

Data Integrity



Research Roundtable
February 2024
Florida Atlantic University
Research Integrity Office



Data Integrity vs Data Management

Data Integrity:

The accuracy, reliability, and consistency of data over its entire life-cycle.

Ensures the accuracy, completeness, consistency, and validity of data.

Data Management:

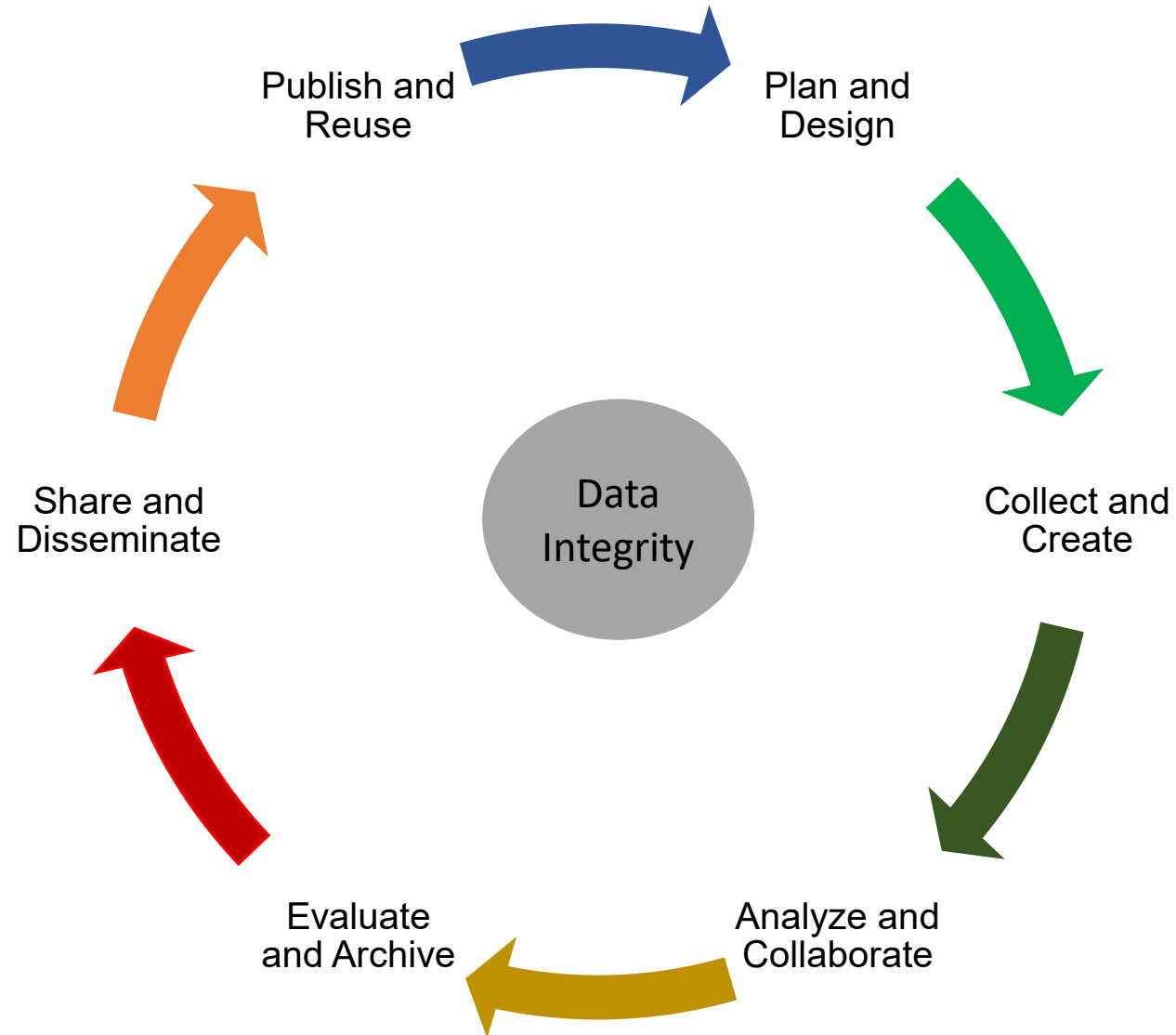
The practice of collecting, organizing, and accessing data to support productivity, efficiency, and decision-making.



Research Data

FAU DOR Policy 10.1.6

- Recorded factual information commonly accepted in the scientific community as necessary to reconstruct, evaluate, and validate research findings and results, regardless of the media on which it may be recorded.
- Examples of Research Data include, but are not limited to, laboratory notebooks, notes of any type including printouts, specimens of any type including organisms, photographs, reagents, digital images, protocols, numbers, graphs, charts, numerical raw experimental results, instrumental outputs from which Research Data can be derived and other deliverables under sponsored agreements.

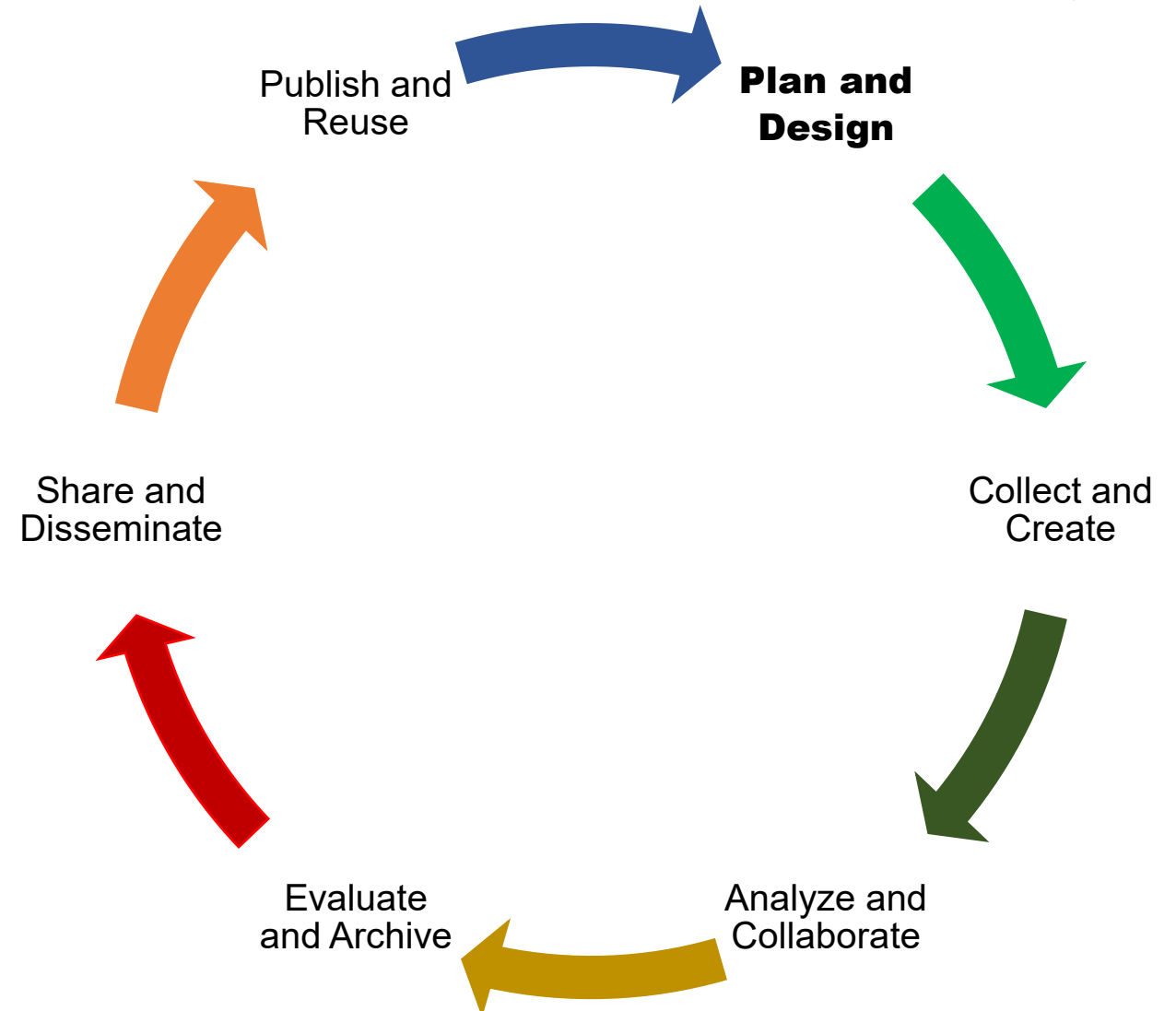




Plan and Design

- Data Management Plans
- Data Policies and Compliance
- Directory Structures
- Roles and Responsibilities
- File Naming Conventions

<https://dmptool.org/>



Publish and Reuse

Plan and Design

Collect and Create

Analyze and Collaborate

Evaluate and Archive

Share and Disseminate



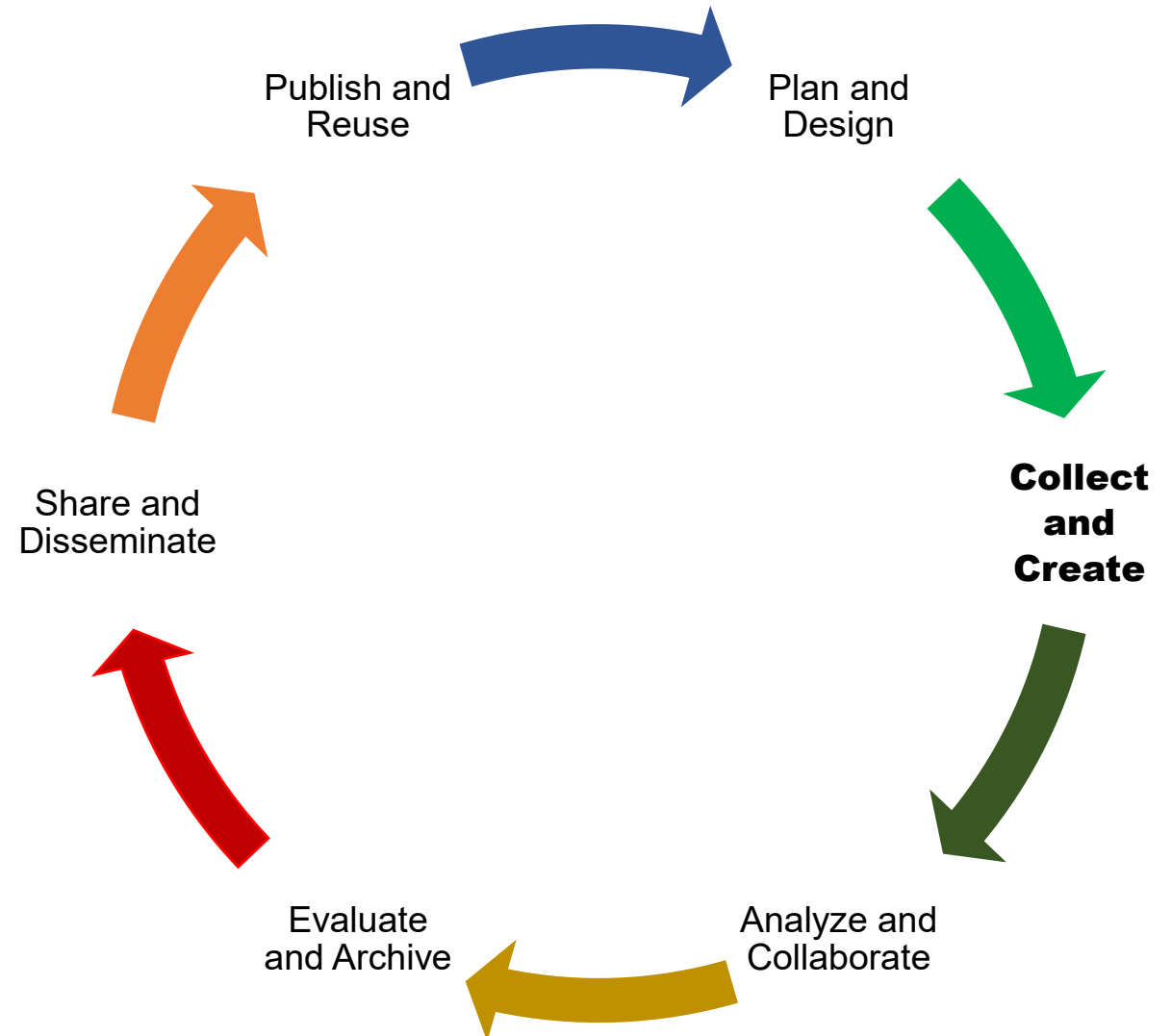
Collect and Create

FAU DOR Policy 10.1.6:

Collecting project data in a consistent and systematic manner.

Requirements for the recording and storage of Research Data and material will vary by discipline.

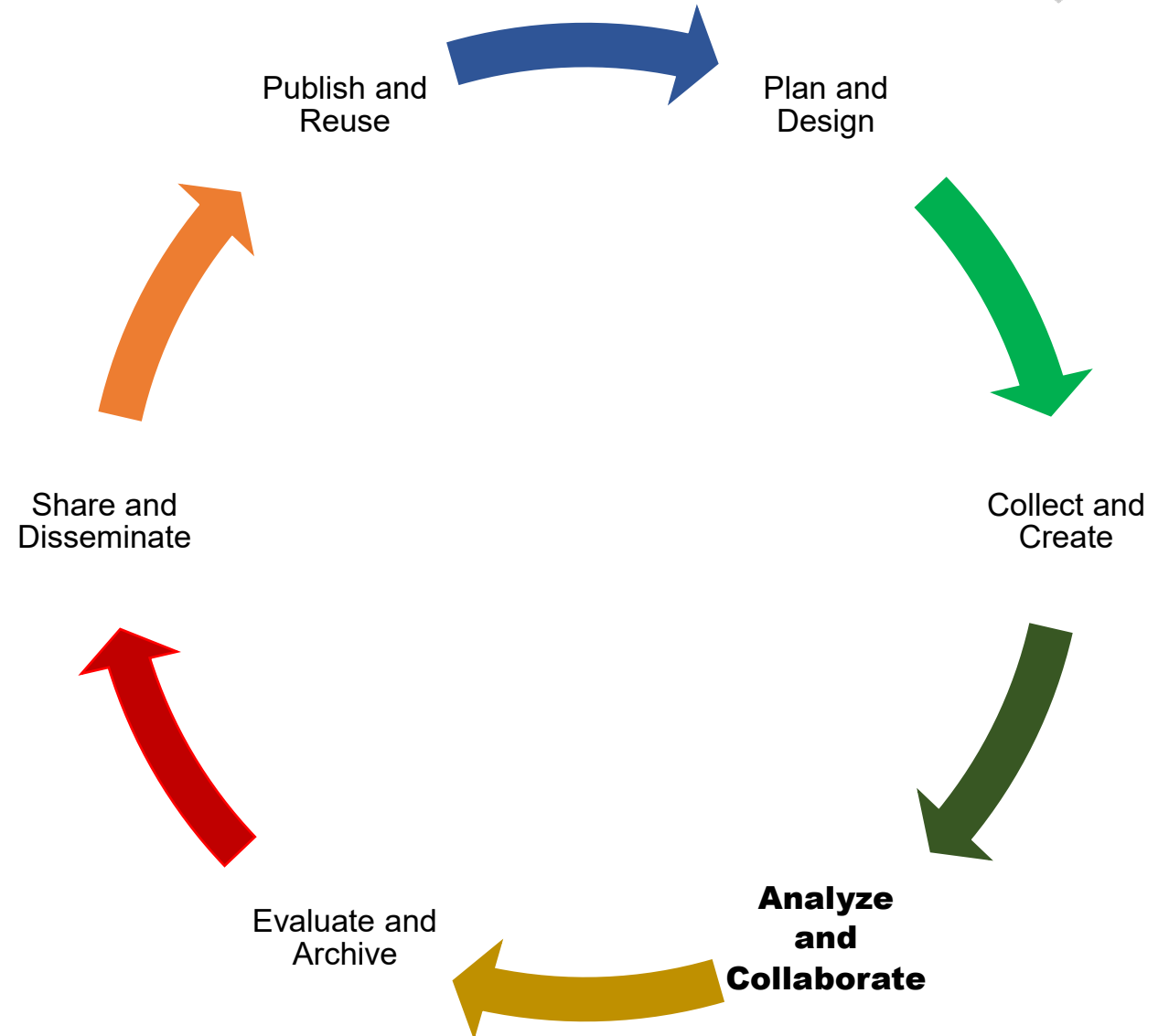
PIs should always adhere to requirements of funding agencies, standards of the applicable industry, professional guidance where available, any principles set out on the College level as well as FAU recommendation as outlined in compliance documents.





Analyze and Collaborate

- Inspecting, cleaning, transforming, and modeling data with the goal of discovering useful information, informing conclusions and supporting decision-making.
- Collaborative tools and software
- Documentation and Metadata
- Reproducibility
- Analysis ready datasets
- Image management
- Version control





Evaluate and Archive

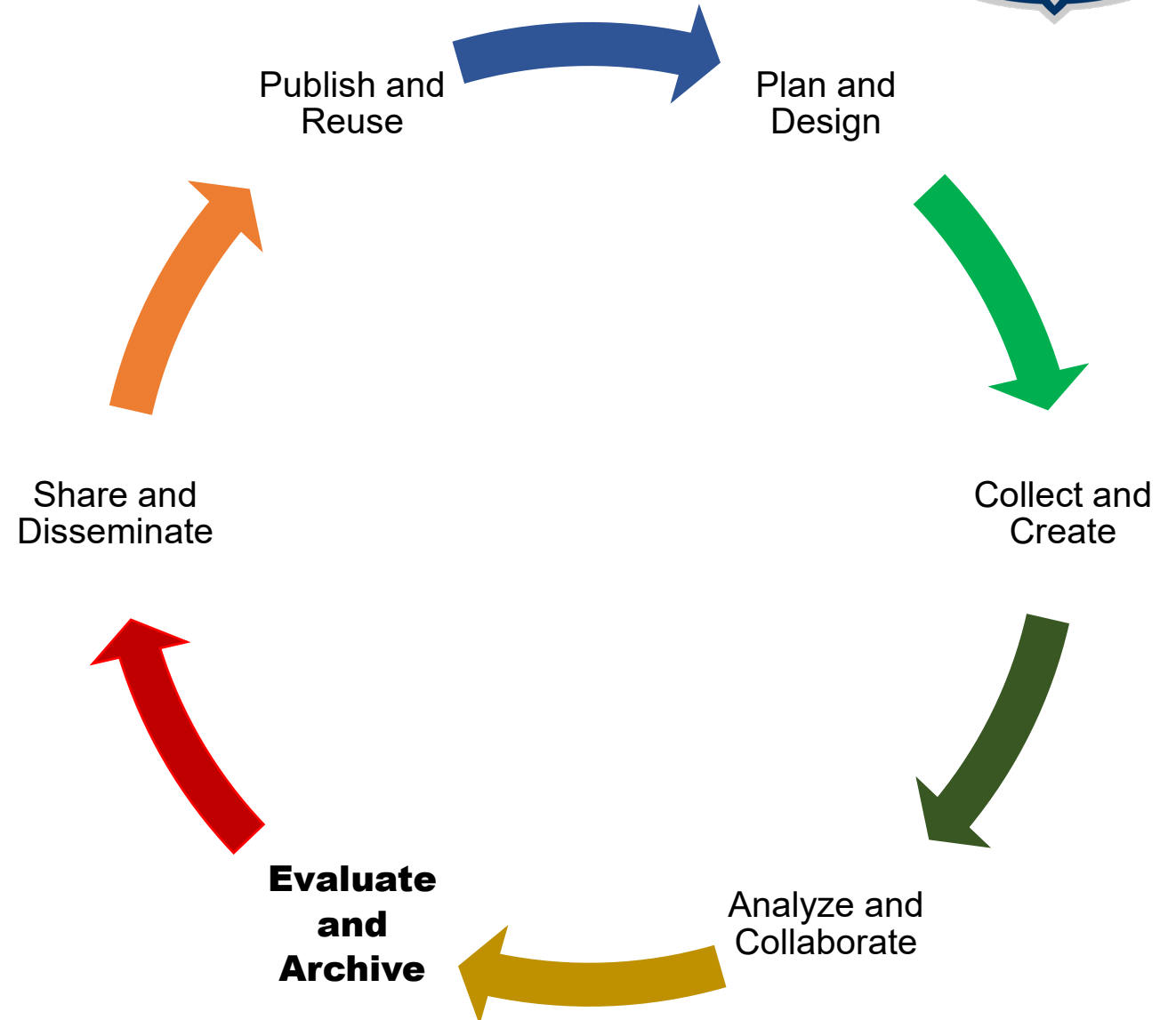
- Security,
- Retention,
- Destruction,
- Archive/ records management

FAU DOR Policy 10.1.6:

Research Data should be stored using a method that permits a complete retrospective audit if necessary.

The PI will have access to the Research Data generated by the project. Any other faculty, staff, student or person involved in the creation of Research Data may have the ability to review that portion of the Research Data that they created.

Report any Research Data integrity breaches to the appropriate FAU oversight entity.



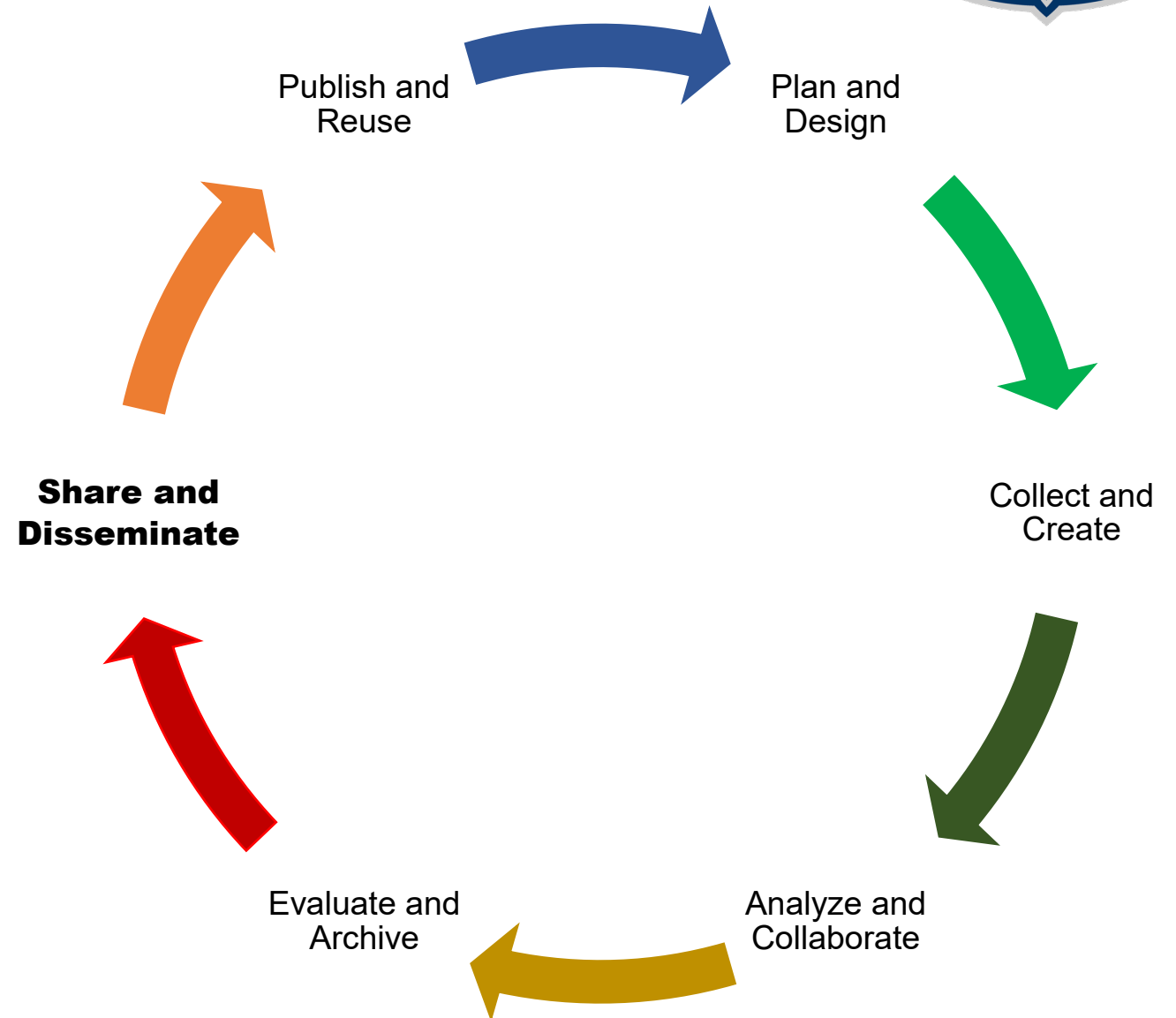


Share and Disseminate

- Data sharing
- Open access
- DUAs
- Intellectual property

FAU DOR Policy 10.1.6:

Details on how, when, to and by whom data will be shared with other researchers and for generalizable knowledge should be detailed in research plans, including but not limited to protocols, data sharing plans, consent documents, and data use agreements.





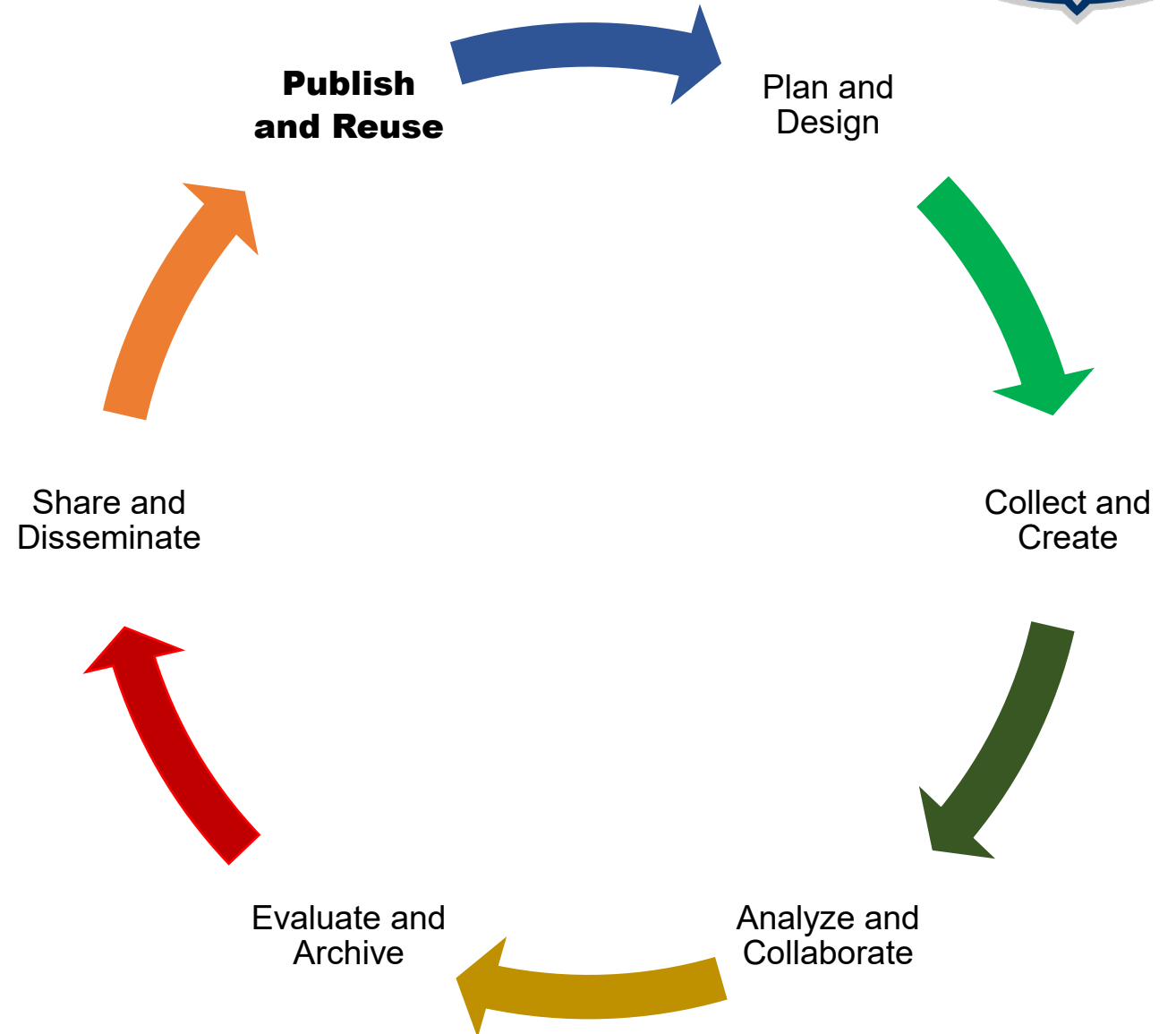
Publish and Reuse

- Scholarly products
- Preprints and publishing
- Data repositories

Data accessibility is the degree to which other researchers, and you yourself can use data.

Data isn't just available, but also usable. Make your data accessible by ensuring it:

- Is in a reliable storage location
- Is retrievable online using standardized protocols
- Has restrictions in place as necessary





Resources

NIH: <https://grants.nih.gov/grants/guide/notice-files/NOT-OD-21-013.html>

NSF: <https://new.nsf.gov/funding/data-management-plan#nsfs-data-sharing-policy-1c8>

NOAA: <https://nosc.noaa.gov/EDMC/PD.DSP.php>

FAU DOR Policies: <https://www.fau.edu/research/policies-and-procedures/>



Questions and Discussion

FAU Office of Information Technology
<https://www.fau.edu/oit/>

FAU Human Research Protection Program
researchintegrity@fau.edu

<https://www.fau.edu/research-admin/research-integrity/human-subjects-irb/>

FAU Responsible Conduct of Research

<https://www.fau.edu/research-admin/research-integrity/responsible-conduct-of-research/>



FAU Research Computing

RESEARCH COMPUTING AT FLORIDA ATLANTIC UNIVERSITY

OFFICE OF INFORMATION TECHNOLOGY

Services



General

- ▶ 10 Gbps Network Uplink to Florida Lambda Rail
- ▶ 100 Gbps Core
- ▶ Various Intel CPU's
- ▶ AMD – EPYC (6,500 cores)
- ▶ NVIDIA A100 - ~18
- ▶ NVIDIA V100 - 48
- ▶ SLURM SCHEDULING
- ▶ Open OnDemand
- ▶ SSH Console Access

HPC Cluster KOKO



Team



- ▶ James Mauser
Systems Administrator
- ▶ Skyler Paulus
Systems Administrator
- ▶ Bahareh Yaseen Saadatmand-Mashhadi
Research Facilitator, BioInformatics
- ▶ Chris Johnson
Form Development
- ▶ Rhian Resnick
Director

Open OnDemand



- Provides a web UI to the clusters.

A screenshot of a web-based file manager interface. The left sidebar shows a 'Home Directory' with various folders like '2bRAD', '2bRAD_denovo', 'AI', 'Adlm', 'Agents', 'CovMutation', 'Desktop', 'Documents', 'Downloads', 'Grais', 'IBM', 'ISM 4212 Database Management', 'MATLAB', 'MATLAB2', 'Music', 'NetBeansProjects', 'New folder', and 'COV'. The main area shows the current directory path as '/mnt/beegfs/home/rresnick/'. Below the path are action buttons: View, Edit, Rename/Move, Download, Copy, Paste, (Un)Select All, and Delete. A table lists files and directories with columns for 'name', 'size', and 'modified date'.

name	size	modified date
..	dir	
2bRAD	dir	10/30/2019
2bRAD_denovo	dir	03/30/2021
AI	dir	03/31/2021
Adlm	dir	10/09/2020
Agents	dir	
CovMutation	dir	01/28/2021
Desktop		
Documents		
Downloads		
Grais		
IBM		
ISM 4212 Database Management		
MATLAB		

A screenshot of the Open OnDemand landing page. The page features the 'OPEN OnDemand' logo and the text: 'OnDemand provides an integrated, single access point for all of your HPC resources.' The top navigation bar includes links for Clusters, Interactive Apps, My Interactive Sessions, Develop, Help, Logged in as rresnick, and Log Out.

A screenshot of a terminal window accessed via Open OnDemand. The browser address bar shows 'ondemand.hpc.fau.edu/pun/sys/shell/ssh/koko-login.hpc.fau.edu'. The terminal output shows the last login time and the user prompt: 'rresnick@koko-login004 ~]\$'. The terminal content is mostly black, indicating a shell session.

SSH



```
[rresnick@koko-login003 ~]$ pwd
/mnt/beegfs/home/rresnick
[rresnick@koko-login003 ~]$
```

```
[rresnick@koko-login003 ~]$ sinfo -p debug
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
debug      up       1:00:00     2 drain* nodeamd[037-038]
debug      up       1:00:00     1  drng  nodeamd034
debug      up       1:00:00     1   mix  nodeamd039
debug      up       1:00:00     4 alloc  nodeamd[017,033,035-036]
debug      up       1:00:00    15  idle  nodeamd[018-032]
[rresnick@koko-login003 ~]$
```


Storage (PowerScale)



- ▶ Home & Scratch
 - ▶ 60TB NVME
- ▶ Archive
 - ▶ 822 TB of storage
- ▶ Users – 50 GB quota
- ▶ Scratch – 300 GB quota deleted after 90 days

Storage (Cloud Nas)



- ▶ Archive
 - ▶ 60TB NVME
 - ▶ Basically Unlimited Cloud Storage
- ▶ Archive
 - ▶ No Backups: \$13.33 / TB / Month
 - ▶ With Backups: \$31.50 / TB / Month
 - ▶ With Backups and Replication: \$63 / TB / Month
- ▶ Most users will receive 300 GB of complimentary storage on archive as long as they are connected to a new or funded research activity. (as determined by the Research Computing Team, we are very liberal with this definition, it just protects our storage system from abuse)

Software



- ▶ Machine Learning
- ▶ Big Data
- ▶ Intel Compilers
- ▶ MPI
- ▶ OpenMP
- ▶ HPC, HTC, Graphics
- ▶ Install to your home directory
- ▶ Install to your group directory
- ▶ Install to entire cluster for sharing with others (upon request)

Remote Desktop via OnDemand



The screenshot displays a remote desktop environment for a CentOS system. The desktop includes a Firefox browser window showing the CentOS website, a File Manager window displaying the file system structure, and a terminal window with a shell prompt.

Home / My Interactive Sessions / KoKo 3 Desktop

Interactive Apps

- Desktops
 - KoKo 3 Desktop**
- GUIs
 - ANSYS Workbench
 - MATLAB
- Servers
 - Jupyter Notebook
 - Jupyter With Additional Tools

KoKo 3 Desktop

This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.

Partition

- shortq7 - Limited to 6 hours of use
- mediumq7 - Limited to 3 days of use
- longq7 - Limited to 7 days of use

Number of hours

Node type

- any - (20 - 64 cores) Use any available KoKo node. This reduces the wait time as there are no node requirements.
- v100 - Limit to v100 nodes
- a100 - Limit to a100 nodes

Number of Cores

Memory (GB)

Exclusive access to node?

I would like to receive an email when the session starts

Launch

* The KoKo 3 Desktop session data for this session can be accessed under the [data root directory](#).

Email Notifications



Dear Rhian Resnick,

Your job 4346736 has started on koko.

Details about the job can be found in the table below:

ID: 4346736
Name: sys/dash
Partition: shortq7
Nodes: 1
Wallclock: 4:00:00
Std out: /mnt/beegfs/home/rresnick/ondemand/data/sys/dashboard/batch_connect/sys/bc_desktop/koko3/output/58d8ac79-0a8b-404e-b3ab-217a2f7b48fe/output.log
Std err: /mnt/beegfs/home/rresnick/ondemand/data/sys/dashboard/batch_connect/sys/bc_desktop/koko3/output/58d8ac79-0a8b-404e-b3ab-217a2f7b48fe/output.log
Work dir: /mnt/beegfs/home/rresnick/ondemand/data/sys/dashboard/batch_connect/sys/bc_desktop/koko3/output/58d8ac79-0a8b-404e-b3ab-217a2f7b48fe
Comment:
Start: 23/08/2022 13:40:08

Regards,

Slurm Admin

Note: This is an automated e-mail.

Costs



- ▶ Everything we offer has a free introductory tier to help spring board research.
- ▶ But some things have a cost regardless.
 1. Secure Virtual Desktop at the cost of \$168.50 per core per year (Includes 4GB of memory per core)
 2. Storage over 300 GB \$160 / TB / Year
 3. Prioritized Compute \$116 / CPU Core / Year
 4. Prioritized GPU \$1,024 / GPU Per / Year (this gets interesting when comparing models, so reach out to us. Our model is based on UF's GPU unit model, more information on request)
 5. Consultation: \$60 per hour
 6. Data Center Hosting: \$16 per U minimum of 4U

Links and Disclaimers



- ▶ Cyber Infrastructure Plan 2017-2022:
<https://helpdesk.fau.edu/TDClient/2061/Portal/KB/ArticleDet?ID=141481>
- ▶ Services:
<https://helpdesk.fau.edu/TDClient/2061/Portal/KB/ArticleDet?ID=142149>
All costs were FAU internal costs, fees are ~20% higher for external entities.
We are working on new grant funded research pricing. This is still a work in progress.
- ▶ Docs: <https://hpc.fau.edu>