From cluster managers to scientific software build & installation frameworks, one day working on HPCNow!

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About HPCNow!

- Young company (born in 2012)
- Staff: 39 HPC folks and growing
- No financial dependencies
- Strong growth
- EU Alliance

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HPC Services

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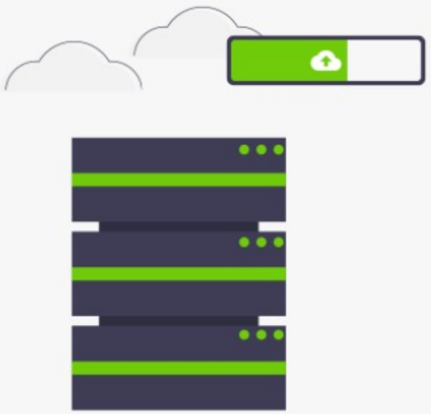
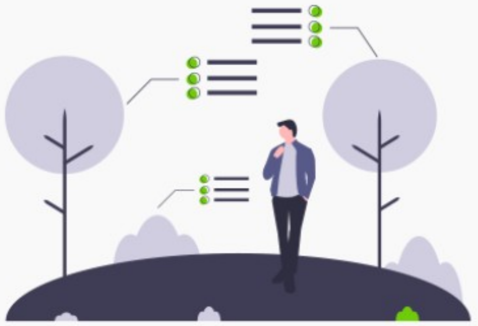
We are passionate about new challenges and HPC technologies enthusiasts. Our goal is to take full advantage of supercomputing to provide solutions to our customers' scientific or engineering dares.

User-oriented company

HPC services and solutions



SW & HW & Cloud agnostics



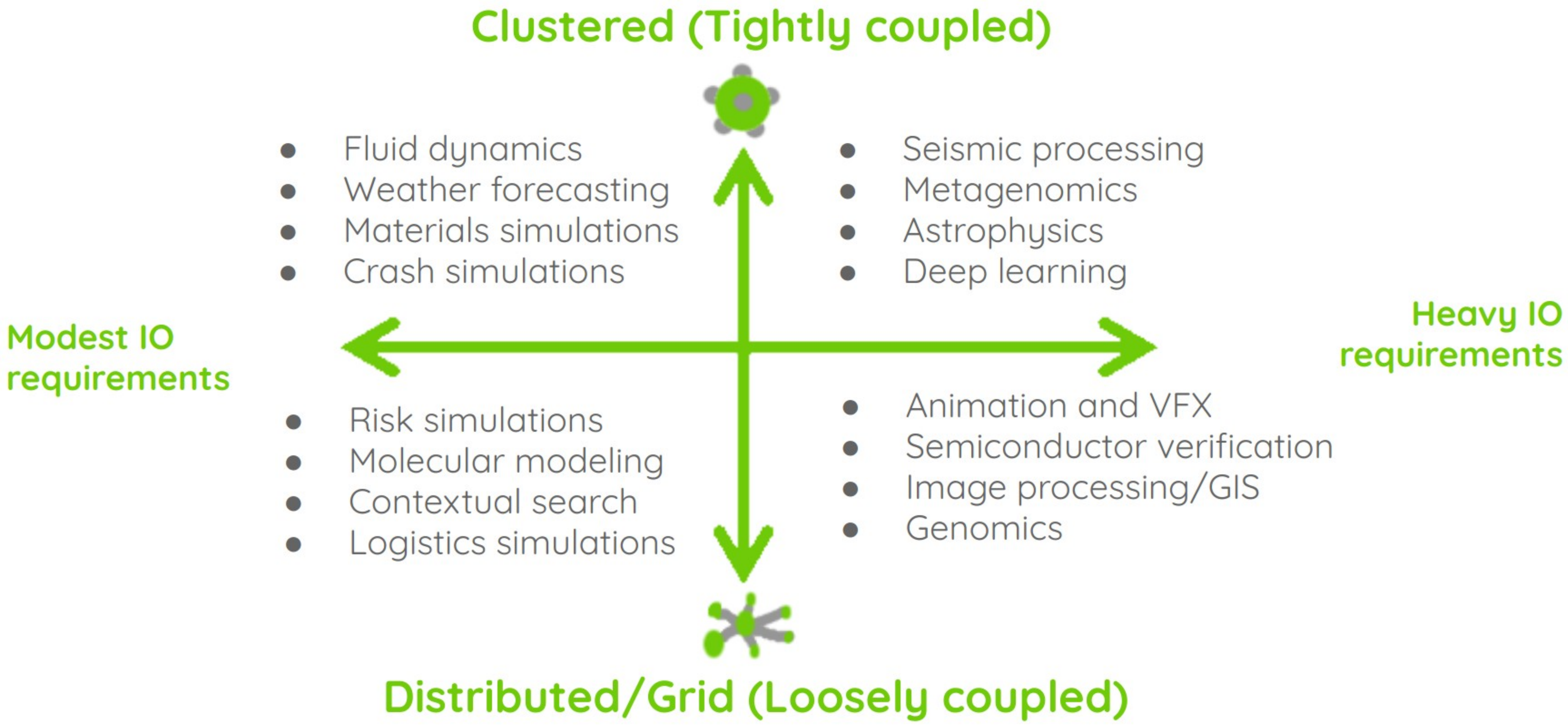
IT + scientific background

www.hpcnow.com

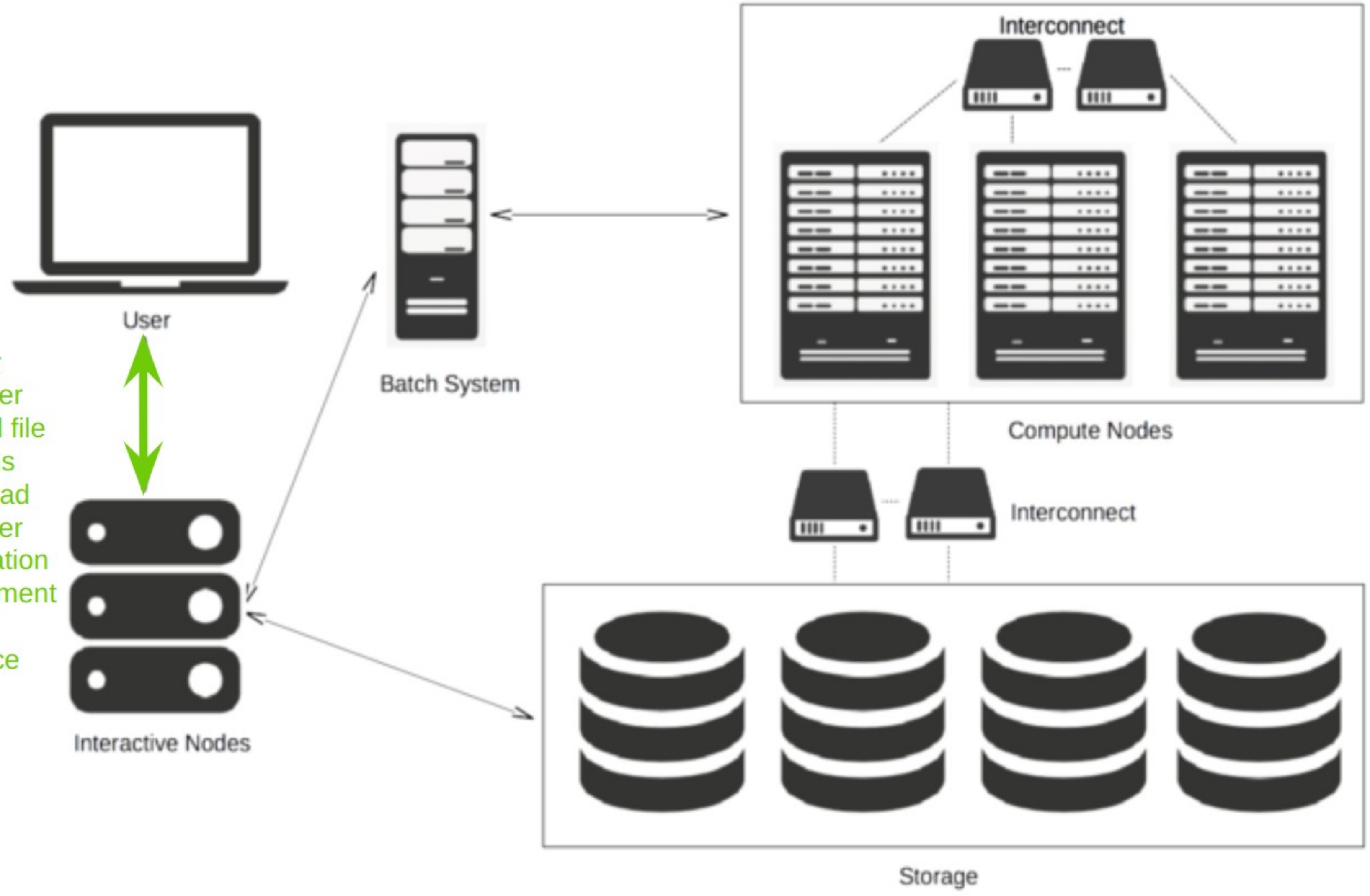
The key goal is to solve the problems faster.

- Speed → Split the work between several processors : the program will run N-ish times faster by using N processors.
- Volume → large data analyses
- Cost → faster results, reduced wet lab analyses
- Efficiency and convenience → shared resources used 24/7, no need to use all resources of your own PC

Main Use Cases for HPC



Our job ...



Many layers:

- ➔ Cluster manager
- ➔ Shared file systems
- ➔ Workload manager
- ➔ Application deployment
- ➔ User interface

Cluster managers

Cluster managers in high-performance computing (HPC) are essential software tools that facilitate the efficient operation and management of a group of interconnected computers, or nodes, that work together to solve complex computational problems.

Key Features of Cluster Managers:

By using effective cluster administration tools, HPC administrators can optimize resource utilization, improve performance, and ensure the reliability of their clusters.

A single point of control for managing the entire cluster.
Centralized Management

Integration with other tools and systems, such as network management and storage systems.
Integration

Scripts and workflows to automate routine tasks.
Automation

Ability to handle large-scale clusters with thousands of nodes.
Scalability

Examples

- xCAT/Confluent
- Warewulf
- Bright Cluster Manager (Nvidia BCM)
- HPE Performance Cluster Manager (HPCM)
- ...

- MAAS
- Cobbler
- ...

\+ **Automation tools:**
Ansible, Chef, Puppet, SALT, Juju integration

xCAT/Confluence

- xCAT stands for **Extreme Cloud Administration Toolkit**.
- **Open Source** with Eclipse Public License
- First release in 31/10/1999
- **Developed by IBM**. Lenovo involved since an IBM division acquisition. Now maintained by the **xCAT consortium**.
- Offers **complete management** of clouds, clusters, HPC, grids, datacenters, renderfarms, online gaming infrastructure, etc.
- Main page: http://xcat.org
- Main repos: https://github.com/xcat2
- Now in maintenance mode, for new deployments they recommend using confluent instead: https://github.com/xcat2/confluent

Warewulf 4

Warewulf is an open-source cluster manager with OS provision, hardware control and infrastructure discovery.

- Based on the design of the original Beowulf Cluster design (and thus the name, soft**WARE** implementation of the beo**WULF**).
- Released in 2001.
- Open source *(from october, 2023 3-clause BSD License is used).*
- Project Charter and Warewulf Technical Steering Committee (TSC) in 2023.
- **Lightweight, simple and flexible.**
- **Agnostic from the hardware and the OS**.
- Secure as it supports SELinux out of the box.
- Warewulf v4 is a complete WW3 rewrite in GoLang.

Main page: https://warewulf.org
Other useful links: https://warewulf.org/help/

Bright Computing

BRIGHT SOFTWARE MAKES THE ADMINISTRATOR'S JOB EASIER, AND THE CLUSTER MORE AGILE

Bright automates the cluster build process	• Provisions nodes from bare metal • Pre-checks hardware to ensure it's working properly • Sets-up network, user directory & security • Deploys workload managers & frameworks • Supports mixed platform HW/OS combinations
Bright allows you to quickly diagnose & resolve failures and performance problems	• Provides detailed metrics & health-checks • Reports resource usage by job and user • Allows automated corrective actions to be taken • Automatically detects and images replacement nodes
Bright makes it easy to deploy software updates and changes across the entire cluster	• 1-step propagation of updates • Auto-update nodes without reimaging • Easily add more servers & new components • Replace failing nodes without disruption • Prevents image-drift amongst nodes
Bright makes your cluster application-friendly and flexible	• Run on bare-metal, VMs or containers within the same cluster • Extend to the public cloud • Dynamically allocate resources where they're needed • Re-image nodes on the fly to host new applications

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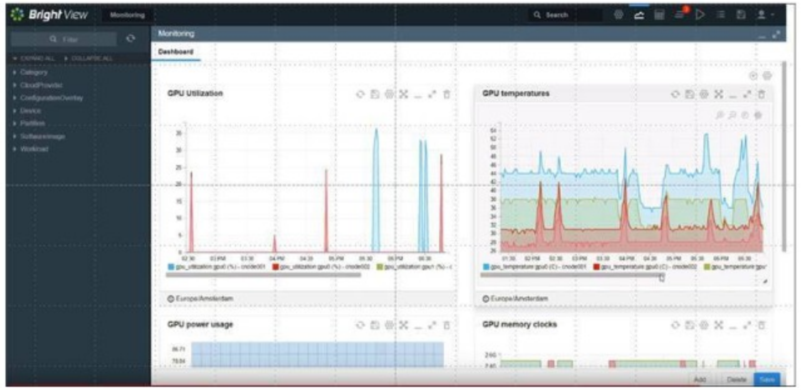
Bright Cluster Manager

Bright Computing provides comprehensive software solutions for deploying and managing enterprise-grade Linux clusters. Bright provisions, monitors and manages GPU clusters, and makes it an ongoing practice to incorporate the latest enhancements in NVIDIA GPU technology into its products, enabling Bright customers to seamlessly use NVIDIA technology.

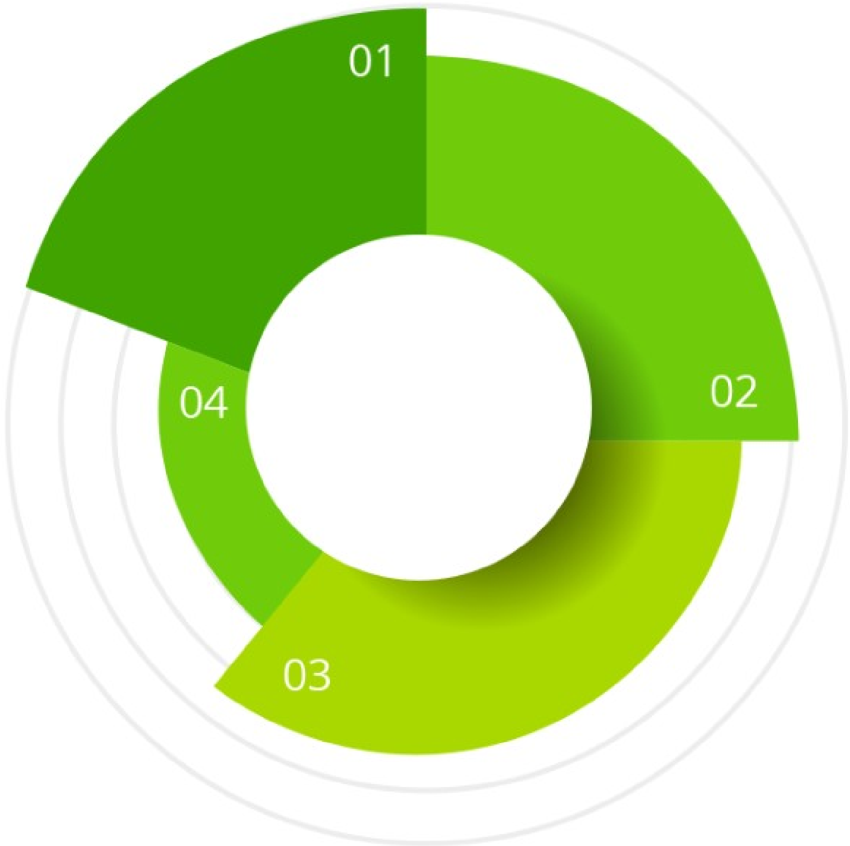
Key Features

- Intuitive web interface provides comprehensive view of GPU and cluster metrics
- Powerful Cluster Management Shell (CMSH) as alternative administrative interface
- Full support for NVIDIA libraries, CUDA, OpenCL, OpenACC, CUDA-aware libraries, NCCL, and CUB
- Comprehensive GPU monitoring and health checking
- Provisions GPU resources from public (AWS, Azure) and private (OpenStack) clouds within minutes
- Auto scaling hybrid cloud based on workload and configured policies
- Supports several popular Linux distributions: RHEL and derivatives, SUSE SLES and Ubuntu LTS
- GPU-enabled Kubernetes and Singularity for running containers
- Offers a complete machine learning stack
- Deployment for popular HPC file systems and management of fast interconnects
- Gives insight into how jobs utilize the resources that were allocated (e.g. GPU usage throughout a job's runtime)
- Provides reporting to administrators to identify users or groups of users that are consistently underutilizing the resources (e.g. GPUs) that they allocate for their jobs.

Bright Cluster Manager can sample and monitor metrics from supported GPUs and GPU Computing Systems, such as the NVIDIA Tesla A100, V100, P100, and T4 GPUs as well as commodity GPUs.



Cluster Managers: Not a best/worst option



Sometimes not an option

- Hardware/infrastructure support
- Community support
- Set of managed services
- OS support

High performance storage

Designed to provide high-performance and scalable file storage for large-scale computing environments

Examples of PDFS:

- **Lustre**: A widely used PDFS known for its scalability and performance.
- **GPFS**: A PDFS offered by IBM, known for its enterprise-class features and reliability.
- **BeeGFS**: An open-source PDFS designed for high-performance computing environments.
- **Ceph**: A distributed object storage system that can also be used as a PDFS.

Key Features of the Parallel distributed file systems:

PDFS are essential components of modern HPC systems, providing the foundation for scalable and high-performance data storage.

Support available from the vendor or community
Support

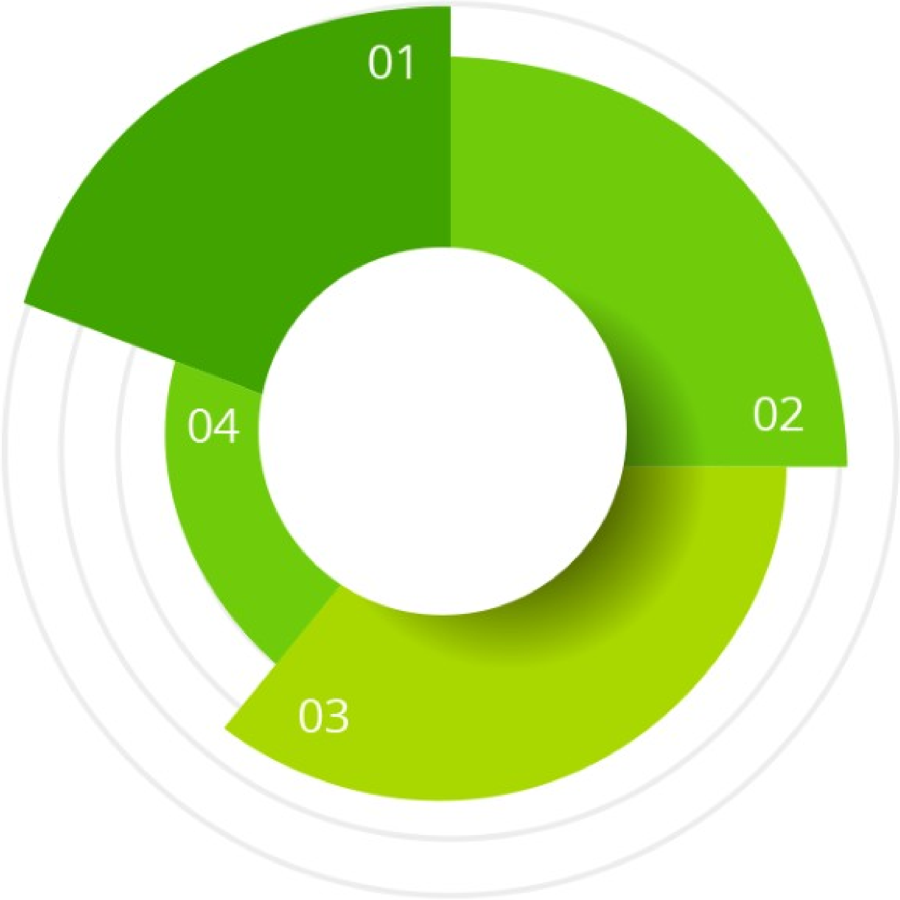
Parallel IO / Low latency / High throughput
High Performance

Specific features and capabilities that are important for your use case.
Features

Horizontal scaling/Large datasets.
Scalability

Parallel distributed file systems

Parallel distributed file systems



Support: both commercial and community

Flexibility

Performance

OS support

Workload managers

Workload managers in high-performance computing (HPC) are essential software tools that handle tasks such as resource allocation, job scheduling, and monitoring system health, ensuring that **computational resources are utilized effectively**.

By managing workloads and distributing tasks across the cluster, these tools optimize performance and reduce downtime. Popular cluster managers include **Slurm, PBS (Portable Batch System), LSF and Grid Engine**, each offering unique features tailored to different HPC environments. As HPC continues to evolve, workload managers play a crucial role in enhancing productivity and enabling researchers to tackle increasingly sophisticated scientific challenges.

Key Features of Workload Managers:

A versatile tool for managing HPC workloads, ensuring efficient resource utilization and maximizing the performance of cluster environments.

.Node, Queue/Partition and Quota Management .

Resource Management

Job Submission, Scheduling and Accounting

Job Management

Task Distribution and Dependency Management

Parallelism

Performance Metrics and Logging

Monitoring and Reporting

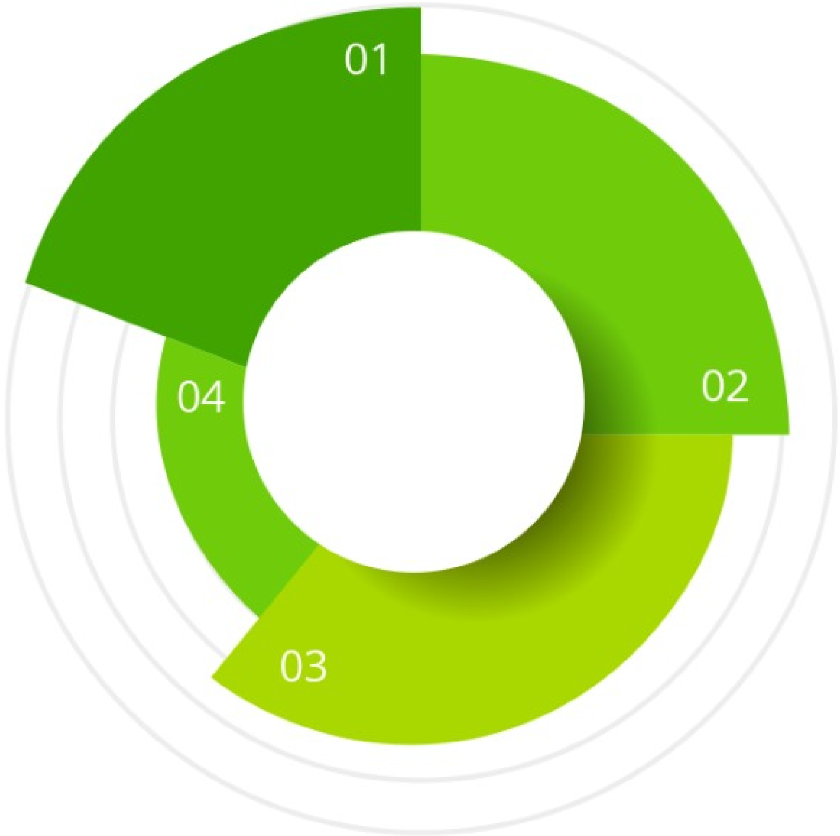
Workload managers: Extra features

Plugin Architecture: Allows for customization and integration with other systems through plugins.
API: Provides an API for programmatic interaction and automation..

License management: Integration with License Servers giving the possibility of license enforcement, license usage Tracking and license optimization.

Multi site, edge support: jobs are executed across geographically distributed clusters, **optimizing data staging**

Workload managers



Slurm as default option

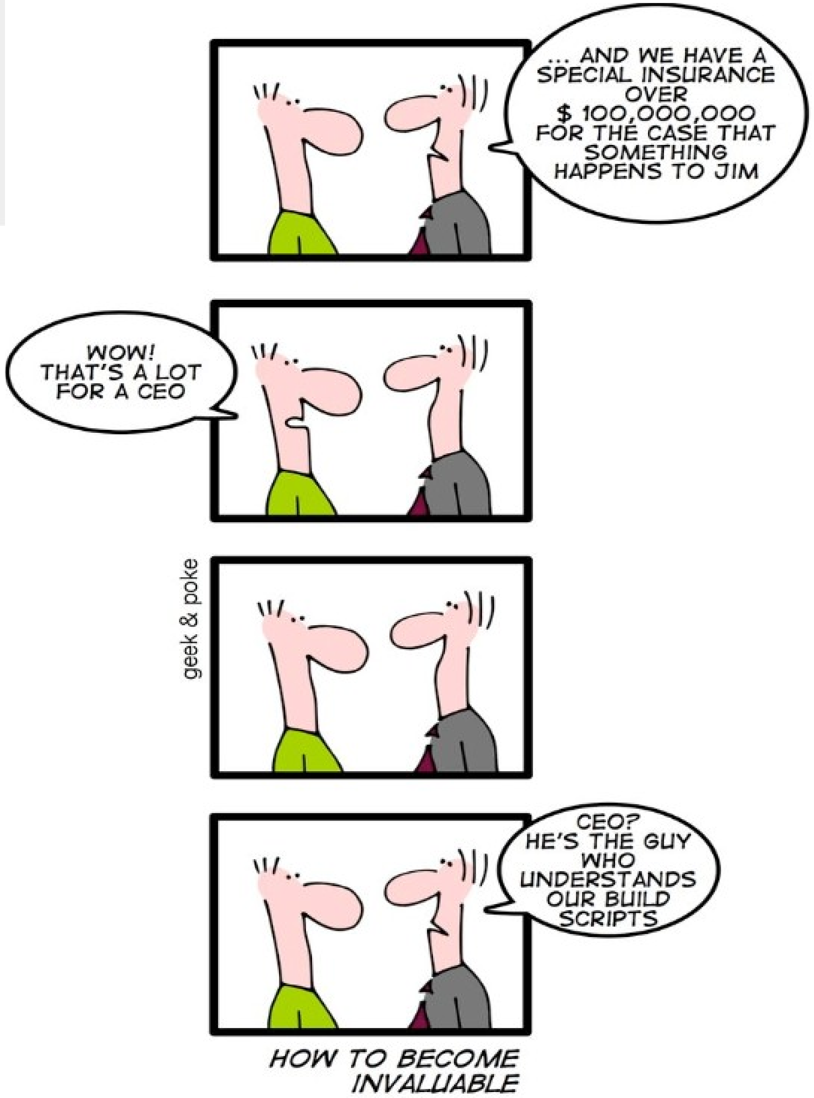
- Support vs. cost
- Extra features
- Scalability
- Application integration

Scientific applications installation

Common issues installing scientific software on HPC:

- Incomplete build procedures
- Requiring human interaction
- Heavily customised and non-standard
- Uses hard-coded parameters
- Poor or outdated documentation
- Any given version will have its own set of dependencies
- **Very time-consuming for user support teams**

It is needed to simplify the process of installing and managing scientific software packages, making it easier for researchers and system administrators to access and utilize their applications.



User software installation: Available tools

EasyBuild focus:
- building from source
- easy installation of software
- good performance

Spack focus:
- building from source
- flexibility
- cross-platform

CONDA/Mamba focus:
- binary packages
- quick & easy software installation
- cross-platform

Nix focus:
- binary installations
- isolated build environment
- portability

GuixHPC focus:
- binary installations
- isolated build environment
- free software & GNU philosophy

And more ...

Key Features of user software installation and management tools:

Aiming to simplify the process of installing and managing scientific software packages.

Streamline the process of installing software packages,.

Simplified software installation

Managing dependencies and configurations ensure software installations reproducibility.

Improved reproducibility

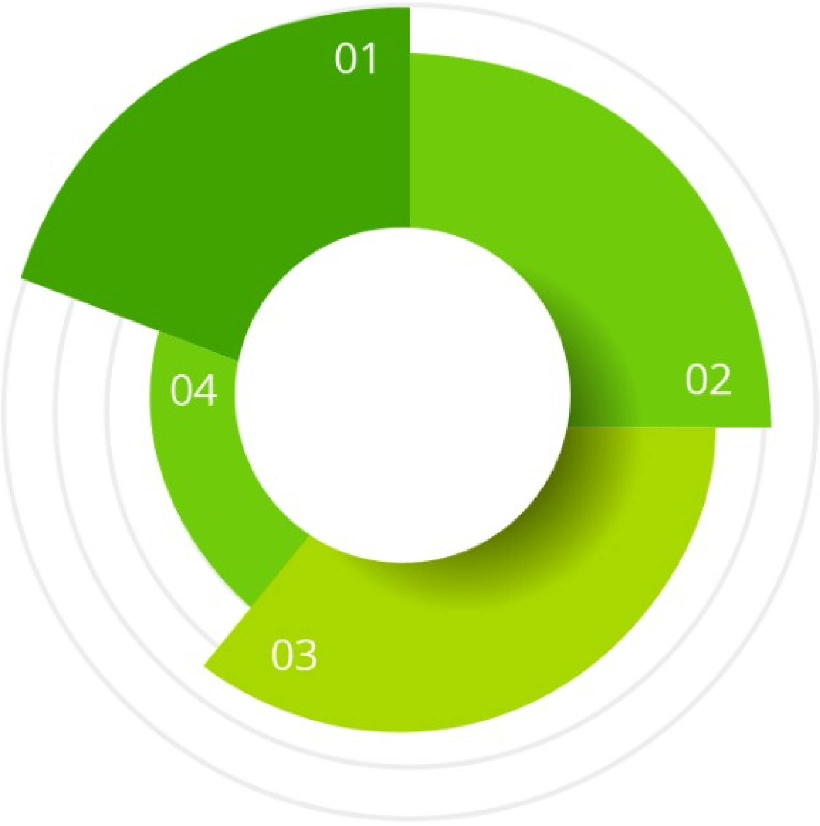
Building software from source.
Software optimized for the processor architecture.

Performance

Tailor the installation process to site specific requirements and preferences.

Customizability

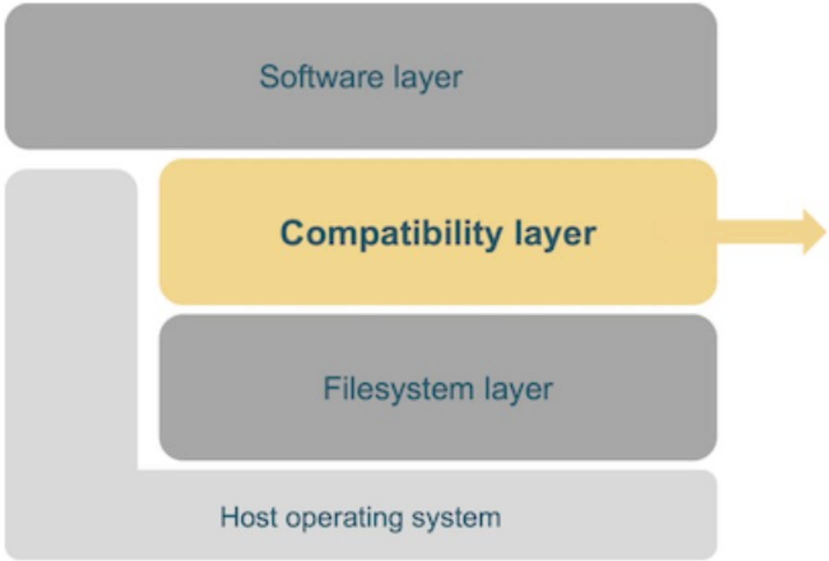
User software installation tools



Not a single option

- Community support
- Customization support
- Building from source
- Time to solution
- Base OS independence

Compatibility layer



gentoo

EESSI
EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

The middle layer of the EESSI project is the **compatibility layer**, which ensures that our scientific software stack is compatible with different client operating systems (different Linux distributions, macOS and even Windows via WSL).

User interfaces

AIM: Provide a user-friendly way to access and manage HPC resources.

Advanced web platforms like **Open OnDemand** or **NICE DCV** integrated with HPC resources improve HPC users accessibility and reduce learning curves.

Key Features of user environments:

User-friendly way to access and manage HPC resources. Simplify the process of submitting jobs, monitoring their progress, and interacting with the HPC environment.

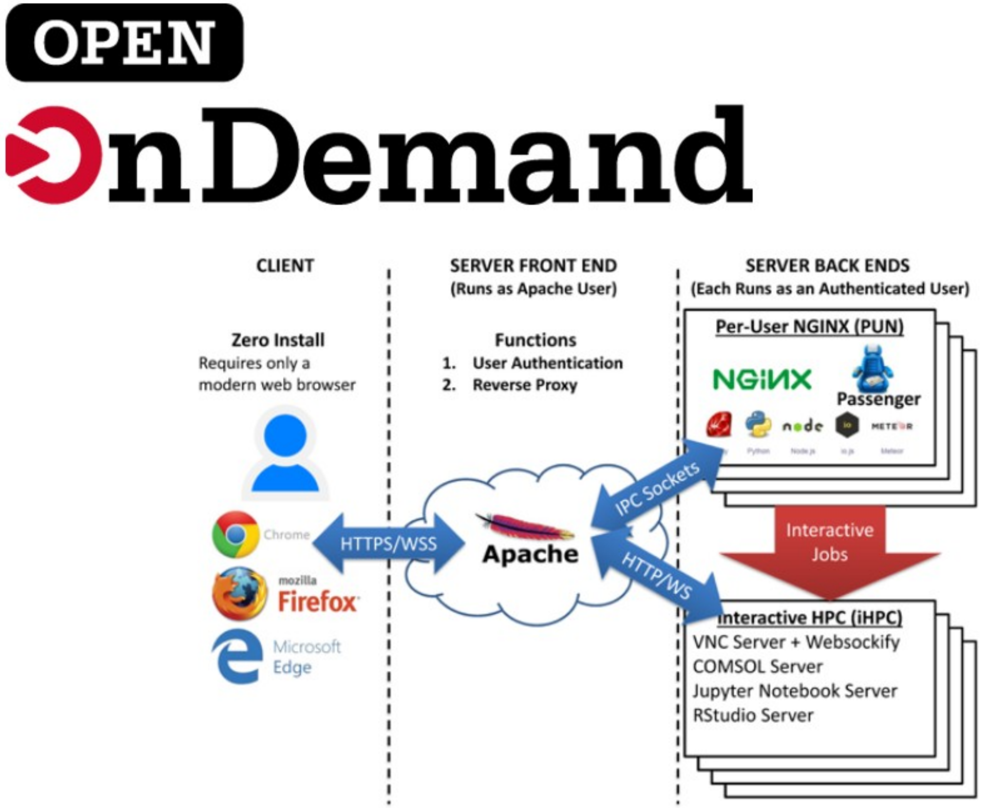
No client software installation required. Web interface
Simplified User Experience

Rapid uptake of HPC by new users: less mistakes
Improved Resource Utilization

Automating tasks / centralized platform for job management
Increased Productivity

Shared workspaces / Integrated tools
Enhanced Collaboration

Open OnDemand, using your cluster with clicks

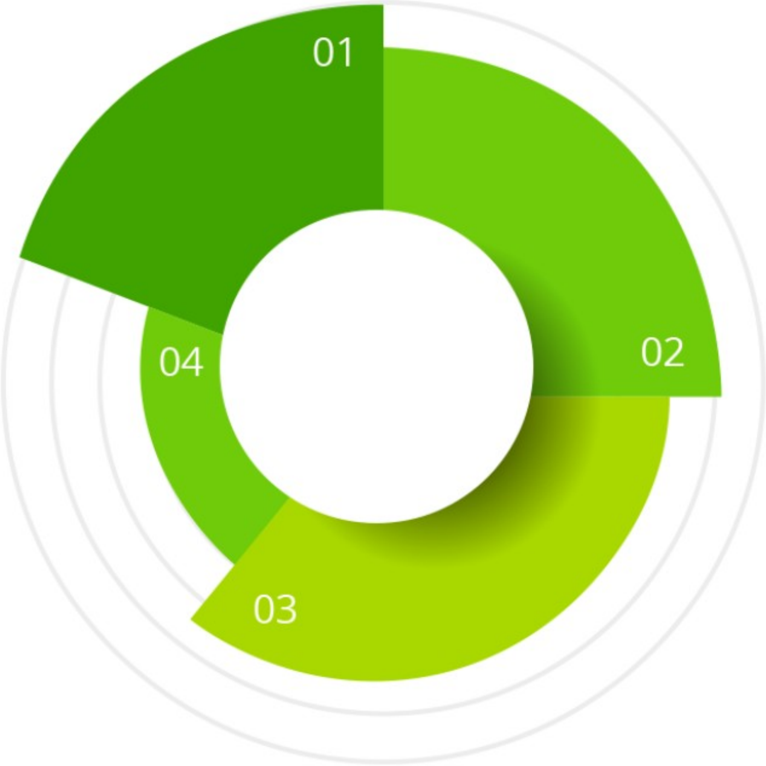


- Founded in 2007 at the Ohio Supercomputing center
- Continuous development and active community
- Satisfies the requirements of a wide range of users

Hudak et al., (2018). Open OnDemand: A web-based client portal for HPC centers. Journal of Open Source Software, 3(25), 622, https://doi.org/10.21105/joss.00622

User environments

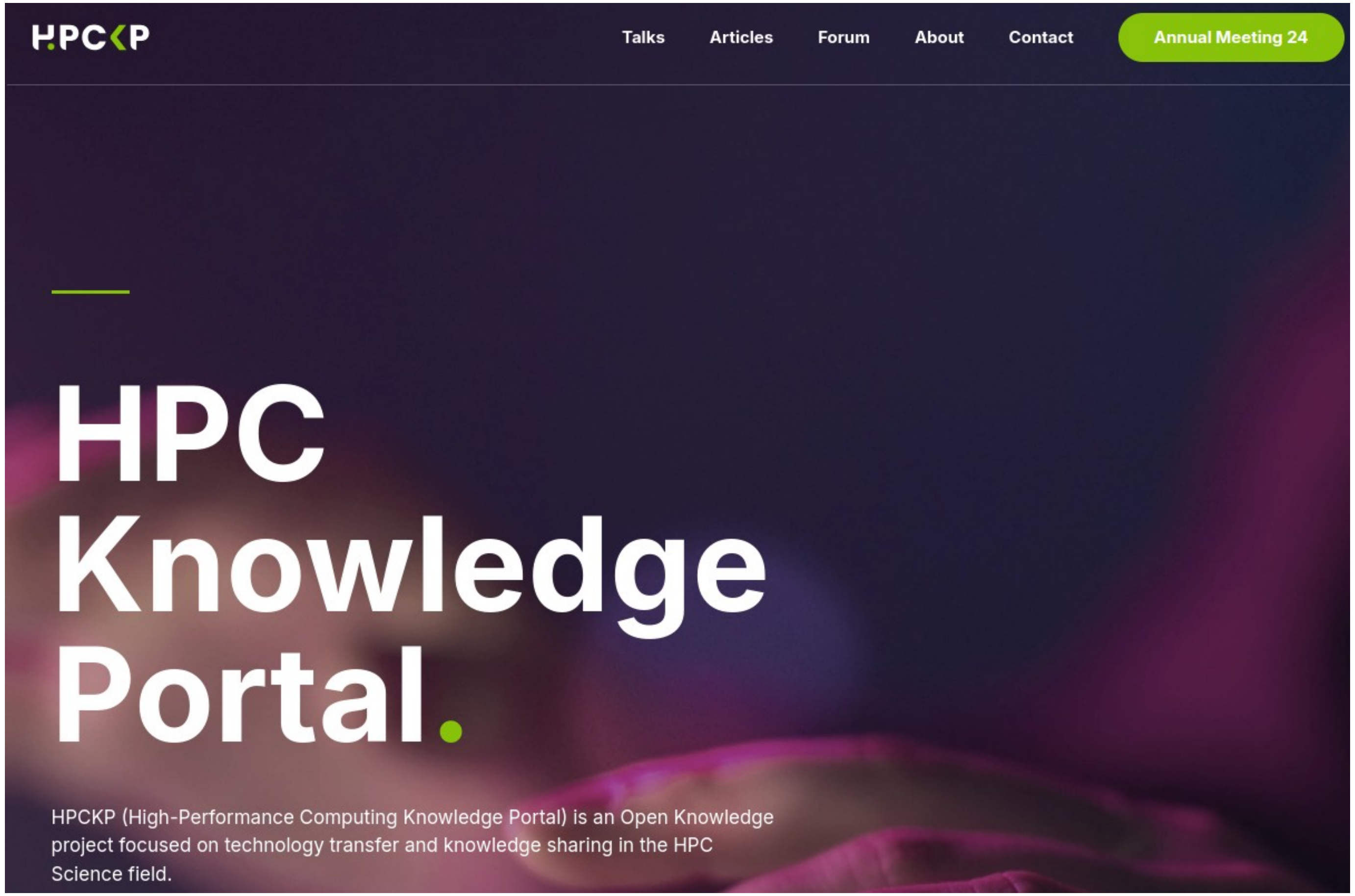
User environments



General web portal?
Science gateway?

- Community support
- Customization support
- Graphics acceleration
- Application integration

Multilayer work	Multidisciplinary team, from the network expert to the application expert
Performance is key Stable service is key Flexibility is key	**Not a unique best solution.** Depends on site and user community
Reduce user learning curve/increase usability	A general web portal helps to improve it



https://hpckp.org