

The future of extreme compute and data

Swiss SKA Days 2022 Maxime Martinasso, CSCS Oct 3rd, 2022

Extreme compute

- Today's world compute capability?
 - EFlops sum of top 10 systems (~0.5 EFlops/year):
 - Jun 2022 2.25 EFlops
 - Nov 2018 0.5 EFlops
 - Not listed machines: how many exaflops machines in China or in the industry?
- Technology
 - We are in the silicon era with the use of accelerators
 - Changing era?
 - Nanotechnology, carbon nanotubes instead of silicon transistor
 - Photonics, photons instead of electrons
 - When for large-scale manufacturing?
 - Quantum computing: might be a specific accelerator?





Extreme compute challenges

- Power efficiency barrier
 - 1 Eflops ~= 20 MW
 - Large hydropower plant: ~30-50 MW
 - Nuclear plant: ~500-1000 MW
 - Reduce power needs, moving large HPC systems to colder countries
- Money challenge
 - Frontier 1.1 EFlops = \$600 Million to build
 - Operational cost over the supercomputer lifetime 20-30% of building cost
 - Variability of power cost
- Usability and programming
 - Build programming abstraction in scientific software
 - DSL / specialized libraries / hardware-specific back-end
 - Refactoring existing codes takes many years of development
 - Performance engineering

For most countries sustaining a unique 1-Eflops machine is today's limit



Extreme data

Scientific data explosion

- New scientific instrument, more precise
- International collaboration, distributed instruments, aggregation of data
- Scientific challenges for finer resolution simulations

Example of dataset sizes

Insitution	Scientific domain	Workflows	Data size
European Centre for Medium-Range Weather Forecasts (ECMWF)	Weather Forecast	Ensemble forecasts, data assimilation,	12 PB/year
Paul Scherrer Institute (PSI)	Synchrotron imaging	X-ray spectroscopy, high resolution microscopy,	10-20 PB/year
CERN	High-energy particle collider	LHC Run 2	1PB/day





Extreme data challenges

- Technology
 - Transfer rate: still orders of magnitude lower than needed
 - 120 TB over internet = 111 days
 - 120 TB sent as discs by Fedex = 1 day
 - Need to build dedicated link with multiple 100Gbps to connect data producers to consumers
 - Transfer only what is relevant for the consumers
 - Storing/presisting PB of data
 - Tapes is still the solution, poor access time
 - Keeping data accessible in near-compute storage is more expensive

Don't move the data move the compute!





Versatile software-defined cluster (vCluster)

Deploy an identical platform on several system technologies

In development

- The platform is defined as a set of config files
 - Each service is a config file (IAM, batch scheduling, data managers, accounting,...)
- Abstraction layer to be system independent
- Provide an engine to deploy such software-defined platforms
- Use Infrastructure-as-Code to implement specific instance of the engine back-end
- Transfer scientific software stack and ensure performance
 - Use containers to store the software stack
 - Use OCI Hooks to expose host HPC-capable stack in the container



- Enable programmatic and web access to the platform
 - Create a RESTful API to access services on the machine
 - Build community portal / scientific workflows using that API







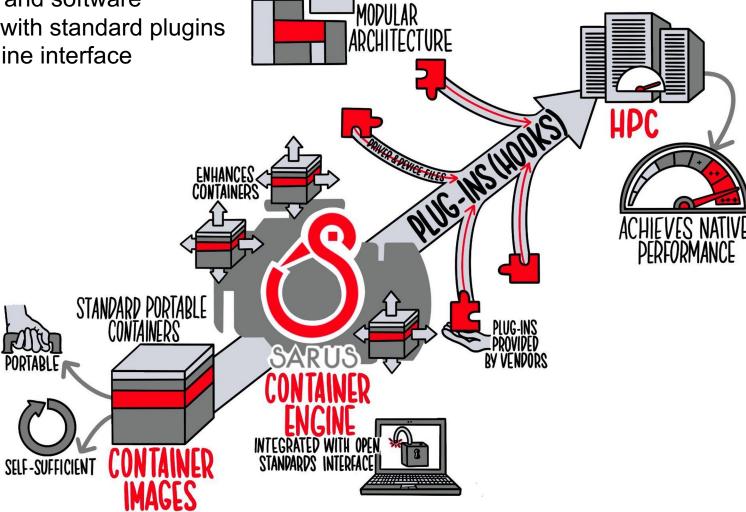
Sarus concept

Combines container portability with native HPC performance

Integrates with HPC infrastructure and software

Customizes containers at runtime with standard plugins

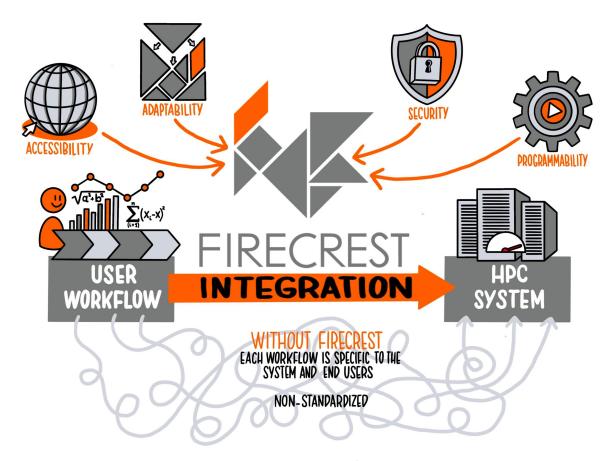
Provides a Docker-like command line interface





FirecREST concepts

- Accessibility: opens web access to HPC from any device
- Adaptability: modular design to support diverse HPC ecosystems
- Security: provides multiple authorization control layers
- Programmability: uses standard interface for a simplified automation





Next steps

- CSCS is committed in the development of the vCluster solution
 - vCluster v1.0, Sarus v2.0, FirecREST v2.0
 - Alps will exclusively use the vCluster technology



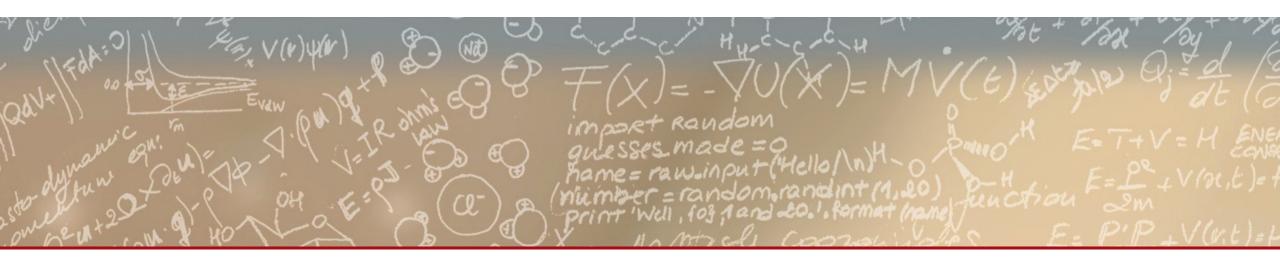
- Identify use cases and partners
 - With EPFL/SCITAS looking into the abstraction layer of the vCluster
 - With PSI enhancing vCluster to enable laaS, tenant-managed vCluster
- Promote and disseminate the vCluster technology
 - Find new use cases and opportunities











Thank you for your attention.