ENDF report

G.P.A. Nobre[1]

[1]National Nuclear Data Center, Brookhaven National Laboratory

Nuclear Data Week - USNDP Meeting
November 13th, 2023

Outline - Fix

- ENDF/B-VIII.1 release status
  - Beta releases
  - mini-CSEWG
  - Hackathon
  - Reviews
  - Preparing for release
- “Big Paper”
- Metrics
  - GitLab
  - Evaluations, fixes, reviews

ENDF release status

ENDF/B-VIII.1 release

The next release of the ENDF/B library is scheduled for **February 2024!**

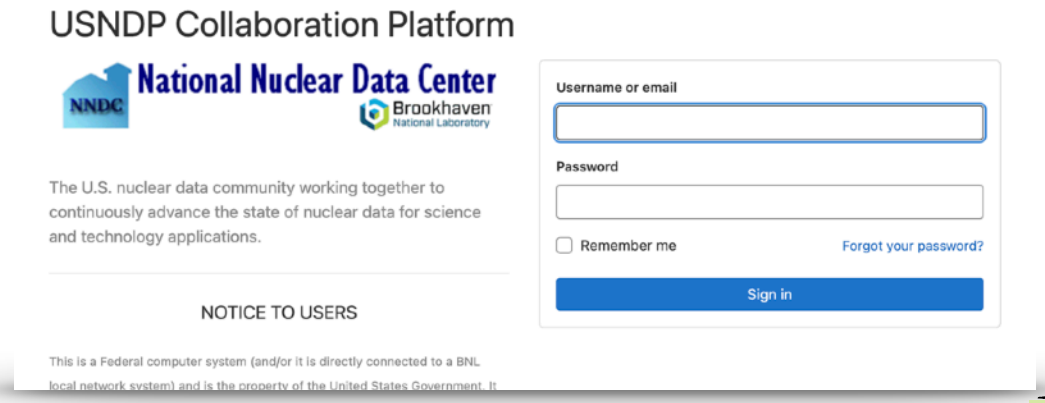
Although technically “minor”, it will have major impact.

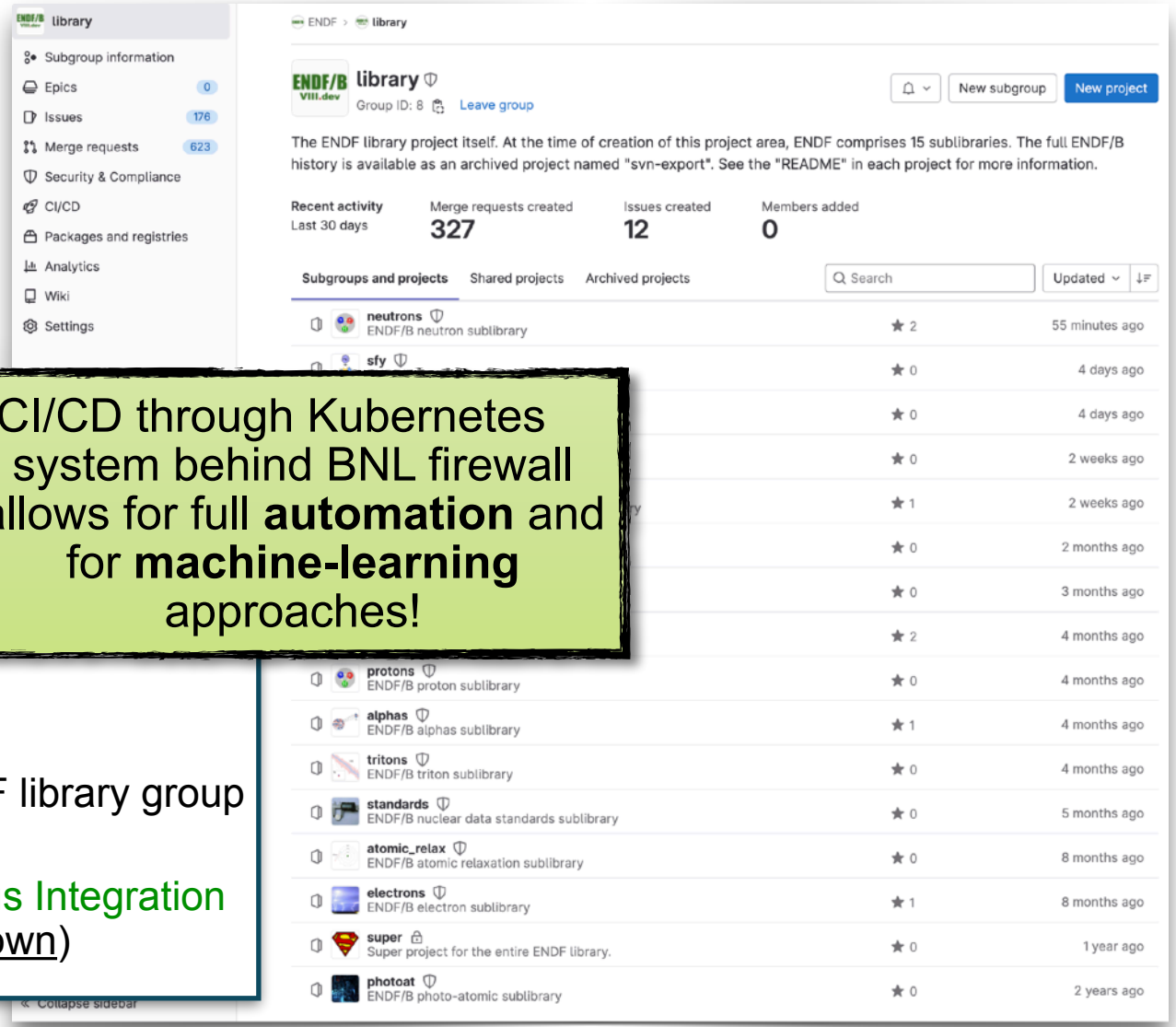
- Why **VIII.1** and not **IX**?
  - There are no planned updates of the standards library for this release
  - Standards are well-stablished cross sections, in specific energy ranges, used in ratios with other measurements
  - However, many, many important and impactful changes are on the way!!
- Next release will be in both legacy **ENDF-6** format and **GNDS-2.0**
- Will have an accompanying **“Big Paper”**
- Implemented review system: Multiple VIII.1 Beta versions have been released
- Preliminary validation indicate that this will be the best-performing library ever!

ENDF/B VIII.1-β2

Brookhaven National Laboratory

ENDF versioned repository: GitLab





- Constantly updated and maintained
- Keeps track of
  - Any changes
  - Development, review and release branches
  - Issue trackers
  - etc…
- Usage is growing! Currently ~60 active members in ENDF library group (unfortunately there's a seat limit)
- Integration of library repository in GitLab with a Continuous Integration system: **ADVANCE** (R. Arcilla, R. Coles, B. Shu, D. Brown)

CI/CD through Kubernetes system behind BNL firewall allows for full **automation** and for **machine-learning** approaches!

What to expect when expecting…
… the ENDF/B-VIII.1 release

Neutrons:

- Many INDEN contributions
- Actinides:
  - ^{239}**Pu**: multi-institution effort, with important updates to fission, nubar, PFNS, capture, URR, RRR, (n,2n)
  - ^{235}**U**: resonances, nubar, covariances,
  - ^{238}**U**: resonance update to improve performance on depletion benchmarks
  - ^{240,241}**Pu**: work in concert with changes in ^{239}Pu and ^{238}U to recover burnup performance
- Stainless steel & other structure materials:
  - ^{54,56,57}**Fe**: Corrects leakage deficiency from ENDF/B-VIII.0
  - ^{50,52,53,54}**Cr**: Thorough re-evaluation, impact in criticality and leakage benchmarks
  - ^{206,207,208}**Pb**: complete evaluations (RPI/LANL)
  - ^{63,65}**Cu**: improved performance
  - ^{55}**Mn**: Gamma spectra
  - ^{28,29,30}**Si**: resonance evaluations
- Others:
  - ^{6}**Li**, ^{9}**Be** (LANL)
  - ^{234,236}**U** (LANL)
  - ^{140,142}**Ce** (ORNL)
  - ^{103}**Rh** (RPI/IRSN)
  - ^{86}**Kr** (BNL)
  - ^{181}**Ta** (RPI/ORNL/LANL)
  - ^{95}**Mo** (IRSN/LANL)
  - Many, many, many more…

What to expect when expecting the ENDF/B-VIII.1 release

TSL:

- 70+ new updated/files
- **Polystyrene**, **zirconium hydride**, **UC**, **UN**, **UO_2**, **sapphire**, **lucite**, **FLiBe**, **etc…**
- Fuel materials with different enrichments
- So many new evaluations that we had to re-think how to identify them.
- Low-temperature extrapolations to light water
- Community-wide review and validation

Fission Yields:

- Many fixes

Photo-nuclear:

- **200+** updates coming from IAEA CRP

Charged particles:

- A few improvements and fixes

Progress towards ENDF/B-VIII.1

- **Beta1** was released on March 1st, 2023:
  - Mostly neutrons sublibraries
  - Mostly INDEN
- **Beta1.1** was released on April 18th, 2023:
  - Mostly TSL files
  - Some few specific neutrons fixes
- Mini-CSEWG (LLNL): April 24-28, 2023

- **Beta2** was released on August 4, 2023
  - All neutrons contributions incorporated
  - New ^{239}Pu that restores depletion performance, following feedback from mini-CSEWG
  - Many updates on photonuclear library based on IAEA CRP
- Hackathon (LANL): August 6-8, 2023

ENDF/B VIII.1-β1

ENDF/B VIII.1-β1.1

ENDF/B VIII.1-β2

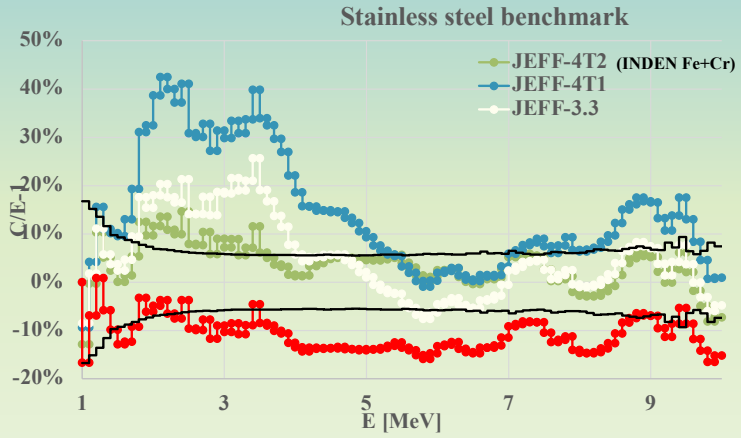
Brookhaven National Laboratory

Results sensitive to stainless steel

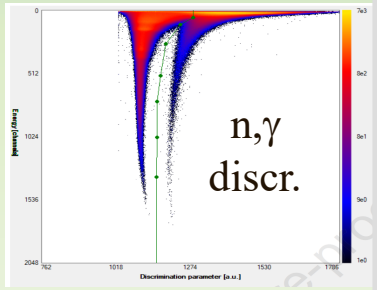
INDEN updated "structural" evaluations:

see nds.iaea.org/INDEN/ - **Validation**

- ✓ Fe isotopes (IAEA/JSI), fe54e80o, fe56e80X29r41, fe54e80o
- ✓ Cr isotopes, BNL/ORNL/IAEA/JSI/CEA, v2.3.2



Kostal et al, priv. com. stilbene meas.



Stainless steel, neutron leakage (Rez, CZ, 11/2021)

Roberto Capote, IAEA Nuclear Data Section
e-mail: R.CapoteNoy@iaea.org
Web: http://www-nds.iaea.org

The Pool Critical Assembly (PCA) Pressure Vessel Simulator experiment was performed in the early 1980s as part of the NRC's LWR Pressure Vessel Surveillance Dosimetry Improvement Program (LWR-PV-SDIP)

Benchmark was recently re-analyzed with exact geometry by Dr. Kulesza (LANL/X-5), and MCNP inputs were published and available for use:
- NUCLEAR TECHNOLOGY · VOLUME 197 · 284–295 · MARCH 2017
- Paper: https://doi.org/10.1080/00295450.2016.1273711
- MCNP Inputs: https://doi.org/10.2172/1601379

Pool Critical Assembly Benchmarking

- C/E Results (ENDF/B-VIII.1b1):
  - MC uncertainty ~= 1%

Depends on U-235, water & SS

	al27a	ni48p	rh103n	in115n	u238f	np237f	avg	std dev
	0.97	0.96	1.04	1.00			**0.99**	**3.9%**
	1.02	0.98	1.08	1.01			**1.02**	**4.3%**
	1.05	1.01	1.07	1.06			**1.05**	**2.5%**
	1.03	0.96	1.00	1.01	0.98	1.03	**1.00**	**2.7%**
	1.03	0.96	0.95	1.00	0.98	1.05	**0.99**	**4.0%**
	1.04	1.02	0.93	1.03	0.98	1.03	**1.00**	**4.1%**
			0.96	0.99	0.99	1.13	**1.02**	**7.6%**
avg	**1.02**	**0.98**	**1.01**	**1.01**	**0.98**	**1.06**	**1.01**	
std dev	**2.8%**	**2.9%**	**6.4%**	**2.1%**	**0.1%**	**1.0%**		**4.2%**

Presented by Greg Fischer, Westinghouse @ miniCSWEG April 2023

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Slides taken from Roberto Capotes's talk at 2023 mini-CSEWG

- Significant performance improvements in SS (Fe and Cr)
- Users are happy with new files!

Results sensitive to stainless steel

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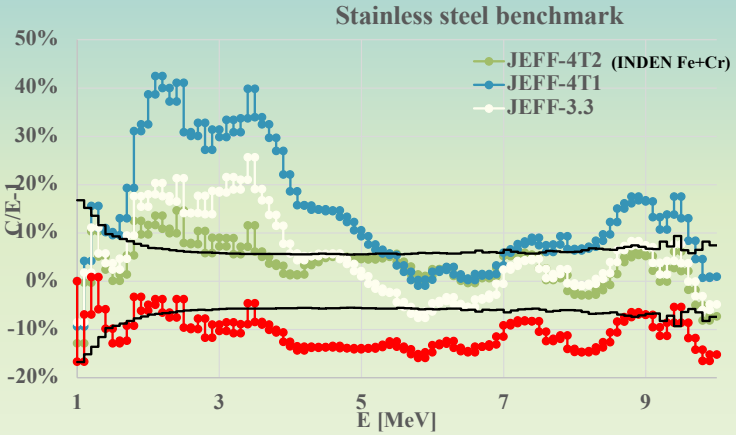

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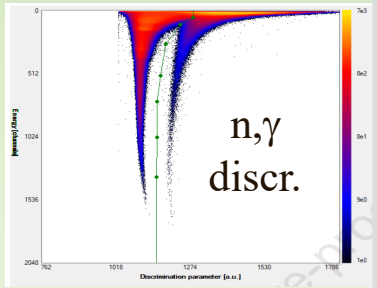

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- Significant performance improvements in SS (Fe and Cr)
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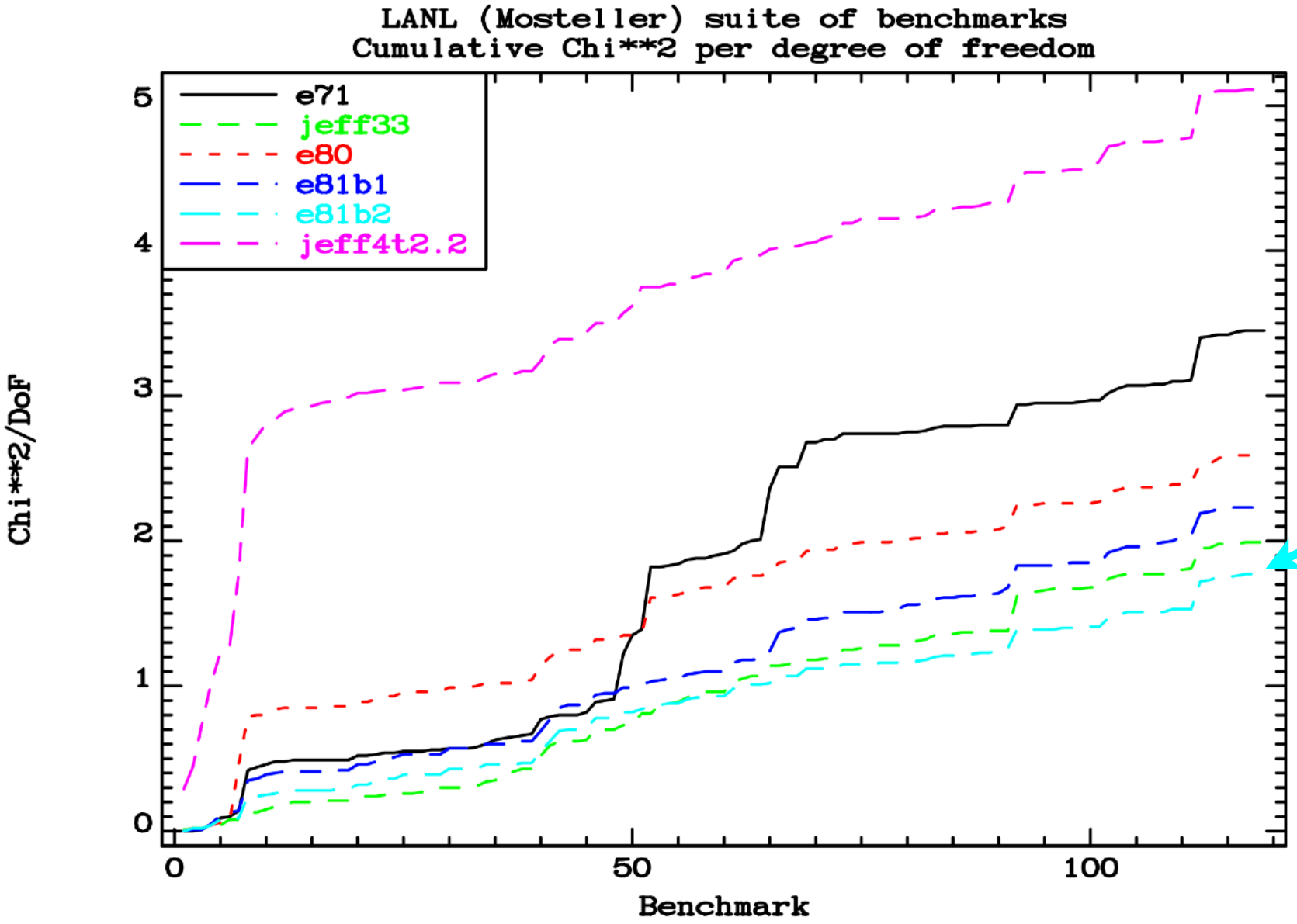
Preliminary validation on Beta2, by Andrej Trkov (JSI)



ENDF/BVIII.1 is on track to be the best-performing library to-date!

Caveat: Cumulative χ^2 of benchmarks provide only a global view. Detailed investigation of performance on specific benchmark are also important.

What to expect for Beta3

- **TSL:**
  - New MAT number assignments
  - Reviewed and new files
  - Extension of light water to low temperatures
- **Neutrons:**
  - Exit distributions form LANL/KAERI
  - Many fixes
  - Improved ^{239,240,241}Pu set with better criticality/depletion performance
- **Photonuclear:**
  - Reverted ^{180,182,183}W to VIII.0
  - ^{242}Pu from JENDL-5.0
  - ^{9}Be from IAEA CRP
- **Atomic sublibraries:**
  - Taken from EPICS-2023
    - Atomic relaxation sublibrary (EADL)
    - Electrons sublibrary (EEDL)
    - Photoatomic sublibrary (EPDL)

Status of Big Paper

Big Paper updates

- Many contributions have been sent but there are still gaps that will be addressed after CSEWG Meeting
- Circulated author tiering draft and collected feedback
- Defined preliminary full list and ordering
- Aiming to have a complete manuscript soon

FIXME: Full title of ENDF/B-VIII.1 paper

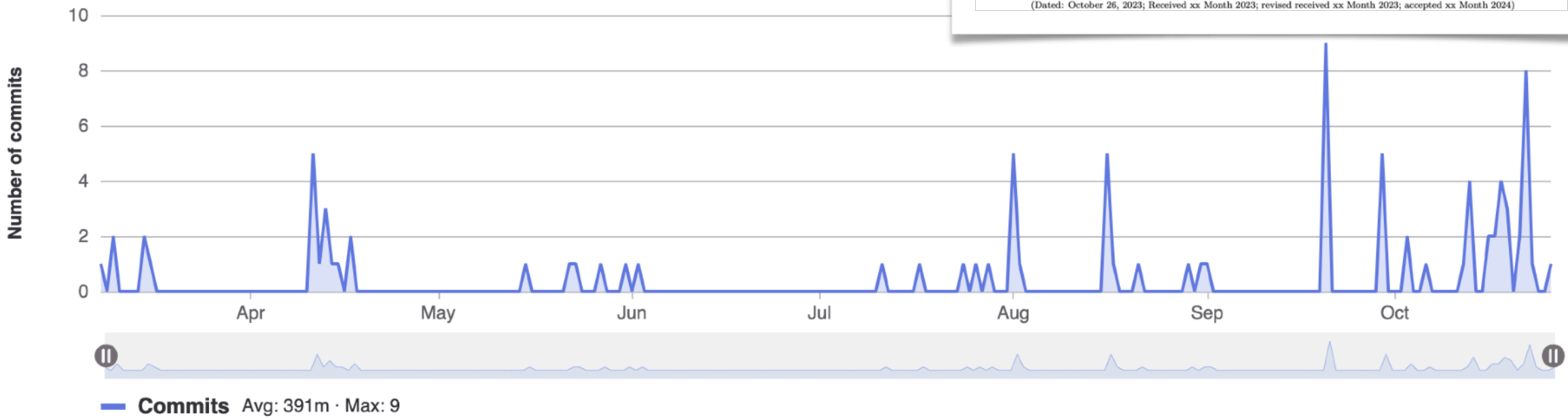
FIXME: WARNING: This is a preliminary, draft, author list. It is not complete, it is not in order![1] G.P.A. Nobre,[1,*] P.K. Romano,[2] M. Cornock,[3] T. Gaines,[3] D.A. Brown,[1] A. Mattera,[1] A.A. Sonzogni,[1] R. Arcilla,[1] B. Pritychenko,[1] A. Lauer-Coles,[1] R. Coles,[1] E.V. Chimanski,[1] G. Noguere,[4] D. Bernard,[4] D. Roubtsov,[5] J.I. MÃąrquez DamiÃąn,[6] G. Muhrer,[6] D.D. DiJulio,[6] R. Capote,[7] G. Schnabel,[7] P. Dimitriou,[7] D.E. Cullen,[7] A. Trkov,[8] J. Malec,[8] H.I. Kim,[9] V.G. Pronyaev,[10] D. Neudecker,[11] M.W. Paris,[11] M.B. Chadwick,[11] I. Stetcu,[11] M.W. Herman,[11] A.C. Kahler,[11] T. Kawano,[11] N.A. Kleedtke,[11] N.A. Gibson,[11] A.E. Lovell,[11] M.R. Mumpower,[11] G.M. Hale,[11] H.Y. Lee,[11] W. Haeck,[11] D.K. Parsons,[11] P.E. Koehler,[11] P. Talou,[11] K. Kelly,[11] M. White,[11] B. Beck,[12] C.M. Mattoon,[12] I.J. Thompson,[12] G. Gert,[12] R.J. Casperson,[12] C.M. Percher,[12] M.-A. Descalle,[12] S. Quaglioni,[12] G. Potel Aguilar,[12] J.J. Ressler,[12] A.C. Dreyfuss,[12] K. Kravvaris,[12] K.A. Wendt,[12] W.E. Ormand,[12] A.I. Hawari,[13] N.C. Fleming,[13] B.K. Laramee,[13] J.P.W. Crozier,[13] A.D. Carlson,[14] D.P. Barry,[15] M. Zerkle,[15] T.H. Trumbull,[15] J. Thompson,[15] J.L. Wormald,[15] A.M. Lewis,[15] J. Holmes,[15] M. Rapp,[15] A. Daskalakis,[15] J. Cotchen,[15] J.D. Haverkamp,[15] A. Ney,[15] M.T. Pigni,[16] L. Leal,[16,17] J.M. Brown,[16] D. Wiarda,[16] C.W. Chapman,[16] J.D. McDonnell,[16] K. Ramić,[16] W.J. Marshall,[16] R. Beyer,[18] A.R. Junghans,[18] M. Schulc,[19] M. Koštál,[19] Y. Danon,[20] P. Brain,[20] M. Dunn,[21] C. Wemple,[22] R. Ferrer,[22] O. Cabellos,[23] R.Q. Wright,[24] and FIXME: Ignacio Duran[25]

[1] *Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[2] *Argonne National Laboratory, Argonne, IL 60439-4842 USA*
[3] *AWE.plc Aldermaston, Reading, BERKSHIRE, RG7 4PR.*
[4] *CEA, DEN, DER, SPRC, Cadarache, 13108 Saint-Paul-lèz-Durance, France*
[5] *Canadian Nuclear Laboratories, Chalk River, Ontario, Canada*
[6] *European Spallation Source ERIC, Lund, Sweden*
[7] *International Atomic Energy Agency, Vienna-A-1400, PO Box 100, Austria*
[8] *Jožef Stefan Institute, Jamova 39, SI-1000, Ljubljana, Slovenia*
[9] *Korea Atomic Energy Research Institute, Daejeon, Republic of Korea*
[10] *International Atomic Energy Agency (consultant), Vienna-A-1400, PO Box 100, Austria*
[11] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[12] *Lawrence Livermore National Laboratory, Livermore, CA 94551-0808, USA*
[13] *North Carolina State University, Department of Nuclear Engineering, Raleigh, North Carolina 27695*
[14] *National Institute of Standards and Technology, Gaithersburg, MD 20899-8463, USA*
[15] *Naval Nuclear Laboratory, Schenectady, New York 12301-1072, USA*
[16] *Oak Ridge National Laboratory, Oak Ridge, TN 37831-6171, USA*
[17] *Institut de Radioprotection et de Sûreté Nucléaire, 92262 Fontenay aux Roses, Cedex, France*
[18] *Physikalisch-Technische Bundesanstalt, Department 6.4 - Ion and Neutron Radiation, Bundesallee 100, 38116 Braunschweig, Germany*
[19] *Research Centre Řež Ltd, Husinec-Řež, Czech Republic*
[20] *Rensselaer Polytechnic Institute, Troy, NY 12180, USA*
[21] *Spectra Tech, Inc., Oak Ridge, TN 37830, USA*
[22] *FIXME: Studvisk*
[23] *Universidad Politécnica de Madrid, José Gutiérrez Abascal, 2 28006, Madrid, Spain*
[24] *FIXME: Missing Affiliation 1*
[25] *FIXME: Missing Affiliation 2*

(Dated: October 26, 2023; Received xx Month 2023; revised received xx Month 2023; accepted xx Month 2024)

Commits to development

Excluding merge commits. Limited to 6,000 commits.



ENDF metrics for FY23

ENDF evaluation metrics

- This is **challenge**
- Not all evaluation contributions are created equal
- *All* linear combinations of **“size”** and **“impact”** of contribution are possible
- There is some degree of intrinsic arbitrariness
- Looked at all repository commits in FY23, separated by lab and “weighed” the contributions

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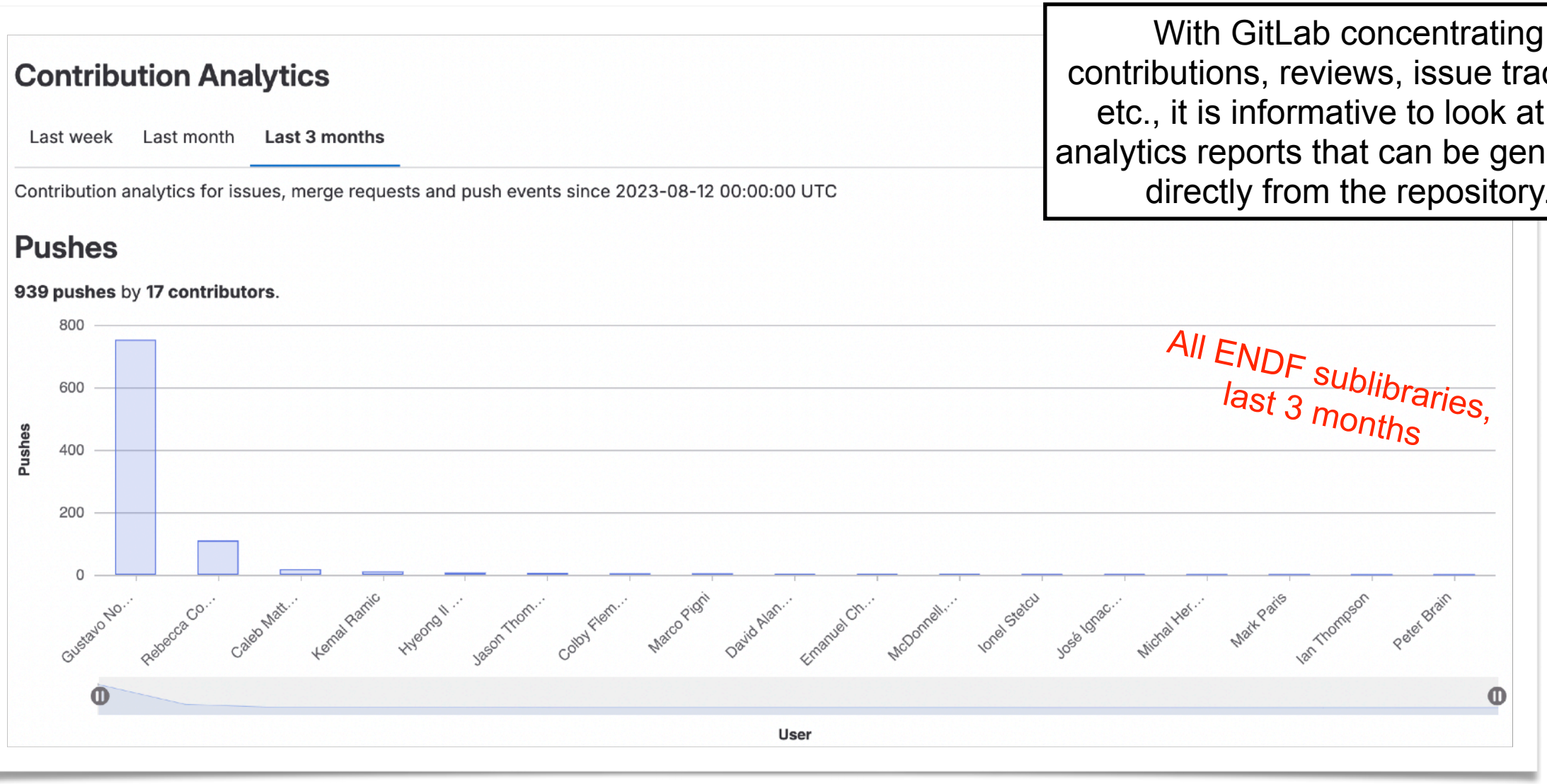
	“number of evaluations”
BNL	8.4
LLNL	14.5
LANL	2.8
ORNL	3.0

Some other metrics from GitLab

With GitLab concentrating contributions, reviews, issue tracking, etc., it is informative to look at the analytics reports that can be generated directly from the repository.



Same thing, but without Gustavo and Rebecca

Contribution Analytics

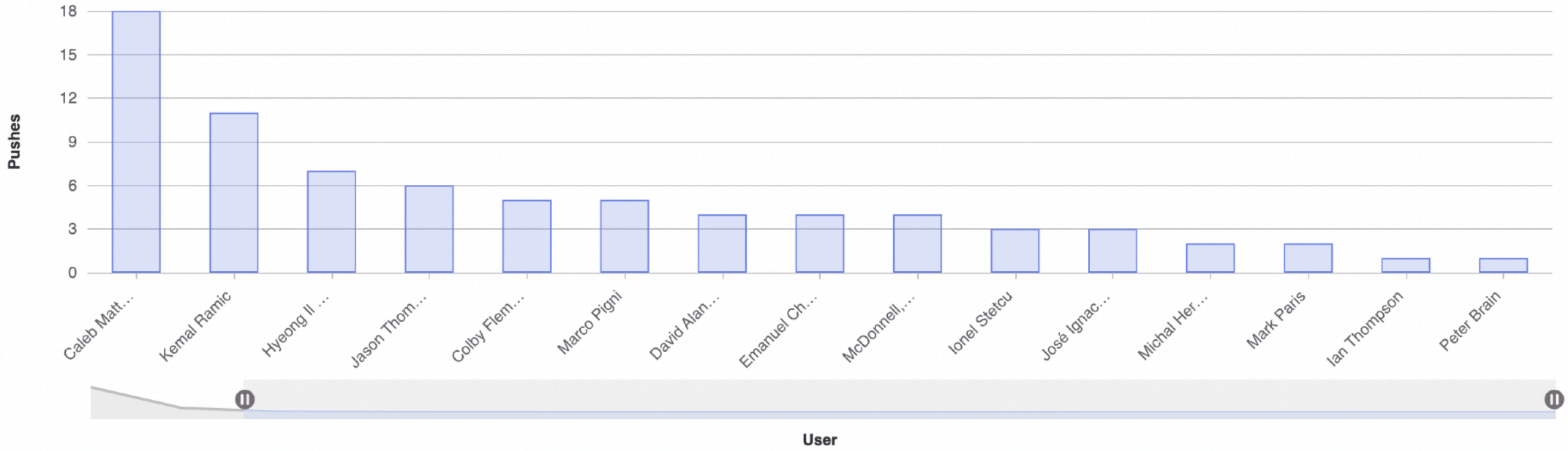
Last week | Last month | **Last 3 months**

Contribution analytics for issues, merge requests and push events since 2023-08-12 00:00:00 UTC

All ENDF sublibraries, last 3 months

Pushes

939 pushes by **17 contributors**.

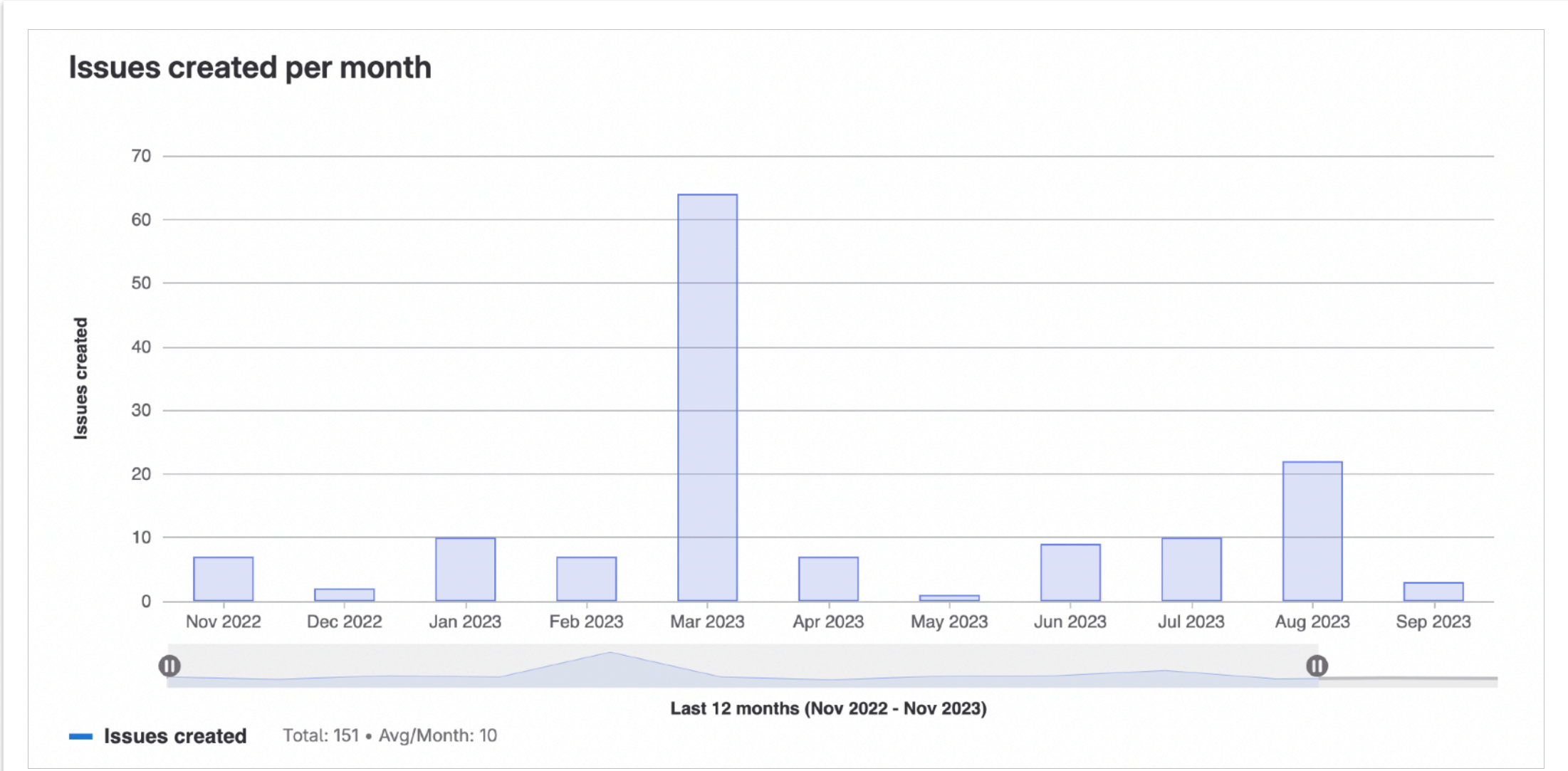


Contributions per group member

Name	Pushed	Opened issues	Closed issues	Opened MRs	Approved MRs	Merged MRs	Closed MRs	Total Contributions
Gustavo Nobre	753	8	2	161	119	119	1	1163
Rebecca Coles	110	0	0	2	0	1	0	113
Caleb Mattoon	18	4	3	0	0	0	0	25
Kemal Ramic	11	0	0	0	0	0	0	11
McDonnell, Jordan	4	0	2	0	0	2	0	8
David Alan Brown	4	2	0	0	0	1	0	7
Hyeong Il Kim	7	0	0	0	0	0	0	7
Jason Thompson	6	0	0	0	0	0	0	6
Marco Pigni	5	0	0	0	0	0	0	5
Colby Fleming	5	0	0	0	0	0	0	5
Emanuel Chimanski	4	0	0	0	0	0	0	4
José Ignacio Marquez Damian	3	0	0	0	0	0	0	3
Ionel Stetcu	3	0	0	0	0	0	0	3
Peter Brain	1	0	0	1	0	0	0	2
Mark Paris	2	0	0	0	0	0	0	2
Michal Herman	2	0	0	0	0	0	0	2
Andrej Trkov	0	0	1	0	0	0	0	1

Some more analytics from all sublibraries in the last 3 months…

Issues created in FY23, all sublibraries



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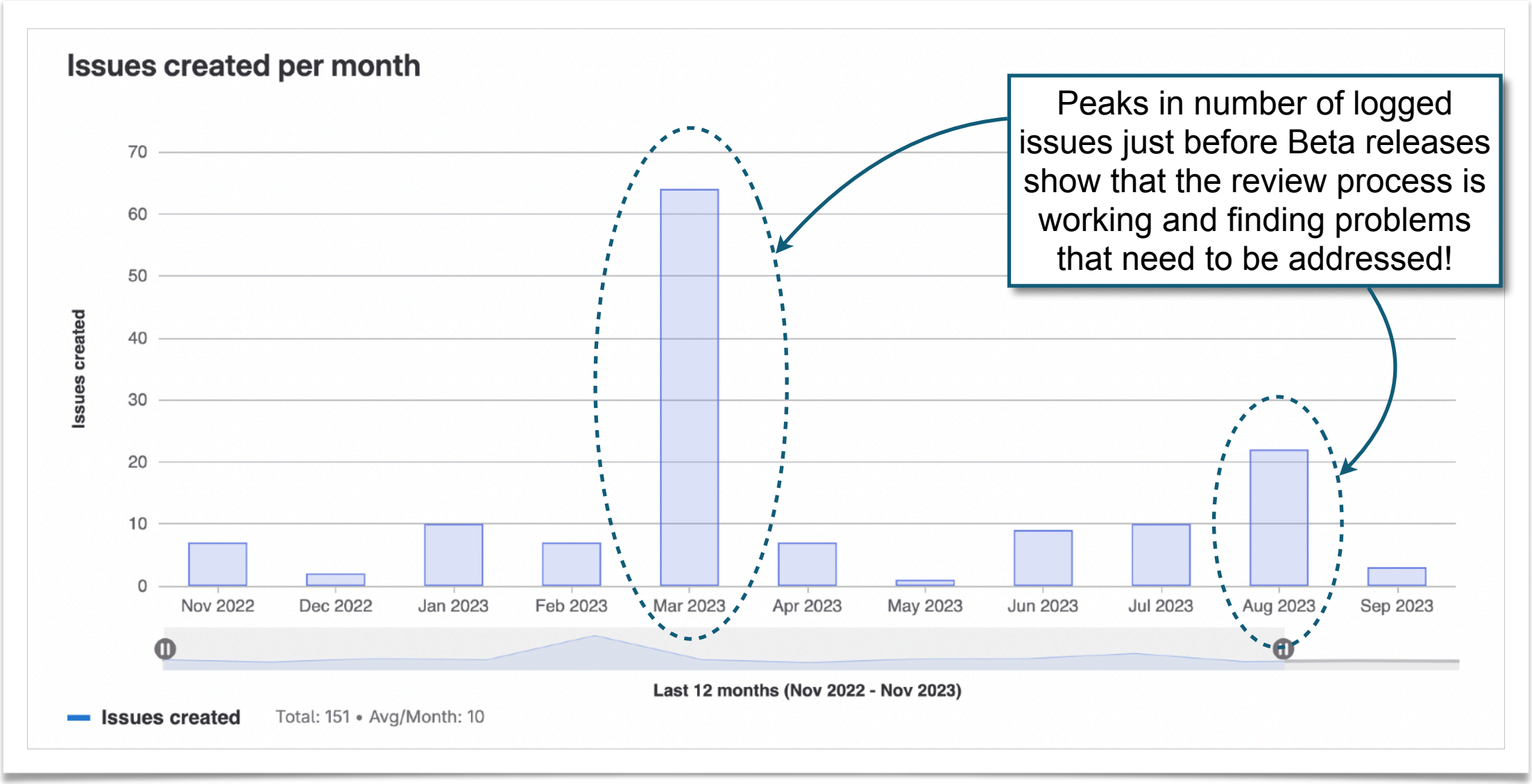

Neutrons: reviews completed

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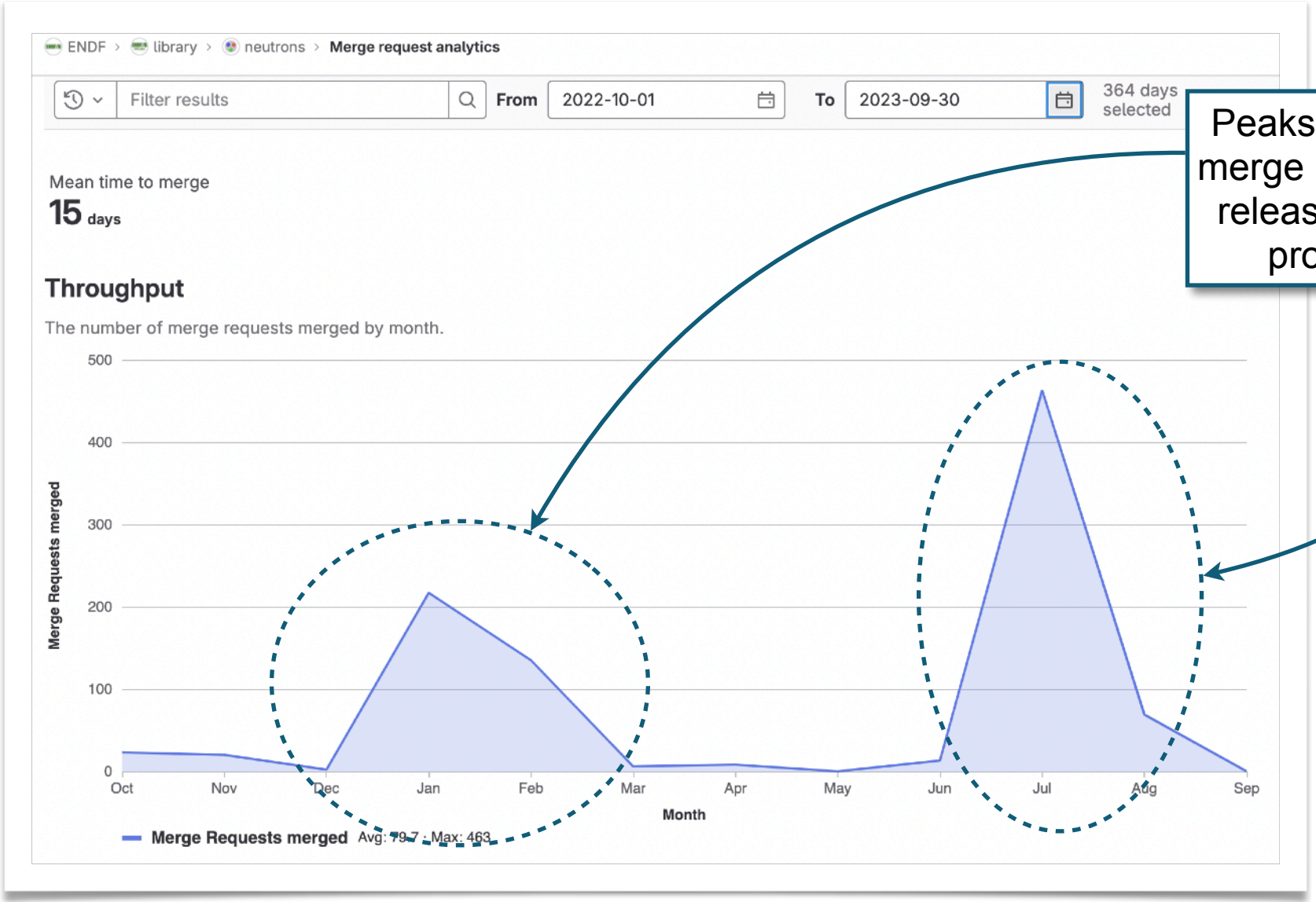
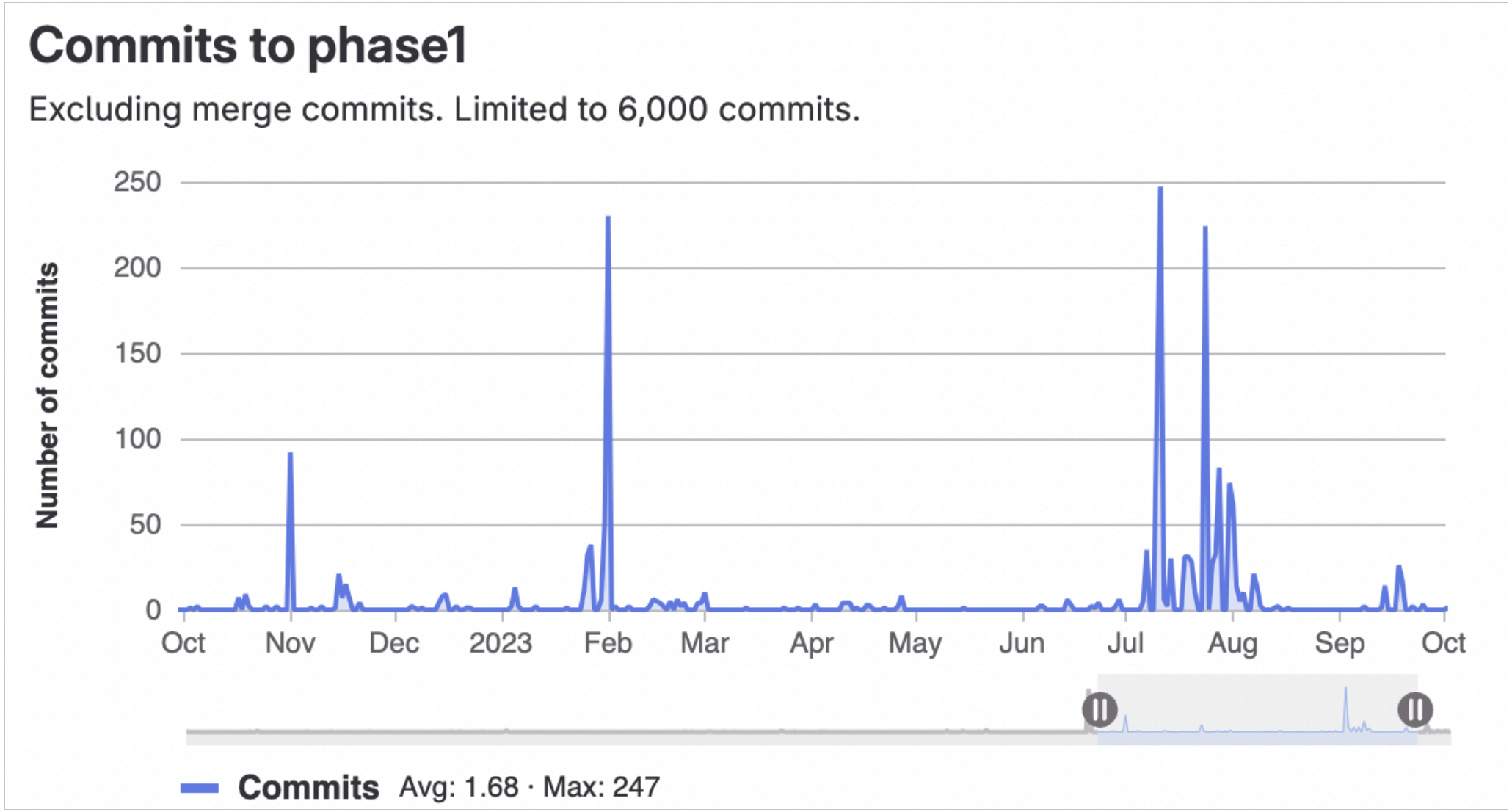


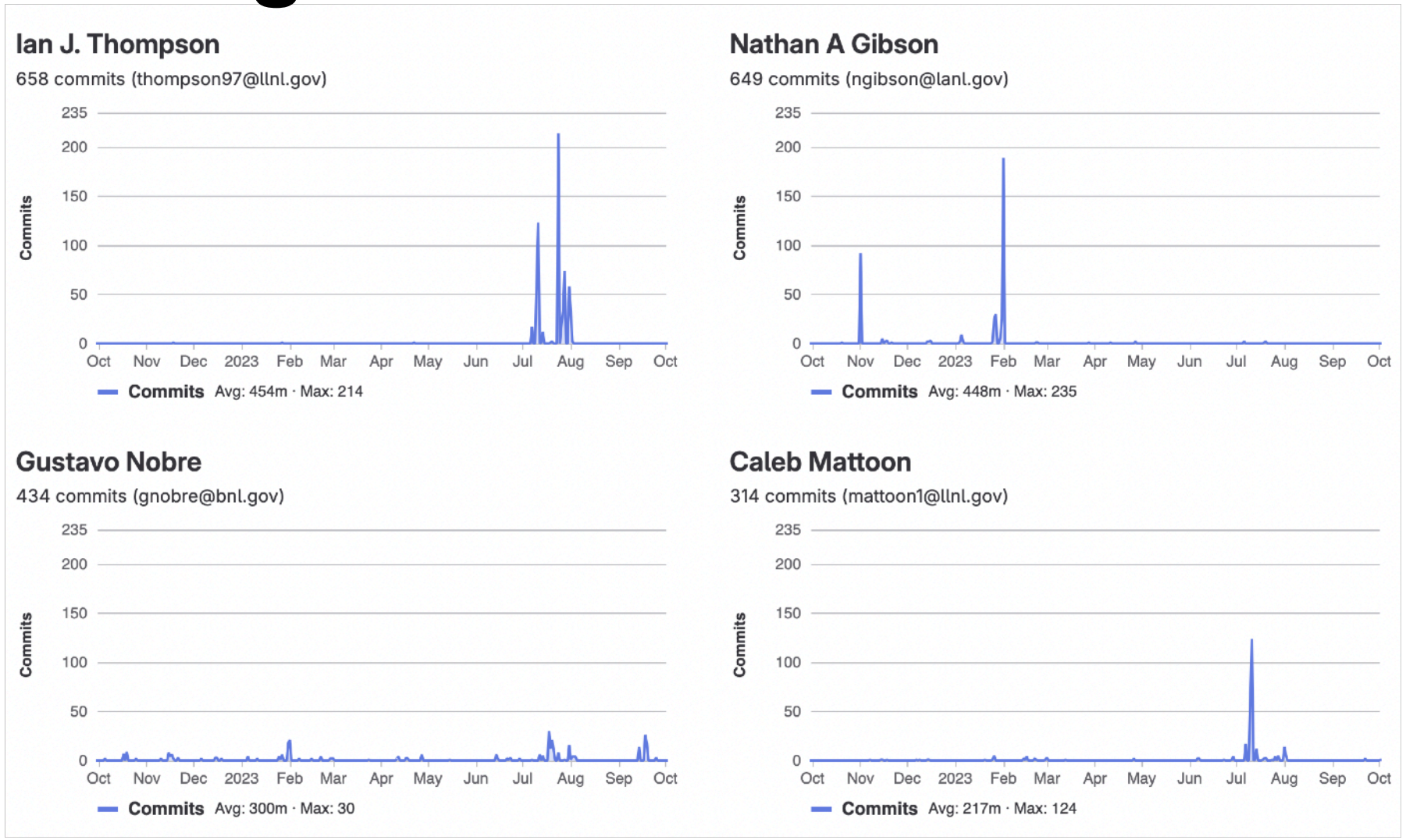
Peaks in number of completed merge requests just before Beta releases show that the review process is working well!

Larger peak shows that many more files were reviewed and incorporated into Beta2

Neutrons: commits contributed



Top committers in neutrons sublibrary during FY23



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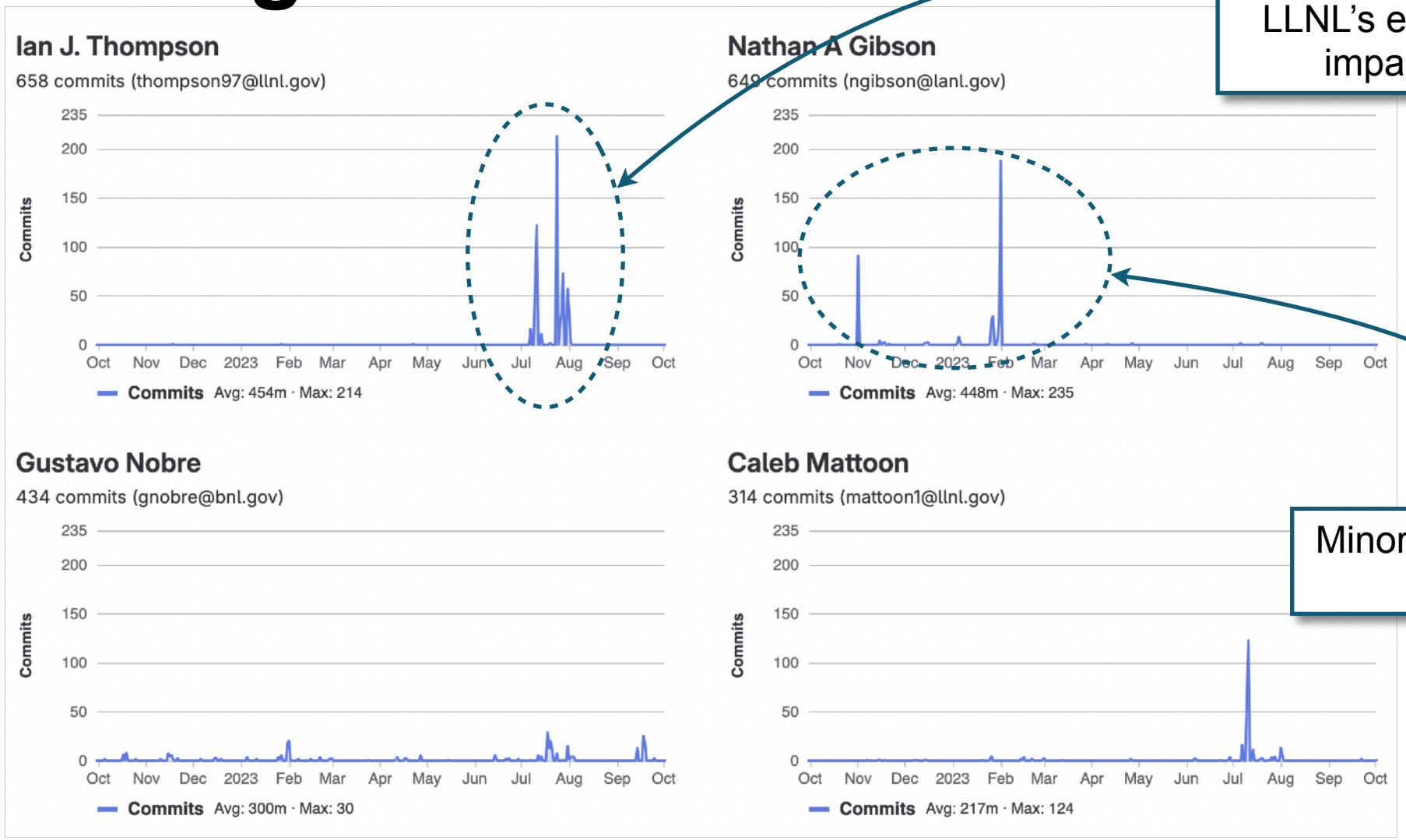
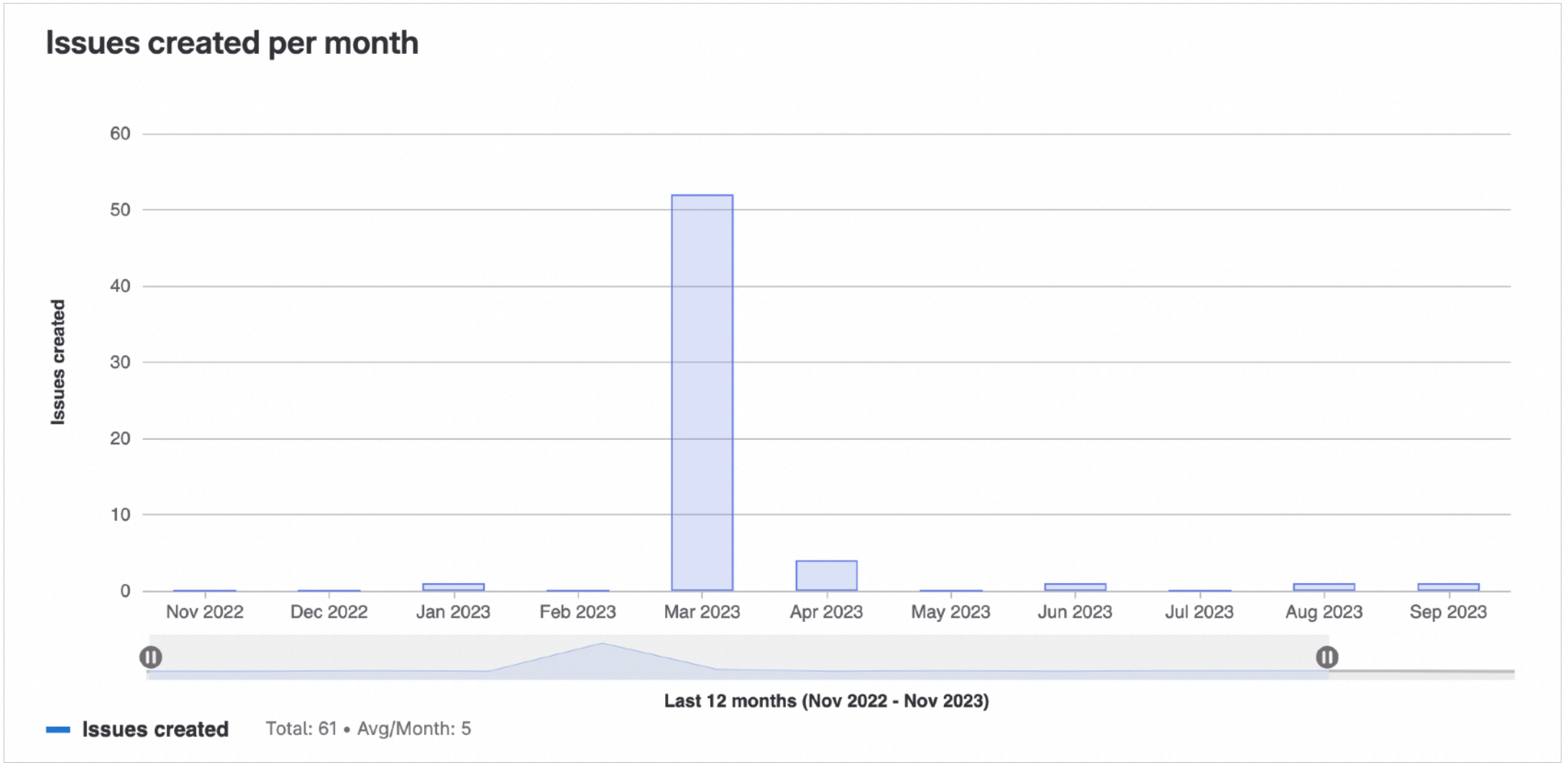


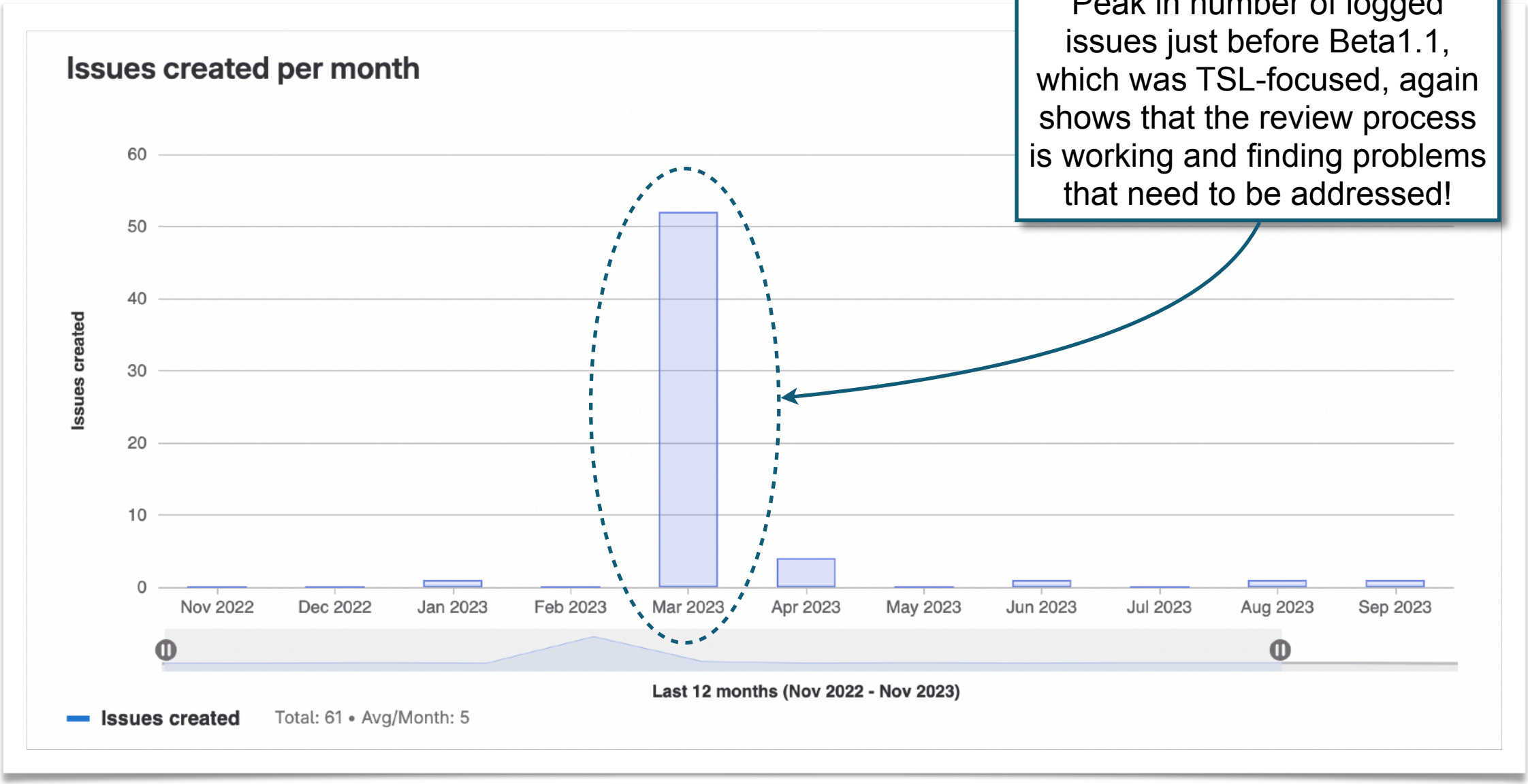
LLNL's exit distribution work impacting many files

Minor format correction across all files

TSL: issues created

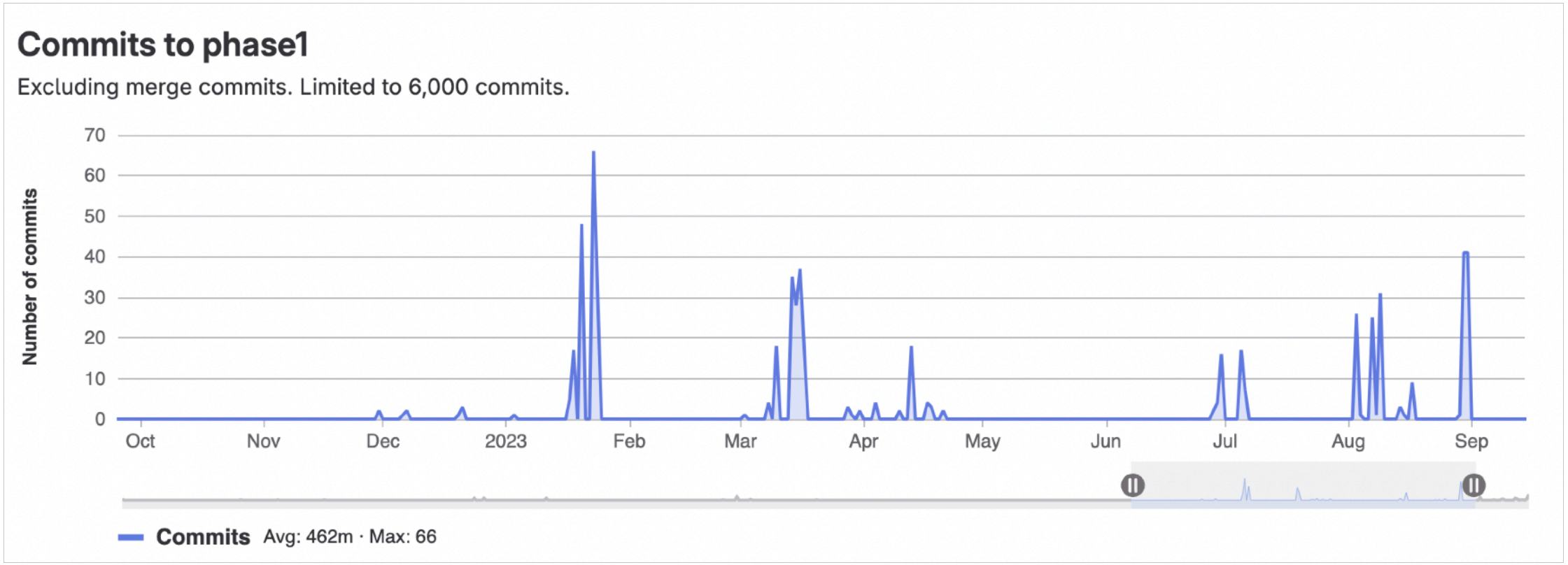


TSL: issues created

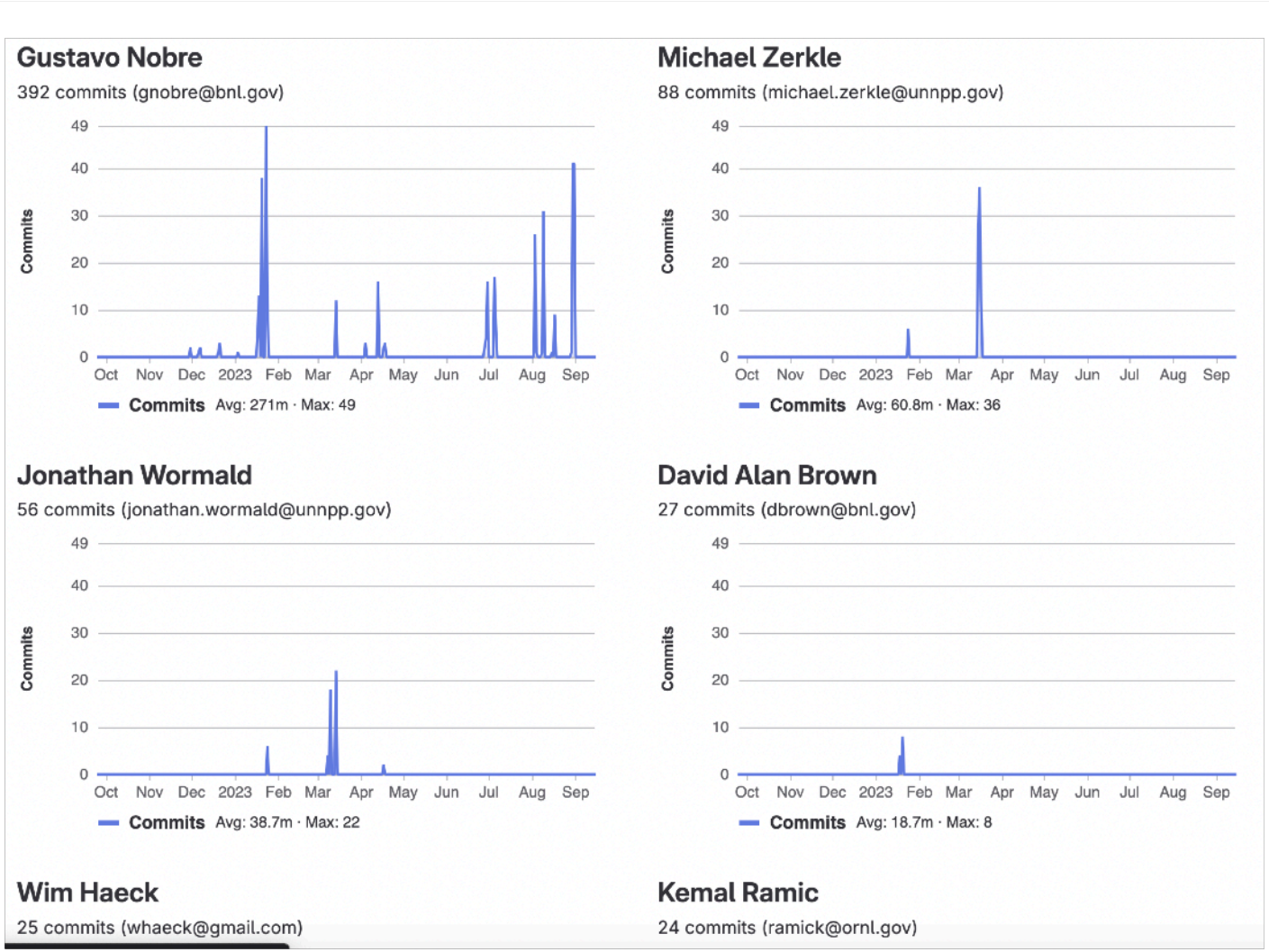


Peak in number of logged issues just before Beta1.1, which was TSL-focused, again shows that the review process is working and finding problems that need to be addressed!

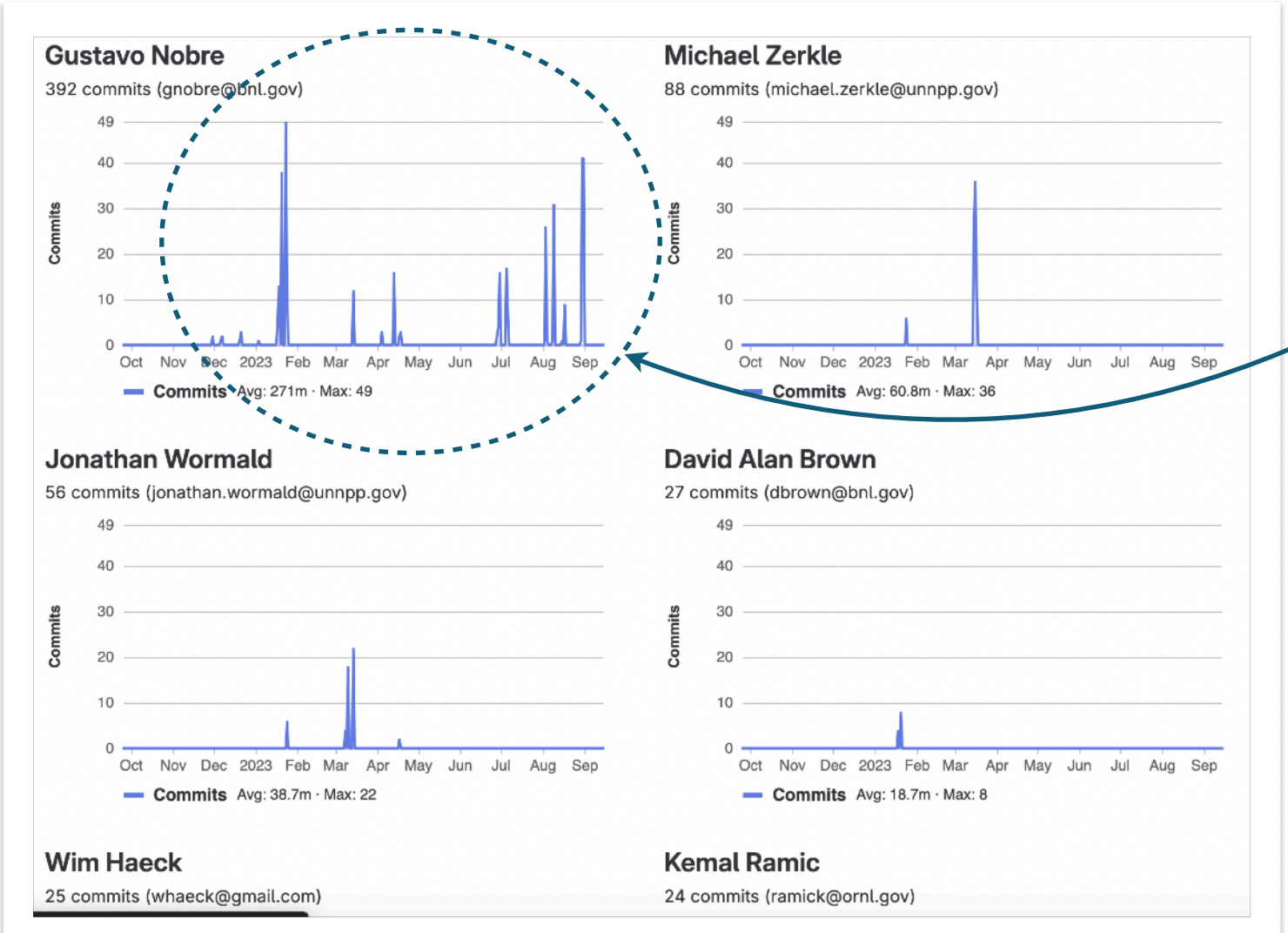
TSL: commits contributed



Top committers in TSL sublibrary during FY23 (phase1 branch)



Top committers in TSL sublibrary during FY23 (phase1 branch)



A large number of these are on behalf of NCSU

Conclusion

- Infrastructure development
  - Set up evaluation review process
  - Tracking issues
  - ADVANCE CI/CD system is live
- Process for the next ENDF/B release is moving along
  - Multiple Beta versions released
  - Most recent (Beta2) released in august, being broadly tested
  - Finishing the next one (Beta3)
    - Validation feedback from Beta1.1/ Beta2 is generally positive with specific improvement needs (that are already being addressed)
    - Expect to have addressed main issues now with Beta2, but still awaiting more validation feedback
    - Beta3 should be very close to final release
- Collaborative effort on evaluation, review and issue fixing have been very successful

Acknowledgements

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