AutoAppendix: Towards One-Click Reproducibility of Computational Artifacts

Chameleon User Meeting 2024

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Outline

1. Motivation
2. AutoAppendix
3. Reproducibility Challenges and Proposed Solutions
4. Chameleon Cloud Jupyter Notebook Templates

Motivation

Supercomputing Conference (SC) Reproducibility Initiative

- Introduced at SC15
- Paper authors submit Artifact Description (AD) and Artifact Evaluation (AE) appendices
  - AD: Relation between contributions and artifacts, necessary information to reproduce results
  - AE (optional): Concrete reproduction instructions
- Authors apply for *reproducibility badges*
  - Artifacts Available
  - Artifacts Evaluated – Functional
  - Results Replicated
- Reproducibility Committee evaluates artifacts and awards badges
  - 8-hour evaluation period
  - Downgrades (e.g., from RR to AF) possible

Badge Verdicts at SC24

Applied / Verdict	Artifacts Available	Artifacts Functional	Results Replicated	Total
Artifacts Available	20	1	0	21
Artifacts Functional	**6**	6	1	13
Results Replicated	**7**	**14**	24	45
Total	33	21	25	79

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How can this be improved?

AutoAppendix

AutoAppendix

- 2-month project conducted during the UCSC Summer of Reproducibility program
- Survey of the *state of reproducibility* of SC'24 papers.
- **Goals**:
  - Understand current challenges in achieving reproducibility
  - Identify best practices and potential for automation
- **Approach**: Select papers *without* special hardware requirements
  $\rightarrow$ Reproducibility depends on software stack and documentation

Paper Selection Criteria

- Select only from papers applying for *Results Replicated* badge
- No special hardware setup (e.g. specific clusters)
- Free software stack
- Experiments reproducible on *a single* ***Chameleon Cloud*** *node*
- Final Selection: **18 papers**

ID	Node Type	Site	Project Type
111	skylake	TACC	Simulator
174	skylake	TACC	Plotting
190	skylake	TACC	Plotting
191	icelake_r650	TACC	OpenMP
202	icelake_r650	TACC	Algorithm/Study
227	v100	UC	CUDA
332	gtx_6000	UC	CUDA
362	gtx_6000	UC	CUDA
368	icelake_r650	TACC	Framework
376	p100	TACC	CUDA
407	mi100	TACC	OpenCL
428	icelake_r650	TACC	Study
466	v100	UC	Study
467	p100	TACC	Framework
482	icelake_r650	TACC	Algorithm/Study
483	icelake_r650	TACC	Framework
496	icelake_r650	TACC	Algorithm
506	icelake_r650	TACC	Compiler

Reproducibility Challenges and Proposed Solutions

Challenge (I): Software Setup

Problem

- Failing builds due to missing dependencies
- Incompatible software versions
- Insufficient documentation

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Solution Ideas:

- State operating system and software versions for all relevant components
- Use reproducible software environments
  - Containerization Solutions: Docker, Singularity, ...
  - Reproducible Builds: Spack, Guix, Nix

Challenges (II): Data Availability

Problem:

- Artifact repositories have limited storage, not sufficient for certain datasets (e.g. ML training data)

→ Data has to be stored externally

- Data may *not be available* anymore
- Download may be slow

Challenges (II): Data Availability

Problem:

- Artifact repositories have limited storage, not sufficient for certain datasets (e.g. ML training data)

→ Data has to be stored externally

  - Data may *not be available* anymore
  - Download may be slow

Solution Ideas:

- Ensure data availability, most importantly in the evaluation period
- Ensure reasonable download times and provide estimates

Challenges (III): Long-Running Operations

Problem:

- Experiment takes a long time, documentation is not clear about how long the operation should take
- No output $\rightarrow$ user does not know if the application is still running
- Too much output may cause performance issues/inconsistencies

Challenges (III): Long-Running Operations

Problem:

- Experiment takes a long time, documentation is not clear about how long the operation should take
- No output $\rightarrow$ user does not know if the application is still running
- Too much output may cause performance issues/inconsistencies

Solution Ideas:

- State expected run time on the *evaluation hardware* for all long-running steps
- If applicable, provide *progress output* to the user

Challenges: Summary

- **Software Setup**: Document software versions and use reproducible environments
- **Data Availability**: Ensure data is available and provide download estimates
- **Long-Running Operations**: State expected run times and provide progress output

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- **Software Setup**: Document software versions and use reproducible environments
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- **Long-Running Operations**: State expected run times and provide progress output

These are only a few examples of the faced challenges, others include:

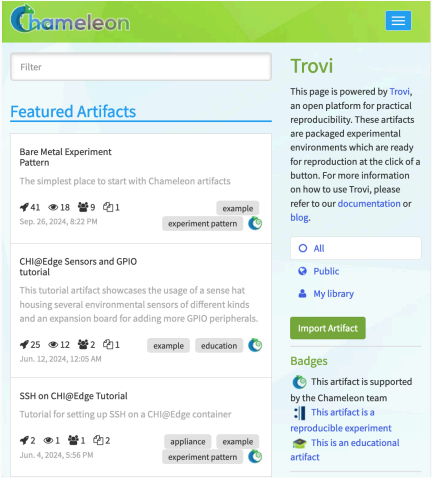
- **Documentation**: Clear and self-contained
- **Hardware Compatibility**: Reproducible on common hardware
- **Expected Results**: State expected behavior and (intermediate) results

Results were compiled into a set of **guidelines** and **best practices**

Chameleon Cloud Jupyter Notebook Templates

Chameleon Cloud Jupyter interface

- Allows for automated node provisioning and setup over `python-chi`
- Experiments can be executed fully automatically without manual intervention
- *Trovi* enables easy artifact sharing

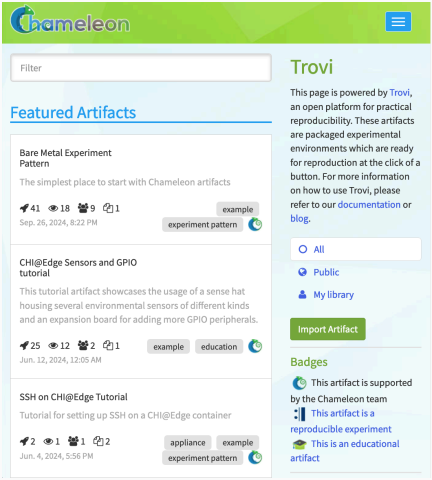


Chameleon Cloud Jupyter interface

- Allows for automated node provisioning and setup over `python-chi`
- Experiments can be executed fully automatically without manual intervention
- *Trovi* enables easy artifact sharing

→ **Very useful for artifact evaluation!**

- No need for manual node setup
- Transparency in software setup and steps



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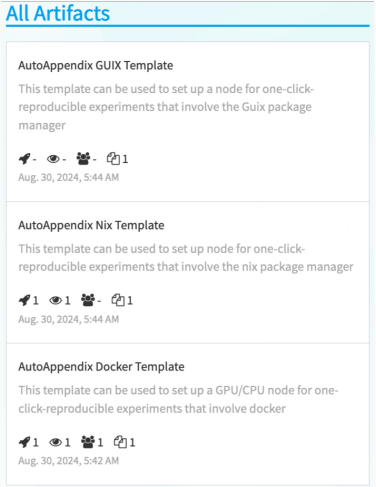
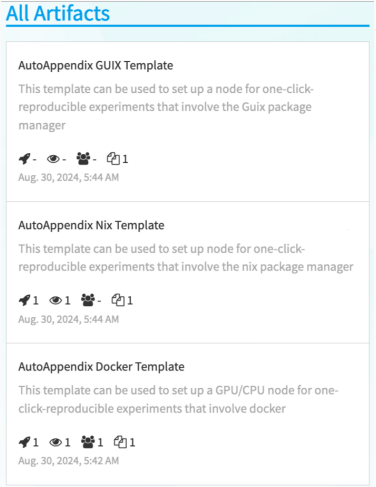
- **How can we make this more accessible?**
- Three new Jupyter Notebook templates on *Trovi*
  - Docker
  - Nix
  - Guix



Jupyter Notebook Templates

- Only 1 submission for SC24 used this approach
- **How can we make this more accessible?**
- Three new Jupyter Notebook templates on *Trovi*
  - Docker
  - Nix
  - Guix
- **Features**:
  - Thorough documentation
  - Centralized Configuration
  - Sample Experiments



Summary

- **AutoAppendix** project aimed to identify challenges in achieving reproducibility
- **Guidelines** and **best practices** were compiled from the challenges encountered
- **Jupyter Notebook Templates** were created to encourage the use of Chameleon Cloud's Jupyter Interface
- **Future Work**:
  - Refine guidelines and best practices
  - Evaluate the impact of the templates and refine
  - Create templates for other software environments

Thank you for your attention!

Questions?

Find the AutoAppendix {Docker, Nix, Guix} Templates on *Trovi*:

`https://www.chameleoncloud.org/experiment/share/?filter=autoappendix`