	macgowan1@llnl.gov
Beam pointing, TASPOS setup	Pascale Di Nicola	423-1336	dinicola3@llnl.gov	Tom Zobrist	422-2614	zobrist3@llnl.gov
Unconverted light mitigation	Dan Kalantar	422-6147	kalantar1@llnl.gov	Brian MacGowan	422-2250	macgowan1@llnl.gov
TaLIS, Beam stayout zones	Gayatri Gururangan	423-7832	gururangan1@llnl.gov	Brian MacGowan, Nathan Masters	422-2250 422-5236	macgowan1@llnl.gov, masters6@llnl.gov
Target Fielding	Tom Kohut	424-3242	kohut2@llnl.gov	Alex Hamza	423-9198	hamza1@llnl.gov
Target Production	Alex Hamza	423-9198	hamza1@llnl.gov	Dave Trummer	423-8848	trummer1@llnl.gov
Target positioning	Pascale Di Nicola	423-1336	dinicola3@llnl.gov			
Target metrology	Maxine Emerich	422-7288	emerich1@llnl.gov	Pascale Di Nicola	423-1336	dinicola3@llnl.gov
Target RVP	Ethan Alger	423-0831	alger5@llnl.gov	Chris Choate	423-3857	choate3@llnl.gov
Target alignment	Tom Zobrist	422-2614	zobrist3@llnl.gov	Pascale Di Nicola	423-1336	dinicola3@llnl.gov
Target diagnostic rule-set	Bob Kauffman	422-0419	kauffman2@llnl.gov	Bob Ehrlich	422-7650	ehrlich1@llnl.gov
Diagnostics	Bob Ehrlich	422-7650	ehrlich1@llnl.gov	Bob Ehrlich	422-7650	ehrlich1@llnl.gov
DIM based diagnostics	Chris Bailey	422-0578	bailey38@llnl.gov	Bob Ehrlich	422-5862	ehrlich1@llnl.gov
GXD, HGXD	Joe Holder	422-2276	holder4@llnl.gov	Bob Ehrlich	422-7650	ehrlich1@llnl.gov
DISC, SPIDER	Shahab Khan	423-1806	khan9@llnl.gov	Bob Ehrlich	422-7650	ehrlich1@llnl.gov
Dante	Alastair Moore	422-4066	moore212@llnl.gov	Bob Ehrlich	422-7650	ehrlich1@llnl.gov
FABS/NBI	Joe Ralph	423-3932	ralph5@llnl.gov	David Turnbull	422-7650	turnbull2@llnl.gov
VISAR	Marius Millot	422-6359	millot1@llnl.gov	Peter Celliers	424-6977	celliers1@llnl.gov
NIS	David Fittinghoff	422-5188	fittinghoff1@llnl.gov	Bob Ehrlich	422-7650	ehrlich1@llnl.gov
TD factory	tdf-supervisors@llnl.gov			Tim Sarginson, Bob Ehrlich	422-7650 424-4437	sarginson2@llnl.gov, ehrlich1@llnl.gov
Snout, filter and New capability requests, RVP	Chris Bailey	422-0578	bailey38@llnl.gov	Bob Ehrlich, Bob Kauffman, Tim Sarginson	422-7650 422-0419 424-4437	ehrlich1@llnl.gov, kauffman2@llnl.gov, sarginson2@llnl.gov
Snout alignment data & calcs	Reg Wood	423-4691	wood11@llnl.gov	Reg Wood, Nick Shingleton	422-7650, 422-0	wood11@llnl.gov, shingleton3@llnl.gov

As of 2/19/2015

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Shot RI training

- There are two aspects to the NIF Shot RI training program
  - Facility required training (defined classes)
  - Program training (mentoring)
- Facility required training
  - Introduction to Shot RI Training
  - Introduction to CMT
  - Laser Performance
  - Target Fabrication
  - NIF Operations
  - Target Fielding
  - Diagnostics
  - Alignment
  - NIF User Office

	Training Category and Description	Point of Contact
1	**Introduction to Shot RI Training, Shot Setup, and Review Process**	Mathew Snyder snyder41@llnl.gov 925-424-3165
	Training process, tracking (incl qual card and platform approvals), FLIP (scheduling), expert groups (BLIP, NOL, TaLIS, HRG, Diagnostics, Target Fab), review process, approvals, change process (CCBs)	
2	**NIF User Office and Shot RI Resources**	
	User Office organization and mission, Shot RI tools, reference documents, shot surveys, and other resources	
3	**Introduction to CMT, Shot Planning Tools, Visualization, and Data**	Mentor
4	**Laser Performance (BLIP, NOL, TaLIS)**	Brian MacGowan macgowan1@llnl.gov 925-422-2250
	Power and energy limits, power and energy performance (balance), beam conditioning (bandwidth, wavelength, CPPs), bundle/quad/beam use constraints and ROEs (RMDE) and compensation for BLs, beam pointing definition, range, and constraints, laser timing and constraints, tradeoffs such as optics inspection, optics use rates, CPP exchanges, etc, backscatter issues and concerns	
5	**Target Fabrication Tools**	Chris Choate choate3@llnl.gov 925-423-3857
	Intro to tools: PORT, ECMS, LoCoS, target metrology plan, target RVP	
6	**Introduction to NIF Operations**	Tom Kohut kohut2@llnl.gov 925-424-3242
	NIF Operations staffing and shift schedules, working in the facility/facility access, shot cycle/ RI interface to operators and Shot Director, Control Room access/rules, Shot RI roles and responsibilities including shift briefings, Approval Manager annotations; shot time change limitations, Safety System implications for shots	
7	**Introduction to Target Fielding**	
	Target operations group interactions, target fielding capabilities and limitations; target prep times and approvals, yield control, shot categories	
8	**Diagnostics, factory, and RVP**	Bob Ehrlich ehrlich1@llnl.gov 925-422-7650
	Optical, x-ray, nuclear instruments, snouts and pinholes, design and fielding constraints (stayout zones, standoff, debris wind, etc), target diagnostic factory (incl assembly, disassembly, film, long lead items, etc), diagnostic alignment, diagnostic timing and cross timing, tradeoffs such as standoff vs field of view, diagnostic RS, diagnostic RVP	
9	**Alignment Classes and Discussion**	Dan Kalantar kalantar1@llnl.gov 925-422-6147
	Classes: Target Alignment, DIM Alignment, and TAS Alignment, followed by alignment observation during shot cycle Discussion: Diagnostic and target alignment review, target configuration design constraints (debris/shrapnel, 1w, backscatter,	

Example – TD RS/RI role in specifying diagnostic configuration

- RS/RI is responsible for defining the standard operating mode for the diagnostic
  - Standard calibration, safe operation, golden templates
- RS/RI is responsible for reviewing the use for safety
  - Evaluating the configuration and use, not validity for data acquisition
- The RS/RI is a resource for guidance but not to engage the design aspects of the experiments
  - If the use falls outside the normal range of operation then it requires negotiation, priority, funding to establish a collaboration with the RS/RI
- Examples
  - Dante

Example – BLIP role in specifying laser setup

- BLIP has defined standard configurations for laser operation and rule-sets that are applied through CMT
- BLIP manages the laser model to meet standard performance
- BLIP reviewers verify the safe operation of the laser, do not review for consistency with physics goals or requirements
  - If the use falls outside the normal range of operation then it requires negotiation, priority, funding to establish a collaboration with BLIP scientists
- Examples
  - Large numbers of rod shots due to poor selection of amp configuration
  - Timing variability with 300 ps gaussian pulses

NIF User Office

- The User Office serves as an interface between all users and the facility
  - Solicitations, performance surveys, tracking
  - Maintains priorities for tools and capabilities
  - Optimizing and managing the schedule
- Senior scientist serves as a point of contact for information
  - Sometimes the source of information is from the program!

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NIF data trends tool

NIF User Forum

Andrew MacPhee

10th / 11th November 2015

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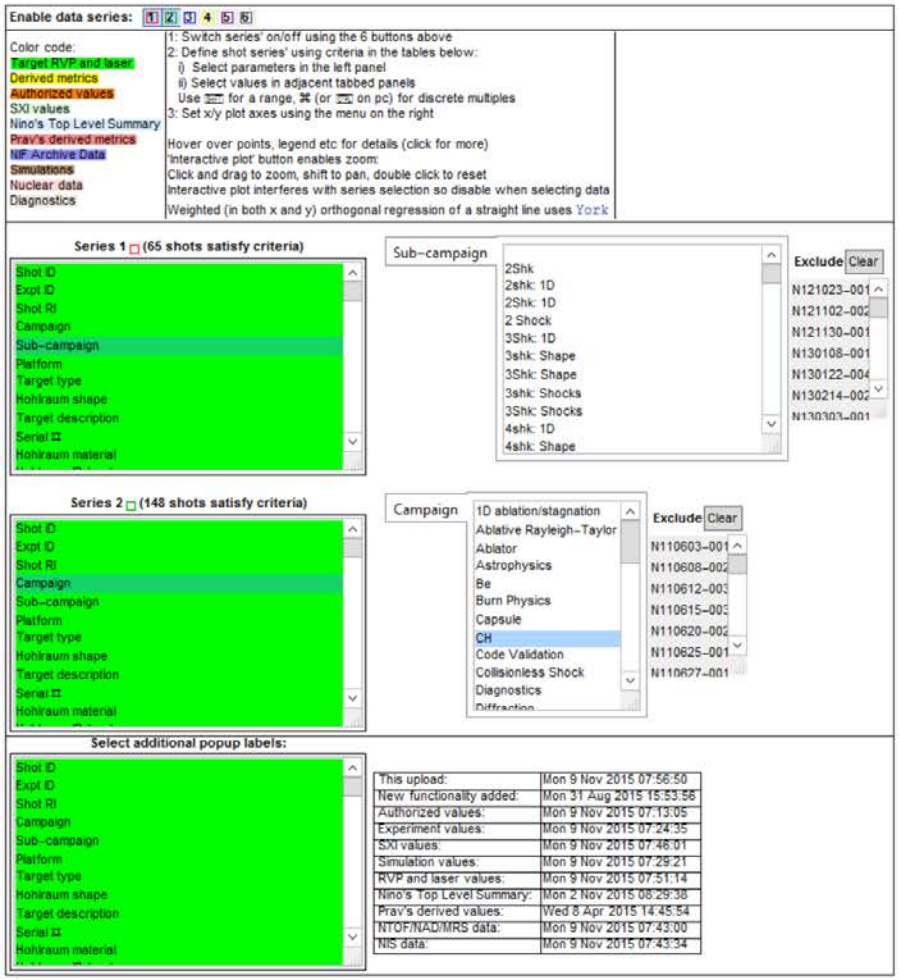
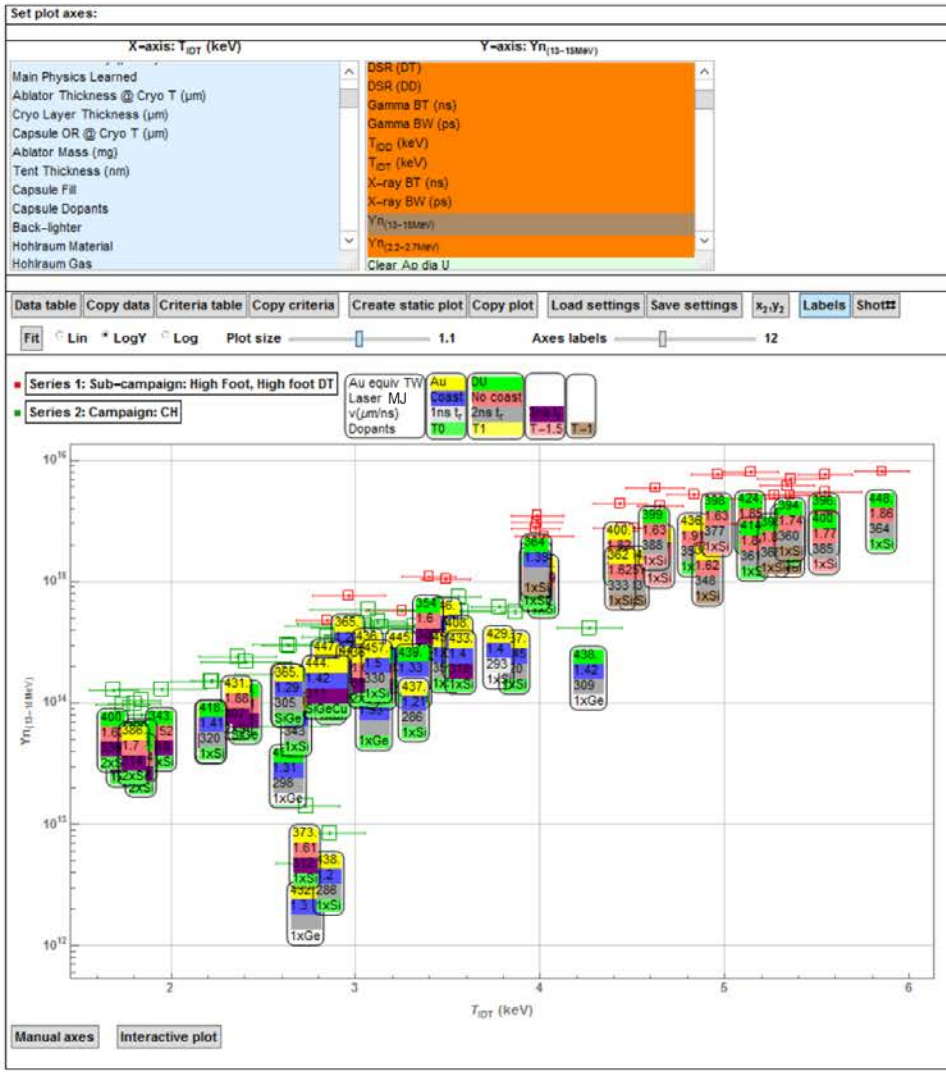
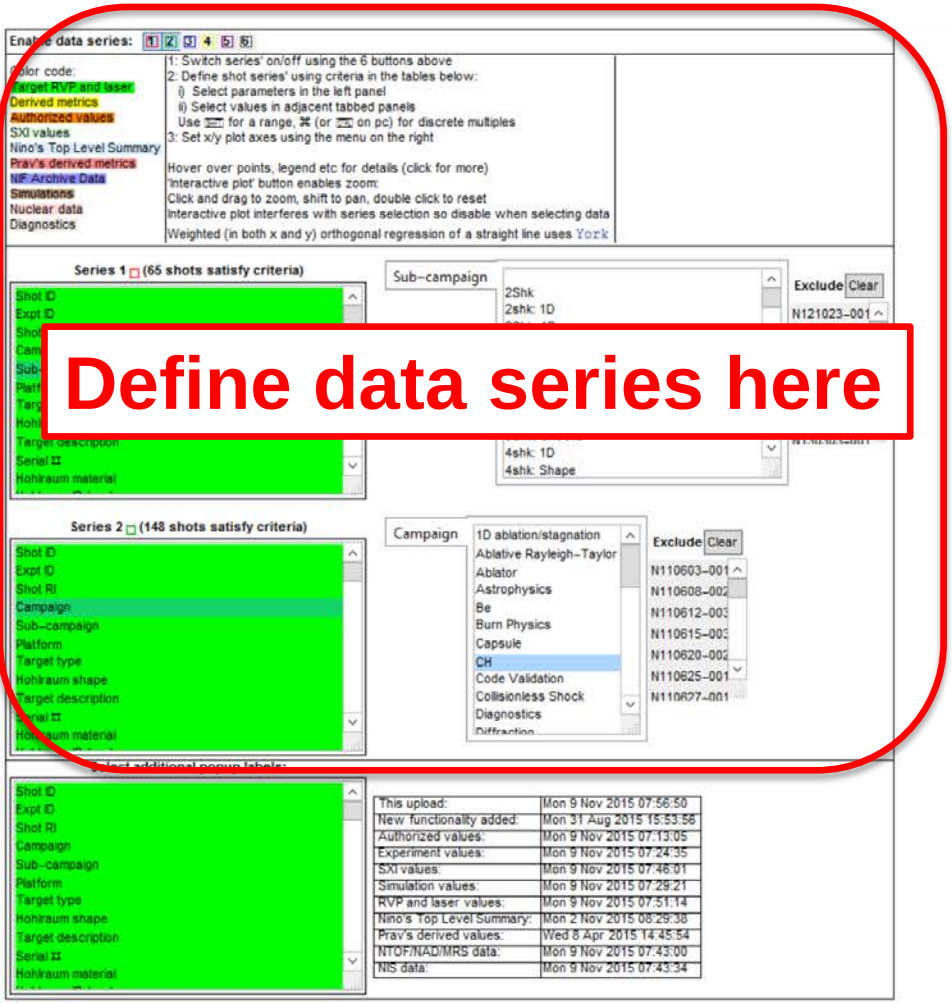
The NIF data trends tool provides a convenient way to visualize (and extract) scalar NIF data



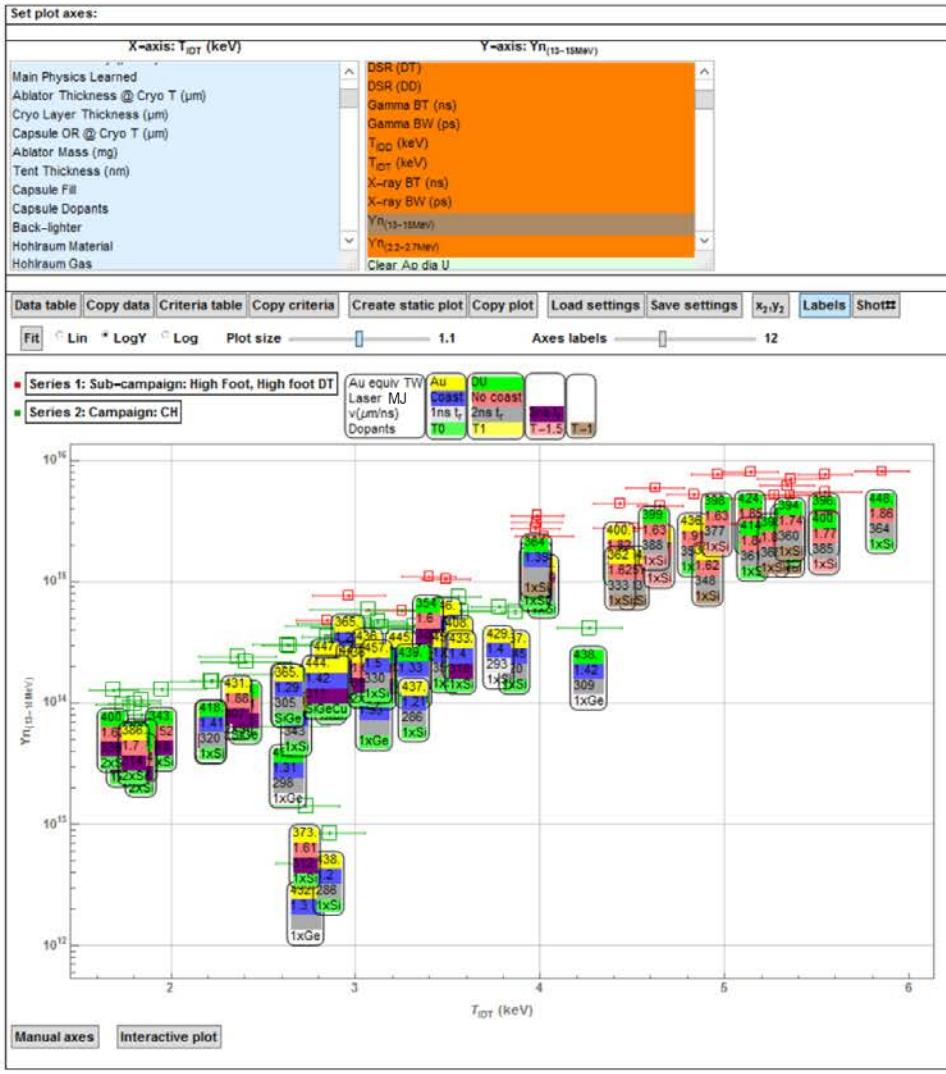


Available on the NIF wiki, runs in free Mathematica viewer

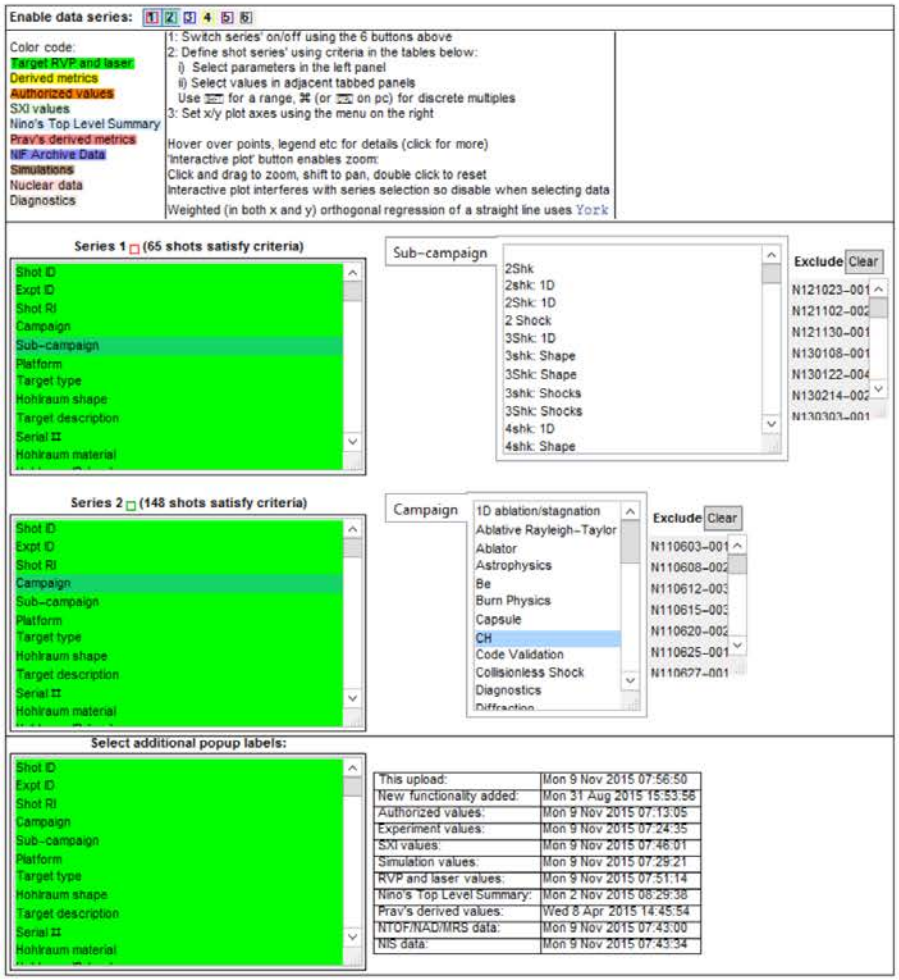
First define the data series

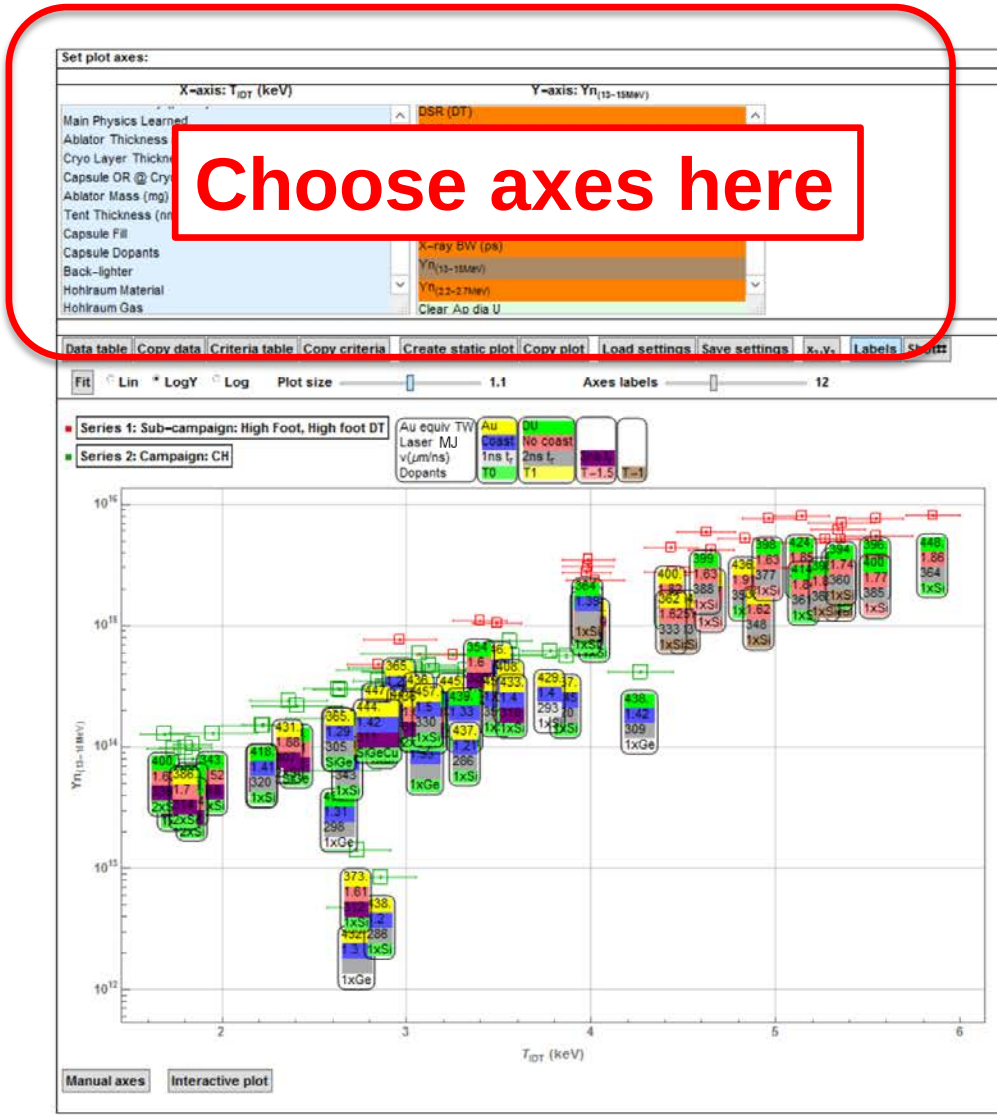


Define data series here

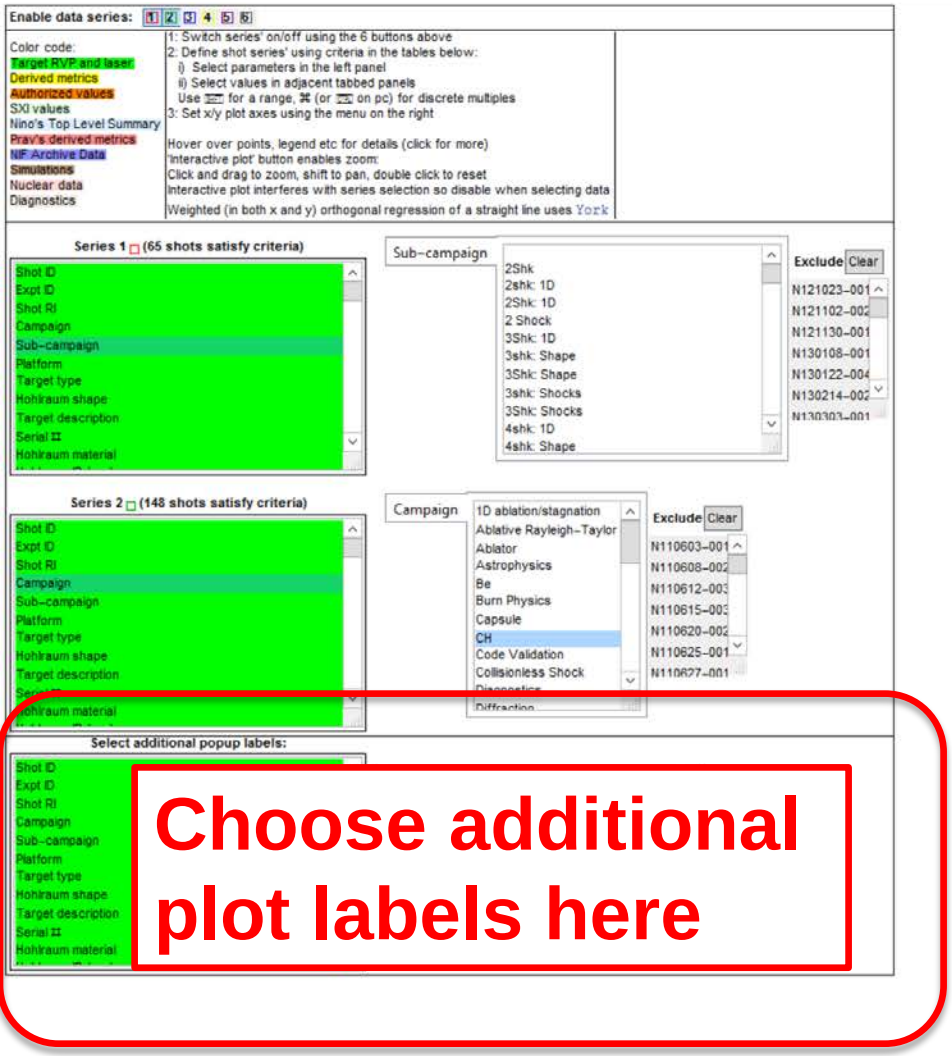


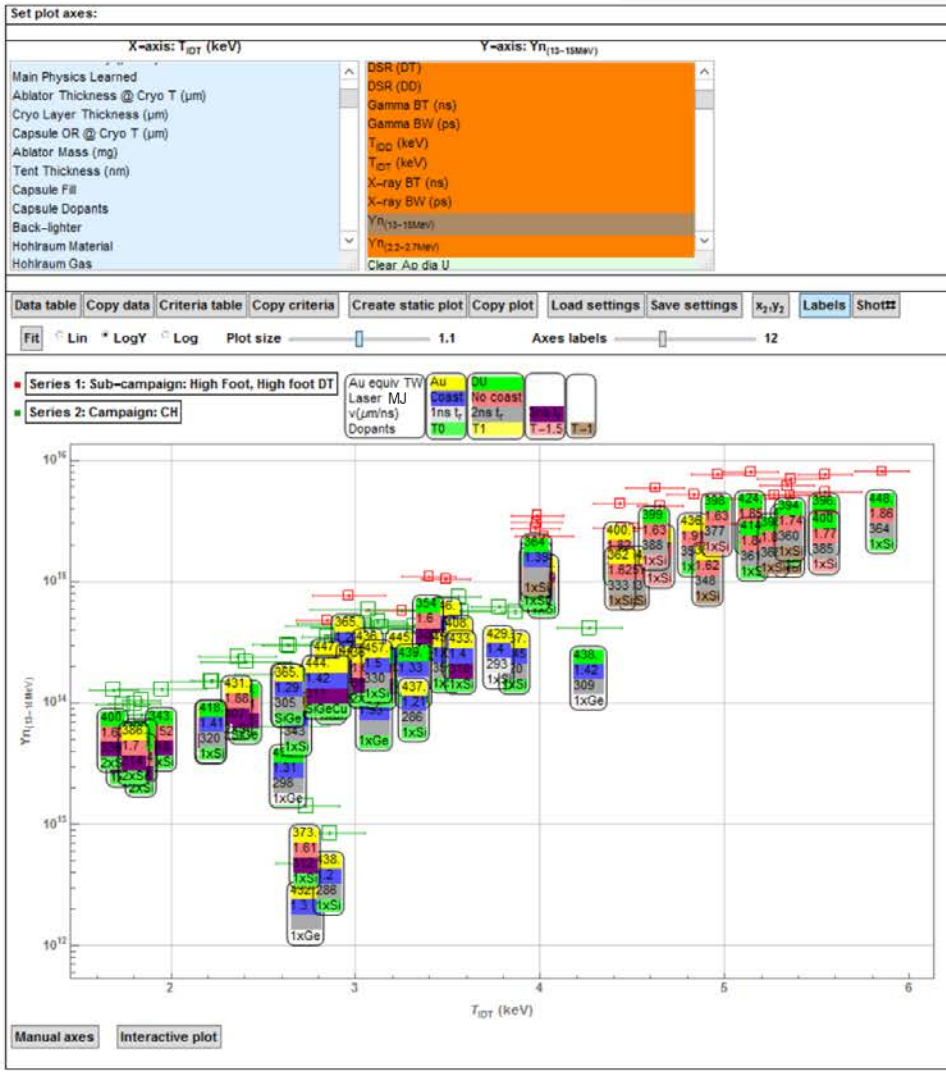
Then select the X-Y axes for the plot



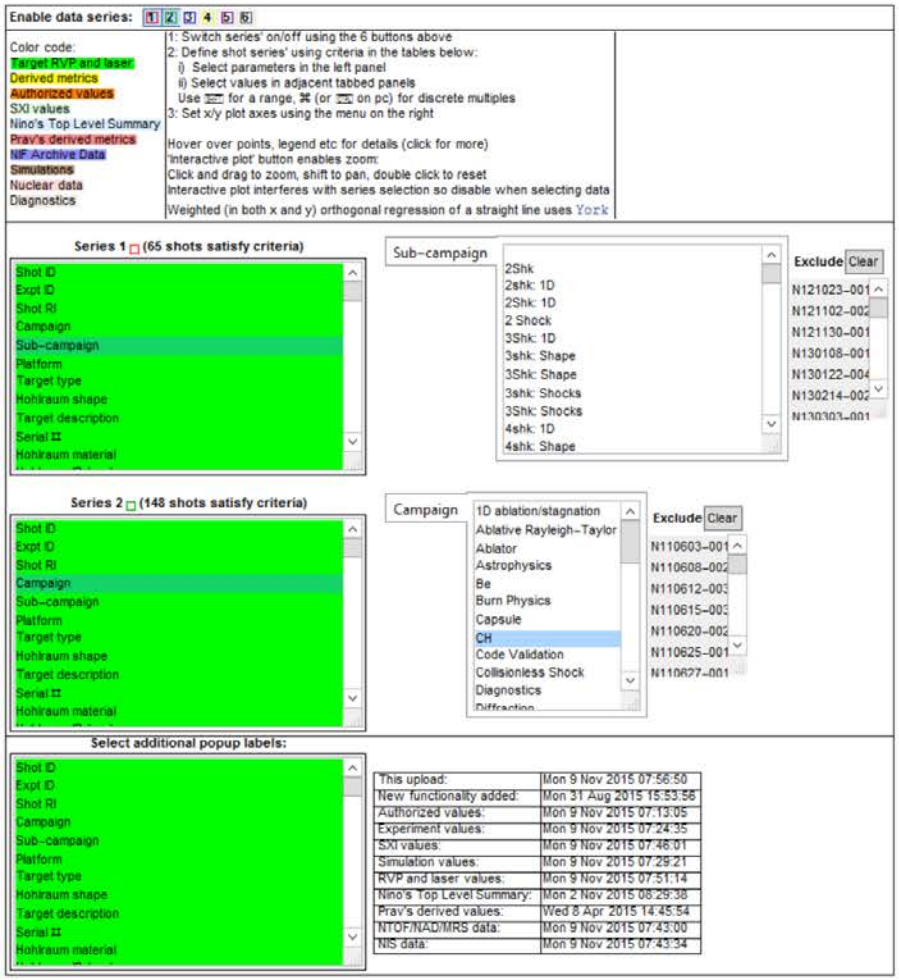


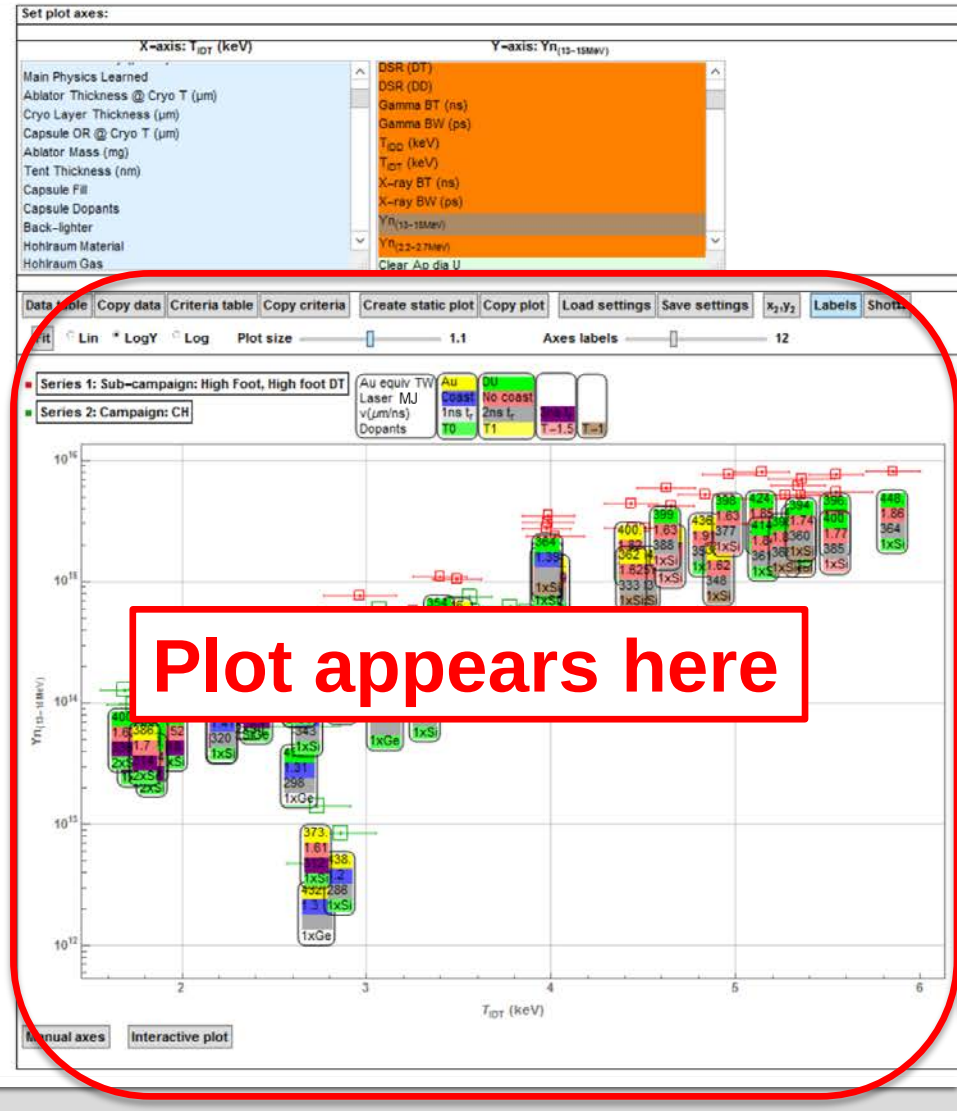
Add additional labels to appear below the default labels



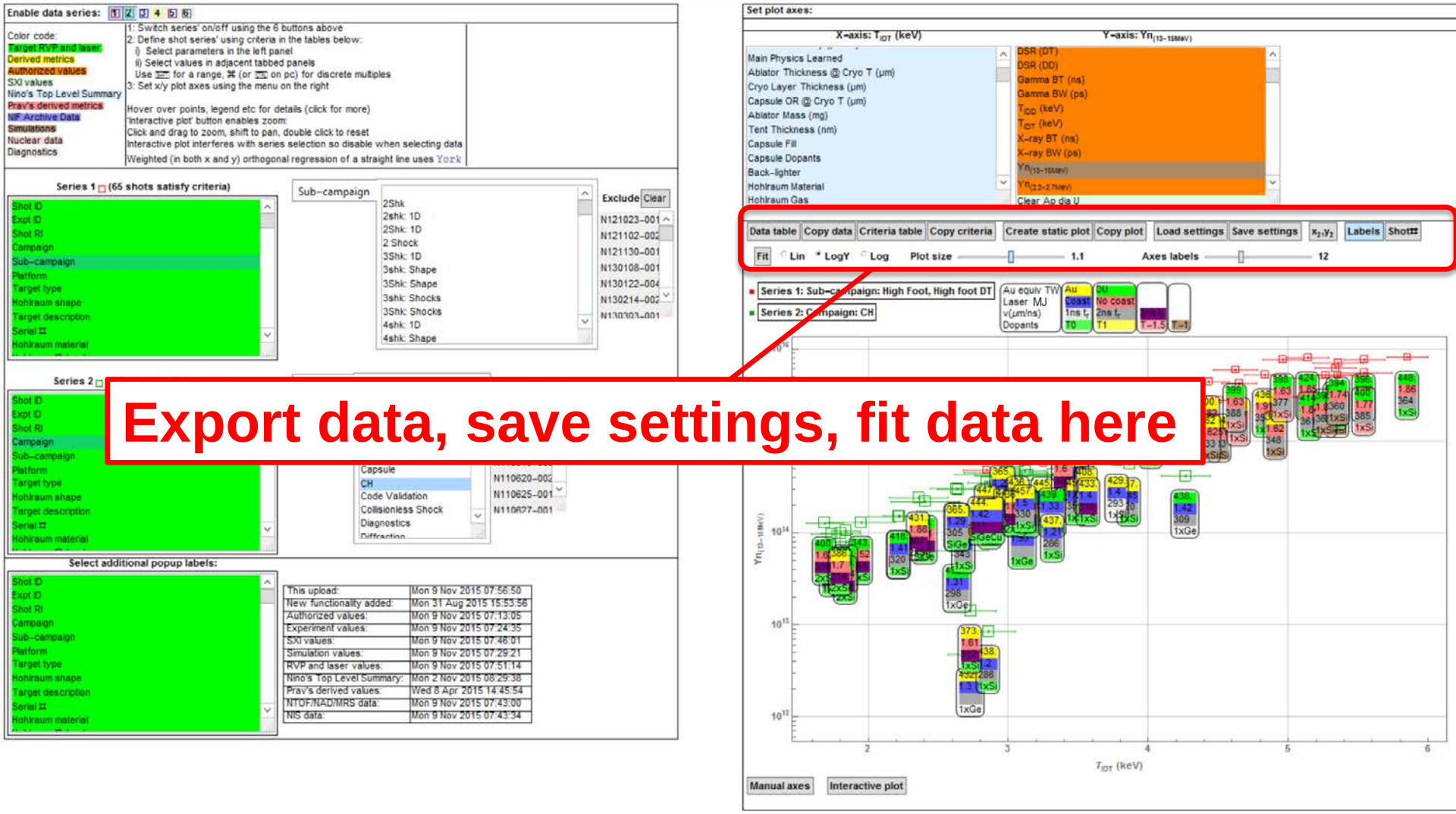


The plot updates as you go along





Export series data, save settings, overlay least-squares fits, choose axes type, copy plot



Export data, save settings, fit data here

Example:
First choose how many data series to plot

Select number of series to plot

Enable data series: 1 2 3 4 5 6

Color code:
Target RVP data
Derived metrics
Authorized values
SXI values
Nino's Top Level Summary
Prav's derived metrics
NIF Archive Data
Simulations
Nuclear data
Diagnostics

1: Switch series' on/off using the 6 buttons above
2: Define shot series' using criteria in the tables below:
i) Select parameters in the left panel
ii) Select values in adjacent tabbed panels
Use ⇧ for a range, ⌘ (or ⊞ on pc) for discrete multi
3: Set x/y plot axes using the menu on the right

Hover over points, legend etc for details (click for more)
'Interactive plot' button enables zoom:
Click and drag to zoom, shift to pan, double click to reset
Interactive plot interferes with series selection so disable when selecting data
Weighted (in both x and y) orthogonal regression of a straight line uses York

Series 1 (65 shots satisfy criteria)

Shot ID
Expt ID
Shot RI
Campaign
Sub-campaign
Platform
Target type
Hohlraum shape
Target description
Serial #
Hohlraum material

Sub-campaign

2Shk
2shk: 1D
2Shk: 1D
2 Shock
3Shk: 1D
3shk: Shape
3Shk: Shape
3shk: Shocks
3Shk: Shocks
4shk: 1D
4shk: Shape

Exclude Clear

N121023-001
N121102-002
N121130-001
N130108-001
N130122-004
N130214-002
N130303-001

Series 2 (148 shots satisfy criteria)

Shot ID
Expt ID
Shot RI
Campaign
Sub-campaign
Platform
Target type
Hohlraum shape
Target description
Serial #
Hohlraum material

Campaign

1D ablation/stagnation
Ablative Rayleigh-Taylor
Ablator
Astrophysics
Be
Burn Physics
Capsule
CH
Code Validation
Collisionless Shock
Diagnostics
Diffraction

Exclude Clear

N110603-001
N110608-002
N110612-003
N110615-003
N110620-002
N110625-001
N110627-001

Select additional popup labels:

Shot ID
Expt ID
Shot RI
Campaign
Sub-campaign
Platform
Target type
Hohlraum shape
Target description
Serial #
Hohlraum material

This upload:	Mon 9 Nov 2015 07:56:50
New functionality added:	Mon 31 Aug 2015 15:53:56
Authorized values:	Mon 9 Nov 2015 07:13:05
Experiment values:	Mon 9 Nov 2015 07:24:35
SXI values:	Mon 9 Nov 2015 07:46:01
Simulation values:	Mon 9 Nov 2015 07:29:21
RVP and laser values:	Mon 9 Nov 2015 07:51:14
Nino's Top Level Summary:	Mon 2 Nov 2015 08:29:38
Prav's derived values:	Wed 8 Apr 2015 14:45:54
NTOF/NAD/MRS data:	Mon 9 Nov 2015 07:43:00
NIS data:	Mon 9 Nov 2015 07:43:34

Set plot axes:

Y-axis: $Yn_{(13-15MeV)}$

Capsule OR @ Cryo T (μm)
Ablator Mass (mg)
Tent Thickness (nm)
Capsule Fill
Capsule Dopants
Back-lighter
Hohlraum Material
Hohlraum Gas

DSR (DT)
DSR (DD)
Gamma BT (ns)
Gamma BW (ps)
T_{DD} (keV)
T_{DT} (keV)
X-ray BT (ns)
X-ray BW (ps)
$Yn_{(13-15MeV)}$
$Yn_{(22-27MeV)}$
Clear Ap dia U

Data table | Copy data | Criteria table | Copy criteria | Create static plot | Copy plot | Load settings | Save settings | x_2,y_2 | Labels | Shot#

Fit | Lin | LogY | Log | Plot size 1.1 | Axes labels 12

Series 1: Sub-campaign: High Foot, High foot DT
Series 2: Campaign: CH

Au equiv TW | Laser MJ | v(μm/ns) | Dopants | Au | coast | 1ns t_r | T0 | DU | No coast | 2ns t_r | T1 | T-1.5 | T-1

$Yn_{(13-15MeV)}$

T_{DT} (keV)

Manual axes | Interactive plot

Define up to 6 series (overlapping series points are progressively larger and distinguishable)

Series 1 and 2 are enabled in this example

Enable data series: 1 2 3 4 5 6

Color code:
- Target RVP and laser
- Derived metrics
- Authorized values
- SXI values
- Nino's Top Level Summary
- Prav's derived metrics
- NIF Archive Data
- Simulations
- Nuclear data
- Diagnostics

1: Switch series' on/off using the 6 buttons above
2: Define shot series' using criteria in the tables below:
  i) Select parameters in the left panel
  ii) Select values in adjacent tabbed panels
  Use SHIFT for a range, ⌘ (or CTRL on pc) for discrete multiples
3: Set x/y plot axes using the menu on the right

Hover over points, legend etc for details (click for more)
'Interactive plot' button enables zoom:
Click and drag to zoom, shift to pan, double click to reset
Interactive plot interferes with series selection so disable when selecting data
Weighted (in both x and y) orthogonal regression of a straight line uses York

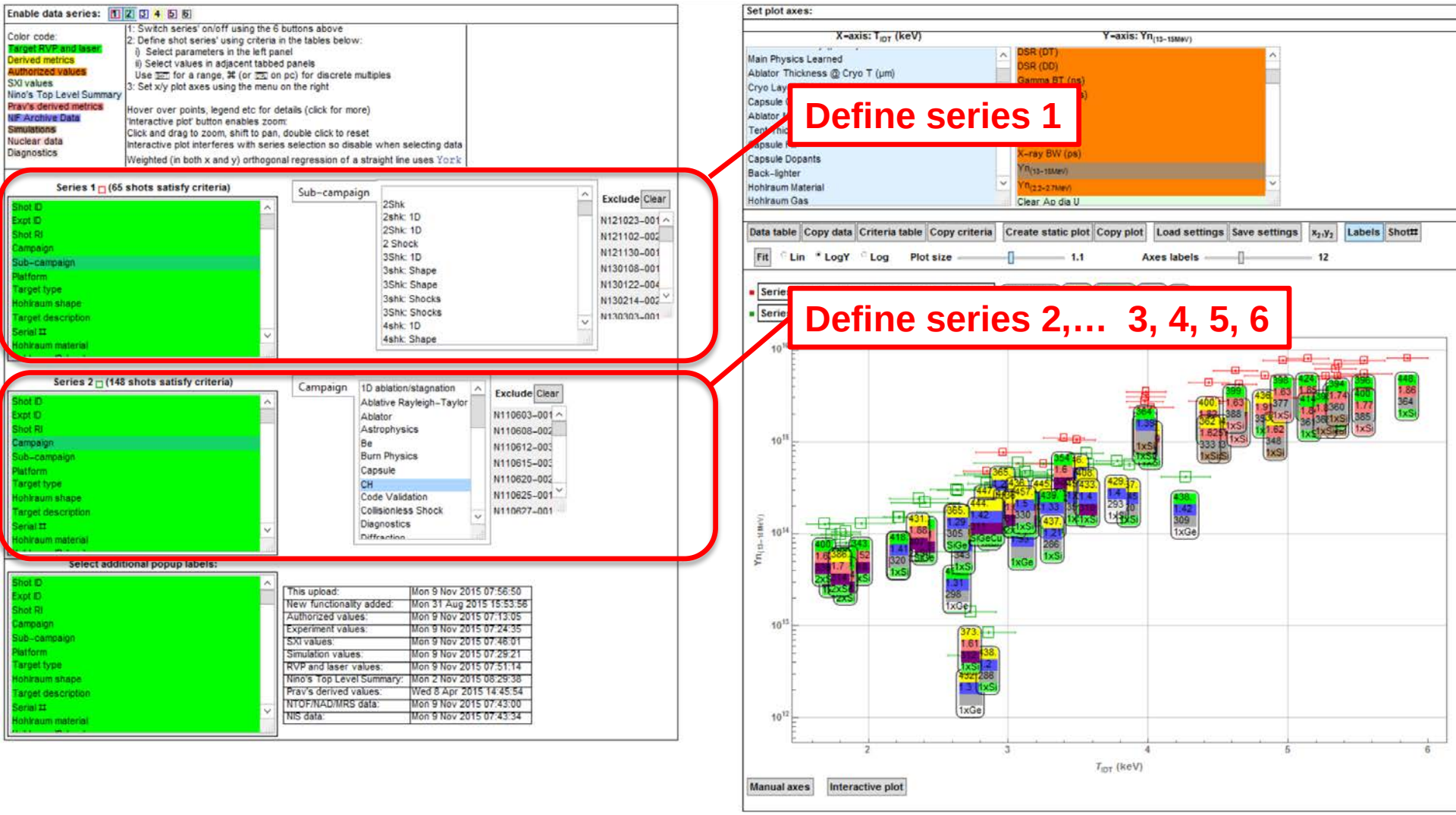
Series 1 (65 shots satisfy criteria)

- Shot ID
- Expt ID
- Shot RI
- Campaign
- Sub–campaign
- Platform
- Target type
- Hohlraum shape
- Target description

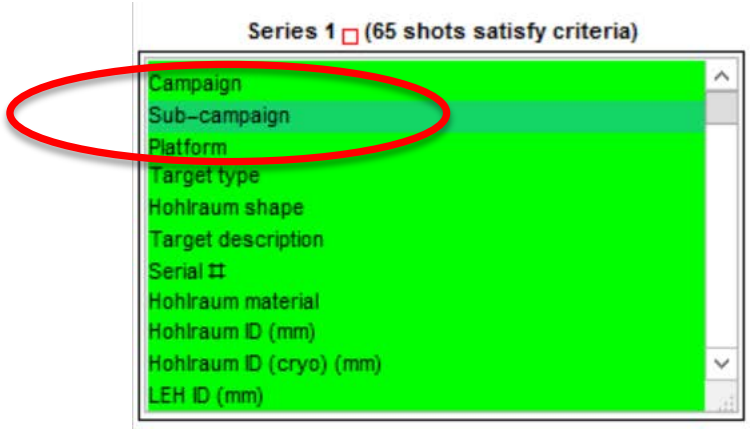
Sub–campaign

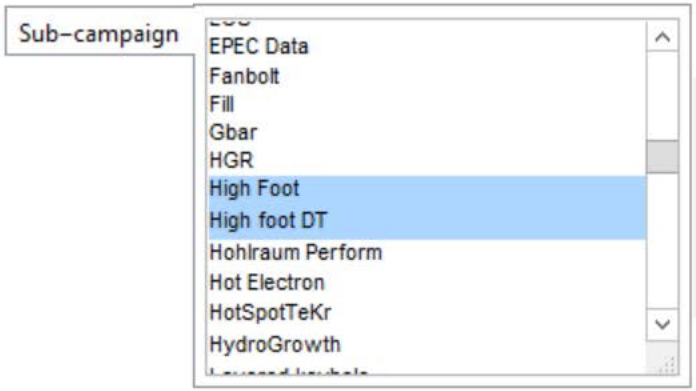
- 2Shk
- 2shk: 1D
- 2Shk: 1D
- 2 Shock
- 3Shk: 1D
- 3shk: Shape
- 3Shk: Shape
- 3shk: Shocks
- 3Shk: Shocks

Filter shots to include in each series from all target shots since NIC shock timing (N110603)

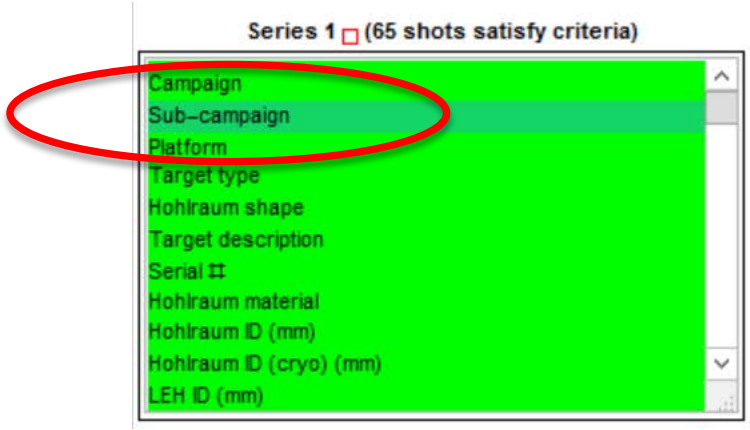


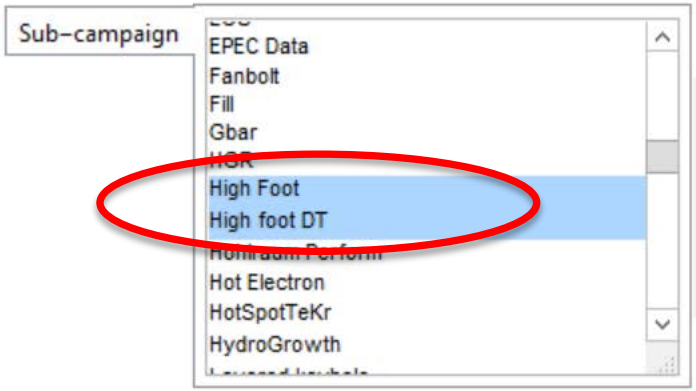
Choose one or more parameter to filter shots by For example, filter by “Sub-campaign” name:



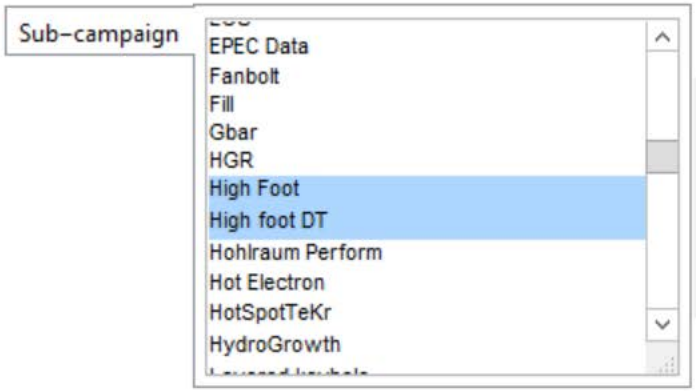


Select which “sub-campaign” names to include e.g., all “High Foot” and “High foot DT” shots

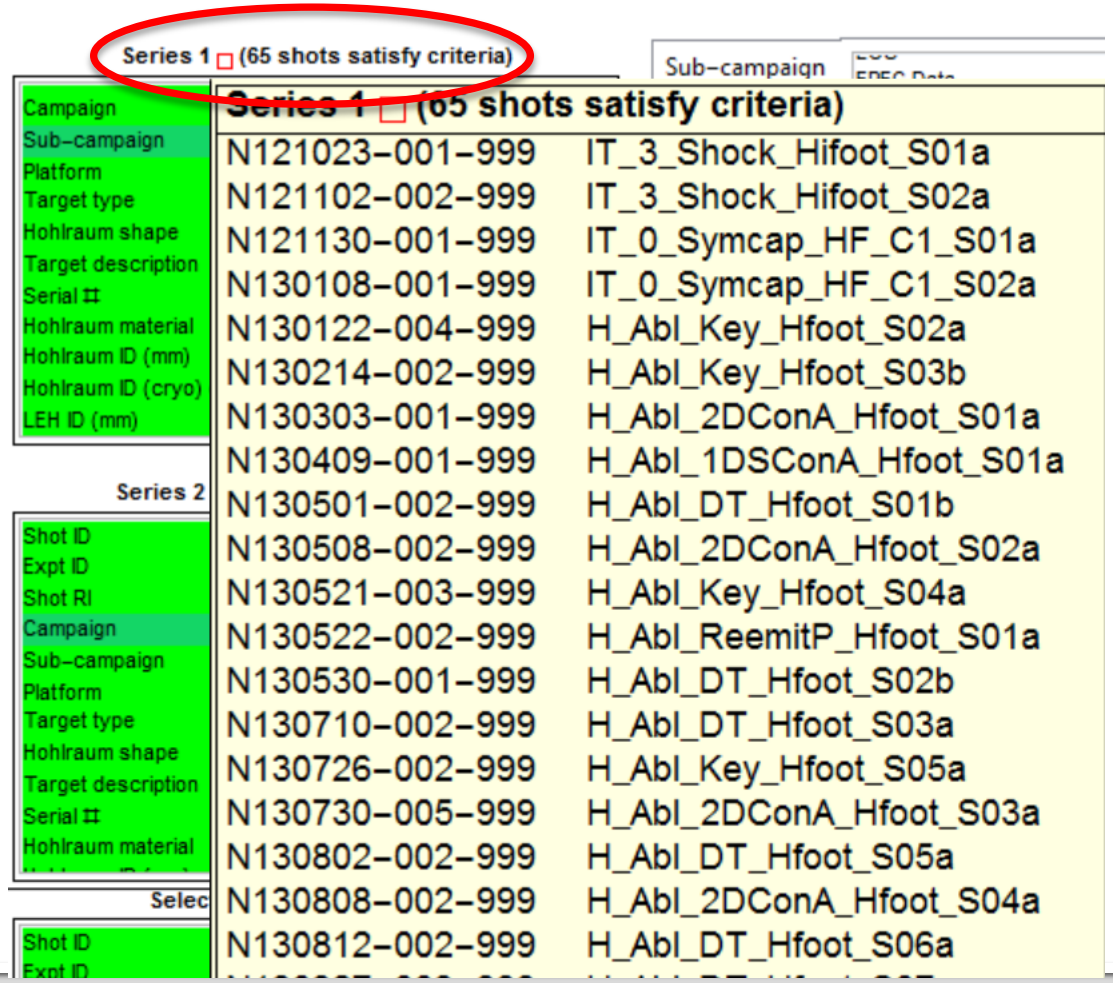




This filter returns 65 shots:

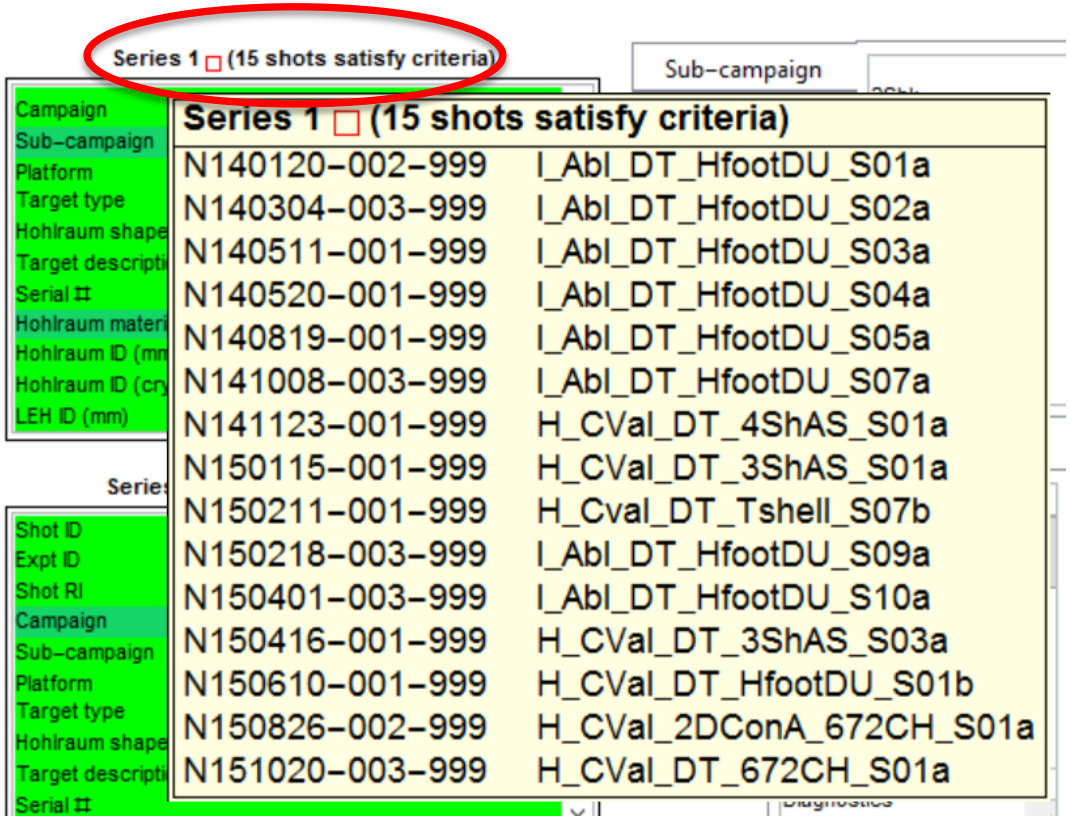


Hover over series name to see the list of shots that match the filter (click for table and copy/paste)



Include additional parameter to further refine the filter
For example, include all “AuDU” hohlraums

This refined filter returns 15 shots



i.e., 15 shots since N110603 were in Sub-campaigns “High foot” and “High foot DT”, and also used a “AuDU” hohlraum

Select X and Y axes for the plot:
Example: X axis: $T_{ion\ DT}$, Y axis: 13-15MeV yield

Set plot axes:

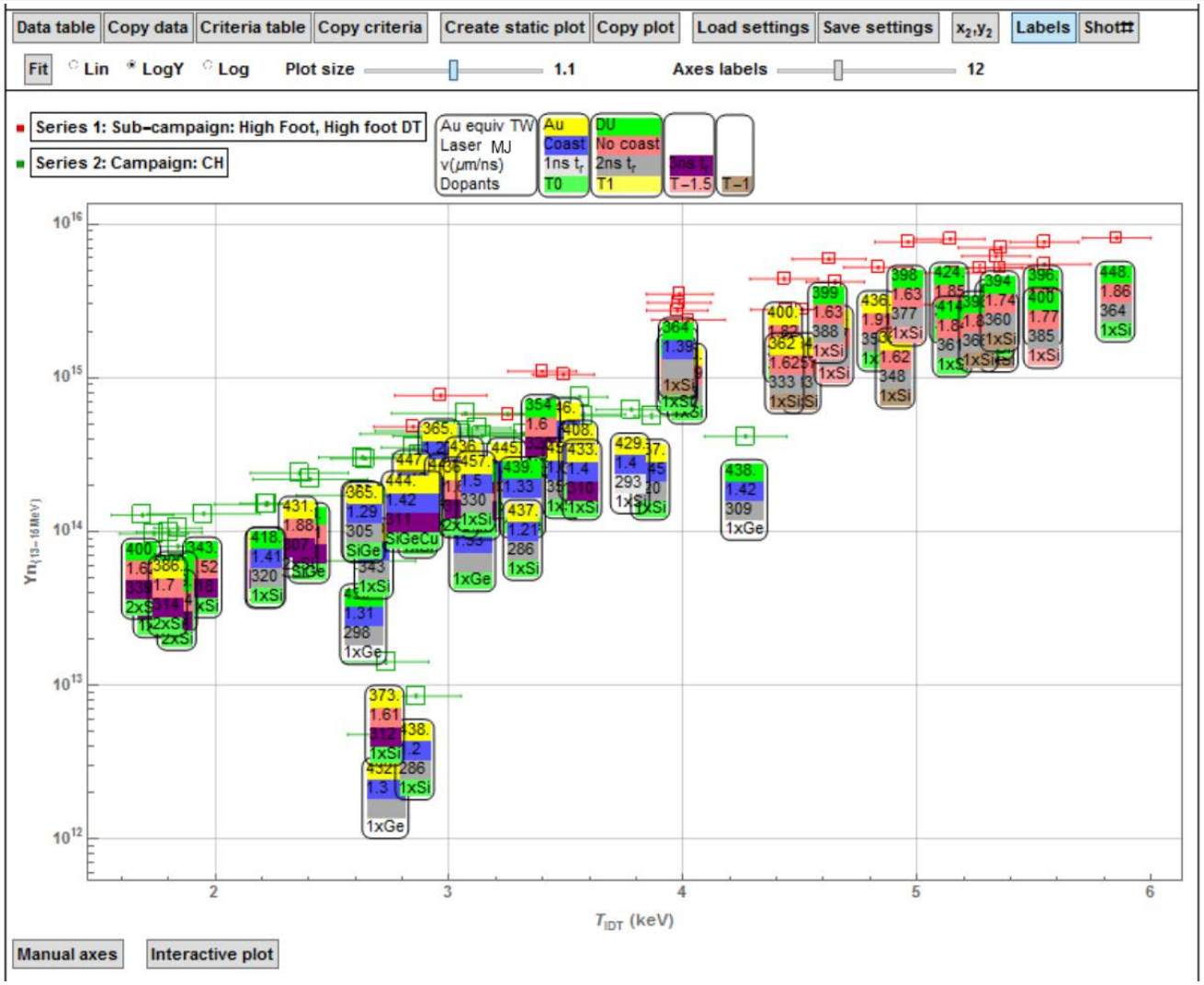
X–axis: T_{IDT} (keV)

- Layered fuel thickness (μm)
- Final rise class (ns)
- Coast time (ns)
- ΔBT_{x-y} (ps)
- $\Delta T_{I\,(DT-DD)}$
- $Y_{n,DT}/Y_{n,DD}$
- $Y_{n,DT}/Y_{n,DD}$ Exp(8.0*DSR)
- $Y_{n,DT}$ Exp(4.0*DSR)
- $Y_{n,DD}$ Exp(12.0*DSR)
- Fuel ρR (g/cm^2)
- DSR (DT)
- DSR (DD)
- Gamma BT (ns)
- Gamma BW (ps)
- T_{IDD} (keV)
- T_{IDT} (keV)

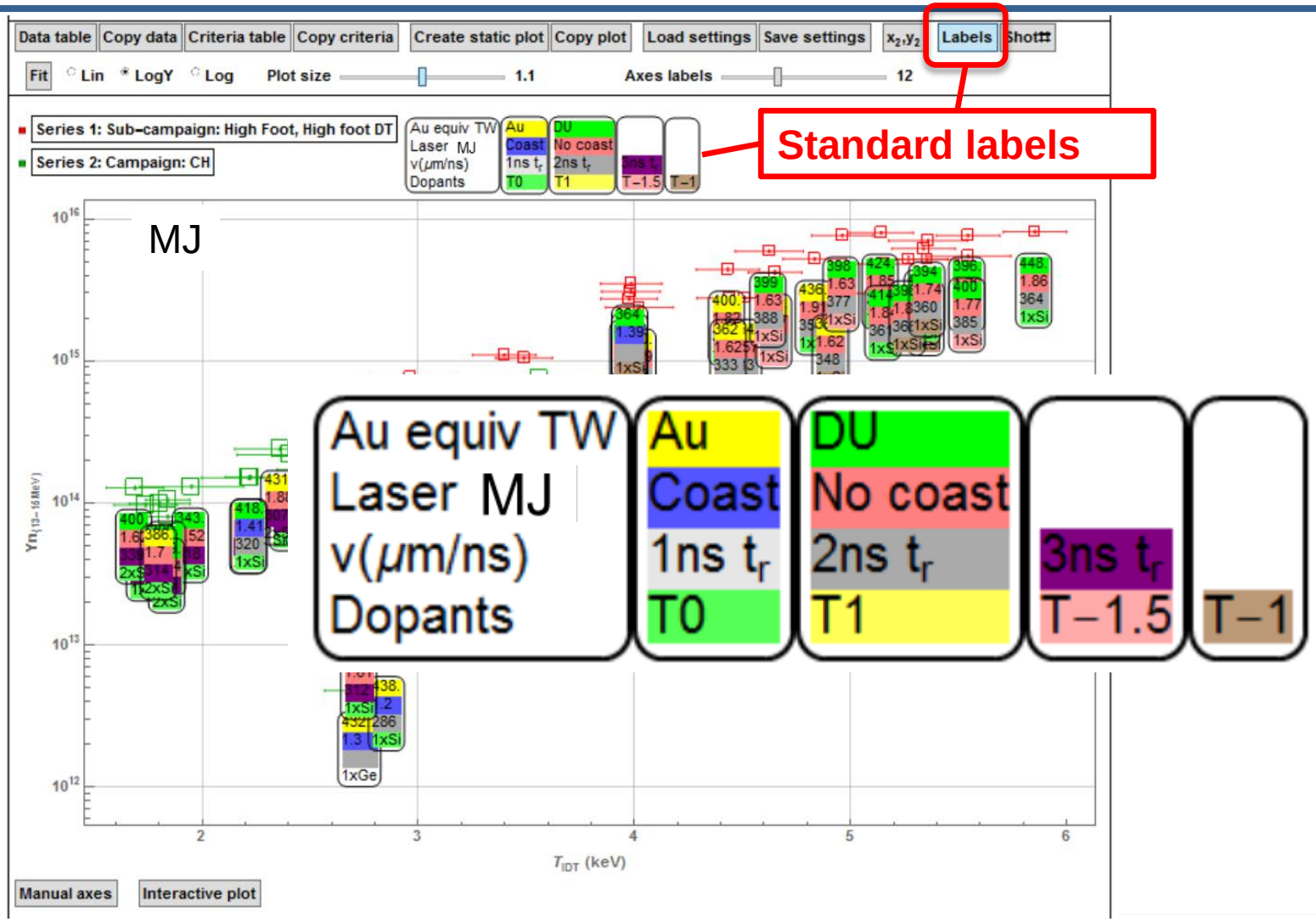
Y–axis: $Yn_{(13-15MeV)}$

- $Y_{n,DT}$ Exp(4.0*DSR)
- $Y_{n,DD}$ Exp(12.0*DSR)
- Fuel ρR (g/cm^2)
- DSR (DT)
- DSR (DD)
- Gamma BT (ns)
- Gamma BW (ps)
- T_{IDD} (keV)
- T_{IDT} (keV)
- X–ray BT (ns)
- X–ray BW (ps)
- $Yn_{(13-15MeV)}$
- $Yn_{(2.2-2.7MeV)}$
- Clear Ap dia U
- Soft x–ray dia U
- Frac in Cl Ap dis U
- Dia for Frac U

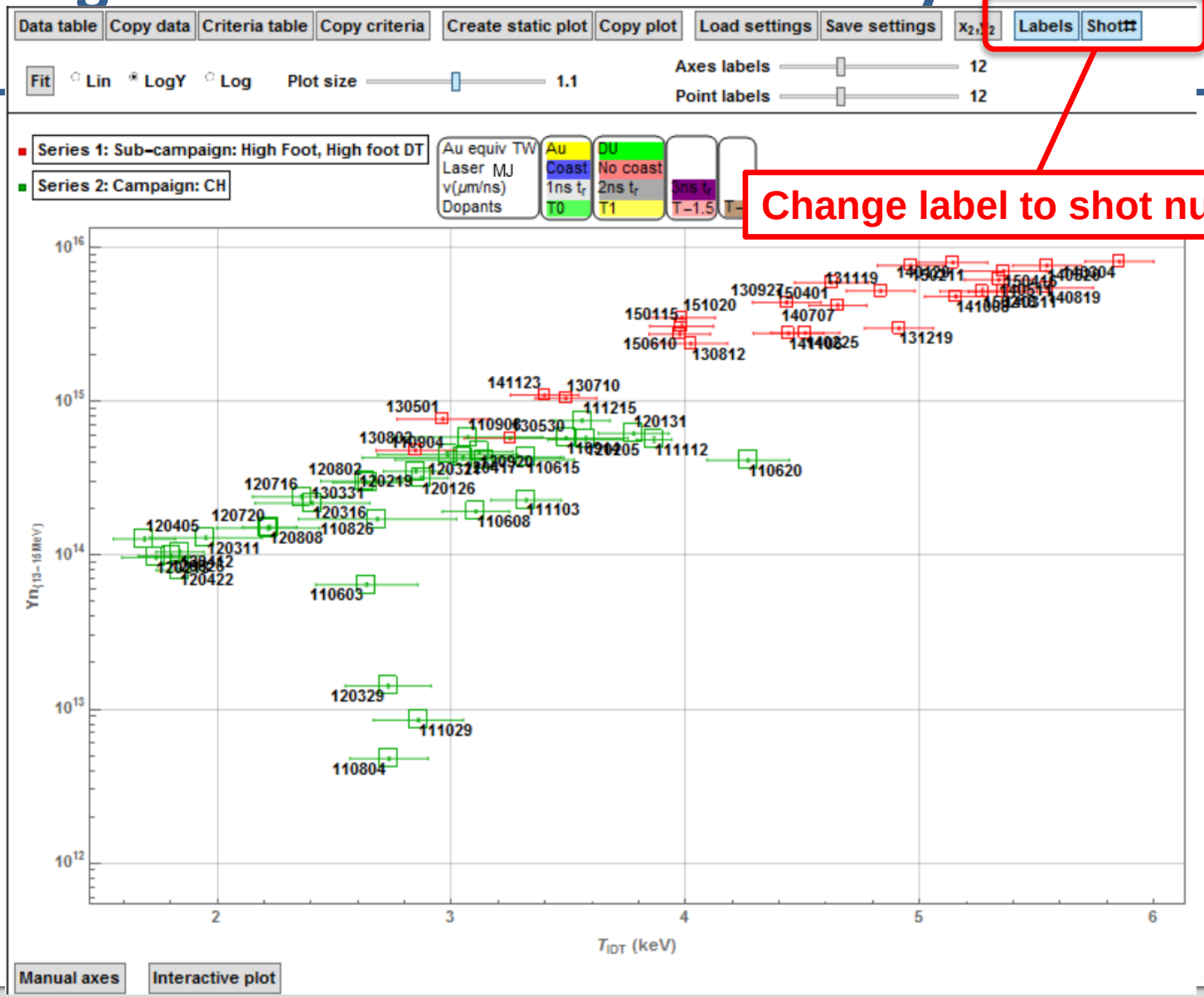
…gives this plot.



By default the plots are labelled with a few key parameters



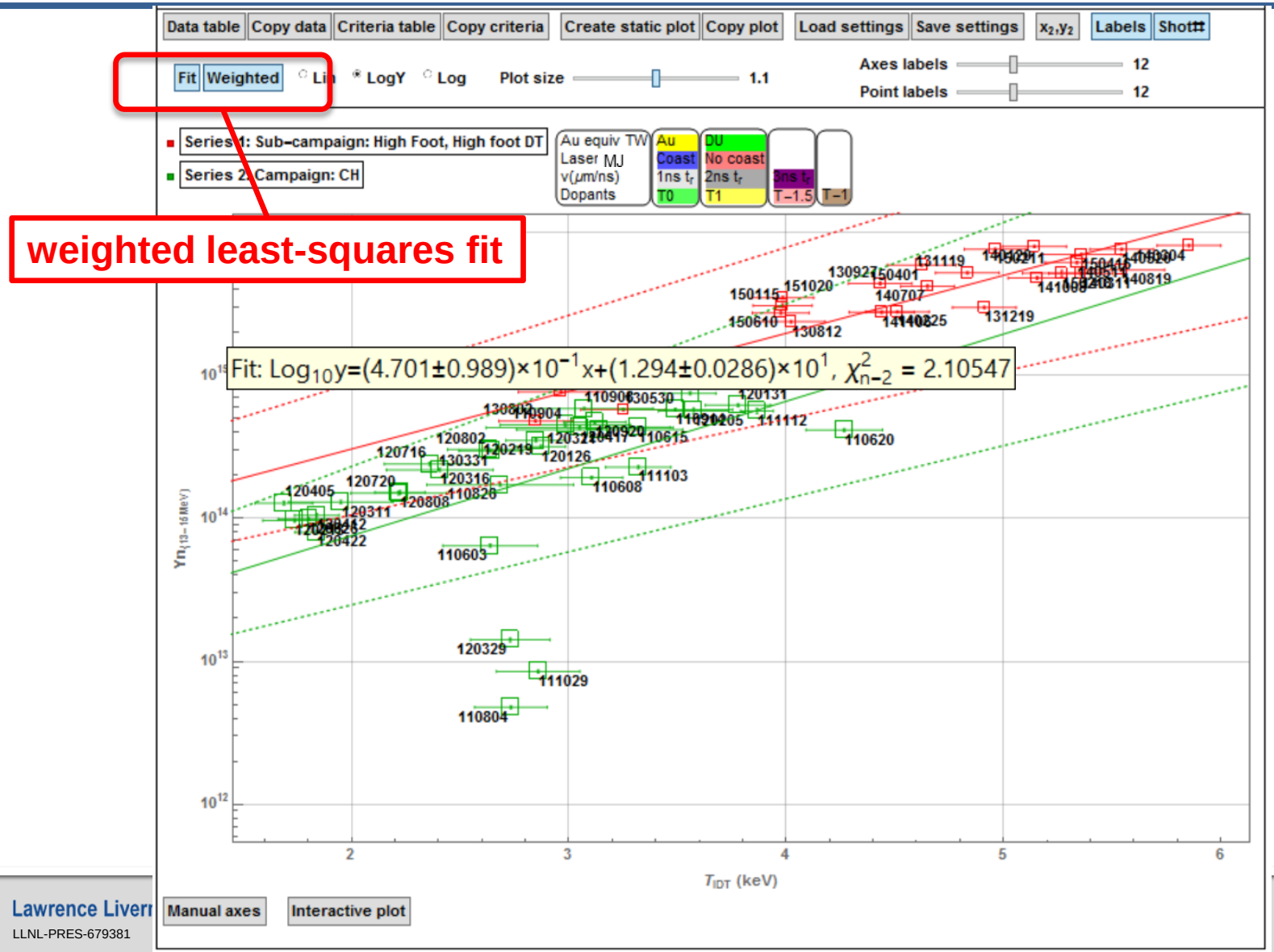
Change labels to shot number only:



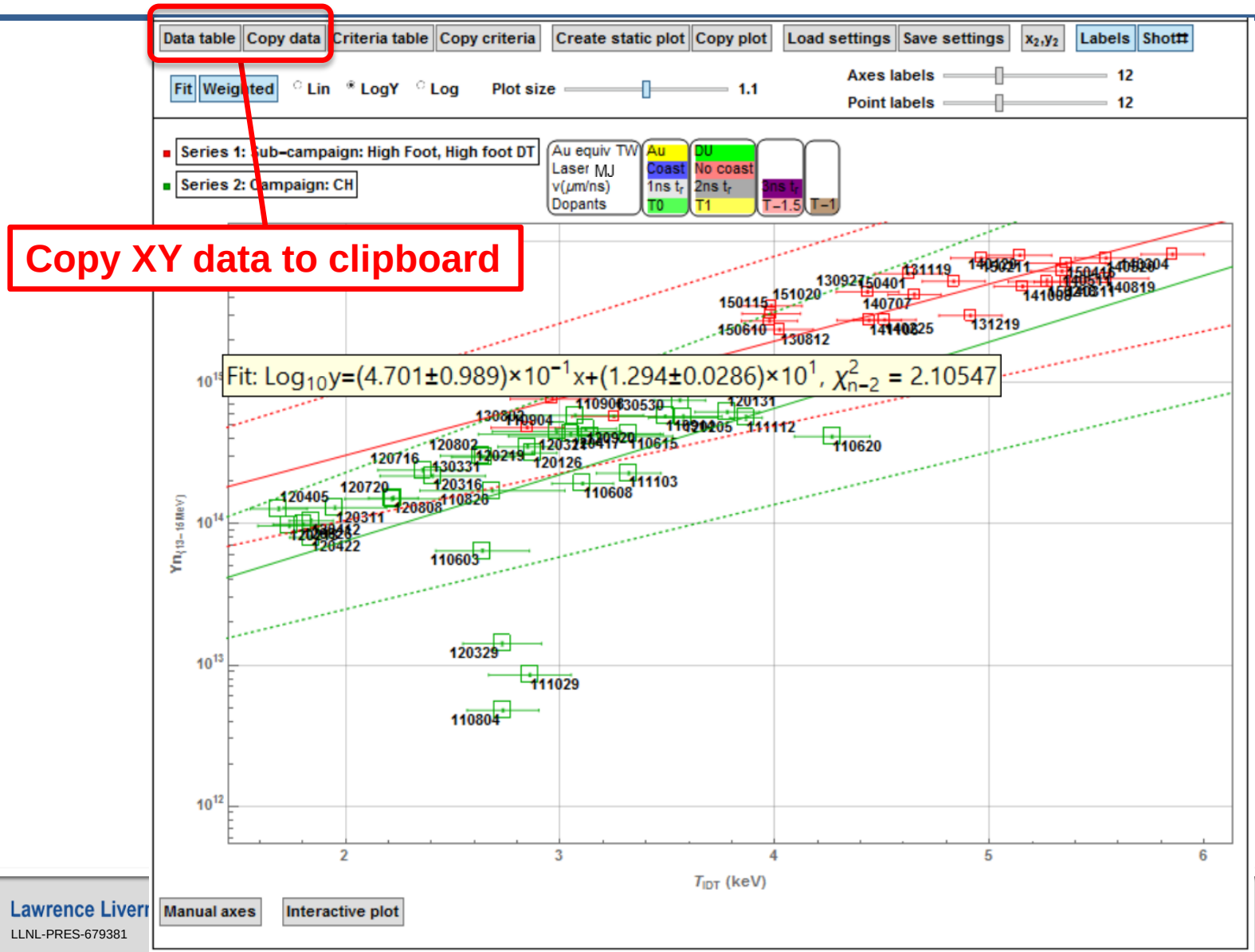
Change label to shot number

Weighted least-squares fit, hover for fit parameters. Uses method of D. York

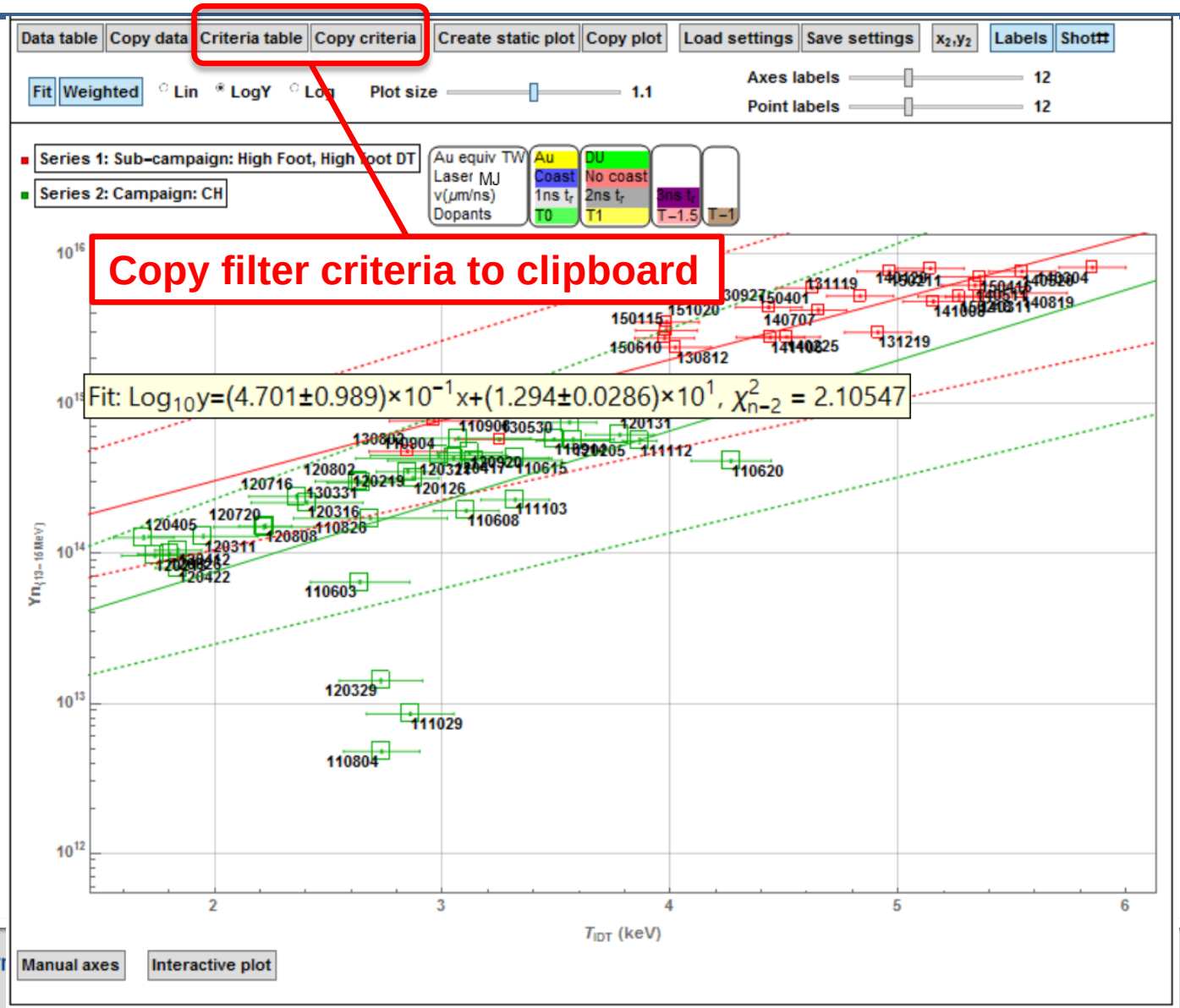
Am. J. Phys. **72** (3), March 2004



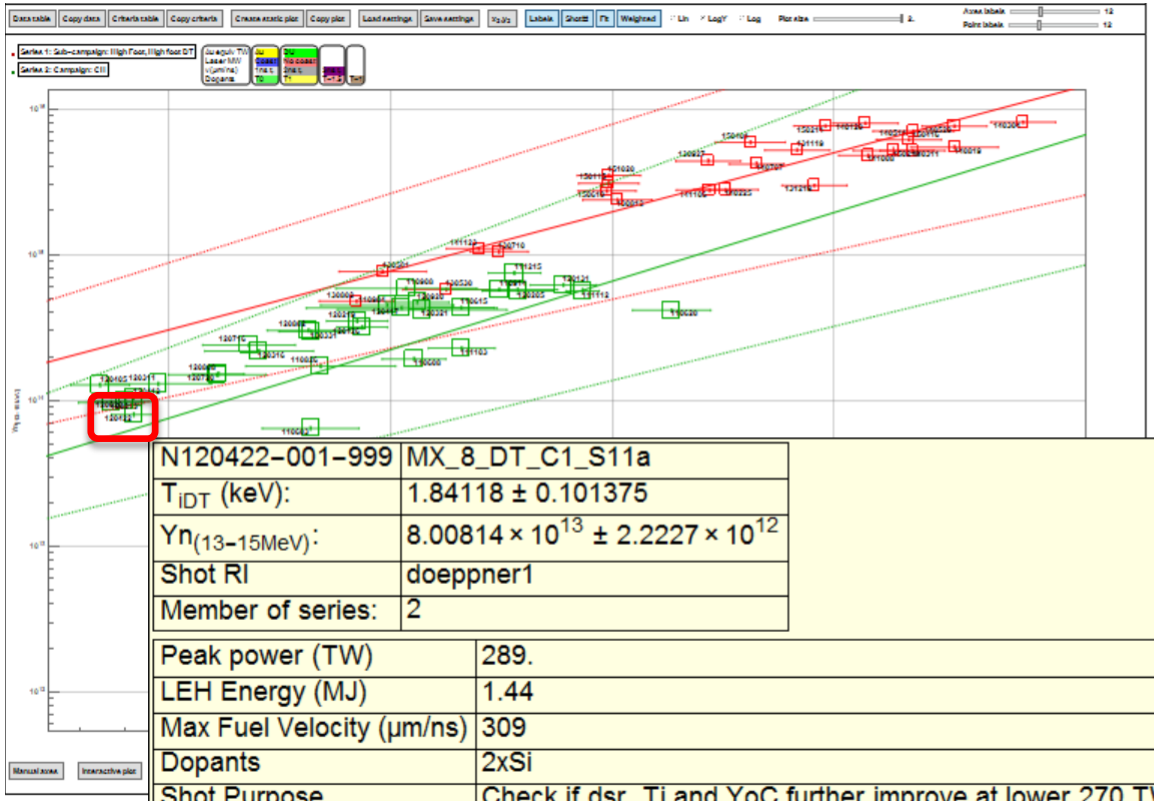
Copy data for all series to the clipboard



Copy filter criteria to clipboard



Hover over XY points for more detailed shot info: Includes “Shot Purpose” and “Main Physics Learned” cells from Nino’s spreadsheet



N120422-001-999	MX_8_DT_C1_S11a
T_{iDT} (keV):	1.84118 ± 0.101375
$Yn_{(13-15MeV)}$:	$8.00814 \times 10^{13} \pm 2.2227 \times 10^{12}$
Shot RI	doeppner1
Member of series:	2

Peak power (TW)	289.
LEH Energy (MJ)	1.44
Max Fuel Velocity (μm/ns)	309
Dopants	2xSi
Shot Purpose	Check if dsr, Ti and YoC further improve at lower 270 TW power with 3 ns rise 2x Si capsule
Main Physics Learned	Ti and yield dropped faster expected for 1D performance, suggesting less density gradient stabilization?

The tool combines data from several sources: Webdav (archive), Nino's spreadsheet, Prav's derived metrics pressure etc, Target RVP, other derived metrics i.e. coast time, $\Delta BT_{x-\gamma}$ etc…

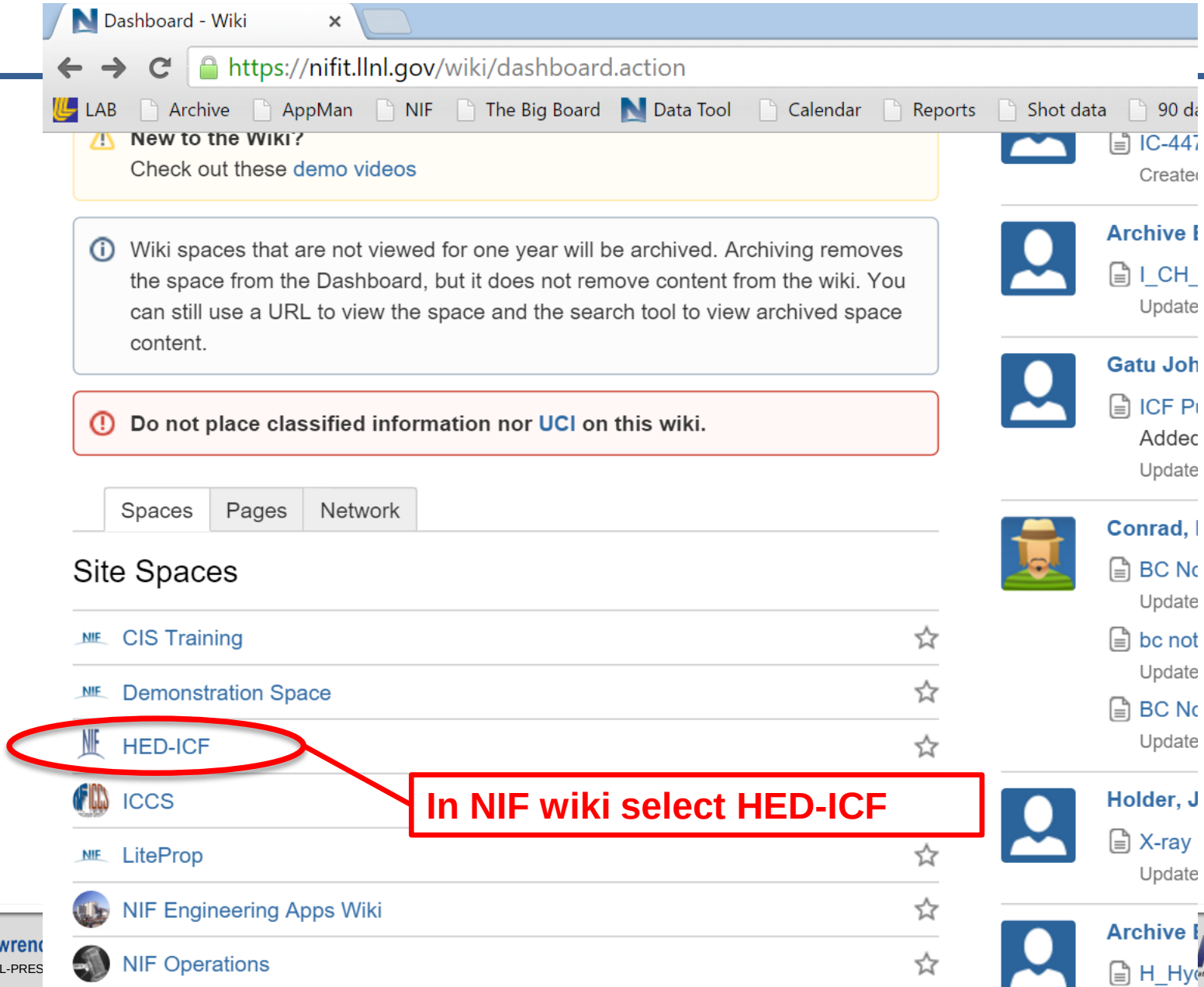
Enable data series: 1 2 3 4 5 6

Color code:
- Target RVP and laser
- Derived metrics
- Authorized values
- SXI values
- Nino's Top Level Summary
- Prav's derived metrics
- NIF Archive Data
- Simulations
- Nuclear data
- Diagnostics

1: Switch series' on/off using the 6 buttons above
2: Define shot series' using criteria in the tables below:
  i) Select parameters in the left panel
  ii) Select values in adjacent tabbed panels
  Use SHIFT for a range, ⌘ (or CTRL on pc) for discrete multiples
3: Set x/y plot axes using the menu on the right

Hover over points, legend etc for details (click for more)
'Interactive plot' button enables zoom:
Click and drag to zoom, shift to pan, double click to reset
Interactive plot interferes with
  series selection so disable when selecting data
Weighted (in both x and y) orthogonal
  regression of a straight line uses York

You can find the data trends tool in the NIF wiki under HED-ICF



Select NIF Data Trends Tool in left panel

NIF Data Trends Tool - HE

https://nifit.llnl.gov/wiki/display/vc/NIF+Data+Trends+Tool

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Shot Data

Preshot Reviews

Postshot Reviews

Laser & Target Files

Lasereq Files

Cryo Reports (at shot)

Layering Reports

HED-ICF

NIF Data Trends Tool

Created by Hutton, Matthew S., last modified by MacPhee, Andrew on Nov 05, 2015

Generate exportable interactive plots of NIF data using var

Download the latest version of the interactive NIF Data Trends Tool here

You can run the tool using the FREE Mathematica CDF Player v10, you don't need

(although it will also work with Mathematica v10 installed)

A new version of the tool is built every morning using freshly downloaded data back

(so if a bunch of values get retroactively updated as happens from time to time, this

Build starts at 7am and is usually available by ~8.10am. The date in the box below t

The tool works cross-platform on OSX, Window and Linux

Here's a zip file of the raw data embedded in the tool (not needed to run the tool)

Email me if you have any questions or if you would lik

Andrew MacPhee

Enable data series: 1 2 3 4 5 6

Color code: 1: Switch series' on/off using the 6 buttons above

NIF Data Trends Tool - HE

https://nifit.llnl.gov/wiki/display/vc/NIF+Data+Trends+Tool

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Also runs in the full Mathematica version

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Andrew MacPhee

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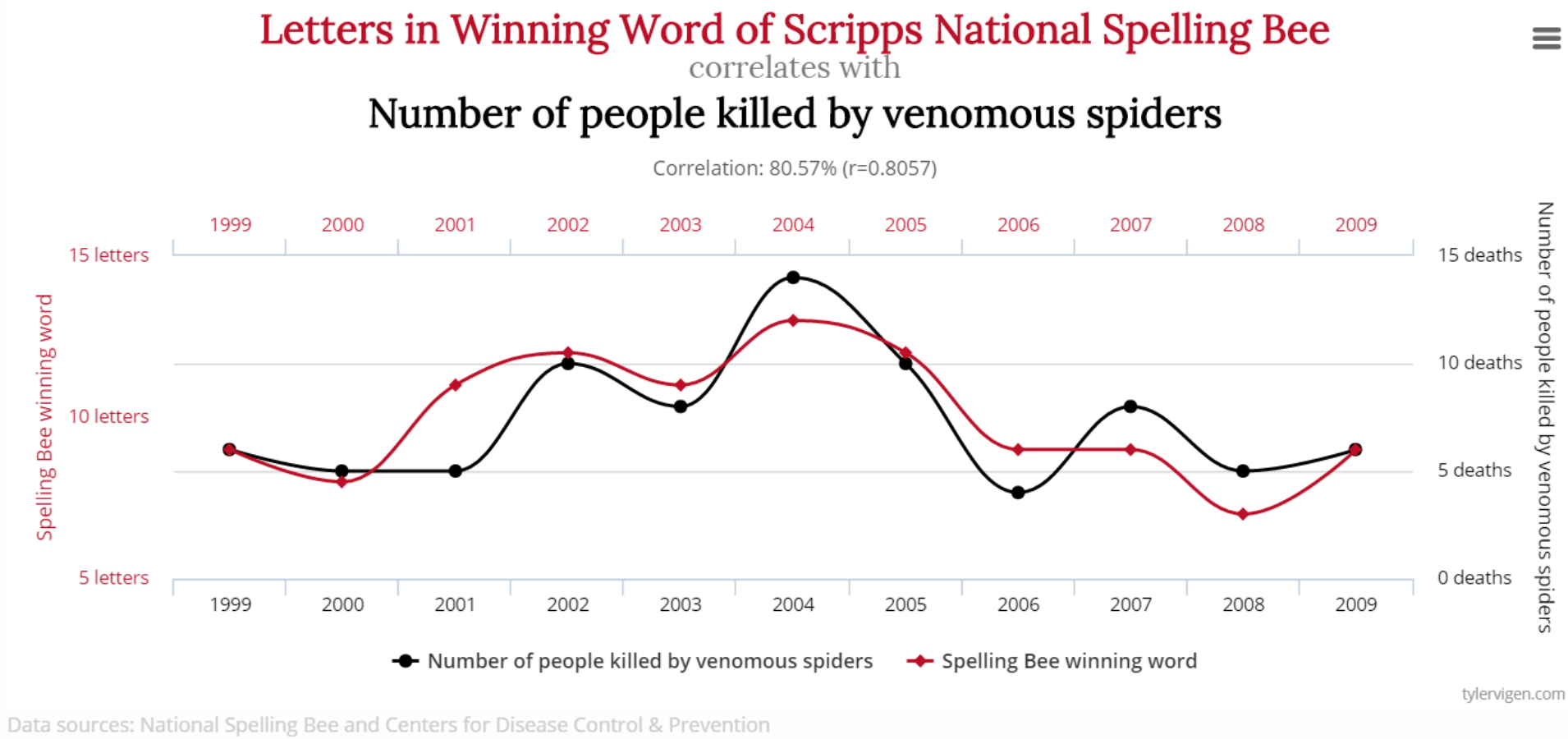
Color code: 1: Switch series' on/off using the 6 buttons above

Beware spurious correlations:



From: http://www.tylervigen.com/spurious-correlations

Lawrence Livermore
National Laboratory

Most of the data is pulled from the archive daily on the fly using WebDav, hence always up to date

http://nifitservices.llnl.gov/ArchiveWebDav/export/shotdata/tags
Requires a webdav username and password (Steve Hahn, B671, x4-5542)

"tags" define the list of shots retrieved:
DT_shots, Target_shots_since_shock_timing,…

"reports" define what data is retrieved:
Authorized_values, Shot_inputs,…

The list of available reports has grown over the years. Clicking a link fires up a script that goes and builds the .csv for that tag

nifitservices.llnl.gov/ArchiveWebDav/export/shotdata/tags/DT%20Shots/reports

reports

Parent Directory

AUTH-INSTR-BANGTIME_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
AUTH-INSTR-BURNWIDTH_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
AUTH-INSTR-DSR_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
AUTH-INSTR-TION_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
AUTH-INSTR-YN_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
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CRYO-SUMMARY_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
DERIVED-METRICS_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
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NEUT-ALLDIAG-VALUES_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
NIS_VALUES_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
POSTSHOT-REVIEW_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
SHOT-INPUTS_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
SIM-HEADERS_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
SIM-VALUES_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
SXI-METRICS_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
TARGET-FUEL-MIX_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
TARGET-VALUES_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
TD-USE_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015
UNAUTH-BANGTIME_DT+Shots.csv	Mon Nov 09 13:28:28 PST 2015

Target Gas Density Calculator Concept, Usage & Limitations

NIF Users' Forum

Dean Holunga, PhD
Cryo Ops Process Engineer

Originally authored by Jim Fair, PhD
Mac conversion by Curtis Walters, PhD

November 10, 2015

LLNL-PRES-679381
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

Why Have a Gas Density Calculator?

- In 2012, it was realized that the non-ideality of subcritical THD gas mixtures exceeded the allowable uncertainty of the capsule density.
  - Why? Conversion from density to pressure was not accurate using the Ideal Gas Law alone.
  - Jim Fair authored the first calculator that calculated the density of the isotopic mixtures of hydrogen and helium.
    - Other gases & gas mixtures being shot are similarly non-ideal. E.g., Neopentane.

- Primary purpose
  - To calculate an accurate conversion of density (mg/cm^3) to pressure (torr) in target gas fill requests.
    - To quantify the non-ideal behavior of subcritical or high pressure gases and gas mixtures.

- Secondary purposes
  - To predict the equilibrium of THD mixtures (H_2, D_2, T_2, HD, HT, DT) from cryogenic to room temperature.
  - To predict the atomic particle density ($atoms/cm^3$).

Model Approach To Non-Ideality Corrections

- Virial Coefficient Corrections to the Ideal Gas Law
  - $z = \frac{P}{RT\rho_m} \approx 1 + B\rho_m + C{\rho_m}^2 + \ldots$
  - Mixing Rules (generally accepted for B, but not universally accepted for C)
    - 2nd Virial Coefficient – for low pressure, low temp or moderate pressure, high temperature gases
      - $B_{ij} = \frac{(B_i + B_j)}{2}$
      - $B_{mix} = \sum_{i=1}^{N} y_i B_{ii} + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \delta_{ij}$
      - $\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj}$
    - 3rd Virial Coefficient – for high pressure gases near critical temperature
      - $C_{ijk} = \frac{(C_i + C_j + C_k)}{3}$
      - $C_{mix} = \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} y_i y_j y_k C_{ijk}$

Caveats

- How good are the predictions? As good as the data.
  - E.g., Vapor pressure. Sources include:
    - Correlations from NIST
    - Compilation of literature data – polynomial fit
    - Antoine equation
  - THD Virial Coefficients
    - 2nd VC - High Confidence:
      - From PIMC models, which match historical data from Souers, Sherwood, Reed, Grilly and others, and is valid from 15K through RT.
    - 3rd VC - Unproven:
      - Is estimated using H_2 3rd VC data and a corresponding states mapping (about T_r) from the 2nd VCs.

- Programming sanity checks is time consuming
  - Use your own judgment and knowledge of the materials being studied.
  - When in doubt, call me.

Using the Density Calculator (Demo)

- V2.5 & above:
  - On a PC: Open the document, accept that Macros need to be run.
  - Navigate to the “Calculator” tab.
  - Enter the desired mass density & shot temperature.
  - Adjust the composition.
  - Check the right hand fields.
  - Find the pressure alongside the desired composition

- V2.4 (Mac)
  - Open the document.
  - Navigate to the “Calculator” tab.
  - Enter the desired mass density & shot temperature
  - Adjust the composition.
  - For THD Mixtures ONLY:
    - N.B. Click the “THD Mixture Calculate” button. Wait for convergence.
      - If there is no convergence, navigate to the “THD EquilibriumCalculator” tab
        - Click “Reset” and “Solve” buttons.
        - Adjust “initial value factor” if necessary.
        - Re-click “Solve” to increase the number of solver iterations.
  - Check the right hand fields.
  - Find the pressure alongside the desired composition

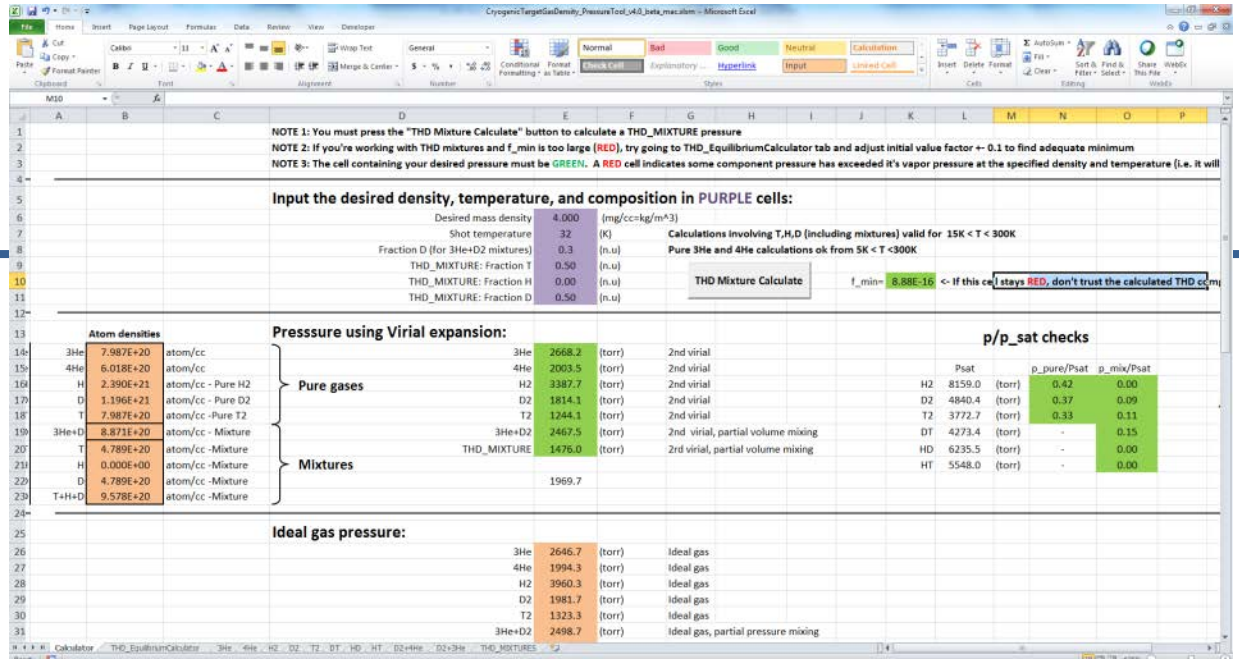
- V2.6 beta
  - Working to resolve the issue of porting VB from PC to Mac version.

Using the Density Calculator (Demo)

- Case 1: Recent D_2-Filled HDC Symcap shot (N151025-001)
- Case 2: How do I request a specific density/mixture?
- Case 3: Post shot re-verification

Using the Density Calculator – Case 1

- Recent D_2-Filled HDC Symcap shot (N151025-001)
  - Original desired density:
    - 4 mg/cc at 32K
  - AppMan Request
    - 1486 Torr at 24K
  - Fielded Capsule
    - Liquid Deuterium
  - What red flags existed?



NOTE 1: You must press the "THD Mixture Calculate" button to calculate a THD_MIXTURE pressure
NOTE 2: If you're working with THD mixtures and f_min is too large (RED), try going to THD_EquilibriumCalculator tab and adjust initial value factor +- 0.1 to find adequate minimum
NOTE 3: The cell containing your desired pressure must be GREEN. A RED cell indicates some component pressure has exceeded it's vapor pressure at the specified density and temperature (i.e. it will

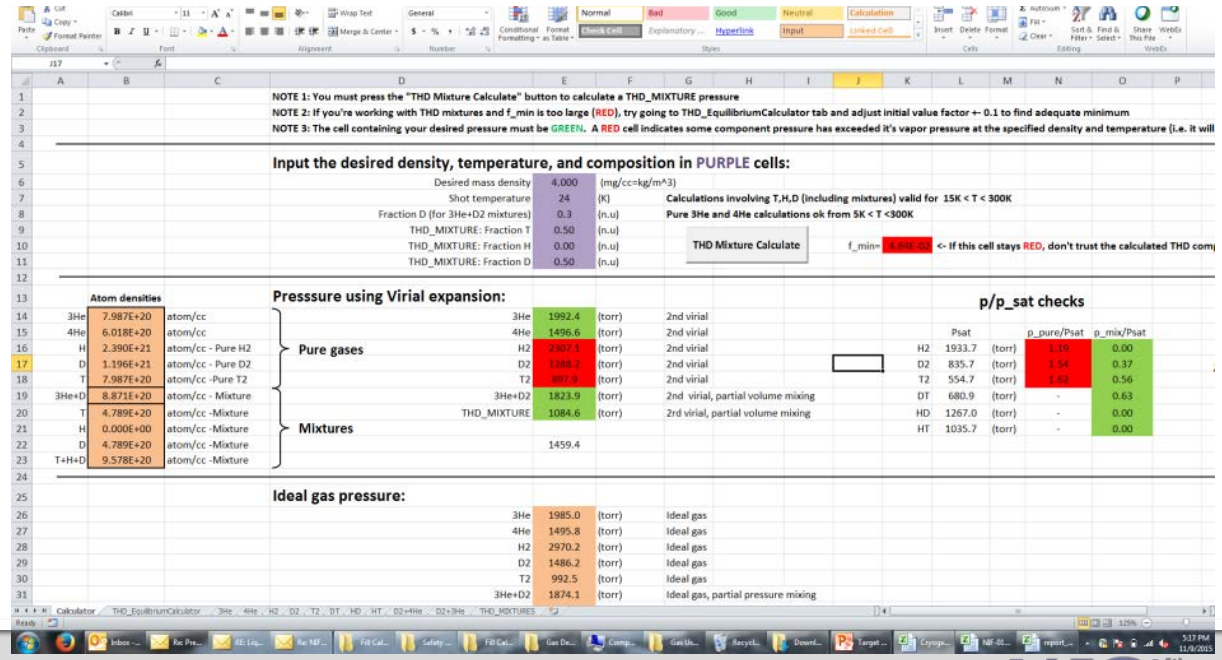
Input the desired density, temperature, and composition in PURPLE cells:

Desired mass density	4.000	(mg/cc=kg/m^3)	
Shot temperature	32	(K)	Calculations involving T,H,D (including mixtures) valid for 15K < T < 300K
Fraction D (for 3He+D2 mixtures)	0.3	(n.u)	Pure 3He and 4He calculations ok from 5K < T <300K
THD_MIXTURE: Fraction T	0.50	(n.u)	
THD_MIXTURE: Fraction H	0.00	(n.u)	THD Mixture Calculate — f_min= 8.88E-16 <- If this cell stays RED, don't trust the calculated THD comp
THD_MIXTURE: Fraction D	0.50	(n.u)	

Atom densities				Presssure using Virial expansion:					p/p_sat checks				
										Psat		p_pure/Psat	p_mix/Psat
3He	7.987E+20	atom/cc	Pure gases	3He	2668.2	(torr)	2nd virial						
4He	6.018E+20	atom/cc		4He	2003.5	(torr)	2nd virial						
H	2.390E+21	atom/cc - Pure H2		H2	3387.7	(torr)	2nd virial		H2	8159.0	(torr)	0.42	0.00
D	1.196E+21	atom/cc - Pure D2		D2	1814.1	(torr)	2nd virial		D2	4840.4	(torr)	0.37	0.09
T	7.987E+20	atom/cc -Pure T2		T2	1244.1	(torr)	2nd virial		T2	3772.7	(torr)	0.33	0.11
3He+D	8.871E+20	atom/cc - Mixture	Mixtures	3He+D2	2467.5	(torr)	2nd virial, partial volume mixing		DT	4273.4	(torr)	-	0.15
T	4.789E+20	atom/cc -Mixture		THD_MIXTURE	1476.0	(torr)	2rd virial, partial volume mixing		HD	6235.5	(torr)	-	0.00
H	0.000E+00	atom/cc -Mixture							HT	5548.0	(torr)	-	0.00
D	4.789E+20	atom/cc -Mixture			1969.7								
T+H+D	9.578E+20	atom/cc -Mixture											

Ideal gas pressure:

3He	2646.7	(torr)	Ideal gas
4He	1994.3	(torr)	Ideal gas
H2	3960.3	(torr)	Ideal gas
D2	1981.7	(torr)	Ideal gas
T2	1323.3	(torr)	Ideal gas
3He+D2	2498.7	(torr)	Ideal gas, partial pressure mixing



NOTE 1: You must press the "THD Mixture Calculate" button to calculate a THD_MIXTURE pressure
NOTE 2: If you're working with THD mixtures and f_min is too large (RED), try going to THD_EquilibriumCalculator tab and adjust initial value factor +- 0.1 to find adequate minimum
NOTE 3: The cell containing your desired pressure must be GREEN. A RED cell indicates some component pressure has exceeded it's vapor pressure at the specified density and temperature (i.e. it will

Input the desired density, temperature, and composition in PURPLE cells:

Desired mass density	4.000	(mg/cc=kg/m^3)	
Shot temperature	24	(K)	Calculations involving T,H,D (including mixtures) valid for 15K < T < 300K
Fraction D (for 3He+D2 mixtures)	0.3	(n.u)	Pure 3He and 4He calculations ok from 5K < T <300K
THD_MIXTURE: Fraction T	0.50	(n.u)	
THD_MIXTURE: Fraction H	0.00	(n.u)	THD Mixture Calculate — f_min= 4.94E-02 <- If this cell stays RED, don't trust the calculated THD comp
THD_MIXTURE: Fraction D	0.50	(n.u)	

Atom densities				Presssure using Virial expansion:					p/p_sat checks				
										Psat		p_pure/Psat	p_mix/Psat
3He	7.987E+20	atom/cc	Pure gases	3He	1992.4	(torr)	2nd virial						
4He	6.018E+20	atom/cc		4He	1496.6	(torr)	2nd virial						
H	2.390E+21	atom/cc - Pure H2		H2	2307.1	(torr)	2nd virial		H2	1933.7	(torr)	1.19	0.00
D	1.196E+21	atom/cc - Pure D2		D2	1288.2	(torr)	2nd virial		D2	835.7	(torr)	1.54	0.37
T	7.987E+20	atom/cc -Pure T2		T2	897.9	(torr)	2nd virial		T2	554.7	(torr)	1.62	0.56
3He+D	8.871E+20	atom/cc - Mixture	Mixtures	3He+D2	1823.9	(torr)	2nd virial, partial volume mixing		DT	680.9	(torr)	-	0.63
T	4.789E+20	atom/cc -Mixture		THD_MIXTURE	1084.6	(torr)	2rd virial, partial volume mixing		HD	1267.0	(torr)	-	0.00
H	0.000E+00	atom/cc -Mixture							HT	1035.7	(torr)	-	0.00
D	4.789E+20	atom/cc -Mixture			1459.4								
T+H+D	9.578E+20	atom/cc -Mixture											

Ideal gas pressure:

3He	1985.0	(torr)	Ideal gas
4He	1495.8	(torr)	Ideal gas
H2	2970.2	(torr)	Ideal gas
D2	1486.2	(torr)	Ideal gas
T2	992.5	(torr)	Ideal gas
3He+D2	1874.1	(torr)	Ideal gas, partial pressure mixing

Using the Density Calculator (Case 2)

- Case 2: How do I request a specific density/mixture?
  - 10 mg/cc of D_2 at 32K
    - Answer should be immediately available
  - 10 mg/cc of 0.4 at% D-^{3}He at 32K
  - 10 mg/cc of 50:50 DT at 32K
    - Mac: must click solver button
  - 10 mg/cc of 2/24/74 HDT at 32K
    - Mac: must click solver button

Using the Density Calculator (Demo)

- Case 3: Post shot analysis
  - Requested: 10 mg/cc of 0.75/0.25 HT at 32K
    - Calculator indicates: 5022 Torr at 32K.

  - Cryo Reports on !DATA:
    - 5069 Torr
    - Mass Spec Analysis
      - 74% H
      - 25% T
      - 1% D

    - Calculator (trial & error)
      - 10.21 mg/cc at 32K

      - NOTE: 75/25 from calculator is 10.13 mg/cc

Current ELM Version is NIF-0135638-AF or v2.5

- Recently added/changed features
  - On the PC version, the THD Equilibrium Calculator is now "live," no need to hit a reset & run-macro button
    - Seems to work for three-component THD mixtures.
    - Uses a pragmatic "forced-mass-balance" scheme to converge the equilibrium expressions.
  - Science fiction checks
    - Polynomial correlation of saturated vapor density of THD.
    - Color coding: an indication of when an estimate is violating something
      - **Green** is good
      - **Red** is bad
      - Any other color: **Use with Caution**
        - Data may be extrapolated or near some critical value (e.g., saturation temp, valid range of vapor pressure expression, etc.)

- If its broken, or if the calculator doesn't have a mixture or material that is of interest, contact me.

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