

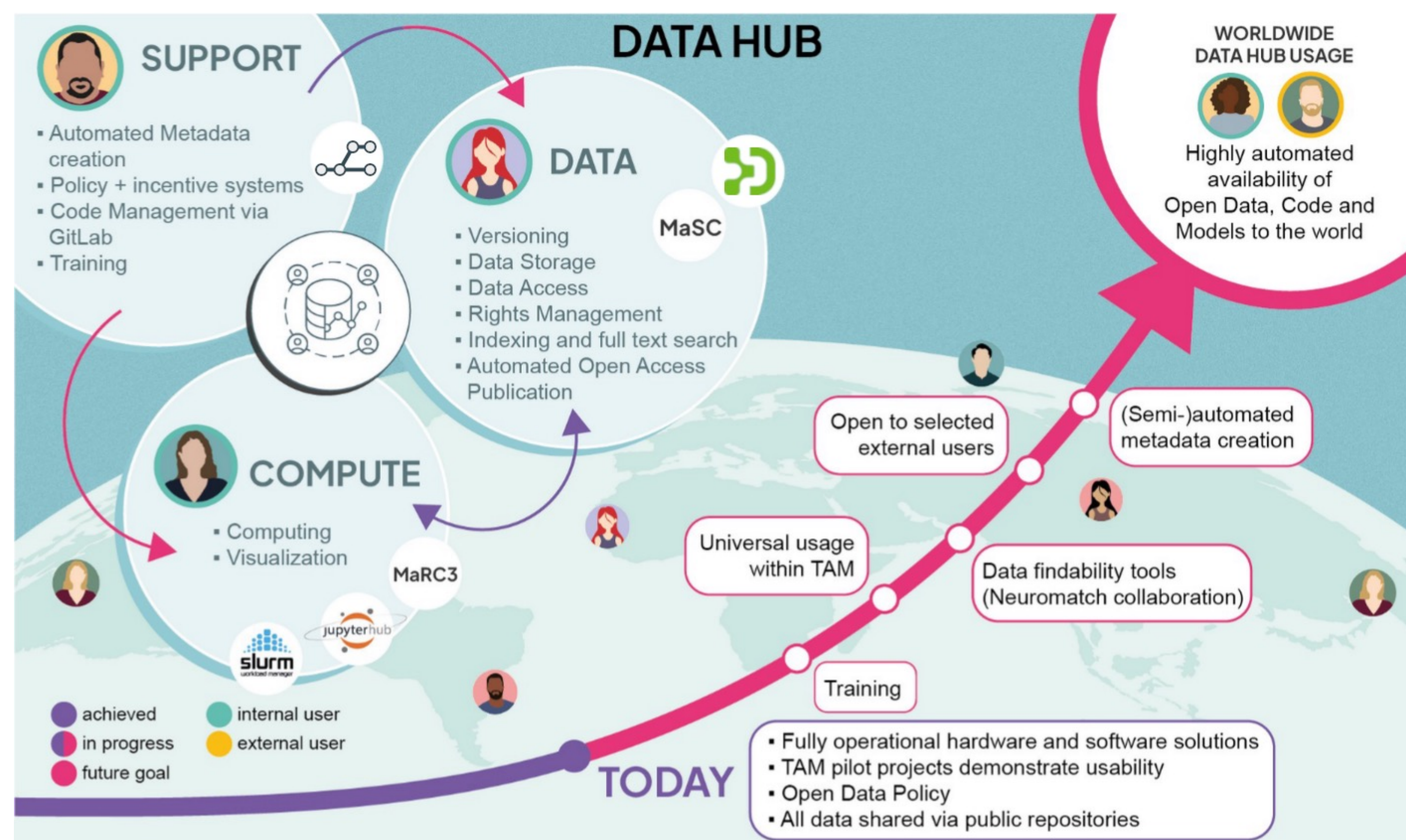
The DataHub: Your Gateway to Effective and Efficient High-Performance Computing in Psychology and Neuroscience Research

Nick Augustat, Stefan Lenze, Tobias Ortwein, Ortrun Brand, Bernd Nicklas, Dominik Endres
Philipps-Universität Marburg

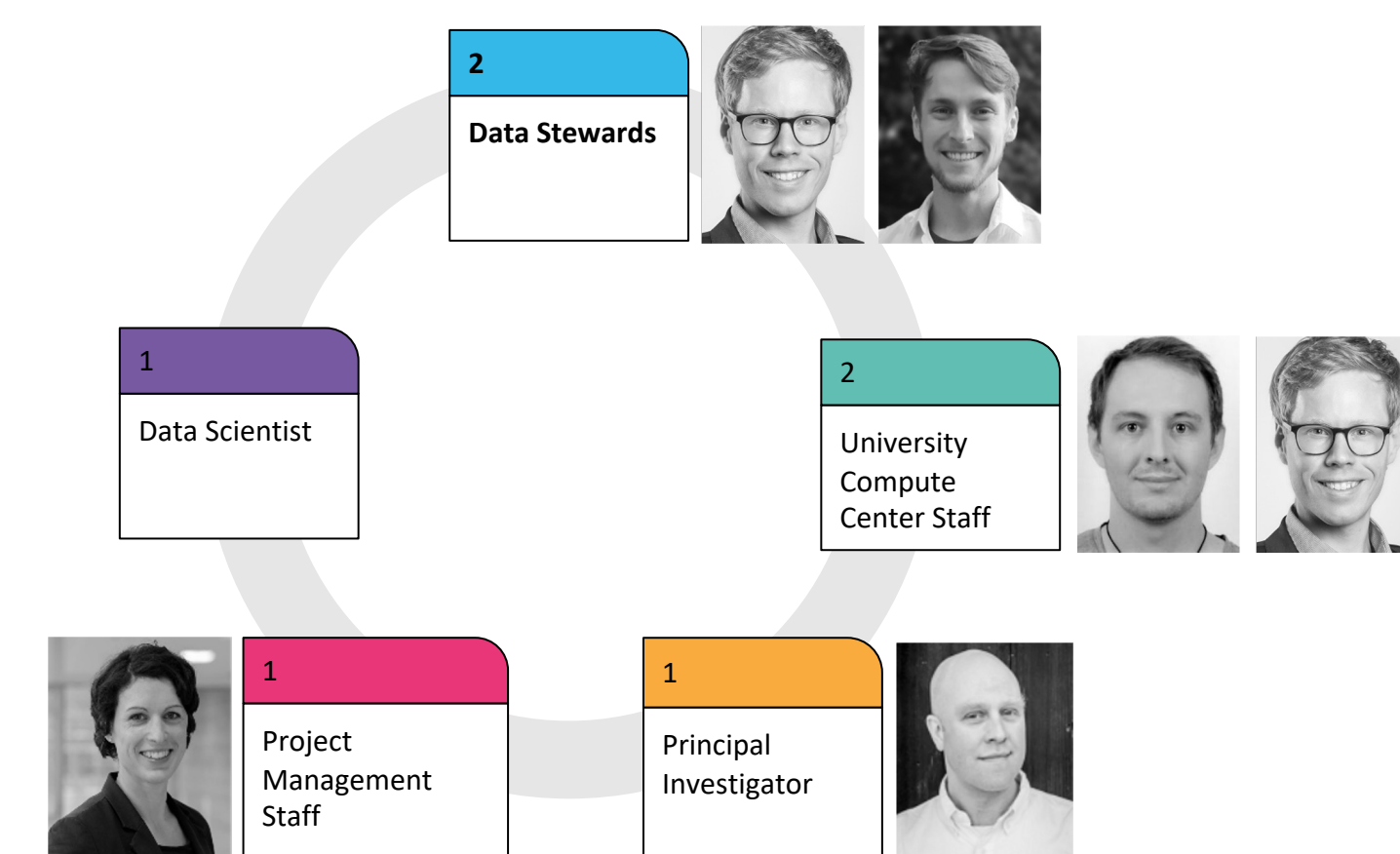


datahub@uni-marburg.de
DataHub Support

Vision, team & collaboration



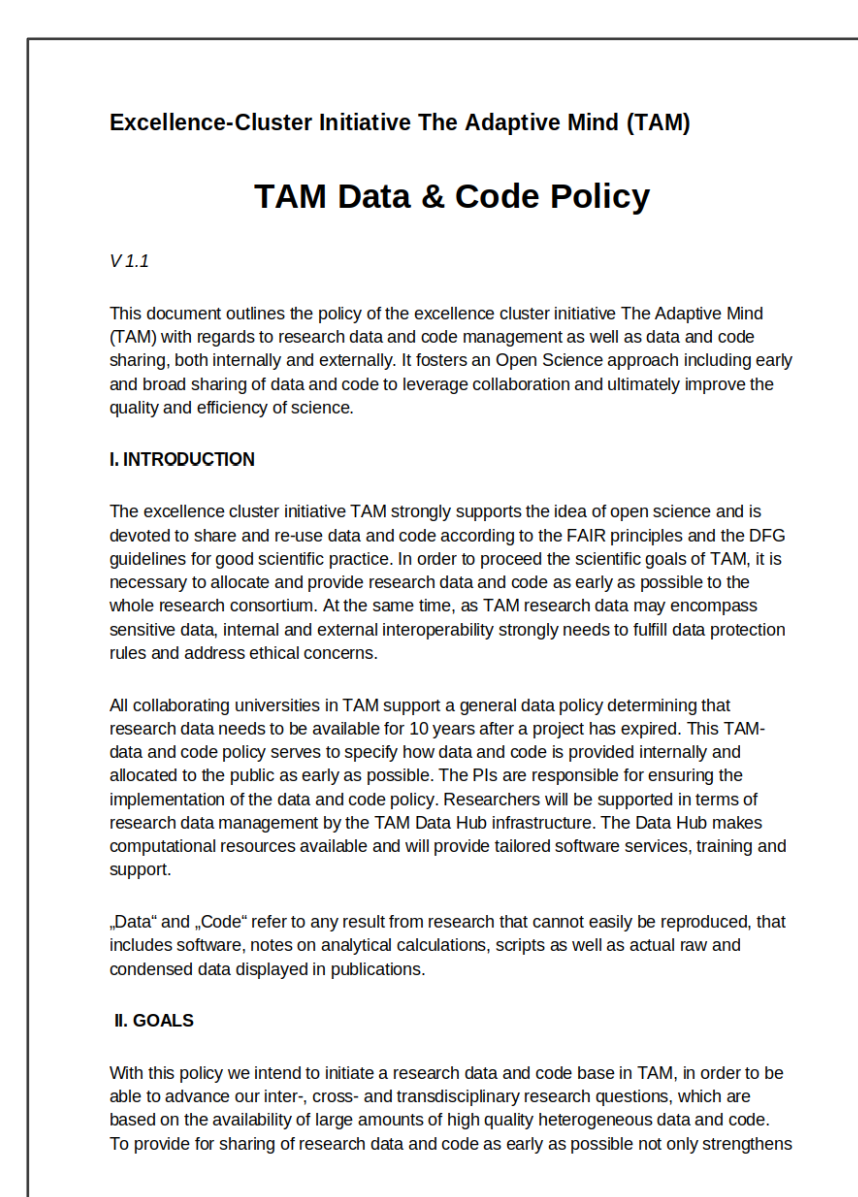
DataHub team



Collaboration



Policy, training & support



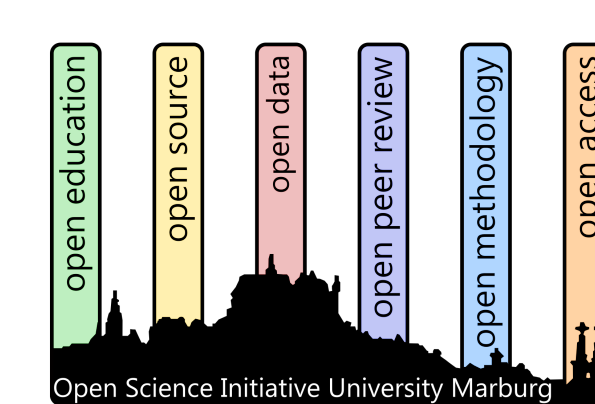
Principles of the TAM policy

- Use shared hardware, services and support.
- Share data and code as early as possible.
- Practice FAIR principles and common standards.
- Make results more transparent and reproducible.
- Prepare for long-term accessibility and publish.
- **To do:** frictionless workflow for international students subject to dual-use concerns

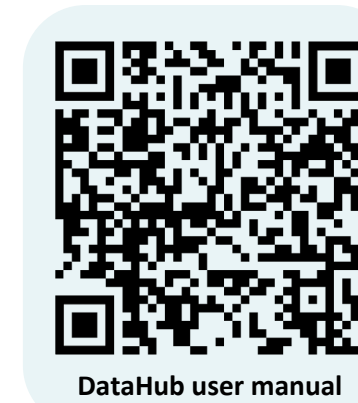
Enhance collaboration and re-use of scientific work.



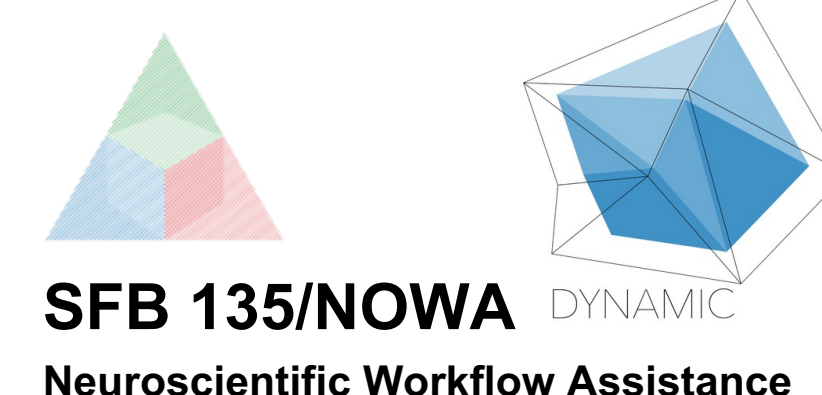
- Access & onboarding
- DataHub workflow
- Service descriptions
- Data & code management
- Git and GitLab tutorial
- Recorded workshops
- FAQ & troubleshoot



Workshops and Summer Schools:
• Fostering open science practices
• **Brainhack Summer School**



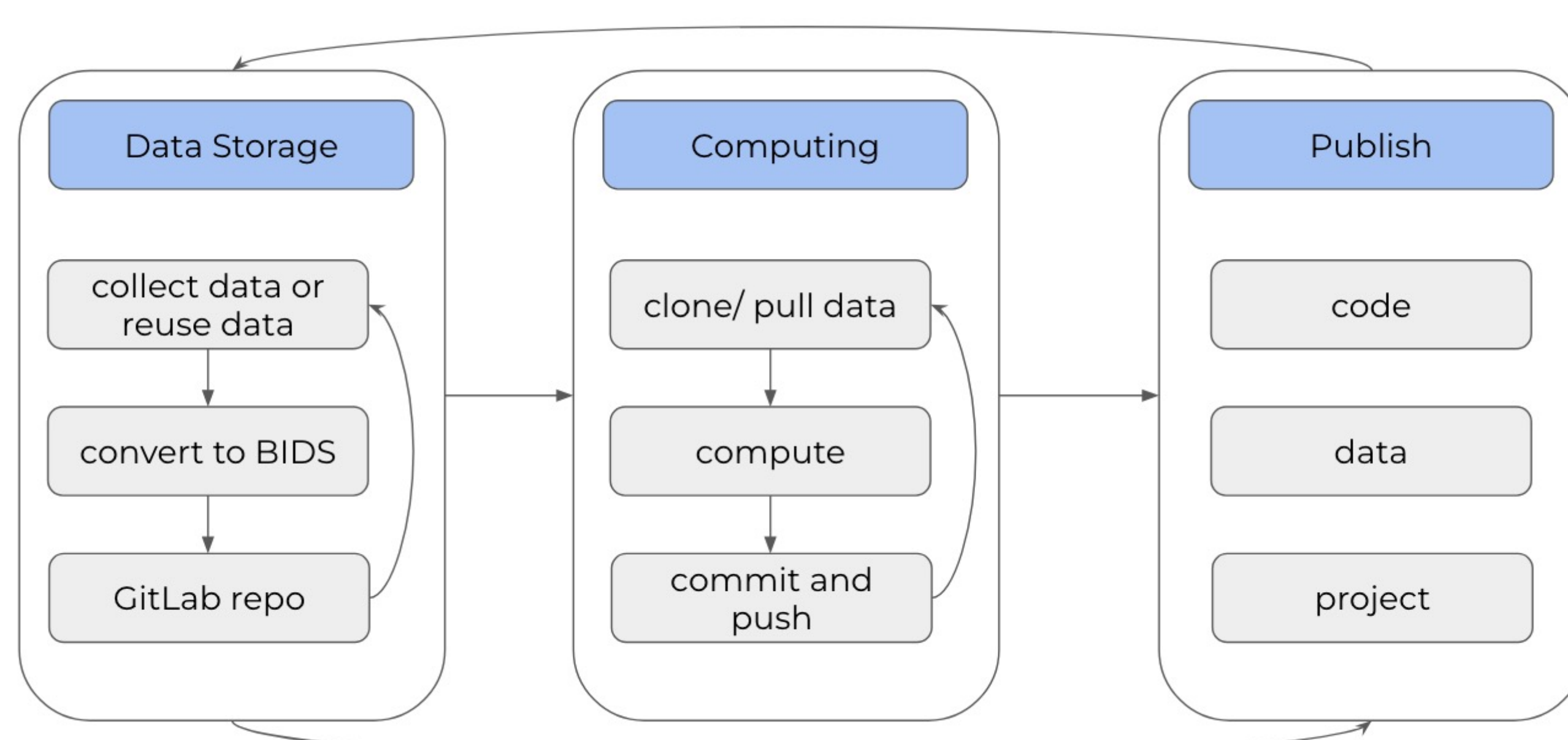
Register now!



Recorded tutorials, materials and instructions, websites and JupyterBooks on:
• Git & GitLab,
• Clean and reusable rode
• Continuous integration, code review, etc.

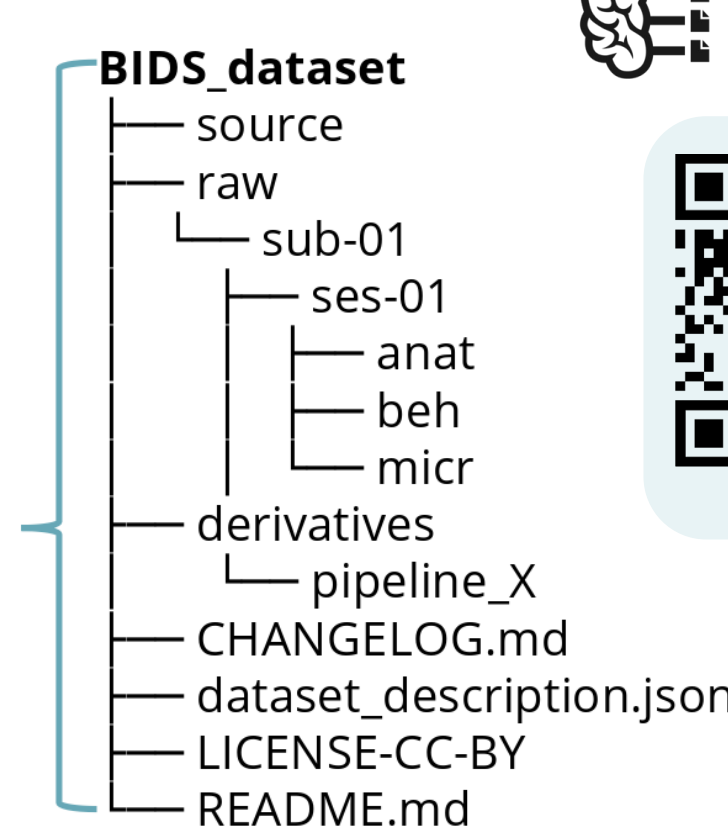
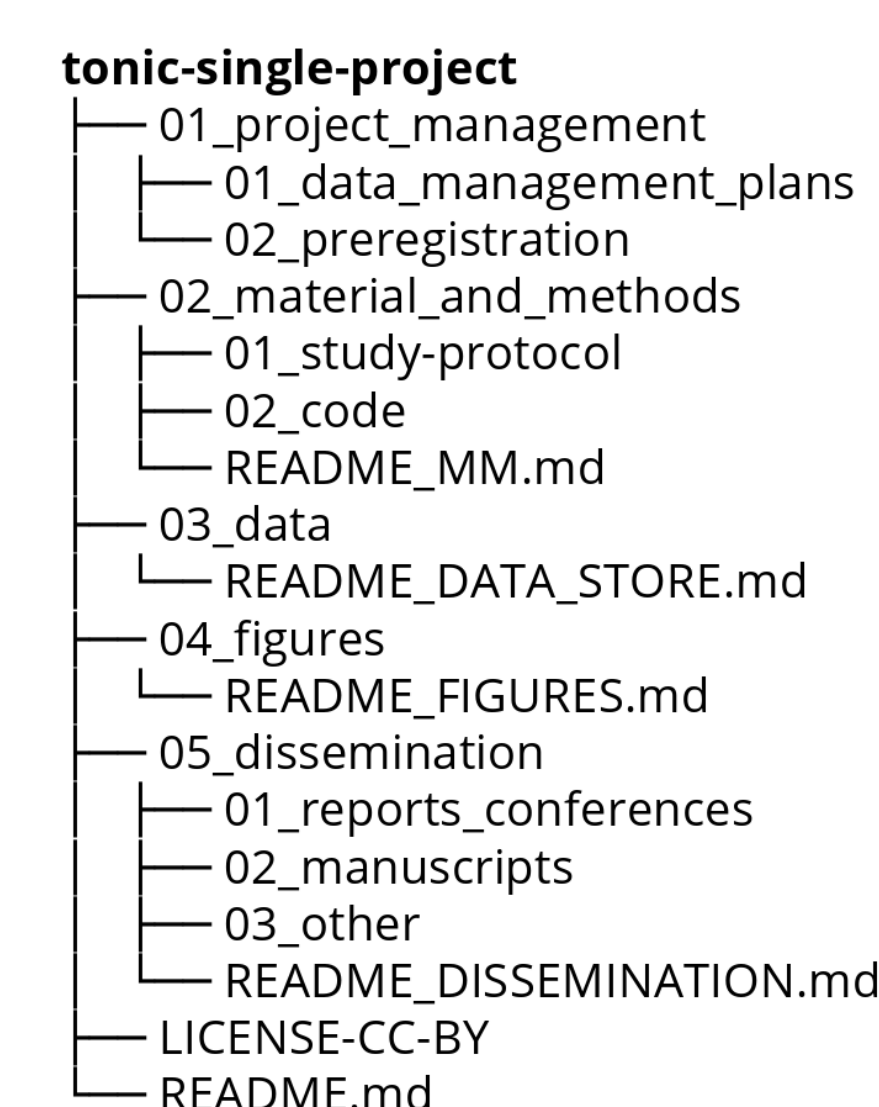
Workflows & standards

Common workflow

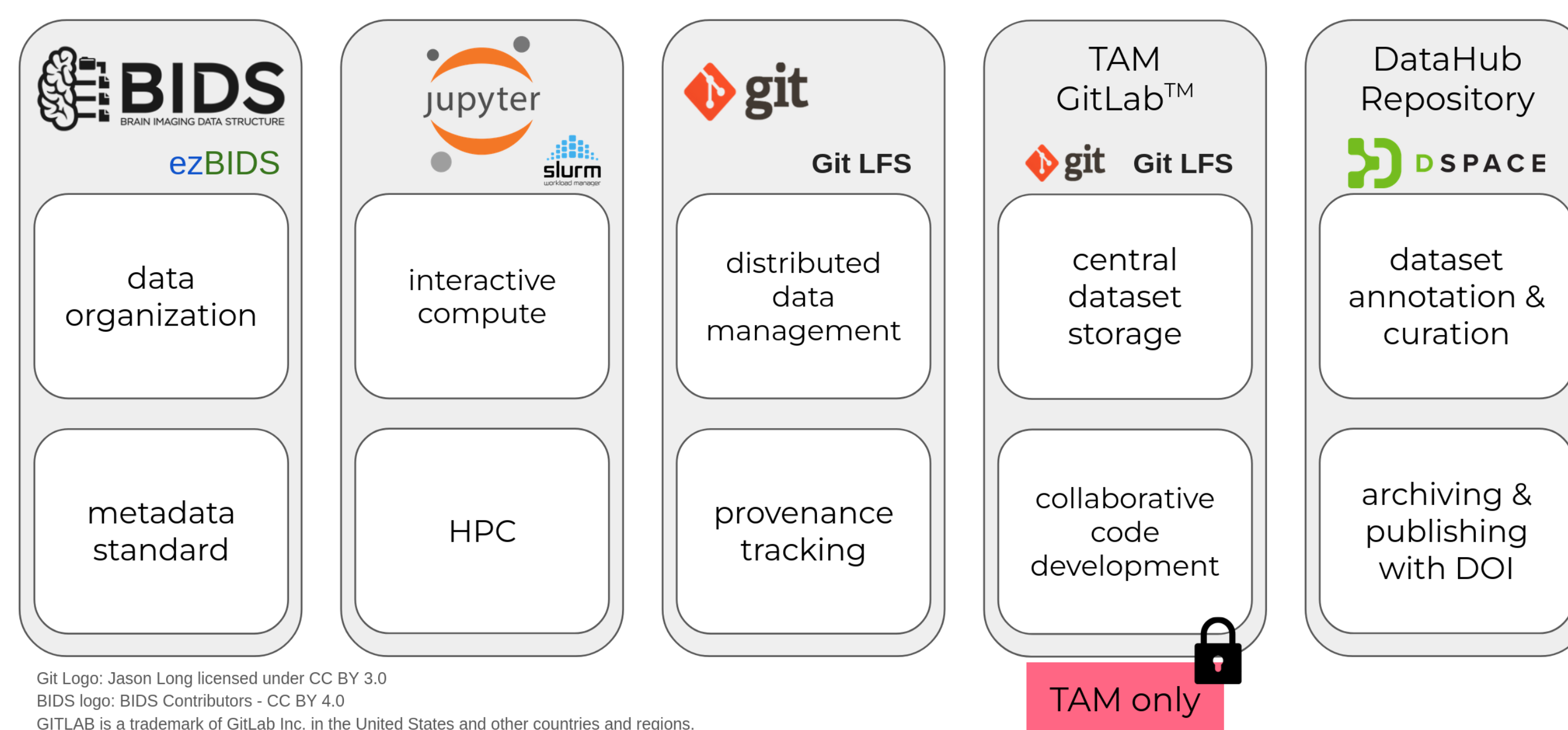


Tonic research folder template

Available from TAM-GitLab



Technical services



DataHub status and latest features

Technical services

- HPC integration: **Production**
- **JupyterHub**: **Production** (new hardware and profiles)
- **TAM GitLab**: **Production** (advanced access management)
- **Git + Git-LFS workflow integration**: **Production**
- TAM DataHub repository: **Pilot**
- **GitLab - DSpace publication pipeline**: **Planned**
- **ezBIDS**: **Test**

Support services

- User manual (GitLab pages): **Production**
- Support queue (request tracker): **Production**
- Curation service (DSpace & GitLab): **Pilot**
- **Data protection policy**

Technical resources & architecture

MaRC3 total resources

- 51 compute nodes, 3264 CPU cores
- 26x AMD EPYC 7702P, 64 cores, 2 GHz
- 23x AMD EPYC 7713, 64 cores, 2 GHz
- 2x AMD EPYC 9334, 2x32 cores, 2.7 GHz
- 256-1024 GB RAM
- 12x V100S, 16x A100 40 GB, 70x A100 80 GB, 6x A40, 4x L40S
- 1.7-7.2 TB local, 134 TB shared scratch, 134 TB home storage
- 25 Gbit Ethernet network (storage: 200 Gbit)

TAM nodes in MaRC3

- 14 nodes / 896 cores + 4 GPUs (A100 80GB)
- 4 nodes / 192 cores (CPU-only)

TAM storage in MaSC

- 703 TB total usable capacity

