

Imaging with Neutrons

Hassina Bilheux VENUS Instrument Scientist

Yuxuan Zhang MARS Instrument Scientist

Jean Bilheux Computational Instrument Scientist

August 7, 2024



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







The Neutron Imaging Team for the General User



Yuxuan Zhang, HFIR MARS Scientist



James Torres, HFIR MARS Scientist



Jean Bilheux, Computational Instrument Scientist



Shimin Tang, Artificial Intelligence, Machine Learning, Hyperspectral Imaging



Chen Zhang Imaging Software Developer

SPALLATION NEUTRON SOURCE



Roger Hobbs, Imaging Scientific Associate (SA)

Kevin Yahne, Imaging SA



Harley Skorpenske, SNS Group Leader



Hassina Bilheux, SNS VENUS Scientist



Yuxuar

Outline

- Imaging at the High Flux Isotope Reactor MARS beamline:
 - Principle of neutron radiography and computed tomography at a continuous source
 - The CG-1D imaging beamline
 - Examples

- Imaging at the Spallation Neutron Source:
 - Principle of neutron radiography at a pulsed source
 - Examples
 - The VENUS !!!construction project

• Scientific programming



Outline

- Imaging at the High Flux Isotope Reactor MARS beamline:
 - Principle of neutron radiography and computed tomography at a continuous source
 - The CG-1D imaging beamline
 - Examples

- Imaging at the Spallation Neutron Source:
 - Principle of neutron radiography at a pulsed source
 - Examples

SPALLATION Neutron National Laboratory

- The VENUS !!!construction project

• Scientific programming



Hassin

Yuxua

Neutron imaging measures the transmitted neutrons though an object







(Figure source: aven.amritalearning.com,. (2013). Shadows and Pin Hole Camera.)

Transmitted neutrons recorded as image/images







Neutrons interact uniquely with matter



CAK RIDGE National Laboratory

Neutrons interact uniquely with matter (cont'd)









Gupta, D., Zhang, Y., Nie, Z., & Koenig, G. M. (2024). Journal of Industrial and Engineering Chemistry





Neutrons interact uniquely with matter (cont'd)







The MARS instrument at HFIR









Example: visualize live root system





(J. Warren (PI), H, Bilheux, M. Kang, S. Voisin, C. Cheng, J. Horita, E. Perfect, Plant Soil, 2013)

Resolve the composition gradient in graded superalloy





Huang S., Shen C., An K., Zhang Y., Spinelli I., Brennan M., Yu D., *Frontiers in Metals and Alloys*, 1, 1070562 (2022)



Transmission image



Reconstructed 3D volume (virtual slicing location in orange) Cross-sectional view atter virtually slicing

[mm]



Measures molten salt densities at MSR operating temperatures





Moon J., Andrews H.B., Agca C., Bilheux J., Braatz A.D., McAlister A., McFarlane J., McMurray J.W., Robb K.R., Zhang Y., Industrial Engineering Chemistry Research, 61, 17665-17673 (2022)

Resolutions and FOVs

Type of detector	Field-of-view (FOV)	Pixel size (µm)	Highest spatial resolution (µm)	Typical acquisition time of 1 radiograph	Maximum speed @16 bit
High-res (1x)	36 x 24 mm ²	3.8	10-15	900 s	1 image/second
High-res (.5x)	50 x 48 mm ²	7.63	20-25	300 s	1 image/second
High-speed	88 x 88 mm²	43	~100	_	74 image/second
Balanced	88 x 88 mm ²	16	~50	30-90 s	1 image/second





(Sample credit: George Williams)

15



IPTS-27734, Y. Zhang, 2022

Resolutions and FOVs





IPTS-27734, Y. Zhang, 2022

RIDGE SPALLATION

What is neutron grating interferometry (nGI)?

A neutron imaging instrumentation that enable the utilization the **wave properties of neutron**, to spatially resolve sub µm internal features



Raw data resulted from a step-wise scan



T. Reimann et al., J. Applied Crystallography. (2016)



Transmission Image (TI)



Y. Kim et al., Applied Sciences (2022). (Sample courtesy of Dr. Chris Fancher)

17

CAK RIDGE National Laboratory

What is neutron grating interferometry (nGI)?

A neutron imaging instrumentation that enable the utilization the **wave properties of neutron**, to spatially resolve sub µm internal features



(Sample courtesy of Dr. Chris Fancher)

Intensity a¹ G₀ position T. Reimann et al., J. Applied Crystallography. (2016)

Raw data resulted from a step-wise scan





10

CAK RIDGE National Laboratory

More about this sample along with the nGI results



(Sample courtesy of Dr. Chris Fancher)

EBSD image is from Plotkowski et al., Additive Manufacturing. 46, 102092, (2021).

CAK RIDGE National Laboratory



More about this sample along with the nGI results



SANS from feature

in certain sizes

(Sample courtesy of Dr. Chris Fancher)

EBSD image is from Plotkowski et al., Additive Manufacturing. 46, 102092, (2021).

Actional Laboratory

Scan through various correlation lengths to understand the length scale



Y. Kim et al., Applied Sciences (2022).

(Sample courtesy of Dr. Chris Fancher)

 $\xi = \lambda L_s/p$

Autocorrelation length

Neutron



Scan through various correlation lengths to understand the length scale



Y. Kim et al., Applied Sciences (2022).

(Sample courtesy of Dr. Chris Fancher)







 $\xi = 580 \text{ nm}$ $\xi = 670 \text{ nm}$ $\xi = 759 \text{ nm}$ $\xi = 848 \text{ nm}$



SPALLATION National Laboratory

Plotting the dark field intensity vs. ξ in region-of-interest (ROI)



0.8 Dark field intensity 0.6 0.4 0.2 -ROI#1 -ROI#2 -ROI#1 -ROI#2 0 1000 2000 3000 4000 0 Autocorrelation length (nm)

 Indicating different microstructures between selected ROIs



(Sample courtesy of Dr. Chris Fancher)

CAK RIDGE SPALLATION National Laboratory SOURCE



Measurement of suspended PMMA spheres in solution as a calibration standard



TI DFI

(Sample courtesy of Dr. Fankang Li)



- The curves indicate the size of the PMMA spheres, which match well with the spec. (~100 nm in the top cell, ~150 nm in the bottom cell)
- Some settling observed in the bottom cell, resulted difference in number density of PMMA can be observed



CAK RIDGE National Laboratory

nGI capability at MARS

Two setups to cover ACL ranges from ~40 nm to ~3400 nm







ACL Coverage for 2.5 Å



25

(Sample courtesy of R. Dehoff)

Yuxuar

Outline

- Imaging at the High Flux Isotope Reactor MARS beamline:
 - Principle of neutron radiography and computed tomography at a continuous source
 - The CG-1D imaging beamline
 - Examples

- Imaging at the Spallation Neutron Source:
 - Principle of neutron radiography at a pulsed source
 - Examples
 - The VENUS !!!construction project

• Scientific programming



Imaging at a pulsed source (SNS)



CAK RIDGE National Laboratory

Higher energy neutrons can also be used for imaging (neutrons of <u>energies</u> higher than 1 eV): Resonance Imaging



National Laboratory | SOURCE

28

Resonance imaging (> 1eV or < 0.286 Å): preparing your experiment

- Soil surveys, contaminants in soil, etc.:
 - transmission through 0.01 mm thickness of ^{nat}Co (between 1 and 5 Å) = 99.5 \%
 - transmission through 1 mm thickness of ^{nat}Zn (between 1 and 5 Å) = 96.4 \%



Simulated resonance for elements of interest(*)



CAK RIDGE National Laboratory

29

(*) Soil surveys in UK (1978-1983, 2000, 2011-2012)

Resonance imaging: preparing your experiment (cont'd)

- Hg contamination in soil
 - Assumptions: 0.1 mm Hg (13.6 g/cm³) + 12.5 mm SiC (with 1.5 g/cm³)
 - Transmission (1 and 5 Å) = 66.4 %





Using epithermal neutrons (energy > 1 eV), resonance imaging can map the isotopic content in advanced nuclear fuel materials in 3D

Distribution of elements drive the performance of the novel advanced nuclear fuel materials





Quantitative analysis is being developed using in-house open-source Python package (ResoFit)

SPALLATION National Laboratory Myhre K.G., Zhang Y., Bilheux H.Z., Johnson J.A., Bilheux J., Miskowiec A., Hunt R.D., "Nondestructive Tomographic Mapping of Uranium and Gadolinium Using Energy-Resolved Neutron Imaging", *Transactions of the American Nuclear Society*, (2018).

Bragg edge imaging: how does it work?



Principle of Bragg edge Transmission

✓ Utilizes thermal and cold neutrons (approximately between 1 and 10 Å) ✓ Obeys Bragg's Law $\lambda_{hkl} = 2d_{hkl} \sin \theta_{hkl}$ simplifies: $\lambda_{hkl} = 2d_{hkl}$



The perfect case study: powders

34



Song G., Lin J.Y., Bilheux J., Xie Q., Santodonato L., Molaison J.J., Skorpenske H.D., dos Santos A.M., Tulk C.A., An K., Stoica A.D., Kirka M.M., Dehoff R.R., Tremsin A.S., Bunn J.R., Sochalski-Kolbus L.M., Bilheux H.Z., "Characterization of Crystallographic Structures Using Bragg-Edge Neutron Bullation Neutron Source", Journal of Imaging, **3**, 4, 65 (2017). Materials Behavior: Monitoring residual strain relaxation and preferred grain orientation of additively manufactured Inconel 625 by in-situ neutron imaging



Fig. 8. Strain distribution (in microstrain) at the (111) Bragg edge measured at room temperature along the sample thickness direction X. SNAP beamline. The image integration time was about 2 h at SNAP. λ_0 value is taken from the annealed sample #1–8 (average across the entire sample). The legend indicates the strain values in microstrain.

CAK RIDGE SPALLATION NEUTRON SOURCE



Engineered Materials: Monitoring residual strain relaxation and preferred grain orientation of additively manufactured Inconel 625 by in-situ neutron imaging (10 min measurements)







Modeled and experimental results.

AM Inconel 625 strain evolution as a function of temperature







Fig. 16. Variation of the standard deviation of the reconstructed strain as a function of image integration time. Three different sizes of the area used for pixel grouping are used for strain reconstruction, as indicated by the legend (in mm²).

Tremsin et al, Nuc. Instr. Methods in Phys. Res. A, 2021.



Tremsin et al, Additive Manufacturing, 2021.

Autonomous Hyperspectral Neutron CT Experiment at ORNL



Up to factor 5 improvement in time

Optimization of the scan based on the unique

Ability to provide real-time reconstructed data

using advanced iterative reconstruction

Light scan and preselection of projection angles









CAK RIDGE National Laboratory



methods

sample geometry



(active learning)
<311> Bragg edge reconstruction at ~ 2.17 Å ± 0.2 Å **Conventional reconstruction methods** Our advanced algorithms/methods



MSE along reconstructions

SSIM along reconstructions



Cu

	Thresholds
MSE ¹	5.689x 10 ⁻³
SSIM ²	0.634

¹Zhou Wang; Bovik, A.C.; ,"Mean squared error: Love it or leave it? A new look at Signal Fidelity Measures," Signal Processing Magazine, IEEE, vol. 26, no. 1, pp. 98-117, Jan. 2009.

¹Z. Wana, A. C. Bovik, H. R. Sheikh and E. P. Simoncelli, "Image quality assessment: From error visibility to structural similarity," IEEE Transactions on Image Processing, vol. 13, no. 4, pp. 600-612, Apr. 2004.



Neutron Imaging Capabilities at VENUS

- Bragg edge imaging
- Resonance imaging
- Epithermal imaging
- Largest field-of-view thermal/cold imaging
- Neutron grating interferometry (to be implemented)
- Polarized imaging (to be implemented)





https://neutrons.ornl.gov/venus





Largest field of view: 20 x 20 cm²

CAK RIDGE National Laboratory

41

Imaging detector at VENUS Spatial resolution mask First 20x20 cm² large field-of-view radiograph measured at VENUS (July 24, 2024)!!!

20 cm

Resonance radiography demonstrated with Tantalum foil and the microchannel plate (MCP) Timepix (TPX) detector



SPALLATION NEUTRON

Bragg edge radiography demonstrated with Nickel powder and the microchannel plate (MCP) Timepix (TPX) detector



SPALLATION Neutron Source

*****OAK RIDGE National Laboratory We hope to see you at VENUS!

The VENUS control hutch



VENUS



Yuxuar

Outline

- Imaging at the High Flux Isotope Reactor MARS beamline:
 - Principle of neutron radiography and computed tomography at a continuous source
 - The CG-1D imaging beamline
 - Examples

- Imaging at the Spallation Neutron Source:
 - Principle of neutron radiography at a pulsed source
 - Examples
 - The VENUS !!!construction project

• Scientific programming





Scientific programming 5 things you must know

Jean Bilheux

Neutron Imaging Computer Instrument Scientist

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







1 Pick the right language





Which language ?





https://www.tiobe.com/tiobe-index/

Which language ?

Jul 2024	Jul 2023	Change	Program	ning Language	Ratings	Change
1	1		e	Python	16.12%	+2.70%
2	3	^	0	C++	10.34%	-0.46%
3	2	•	Θ	С	9.48%	-2.08%
4	4			Java	8.59%	-1.91%
5	5		0	C#	6.72%	-0.15%
6	6		JS	JavaScript	3.79%	+0.68%
7	13	*	-60	Go	2.19%	+1.12%
8	7	*	VB	Visual Basic	2.08%	-0.82%
9	11	^	F	Fortran	2.05%	+0.80%
10	8	*	SQL	SQL	2.04%	+0.57%
11	15	*	3	Delphi/Object Pascal	1.89%	+0.91%
12	10	•	-	MATLAB	1.34%	+0.08%
13	17	*	ß	Rust	1.18%	+0.29%
14	16	^		Ruby	1.16%	+0.25%
15	12	*		Scratch	1.15%	+0.08%
16	9	*	php	РНР	1.15%	-0.27%
17	18	^	8	Swift	1.13%	+0.25%



SPALLATION National Laboratory



- Huge community (help, libraries, ...)
- Easy to learn (no compiler needed)
- Easy to build GUI (standalone application, Web interface)
- Run on any platform (🚑 📹 🧳 🛋:os ...)
- Notebooks



Notebooks



So... how much is a TB, really?

We have been talking about different data amounts of MB, GB, and TB. But, what does that really mean in reality? Let us explore what is a TB.

If you looked at one image with 1024 x 1024 pixels (1 Mpixels)

Here we create one image with 1000x1000 pixels with random values form a uniform distribution [0,1] and show it.

In [2]: %matplotlib inline import matplotlib.pyplot as plt import numpy as np

> > 1k x 1k random image







Notebooks

Do not know how to run this notebook? Click ME!





SPALLATION National Laboratory

Notebooks









CAK RIDGE SPALLATION Neutron Source

1 Pick the right language

2 Stay green





Stay green

We need to preserve our **environment!**









- **1** Pick the right language
- 2 Stay green
- **3** Write good code





Naming & Documentation

Write good code



There is a good chance that later, you will be the one trying to understand your own code.





Write good code

- Name of variable is what they represent
- Name of method indicates what they do
- Explain strange choices
- Add examples at top of methods/classes







REAL PROPERTY OF THE REAL PROP

Naming & Documentation

SPALLATION National Laboratory

59

https://www.youtube.com/results?search_query=clean+code+uncle+bob

Write good code

Workflow

- decide the code to write
- Write the test
- It should fail
- Write the code to pass the test
- It should pass
- Move on to the next one



Unit Test

Advantages

- The unit tests are often used as documentation to learn how the software works
- You write better code (simpler)
- People will trust your code
- You can check the unit test coverage
- Later on, when you make changes, you will quickly find out if the software still works
- If someone report a bug, first write a unit test to reproduce the bug, then fix it!

Disadvantages

• It seems slower to code (but overall, it's not)



Write good code







. . .



Getting a publication out of your software !

F1000Research





- **1** Pick the right language
- 2 Stay green
- 3 Write good code
- 4 How to keep your job!





iBeatles

- Program that perform automatic strain mapping calculation
- 1 million lines of code
- 5 years development
- Kept top secret until today (only copy is on this machine!)





iBeatles

Demo time !



iBeatles

Demo time !





Press any key to continue







Repositories



- Backup of your project
- Provide a full history (easy to reverse changes, ...)
- Ideal for collaboration (parallel work, ...)
- Documentation
- Necessary tool for publication of the code
- Easy to share code (web interface, ...)
- GitAction (automatic test, deployment, build documentation)



ucket Projects Rep	ositories v			Search for code, commits or repositories	a @ 0	0 03 🚯	
ly Awesome Project ommit-graph	My Awesome Project Commits	t / commit-graph					J L.
	\$9 master ~	Show All					
e branch	66 A	luthor	Commit	Message	Commit date	Issues	IUN
e pull request	1 4	💁 Dennis Wong	##5555ac05564 [M]	Margari in GRAPH-142 (pull request #52) GRAPH- Praster		GRAPH-142	
e fork	4	Dennis Wong	ofintentile [M]	Marged in GRAPH-141 window 5 (pull request #10) GRAPH-141		GRAPH-141	
	£ 1	Dennis Wong	effc767d9d7	GRAPH-141 make more css loaded or \$9 GRAPH-141-versi	Yesterday	GRAPH-141	
e nite		🐌 Dennis Wong	b01b7eb91c0	GRAPH-141 added css fixes to make tag labels looks correctly in	2 days ago	GRAPH-141	
hes		S Dennis Wong	159c26f1b64	GRAPH-142 added license changed event han: \$9 GRAPH-142	2 days ago	GRAPH-142	
15	+ 4	🛃 Dennis Wong	54accbdc446	GRAPH-142 fixed react to not call api if license is not present	2 days ago	GRAPH-142	
equests	+ 4	🛃 Dennis Wong	bb91db98c85	GRAPH-142 initial implementation	3 days ago	GRAPH-142	
		Mohammed Davoodi	1ed71:5e605				
E.	G .	🐌 Dennis Wong	512ede#0104	Merged in GRAPH-140 (pull request #50) GRAPH-140 edded Torn		GRAPH-140	
nortcut		Mohammed Davoodi	8d19aee8e20	GRAPH-144 Added screenshot to use pricesing-impro. 15	5 days ago	GRAPH-144	
sitory settings	lt d	Mohammed Davoodi	4a36b4ba6e5	GRAPH-144 Licnesing updates for repository contributions.	6 days ago	GRAPH-144	
	2	S Dennis Wong	4b26ecede43	GRAPH-140 added fix to rest branch property 29 GRAPH-140 dd	5 days ago	GRAPH-140	
		Mohammed Davoodi	b7ef13935cc (#	Merged in GRAPH-98 merving but request #40 GRAPH-98 %		GRAPH-98	
	f	Mohammed Davoodi	Scca41e437b	GRAPH-98 Added instructions for de 19 GRAPH-98-cestyl.	07 Jun 2018	GRAPH-98	

Pull

🗢 🗢 🔹 📿 Giti	Hub - ornineutronimaging/ × +			•
€ → C @	1 github.com/ornineutronimaging/NeuN	sm ६९४) 🛊 🚜	N R 4	📸 🕫 🔊 🗉 🖸 速 🚇 🖬 Finish update 🗄
💡 Google Maps 🛛 🕅	Gmail 👗 Google Contacts 🔝 Google Calendar	🗅 List of Bookmarks 🛄 TasksManager 🗅 Bass Prac	tice 📓 TweetDeci	k 🥝 GitLab 🔄 🗅 Al Bookmarks
Product ~	 Solutions Resources Open Source 	✓ Enterprise ✓ Pricing	Q. Search	h or jump to 7 Sign in Sign up
G ornineutroni	imaging / NeuNorm (Public)			Q. Notifications ♀ Fork 0 ♀ Star 1 +
0.00	a b barrent a C brend	en O Antiere III Breitente III Breuter III bei	***	
0.000	isues (i) 11 Pullieduests (ii) VV Liscussio	na 🕗 Actiona 🔛 Projecta 🔍 Security 🗠 Inaig	ns	
P	next 👻 🥲 🕏 Branches 🛇 🛚 Tags	Q. Go to file	↔ Code +	About
4	JeanBilheux Update README.md 🚥 🗸	0730857 - 5 months ago	🕙 24 Commits	Neutron Imaging Loading and Normalization Tools
	.github/workflows	fix conda build path type	6 months ago	Readme
	conde.recipe	fix version and build number in meta.yaml	6 months ago	Activity
	data	brinbing back NeuNorm home.	6 months ago	Custom properties
	documentation	fix pre-commit located issues	6 months ago	17 1 star ⊙ 2 watching
	notebooks	brinbing back NeuNorm home.	6 months ago	약 @ forks
	paper	fix pre-commit located issues	6 months ago	Report repository
	scripts	remove deprecated conf files	6 months ago	Releases
	src/NeuNorm	removed file, this refs #17	5 months ago	⊗ 8 tags
•	tests	fix pre-commit located issues	6 months ago	Packages
C	j .gitignore	cleanup gitignore	6 months ago	No packages published
C	pre-commit-config.yaml	fix pre-commit located issues	6 months ago	Contributors
e	j .readthedocs.yaml	rename files	6 months ago	
C	CONTRIBUTING.md	fix pre-commit located issues	6 months ago	Anaphiliberry loss Dilberry
C	LICENSE	rename files	6 months ago	A new complexitient
C	README.md	Update README.md	5 months ago	A bre-commercified
C) codecoxyaml	fix pre-commit located issues	6 months ago	Languages
C	environment.yml	add missing anaconda client to env	6 months ago	 Bushes (2) (3)
C	pyproject.tomi	remove invalid entry	6 months ago	Jupyter Notebook 38.5% Other 0.7%
œ	README BSD-3-Clause license		=	
	Employee 2013 Exemption of the effect o	and the second s	n close by st take, in moved but allows to following	



- **1** Pick the right language
- 2 Stay green
- 3 Write good code
- 4 How to keep your job!
- 5 Use the best debugging tool







Each of you will leave today with that tool!



- Any computing language
- It takes no time to learn how to use it
- It never needs any software update
- It has a very small carbon footprint







Best debugging tool



 Tell your new friend what your program does, and you will find what is wrong with it !



The Yellow Duck





- 1 Python
- 2 use environments
- **3** Good naming & unit tests
- 4 Repository
- 5 Talk to your yellow duck





Acknowledgements



Research sponsored by the **Laboratory Directed Research and Development Program** of Oak Ridge National Laboratory, managed by UT-Battelle LLC, for DOE.

Resources at the **High Flux Isotope Reactor (HFIR)** and **Spallation Neutron source (SNS)**, U.S. DOE Office of Science User Facilities operated by ORNL, were used in the research.






Thank you



https://forms.office.com/g/gtdnJGM87r

NXS Lecture - Yuxuan Zhang, Hassina Bilheux & Jean Bilheux: "Neutron Imaging"



Questions

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



