



# DRI WorkShop - Data Analysis

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Digital Research Alliance of Canada

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# Session Overview

- Introduction to the arc and VM
- Machine learning and LLMs
- **Introduction to data analysis**
- **What to do when your laptop isn't enough**
- **The Digital Research Alliance of Canada (ARC)**
- **Demo**
- **Using resources - Workshop**
- **Data analysis Demo**



Business  
Question



Get Data



Explore Data



Prepare Data



Present  
Findings



Analyze Data

# Data Analysis

The process of examining, cleaning, transforming, and modeling data to uncover insights and support decision-making.



**Premise:** Turn raw data into actionable insights that drive informed decisions.

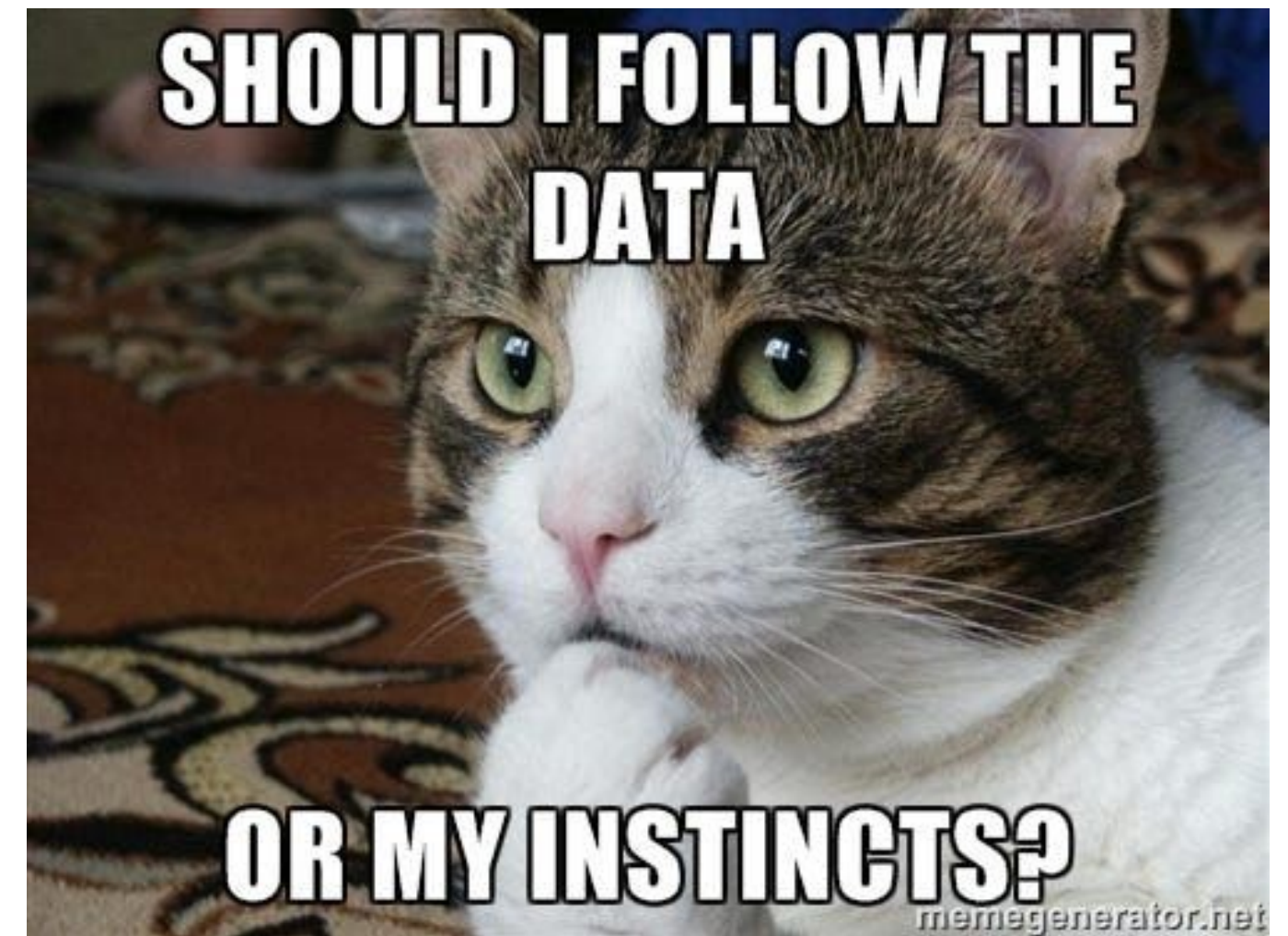
# Data Visualization

Graphical representation of data to make complex information easy to understand and insights more accessible.

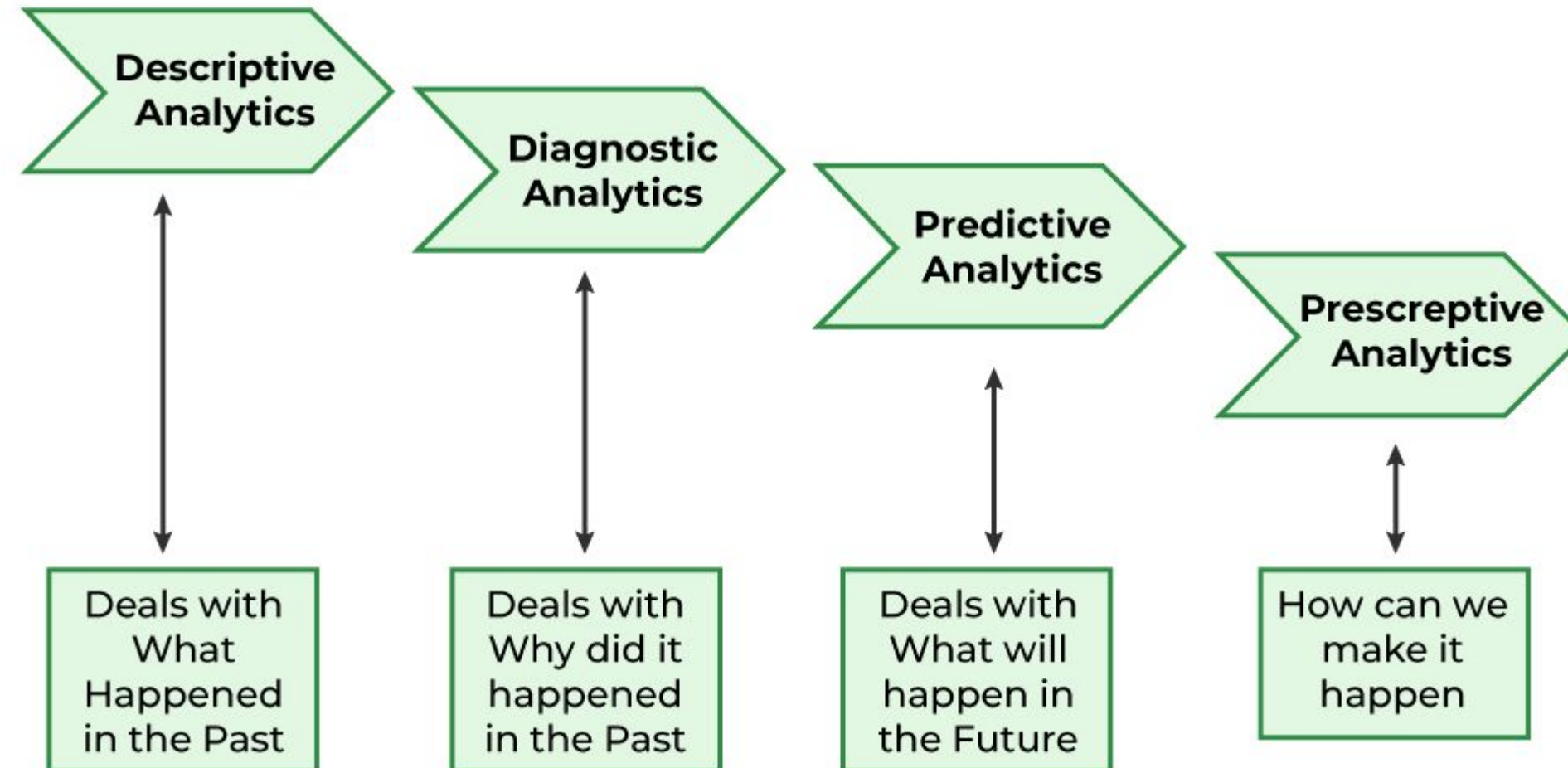
- Simplifies complex data, make it understandable
- Identifies trends and patterns at a glance for quick decision-making
- Improves data-driven communication, making findings more persuasive
- Reveals relationships between variables that may be hard to see in raw data

# Importance

- **Era of digital transformation :Explosion of data generated by digital technologies**
  - **Improves Decision-Making**
  - **Reveals inefficiencies in processes**
  - **Allows for better resource allocation and cost savings**
  - **Forecasts Trends and Risks**
  - **Supports Customer Experience**
  - **Provides insights that inspire new products**
  - ...



# Types

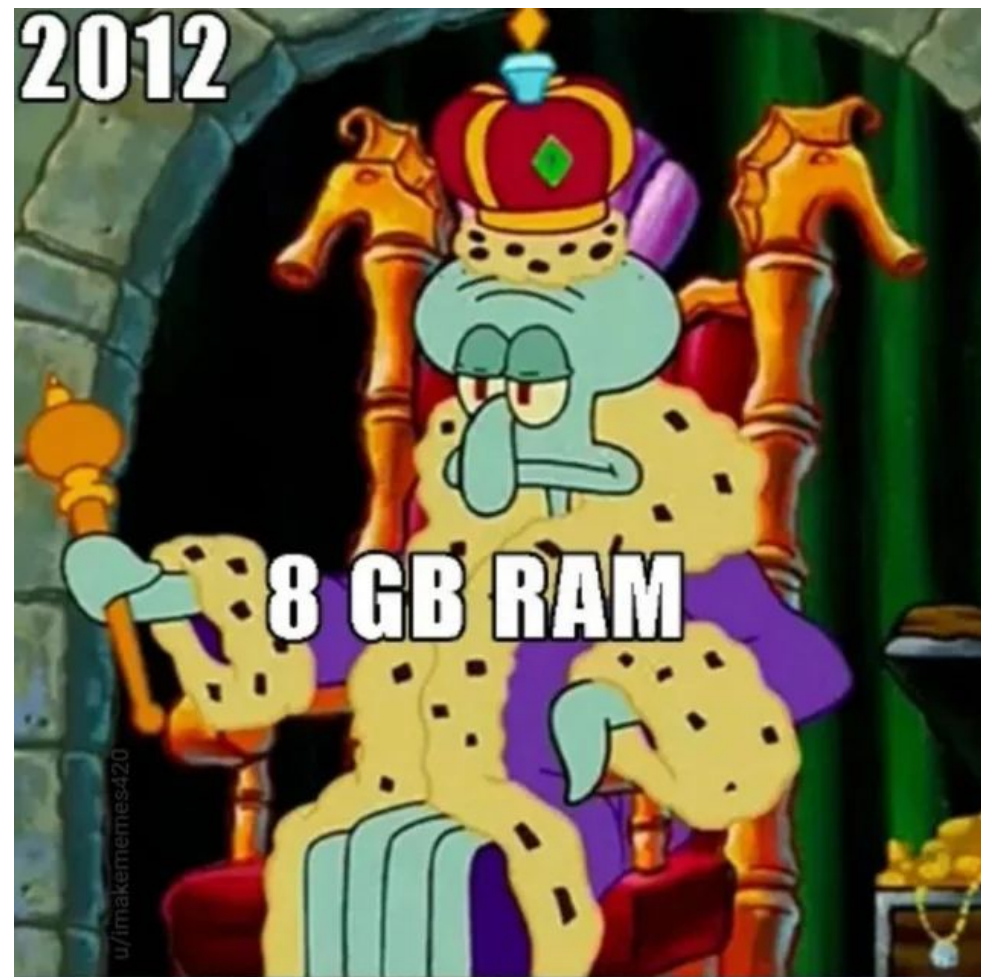


# Laptop not enough

- **Self-purchased**
- **Digital Research Alliance of Canada**
- **Cloud**
- **UBC resources (UBC ARC)**



2012



# Not Enough Resource

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- Analysis taking to long
- Not enough computing power
- Not enough storage

2021





**It doesn't matter how many  
resources you have...**



**If you don't know how to use  
them, it will never be enough.**



# The Digital Research Alliance of Canada (ARC)

- **Mission:** To provide Canadian researchers with the tools and infrastructure needed to conduct world-class research.
- **Key Services:**
  - **Advanced Research Computing (ARC):** Provides high-performance computing resources, data storage, and software tools to support computationally intensive research.
  - **Research Data Management (RDM):** Offers services to help researchers manage and preserve their research data.
  - **Research Software (RS):** Supports the development and dissemination of research software.

# Account

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- Create an account

<https://alliancecan.ca/en/services/advanced-research-computing/account-management/apply-account>

- Provide:

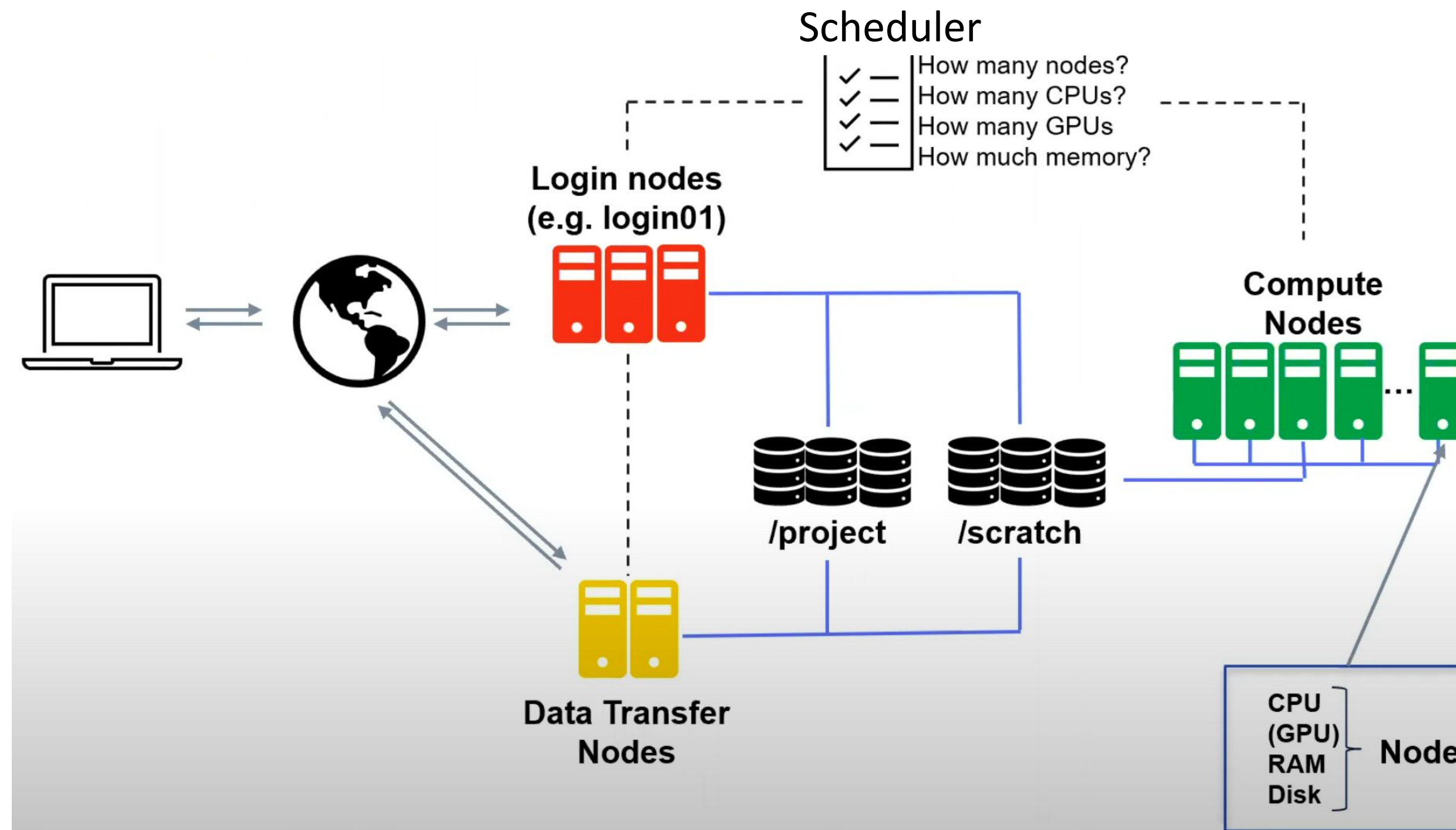
- Your institutional credentials (e.g., university email).
- Contact information for your sponsor (usually a supervisor or research lead).
- **Sponsor Account:** Required to access DRI resources.
- Sponsor information (e.g., name)

- Once submitted, you'll receive credentials and details about your assigned resources.

- Logging in

<https://www.alliancecan.ca/en>

# ARC Structure



# Structure

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- Cluster:
  - A cluster is a group of interconnected computers (nodes) that work together to perform tasks.
  - To handle large-scale computational tasks that a single computer cannot.
  - To divide tasks among multiple nodes for faster processing.
- Node:
  - A node is an individual computer within a cluster.
  - Types of nodes:
    - Login Nodes: Entry points for users to access the cluster. Used for submitting jobs, transferring files, and setting up environments.
    - Compute Nodes: Perform the actual computation. Jobs are executed here.
    - Storage Nodes: Dedicated to managing and storing data.



# Structure

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- Job:
  - A job is a task or set of tasks submitted to a cluster's scheduler for execution on the compute nodes.
  - Jobs represent the work you want the system to perform, such as running a program, processing data, or training a machine learning model.
- Scheduler:
  - A scheduler manages how jobs are distributed and executed on the cluster's compute nodes.
  - Slurm (Simple Linux Utility for Resource Management): Widely used on DRI clusters.
  - Prevent resource conflicts between users.
  - Efficiently allocate resources to users.
  - Manage queues for job execution.



# Let's Start

# Connection

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- Terminal

- The terminal (or command line) is a text-based interface to interact with your computer.

- search for `cmd(windows)/terminal(mac/linux)`

- Host: The server you're connecting to.

- Username: Your account name on the server.

- Authentication: Password or SSH keys.

- SSH: SSH (Secure Shell) is a protocol to securely connect to remote servers (DRI)

# Connection

- SSH

`ssh username@cluster_name.dri.ca`

`okpas30@beluga.computecanada.ca`

```
Success. Logging you in...
#####

  _ _ _ _ _      Grappe de calcul Béluga / Béluga cluster
 | | _ / _ | | _ _ _ _ _
 | ' _ \ / _ \ | | | / _ \ |
 | | _ | _ / | | | ( | | ( | | Aide/Support: support@tech.alliancecan.ca
 | _ _ \ _ \ | | \ , _ \ , | \ , _ | Globus Collection: computecanada#beluga-dtn
                                     | _ / Documentation: docs.alliancecan.ca
                                     Portail/Portal: portail.beluga.calculquebec.ca
#####
```



# Connection

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- Terminal

- Connect to the host
- for this workshop
- password

ssh username@hostname

[username@champions.c3.ca](mailto:username@champions.c3.ca)

champions-24

```
➔ ~ ssh user01@champions.c3.ca
(user01@champions.c3.ca) Password:
[user01@login1 ~]$ ls
bert_complete.txt  projects  script_test.py  test.py
poynter_data.csv  scratch  script_test.sh  Untitled.ipynb
```

# Connection

---

```
➔ ~ ssh user01@champions.c3.ca  
(user01@champions.c3.ca) Password:  
[user01@login1 ~]$ ls  
bert_complete.txt  projects  script_test.py  test.py  
poynter_data.csv   scratch  script_test.sh  Untitled.ipynb
```

- projects: A directory (folder) -> A place where related files and scripts are grouped together.
- scratch: A directory -> Often used as temporary storage for work in progress.

# Data/File types



Data



Script/Code



Intermediate  
files/Data



Results



Log files

- How big are the files?
- Would you like others to access these files?

# Commands

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- Create link for project space  
`ln -s /arc/project/tr-bootcamp-1 project`
- Create personal directory  
`mkdir < personal-directory-name>`
- Transfer local file to your directory  
`scp /local-path/local-file-name user-name@cluster<host>:/file-path`
- Transfer the whole directory  
`scp-r/local-path/local-directory user-name@cluster<host>:/directory-path`



# Commands

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- Upload scripts to the cluster:

- In your local machine run below command

scp "local file" username@cluster.computecanada.ca:"path of destination"

scp samplefile.py okpas30@beluga.computecanada.ca:/home/okpas30/

```
→ Downloads scp samplefile.py okpas30@beluga.computecanada.ca:/home/okpas30/
Multifactor authentication is now mandatory to connect to this cluster.
You can enroll your account into multifactor authentication on this page:
https://ccdb.alliancecan.ca/multi_factor_authentications
by following the instructions available here:
https://docs.alliancecan.ca/wiki/Multifactor_authentication

=====

L'authentification multifacteur est maintenant obligatoire pour vous connecter
à cette grappe. Configurez votre compte sur
https://ccdb.alliancecan.ca/multi_factor_authentications
et suivez les directives dans
https://docs.alliancecan.ca/wiki/Multifactor_authentication/fr.
(okpas30@beluga.computecanada.ca) Password:
```

# Access Files

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- cat, nano, ....

nano filename

nano samplefile.py

```
GNU nano 7.2 samplefile.py
print('Hello world!!!')
print('Welcome to the workshop')
print('The job is running:')
print('The job is completed')
```

# Create a Job

---

- Create a new job script

nano submit\_job.sh

```
GNU nano 7.2 submit_job.sh Modified
#!/bin/bash
#SBATCH --job-name=python_job      # Job name
#SBATCH --output=job_output.txt    # Standard output and error log
#SBATCH --time=00:10:00            # Runtime limit (HH:MM:SS)
#SBATCH --ntasks=1                 # Number of tasks (processes)
#SBATCH --cpus-per-task=1          # CPUs per task
#SBATCH --mem=2GB                  # Memory per node

# Load necessary modules
module load python/3.8

# Run your Python script
python samplefile.py
█
```

# Submit The Job

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- Submit the job script using the sbatch command
- After submitting, Slurm will provide a job ID
- output

`sbatch submit_job.sh`

```
[okpas30@beluga1 ~]$ sbatch submit_job.sh  
Submitted batch job 52669520
```

`cat job_output.txt`

```
#!/Module  
  
Hello world!!!  
Welcome to the workshop  
The job is running:  
The job is completed
```



# Prepare Environment

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- Module

- Modules are used to load software or tools you need for your project.
- Check loaded module
- Make a directory (folder)
- move between directories(cd)

`module load python/3.8`

`module list`

`mkdir data_analysis_project`

`cd data_analysis_project`

# Virtual Environment

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- Avoid Conflicts:
  - Different projects might require different versions of the same library.
  - Without a virtual environment, installing a new version of a library globally could break existing projects.
  - Example:
    - Project A requires `pandas==1.2.0`.
    - Project B requires `pandas==1.3.0`.
  - A virtual environment ensures each project uses its required version.

# Virtual Environment

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- Avoid Conflicts
- Keeps Global Environment Clean:
  - Prevents unnecessary clutter in the global Python environment.
  - Avoids polluting the global Python installation with libraries that might only be used for a single project.
- Easier Debugging:
  - Isolated environments reduce the risk of unforeseen bugs caused by mismatched dependencies.

# Virtual Environment

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- Avoid Conflicts
- Keeps Global Environment Clean
- Easier Debugging

1. Create a virtual environment:

```
python -m venv myenv
```

2. Activate virtual environment

```
source myenv/bin/activate
```

3. Closing virtual environment

```
deactivate
```

4. remove virtual environment

```
rm -r myenv
```

# Install Requirements

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1. Create a virtual environment:

```
python -m venv myenv
```

2. Activate virtual environment

```
source myenv/bin/activate
```

- Install libraries:

- pandas
- matplotlib

- Freeze and install them at once

```
pip freeze > requirements.txt
```

- Use

```
pip install -r requirements.txt
```

# Connect to Jupyter Notebook

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- Install jupyter notebook **if not already installed**

`pip install notebook ipykernel`

- Add the VE to the jupyter notebook

`python -m ipykernel install --user --name=myenv--display-name "Python (myenv)"`

- Restart jupyter notebook

`pkill jupyter`

- Start again

`jupyter notebook`

- Open your Jupyter Notebook in the browser. If you're using a web-based Jupyter setup, log back in as needed.
- Choose the kernel tab and change kernel



# Data Analysis

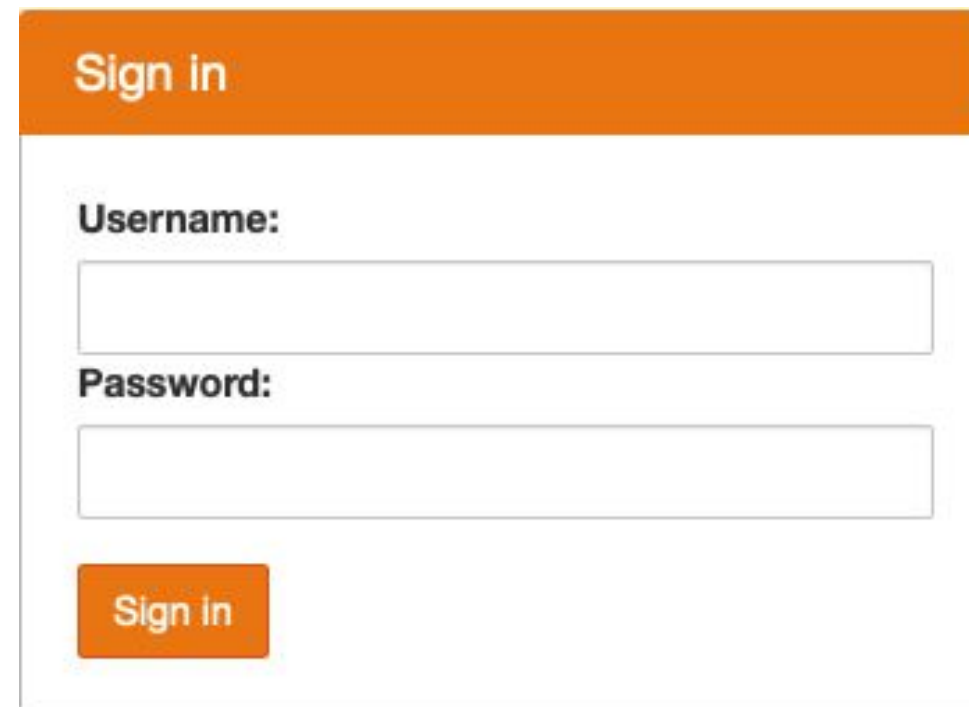
# Connection

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- Web

- In your browser

<https://jupyter.champions.c3.ca/hub/login>

A screenshot of a web login form. It has an orange header bar with the text "Sign in". Below the header, there are two input fields: "Username:" and "Password:". Below the password field is an orange button with the text "Sign in".

Sign in

Username:

Password:

Sign in

- username
- password

user01

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# Libraries

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- Python libraries
  - A Python library is a collection of related modules.
  - It makes Python Programming simpler and convenient for the programmer.
- List of Libraries

<https://docs.python.org/3/library/index.html>

<https://www.geeksforgeeks.org/libraries-in-python/>

# Load Data

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- Load data from web and different libraries

```
penguins = sns.load_dataset('penguins')
```

- Upload data using scp into server.

```
scp "local file" username@cluster.computecanada.ca:"path of destination"
```

- Check data

- head(n): prints the n first columns of the dataset.
- penguins.info(): prints information about the columns of the dataset.
- penguins.isnull().sum(): Check for missing values.

# Handling missing values

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- Why?
  - Missing values can lead to biased or invalid results.
  - Many machine learning algorithms do not handle missing data well.
  - incorrect handling of missing data can distort statistical calculations.
- Solution
  - Remove Missing Data: The dataset is large, and the missing data is minimal.
  - Impute Missing Data: Missing values are not random or constitute a significant part of the dataset.
  - Predict Missing Value: Complex relationships exist between features, and simple imputation isn't sufficient.
  - ...

# Analyse

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- Scatterplot:
  - Purpose: Visualizes the relationship between two numerical variables.
  - Example: Flipper length vs. body mass, with points colored by penguin species.
  - Insights: Highlights trends, clusters, or correlations between variables.
- Boxplot:
  - Purpose: Shows the distribution of a numerical variable across categories.
  - Example: Bill depth by species.
  - Insights: Identifies medians, spread, and potential outliers.



# Analyse

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- Pairplot:

- Purpose: Provides pairwise scatterplots of all numerical variables.
- Example: Pairwise relationships of features (e.g., body mass, bill length).
- Insights: Comprehensive overview of correlations and distributions.

- Heatmap

- Purpose: Displays the correlation matrix between numerical variables.
- Example: Correlation matrix of penguin features.
- Insights: Shows how strongly numerical variables are related.

# Outliers

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- Outliers can significantly influence data analysis.
- Detecting and handling them ensures more reliable insights.
- Different methods of outlier detection
  - Here for simplicity we use the same boxplot
- Handling outliers
  - Removing outliers
  - Capping Outliers: Replace with nearest acceptable value.
  - Transform Data (log,etc): Reduce the impact of outliers.

# Questions