

Information Infrastructure for Data Assimilation

Z03



Hi. This is us.

We want your data to matter! We want...

- to facilitate the sharing of data, algorithms, and results
- to safeguard the sustainable handling of digital artefacts
- to ensure good publication practice

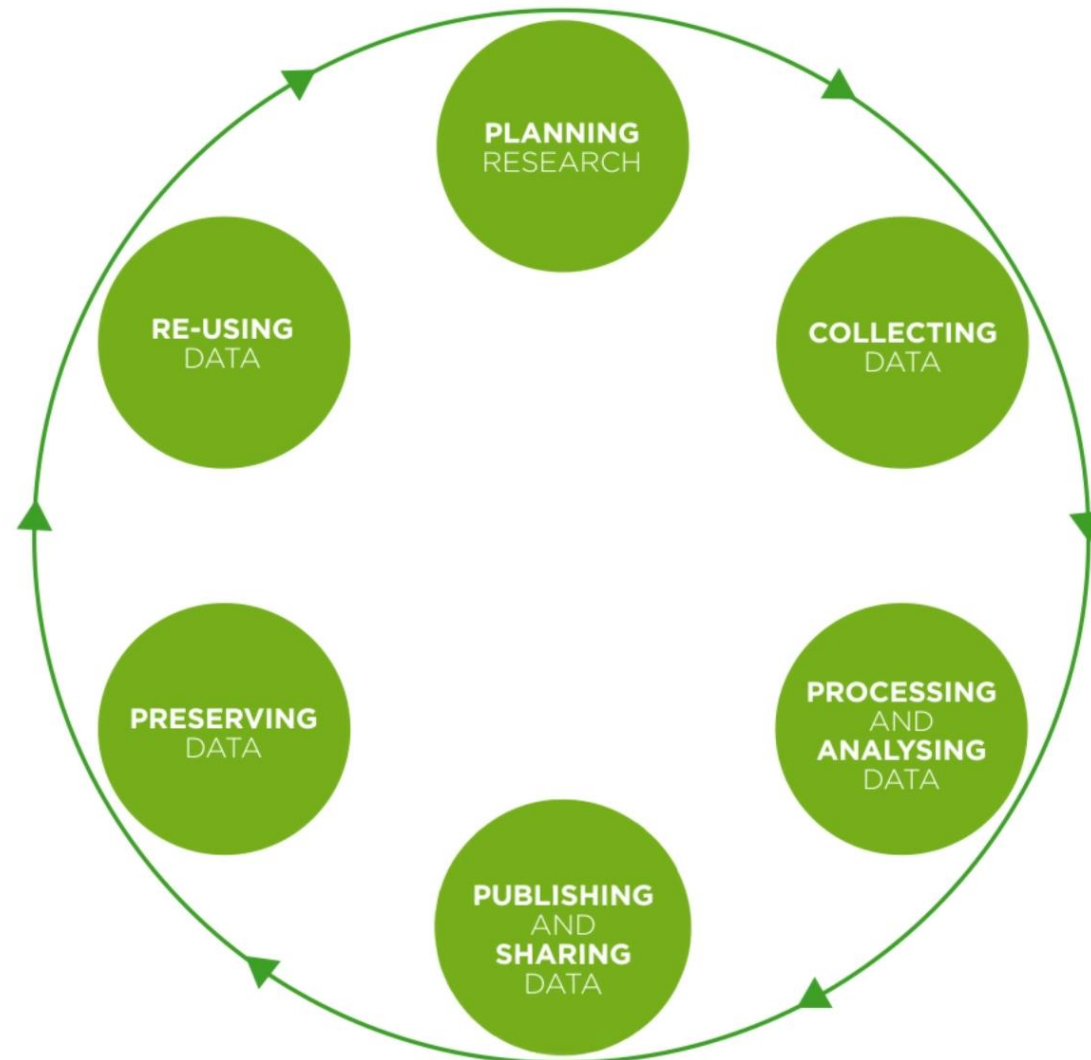
PIs: Prof. Dr. Ulrike Lucke, Prof. Dr. Ralf Engbert,

Staff: Dr. Christian Riedel (Researcher), N.N. (Technician)

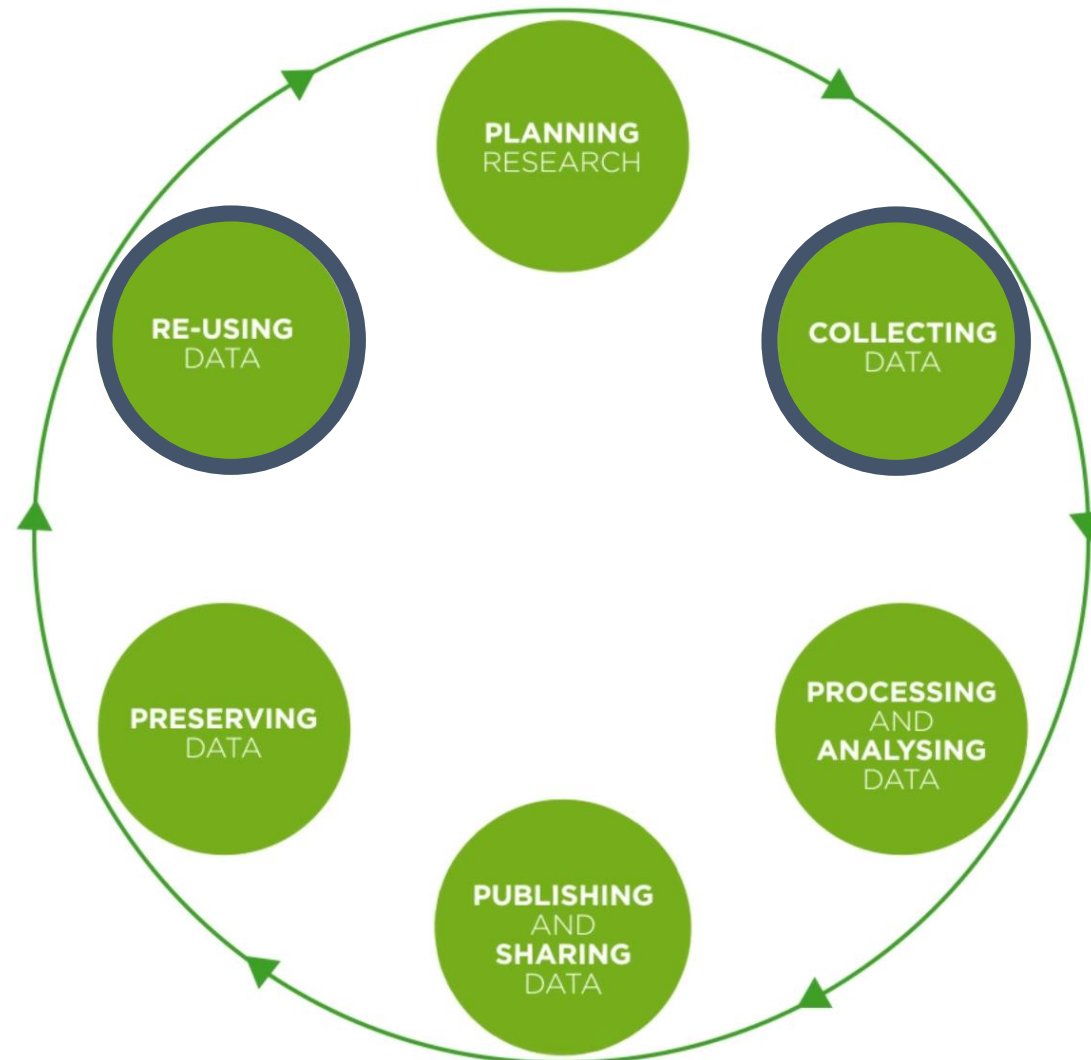
Stud. Assist.: Safial Islam Ayon, Shafayet Hossen Chowdhury



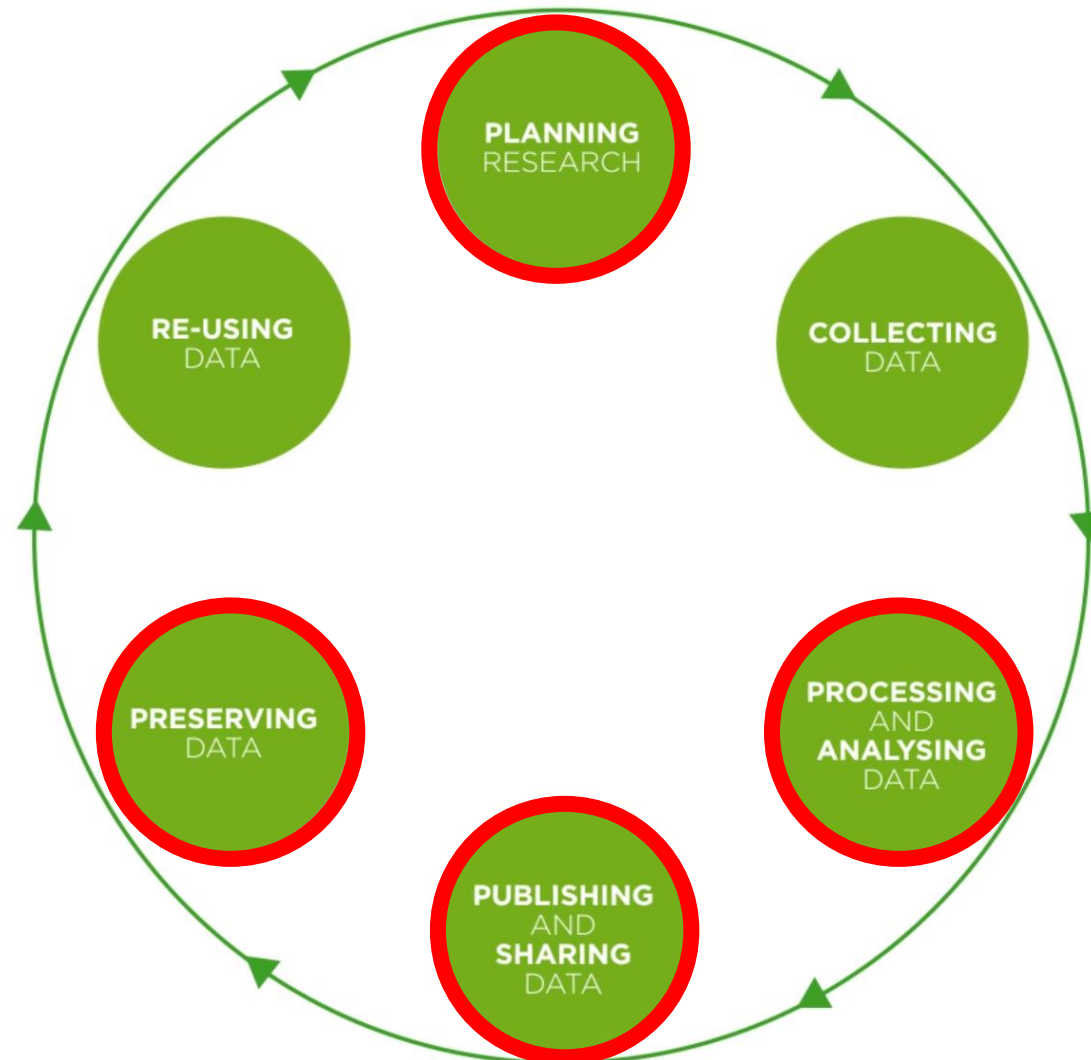
Research Data Lifecycle



Research Data Lifecycle: Specific Aspects



Research Data Lifecycle: Generic Aspects



Managing your Research Process

Planning

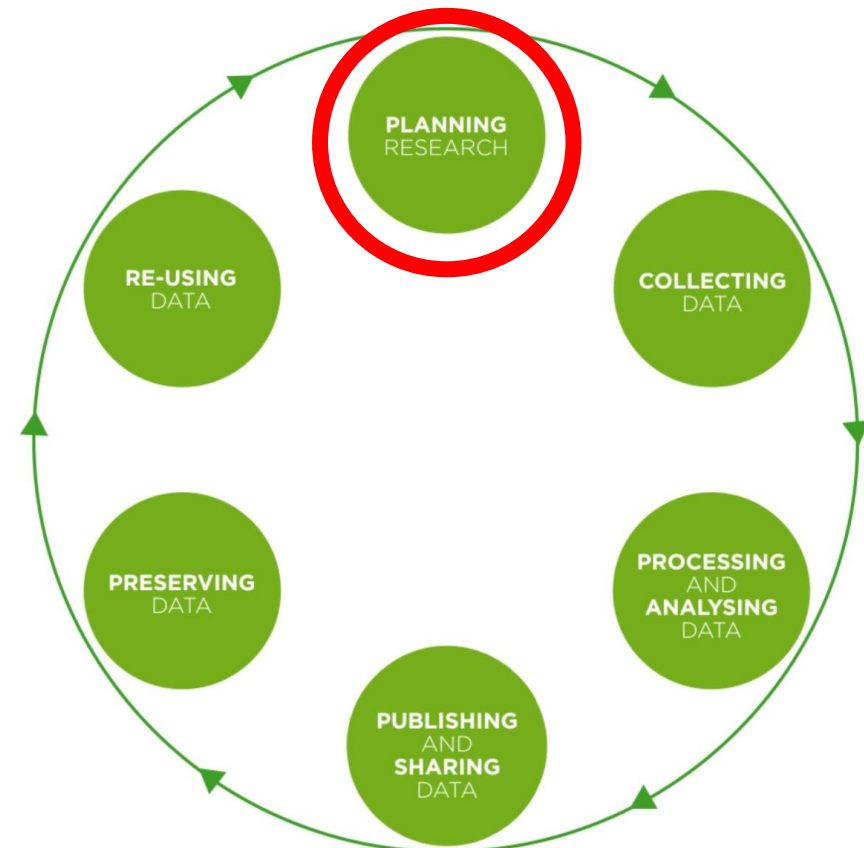
- RDMO.UP

Quality Checks

- ConQuaire

RDMO.UP

ConQuaire



Planning Research

Project Planning

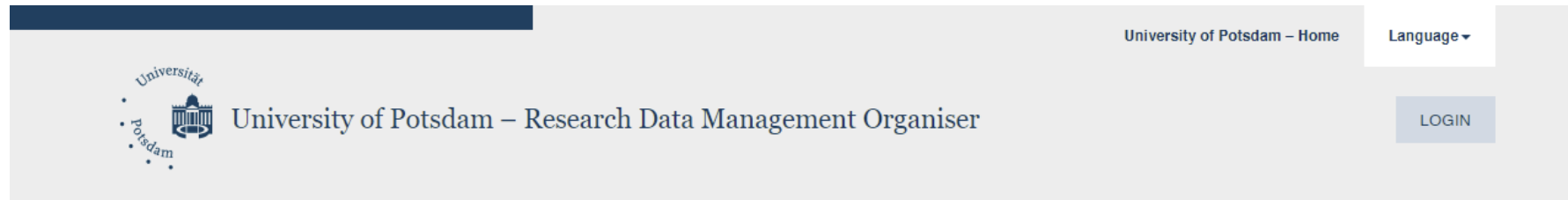
Applicants should [...] detail in the proposal **what research data will be generated or evaluated** during a scientific research project.

- Required by funding agencies (depends on the programme)
- Tool for quality management in research data management

To record the intended handling of research data includes:

- activities during the research process & subsequent handling
- information about data collection, preparation, archiving, and publication

Research Data Management Organizer



Welcome to RDMO.UP

You can use RDMO.UP – University of Potsdam's Research Data Management Organizer – for the following tasks:

- Plan and document data management for your research project in a structured way. To that end, you can choose from several questionnaires.
- Share data management plans with other users and edit them collaboratively.
- Create versions of data management plans to make changes and account for changing circumstances during project progression.
- Export different views on your answer to generate documents that fulfill particular funder requirements regarding data management plans.

RDMO.UP is a service of University of Potsdam's Research Data Management Team, staffed collaboratively by the University Library (UB) and the Centre for Information Technology and Media Management (ZIM). The service currently operates in test mode. It is available for testing by University of Potsdam researchers and their external collaborators. If this does not apply to you, please do not use RDMO.UP for testing and make use of AIP's public RDMO demo installation instead.

RDMO.UP is not currently integrated with University of Potsdam's single sign-on. To use it you need to register.

Login

Username

christian.riedel

Password

.....

☐ Remember Me

Login

If you have not created an account yet, then please [sign up](#) first.

If you forgot your password and want to reset it, [click here](#).

Alternatively, you can login using one of the following third party accounts:



<https://rdmo.uni-potsdam.de/>

Research Data Management Organizer



[University of Potsdam – Home](#)

[Language](#) ▼



University of Potsdam – Research Data Management Organiser

[LOGIN](#)

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christian.riedel

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Alternatively, you can login using one of the following third party accounts:

 SIGN IN with **ORCID** 

Continuous Quality Control for Research Data

... to ensure reproducibility



- Git integration
- Automatic tests: e.g., whether a particular result can be reproduced
- Implementation of CI Runner in Git.UP

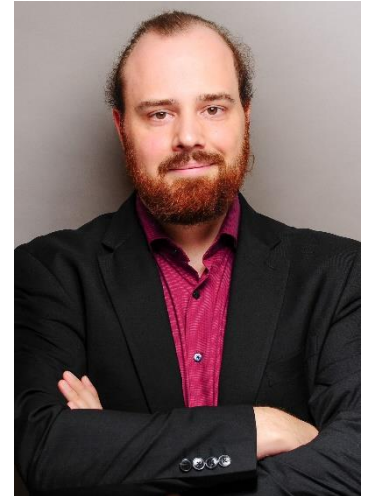
→ Please let us know, if you want to include this in your research!

→ Experiences in CI/CD pipelines are highly valued in the industry!

We are not alone!

Services provided by ZIM and UB

Hendrik Geßner,
Team Leader Application Operation



Services for Research Data and Code

Processing and analysing

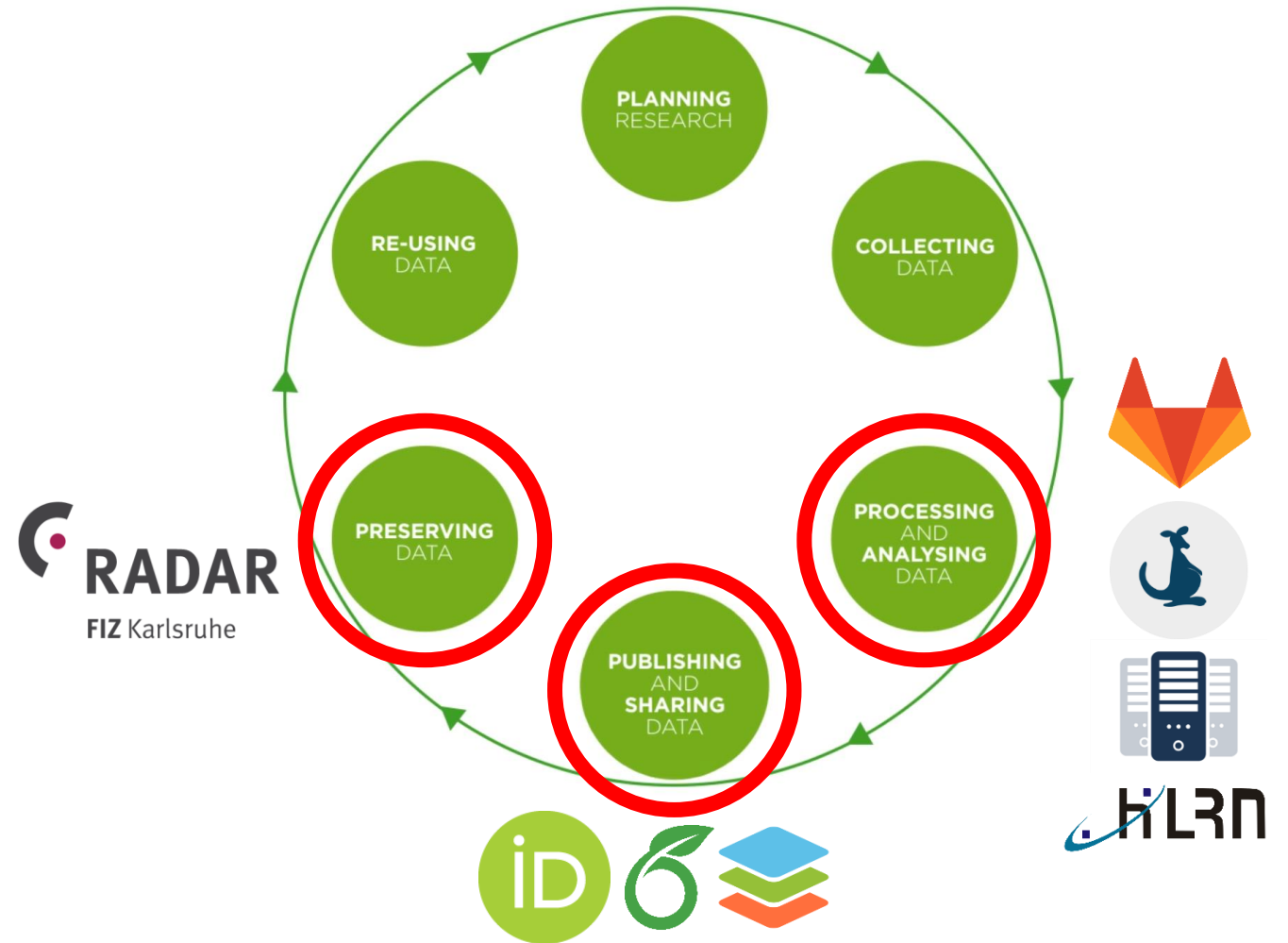
- Git.UP, Box.UP, HPC.UP, HLRN

Publishing and sharing

- ORCID, Overleaf, OnlyOffice

Preserving

- DSpace, RADAR.UP



Services for Research Data and Code

Processing and analysing

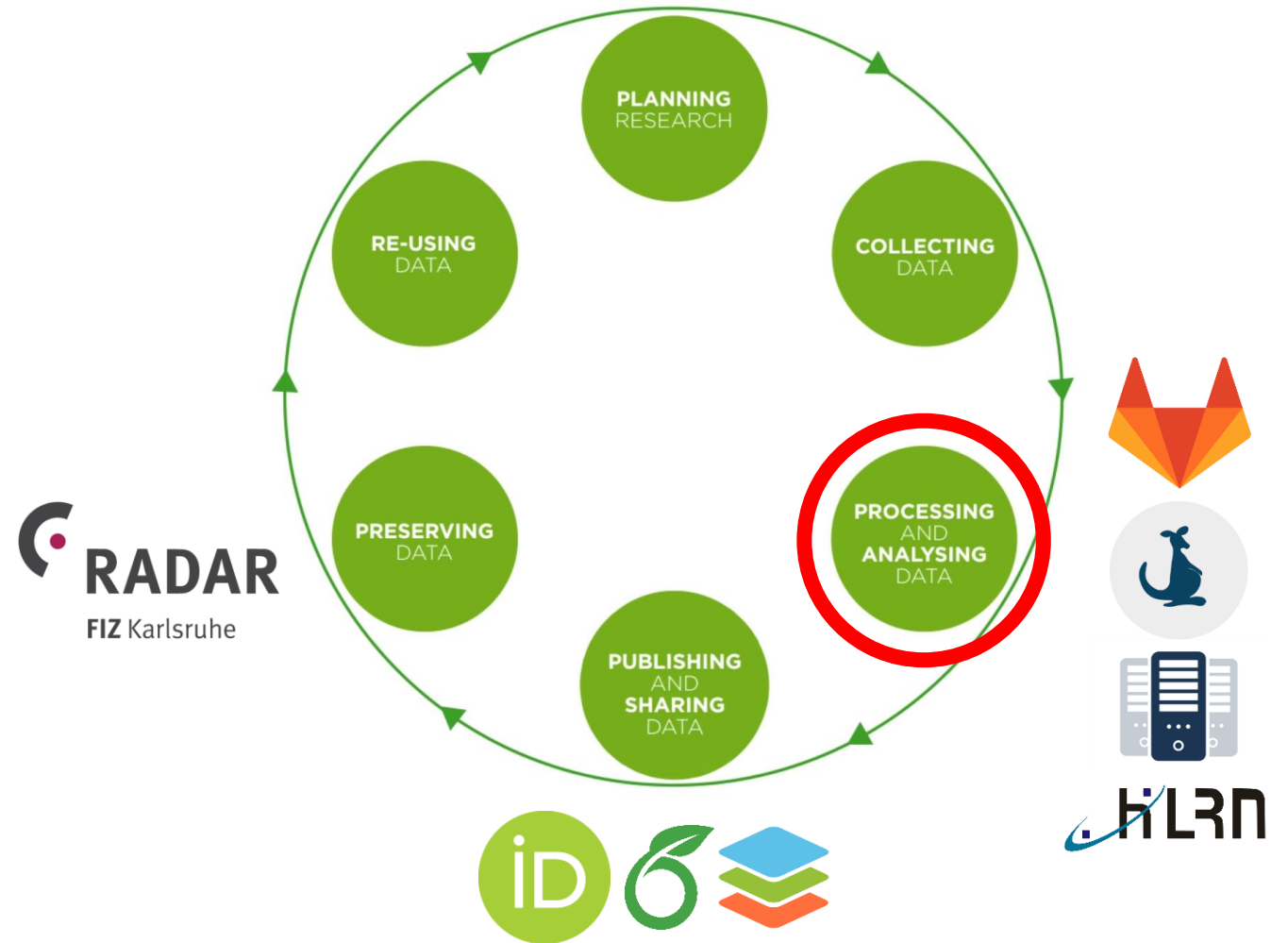
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Storage and Backup



Servers and Services

- ✓ Box.UP
- ✓ Git.UP
- ✓ CRC Wiki + Archive

- ? Your external HDD
- ? Your server

Setting up a backup (3-2-1 rule)

- *At least 3 copies per file*
- *On at least 2 different media*
- *Of which at least 1 is remote*



Storing Data and Documents: Box.UP



Personal Storage

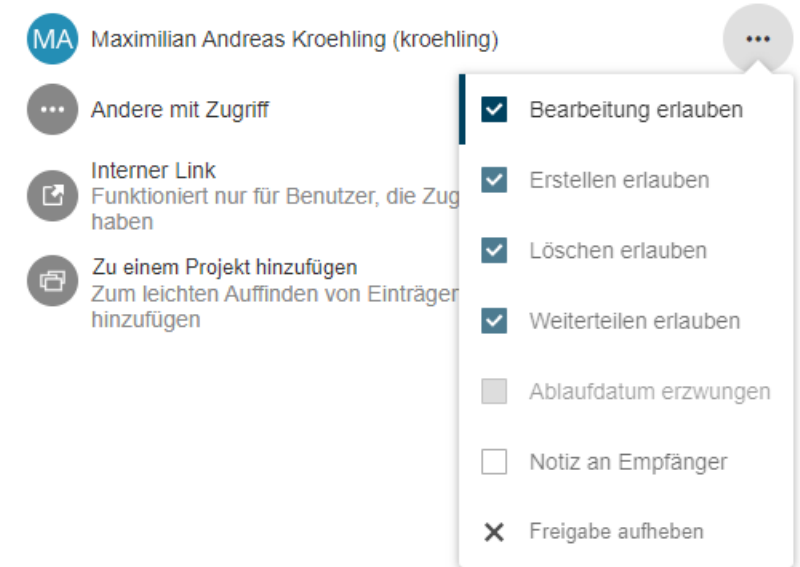
- „Dropbox@UP“
- 30 GB cloud storage
- Web interface, clients for desktop and mobile devices

CRC 1294 folder

- 20 TB cloud storage
- Professional backup

Sharing

- Link (with password, 365 days)
- With Accounts (unlimited)



Storing Data and Code: Git.UP



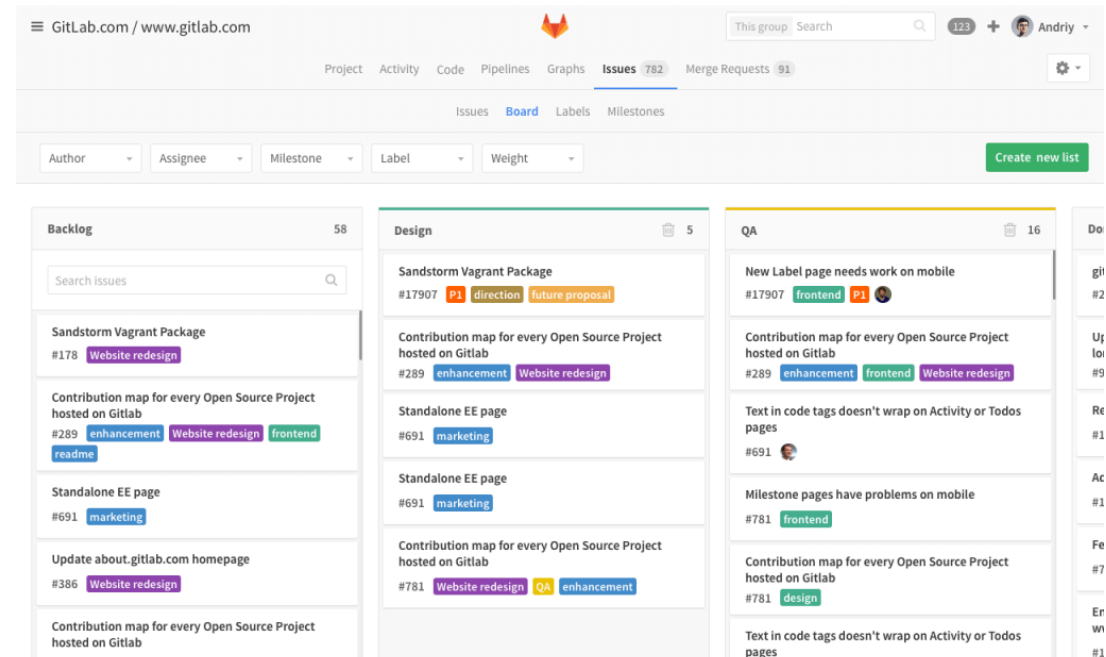
Project management

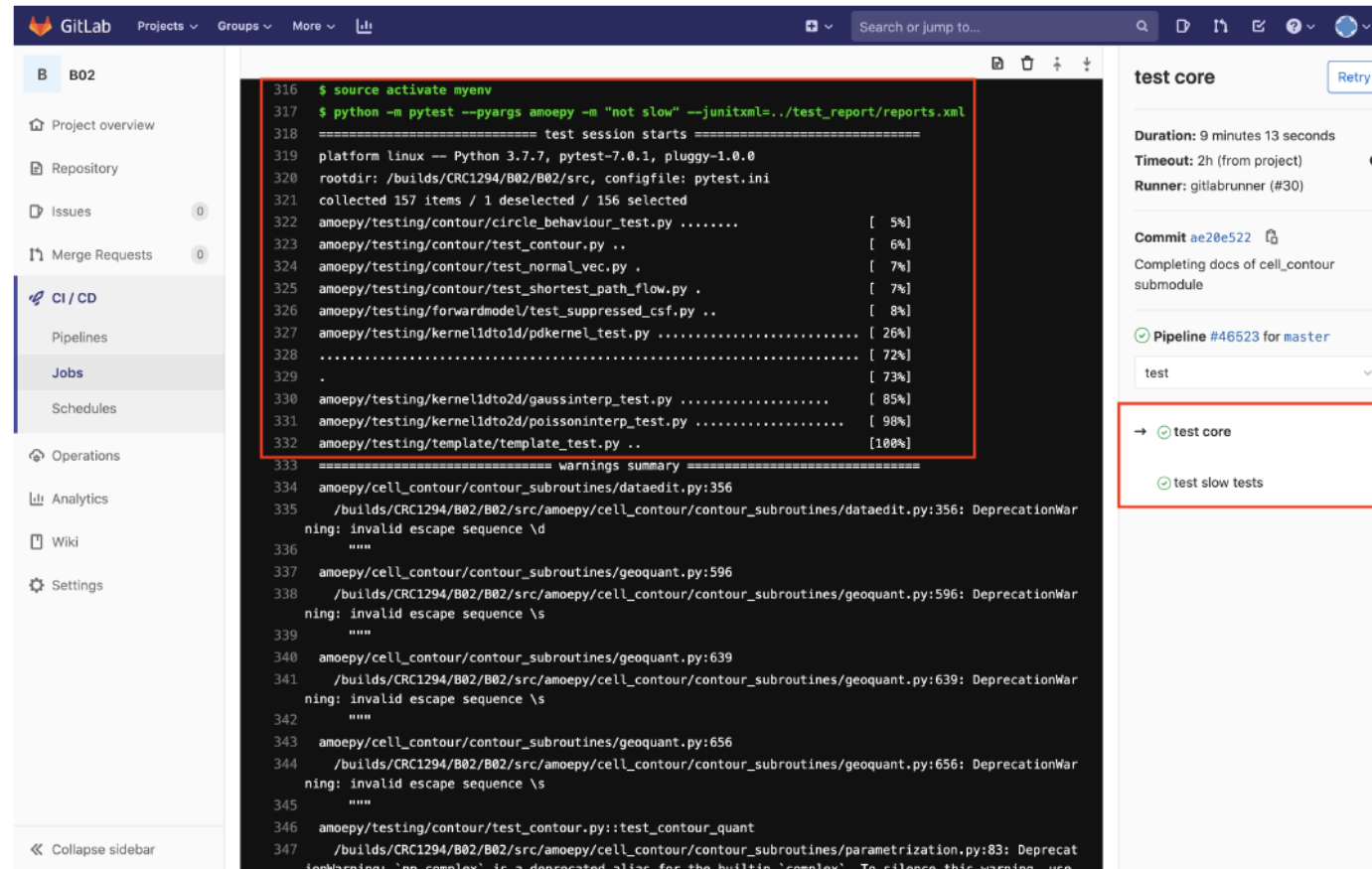
- Tasks, milestones, tags and keywords, time spent, ...

Integrated tools

- Git
- Issues
- Wiki
- CI/CD and automation

Kanban boards in Git.UP





The screenshot displays the GitLab CI/CD interface for a project named 'B02'. The left sidebar shows navigation options: Project overview, Repository, Issues, Merge Requests, CI/CD (selected), Pipelines, Jobs, Schedules, Operations, Analytics, Wiki, and Settings. The main area shows the details of a pipeline run for the 'test' job. The terminal output is as follows:

```

316 $ source activate myenv
317 $ python -m pytest --pyargs amoepy -m "not slow" --junitxml=../test_report/reports.xml
318 ===== test session starts =====
319 platform linux -- Python 3.7.7, pytest-7.0.1, pluggy-1.0.0
320 rootdir: /builds/CRC1294/B02/B02/src, configfile: pytest.ini
321 collected 157 items / 1 deselected / 156 selected
322 amoepy/testing/contour/circle_behaviour_test.py ..... [ 5%]
323 amoepy/testing/contour/test_contour.py .. [ 6%]
324 amoepy/testing/contour/test_normal_vec.py . [ 7%]
325 amoepy/testing/contour/test_shortest_path_flow.py . [ 7%]
326 amoepy/testing/forwardmodel/test_suppressed_csf.py .. [ 8%]
327 amoepy/testing/kernelldto2d/pdkernel_test.py ..... [ 26%]
328 ..... [ 72%]
329 . [ 73%]
330 amoepy/testing/kernelldto2d/gaussinterp_test.py ..... [ 85%]
331 amoepy/testing/kernelldto2d/poissoninterp_test.py ..... [ 98%]
332 amoepy/testing/template/template_test.py .. [100%]
333 ===== warnings summary =====
334 amoepy/cell_contour/contour_subroutines/dataedit.py:356
335 /builds/CRC1294/B02/B02/src/amoepy/cell_contour/contour_subroutines/dataedit.py:356: DeprecationWarning: invalid escape sequence \d
336     ....
337 amoepy/cell_contour/contour_subroutines/geoquant.py:596
338 /builds/CRC1294/B02/B02/src/amoepy/cell_contour/contour_subroutines/geoquant.py:596: DeprecationWarning: invalid escape sequence \s
339     ....
340 amoepy/cell_contour/contour_subroutines/geoquant.py:639
341 /builds/CRC1294/B02/B02/src/amoepy/cell_contour/contour_subroutines/geoquant.py:639: DeprecationWarning: invalid escape sequence \s
342     ....
343 amoepy/cell_contour/contour_subroutines/geoquant.py:656
344 /builds/CRC1294/B02/B02/src/amoepy/cell_contour/contour_subroutines/geoquant.py:656: DeprecationWarning: invalid escape sequence \s
345     ....
346 amoepy/testing/contour/test_contour.py::test_contour_quant
347 /builds/CRC1294/B02/B02/src/amoepy/cell_contour/contour_subroutines/parametrization.py:83: DeprecationWarning: 'nn.complex' is a deprecated alias for the builtin 'complex'. To silence this warning, use
  
```

On the right side, the 'test core' job details are shown, including a 'Retry' button, duration (9 minutes 13 seconds), timeout (2h), and runner (gitlabrunner (#30)). Below this, the commit 'ae20e522' is listed with the message 'Completing docs of cell_contour submodule'. A 'Pipeline #46523 for master' is also shown. At the bottom, a list of jobs is displayed, with 'test core' and 'test slow tests' highlighted by a red box.

Figure 10. All dependency cycles in Amoepy

```
class DynQuant(object):
    """
    Methods of :class:`amoepy.cell_contour.contour.Contour`
    regarding the computation of dynamics quantities such as:
    - local dispersion
    - normal velocity
    - normal vectors/Frenet vectors between contours
    """
    def __init__(self):
        """
        Constructor of
        :class:`amoepy.cell_contour.contour_subroutines.dynquant.DynQuant`
        """
        Note
        -----
        However, this class is not meant to be used separately.
        Its purpose is a better organization of all functions of
        :class:`amoepy.cell_contour.contour.Contour`.
        """
        pass

    def frenet_vectors(self, r, sigma, n_clip=None):
        """
        Compute the x- and y-coordinates of virtual markers
        based on GPR smoothing and the corresponding Frenet vectors
        (normalized tangent and normal vectors)
        and the curvature.

        The Frenet vectors are given by the formula:

        .. math ::
            \begin{aligned}
            \vec{e}_1(\theta) &= \Phi'(\theta) \\
            \vec{e}_2(\theta) &= \Phi''(\theta) - \langle \Phi''(\theta), \vec{e}_1(\theta) \rangle \vec{e}_1(\theta) \\
            \vec{t}(\theta) &= \frac{\vec{e}_1(\theta)}{\|\vec{e}_1(\theta)\|_2} \\
            \vec{n}(\theta) &= \frac{\vec{e}_2(\theta)}{\|\vec{e}_2(\theta)\|_2}
            \end{aligned}
            LaTeX formulas

        The sign of Frenet vectors are depending on the convexity of the
        contour.

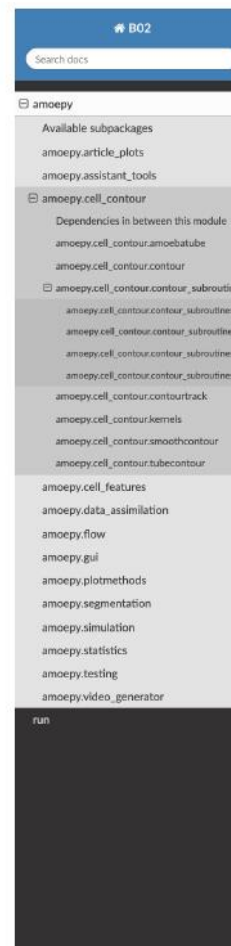
        .. image:: ../static/frenetvec.*
            Images

        :param r: Radius parameter of Poisson kernel :math:`0 < r < 1`
        :type r: float
        :param sigma: GPR noise parameter :math:`\sigma > 0`
        :type sigma: float
        :param n_clip: Minimal (included) and maximal (excluded) index
            of cell contours for which this method is used on
        :type n_clip: tuple or list with two int

        :return: tuple of
            1-2) x- and y-components of unit normal vectors,
            3-4) x- and y-coordinates of virtual markers,
            5-6) x- and y-components of unit tangent vectors,
            7) contour curvature
        :rtype: tuple

        Parameter descriptions

        if n_clip:
            n_min = n_clip[0]
            n_max = n_clip[1]
        else:
            n_min = 0
            n_max = self.n_cells()
        """
```



normal_velocity [r, sigma, center]	Compute the normal velocity for all contours at each v
shortest_path_backward [r, sigma, m_ip]	Compute contour mapping based on shortest path flo
shortest_path_forward [r, sigma, m_ip]	Compute contour mapping based on shortest path flo

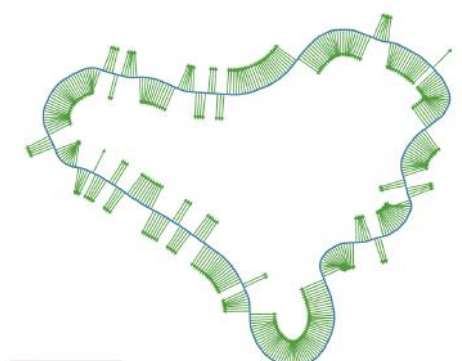
frenet_vectors(r, sigma, n_clip=None)

Compute the x- and y-coordinates of virtual markers based on GPR smoothing and the corresponding Frenet vectors (normalized tangent and normal vectors) and the curvature.

The Frenet vectors are given by the formula:

$$\begin{aligned} \vec{e}_1(\theta) &= \Phi'(\theta) \\ \vec{e}_2(\theta) &= \Phi''(\theta) - \langle \Phi''(\theta), \vec{e}_1(\theta) \rangle \vec{e}_1(\theta) \\ \vec{t}(\theta) &= \frac{\vec{e}_1(\theta)}{\|\vec{e}_1(\theta)\|_2} \\ \vec{n}(\theta) &= \frac{\vec{e}_2(\theta)}{\|\vec{e}_2(\theta)\|_2} \end{aligned}$$

The sign of Frenet vectors are depending on the convexity of the contour.



Parameters:

- r** (float) – Radius parameter of Poisson kernel ($0 < r < 1$)
- sigma** (float) – GPR noise parameter :math>\sigma > 0
- n_clip** (tuple or list with two int) – Minimal (included) and maximal (excluded) index of cell contours for which this method is used on

Returns: tuple of 1-2) x- and y-components of unit normal vectors, 3-4) x- and y-coordinates of virtual markers, 5-6) x- and y-components of unit tangent vectors, 7) contour curvature

Return type: tuple

Figure 17. Code (left) and corresponding Sphinx documentation (right)

High Performance Computing



HPC.UP

- Supports Matlabs, Python, R and more
- Strongest cluster at the University of Potsdam
- Easy access, practically no administrative process

HLRN

Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen

- Two HPC centers for Northern Germany
- Very high performance
- Long administrative process

Workshop wanted?



Services for Research Data and Code

Processing and analysing

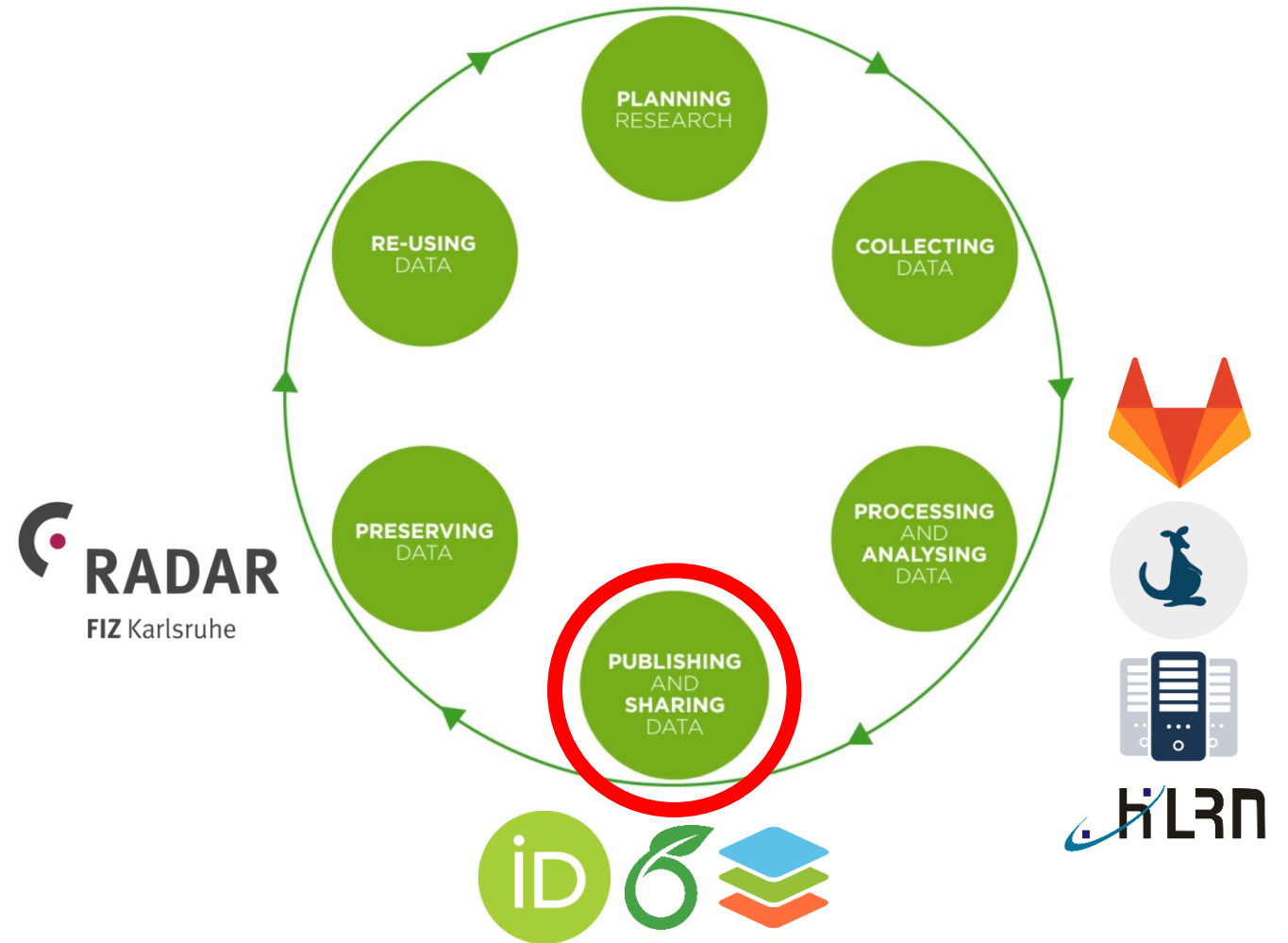
- Git.UP, Box.UP, HPC.UP, HLRN

Publishing and sharing

- ORCID, Overleaf, OnlyOffice

Preserving

- DSpace, RADAR.UP

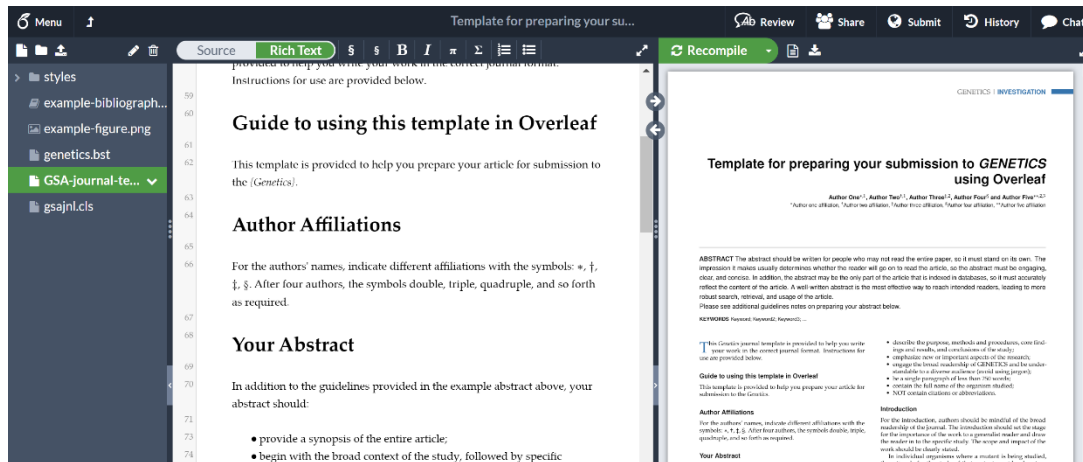


Collaborative Editing



Overleaf

- Real-time LaTeX editor
- **Offers Git integration**
- CRC 1294 only



OnlyOffice

- Real-time document editor
- **Fully integrated with Box.UP**
- Publicly available from April



Publishing Research

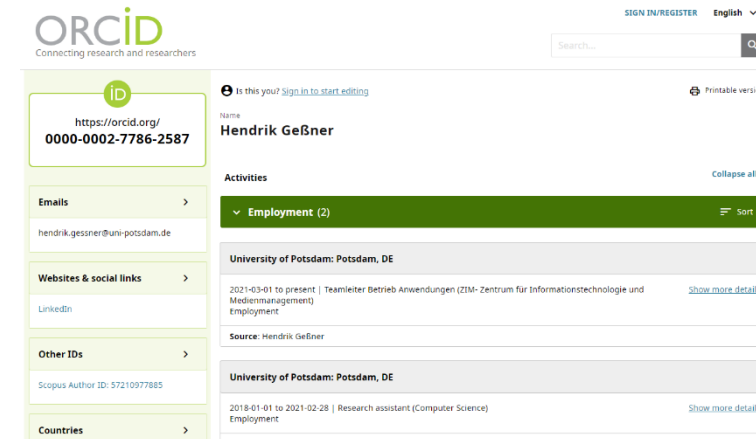
Research data repositories

- Gives *DOI* for data and code
- Goal: Long-term findability
- Search **re3data.org** portal for fitting repository
- Use **Zenodo** (by CERN)



ORCID

- „DOI for humans“
- For entire research career
- Enables automation



Publish

Research &

- Gives *DOI*
- Goal: Long

- Search re
portal for
repositor

- Use **Zenodo**
(by CERN)

The screenshot shows the Box.UP Support website for the University of Potsdam. The header includes the university logo, navigation menus for 'STUDIUM', 'FORSCHUNG', 'UNIVERSITÄT', and 'ONLINE-DIENSTE', and a language selector set to 'Deutsch'. Below the header, there are five main navigation buttons: 'UP entdecken', 'Fakultäten', 'Organisation', 'Campus International', and 'Wirtschaft, Transfer und Gesellschaft'. The breadcrumb trail indicates the user is in 'Box.UP Support / Ansprechpartner'.

On the left sidebar, there are three menu items: 'Übersicht', 'Installation', and 'Ansprechpartner', with 'Ansprechpartner' being the active selection.

The main profile area for Hendrik Geßner, Teamleiter Betrieb Anwendungen, includes a profile picture, contact information (phone: 0331 977-1039, 0331 977-1750; email: hendrik.gessner@uni-potsdam.de), location (Campus Griebnitzsee, August-Bebel-Straße 89, Haus 1, Raum 1.64), and office hours (Sprechzeiten auf Anfrage).

The 'Publikationen' section lists six publications:

- [1] Geßner, H. and Kiy, A. 2019. A mobile campus application as a sensor node for Personal Learning Environments: Hybrid cross-platform User Contextualization. *Lecture Notes in Informatics (LNI), Proceedings - Series of the Gesellschaft für Informatik (GI)*. P-297, (2019), 187–192. DOI: https://doi.org/10.18420/delfi2019_356.
- [2] Geßner, H. and Sass, K. 2016. Context-based E-Learning for the diagnosis and rectification of network errors using the App ThermoFind as an example, Kontextbasiertes E-Learning zur Diagnose und Behebung von Netzwerkfehlern am Beispiel der App ThermoFind. *Lecture Notes in Informatics (LNI), Proceedings - Series of the Gesellschaft für Informatik (GI)*. 262, (2016), 15–17.
- [3] Geßner, H. and Weise, M. 2014. 3D-Rekonstruktion mit der AR.Drone 2.0. *44. Jahrestagung der Gesellschaft für Informatik, Big Data - Komplexität meistern, INFORMATIK 2014, Stuttgart, Germany, September 22-26, 2014* (2014), 2497.
- [4] Kiy, A. et al. 2015. A Hybrid and Modular Framework for Mobile Campus Applications. *i-com*. 14, 1 (2015), 63–73.
- [5] Universität Potsdam, I.F.I.U.C.S. 2021. Transparently Safeguarding Good Research Data Management with the Lean Process Assessment Model. (2021). DOI: <https://doi.org/10.11588/HEIDOK.00029719>.
- [6] Zender, R. et al. 2013. RouteMe - Routing in Ad-hoc-Netzen als pervasives Lernspiel. *i-com*. 12, 1 (2013), 45–52. DOI: <https://doi.org/10.1524/icom.2013.0007>.

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Services for Research Data and Code

Processing and analysing

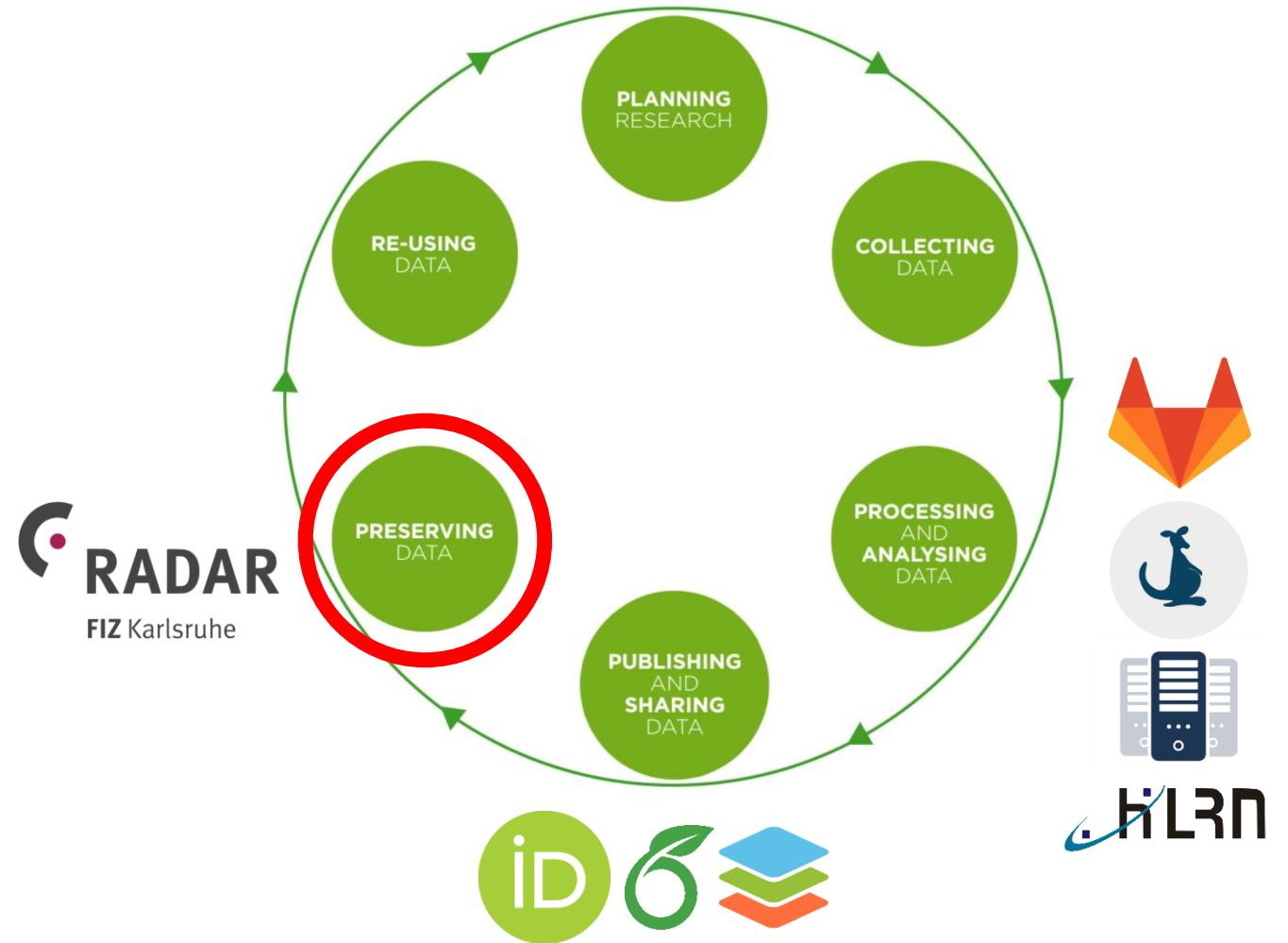
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Publishing and sharing

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Preserving

- DSpace, RADAR.UP



Archiving Research Artifacts

DSpace (CRC 1294 only)

- Required by CRC 1294 archiving policy

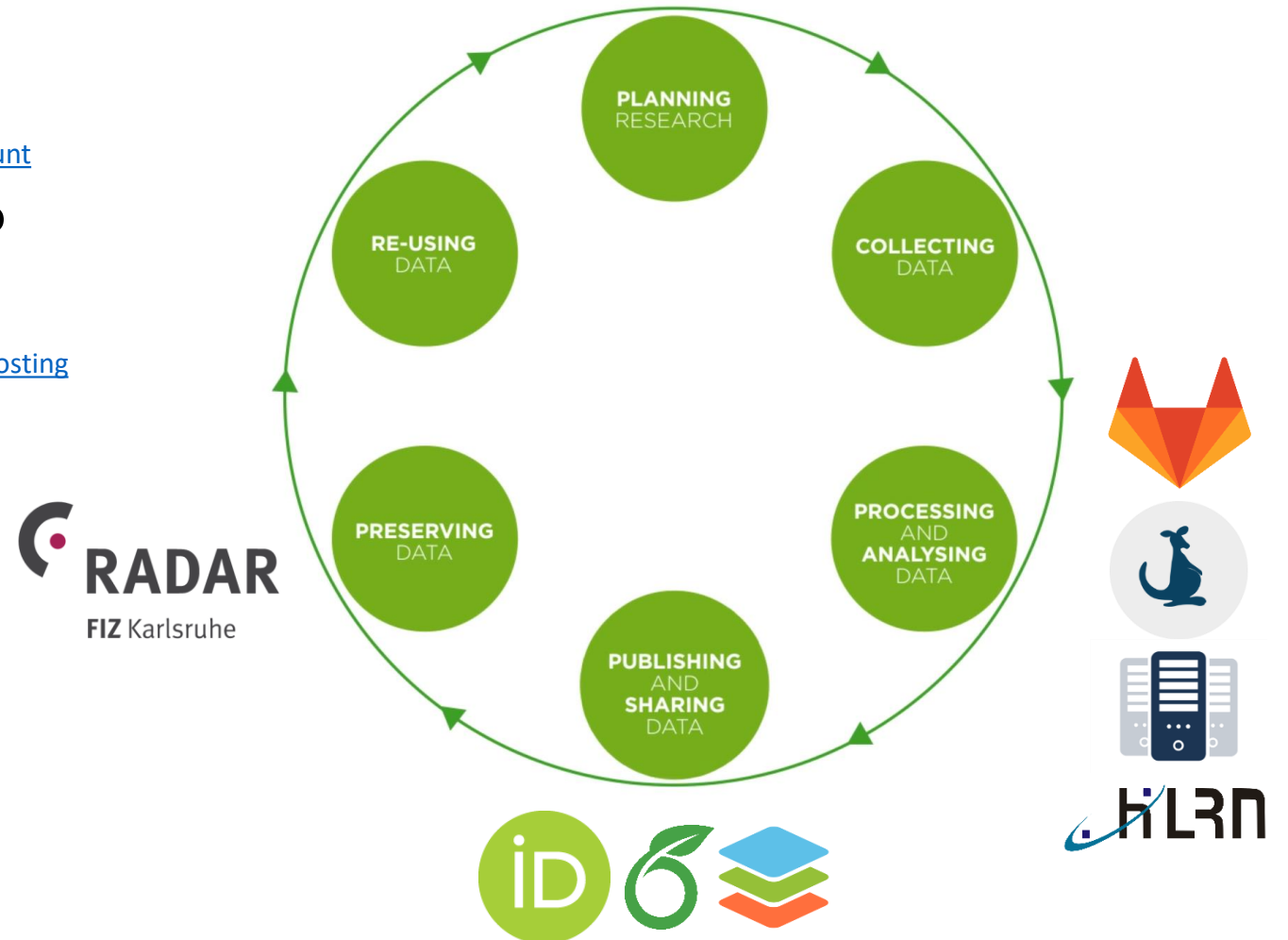
RADAR.UP (still in development)

- Official research data archive at the University of Potsdam
- Launches this year, CRC 1294 will get early access



Additional Services

- Need access?
Get a UP guest account!
<https://www.uni-potsdam.de/de/zim/angebote-loesungen/up-account>
- Need your own server space?
Get a Virtual Machine!
<https://www.uni-potsdam.de/de/zim/angebote-loesungen/server-hosting>
- Need more help?
Attend the PoGS workshop
„Reproducibility in Scientific Publications“!
<https://pogs.uni-potsdam.de/booking/course/7f134c29.html>



Contact us!



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Team Leader
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Thank you!