

Appendix: Artifact Description/Artifact Evaluation

Artifact Description (AD)

Overview of Contributions and Artifacts 1.1

Paper's Main Contributions

Provide a list of all main contributions of the paper.

C1 Framework for storage, sharing and analysis of scientific tools using container as a service on the cloud platform

C2 HPC AI integration to enable adaptive sampling using indigenously developed workflows

Computational Artifacts

List the computational artifacts related to this paper along with their respective DOIs. Note that all computational artifacts may be archived under a single DOI.

A1 Architecture & Hardware Information

A2 Gromacs

A3 Pyemma

A4 Grafana

<https://grafana.com/solutions/kubernetes/>

A5 Ambertools

<https://anaconda.org/conda-forge/ambertools>

A6 Scripts to generate saturation and conformation exploration plot for adaptive sampling

Provide a table with the relevant computational artifacts, high-light their relation to the contributions (from above) and point to the elements in the paper that are reproducible by each artifact, e.g., which figures or tables were generated with the artifact.

Artifact ID	Contributions	Related Supported Paper Elements
A1	C1	Table 1 Figure 1
A2,A3,A4,A5,A6	C2	Figures 2,3,4,7

Computational Artifact A1

Relation To Contributions

C1 Framework for storage, sharing and analysis of scientific tools using container as a service on the cloud platform

Artifact Setup (incl. Inputs)

Hardware details : Given in the table 1 of the manuscript

<https://nsmindia.in/infrastructure/nsm-systems/param-rudra-iuac-new-delhi/>

Artifact Execution

<https://icecloud.in>

Username: testuser

Password: testuser123

Expected Results

User can explore and access icecloud

Computational Artifact A2 to A6

Relation To Contributions

C2 HPC AI integration to enable adaptive sampling using indigenously developed workflows

Artifact Setup (incl. Inputs)

Software.

Gromacs

<https://manual.gromacs.org/2024.4/download.html>

Pyemma

<https://emma-project.org/latest/>

Grafana

<https://grafana.com/solutions/kubernetes/>

Ambertools

<https://anaconda.org/conda-forge/ambertools>

Datasets/Inputs.

Penta-peptide data available at github:

https://github.com/bioinformatics-cdac/ICE_SC25/tree/main/inputs_pentapeptide

All tools are available as container on ICE cloud

<https://icecloud.in>

Artifact Execution

Steps for running the adaptive sampling for a model system of pentapeptide has been given in the link below,

https://github.com/bioinformatics-cdac/ICE_SC25/blob/main/Artefact_Manual.pdf

Expected Results

Pentapeptide output data available at github:

https://github.com/bioinformatics-cdac/ICE_SC25/tree/main/outputs_pentapeptide

Expected Reproduction Time (in Minutes)

The expected computational time of this artifact is 20mins per cycle.

Artifact Evaluation (AE)

2.1 Computational Artifact A1

Artifact Setup (incl. Inputs)

Provide instructions for installing and compiling libraries and code. Offer guidelines on deploying the code to resources.

Artifact Execution

Describe the experiment workflow. If encapsulated within a work-flow description or equivalent (such as a makefile or script), clearly outline the primary tasks and their interdependencies. Detail the main steps in the workflow. Merely instructing to “Run script.sh” is inadequate.

Artifact Analysis (incl. Outputs)

- Provide a description of the expected results and a methodology for evaluating these results.

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Explain how the expected results from the experiment workflow correlate with the contributions stated in the article.

- For example, if the article presents results in a figure, the artifact evaluation should also produce a similar figure, depicting the same generalizable outcome. Authors must focus on these aspects to reduce the time required for others to understand and verify an artifact.

2.2 Computational Artifact A2

Artifact Setup (incl. Inputs)

Artifact Execution

Artifact Analysis (incl. Outputs)