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Sustainable Research Software and Infrastructure for HPC: Practices, Challenges, and Community

Wednesday, 3 December 2025 11:00 (1h 30m)

Motivation

Around the world, the Research Software Engineering (RSE) movement has shown how professionalising research software practices and building RSE communities can strengthen the sustainability of HPC-enabled research. Many HPC users are writing their own code, often without formal training or long-term support, which raises challenges for efficiency, portability, reproducibility, and maintenance, all of which are foundational to sustainable research software. This workshop, the first of its kind in Africa, creates a space to showcase local software projects, share sustainability challenges, opportunities and practices, and strengthen our collective capacity for impactful computational research. Similar events have been held at computational conferences, such as ISC 2023 (where MS was an invited speaker) and SC, for the last five years.

Objectives

- Raise **awareness** of the global movement related to research software sustainability, with a specific focus on RSEs and HPC.
- Highlight the crucial role of **research software in leveraging HPC systems** for scientific discovery.
- Showcase participant **HPC-related software projects** with a focus on sustainability and scalability.
- Discuss **challenges** unique to research software that runs on HPC systems (e.g. portability, optimisation, reproducibility).
- Strengthen the **RSE community** within the HPC ecosystem in South Africa and across Africa.

Structure (90 minutes)

1. Welcome & Framing (10 min)

- RSE as the "missing link" between HPC infrastructure and impactful research.
- Why software sustainability is crucial for HPC environments:
- Code must be portable across architectures (clusters, GPUs, cloud/HPC hybrids).
- Performance tuning and scaling.
- Dependency management and containerisation (Singularity/Apptainer, Docker → HPC).
- Long-term usability beyond initial grants.
- Outline of session flow.

2. Lightning HPC Project Presentations (45 min)   Participants deliver **3–4 minute lightning talks** about their research software projects, following a **structured template**, with a focus on **software sustainability** in an HPC context.

Template prompts (HPC-focused):

- Project name & research domain
- Software function (how it supports/accelerates research)
- Where it runs (e.g., CHPC, regional facility (e.g. ilifu), institutional cluster, international facility)
- Development & maintenance team (single student? research group? cross-institution?)
- Sustainability considerations
- Portability & scaling: Can it run on different HPC systems? GPU/CPU optimisations?
- Documentation & training: Is it accessible to new users? HPC-specific usage guides?
- Community & adoption: Who uses it, and how can they contribute?
- Dependencies & environment: How are software stacks managed (modules, containers, Conda)?
- Identifiers & citations: DOI for code/data, ORCID/ROR for credit.
- Funding & longevity: Beyond project lifetime, who maintains it?
- Biggest HPC-related sustainability challenge (e.g., scaling beyond a local cluster, lack of developer time, rapid hardware changes).

We will provide a **slide template** in advance with these fields for participants to populate with their content. The slide template is attached to this submission for reference.

3. Group Reflection & Discussion (25 min)   Facilitated conversation drawing out common themes:

- Which HPC-related sustainability challenges recur (e.g., portability, performance, lack of maintainers)?
- What practices are helping (e.g., using containers, joining global open-source communities, institutional RSE support)?
- How can CHPC, universities, and RSSE-Africa support the sustainability of HPC software?
- Is there a need for a shared HPC-RSE knowledge base/training programme?

4. Next Steps & Closing (10 min)

- Summarise takeaways: recurring issues + promising solutions.
- Announce possible follow-up:
- An HPC–RSE community of practice under CHPC.
- A repository of HPC software projects in South Africa.
- Training opportunities (e.g., Carpentries HPC lessons, RSSE Africa workshops).
- Share resource links (e.g., FAIR4RS principles, Software Sustainability
- Institute guides, containerisation best practices for HPC).

Deliverables / Follow-up

- Shared **slide deck/Zenodo** collection of participant projects.
- Post-session **blog/summary** for CHPC website/newsletter.
- Potential to propose a **recurring HPC Software Sustainability SIG** at future CHPCconf.

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No. Not a student nor Postdoc.

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No

CHPC User

No

CHPC Research Programme

Not applicable

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