

Cover image: twenty word clouds based on country-specific neutron vocabulary, projected on the flags of country-members of ENSA (described in the last paragraph of chapter 7).



1. Project Deliverable Information Sheet

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2. Document Control Sheet

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3. List of Abbreviations and Acronyms

AI	Artificial Intelligence
API	Application Program Interface
ENSA	European Neutron Scattering Association
ESFRI	European Strategy Forum on Research Infrastructures
ESS	European Spallation Source
LDA	Latent Dirichlet Allocation
NLP	Natural Language Processing
TU Delft	Technische Universiteit Delft

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5. Executive Summary

Here we report on “Future Needs” of scientists that use neutrons for their research. This ‘neutron community’ is represented by the European Neutron Scattering Association, ENSA, through 20 European national delegates in the association. As such, both the community and ENSA express the Future Needs in this report; a product of execution of Task 2.2 of the Brightness² Work Package 2.

We introduce a novel method to describe the community of neutron scientists, by applying Artificial Intelligence (AI) analysis on the published work of neutron scientists. This approach has delivered new insights to this community, to the European neutron facilities and the Brightness² consortium. The AI analysis also serves as the starting point to assess the needs of the European neutron science community for new neutron-based methods.

The neutron science community expressed their Future Needs for the ESS and the European infrastructure of neutron sources. Central to neutron science is the Experiment performed at the neutron facility, where the neutron scientists mostly request for improvement at the stages ‘before Experiment’ and ‘after Experiment’. These two Future Needs can be condensed into improvements concerning respectively Experiment Optimization, Access Modes, Neutron Facility Staffing, and Software & Analysis. Such improvements will most likely also attract more Industrial application of neutron science.

The use of Artificial Intelligence to analyse neutron science over many decades has proven very valuable to assess the many fields of science from fundamental physics to engineering applications.



6. Introduction

Task 2.2 of Brightness² is summarized as *Assessing the needs of the European science community for new neutron-based methods*. This scientific community is strongly affected by the current and future changes to the neutron landscape as described in the [ESRF report](#). The European Neutron Scattering Association (ENSA) represents this scientific community and leads the execution of Task 2.2 to assess the needs of its community.

The unique properties of neutrons and the professional developments at neutron science facilities have resulted in a very broad field of science that benefits from neutron scattering. Neutron science involves research in fundamental interactions in sub-atomic particles, in magnetism and solid state and soft matter physics and chemistry, as well as biology and engineering applications. By developing AI algorithms to search and categorize published **work since 1960**, we were able to visualize what neutron science is and how it develops over time, covering so many scientific communities that benefit from neutrons.

This rather broad group of scientists across Europe was approached via their national ENSA delegates through a web survey specific for each country. The web survey itself starts with a summary of the AI analysis of published work in that particular country, serving as a seeding point for assessing current scientific use of neutrons and future needs.

ENSA is leading this work package, but since it holds no (single) office in a country, the execution of the project is centred at the Technische Universiteit Delft (NL), the affiliation of the vice-chair of ENSA, Lambert van Eijck. Dr. Evgenii Velichko is data scientist employed by TU Delft on this Brightness² project. Together with the chair, Prof. Henrik Rønnow, they are in close collaboration with the Brightness² consortium members and its Steering Board. The communication with the European neutron scientists community is organized via the 20 ENSA delegates that interact with their respective national (European) scientific communities. Although the computing work related the AI analysis is performed at TU Delft, the national delegates in ENSA are strongly involved in the whole processes of WP2.2, with more than 10 ENSA meetings held to deliver this Report.

This Report builds on the Intermediate Report D2.3a which was submitted as a deliverable to Brightness² in August 2020. The Intermediate Report described the use of Artificial Intelligence and Natural Language Processing to describe the community of Neutron Science through their scientific output by analysis of the published work. This approach enables to ‘visualize’ the broad community of scientists ranging from biologists and engineers to researchers in material science, magnetism and fundamental physics on elementary particles and interactions. The analysis served as a starting point of the web-based country-specific survey sent to the community through their national delegates. The current report focusses on Future Needs for Neutron Science as expressed by the community and their national delegates in ENSA.



7. Artificial Intelligence analysis of published work

Considering the large number of publications on the research performed with the help of neutrons, the task of keeping up to date becomes increasingly challenging, even for experts in a particular field. Fast developments in Artificial Intelligence, on the other hand, facilitate multiple steps in the research process. Natural Language Processing - a branch of artificial intelligence that deals with the interaction between computers and humans - can allow scientists to delegate part of the routine tasks related to handling unstructured data, e.g. reading large volumes of research publications to extract valuable information for their research. In order to accomplish the task of defining and reporting the needs of European neutron scientists, we developed a two-step approach. At the first step, we analyse the published research performed with the help of neutrons. At this step our goal is to gain the insight into most common research topics benefiting from the application of neutrons. Correlations between the research topics and specific neutron techniques are established at this stage. The results of this analysis were used as an input in preparation of the survey which was sent out to the European neutron scientists at the second step of our approach.

In order to ascertain representability of the data used for the NLP analysis, we chose a Scopus database as one of the most inclusive collections of scientific publications¹ with a user-friendly API. For accessing the database we used a pybliometrics wrapper². Retrieval of metadata for all the publications from institutions related to neutron research has yielded about 1.3M results, among which about 50k contained the word “neutron” either in the title or in the abstract. A closer look at the meta-data of the “neutron” publications revealed a collection of entries related to e.g. neutron stars and particle physics, which are not relevant to our goal. In order to clean the metadata, all the publications containing terms 'tokamak', 'lhc', 'stellar', 'neutron star', 'gravitational', 'blanket' were filtered out. We anticipate that the fraction of relevant publications lost due to this filtering step is small. The thus filtered metadata set contained about 46k entries and was further utilized for a topic modelling by means of Natural Language Processing (NLP).

An unsupervised machine learning technique based on Latent Dirichlet Allocation³ was utilized to retrieve a typical set of topics frequently appearing in the “neutron” publications. Unsupervised machine learning is a powerful technique allowing humans to delegate large time-consuming classification tasks to computers without providing much preliminary information. However, there are some drawbacks with this technique. Firstly, the number of topics for classification needs be set beforehand. No matter what the number is, the algorithm will always satisfy this criterion, sometimes at a cost of quality of the result. Secondly, the classification criteria used by the learning algorithm are not always easy to identify *a posteriori* from the classification results. In case of topic modelling and text classification tasks, these drawbacks might lead to the algorithm merging some of

¹ A. Martín-Martín, E. Orduna-Malea, M. Thelwall, E. Delgado López-Cózar, Google Scholar, Web of Science, and Scopus: A systematic comparison of citations in 252 subject categories, J. Informetr. 12 (2018) 1160–1177. doi:10.1016/j.joi.2018.09.002.

² M.E. Rose, J.R. Kitchin, pybliometrics: Scriptable bibliometrics using a Python interface to Scopus, SoftwareX. 10 (2019) 100263. doi:10.1016/j.softx.2019.100263.

³ M.D. Hoffman, D.M. Blei, F. Bach, Online learning for Latent Dirichlet Allocation, Adv. Neural Inf. Process. Syst. 23 24th Annu. Conf. Neural Inf. Process. Syst. 2010, NIPS 2010. (2010) 1–9.

the under-represented non-related topics into one topic, due to a small number of requested topics, or, to split some of the over-represented topics into smaller bits due to a high number of requested topics. Therefore, it is common to perform the modelling with several numbers of topics and pick the most meaningful number based on an expert analysis of the result. In order to make the topic modelling results easily accessible to a wide group of neutron scientists, we created interactive topics visualisation tools using LDAvis method⁴.

The outcome of this analysis then served as a starting point of survey, by addressing the analysis at the national level of each of the ENSA member countries. Through the delegates, the per-country surveys were then sent to the communities as web-based surveys with statistical information about research performed with the help of neutrons in Europe as a whole, and in the individual European country. Each page of the web survey contained a word cloud representation of the most relevant terms for the publications from the target country, an interactive tool for description of the found topics and statistical country-related results of our analysis. The word clouds are made in colours and shapes of the country flags (see the title page for example). These pages served as a starting point to the survey of the European neutron scientist's needs. Moreover, the direct involvement of the national delegates in the interactions with their communities renders the request "more personalized" without breaching any GDPR rules.

8. Statistics and NLP analysis

In order to focus our research on the European neutron scientists, our dataset was divided into two categories: publications written with at least one European (co-)author (in the following text named "European publications") and publications written without any European (co-)authors (in the following text named "non-European publications"). For some basic statistics, we compare the two publications categories, while for further analysis we focus on the former one.

Statistical analysis of metadata shows a clear increasing trend in the number of neutron publications per year with most publications including at least one European (co-)author (Figure 1). It is worth mentioning that the first significant increase of the number of European publications above non-European ones appears around 1967. This could be related to the foundation of the Institut Laue-Langevin. However, there might be other direct and indirect causes for this phenomenon. Another important trend is an increase in the average number of (co-)authors per neutron publication (Figure 2). We interpret this trend as an indication of an increasing complexity of research performed with the help of neutrons, as the scientific field that benefits from neutrons broadens with time and increasingly multidisciplinary synergetic science emerges. Noticeably, the European publications tend to have more (co-)authors on average than non-European ones and this tendency seems to hold since around 2004.

⁴ C. Sievert, K. Shirley, LDAvis: A method for visualizing and interpreting topics, (2015) 63–70. doi:10.3115/v1/w14-3110.

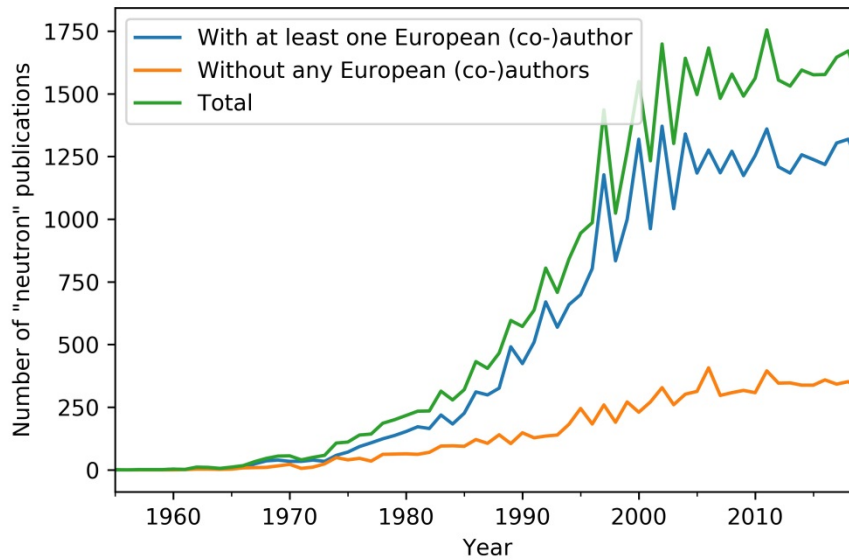


Figure 1: The increase in the number of "neutron" publications per year, as derived from the corpus of collected publications.

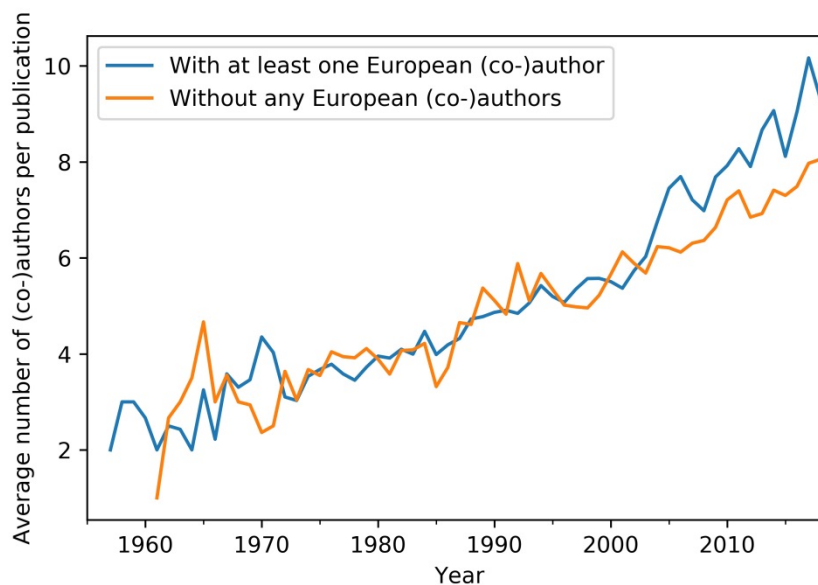


Figure 2: Increase in the number of authors per publication per year.

The entire dataset of "neutron" metadata was used for training our NLP topic modelling algorithm. The algorithm categorizes the corpus of publication into a pre-defined number of topics, where each topic is defined by the vocabulary of the publications and the assignment of a single publication is done using a probability distribution over the topics. Because of the multidimensionality of the vocabulary of the corpus, the visualization of the NLP outcome deserves some explanation.

8.1. Visualization tool for NLP analysis

Figure 3 is an explanation of the graphical representation of the 3-topics NLP analysis. The corpus of publications is converted to a multi-dimensional space where each publication is a single vector, with its vocabulary as vector components. The NLP analysis groups the publications (here into 3 topics) according to similarity in the vector components. To visualize the multi-dimensional space with only 2D graphics, the publications are projected onto a Principle Components diagram, indicated with **PC1** and **PC2**. Each of the topics is depicted as separate **circles** with the relative distance between the circles expressing how distinct the topics are, and the circle radius expressing the relative weight of the topic in the corpus. If one selects one of these circles (in the interactive version of these graphics accessible at footnote ⁵), the **30 most salient terms** appear on the right half of the graphics, describing the "content" of the topic. Human intelligence is needed to (e.g.) replace topic "3" in the NLP algorithm numbering with topic (or container) "instrumentation", after inspection of these **30 terms**. The collection of 30 terms depends on the choice of the **relevance metric**: set to 0 (zero), the 30 terms are shown which are unique to the chosen topic. By selecting non-zero values on the **relevance metric slide bar** the 30 terms will be shown that also appear with some fraction in other topics. The fraction itself can be read from the horizontal bar plot to the right of the term; it is the ratio "red / blue". By then selecting any single term, the left PC diagram will show how the selected term appears in all the different topics. The interactive web-version of these graphics are very helpful to grasp the idea behind the visualization.



Figure 3: Visualization in 2D of multi-dimensional clustering of the publication corpus into topics (here 3). The Principle Component (PC) axes of the 2D representation are underlined in purple, the **topic** size and 'distinctness' in the 2D plot (red dashed line circle), the group of NLP **terms** (green box), here related to topic 1, and the **Relevance Metric** slide bar in the orange box.

⁵ <https://ensa.tudelft.nl/topics/3topics.html>,
<https://ensa.tudelft.nl/topics/11topics.html>

<https://ensa.tudelft.nl/topics/7topics.html>,

8.2. Outcome of the NLP analysis

In order to examine the algorithm's topic resolving power, the modelling was performed with pre-defined numbers of topics: 3, 7 and 11. The resulting graphical representations of found topics by the algorithm are shown in Figure 4 (a, b, c) and the interactive web-version is accessible at footnote ⁶. As can be seen, when imposing the discrimination into three topics, the corpus of published work could be very well resolved into 3 well-separated 'islands', corresponding to what could be termed as containers: "1- hard matter", "2 - soft matter" and "3 - instrumentation", respectively. Increasing the number of topics to 7 also yields a well-resolved and meaningful set of topics, namely, "1 - magnetism", "2 - instrumentation", "3 - fundamental science", "4 - protein dynamics", "5 - surfaces and interfaces", "6 - soft matter", and "7 - biomembranes". Further increase in the number of topics to 11 leads to more ambiguity in topics definition, as can be seen in Figure 4 (c). As a result of this analysis, a model with 7 topics was chosen for further classification of the publications data set.

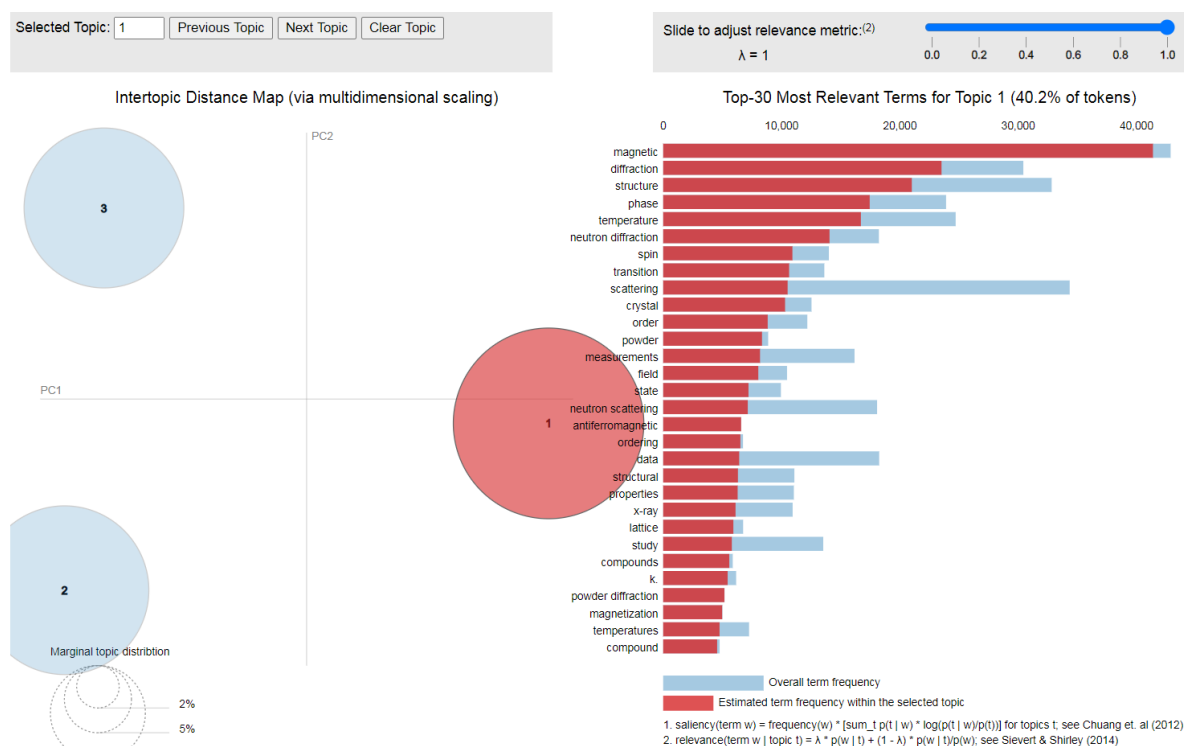


Figure 4(a): Graphical representation of topic models obtained with LDA machine learning algorithm with 3 topics

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<https://ensa.tudelft.nl/topics/3topics.html>,
<https://ensa.tudelft.nl/topics/11topics.html>

<https://ensa.tudelft.nl/topics/7topics.html>,

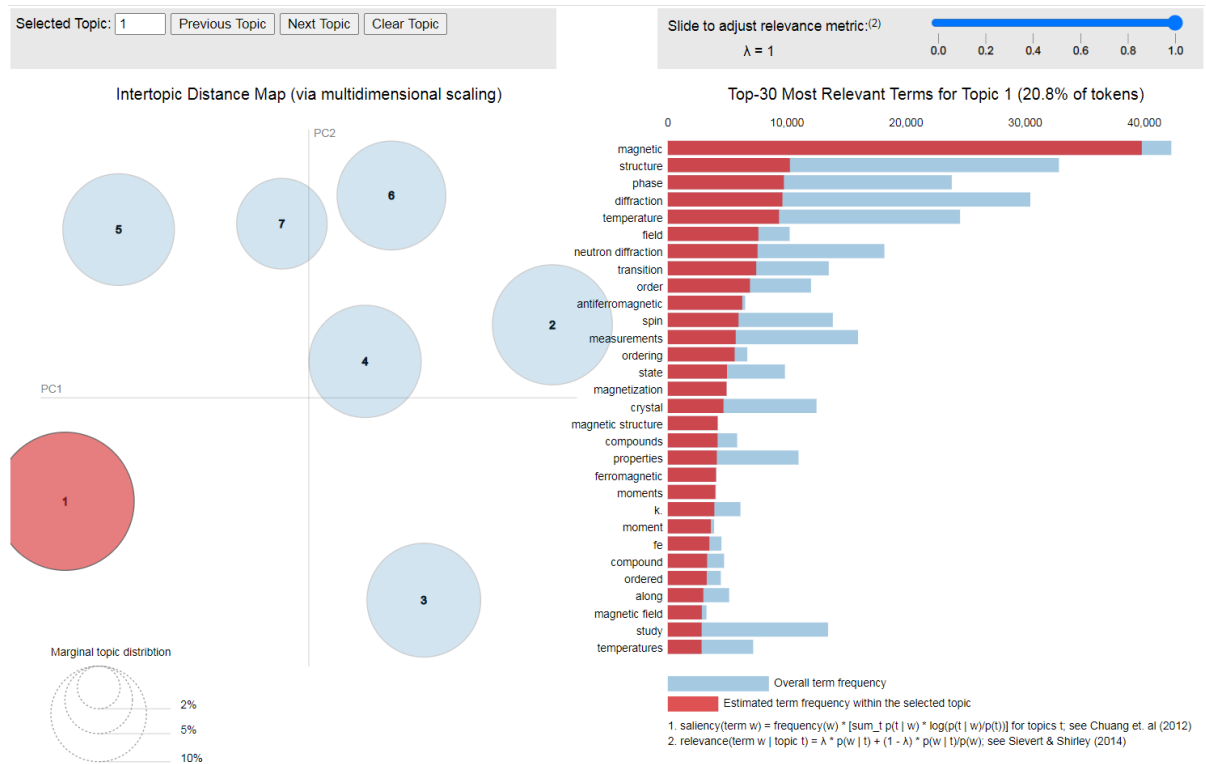


Figure 4 (b): Graphical representation of topic models obtained with LDA machine learning algorithm with 7 topics

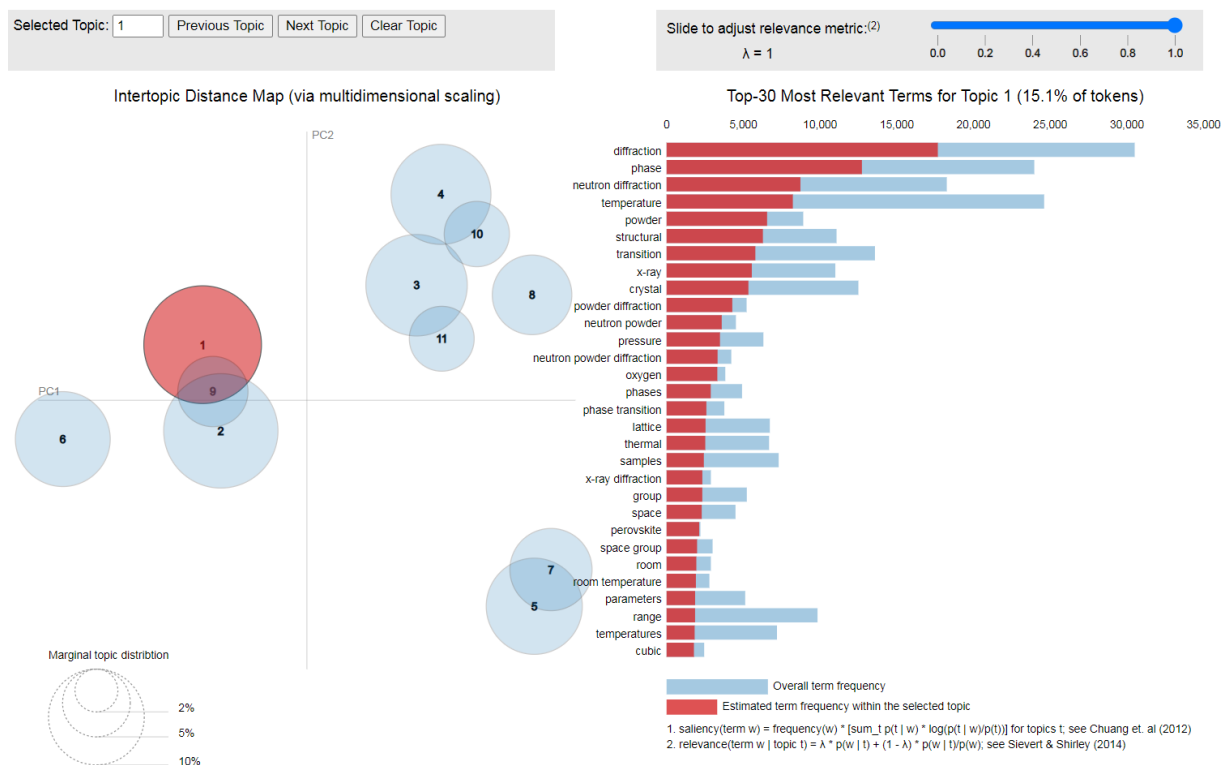


Figure 4 (c): Graphical representation of topic models obtained with LDA machine learning algorithm with 11 topics. Numbered bubbles on the left represent individual topics with the one highlighted in red being currently selected (see footnote 2 for interactive versions). The bar-chart on the right represents frequency of the most relevant terms (in blue – for entire corpus and in red – the term frequency in the selected topic). The slide in the upper right corner allows to adjust the relevance metric for a selection of terms to be shown (0.0: the terms specific for this particular topic, not appearing in the rest of the corpus, 1.0: the most frequent terms in the entire corpus).

By condensing each topic into one or two “container words” for naming purposes, the terms included in it allow us to indicate some specific materials, properties and phenomena, which are being investigated within the topic, as well as, experimental and modelling techniques used in such research. For example, topic “1 - magnetism” contains not only “magnetic structure”, “magnetic phase diagram” and “magnetic order”, but also “rare-earth elements”, “multiferroics”, “susceptibility measurements”, “magnetoresistance”, “Mössbauer spectroscopy”, “neutron diffraction”, and “inelastic neutron scattering”. Appendix 1 contains lists of the most topic-specific terms for each of the topics.

After naming the 7 topics using the ‘container words’, the next step is to categorize the whole corpus of published work by classification according to the chosen 7-topics model, yielding a percentage distribution of all entries between the topics. A pie chart, representing the topic distribution of European publications over the entire time-frame of our dataset (1956-2020) as well as a bar chart for steps of 5 years are shown in the Figure 5. The pie chart shows a nearly equal distribution over the topics with a slightly larger fraction of magnetism-related research and slightly smaller fraction of biomembranes-related research. From the bar chart, on the other hand, one can clearly see a decreasing role of the magnetism-related research over the past 15 years and a growing fraction of the instrumentation-related research since 1995. One could read from this bar chart that the science that is done with neutrons over the last 70 years has become less “fundamental” and more applied, with the increasing fractions of biology and material science related research.

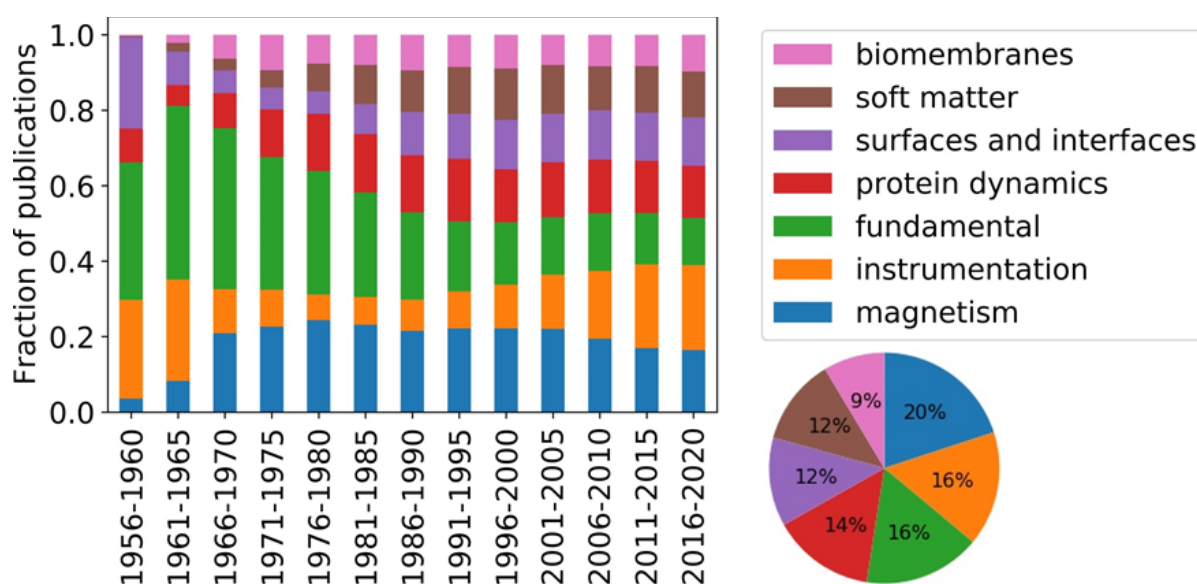


Figure 5: Topic distribution of the "neutron" publications with at least one European (co-)author. The pie chart corresponds to distribution of topics over the entire time span (1956-2020) of the dataset, while the bar diagram shows the evolution of topic distribution in steps of 5 years.

Individual expertise of each of the European countries could be estimated by selecting only the publications with at least one (co-)author from the country. Figure 6 shows pie charts for 20 European countries members of ENSA. From Figure 6, one can clearly see that different countries

have different topics prevailing among their publications. These differences most likely originate from the differences in established neutron science in these countries.

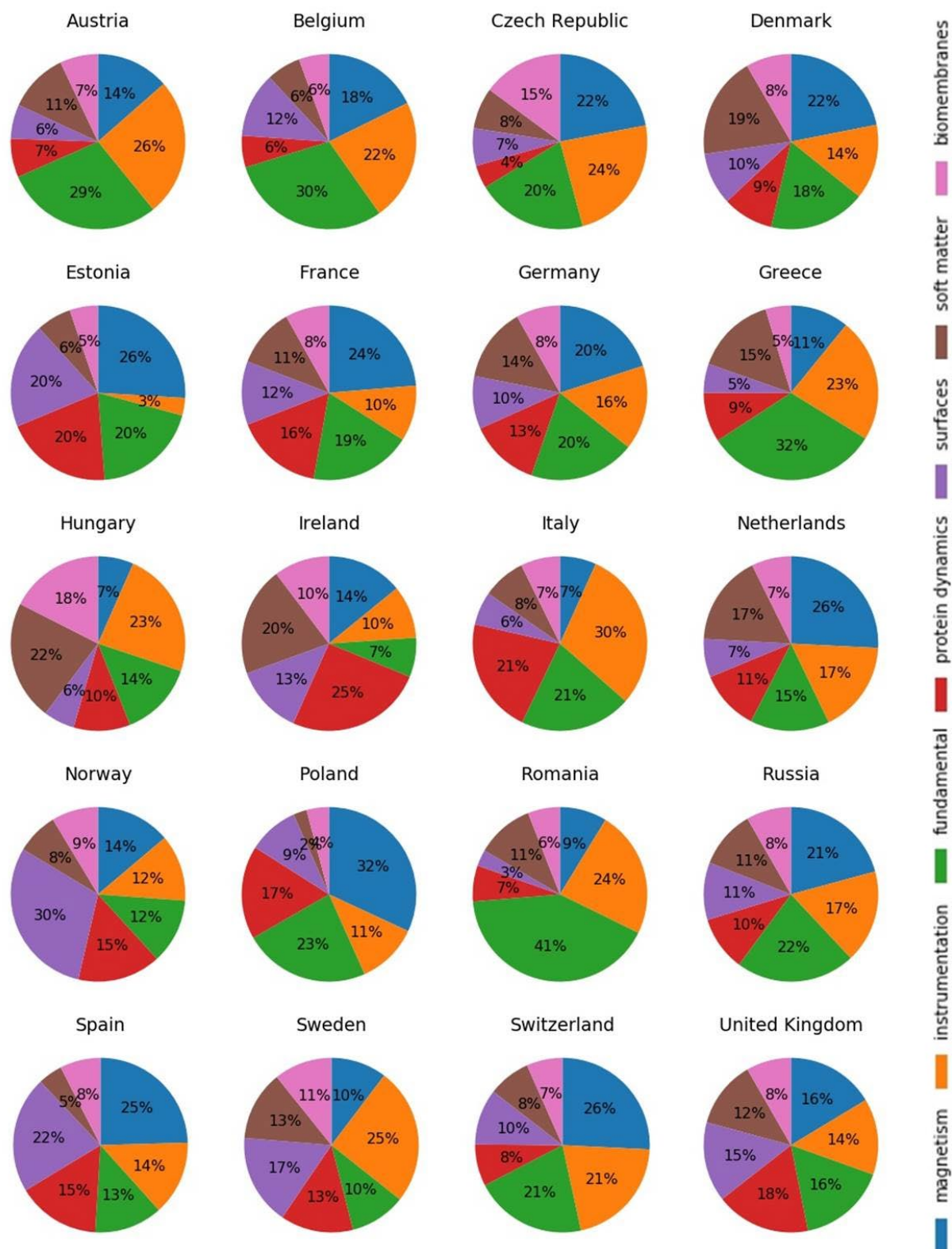


Figure 6: Pie charts of the distribution over 7 topics for the 20 European countries members of ENSA (topic Surfaces representing Surfaces and Interfaces).

Besides the above relative distribution of the topics, for each country, the analysis also allows us to project the topics onto the map of Europe. For this purpose, we identify, for each topic, the authors (at their affiliation) that have at least produced one publication. Figures 7-14 show where authors (at their affiliation) are located for each of these topics, in a "HeatMap" fashion. Inherently, these heat maps are strongly biased by population density (e.g. Netherlands has a particularly high density) and interpretation of the results require a certain level of zoom-in, which is only available in the online interactive versions of the HeatMaps⁷. Nevertheless, the *non-interactive* maps do demonstrate where the science is performed for each topic. The HeatMap shows the density of scientists (at their affiliation) and not the number of publications they produced in the topic.

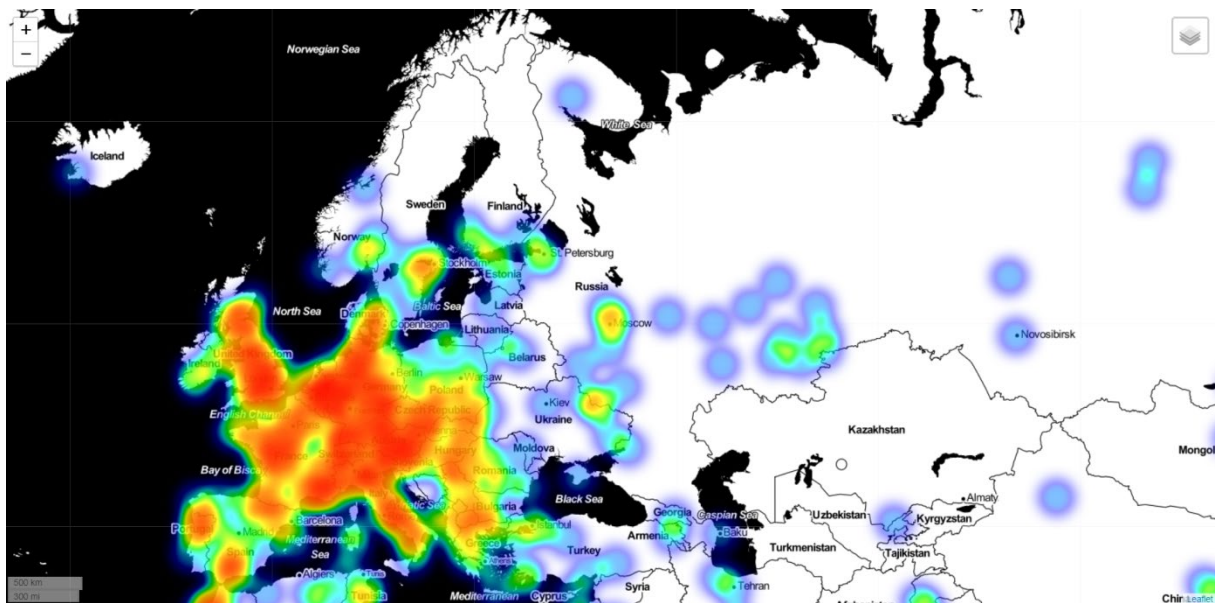


Figure 7: HeatMap for the NLP container "Magnetism". The color map expresses the density using 'rainbow' colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

⁷ https://ensa.tudelft.nl/map/neutron_all_topics_map.html

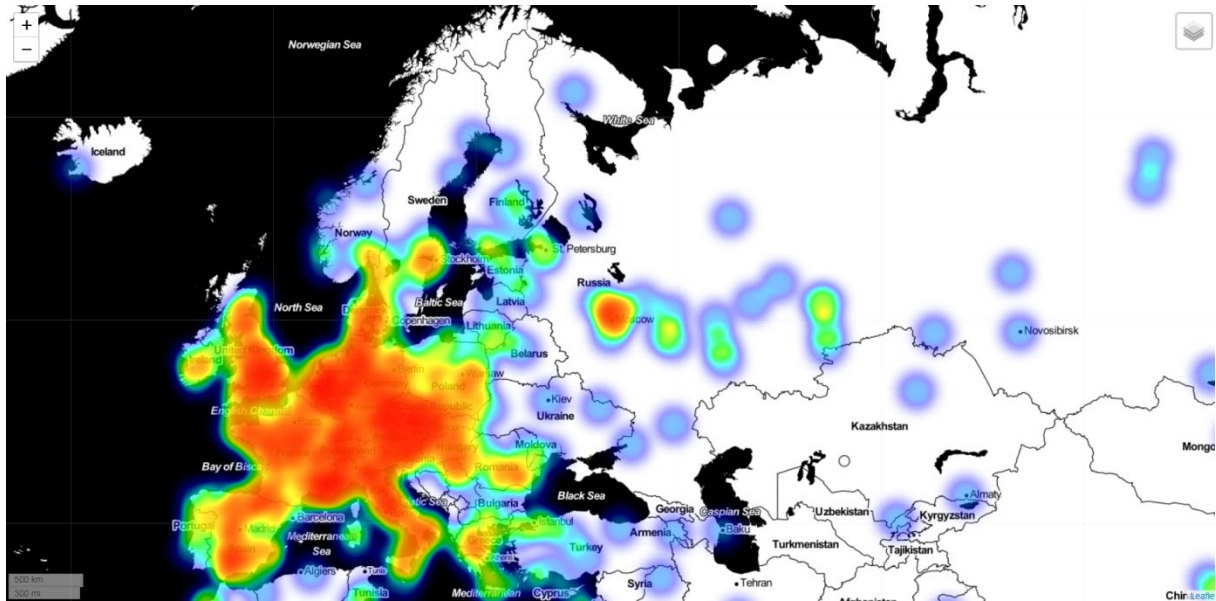


Figure 8: HeatMap for the NLP container “Instrumentation”. The color map expresses the density using ‘rainbow’ colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

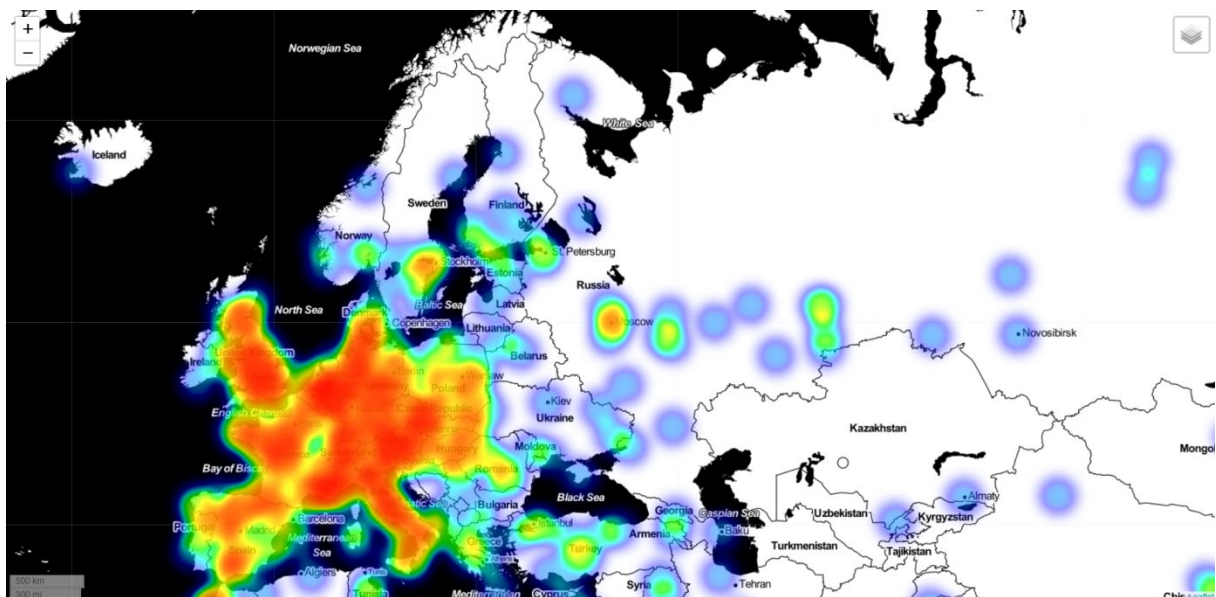


Figure 9: HeatMap for the NLP container “Fundamental science”. The color map expresses the density using ‘rainbow’ colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

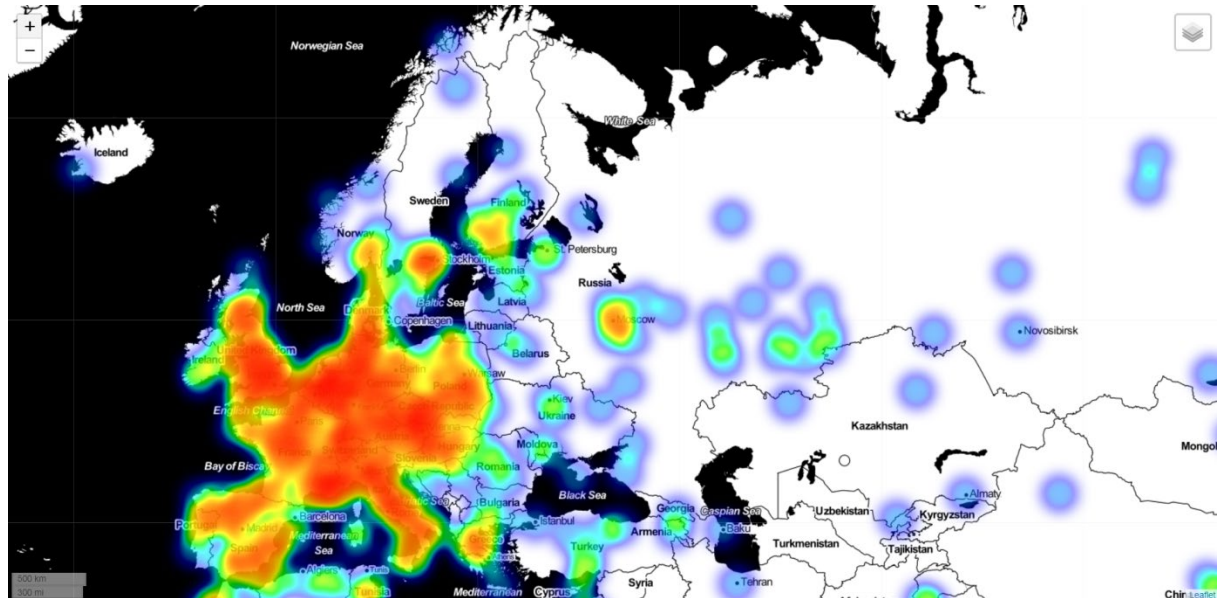


Figure 10: HeatMap for the NLP container "Protein dynamics". The color map expresses the density using 'rainbow' colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

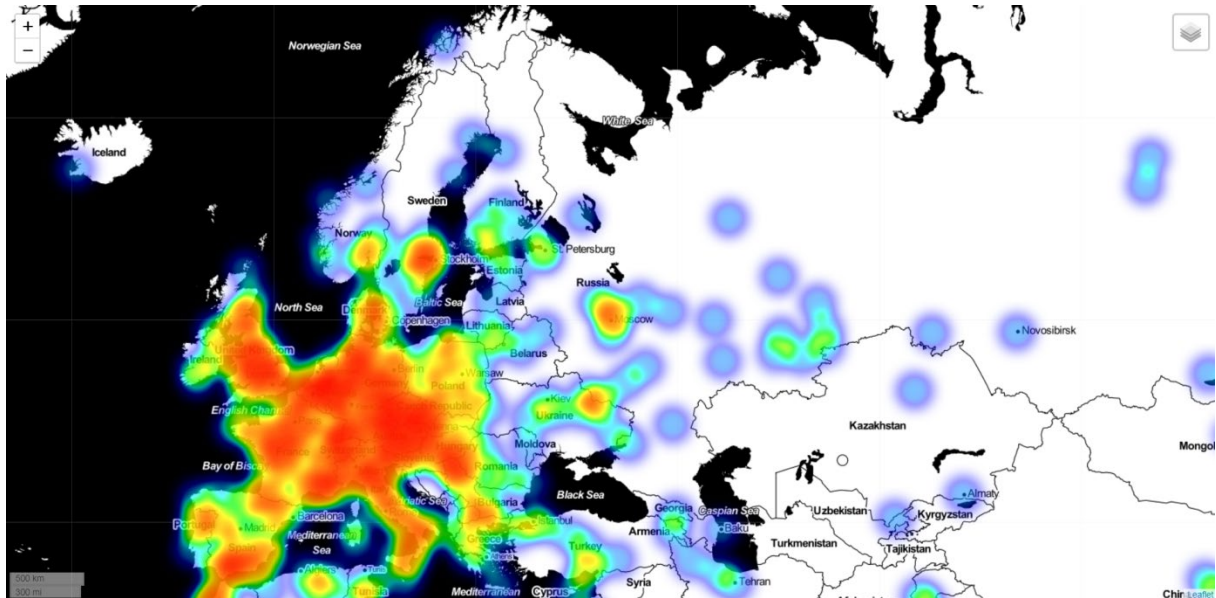


Figure 11: HeatMap for the NLP container "Surfaces and interfaces". The color map expresses the density using 'rainbow' colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

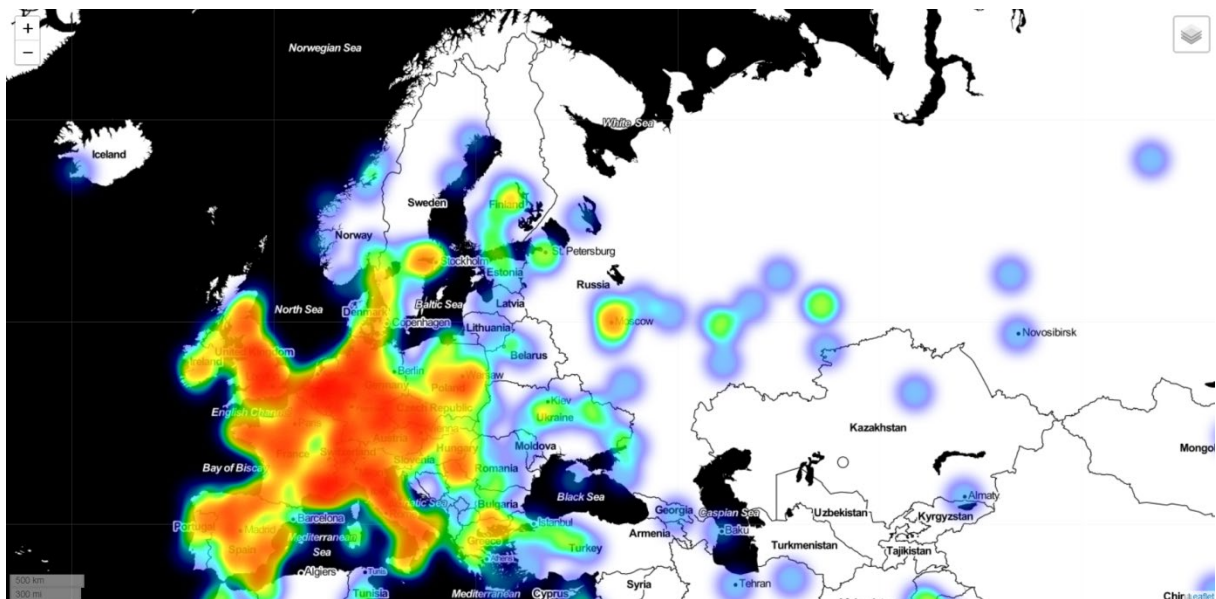


Figure 12: HeatMap for the NLP container "Soft matter". The color map expresses the density using 'rainbow' colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

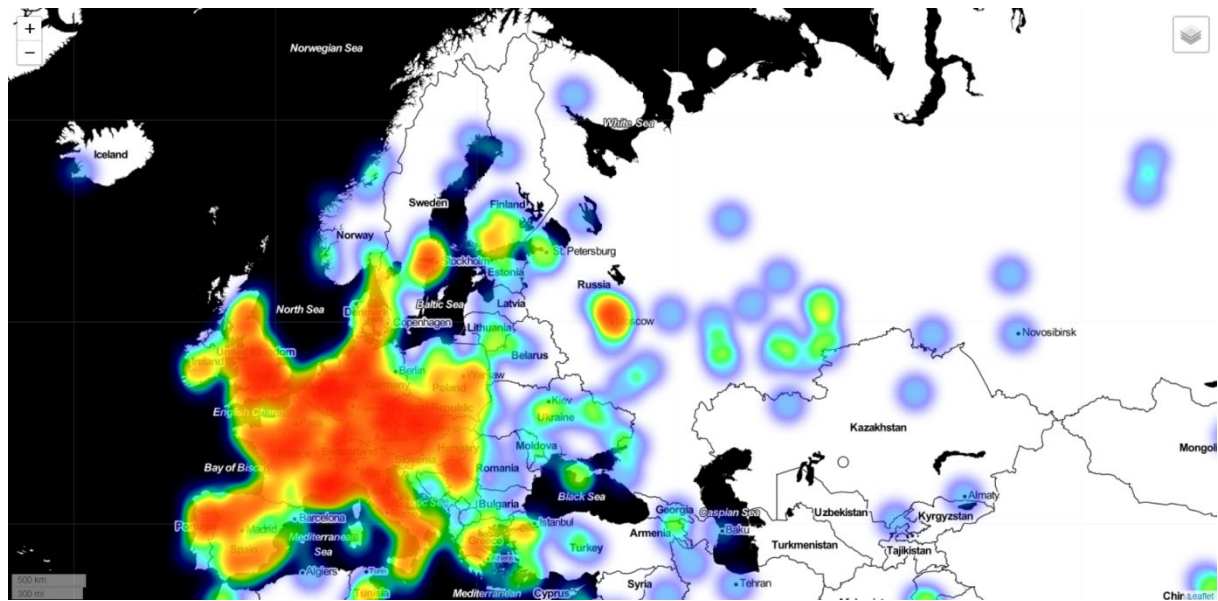


Figure 13: HeatMap for the NLP container "Biomembranes". The color map expresses the density using 'rainbow' colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

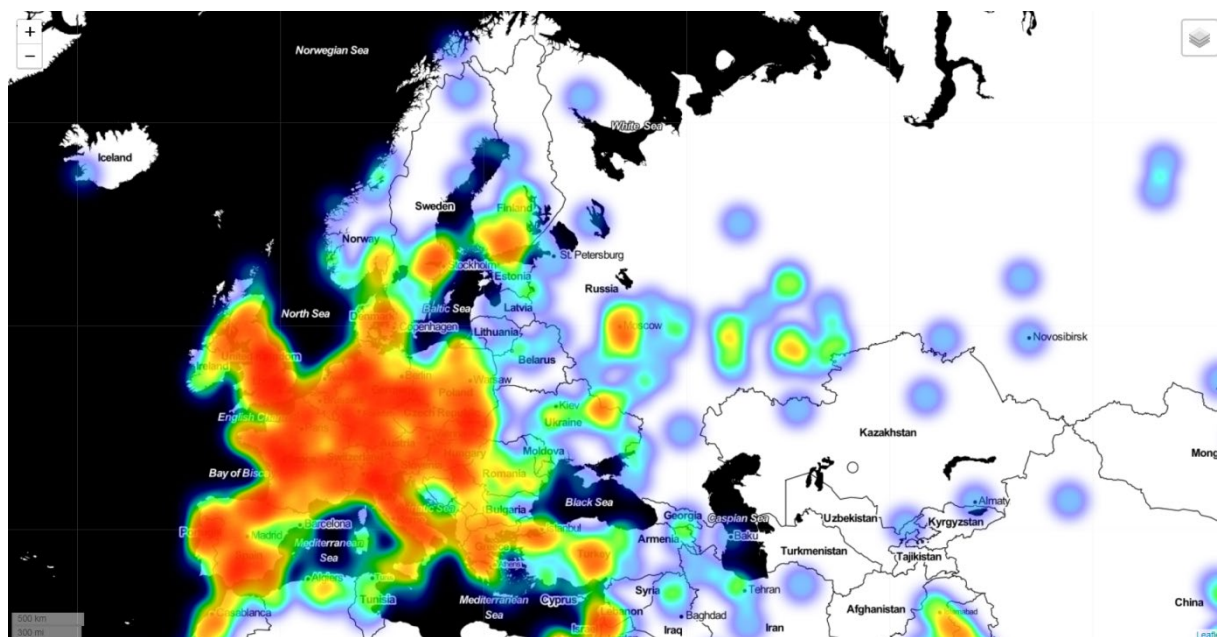


Figure 14: HeatMap of neutron scientists in Europe using the accumulation of all topics. The color map expresses the density using 'rainbow' colors, with purple/blue being low density and red being high density. The maps are not corrected for population density. See footnote 7 for an online interactive version, where a zoom-in will better allow to localize the communities across the continent.

What transpires from the HeatMaps, is that the neutron community is well spread, geographically, over Europe and that many nations or regions are well represented in each of the topics, although one can discern variations in the intensity of the HeatMaps regionally.

In reference to Figure 1, we also present in Figure 15 an impression of how the growth of neutron science is directly related to the growing community geographically, as “neutron science spreads over the continent”.

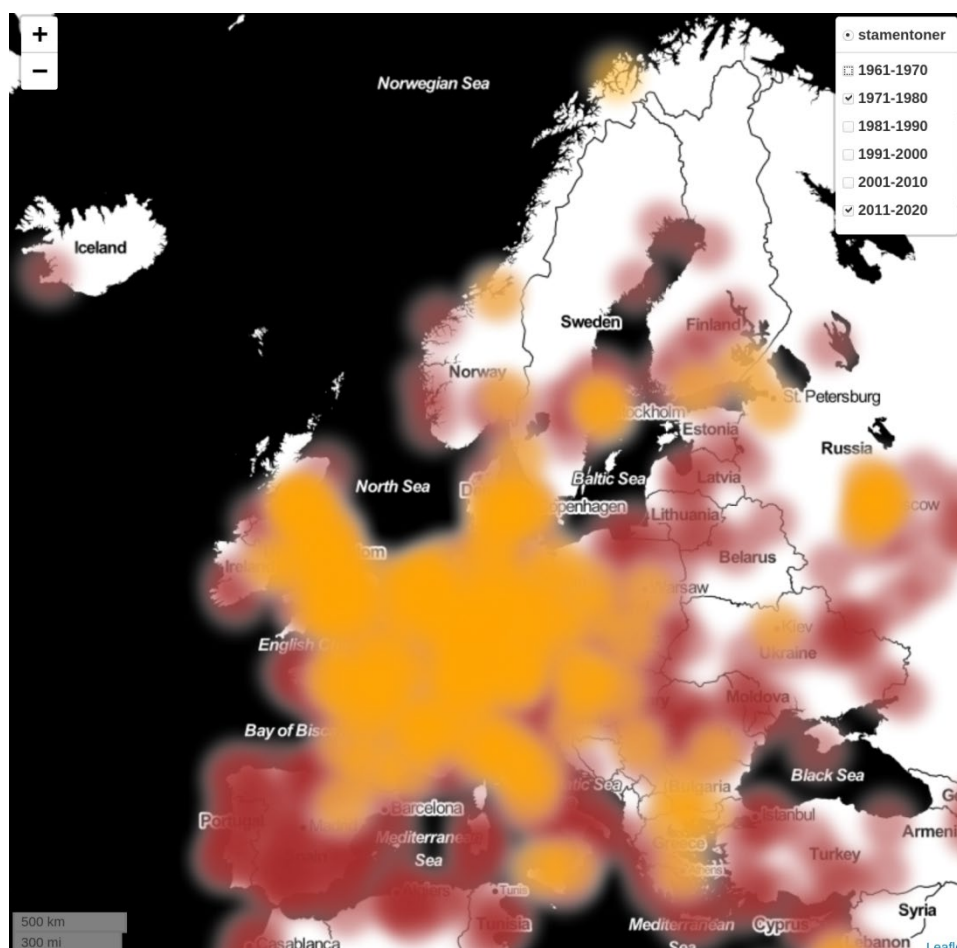


Figure 15: HeatMap of neutron scientists in Europe for the accumulation of all topics together, in the time span 2011-2020 (Bordeaux-red) and in the time span 1971-1980 (yellow/orange). The map is not corrected for population density. See footnote⁸ for an online interactive version.

The scientists at their affiliations as shown above, are involved in more than half of the publications available in the corpus. The accounting of their individual or even national contributions to these topics is not evident, because countries have different conventions of inclusion of scientists in the authors list for publications. Even within different field of science, such convention vary. The weight

⁸ <https://ensa.tudelft.nl/map/evolution.html>

of contributing to a publication can also depend on the position of the author in the author list. Therefore, we present in Figure 16 the distribution of publications over the countries of Europe by assigning each publication to a specific country if the publication contains one or more affiliation from that country.

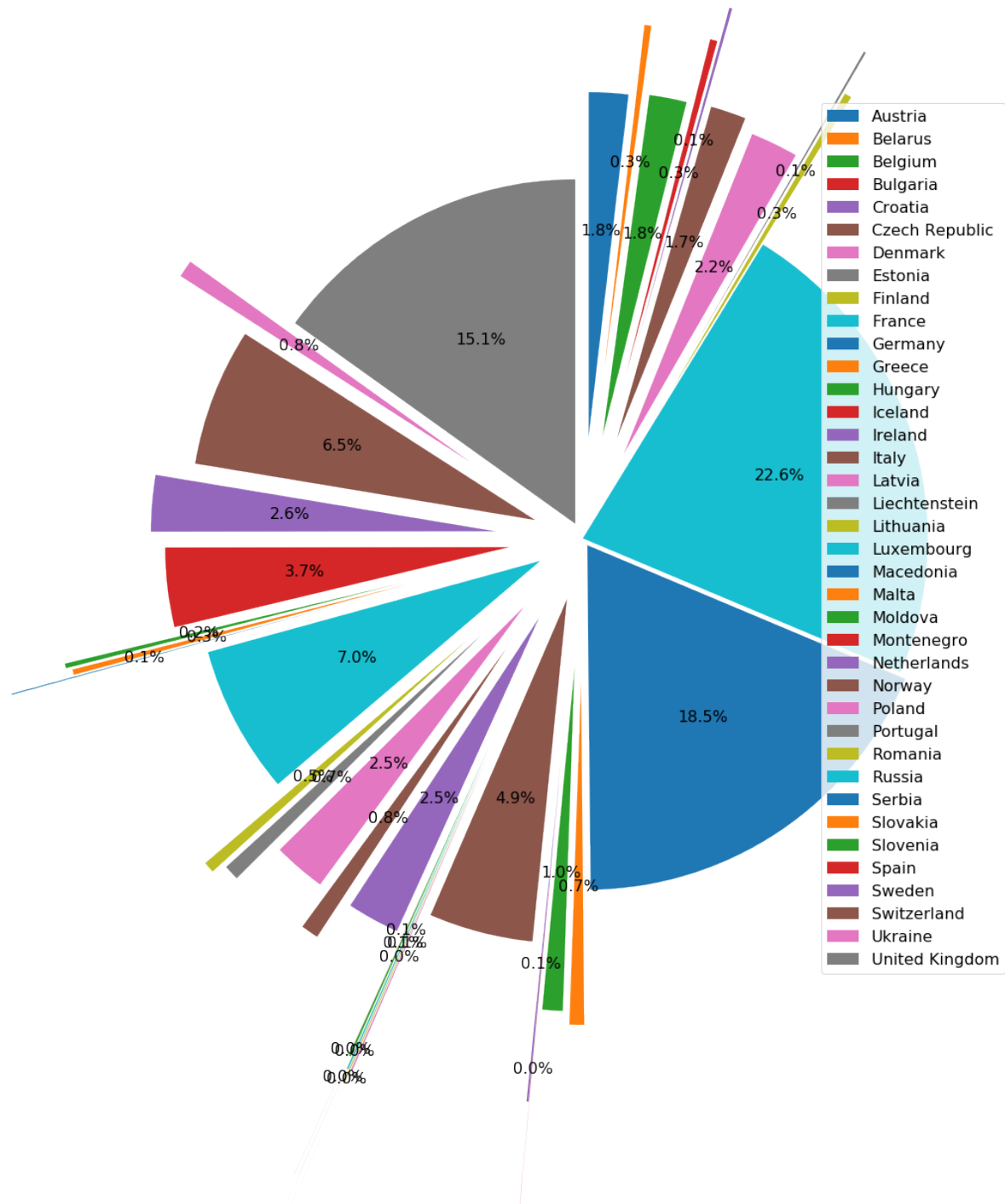


Figure 16: Pie chart of publication distribution over all European countries. In the legend the color coding starts with blue for Austria; in the pie chart, the pie fraction of Austria starts at the '12h position' of the circle and ends 'clockwise' (1.8%). The next country in the legend is Belarus and the pie fraction to the right of the Austria in the pie chart indicates the (linear) angular fraction of publications that Belarus was involved in, within the corpus of European publications. As such, reading the pie chart is done 'clockwise', while the legend is read downwards. With ENSA's 20 delegates, it represents 96.6% of all published science in Europe.

9. Future Needs of the neutron science community

The above NLP analysis of published ‘neutron science’ served as the starting point of the survey. The community uses neutrons among other techniques in their daily science and one can assume a typical respondent to our survey will not have a complete overview of neutron science in her/his country. As such, we hope our analysis will intrigue the respondent and we start the survey asking the respondent their opinion on our analysis, before proceeding to their experience and Future Needs.

The survey was designed as a country-specific and password-protected on-line web form. This allowed the national ENSA delegates to address their communities.

9.1. Survey among neutron scientists

The below paragraphs 9.1.1 until 9.1.4 summarize the questions in the on-line survey. The country-specific graphics are therefore not depicted in this report and the generic questions “Can you elaborate on”, giving the respondent the possibility to express their opinion and comment or questions, are skipped in the below 4 paragraphs.

The lists below can consist of either ‘single choice’ items (depicted as radio button / circles) or ‘several answers possible’ (items depicted as squares). When presenting the survey responses in the following paragraphs using bar charts, we use the term “number of selections” to describe how many respondents selected a certain option. For ‘single choice/radio button’ items the selection of one item rules out the other items, while for ‘several answers possible/squares’ the respondent could select multiple items.

Several questions were conditional, such as “How many PhD students did you introduce to neutron science”. This question was not asked when the respondent is PhD student her/himself. As well, for the ‘several answers possible’ lists, selection of one of the items, typically induces a “Can you elaborate on” question. Such follow-up questions are *not shown below*.

9.1.1. Do you recognize yourself in the following country specific NLP analysis?

(referring to NLP graphics) To make it easier to discuss these topics, we gave them some short labels (“magnetism”, “instrumentation”, “fundamental science”, “protein dynamics”, “surfaces and interfaces”, “soft matter”, and “biomembranes”).

Sticking to these 7 topics found by AI, do you agree with the label names?

- The labels should be changed
- The labels are fine

Based on the modelled topics and publications data from Scopus database, we classified all the publications authored or co-authored by scientists from your country in the last 20 years. In the figure below you can see the distributions of the topics among the publications. A pie chart on the left represents a percentage distribution of all the publications. A bar chart on the right shows a yearly evolution of the number of publications within each of the topics.



Does the development trend in the topics for your country fit to your expectations?

- ☐ No
- ☐ Yes

Based on our analysis we were able to classify all of the neutron scientists from your country we found according to their respective topics and placed them all on the [country map as a HeatMap](#). In the upper right corner of the map, you can choose topics of interest.

Does this Heat Map fit to your expectations, or would you expect a different distribution of neutron scientists in your country?

- ☐ It fits my expectations
- ☐ I expected it to be different

Your opinion and any comments on our neutron publications analysis

(Criticism on the approach, interpretation, etc. Things you want to off your chest before addressing the survey.)

9.1.2. Your experience with neutrons until now

ENSA and Brightness2 would like to get better understanding of the scientist forming the European neutron scattering community.

Please indicate your level of expertise as a "neutron scientist"

(-----scale bar 1-10-----)

Selected Value: 5

(1 = novice, 10 = expert. Expertise can be experimental, interpretation, modelling, instrument design, etc.)

At which stage are you in your scientific career?

- ☐ Student
- ☐ PhD candidate
- ☐ Postdoc
- ☐ Permanent staff member
- ☐ Professor/group leader
- ☐ Other

Which percentage of your research activity is neutron-related?

(-----scale bar 1-100-----)

Selected Value: 50

Including all the time you spend starting from experimental design and including all the steps of data gathering, treatment, modelling and publishing.



Which of the topics found by our AI are related to your research?

- ☐ Magnetism
- ☐ Instrumentation
- ☐ Fundamental science
- ☐ Protein dynamics
- ☐ Surfaces and interfaces
- ☐ Soft matter
- ☐ Biomembranes
- ☐ None of the above

In which of these societal relevance areas does your research fit?

- ☐ Adaptation to climate change, including societal transformation
- ☐ Cancer
- ☐ Soil health and food
- ☐ Climate-neutral and smart cities
- ☐ Healthy oceans, seas, coastal and inland waters
- ☐ Other

In how many neutron experimental campaigns did you participate in the last 10 years?

- ☐ 1-9
- ☐ 10-19
- ☐ 20-29
- ☐ 30-39
- ☐ 40-49
- ☐ 50 and above

An experimental campaign is an entire chain of steps involved in the research with neutrons, starting from experimental design and writing a beam-time proposal and finishing with a publication of the result.

How would you judge whether one of your neutron experiments was successful or not?

What is your experience with the current proposal systems?

- ☐ It is easy and convenient.
- ☐ It is OK
- ☐ It requires quite some effort
- ☐ It is a pain in the neck
- ☐ Not applicable

At which neutron centers have you performed your experiments?

- ☐ ISIS - Rutherford-Appleton Laboratories, The United Kingdom
- ☐ Institut Laue-Langevin, France



- Leon Brillouin Laboratory, France
- Berlin Neutron Scattering Center, Germany
- GEMS at Helmholtz-Zentrum Geesthacht, Germany
- Jülich Center for Neutron Science, Germany
- FRM-II, Germany
- Budapest Neutron Centre, Hungary
- RID, The Netherlands
- SINQ, Paul Scherrer Institut (PSI), Switzerland
- Frank Laboratory of Neutron Physics, Russia
- St. Petersburg Neutron Physics Institute, Russia
- NIST Center for Neutron Research
- Oak Ridge Neutron Facilities (SNS/HFIR)
- Indiana University Cyclotron Facility
- ISSP Neutron Scattering Laboratory, Japan
- JAEA Research Reactors, Japan
- KENS Neutron Scattering Facility, Japan
- Hi-Flux Advanced Neutron Application Reactor, Korea
- Bhabha Atomic Research Centre, India
- Bragg Institute, ANSTO, Australia
- Other

Which instrument type(s) do you use?

- Neutron transmission (imaging)
- Diffraction
- Small Angle Neutron Scattering (SANS)
- Reflectometry
- Quasielastic neutron scattering
- Neutron spin-echo
- Inelastic neutron scattering
- Other

Which type(s) of sample environment do you use?

- Pressure
- Cryostat
- Oven
- Cryofurnace
- Magnetic fields
- Mechanical deformations
- Stopped flow cell
- Humidity chamber
- Automatic sample changer
- Electric fields
- Shear-cell
- In-situ sample stimulus



- In-situ sample analysis
- Other

What are the key factors for you when choosing where to apply for neutron beamtime?

- Neutron flux
- Beamline scientist
- Preliminary experience with the specific instrument
- Accessibility of the location (travel time from your affiliation)
- Availability of sample environment
- Level of competition for beamtime
- Other

Per 1 day of neutron beamtime, how many days do you typically use on conceiving, preparing, analyzing and publishing the project?

Comments concerning the above question.

What kind of software do you use for data analysis?

- Igor
- Matlab
- Origin
- Python
- R
- C / C++
- Facility-provided software
- Method-specific software
- Other

Do you work with industry?

- Yes, often
- Yes, sometimes
- No

Which other analysis methods do you use for your research?

- Microscopy
- Electron microscopy
- NMR
- large-scale X-rays
- lab-based X-rays
- (FT)IR
- Raman
- DLS
- UV/VIS
- Other



Do you work with other large-scale research infrastructures?

- ESRF EBS (European Synchrotron Radiation Facility Extremely Brilliant Source)
- European XFEL (European X-Ray Free-Electron Laser Facility)
- EMFL (European Magnetic Field Laboratory)
- EU-SOLARIS (European Solar Research Infrastructure for Concentrated Solar Power)
- IFMIF-DONES (International Fusion Materials Irradiation Facility - DEMO Oriented NEutron Source)
- MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications)
- WindScanner (European WindScanner Facility)
- ECCSEL ERIC (European Carbon Dioxide Capture and Storage Laboratory Infrastructure)
- EISCAT_3D (Next generation European Incoherent Scatter radar system)
- EMSO ERIC (European Multidisciplinary Seafloor and water-column Observatory)
- EPOS (European Plate Observing System)
- EURO-ARGO ERIC (European contribution to the international Argo Programme)
- IAGOS (In-service Aircraft for a Global Observing System)
- ICOS ERIC (Integrated Carbon Observation System)
- LifeWatch ERIC (e-Infrastructure for Biodiversity and Ecosystem Research)
- ACTRIS (Aerosols, Clouds and Trace gases Research Infrastructure)
- DANUBIUS-RI (International Centre for Advanced Studies on River-Sea Systems)
- DiSSCo (Distributed System of Scientific Collections)
- eLTER (Long-Term Ecosystem Research in Europe)
- AnaEE (Infrastructure for Analysis and Experimentation on Ecosystems)
- EMPHASIS (European Infrastructure for Multi-scale Plant Phenomics and Simulation)
- EU-IBISBA (Industrial Biotechnology Innovation and Synthetic Biology Accelerator)
- ISBE (Infrastructure for System Biology Europe)
- METROFOOD-RI (Infrastructure for promoting Metrology in Food and Nutrition)
- MIRRI (Microbial Resource Research Infrastructure)
- BBMRI ERIC (Biobanking and BioMolecular Resources Research Infrastructure)
- EATRIS ERIC (European Advanced Translational Research Infrastructure in Medicine)
- ECRIN ERIC (European Clinical Research Infrastructure Network)
- ELIXIR (A distributed infrastructure for life-science information)
- EMBRC ERIC (European Marine Biological Resource Centre)
- ERINHA (European Research Infrastructure on Highly Pathogenic Agents)
- EU-OPENSOURCE ERIC (European Infrastructure of Open Screening Platforms for Chemical Biology)
- Euro-BioImaging (European Research Infrastructure for Imaging Technologies in Biological and Biomedical Sciences)
- INFRAFRONTIER (European Research Infrastructure for the generation, phenotyping, archiving and distribution of mouse disease models)
- INSTRUCT ERIC (Integrated Structural Biology Infrastructure)
- ELI (Extreme Light Infrastructure)
- FAIR (Facility for Antiproton and Ion Research)
- HL-LHC (High-Luminosity Large Hadron Collider)



- SKA (Square Kilometre Array)
- SPIRAL2 (Système de Production d'Ions Radioactifs en Ligne de 2e génération)

9.1.3. Your future needs (facility related)

In this block of questions, we would like to collect your thought and expectations for the future of the neutron-based experiments and the way they are organized.

At which stages of neutron-based research would you like to see improvements?

- Before the experiment
- During the experiment
- After the experiment

Which aspects of the pre-experimental stage should be improved?

- Proposal system
- Contact with the facility staff members
- Access options
- Possibilities for sample transportation to the instrument
- Education in neutron science
- Instrument-related training
- Something else

Which aspects of the experimental stage should be improved?

- Experimental support
- Instrument-related
- Accommodation
- Something else

Which aspects of the post-experimental stage should be improved?

- Experimental data treatment support
- Experimental data analysis support
- Possibilities for data modelling and simulations
- User meetings
- Writing the manuscript
- Something else

What would be your dream scenario in regard to future neutron science?

How can the European Spallation Source (ESS) help in realizing this dream?



9.1.4. Your future needs (not facility related)

Science is typically not-for-profit, but acquiring/securing funding can consume a lot of time for a scientist. Here we would like to hear your opinion on such factors that are not directly related to your neutron science, but that can have a large impact on what neutron science you can do.

I want funding schemes improved as follows:

- Small-scale (experiment-specific): [money for travel, accommodation, students joining, colleagues joining]
- Medium-scale (project-specific) [phd-candidate lifetime – 3-4 years, covering all the costs, including salary, equipment and materials]
- Large-scale (topic-specific) [inter-institutional/international/European collaboration in endeavor to solve a global challenge, neutron research presents less than 51% of the whole package]
- Other

Other things that would boost my neutron science:

- Better education/training of students
- Experts in my field at the facility, during the experiment
- AI helping me during the experiment and analyzing the data
- Students joining the experiment
- FAIR data
- Scientific meetings other than the current (workshop, conference, ad-hoc) possibilities
- Better/more collaboration with industry
- Other

What role can ENSA play to boost your future neutron science?

THANK YOU! Your input will serve (anonymously) to the Brightness2 Report on Future User Needs. ENSA will report back to the neutron community through the national ENSA delegates.

[[SUBMIT button]]

The web survey was sent out to the community via the 20 national delegates of ENSA in the beginning of September 2020 and resulted in 450 responses that were analysed by ENSA.

9.2. Statistics of the survey responses

To find cross-correlations in the pool of answers from the 450 respondents on a survey of 30+ questions, we here combine bar-chart statistics with word clouds. Since the survey also inquired about “who the respondent is” in terms of career and neutron methods, we apply word clouds to show cross-correlation (or lack thereof) in the responses. Therefore, it is necessary to condense the survey questions (consisting of one or more sentences) to single “word tags” (see Appendix 2 for



details). As an example, the question in 9.1.2 “At which stage are you in your scientific career?” is tagged to “who_stage_career”, which appears in the graphics like Figure 17 and many of the word clouds.

First, we identified the career stage of the survey responders, depicted in the Figure 17. The largest group of responders is formed by professors and group leaders (194/450), followed by permanent staff members (130/450), postdocs (61/450) and PhD candidates (44/450). With only 2 responses, the students form the smallest group of the responders. The group “other”, represented by 18 responders included mostly scientists working outside of academic institutions, either in industry or consultancies, and retired scientists.

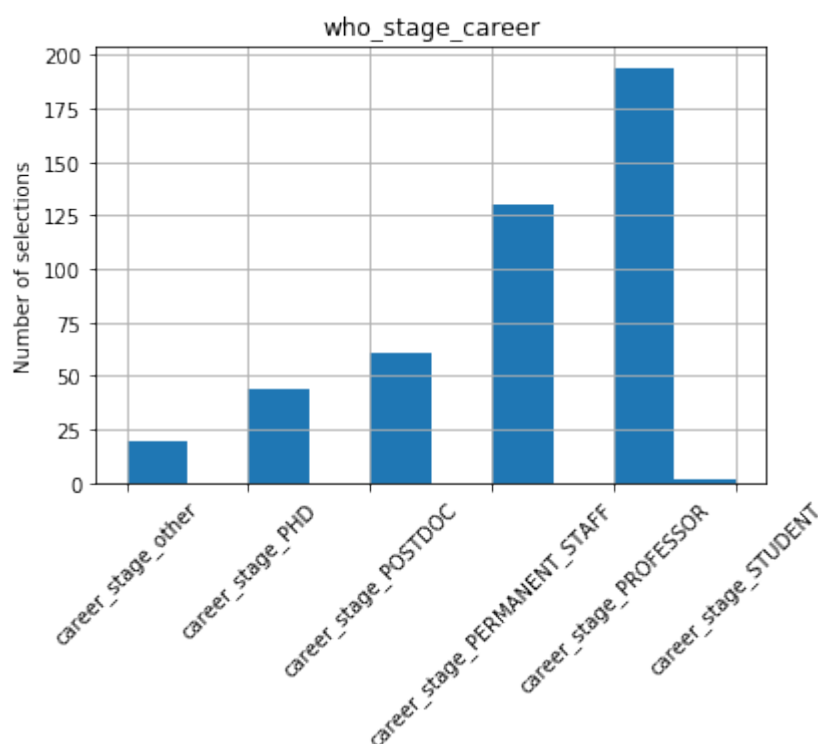


Figure 17: Distribution of respondents career stage, in the survey.

9.2.1. Explanation of the word cloud as a visualization tool of survey answers

The word clouds enable to “project” the pool of answers onto imaginary axes such as “Career Stage”, “Method” and “ESS Instrument”. Although word clouds are not quantitative, they help to identify which are the most important terms that appear in any of the 3 “projections” that we chose. As such, the word cloud is set to a limited 50 terms. Each of the terms that can be found in a word cloud, consists of one **lower_case** word that “represents a question from the survey” (see Appendix 2), combined with a second **_UPPERCASE** answer to that question.

The position of any of the 50 terms is random, the size of the font of each term expresses the importance of the term. For instance, in the below word cloud “Demographics of PhD candidates”, the most prevalent term is “career_stage_PhD” because the respondents (being PhD students) all filled in “PhD” to the survey question “At which stage are you in your scientific career?”. The next-largest term in the word cloud shows that such PhD students usually do not (yet) have any collaboration with industry (see the term “who_industry_collaboration_NO” in the word cloud).

Below the responses are presented as ‘projection onto Career Stage’ in 9.2.2 and as ‘projection onto Method’ in 9.2.3. Within these paragraphs, for each selection (being a tick mark on the imaginary projection axis) two word clouds display the responses unique to that selection. The left-side word cloud shows the (dominant) responses to questions in 9.1.2 and the right-side word cloud shows the (dominant) responses to questions in 9.1.3 and 9.1.4, relating to Future Needs.

The projection onto the imaginary axis “ESS Instrument” has overlap with the below “(Experimental) Method” projection, so these word clouds are placed in Appendix 3.

9.2.2. Word cloud interpretation of the survey responses concerning “Career Stage”



Figure 18: Demographics (left) and requirements for improvements (right) of PhD candidates who responded to survey (44/450)

As can be seen, from the left word cloud (questions about experience up to now), the most frequent answers are “Flux is the main factor in choosing the facility for experiment”, “no collaboration with industry”, “interested in the career in neutrons”, “among the found topics, the fundamental is the most relevant to my research”, “could not associate my research with any of the societal relevance fields of the Horizon Europe”, and “not seeking any collaboration with industry.” We interpreted these answers as follows. Most of the PhD candidates who answered our survey are enthusiastic about neutron science and would like to continue with it in the future. However, their projects are mostly in the field of fundamental science and they do not see how their science could be related to industrial applications, or any of the societal relevance fields within the Horizon Europe.

From the word cloud on the right (questions about the improvements required to facilitate the progress of the science with neutrons), we can see that the main requirement is “education and trainings in neutron science for students”, followed by “medium scale funding,” “presence of students and field experts during the experiments,” “help of AI during the experiment,” and “post-experimental data treatment, data analysis and data modelling and simulations.” We interpret these results as follows. Most of the PhD candidates feel that they do not have enough knowledge for the neutron experiments they perform. It includes the experiments itself, as well as post-experimental data interpretation. As a main solution to this problem, they see more possibilities for education and trainings in neutron science. Alternative solutions they see in presence of experts in their field of science, from whom they could learn on the go. They also assume that the problem could be helped if students could join neutron experiments and learn from it even during their undergraduate

program. This way, they would be much better prepared for the experiments during their PhD projects.

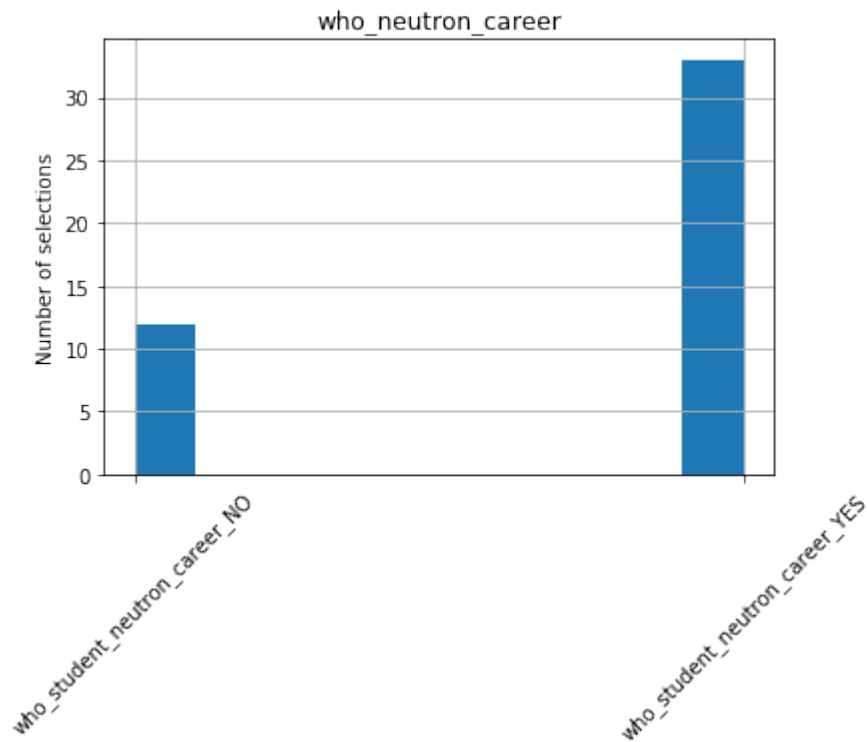


Figure 19: Young scientists see the great potential of neutron scattering as a main tool to develop their research programmes.

From the word clouds for professors and group leaders we can see that the largest terms in the word cloud on the left are “who_neutron_centers_ILL,” “who_factors_facility_choice_FLUX,” and “other_analysis_methods_lab_X_rays.” We interpret these results as follows. Most of the professors use X-rays as well as neutrons for their science and since they are mostly interested in the neutron flux when choosing a neutron source, they mostly go for experiments at ILL, as it provides the highest flux of neutrons.





Figure 21: Demographics (left) and requirements for improvements (right) of postdocs who responded to survey (61/450)

From the word clouds for postdocs, first of all we can see that they give much more diverse answers on the “who” type of questions (there are no outstanding answers in the left word cloud apart from “career_stage_POSTDOC”). We can see that they choose a facility either based on the presence of a specific sample environment, neutron flux, or their previous experience at that facility. Most of them use either neutron diffraction or SANS for their research.

On the required improvements, on the other hand, they are much more consistent. Medium and small-scale funding seems to be the most important improvement factors for them. These factors are followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments and post-experimental data analysis and treatment.

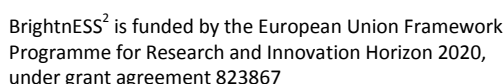




Figure 23: Demographics (left) and requirements for improvements (right) of "other" career group who responded to survey (19/450)

As we noticed earlier, the "other" career group is formed mostly by scientists working in industry and retired scientists. This group seem to perform most of their experiments either at ILL or ISIS. They mostly use neutron diffraction for their experiments, and they couldn't find the societal relevance field related to their research.

Their most required improvements include medium and small scale funding for their research. The funding group of improvements is followed by the requirement for improvements in scientific meetings and industrial collaboration.

9.2.3. Word cloud interpretation of the survey responses concerning “Methods”



Figure 24: Demographics (left) and requirements for improvements (right) of the group using neutron diffraction (258 /450)

From the answers of scientists who use neutron diffraction we could interpret the following. Most of their experiments are performed at ILL, FRM-II and ISIS. Their facility choice is mostly defined by the presence of a specific sample environment, flux and previous experience at that facility. The most often used sample environment by the group is cryostat and among other non-neutron based analysis methods they mostly use laboratory-scale X-ray techniques.

Their most required improvements include medium and small scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students and the possibility for students to join neutron experiments.



Figure 25: Demographics (left) and requirements for improvements (right) of the group using SANS (215/450)

From the word clouds for the group using SANS technique we can see that they perform most of their experiments at ILL, followed by FRM-II and ISIS.

Their most required improvements include medium and small scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments, and the possibility for students to join neutron experiments. The third group of required improvements is related to post-experimental data treatment, analysis, modelling and simulations.



Figure 26: Demographics (left) and requirements for improvements (right) of the group using QENS (123 /450)

From the word clouds for the group using QENS technique we can see that they perform most of their experiments at ILL, followed by FRM-II and ISIS.

Their most required improvements include medium and small scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments, and the possibility for students to join neutron experiments. The third group of required improvements is related to post-experimental data treatment, analysis, modelling and simulations.



Figure 27: Demographics (left) and requirements for improvements (right) of the group using imaging (64/450)

From the word clouds for the group using neutron imaging technique we can see that they perform most of their experiments at FRM-II, followed by ILL, SINQ and HZB. In addition to QENS they often use neutron diffraction and SANS techniques.

Their most required improvements include medium and small scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments, and the possibility for students to join neutron experiments. The third group of required improvements is related to post-experimental data treatment, analysis, modelling and simulations.

From the word clouds for the group using neutron reflectometry technique we can see that they perform most of their experiments at ILL, followed by FRM-II and ISIS. In addition to neutron reflectometry they often use SANS technique.

Their most required improvements include medium and small-scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments, and the possibility for students to join neutron experiments. The third group of required improvements is related to post-experimental data treatment, analysis, modelling and simulations.



Figure 29: Demographics (left) and requirements for improvements (right) of the group using inelastic neutron scattering (162/450)

From the word clouds for the group using inelastic neutron scattering technique we can see that they perform most of their experiments at ILL, followed by ISIS and FRM-II. In addition to inelastic neutron scattering they often use neutron diffraction.

Their most required improvements include medium and small-scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments, and the possibility for students to join neutron experiments. The third group of required improvements is related to post-experimental data treatment, analysis, modelling and simulations.

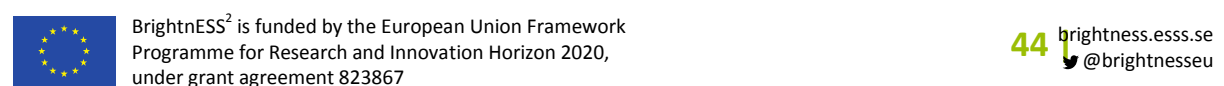




Figure 31: Demographics (left) and requirements for improvements (right) of the group using an instrument other than named above (49/450)

From the word clouds for the group using an instrument other than named above we can see that they are mostly motivated by neutron flux when choosing a facility for their experiments. Among the topics identified by our NLP publications analysis they indicated mostly instrumentation, or fundamental. They perform most of their experiments at ILL, followed by FRM-II.

Their most required improvements include medium and small-scale funding for their research. The funding group of improvements is followed by the neutron-specific education and trainings for students, presence of the field experts during their experiments, and the possibility for students to join neutron experiments. They are also particularly interested in the improvements of the instrumental parameters at the experimental stage of their research.

9.2.4. Improvements requested at the level of “facility”

Among the facility-related improvements, most of the respondents would like to see the improvements at the post-experimental stage of their research (182 responses), followed by improvements during the experiment (161 responses) and pre-experimental stage (132 responses).

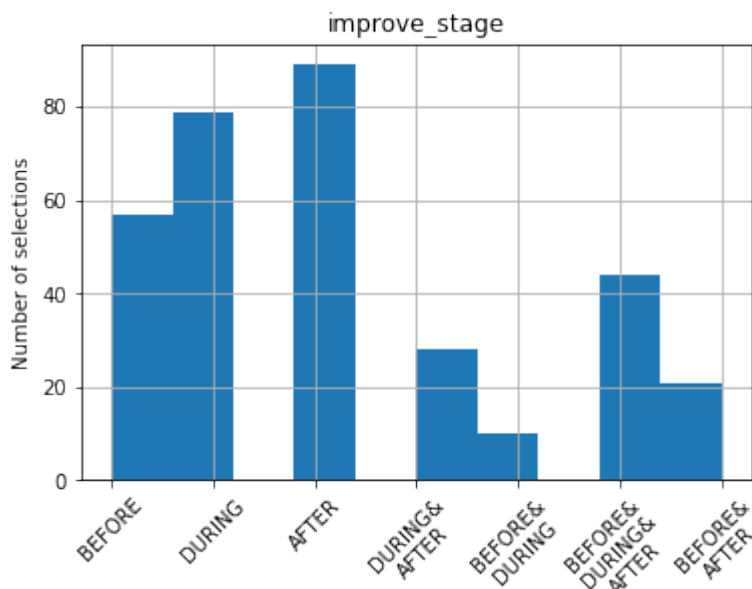


Figure 32: A distribution of answers to the question about the research stage which requires improvements, the possible options being "before", "during", "after" and combinations thereof.

During the pre-experimental stage, the most demanded improvement is instrument-related training (57 responses), followed by facility access options (47 responses), education in neutron science (39 responses), proposal system (33 responses), contact with the facility staff (33 responses), sample transport to the beamline (32 responses).

During the experimental stage, the most demanded improvement is instrument-related (103 responses), followed by the improvements in the experimental support (61 response), and accommodation (28 responses).

During the post-experimental stage, the most demanded improvement is in the experimental data analysis (123 responses) followed by data treatment (112 responses), data modelling and simulations (101 response), with a very little demand for improvements in user meetings (13 responses) and manuscript writing (8 responses).

9.3. ENSA interpretation of community response on Future Needs

For nearly every question that was posed in the survey, the respondents had opportunity to elaborate on their choice or selection. Such 'text field' answers were interpreted by the ENSA delegates and will be summarized in the following 6 paragraphs.

9.3.1. Complementary sources

By far the greatest concern expressed by today's European neutron users was that there would be a much-reduced availability of neutron beam-time over the coming decade⁹, severely limiting the scope for standard, screening, test or exploratory measurements, as well as for teaching purposes, and with the inevitable consequence that there will be a loss of European science leadership in this area. The community is already suffering the consequences of the 2019 closures of three national neutron scattering facilities in France, Germany, and Norway. The users are seeking reassurance that their current long-term research projects involving neutron scattering will not be jeopardized in a few years' time by the loss of available neutron beam time and are calling for an ongoing (and increased) support and augmentation of the existing ILL and ISIS facilities, in tandem with development of a network of smaller neutron facilities, which can operate in synergy with ESS.

At full power operation, fully commissioned ESS instruments will deliver one to two orders of magnitude higher data collection rates at equal resolution than the highest intensity neutron scattering instruments in existence today worldwide. This will be achieved by combining at ESS highest neutron source brightness with most advanced instrument design. Such new capabilities in data rates will lead to breakthroughs-in the study of new phenomena with very weak signals, of new materials that are only available in very small quantities, of broad parametric domains, etc. These are cases, where with the neutron intensities of current instruments, experiments would require beam times of several months or more. In contrast, in studies that require less than a few days beam-time today, ESS will offer little time saving advantage, since there always is an incompressible logistic time need in any experiment, such as alignment, changing sample parameters, controls and – not the least – evaluating the best next steps. ESS capabilities will open up new qualitative opportunities, but will not increase dramatically the number of currently feasible studies one instrument can deliver within a period of time, such as one year. ESS beam-time at full operation with the originally planned 22 ESS financed instruments (i.e. some 10 years from now) will amount to about 4500 beam days per year, i.e. on average 0.5 days per year per neutron user in Europe. In order to serve this community and respond to the broad need for neutron probe results, a top-of-the-line facility needs to be complemented by a synergetic broad network of national and regional neutron sources. This alone will allow for focusing on the most intensity demanding phenomena that wait to be discovered. This synergy is the key to the success for both sides: ESS would not be able to explore unique challenges if it would have to serve too many users all the time. On the other hand, the exploratory progress at the top facilities brings up questions and whole fields of interest that can be perfectly handled by smaller or much smaller neutron sources. For example, exciting new opportunities by novel materials in very small initial quantities will call for very high intensity instruments to be first discovered, but their practical interest goes by their availability in higher quantities that also open up the opportunities to be more widely studied for broad scientific and practical needs at less intense neutron sources.

9.3.2. Neutron Facility Staffing

A recurring theme in the survey responses was that the neutron scientists need increased levels of expert support from the neutron facilities not just for running the neutron instrument during an experiment but for preparing advanced experiments including e.g. in-situ sample environments,

⁹ <https://www.esfri.eu/neutron-landscape-group>

complex data-analysis etc. This need correlates with the findings of the NLP analysis that the average number of authors on articles containing neutron science is increasing. The research is becoming increasingly complex, requiring multiple complementary techniques. As to total number of neutron-using scientists increase, especially the number of scientists that are not neutron science experts increase, which leads to the need for expert support from the facilities.

Currently most facilities operate in a system where each instrument has 1-2 instrument scientists whose main role is to guarantee the technical performances of the instruments, conduct experiments in the most effective way and upgrade the techniques to respond to the needs of the community. Increasing the number of experts at facilities would allow having specialists in several fields with enough time to offer not only a high-level technical support, but continue the collaboration with users to the data treatment and interpretation. In some cases, this can be crucial to enable the final publication of the data, mainly for users who are not neutron science experts. Moreover, ensuring this extended collaboration is probably the best way to open the use of neutron techniques to a wider community as well as to find the means for the education of new users or future specialists. It is also the best way to generate a greater return of value for the investments puts into ESS.

9.3.3. Neutron data software/analysis

From the survey responses concerning the dream scenario of future experiments, data analysis plays an important role. The users see potential for better use of the experimental data in the way the measured results are handled. In general, there is a remarkable need for suitable, well documented, and user-friendly analysis packages, significantly accompanied by the wish that the facilities take responsibility to provide and maintain such packages. The latter would also satisfy the tendency to ask for common/standardized sets of analysis tools, usable for data from all facilities. Often this request is related to simultaneous wishes for modelling and simulation tools, which includes comparison of data with calculations as well as virtual instruments for preparing the experiments.

A part of the community expresses a wish for analysis software having enough capability for a publication-quality data visualisation without further programming. Personal help with data analysis by instrument staff and possible use of AI for on-the-fly data analysis have been mentioned, too.

9.3.4. Facility Access System

The survey responses touched upon several aspects of the neutron access systems, which have also been discussed among stake holders over the past years. These can roughly be grouped into i) types of access, ii) proposal system functions, iii) international access. The biannual peer reviewed proposal rounds through which the majority of beamtime is currently distributed, ensure reasonably fair distribution of beamtime, but may result in delays in the individual science projects. It might benefit the future neutron scientists if e.g. the top 50% proposals could be accepted by a standing committee on a rolling basis without 6 months delay. Most facilities offer a variety of other access modes, including rapid, mail-in programme, collaborating research group, and proprietary paid access for industry. Especially with the massively increased count rates expected at ESS, it would be interesting to explore providing more neutron access in the form of rapid/mail-in/sequential access types, which would however require additional hardware and software provisions for increased automation in experiments, and likely would also require increased staffing at the facilities. Many



neutron scientists are frustrated by the access restrictions to international facilities based on which countries are contributing financially to these facilities. While such restrictions are natural consequences of the complex challenge of funding neutron facilities, they impact individual scientists and science programs in ways out of their control. It would greatly benefit neutron scientists if solutions were found to avoid such nationality barriers, for instance by accounting neutron funding in the broader scheme of international collaborations.

9.3.5. Neutron Experiment Optimization

A common concern of neutron users is what we refer to here as “Experiment Optimization”: preliminary and/or parallel testing on samples to be investigated in a given neutron scattering experiment, together with the optimal use of available or user-provided sample environment for the experiment itself.

Standard laboratory-based sample characterisation is naturally the departure point, but coordination/synchronisation between advanced characterisation techniques based on other large-scale facilities (e.g. synchrotron sources) is often difficult. While the physical proximity of different large-scale facilities is indeed in place in several European science parks (ILL and ESRF in Grenoble, SLS and SINQ in the Paul Scherrer Institut, Max IV and ESS in Lund, etc.), the possibility of joint proposals between the facilities is limited. The accompanying schemes are not widely-known among the European neutron user community. The PSB (Partnership for Structural Biology) SAXS/SANS platform run jointly by the ILL and ESRF and the SLS/SINQ scheme in the Paul Scherrer Institute are two such examples, each limited to a particular scattering technique (or indeed scientific field).

It would be worthwhile to assess the experiences of users and user groups that have benefited from the NFFA (Nanoscience foundries and fine analysis) program (see NFFA.eu) that provided access to laboratory and large-scale facilities in such a way as to make optimal use of complementary techniques on the same samples. From those scientists important input can be gained about the added value of having access to different facilities based on a single proposal.

LINXS (Lund Institute for Advanced Neutron and X-ray Science) should be a fertile ground for promoting a far more general and flexible scheme of X-ray-neutron joint proposals and raising awareness of such schemes among both the neutron and X-ray user communities. Similar partnerships with advanced NMR or microscopy platforms could and should be envisaged. The implementation of two-technique experimental beam-times should be significantly aided by the generalization of the Block Allocation Group (BAG) neutron beam times.

The second aspect of “Experiment Optimization” is the availability and optimisation of sample environments on the neutron scattering beamlines. Very often users discover problems/limitations of the available sample environment, while the neutron experiment is already running, leading naturally to (sometimes significant) beam time loss. For non-standard sample environments, be it facility-provided or user-provided, a testing stage (prior to neutron beam-time) seems to be essential and should be officially integrated into the experiment, together with the availability of experimental space and the necessary technical staff. To some extent the problem could already be alleviated by providing still more specific and detailed information (blueprints of sample holders, pictures of magnet configurations, power supplies, etc.) about the available sample space and environments on the website of the beamline, so that beamline scientists do not have to repeat this information time and again. Especially for new users, such detailed pictures of possible sample configurations (perhaps

even with interactive pictures allowing panning and zooming) would be useful for new and inexperienced users who are unfamiliar with technical terms used at the beamline. Needless to say, under the current number of staff dedicated to each neutron beamline, accompanying an additional experimental team for an “off-beam” set-up of the sample environment is unrealistic. Within the SINE2020 program (www.sine2020.eu) a significant number of e-learning modules about neutron scattering experiments was developed. It should be encouraged to draw the attention to the existing e-tools and to stimulate further development, aiming at the goal of letting users doing simulations of the experiments that they intend to perform, so that they can discover practical and configurational issues well before the actual beam-time.

9.3.6. Neutron science and Industry

Over the last decade, the neutron facilities across Europe have undergone major improvements and additions to their instrument suites with some instruments now more explicitly targeted towards industrial applications. The community's expression of involvement with industry is seen in the ESS Instruments "projections" of the BEER and ODIN word clouds (see appendix 3), and also in the corresponding projections for several other ESS Instruments (NMX, ESTIA, HEIMDAL, VESPA, LoKi). There is a wish for better education of students and better data treatment and/or analysis software, which will also enhance industry involvement, as this typically requires a more extensive resources in staffing 'during and after' the experimental campaign. Together with the dedicated instrumentation for engineering purposes, Industry will definitely profit from such improvements in 'user friendliness' for their R&D, and particularly if the modes of access to neutron facilities also provide the required flexibility. It may be noted too, that the boost in neutron facility instrument performance across Europe has been made possible by industrial partners who have collaborated to deliver components at all stages from particle accelerator to data visualization tools.



10. Possibilities for future applications of the analysis tools developed for this project

All analysis tools developed for this project could be applied for future investigations of the development trends in the research and research communities in Europe and in the world. One of the potential applications of the networks analysis of the neutron scientists could be to catalyse research collaborations. One could think about an online tool for finding a “path” between him/herself and the research group working in a topic of interest or using a specific analytical technique. It could also facilitate the growth of the European and national neutron scattering communities.

Another application could be in discovering the emerging research topics and predicting their future developments. Some of the highly influential publications could be identified at the early stage by faster citation dynamics with respect to the field on average. Such analysis could also serve in establishing connections between specific policies applied in science on the European or national level and the changes in trend developments in a specific research field influenced by such a policy.

It should be noted that the developed approach is not specific for neutron science and could be easily transferred to any scientific field.



11. Appendix 1: Topic/container naming from NLP

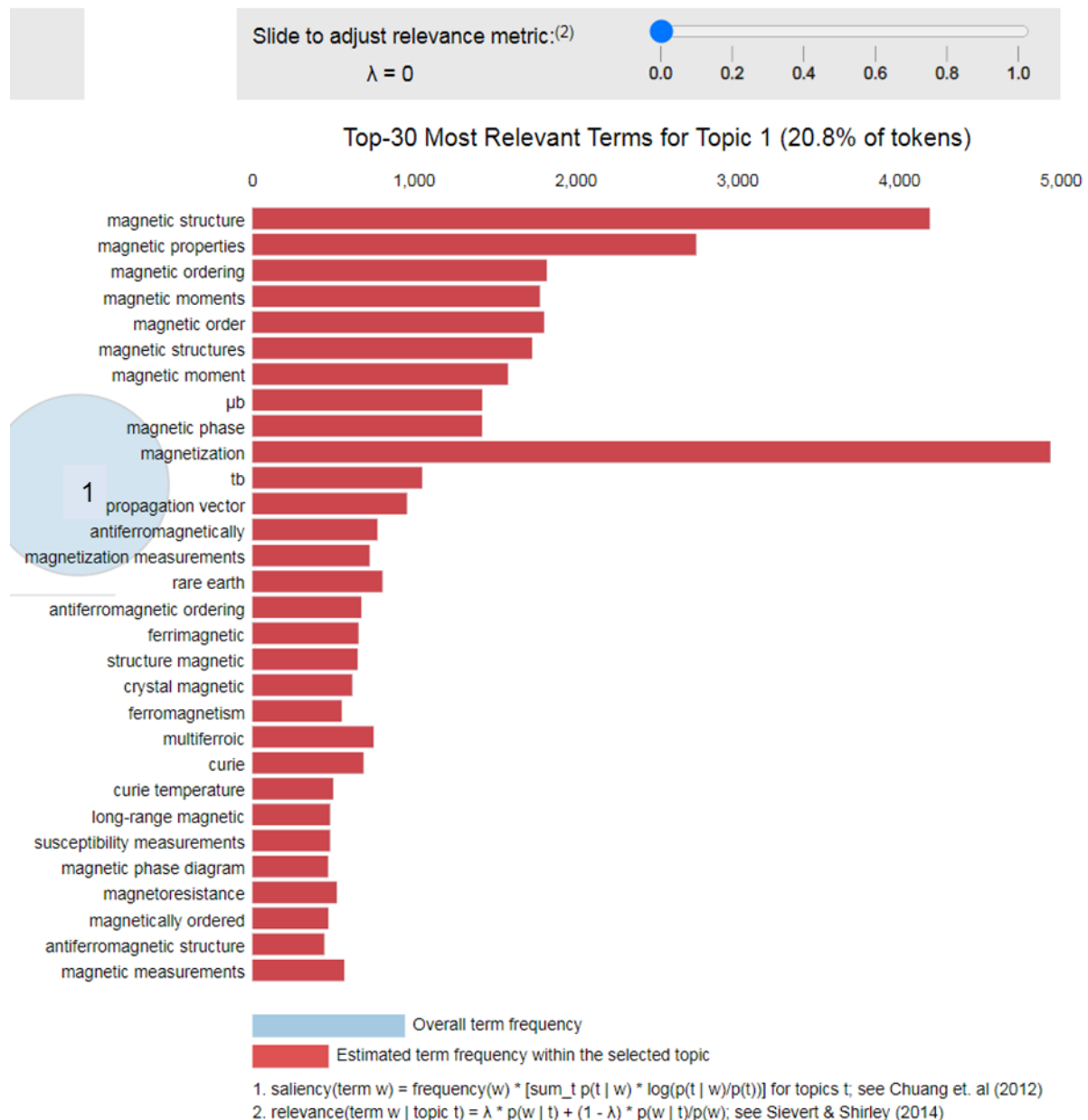


Figure 33: Top 30 most relevant terms for topic 1 out of 7

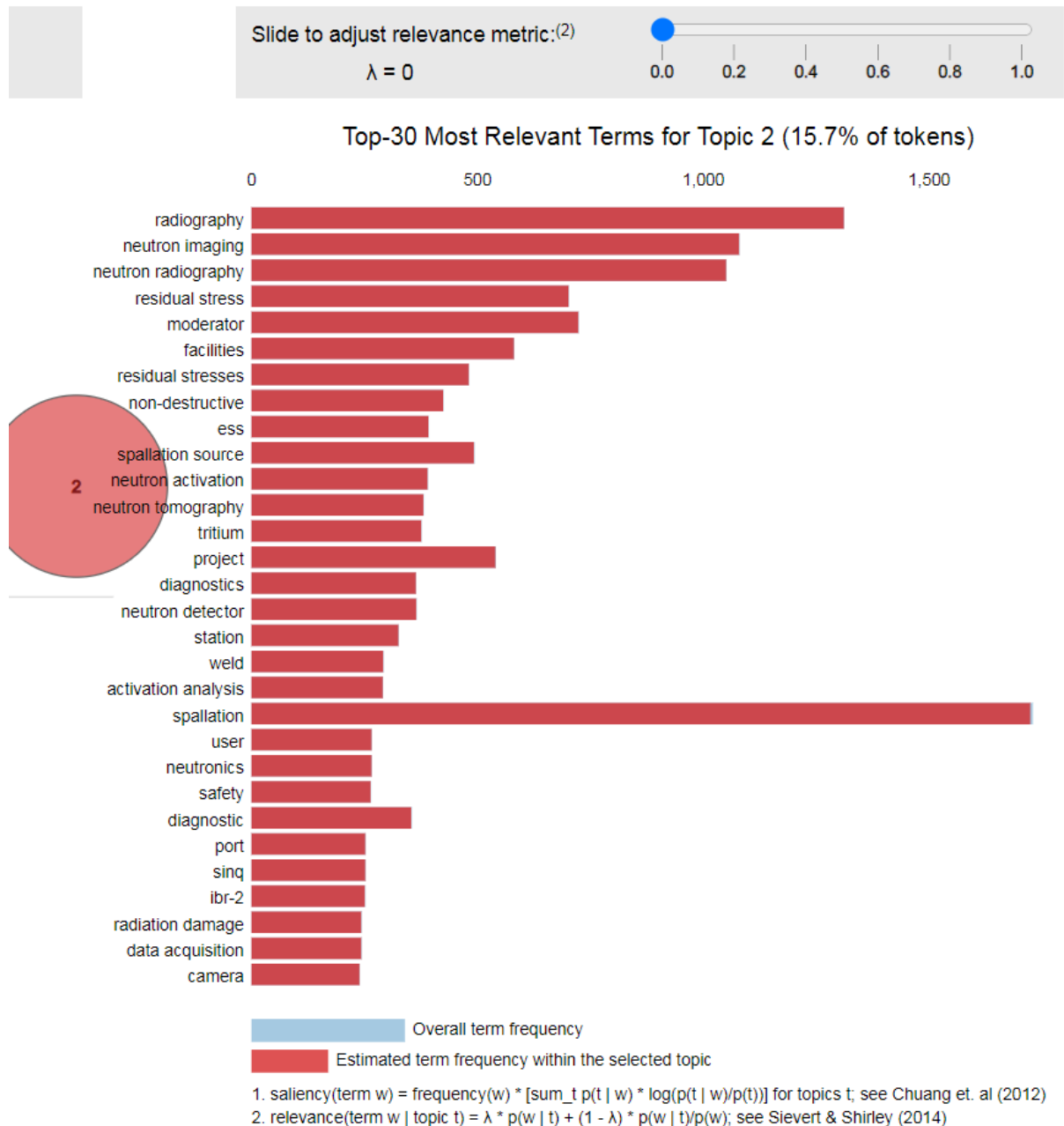


Figure 34: Top 30 most relevant terms for topic 2 out of 7

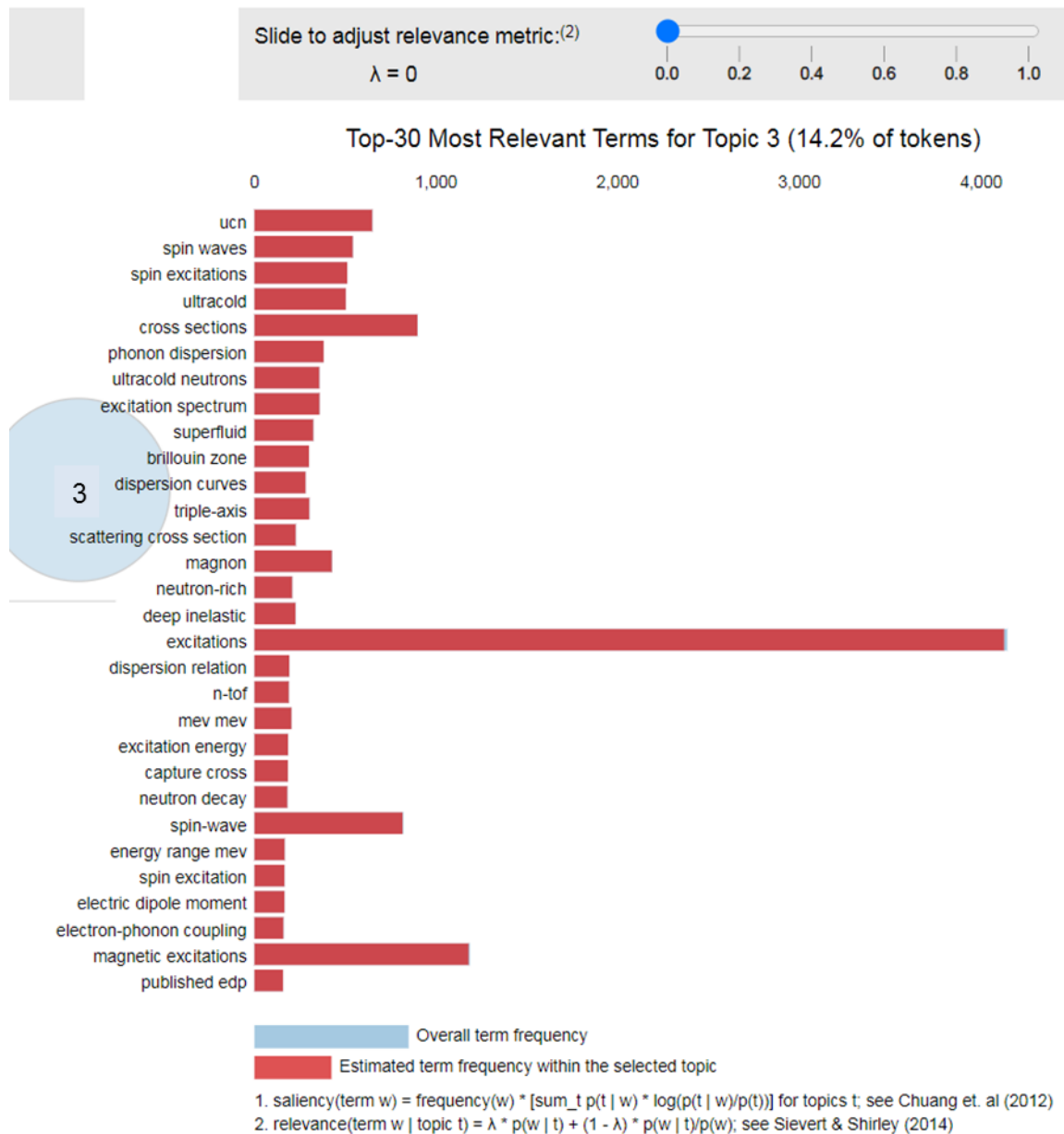


Figure 35: Top 30 most relevant terms for topic 3 out of 7

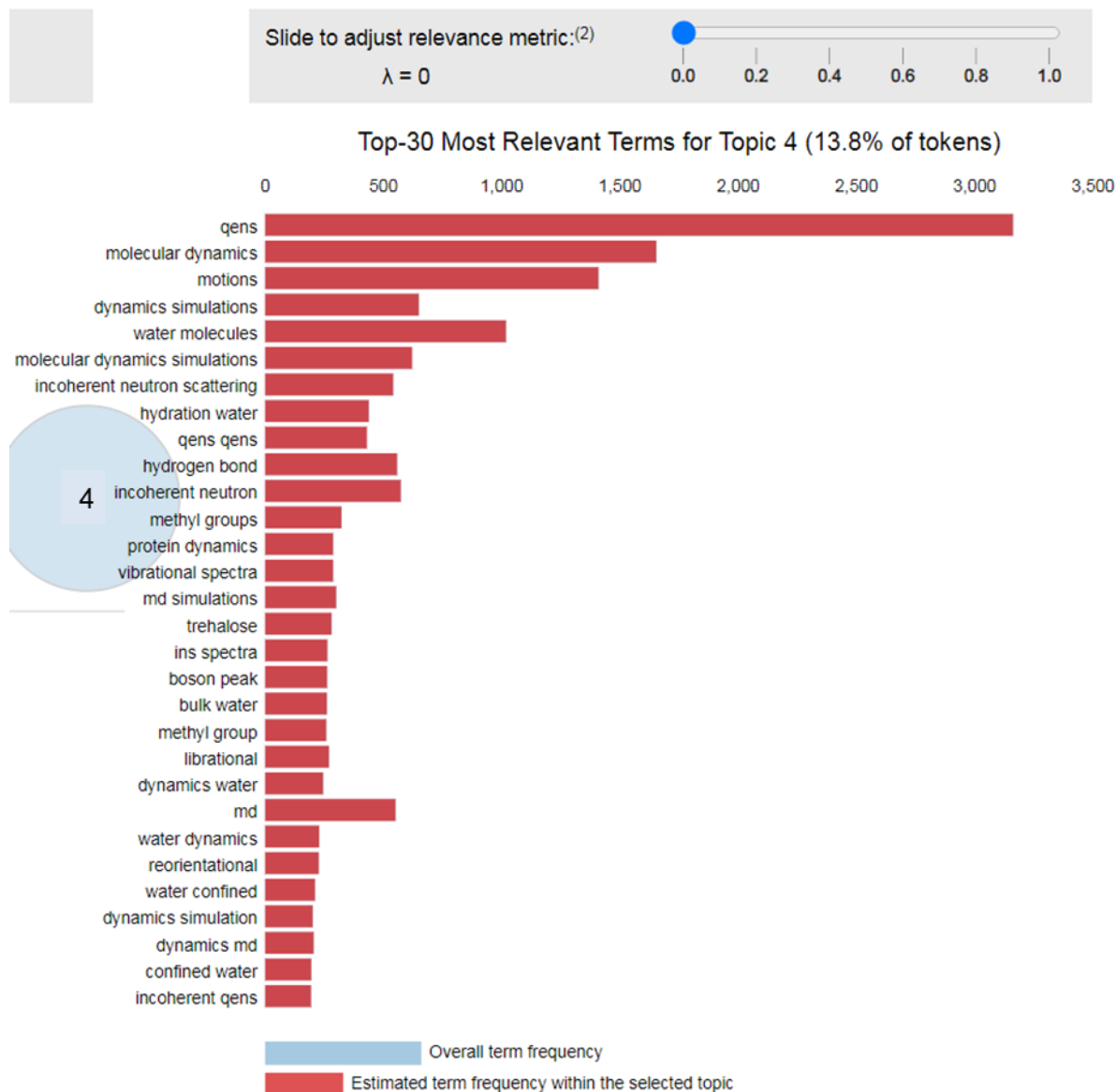


Figure 36: Top 30 most relevant terms for topic 4 out of 7

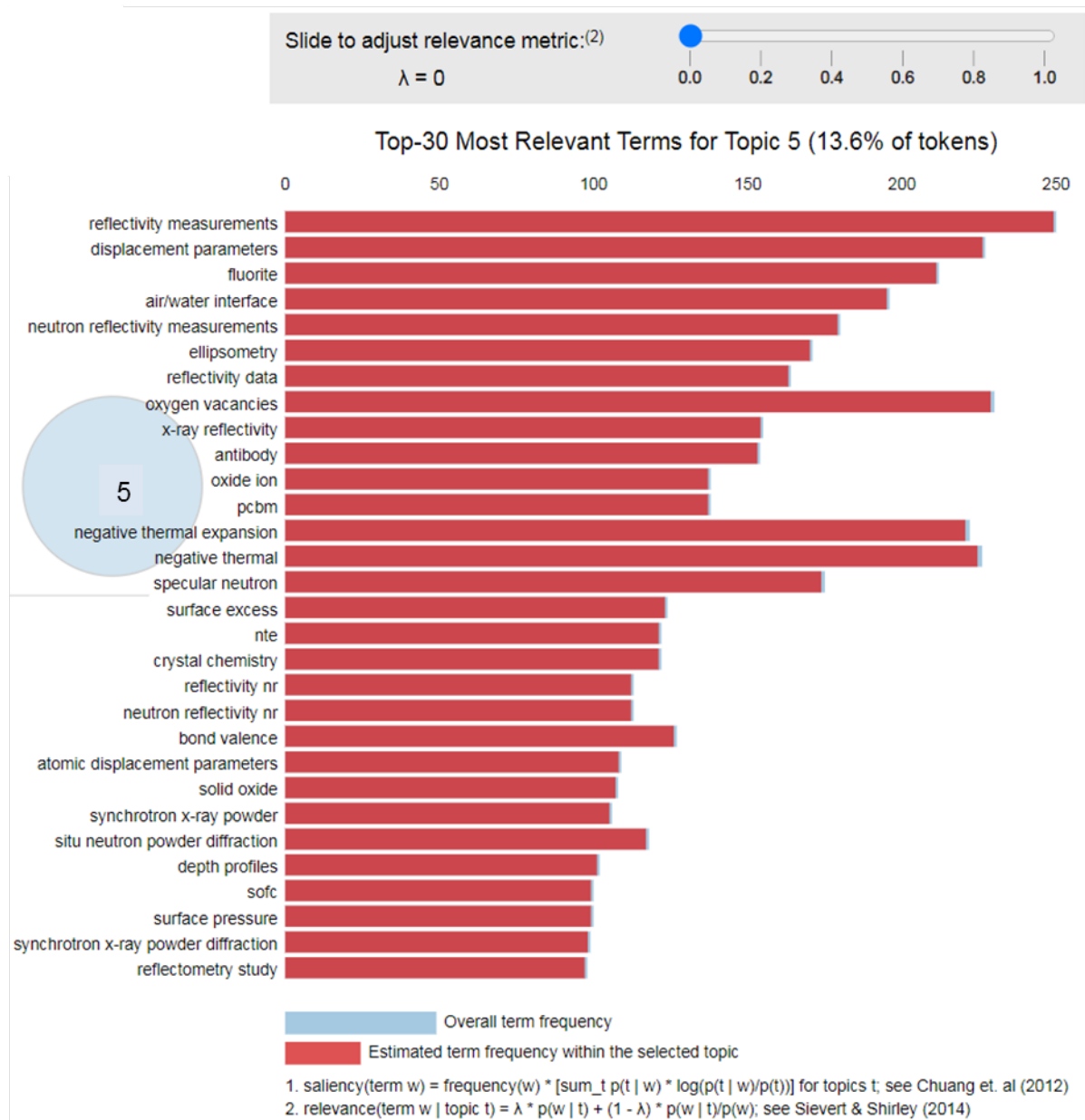


Figure 37: Top 30 most relevant terms for topic 5 out of 7

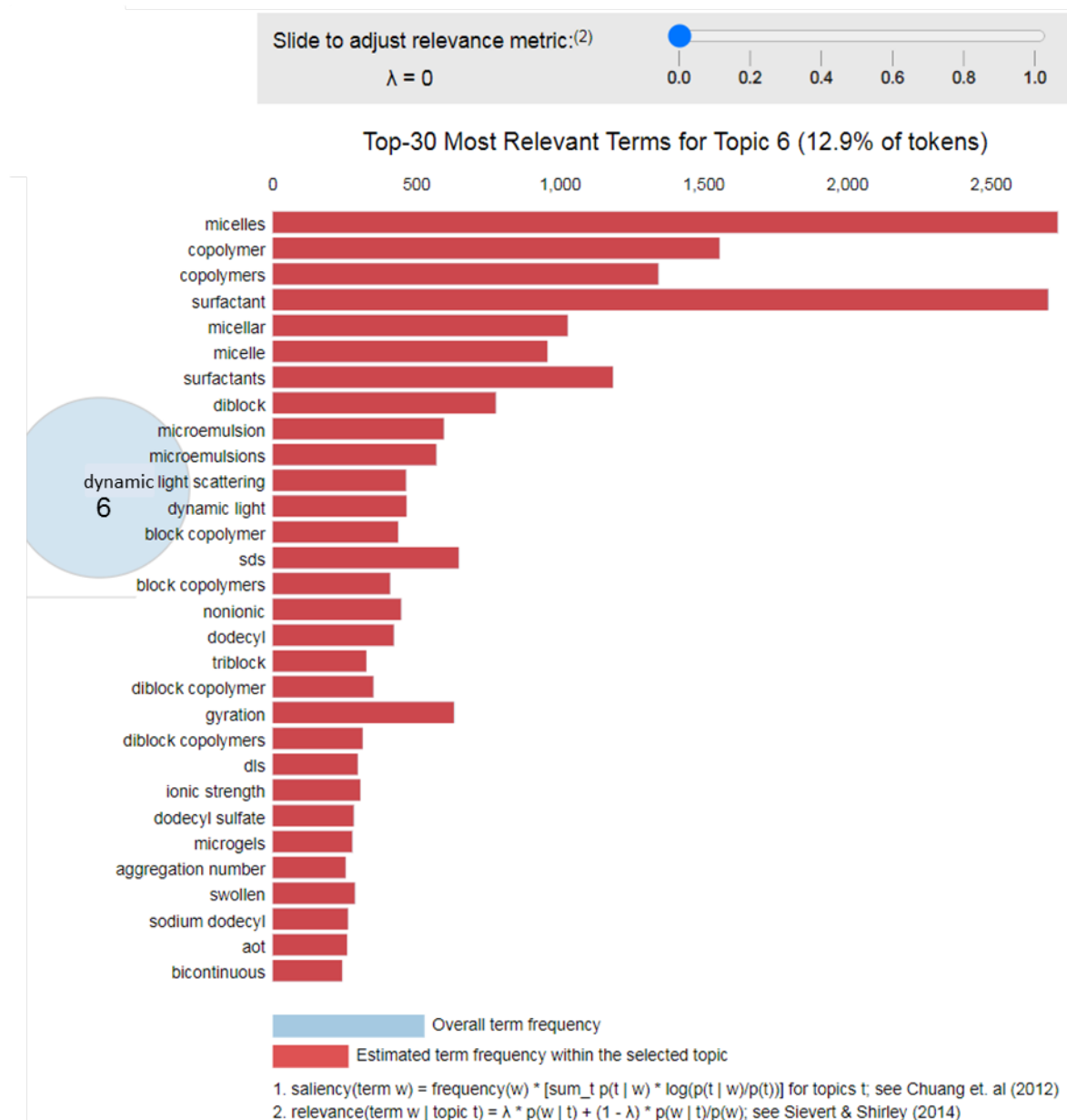


Figure 38: Top 30 most relevant terms for topic 6 out of 7

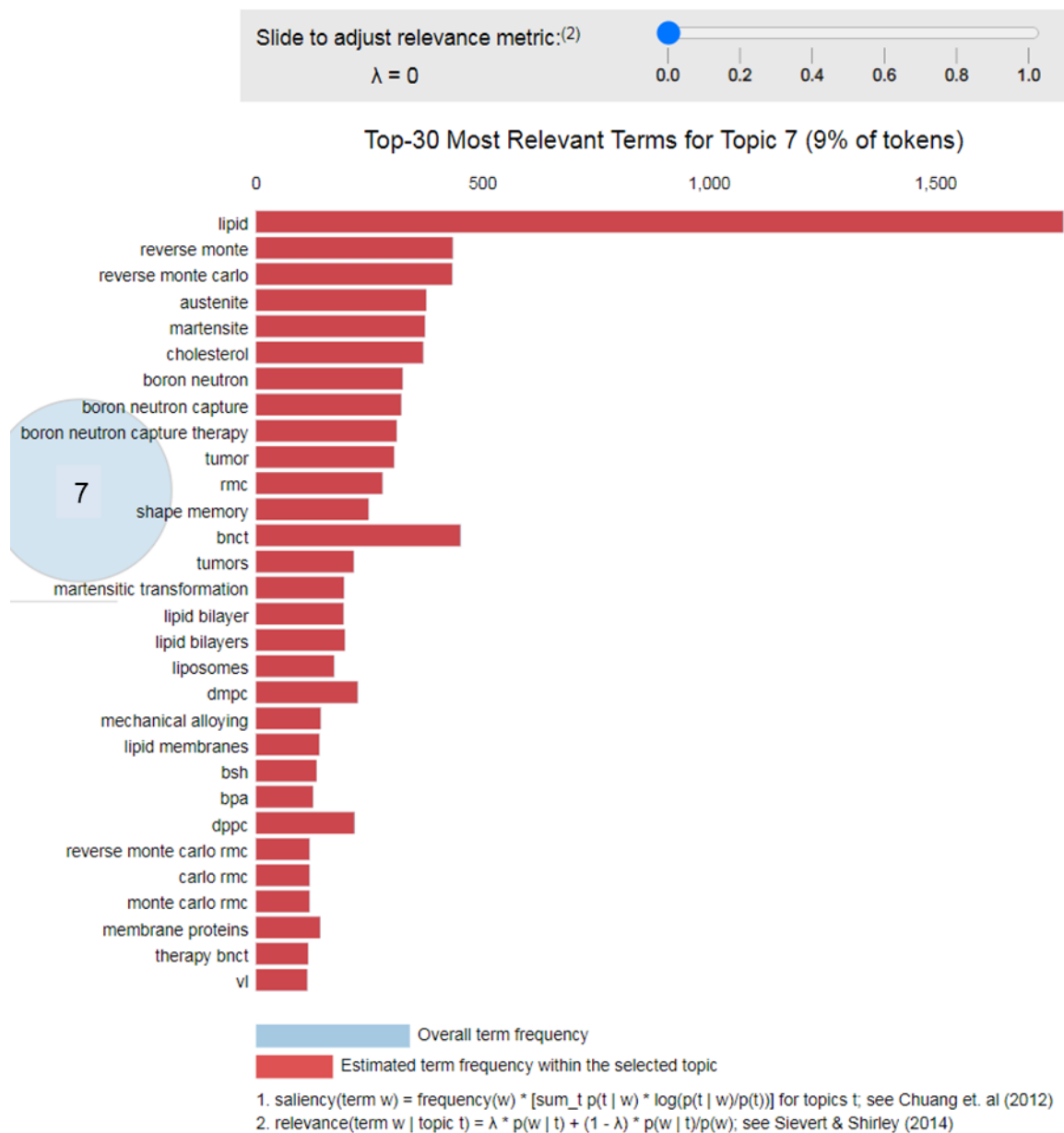


Figure 39: Top 30 most relevant terms for topic 7 out of 7

Table 1: Detailed descriptions of the topics/containers found in our NLP analysis.

	Container name	NLP terms relevant to container	NLP container methods
1	Magnetism	Magnetic structure, magnetic properties, magnetic ordering, magnetic moments, magnetic phase, magnetization, propagation vector, AF/FM ordering, rare earth, ferrimagnetic, crystal, multiferroic, Curie temperature, long-range, magnetic phase diagram, magnetoresistance, Neel temperature, magnetic field, incommensurate, compounds, transition, spin state, along.	Magnetization, susceptibility measurements, Mossbauer, temperature, neutron diffraction.
2	Instrumentation	Neutron radiography, residual stress, moderator, facilities, non-destructive, ESS, spallation source, neutron activation, neutron tomography, tritium, project, diagnostics, neutron detector, station, weld, activation analysis, user, neutronics, safety, port, radiation damage, data acquisition, camera, reactor, instrument, design, operation, diffractometer, research, neutron flux, guide, monochromator, pulse, beam, target, performance, neutrons, neutron irradiation, cold neutron, materials, development, method, analysis, data, nuclear, thermal, energy.	
3	Fundamental	spin waves, spin excitation, cross section, phonon dispersion, super fluid, Brillouin zone, dispersion curves, magnon, neutron-rich, excitations, meV, capture, decay, electric dipole moment, electron-phonon coupling, phonon, magnetic excitations, nuclei, quantum, gap, spin dynamics, energies, momentum, spectrum, resonance, fission, fluctuations, model, mode, data, temperature, magnetic.	UCN, Triple axis, deep-inelastic, neutron-TOF, neutron inelastic scattering.
4	Protein Dynamics	Molecular dynamics, motions, water molecules, hydration water, hydrogen bond, methyl groups, protein dynamics, vibrational spectra, trehalose, boson peak, bulk water, librational, reorientational, confined water, vibrational, translational, intermolecular, self-	QENS, MD simulations, incoherent neutron scattering, INS, vibrational spectroscopy, Raman.

		diffusion, diffusion, molecules, glass transition, ice, relaxation, protein, liquids, density, time, structure, transition, model.	
5	Surfaces & Interfaces	Displacement parameters, fluorite, air/water interface, oxygen vacancies, antibody, oxygen ion, negative thermal expansion, specular, surface excess, crystal chemistry, bond valence, solid oxide, depth profiles, solid oxide fuel cell, surface pressure, electrochemical, impedance, antibody, thin films, vacancies, Lithium, octahedral, conductivity, crystal structure, space group, perovskite, cation, layer, phase, site, atoms.	Reflectivity measurements, ellipsometry, X-ray reflectometry, synchrotron XRD, in-situ neutron powder diffraction, Rietveld refinement.
6	Soft Matter	Micelles, copolymer, surfactant, diblock, microemulsion, non-ionic, dodecyl sulfate, triblock, gyration, ionic strength, microgels, aggregation number, swollen, discontinuous, blends, molecular weight, colloidal, fractal, self-assembly, aggregates, nanoparticles, contrast variation, pH, concentration, solution, solvent, shear, chain, aqueous, surface, structure, phase.	DLS, SANS, SAXS.
7	Biomembranes	Lipid, austenite, martensite, cholesterol, boron neutron capture therapy, tumor, shape memory, martensitic transformation, lipid bilayer, liposomes, mechanical alloying, membrane proteins, precipitates, phospholipid, milling, vortex lattice, membrane, grain, nanocrystalline, alloy, nanocrystalline, glasses, amorphous, vortex, deformation, strain, grain, microstructure, steel, structure, texture, phases, formation, lattice.	Reverse Monte Carlo, neutron diffraction, in-situ, X-ray, SANS.

12. Appendix 2: Conversion vocabulary between the survey questions and lower_case indications for word clouds.

Are you interested in a career in neutrons? : who_neutron_career
 Are you seeking collaboration with industrial partners? : who_industry_seek
 At which neutron centers have you performed your experiments : who_neutron_centers
 At which stage are you in your scientific career? : who_stage_career
 At which stages of neutron-based research would you like to see improvements? : improve_stage
 Do you teach neutron science? : who_teach_neutron
 Do you work with industry? : who_industry_collab
 Do you work with other large-scale research infrastructures? : who_other_lsri
 Does the development trend in the topics for your country fit your expectations? : who_trend_fit
 Does this Heat Map fit to your expectations, or would you expect a different distribution of neutron scientists in your country? : who_heatmap_fit_to
 I want funding schemes improved as follows: : improve_funding_schemes
 In how many neutron experimental campaigns did you participate in the last 10 years? : who_neutron_campaigns
 In which of these societal relevance areas does your research fit? : who_societ_relevance
 Other things that would boost my neutron science: : improve_other_boost
 What are the key factors for you when choosing where to apply for neutron beamtime? : who_factors_facility_choice
 What is your experience with the current proposal systems? : who_proposal_system
 What kind of software do you use for data analysis? : who_software
 Which access option should be improved? : improve_access_options
 Which aspects of the accommodation should be improved? : improve_accomodation_aspects
 Which aspects of the experimental stage should be improved? : improve_experiment_stage_aspects
 Which aspects of the pre-experimental stage should be improved? : improve_pre_experimental_stage_aspects
 Which aspects of the the experimental support should be improved? : improve_experimental_support_aspects
 Which aspects of the the post-experimental stage should be improved? : improve_post_experimental_stage_aspects
 Which instrument type(s) do you use? : who_instrument_types
 Which of the following ESS instruments do you expect to provide such improvements? : improve_ESS_instruments
 Which of the topics found by our AI are related to your research? : who_found_topics
 Which other analysis methods do you use for your research? : who_other_analysis_methods
 Which parameters of the inelastic neutron scattering instrument require improvement? : improve_parameters_INS
 Which parameters of the instrument you use require improvement? : improve_parameters_other
 Which parameters of the neutron diffraction instrument require improvement? : improve_parameters_DIFFRACTION
 Which parameters of the neutron spin-echo spectroscopy instrument require improvement? : improve_parameters_NSE

Which parameters of the neutron transmission (imaging) instrument require improvement? :
improve_parameters_IMAGING

Which parameters of the quasielastic neutron scattering instrument require improvement? :
improve_parameters_QENS

Which parameters of the reflectometry instrument require improvement? :
improve_parameters_REFLECTOMETRY

Which parameters of the small angle neutron scattering (SANS) instrument require improvement? :
improve_parameters_SANS

Which percentage of your research activity is neutron-related? : who_percentage_neutron

Which type(s) of sample environment do you use? : who_sample_environment

Would you like to have a European single access proposal system (nonspecific to an instrument, or a neutron source; beamtime can be granted at an instrument X in country Y)? : improve_single_access

Would you like to have a standard electronic logbook interchangeable between all the facilities? :
improve_standard_logbook

Your level of expertise as a "neutron scientist" : who_expertise_level

Your opinion and any comments on our neutron publications analysis : who_ai_opinion



13. Appendix 3: Word cloud interpretation of survey responses concerning “ESS instrument”

All of the instruments included in the ESS construction project were selected by survey respondents as potential providers of the improvements that the community seeks in the neutron instruments. The terms that appear in the word clouds of the different instruments are rather similar for many instruments. However, in the word clouds below one can find information per instrument about the group of scientists that selected a specific instrument (left word clouds with the answers to “who”-type of questions), as well as the kind of improvements such a group of scientists is seeking (right word clouds with the answers to “improve”-type of questions). These word clouds could be used for better understanding of the potential research done with the instruments, and for selection of the equipment of the laboratories related to the instruments. It should also be noted that in nearly all word clouds, *several* ESS instruments appear, which may be interpreted as an indication of good compatibility of the instruments for science done with the help of neutrons.

Below, the word clouds are shown per ESS instrument, with the left-side word cloud describing the survey respondents, the right-side word cloud expressing what kind of improvements these respondents seek. Each word cloud is appended with a short interpretation.



Figure 40: Demographics (left) and requirements for improvements (right) of the respondents who selected T-REX for their Future Needs

From the word clouds for the group of the respondents who selected T-REX for their Future Needs we can see that they are performed most of their neutron experiments at ILL. The motivation for their facility choice is neutron flux. They are mostly using inelastic neutron scattering technique. Among the other (non-neutron) large scale research infrastructures they mostly use ESRF. As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron background, sample environments, and availability of the instrument. Apart from T-REX, they are also interested in using BIFROST, MAGiC and DREAM instruments at ESS.



Figure 41: Demographics (left) and requirements for improvements (right) of the respondents that selected HEIMDAL for their Future Needs

From the word clouds for the group of the respondents who selected HEIMDAL for their Future Needs we can see that they are motivated by neutron flux when choosing a facility for their experiments. They are mostly using neutron diffraction. Among the other (non-neutron) analysis methods they mostly use lab- or large-scale X-ray techniques.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron background, flux, resolution, sample environment and availability of the instrument. Apart from HEIMDAL, they are also interested in using DREAM, BIFROST and MAGiC instruments at ESS.

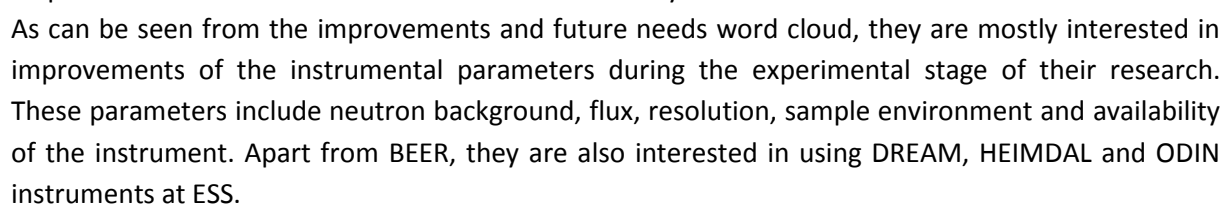
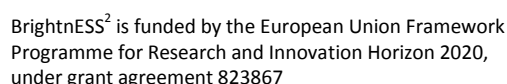




Figure 43: Demographics (left) and requirements for improvements (right) of the respondents that selected CSPEC for their Future Needs

From the word clouds for the group of the respondents who selected CSPEC for their Future Needs we can see that they perform most of their experiments at ILL. They are motivated by sample environment, neutron flux and beamline scientist when choosing a facility for their experiments. They are mostly using neutron diffraction and inelastic neutron scattering techniques. Among the other (non-neutron) analysis methods they mostly use lab- or large-scale X-ray techniques.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron flux, resolution, sample environment and availability of the instrument. Apart from CSPEC, they are also interested in using DREAM, HEIMDAL, MIRACLES, BIFROST and T-REX instruments at ESS.



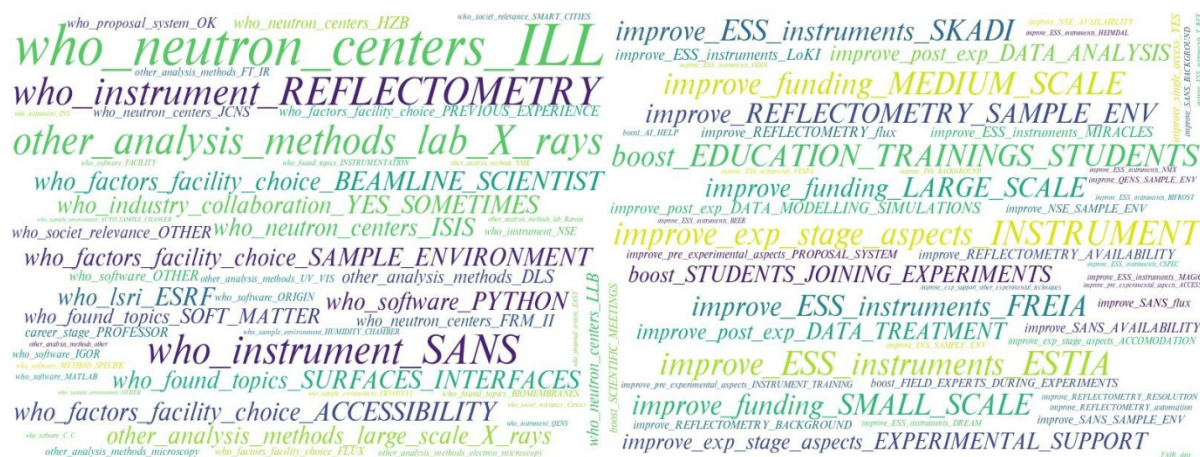


Figure 45: Demographics (left) and requirements for improvements (right) of the respondents that selected ESTIA for their Future Needs

From the word clouds for the group of the respondents who selected ESTIA for their Future Needs we can see that they perform most of their experiments at ILL. They are motivated by sample environment, accessibility and beamline scientist when choosing a facility for their experiments. They are mostly using neutron reflectometry and SANS techniques. Among the other (non-neutron) analysis methods they mostly use lab- or large-scale X-ray techniques.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron flux and sample environment. Apart from ESTIA, they are also interested in using FREIA and SKADI instruments at ESS.



Figure 46: Demographics (left) and requirements for improvements (right) of the respondents who selected MIRACLES for their Future Needs

From the word clouds for the group of the respondents who selected MIRACLES for their Future Needs we can see that they perform most of their experiments at ILL. They are motivated by neutron flux when choosing a facility for their experiments. They are mostly using inelastic neutron scattering technique. Among the other (non-neutron) large scale research infrastructures they usually use ESRF. Among the topics found by our NLP analysis, they identified instrumentation as the most relevant for their research.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron background and sample environment. Apart from MIRACLES, they are also interested in using FREIA, ESTIA, T-REX, LoKI and SKADI instruments at ESS.



Figure 47: Demographics (left) and requirements for improvements (right) of the respondents that selected BIFROST for their Future Needs

From the word clouds for the group of the respondents who selected BIFROST for their Future Needs we can see that they perform most of their experiments at ILL, ISIS or HZB. They are motivated by neutron flux, beamline scientist, previous experience and accessibility when choosing a facility for their experiments. They are mostly using neutron diffraction and inelastic neutron scattering techniques. Among the other (non-neutron) large scale research infrastructures they usually use ESRF.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron background, availability, flux, resolution and sample environment. Apart from BIFROST, they are also interested in using DREAM instrument at ESS.



Figure 48: Demographics (left) and requirements for improvements (right) of the respondents that selected NMX for their Future Needs

From the word clouds for the group of the respondents who selected NMX for their Future Needs we can see that they perform most of their experiments at ILL or FRM-II. They are motivated by neutron flux, accessibility and beamline scientist when choosing a facility for their experiments. They are mostly using neutron diffraction. Among the topics found by our NLP analysis, they identified instrumentation as the most relevant for their research. This group of responders has occasional collaborations with industry.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. Apart from NMX, they are also interested in using HEIMDAL, DREAM, and MAGiC instruments at ESS.



Figure 49: Demographics (left) and requirements for improvements (right) of the respondents that selected MAGiC for their Future Needs

From the word clouds for the group of the respondents who selected MAGiC for their Future Needs we can see that they perform most of their experiments at FRM-II and ILL. They are motivated by neutron flux, sample environment, previous experience and beamline scientist when choosing a facility for their experiments. They are mostly using neutron diffraction. Among the other (non-neutron) analysis methods they usually use lab-scale X-rays.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron background, flux, resolution and sample environment. Apart from MAGiC, they are also interested in using DREAM and BIFROST instruments at ESS.



Figure 50: Demographics (left) and requirements for improvements (right) of the respondents that selected VESPA for their Future Needs

From the word clouds for the group of the respondents who selected VESPA for their Future Needs we can see that they perform most of their experiments at ILL. They are motivated by availability of a specific sample environment, beamline scientist, previous experience and neutron flux when choosing a facility for their experiments. They are mostly using inelastic neutron scattering and neutron diffraction. Among the other (non-neutron) large scale research infrastructures they usually use ESRF. Among the topics found by our NLP analysis, they identified fundamental as the most relevant for their research.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron background, resolution, instrument flexibility and sample environment. Apart from VESPA, they are also interested in using CSPEC and MIRACLES instruments at ESS.



Figure 51: Demographics (left) and requirements for improvements (right) of the respondents that selected LOKI for their Future Needs

From the word clouds for the group of the respondents who selected LoKI for their Future Needs we can see that they perform most of their experiments at ILL. They are motivated by neutron flux, sample environment, beamline scientist and previous experience when choosing a facility for their experiments. They are mostly using SANS technique. Among the other (non-neutron) large scale research infrastructures they usually use ESRF. Among the topics found by our NLP analysis, they identified soft matter as the most relevant for their research.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron flux, availability, sample environment and remote control of the instrument. Apart from LoKI, they are also interested in using SKADI instrument at ESS.



Figure 52: Demographics (left) and requirements for improvements (right) of the respondents that selected SKADI for their Future Needs

From the word clouds for the group of the respondents who selected SKADI for their Future Needs we can see that they perform most of their experiments at ILL. They are motivated by neutron flux, sample environment, beamline scientist and previous experience when choosing a facility for their experiments. They are mostly using SANS technique. Among the other (non-neutron) large scale research infrastructures they usually use ESRF. Among the topics found by our NLP analysis, they identified soft matter as the most relevant for their research.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron flux, availability, sample environment and remote control of the instrument. Apart from SKADI, they are also interested in using LoKI and ESTIA instruments at ESS.



Figure 53: Demographics (left) and requirements for improvements (right) of the respondents that selected ODIN for their Future Needs

From the word clouds for the group of the respondents who selected ODIN for their Future Needs we can see that they performed most of their experiments at HZB. They are motivated by neutron flux, sample environment, beamline scientist and previous experience when choosing a facility for their experiments. They are mostly using neutron diffraction and imaging techniques. Among the other (non-neutron) analysis techniques they mostly use lab-scale X-rays. This group of scientists has collaborations with industry.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron flux, availability, and sample environment. Apart from ODIN, they are also interested in using SKADI and DREAM instruments at ESS.



Figure 54: Demographics (left) and requirements for improvements (right) of the respondents that selected DREAM for their Future Needs

From the word clouds for the group of the respondents who selected DREAM for their Future Needs we can see that they perform most of their experiments at ILL, FRM-II and ISIS. They are motivated by neutron flux, sample environment, beamline scientist and accessibility when choosing a facility for their experiments. They are mostly using neutron diffraction. Among the other (non-neutron) analysis techniques they mostly use lab-scale X-rays.

As can be seen from the improvements and future needs word cloud, they are mostly interested in improvements of the instrumental parameters during the experimental stage of their research. These parameters include neutron flux, background, availability, and sample environment. Apart from DREAM, they are also interested in using HEIMDAL, BIFROST and MAGiC instruments at ESS.