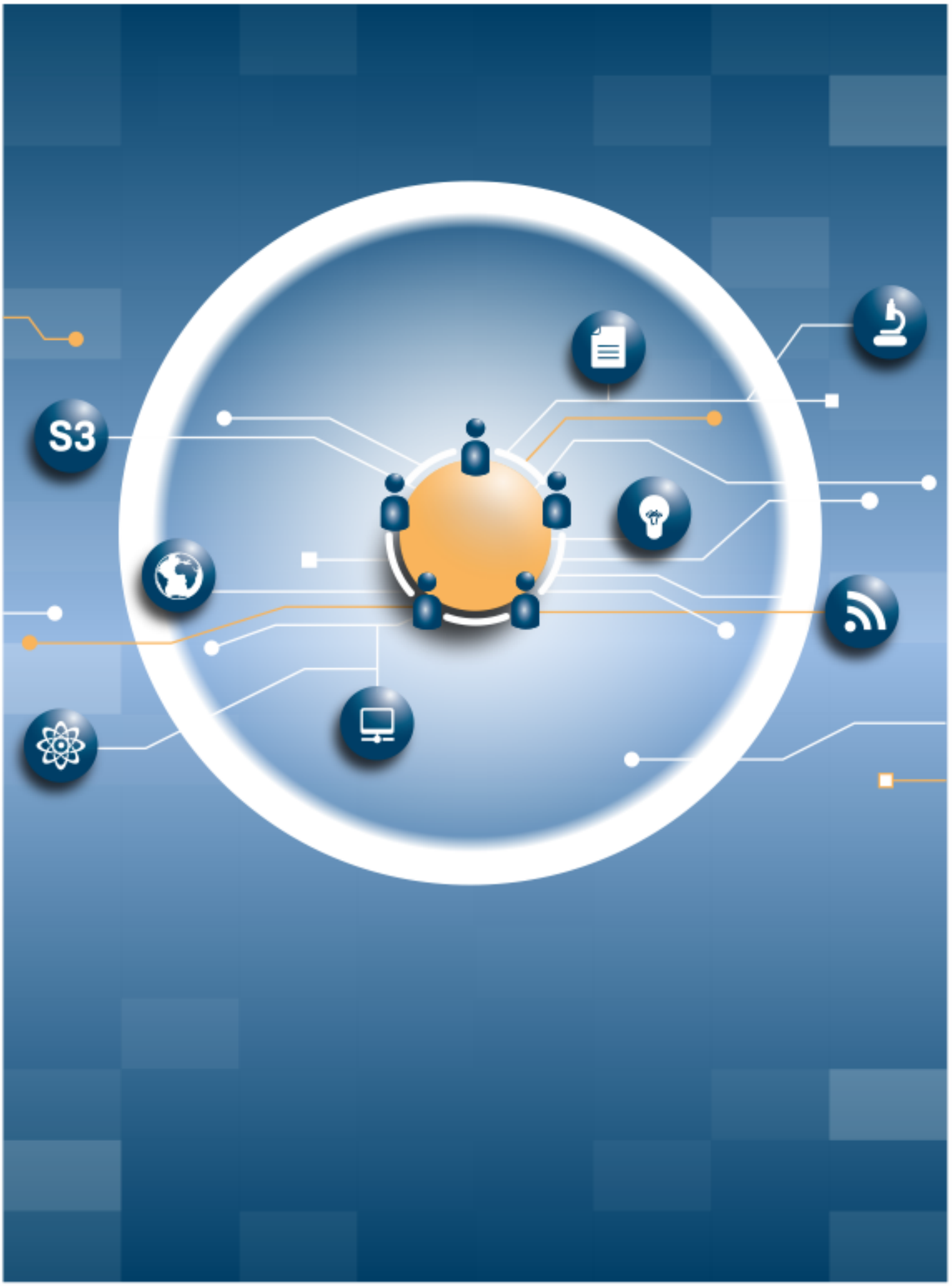



**IT-Newsletter**

"Collaborative work with GitLab"

Edition 4/2020 | 15.09.2020

JÜLICH
Forschungszentrum

# Contents

# IT-Newsletter

**Issue 4/2020**

**Collaborative work with GitLab**

## Editorial

The IT Newsletter is in a state of change. We have a high influx of articles. Our English and German speaking readers* say that they appreciate the information content. We also hear voices telling us that we have left the framework of a newsletter. For this reason, the editorial team has decided to present IT News in future in brief and to publish the detailed articles on IT topics that determine our cooperation or our findings in a separate format, the "IT Magazine". Both media will be linked with cross-references. Last but not least, you will therefore receive a detailed "IT Newsletter" in the character of an IT magazine. In the future, *IT news* will be distributed via the familiar channels. You will continue to find the *IT magazine* in its usual place.
Now enjoy reading the current issue in its old format!

***Brief technical information*** The IT Newsletter contains QR codes that allow access to web content. This also allows easy access to the stored links in printouts and screenshots. The QR codes can also be clicked on like any other conventional link. This is indicated by the hand symbol . Links that lead to an area that is not freely accessible (Intranet) are marked by the lock symbol .

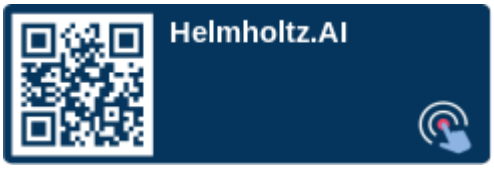
**The action circle "Aktionskreis Auftritt der IT Gremien"**

# Reports / News

## Funding for AI Projects

*Sven Rank*

The Helmholtz Association is funding research projects in the field of applied artificial intelligence (AI) and machine learning (ML) with 7.2 million euros. A panel of experts selected 19 projects for the "Helmholtz AI Cooperation Unit" (Helmholtz.AI), which will be funded with up to €400,000 each. Researchers from Jülich are involved in five projects.



The projects use novel analytical tools to solve pressing social challenges such as climate change or mobility through AI. They promote the testing of new approaches, are supported by several partners and completed in up to three years - thus enabling larger follow-up projects. From Jülich were successful:

### AINX: KI for neutron and X-ray scattering experiments

The project develops AI-supported data reduction and analysis techniques for neutron and X-ray scattering experiments. The goal is to optimize beam time utilization and to accelerate data analysis. Dr. Marina Ganeva (JCNS-FRM-II), E-Mail: m.ganeva@fz-juelich.de

### aN0: Improving simulations on high-performance computers

The goal of AlphaNumerics Zero is to rethink the design of numerical methods on high-performance computers. The project uses reinforcement learning techniques so that the computer independently learns the optimal numerical solution method for a given simulation problem. Dr. Robert Speck (JSC), e-mail: r.speck@fz-juelich.de

### EDARTI: AI approaches for improved electron diffraction inversion

In this project an interdisciplinary team of mathematicians and physicists is dedicated to decoding properties of material scientific and biological samples from 4-D diffraction images by further development of AI methods. Prof. Knut Müller-Caspary (ER-C-1), e-mail: k.mueller-caspary@fz-juelich.de

### i2Batman: Intelligent battery management through spectroscopy and ML

In the i2Batman project, ML techniques for optimised battery management at the battery cell level will be developed and demonstrated. The aim is to achieve optimised fast charging behaviour while at the same time ensuring that the battery life meets or even exceeds the industry standard. Prof. Josef Granwehr (IEK-9), e-mail: j.granwehr@fz-juelich.de

### MOMONANO: ML enables molecular nanorobots

The aim of the project is to build complex functional nanostructures with single molecules like LEGO® building blocks. However, the quantum mechanical simulations required for this are too time-consuming. Momonano combines expertise in ML, molecular simulations

and nanorobotics to accelerate such simulations by orders of magnitude. Dr Christian Wagner (PGI-3), e-mail: c.wagner@fz-juelich.de

The Helmholtz.AI call was promoted among others at the 9th IT Forum. Thank you very much for the strong interest of the community and good luck to the winners in implementing their projects!

## IT-Platforms and Tools directly linked on the homepage of the IT Portal

On the start page of the IT portal you will find a collection of useful IT tools and platforms as icons that can be clicked directly.


An explanation of the respective tools can be found under the respective keyword in the A-Z keyword list.

If you have further suggestions, please post them in the Chat #AK Auftritt IT-Gremien.


## IT-Vacancies now bundled in the IT portal

In the main navigation of the IT portal you can now find all current IT-related job offers directly:


The service is developed in cooperation with P-E.

### Call from P-E: Your feedback on external IT platforms

The Human Resources Development and Recruiting Department (P-E) asks for your feedback on the external IT platforms "Reddit" and "Golem". Are you familiar with these platforms/do you use them yourself? If so, how do you assess the quality of these? Do you think that publishing IT vacancies on these two platforms could be worthwhile for the Research Centre? If so, do you know of any other platforms/forums that you could recommend? Your feedback in the corresponding Gitlab issue would be very welcome for P-E!


## Briefly introduced

### Gebhard Günther

**What do you do at the Research Centre?** I head the *Cross Sectional Group IT* of the IEK-7 (Institute for Energy and Climate research (stratosphere)). Together we operate the workstation group of the Institute and support our users in the area of scientific workflow. Together with colleagues from the JSC's SimLab Climate Science, I operate the "Jülich MeteoCloud", a repository for meteorological operational and reanalysis data, satellite data and climatological and episodic model data.

**What did you do previously?** After studying geophysics and completing my doctorate at the University of Cologne, I joined the research centre at the former ICG-1, now called IEK-7, in 1998. Here I worked within the theory department on the development of the Chemical Lagrange Model of the Stratosphere, which is mainly used for planning, monitoring and interpretation of the measurement campaigns of IEK-7.

**What is important to you in your work in the IT committees?** In the IT committees, the combined know-how of the research centre in the field of IT is concentrated. Here, the problems that every employee faces in connection with his or her (sometimes more, sometimes less) digital workplace are tackled flexibly and unbureaucratically. Important in the IT forums is the respectful interaction at eye level, which keeps the threshold low for many employees to ask questions and participate. I would like to thank the many colleagues who, with a high level of willingness to respond, always react surprisingly quickly and competently to enquiries.

**What do you like to do most in your free time?** When my family allows me time, I love to read and (of course) play computer games.

## Dates

The next Digital IT Forum is scheduled for 6 October 2020, 9:00 - 11:00. Please save the date.

# Good to Know

## Introduction to managing daily tasks with GitLab

*Reimar Bauer*

In linguistic usage, GitLab is a web application for software projects based on Git. It comes with a number of tools that are useful for a variety of other management tasks. In the following, I'll introduce you to some of the possibilities you can use for your daily tasks.

For internal use we use gitlab.fz-juelich.de and for external cooperation we use gitlab-public.fz-juelich.de also called jugit.fz-juelich.de.

In the IT-Forum a thematic action circle has developed dedicated to GitLab. The employees can be reached via #gitlab-users in the Rocket.Chat.


The login to the two provided platforms is done via Shibboleth with the central user name (the first part of the email address before the @) and the central email password.

### Differences gitlab, gitlab-public

**gitlab.fz-juelich.de**


- internal, not available to the outside
- public projects can be viewed from the JuNET

**gitlab-public.fz-juelich.de**


- worldwide, accessible to the outside world

- external users possible
- public projects can be viewed worldwide

### Setting the language

For the platform GitLab there are translations of the interface in different languages. Often the default language is English. Once you have logged in, you can change the language setting to suit your needs.

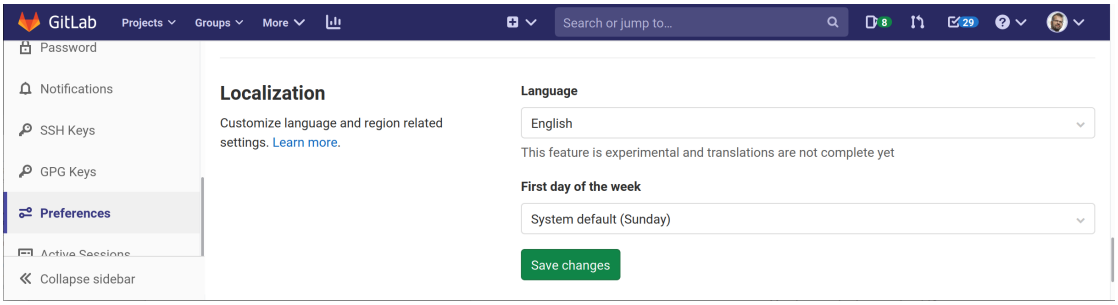



Figure 1: Screenshot "GitLab language setting"

### New Project

Every registered employee can create projects on this platform and configure elements. The ticket system can be designed in many ways.

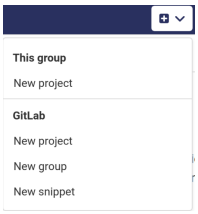



Figure 2: New Ticket, New Project GitLab

### Use of tickets

It is often worth looking at existing public projects for guidance. The tickets can be grouped by labels. Your own participation is shown in the navigation after logging in.

You can see what's happening by looking at the activity indicators and sorting by "Last updated".

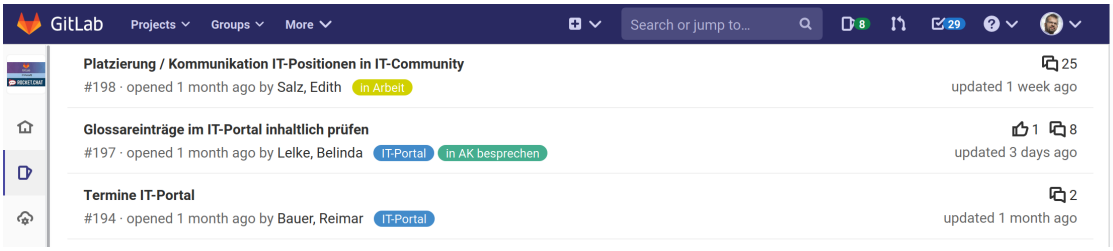



Figure 3: Ticket bar in GitLab

All interested parties can join a discussion in a ticket at any time, discuss the content, contribute to the solution. As soon as the solution is realised, the ticket is closed. The content will not disappear. It is only no longer displayed as an “Open Ticket”.

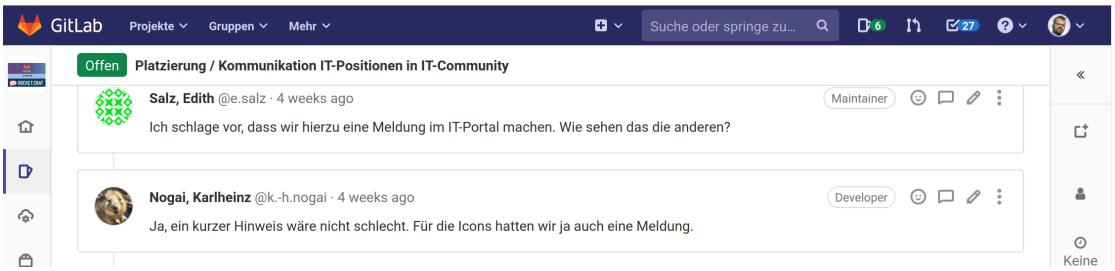
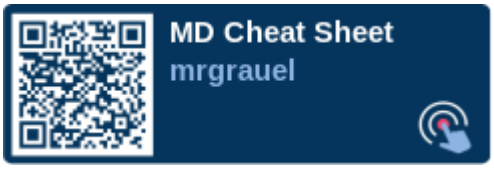



Figure 4: Discussion in a ticket in GitLab

### Text writing

You probably remember the article in the IT newsletter about iffmd. md stands for Markdown. In GitLab you have another possibility to write texts in this way.

Find an overview of the syntax here: Cheat Sheet by mrgrauel, CC-BY-SA 2.0



### Kanban display

The labels are used for grouping. This grouping can be visualised next to the list in a Kanban Board.

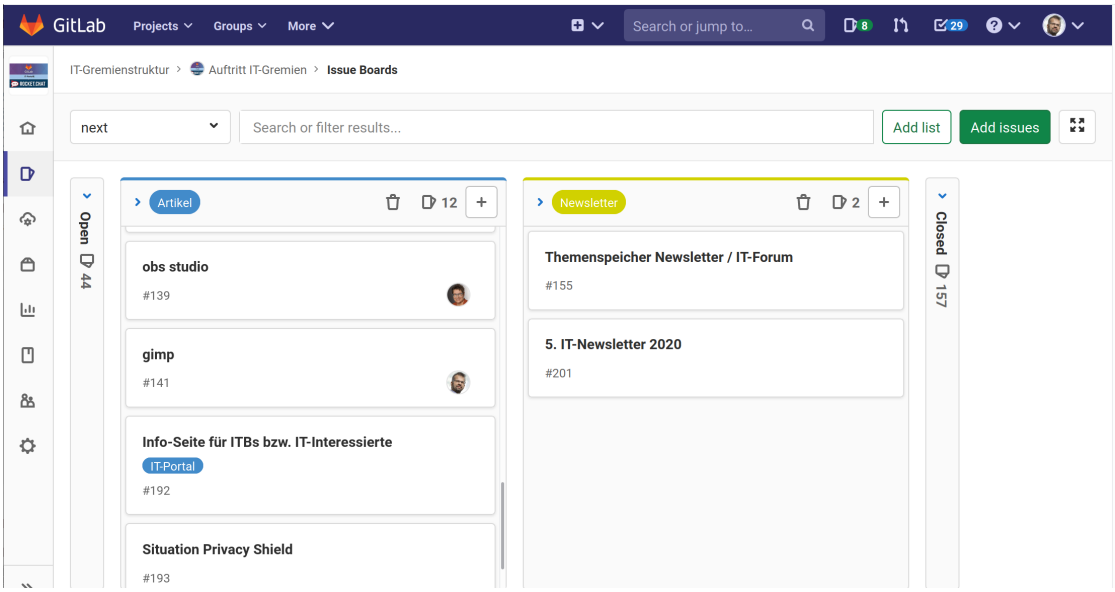



Figure 5: Planning view in Kanban layout

### Shortcuts

The "?" gives you an overview of the key commands.

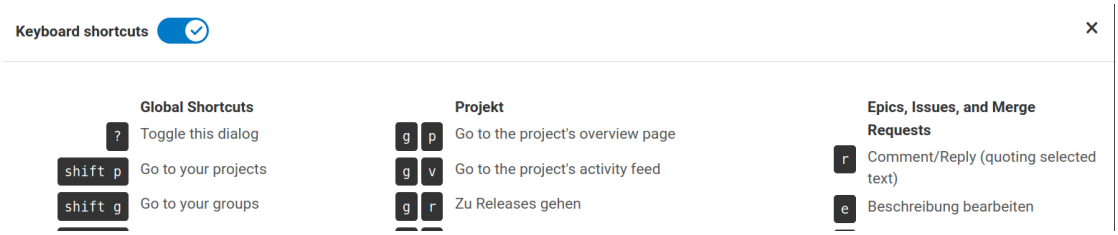



Figure 6: Shortcuts

## GitLab Use Case: Quality Management

*Ulrich Ivens*

GitLab is actually a web application used for software development. And that has little to do with a quality management system according to DIN EN ISO 9001:2015. Of course quality management is also important in software development, but with our use case of GitLab we are miles away from software development or data management or similar things - after all, we are part of the human resources department. And yet, at P-Z (Zentrale Berufsausbildung), we have a great deal to gain from and with GitLab. The ticket system in GitLab described in the previous article is a very powerful tool that, through its ease of use, has literally (positively) turned our already very mature quality management system on its head in a very short time.

Specifically, as the (first) application, we have changed our error handling process (in the QM mind: corrective and preventive actions as well as tracking and implementing improvements) to the ticket system in a closed GitLab project

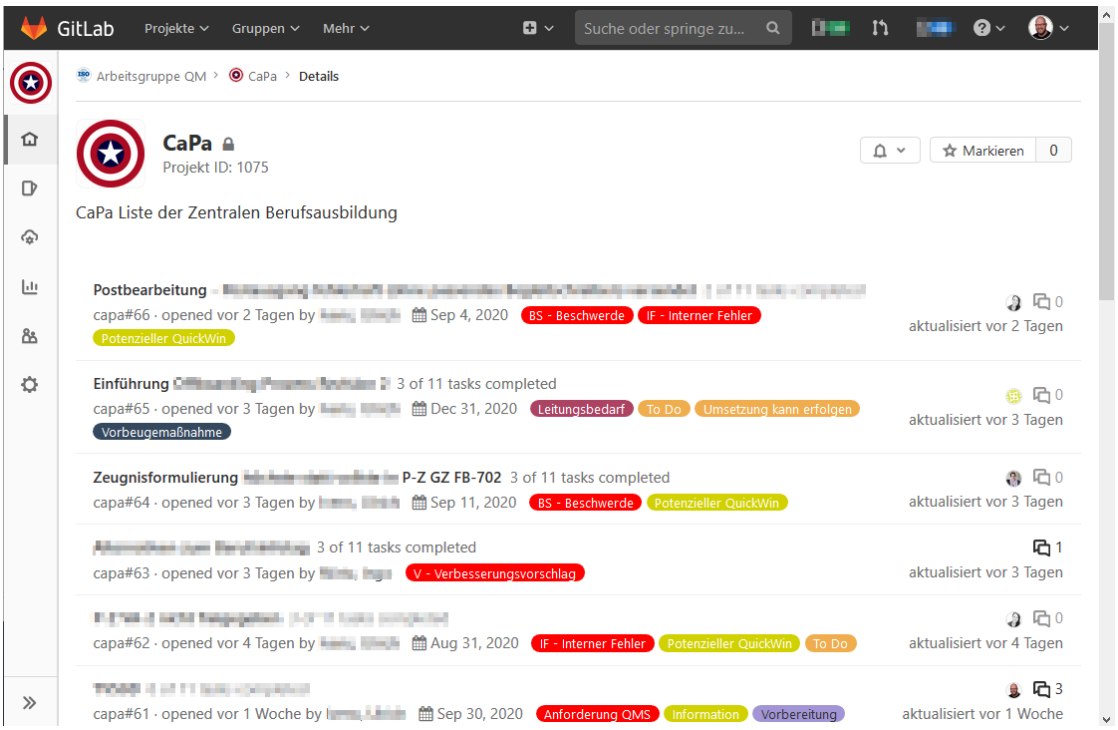



Figure 7: Tickets incl. labels in list view

This was traditionally done via our CaPa list, which was created in Excel and managed with ConSense. We also use the CaPa list for other measures, not only for errors, but also for suggestions for improvement, complaints and the like.

The actual advantages of GitLab in our Use Case are

1. it is very flexible as a web application and works both from the home office and from the company. Apart from a VPN access or the Linux Remote Desktop via Guacamole, nothing is necessary for the server we use.
2. several employees can work in it at the same time, the waiting times are significantly reduced. Colleagues from other OUs can be easily integrated into projects.
3. content and communication are bundled in one place The workflow in the processing of tasks is therefore not disturbed by media breaks.
4. those who continue to favour e-mail also receive all necessary information by e-mail.
5. the documentation is complete and of higher quality than in conventional working formats. It is therefore easier to keep track of and remains persistent, because closing the tickets only removes it from focus, but does not delete it.

In our use case, the previous method has not only been replaced by another format. The new format has been optimised through topic-related communication and knowledge management.

It should be interesting for the managers that the adaptation is also appreciated by almost all employees in my department. The whole thing has almost become independent in a very short time and has become something like a "new work approach" - without any great pain of adaptation. The most difficult thing for some people is probably to get involved in Markdown, but you learn that very quickly.

This newsletter article gives a first overview of the advantages of our Use Case. Further applications in P-Z will follow (or have already been implemented) e.g. the "planning of changes" procedure prescribed in the QMS, digital filing, meeting documentation...


The Use Case is described in detail (especially with the *how*) in a detailed article, which can also be found in iffMD

## What is a "GitLab Runner"?

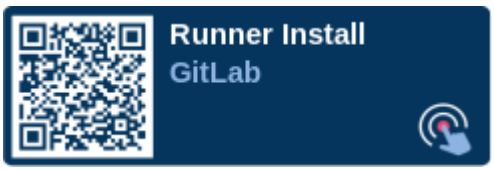
*Jörn Ungermann*

The Continuous Integration (CI) features built into GitLab have many uses: From simple code analysis (checking syntactic correctness and adherence to style guides), to functional correctness testing, to automatic construction of scientific publications (LaTeX), documentation websites, or docker containers. This list also expresses the historical use of IEK-7 through a better understanding of the possibilities of the platform. IEK-7 is now in charge of more than a dozen software projects and even more LaTeX

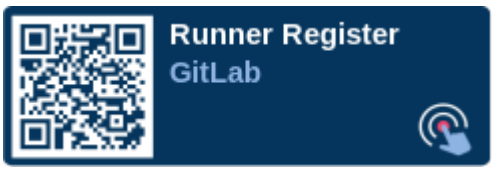
projects, all of which are built and/or tested via CI, and for which a successful run through the CI pipeline is the prerequisite for a merge through the four-eyes principle.

At the beginning of our GitLab use, we had little experience with these systems, and the use of the infrastructure provided by ITS already places relatively high demands on the automation of the software project, which were generally not met. We circumvented the problem in the first phase by using our own Gitlab runner. A runner is a service that communicates with the GitLab server and at its behest commands are executed on the local machine. This allows the software project to be automatically tested directly on the machine, which is also used for development and/or production purposes. The advantages are self-evident: the necessary environment (e.g. obscure C or Fortran libraries or special commercial compilers) for building and deploying the software is directly available and the necessary (test) data is generally available.

Runner Install:




Runner Register:




The installation of the Runner software on the target machine is well documented at https://docs.gitlab.com/runner/install/linux-repository.html and takes only a few minutes. Besides Linux, other operating systems are also supported. Creating the Runner service and registering it on jugit.fz-juelich.de hardly takes any longer (https://docs.gitlab.com/runner/register/; the machine must be accessible via http from jugit.fz-juelich.de!) There are different variants of runners, but for starting it is recommended to use a simple "shell" access, where the commands of the CI pipeline are executed directly in a shell on the target system. This involves a dedicated user with limited rights, but who can in principle gain access to all resources of the system. In this way, we were able to initiate the automated building and testing of a complex C++ software via jugit-CI on our own hardware in half a morning.

Since then, slowly and bit by bit, we have switched to more complex procedures and meanwhile also docker-based containers for encapsulating the development environment, which allow you to easily switch between your own runners and those provided by ITS. Only for tests with extensive data or very long runtimes do we still exclusively use our own runners.

In this way, GitLab allows an easy and immediate entry into the automated testing of your own projects.

## Technical Data Security at Forschungszentrum Jülich

*Frank Rinkens*

The General Data Protection Regulation GDPR placed considerable demands on companies. The somewhat new legal situation has a particular impact on IT security, which is now a fundamental component of data protection and data security, i.e. technical data protection. For technical practice and the handling of data, there are a lot of new obligations for Research Centre Jülich and its own IT landscape.

**New Rules of the GDPR** In the past, IT security and data protection were often considered separately. However, the new regulations of the DSGVO extend the legal requirements for the IT landscape of a company substantially that IT security becomes a fundamental component of data protection. This can have a considerable impact on the IT officers or administrators of the research centre when it comes to new system purchases, in-house designs and their maintenance, as soon as personal data is affected. In retrospect, the rather unusual practice of transferring IT security and data protection to one person thus proves to be forward-looking and goal-oriented. Data protection law now also makes use of the IT security protection goals of confidentiality, integrity, availability and resilience of IT systems.

Article 5 GDPR regulates what is to be observed in this context. This states that personal data must be processed in such a way that "adequate security of the data is ensured, including protection against unauthorised or unlawful processing, loss, destruction or damage". More specifically, Article 32 GDPR, which defines the technical requirements for the processing of personal data, is more specific. According to this article, factors such as "the state of the art, implementation costs, the different probabilities of occurrence and the seriousness of the risk to the rights and freedoms of the data subjects" must be taken into account. The decisive factor for us is therefore what the owners of the data could be threatened with, for example, by a data breach and that this risk is brought to an acceptable level of protection/residual risk by organisational and technical measures. The relationship between risk and package of measures must therefore be consistent and coherent.

At the same time, the GDPR offers some more or less concrete methods to ensure this:

- Pseudonymisation and encryption
- the ability to ensure the confidentiality, integrity, availability and resilience of systems and services over time
- the ability to quickly restore the availability of and access to data in the event of a technical incident

- regular review and evaluation of the effectiveness of the organisational and technical measures to ensure safety.

In practical terms, this means that the obligation to make regular backups is just as much a legal obligation as the regular testing of one's own IT infrastructure, for example through pentesting or nessus scans. However, it is not absolutely necessary to implement all of these exemplary measures. Sufficient is a convincing concept for IT security, which can and should contain these parts, but is not mandatory. The Research Centre ensures this with the IT security guidelines, also with regard to data protection. Nevertheless, this must always be re-evaluated when new acquisitions are made in the IT environment and the technical and organisational measures must be checked for effectiveness.

The TOMs, i.e. the **T**echnical and **O**rganisational **M**easures, play an essential role in the evaluation of the IT security available at the research centre. If business units of the Research Centre act as contract processors for a third party within the meaning of data protection law, the clients always query our TOMs, just as we do with our contractors before the start of the contract. They document how the data of the persons concerned are protected and secured; according to Art. 32 GDPR, a "level of protection appropriate to the risk" must be achieved. The TOMs are particularly important if the state data protection authority of North Rhine-Westphalia investigates a data protection breakdown. In this case, the research centre must also use the TOMs to prove that it had taken appropriate measures to protect the data concerned. Therefore, documentation of the measures taken in the area of IT infrastructure is also essential in this area. For new IT systems - the IT security officer of the research centre is usually involved at an early stage - the data protection officer must therefore also be contacted. He prepares a risk assessment and evaluates the TOMs already taken. For ITBs, a checklist of TOMs is available to prepare the meeting with the DPO. This is the only way to ensure that the existing TOMs can be extended with new measures if necessary. However, the TOMs are not witchcraft.


Forschungszentrum Jülich had already taken the necessary measures before the DSGVO came into force. Now it is important to extend these measures where necessary in the context of risk. In order to be able to test the effectiveness of the TOMs early on in the development phase, the DSGVO stipulates that "privacy by design" (data protection through technology design) or "privacy by default" (data protection through data protection-friendly default settings) must be taken into account when procuring new IT systems. These formulations refer to systems which are already prepared for active data protection in the factory or in development, whether by automatic settings with regard to encryption, pseudonymisation up to deletion of the data or by data-saving programming so that only the data which is required for the purpose of processing is

stored. In this way it is possible, for example, to ensure at an early stage in larger database projects that personal data can be deleted with little effort if necessary. Manufacturers of IT systems have already recognised this as added value and competitive advantage. FZJ project managers should discuss this possibility with the providers at an early stage.

The DPO Frank Rinkens, Tel. 02461 61 9005, f.rinkens@fz-juelich.de, @f.rinkens is available at all times to answer questions and discuss specific projects.

**Data Protection Infos on the IT Portal:**


## ECJ-Ruling: Data protection agreement with USA invalid - research centre also affected

*Text of an internal release to the OU-Heads, dated 2020-08-03*

*The heads of the OUs of the Research Centre were informed about the consequences of the ECJ ruling in a memorandum of the Executive Board at the beginning of August.*

**ECJ Ruling and its consequences**
A decision with far-reaching consequences for companies and research institutions across Europe: the legal basis for the transfer of personal data from Europe to the US has been annulled by the European Court of Justice (ECJ). According to a ruling of the ECJ on 16 July, the EU Commission's previous decision - the so-called EU-US Privacy Shield - is invalid. The reason: the ECJ no longer considers the level of data protection prevailing in the US to be sufficient.

"Many software products and web services that are also used at the research centre are affected by the ruling," says data protection commissioner Frank Rinkens. "This ranges from the use of certain video conferences to cloud solutions whose providers are based in the USA - even if the servers used are located in Europe. In the same way, it can also affect data exchange with US partners in research cooperations.

**Privacy Officer: Assistance needed from OUs**
As the Data Protection Officer, Rinkens is currently preparing an overview of the software and online services used at the Research Centre, where data flows to the USA take place. The Data Protection Officer asks all business units and institutes to identify such data flows - also in the context of cooperation and project work - as quickly as possible and to report them collectively to him via the OU heads - and thus to support him in individual case examinations and in providing an overall overview.

“This is important in order to check which legal basis forms the basis in each case - and whether there is a concrete need for action, which I will support,” said Rinkens. "For the supervisory authority can at any time examine how the research centre has reacted to the changed legal situation.

Central service providers such as Microsoft, Google or AWS (Amazon Web Services) are already being examined.

Rinkens is available to answer any questions by phone: 02461 61-9005 and e-mail: f.rinkens@fz-juelich.de.

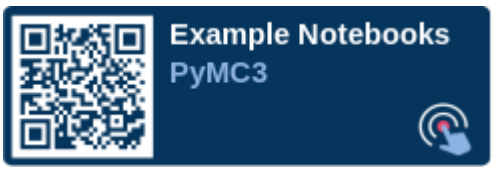
## PyMC3 – Insight through probabilistic programming and domain knowledge

*Michael Osthege*

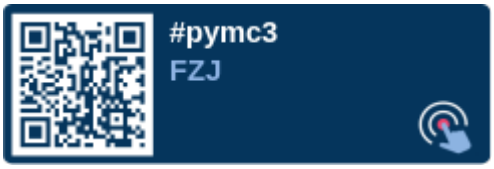
PyMC3 is a probabilistic programming language that enables users to encode their domain knowledge and assumptions as intuitive Python code and run sampling with cutting-edge MCMC algorithms. Via autodifferentiation, PyMC3 automatically calculates gradients, enabling the use of Hamiltonian Monte Carlo (specifically NUTS) sampling that remains efficient even for models with hundreds of dimensions.

Its capabilities range from multivariate, multilevel modeling to Gaussian processes, or variational inference, with applications in astrophysics, biology, finance, sports and epidemiology.


One recent example, with involvement from Forschungszentrum Jülich is the application of PyMC3 for Rt.live and Rtlive.de, where it is used to infer COVID-19 reproductive numbers and case counts while accounting for infectiousness period, testing delay and variations in testing exposure.




Apart from the example gallery, you should take note of the PyMCON 2020 online conference, and you might want to join the #pymc3 channel on the Rocket chat




## New Hardware included in the IT-Standards

*Helmut Timmermanns*

The hardware for the notebooks, the office PC as well as the CAD and standard PC was adapted to the new models of the manufacturers. The devices are thus based on the latest chipsets and processors. Technical details, prices and order templates for this can

be found in the IT standards section of the IT portal. Software Licences and Hardware Standards in the access of the IT portal.


### Displays

Those who use their workstation in combination with a docking station and a current USB-C capable notebook will be pleased about the following technical advancement of the monitors: The docking station moves into the monitor in the future. In addition to the power cable, the network cable and other peripherals, such as keyboard or mouse, will then also be connected directly to the monitor. All that remains is a USB-C cable to the notebook. All communication, screen output and recharging of the notebook runs via this cable. As a result, the workplace will look much tidier in the future and more space will be available on the desk.

### Headsets & Webcams

The availability and delivery situation for headsets is still extremely difficult. Delivery times are often 6 to 8 weeks, and even these figures are still subject to a high degree of uncertainty. Fortunately, prices here are only moderately higher than before. Unfortunately, the situation is completely different for webcams. Simple standard HD cams, which were otherwise available for about 30 €, are now for example as much as 110 €. Even estimated delivery dates are not available here at all. Please feel free to inform Helmut Timmermanns (h.timmermanns@fz-juelich.de) about your requirements. He bundles them and, supported by the purchasing department, takes care of the procurement of technically and price-wise suitable components.

### AK IT-Standardisierung

## Current Topics in the IT Forum: Join the discussion!

IT-Gremien IT-Forum
FZJ Intranet

**Selected topics:**

- Communication tool for projects with external parties (Rocket Chat) #116
- Archiving of forums and wayback access for the readers as a whole in FZJ #172
- Mentimeter / Kahoot alternative for live voting at FZJ #178
- Recruitment of research data managers #179
- New action group: Implementation of a guideline for sustainable research software at Forschungszentrum Jülich (AK Forschungssoftware) #187
- Appointment of representatives of the IT committees for the Aktionskreis IT-Standardisierung from the IT-Forum #188

## IT-Officers

In recent weeks, the following colleagues have been appointed as IT officers for their organisational unit.


Daniel Antons (UK)
@d.antons


Eta Billion (M)
@e.billion


Dr. Daniel Mann (ER-C-3)
@d.mann


Dr. Nils Rosjat (INM-3)
@n.rosjat

**Full list of IT-Officers**

Liste IT-Beauftragte
FZJ Intranet

## Imprint

The IT Newsletter is a format to report on topics and news from the IT committees, especially the IT Forum but also from the action groups. Each issue presents people who are involved in the IT committees. In addition, there are interesting and useful information on a wide range of IT topics. In this way, we are also pursuing the goal of making the IT committees and the new participatory cooperation model better known and encouraging participation. The IT Newsletter is published regularly but not at a fixed rhythm.

Contact person for the IT Newsletter is the Aktionskreis Auftritt der IT Gremien. Editors: Edith Salz (UE, responsible), Reimar Bauer (IEK-7), Arne Graf (IAS-7), Belinda Lelke (ITS), Karlheinz Nogai (IEK-7), Frank Rinkens (DSB), Stephanie Schmitz (TB-P), Horst-Toni Lambertz (IEK-4).

Suggestions, criticism and wishes are expressly requested: it-news@fz-juelich.de or directly in the Rocket.Chat channel of the action circle (if necessary, log in with central username and email password and switch to #ak-auftritt-it-gremien)

Information on the current topics of the IT committees and action groups about GitLab: itg.fz-juelich.de

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