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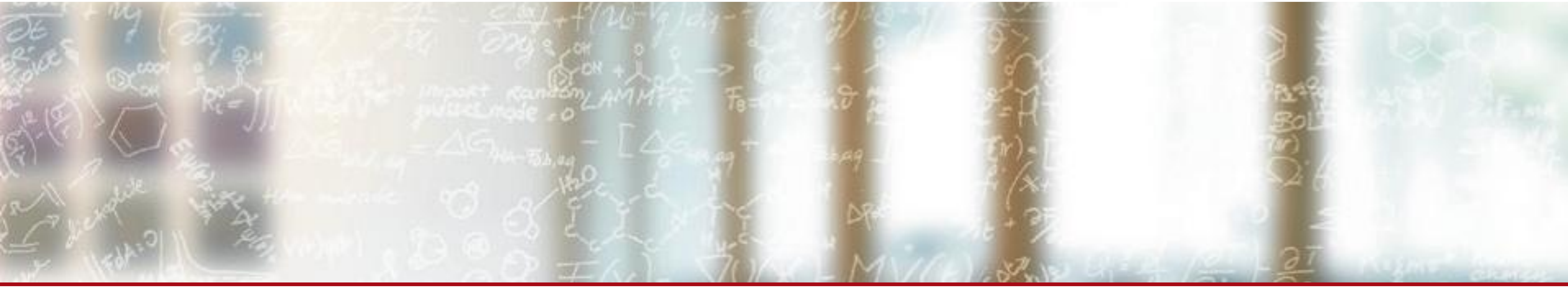

Evolving Sarus to augment Podman for HPC on Cray EX

CUG 2025

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Sarus (2019)

- Combines container portability with native HPC performance
- Supports container specialization and HPC features through OCI hooks (modular plug-in components)
- Adopts OCI-compliant standards and technologies:
  - Runtime (runc)
  - Hooks (e.g. NVIDIA Container Toolkit)
  - Image conversion tools (Skopeo, umoci)

Container Engine (CE) (2023)

- Forward-looking solution implementing “containers as first-class elements”
- Intended to enable containerized user environments on Alps
- Based on significantly modified versions of NVIDIA Enroot and Pyxis software
- Built on knowledge and insights from Sarus

- Paper at CUG 2024 discussing principles, architecture, implementation, use cases.

Containers-first user environments on HPE Cray EX

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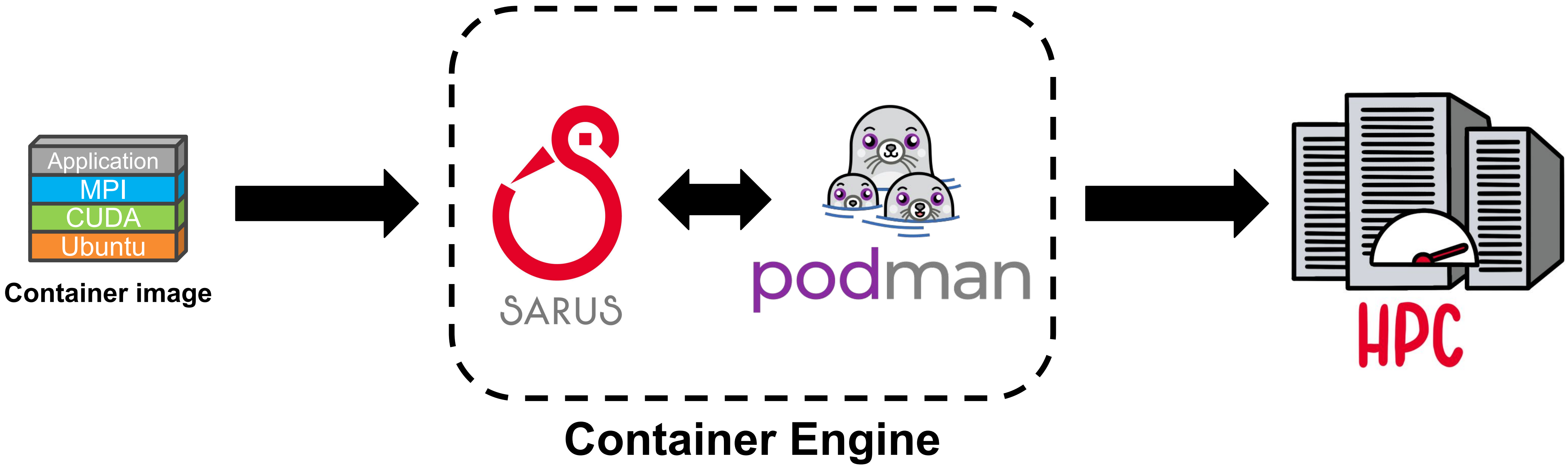
***Abstract*—In High-Performance Computing (HPC), managing the user environment is a critical and complex task. It involves composing a mix of software that includes compilers, libraries, tools, environment settings, and their respective versions, all of which depend on each other in intricate ways. Traditional approaches to managing user environments often struggle with finding a balance between stability and flexibility, especially in large systems serving diverse user needs.**

This work introduces a containers-first approach for HPC, enhancing stability and flexibility in user environments by seamlessly integrating container technologies on an HPE Cray EX system. This approach evolves the user environment management and delivery, enabling customized, fast, and transparent deploy-

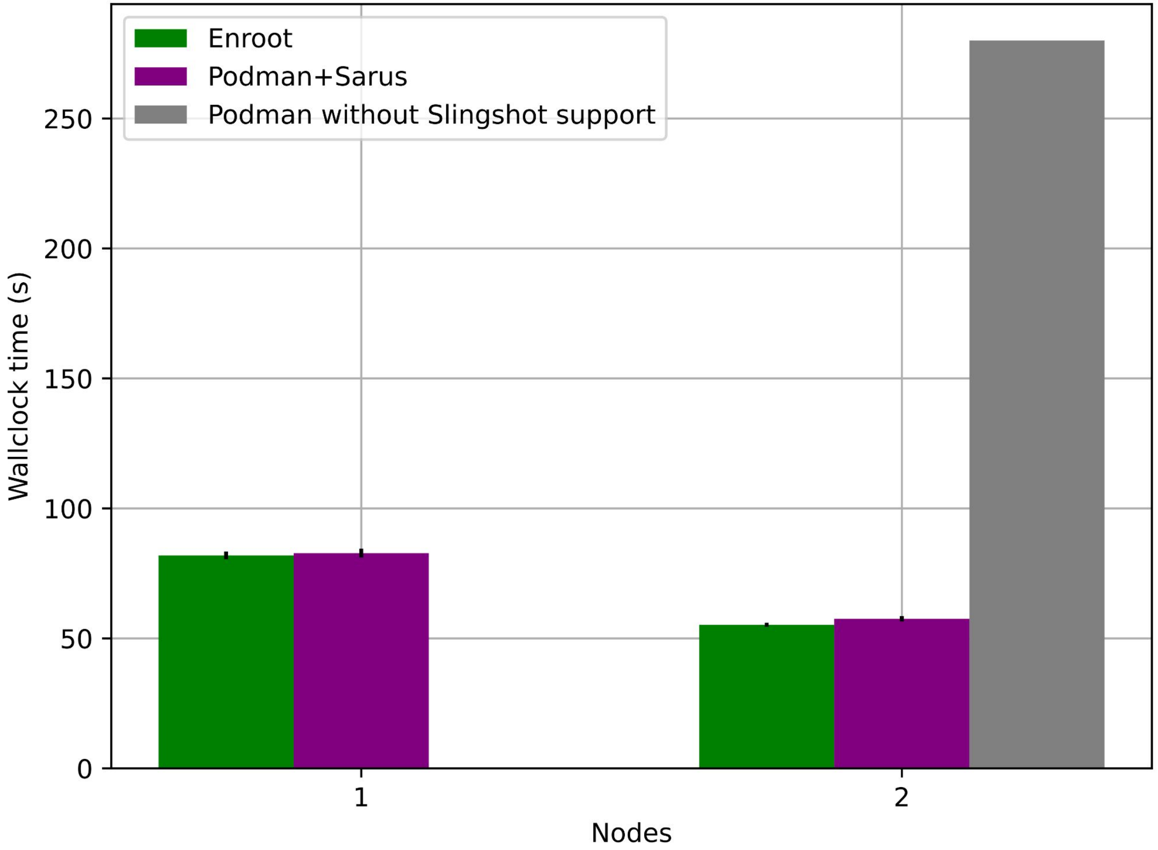
An extensive usage of containers can bring major benefits to HPC users and providers; and could address relevant problems encountered by HPC users and providers alike:

- Decouple user environment from system components: more freedom and flexibility in planning and executing system maintenances, improved robustness and consistency of the user environment as they do not change across maintenance, more informative and meaningful analysis of regressions as user-side components do not change and are reproducible.

Outlook: Augmenting Podman for the next generation Container Engine



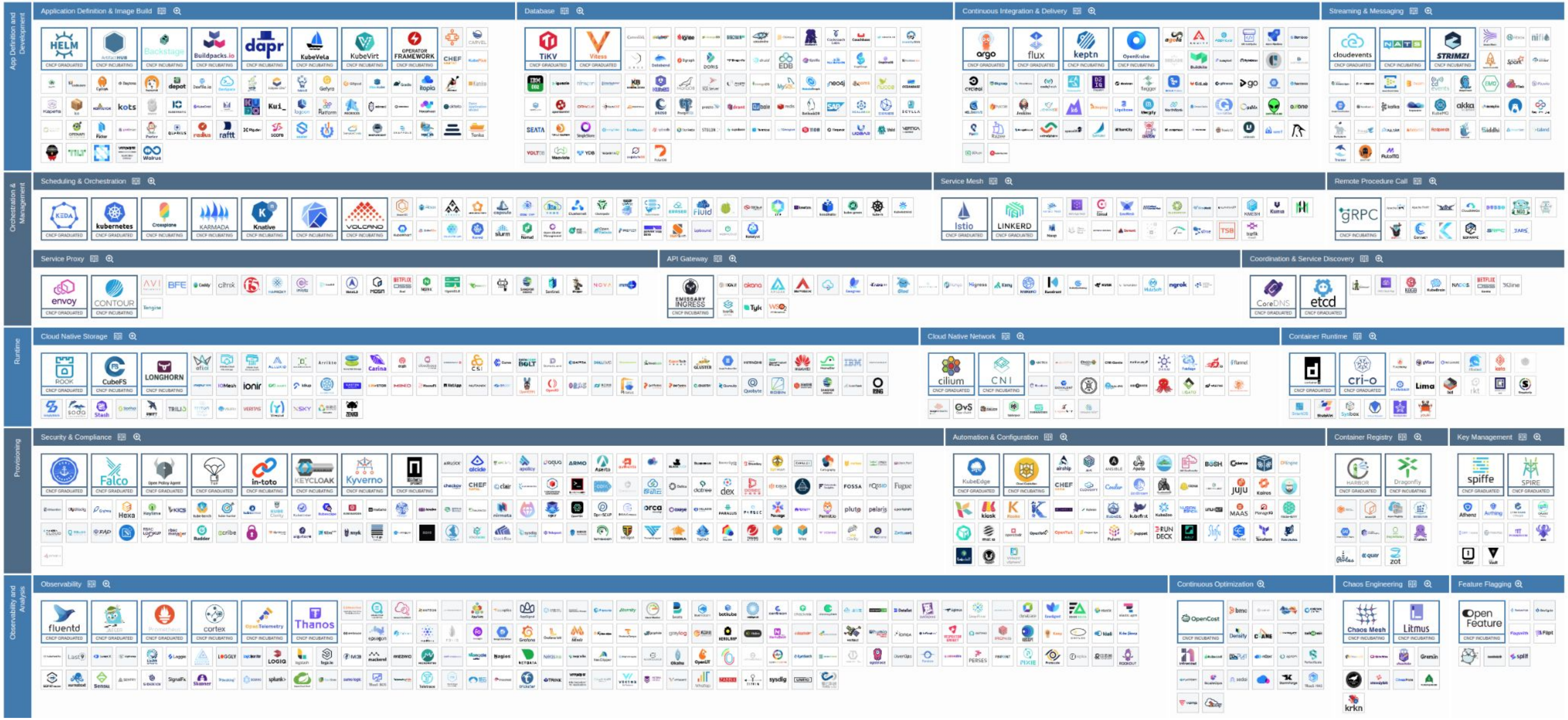
PyFR (Flux Reconstruction CFD)



Container: PyFR 2.1, OpenMPI 5.0.7, CUDA 12.8, Ubuntu 24.04
Test case: 3D Taylor-Green vortex (4 ranks per node, 20 repetitions)
System: Alps Infrastructure - Development vCluster (2 x AMD EPYC 7713, 4 x NVIDIA A100, Slingshot 11 200Gb)

Why are we doing this?

Cloud-native landscape continues to evolve



https://landscape.cncf.io/

Cloud-native evolving to enable AI

- AI is rising as a dominant cloud workload, despite remaining gaps
- Containers are essential building blocks of cloud native, and many container projects are involved
- Aligning and adapting to these innovations can open significant opportunities

CNAI Whitepaper, March 2024

Our current software not in a position to keep up

- Sarus
  - CSCS-developed HPC container engine, in production since 2019
  - Designed primarily to deploy user-defined software stacks and run traditional HPC apps
  - Missing many interactivity and manageability features due to focus on HPC integration
- Container Engine (CE)
  - Pathfinder to demonstrate the “containers as first-class elements” approach
  - Based on NVIDIA’s Enroot + Pyxis software
    - Not officially supported products
    - No significant feature development ongoing or expected
    - No adoption of OCI standards
- Expanding scope of requirements is very demanding in terms of developers time and expertise
- We also want to consolidate work from the two efforts

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Tracing a path forward

Core concepts

- Container portability + native HPC performance
- Container specialization and HPC features through modular components
- Adopt OCI and cloud-native standards and technologies

SARUS
(2019)

- Usability and seamless integration with WLM

CE
(2023)

- Advanced runtime
- Very actively developed and large user community
- Early access to innovative technologies and bleeding-edge developments

podman

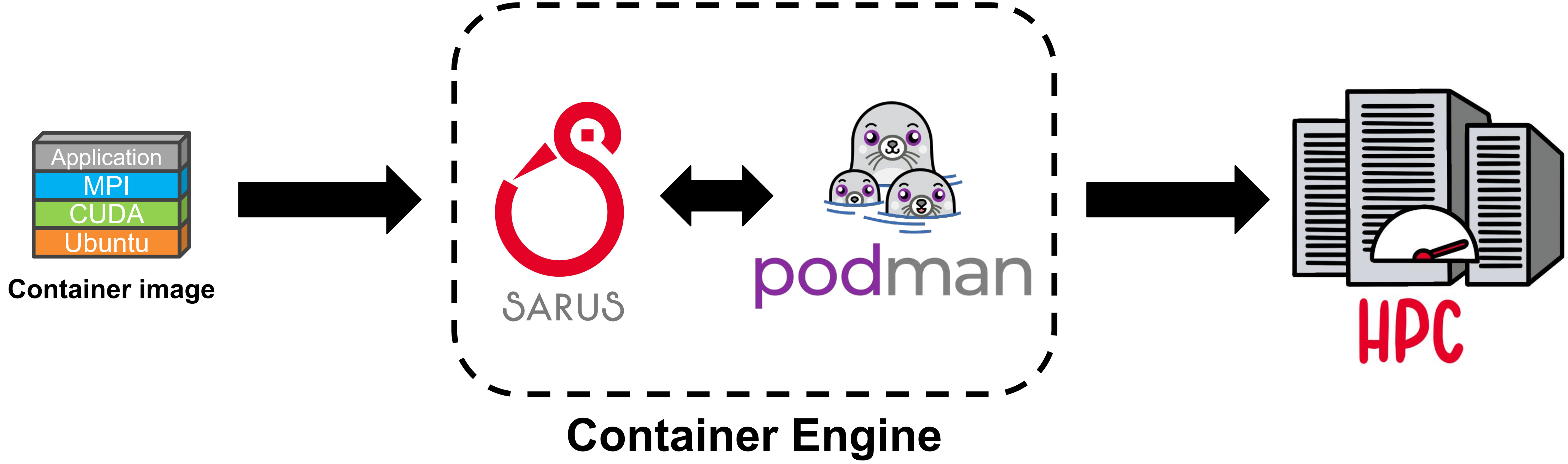
SARUS

Sarus is evolving into a collection of software to unlock the power of HPC for community tools based on open standards.

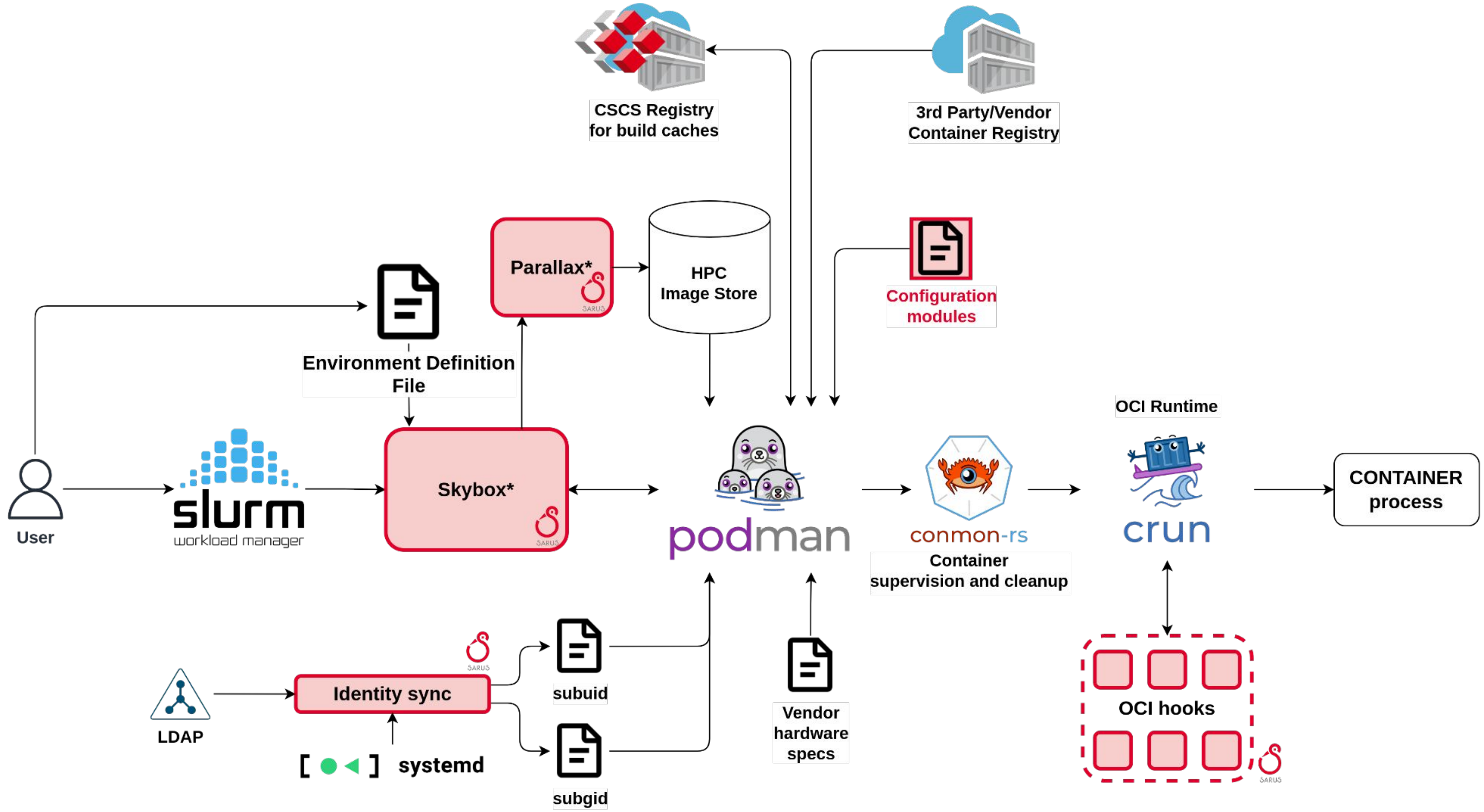
- **Sarus Hooks:** OCI hooks for HPC use cases
- **Parallax*:** Support SquashFS image storage on parallel filesystems
- **Skybox*:** Slurm SPANK plugin for transparent deployment of containers as job environments
- **libsarus:** Foundational C++ library for container tools and OCI hooks
- **rootless-subid-sync:** System-level utility to synchronize Linux subordinate IDs across computing clusters

* : provisional development codenames

Augmenting Podman for the next generation Container Engine



Podman+Sarus Container Engine architecture



*: provisional development codenames

Early tests

Test setup

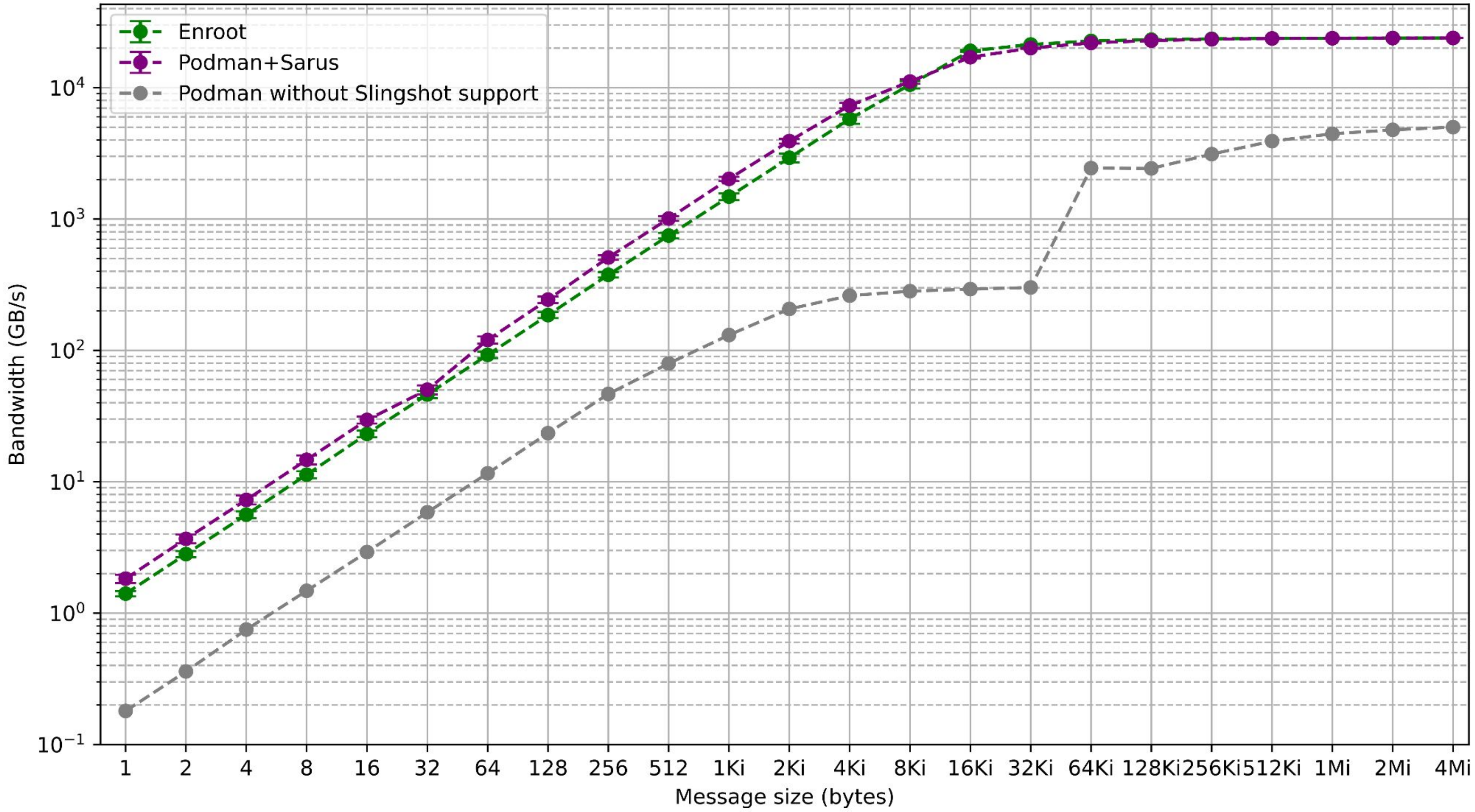
- System: Test & development vCluster within the Alps infrastructure
  - Node architecture: 2x AMD EPYC 7713 (64c) + 4x NVIDIA A100
  - Slingshot 11 200Gb interconnect

- Comparing Enroot (currently used in production) and Podman as internal runtimes within the CE toolset

- HPC feature support for Podman
  - Common “HPC mode” settings: dedicated Podman config module
  - CXI/Slingshot: CSCS-written CDI + Sarus MPI hook
  - GPU: NVIDIA CDI
  - Squashfs images migration and mounting: Parallax

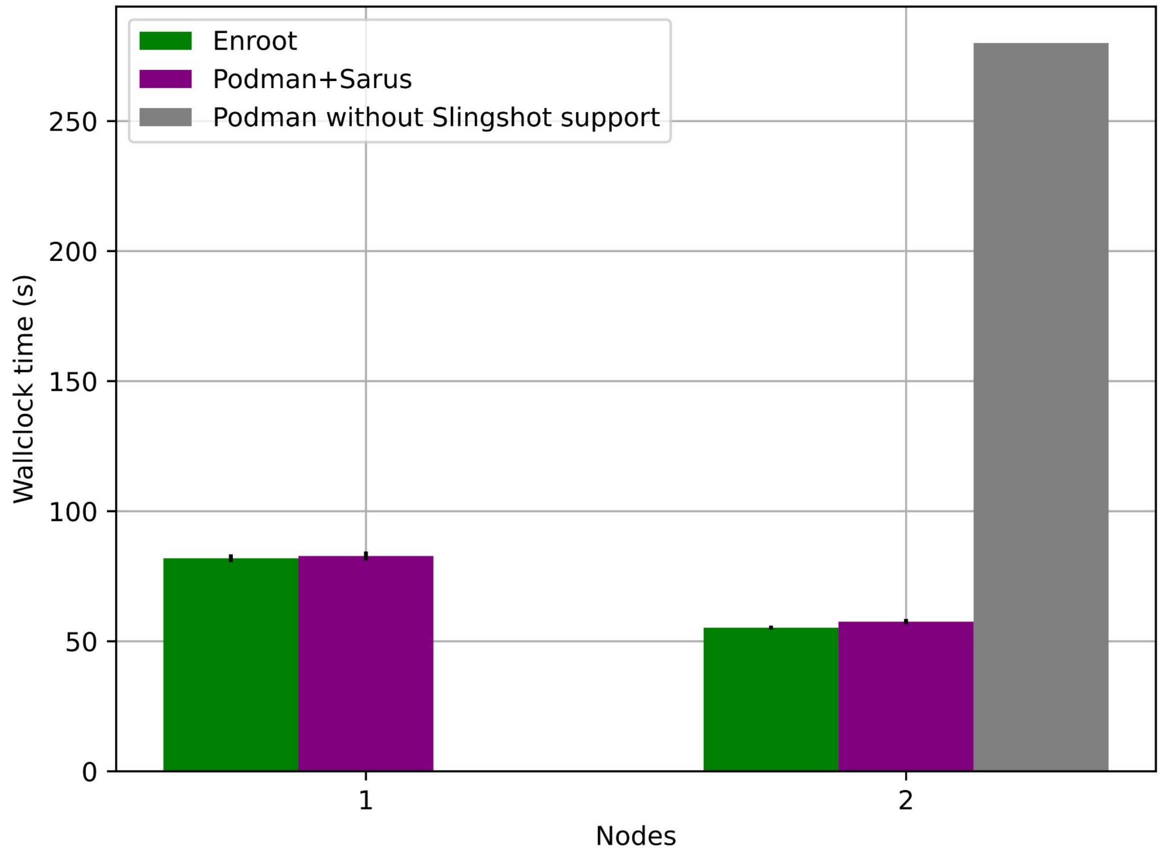
- Using customized Pyxis as SPANK plugin
  - Skybox development not started yet

OSU Bandwidth



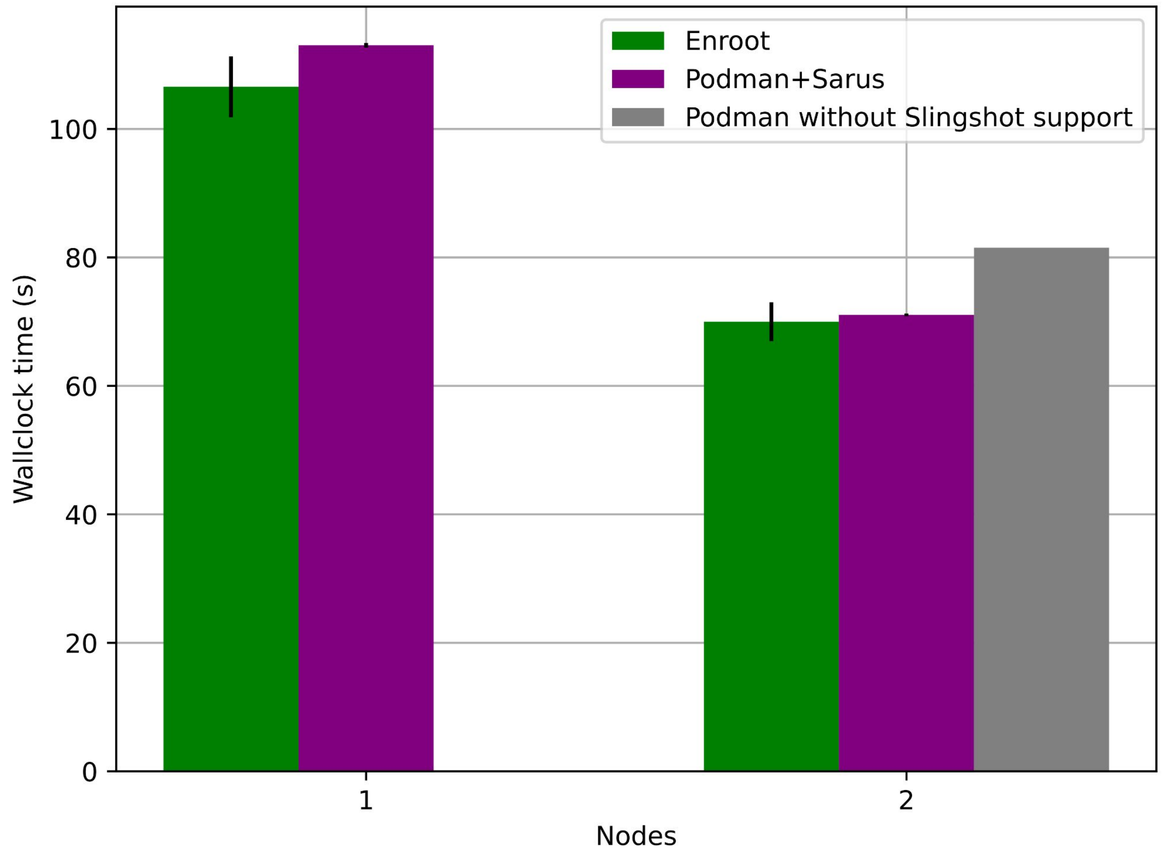
Container: OSU Micro-Benchmarks 7.5, OpenMPI 5.0.7, Ubuntu 24.04
Test case: `osu_bw` benchmark (2 physical nodes, 20 repetitions)
System: Alps Infrastructure - Development vCluster (2 x AMD EPYC 7713, 4 x NVIDIA A100, Slingshot 11 200Gb)

PyFR (Flux Reconstruction CFD)



Container: PyFR 2.1, OpenMPI 5.0.7, CUDA 12.8, Ubuntu 24.04
Test case: 3D Taylor-Green vortex (4 ranks per node, 20 repetitions)
System: Alps Infrastructure - Development vCluster (2 x AMD EPYC 7713, 4 x NVIDIA A100, Slingshot 11 200Gb)

SPH-EXA (Smoothed Particle Hydrodynamics)



Container: SPH-EXA v0.93.1, OpenMPI 5.0.7, CUDA 12.8, Ubuntu 24.04
Test case: Sedov spherical blast wave (4 ranks per node, 20 repetitions)
System: Alps Infrastructure - Development vCluster (2 x AMD EPYC 7713, 4 x NVIDIA A100, Slingshot 11 200Gb)

Runtime startup comparison

	Enroot	Podman
Start function in SPANK plugin	3.7523 ± 0.052 s	1.2821 ± 0.054 s
Time spent in the runtime itself	3.7521 ± 0.052 s	1.2360 ± 0.052 s

Maximum runtime startup times averaged across 20 repetitions of PyFR runs

Container: PyFR 2.1, OpenMPI 5.0.7, CUDA 12.8, Ubuntu 24.04

Including support for CXI/Slingshot, NVIDIA GPUs, AWS NCCL plugin

Conclusions

- Sarus evolving from an engine to a suite of tools
  - Modular, open-source collection of reusable components
  - Continuing to combine HPC with cloud-native flexibility and standards

- Enabling first-class container integration with HPC
  - Containers are transparent, manageable, and fully integrated into HPC

- Strategic shift towards performance-enhanced Podman as runtime
  - CSCS will use Sarus components to enable profitable usage of Podman in HPC

- Forward-looking and OSS-oriented
  - Towards a container stack for adaptability and sustainability
  - Smoother adoption path to other cloud native technologies

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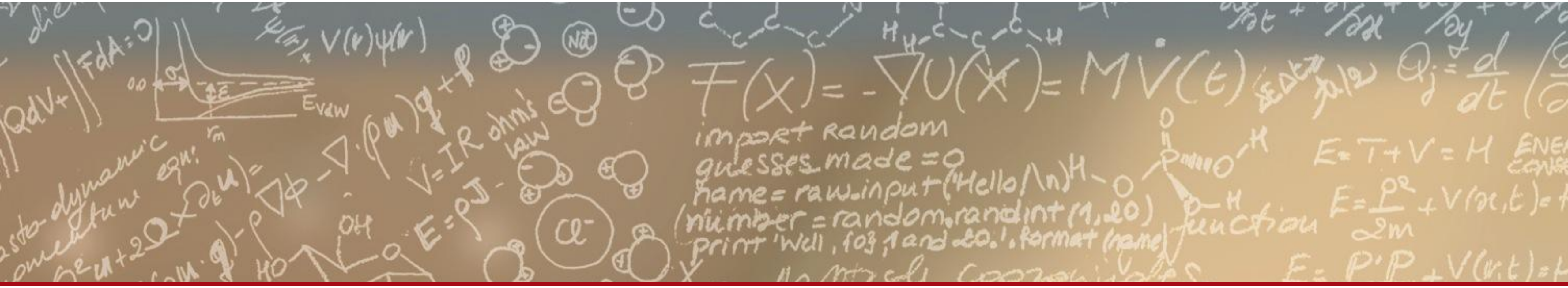

Thank you for your attention.