



MedeA *Instrument*

Skip the Data-Center — High-Performance Computing and Simulation Under Your Control

At-a-Glance

The MedeA^{®1} *Instrument* is a powerful, integrated platform for atomistic simulation. State-of-the-art hardware and design bring affordable, high-performance computing out of the data center and into your office. The MedeA *Environment* is installed and tested with the modules ready to run.

Key Benefits

- Minimal setup time, with little to no IT
- High-Performance Computing without the learning curve of Linux Clusters
- MedeA *Environment* benefits, including job management and performance monitoring
- Remote access from anywhere via configured virtual private network (VPN)
- Quiet enough for the office, and needs no special cooling or electrical requirements
- Fast, integrated support with a single vendor for tech support and scientific consulting on hardware, OS, and MedeA



Figure 1: MedeA Instrument workstation is the size of a standard computer tower

Based on time to solution, and cost of equipment, our MedeA Instrument is about eight times more efficient than our other compute options.

— Chief Scientist, R&D Center

Designed for Performance and Ease of Use

The MedeA *Instrument* arrives preinstalled: Simply unpack it: connect the monitor, keyboard, and mouse; plug it in; and start modeling at a level you never have before, all under your control with — no data center required.

The MedeA *Instrument* is designed to be quiet and energy efficient. It plugs into a standard wall socket, and does not need special cooling — if you are comfortable, then it is too.

Key Features

Performs simulations with all engines supported by the MedeA *Environment*:

- MedeA VASP — Vienna Ab-Initio Simulation Package
- MedeA LAMMPS — Large-scale Atomic/Molecular Massively Parallel Simulator
- MedeA GIBBS — Monte Carlo simulation for Fluid properties and Sorption
- MedeA MOPAC — Molecular Orbital PACKage for fast screening of molecular systems and solids
- MedeA Gaussian GUI — The standard in Computational Chemistry

Configurable stand-alone, or networked with other

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high-performance compute resources:

- 80 cores in standard configuration, providing a peak of over 3 TFLOPS
- Customizable Xeon-based architecture, with up to 176 cores
- Expandable by adding compute nodes
- Accessible via VPN for secure remote access
- Connect from laptop or desktop *MedeA* clients

Reference Specifications

Workstation Tower

A single workstation in a standard tower case with 64 to 128 cores.

Property/Device	Value
Dimensions (W x H x D)	29.8 x 25.6 x 23.6 inches / 25 x 65 x 60 cm
Weight	65 lbs / 29.5 kg (shipping)
Voltage	110-240 V; 50Hz to 60Hz, single phase; 1300W
Operating temperature	50- to 95-degrees F (10- to 35-degrees C)
Processors	2x AMD EPYC 7000-Series processors with up to 64 Cores (per CPU)
Compute cores	64 (standard), or up to 128
Memory	512 GB (standard), or up to 2048 GB
Expansion Slots	3 x PCIe 3.0 x8 (x8 mode)
Storage	SSD System Disk
LAN	10 GB/s Ethernet
Operating System	Ubuntu 20.04 or CentOS
<i>MedeA</i>	Version 3.x (most recent)

Workstation Rack

A single workstation in a 2U rack mount chassis with 64 to 128 cores.

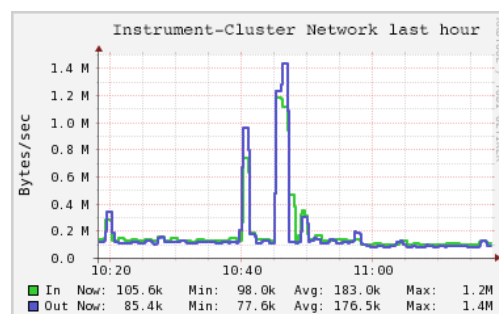
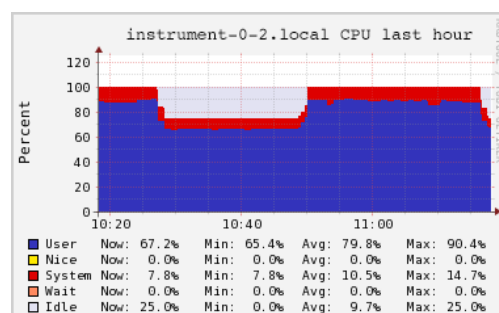
Property/Device	Value
Dimensions (W x H x D)	17.24 x 3.46 x 32.68 inches / 43.8 x 8.78 x 83 cm
Weight	66 lbs / 30 kg (shipping)
Voltage	110-240 V; 50Hz to 60Hz, single phase; 1300W
Operating temperature	50- to 95-degrees F (10- to 35-degrees C)
Processors	2x AMD EPYC 7000-Series processors with up to 64 Cores (per CPU)
Compute cores	64 (standard), or up to 128
Memory	512 GB (standard), or up to 2048 GB
Expansion Slots	3 x PCIe 3.0 x8 (x8 mode)
Storage	SSD System Disk
LAN	10 GB/s Ethernet
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Cluster Rack

A two chassis solution with a dual-core head node and four compute nodes. Runs 80 - 128 compute cores.

Call for additional specs.

Performance Monitoring



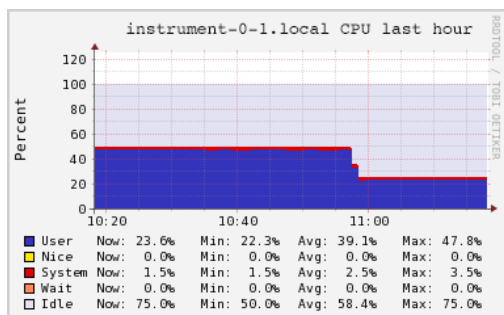


Figure 2: Monitoring compute jobs and resources on the Instrument using Ganglia

- *MedeA MOPAC*
- *MedeA Gaussian GUI*
- *MedeA GIBBS*
- *MedeA HT-Launchpad*

Supported Modules

- All *MedeA* components

Find Out More

Learn more about how *MedeA* can support your work through capabilities such as Databases, Builders, Compute Engines, Forcefields, Property Modules, Analysis Tools, and High-Throughput.

Required Modules

- *MedeA Environment*

Recommended Modules

- *MedeA VASP*