



MedeA Instrument

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

At-a-Glance

Through a partnership with Exxact Corporation, we offer a powerful, integrated platform for *MedeA* atomistic simulations running VASP, LAMMPS and related *MedeA* modules on NVIDIA Graphical Processing Units (GPUs) and Intel or AMD CPUs. State-of-the-art hardware and design bring affordable, high-performance computing out of the data center and into your office. Optionally, the *MedeA* materials simulation environment can be pre-installed on the system prior to shipment and is ready to run.

You can also connect to your HPC hardware from a laptop or desktop running the *MedeA* user interface, where the HPC hardware only hosts the *MedeA* JobServer and TaskServer services.

Key Benefits

- Minimal setup time, with little to no IT support required
- High-Performance GPU Computing without complex hardware setup and Linux system configuration
- *MedeA Environment* benefits, including job management and performance monitoring
- Remote access from anywhere via configured virtual private network (VPN)
- Workstations are quiet enough for the office, and need no special cooling or electrical requirements
- Fast, integrated support for tech support and scientific consulting on hardware, OS, and *MedeA*

Note

We focus here on state-of-the-art GPU-based workstations, but Exxact can also provide HPC data center hardware to run *MedeA* software, such as CPU and GPU clusters.

Our Partnership with Exxact Corporation

Materials Design is proud to partner with Exxact Corporation to supply cost-effective HPC hardware for materials simulations. We collaborate on validating and benchmarking *MedeA* software on Exxact's systems.

Exxact Corporation was founded in 1992, and provides technology solutions that enable many of the world's top national laboratories, research institutes, universities, startups, and Fortune 1000 companies to conduct cutting-edge artificial intelligence, drug discovery, and advanced engineering simulations, while also powering a host of other HPC, datacenter, and visualization applications.

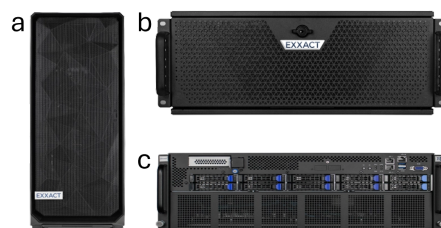


Figure 1: Examples of Exxact VASP Optimized GPU Workstation Tower (a), Rack Mountable GPU Workstation (b), and 4U GPU Server (c)

System Integration

As computational challenges increase in complexity, Materials Design works with Exxact engineers to provide the right balance of computation, networking, storage, and memory in order to deliver cost effective and reliable simulation performance.

Quality Service

Exxact corporation's extensive HPC expertise and unparalleled customer support allows customers

to increase and sustain their computational infrastructure through personalized service, life cycle management, product allocation, and end-of-life product sourcing.

Designed for Performance and Ease of Use

With the MedeA materials simulation environment preinstalled, you can simply unpack your system, connect monitor, keyboard, and mouse, plug it in; and start modeling at a remarkable level of performance, all under your own control, with or without a dedicated data center.

Exact Corporation MedeA configurations can be designed to be quiet and energy efficient, plug into a standard wall socket, and not require special cooling.

Key Features

Exact Corporation systems provide high efficiency for 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
- *MedeA PhaseField*

A typical configuration can provide a peak performance of well over 3 TFLOPS, is expandable through the addition of compute nodes or GPUs, is accessible via a VPN for secure remote access, and supports access to the *MedeA* simulation environment via laptop or desktop *MedeA* clients.

Example Specifications

GPU Tower Workstation

A single workstation in a standard tower case with up to 4 GPUs, up to 56 CPU cores.

Property/Device	Value
CPU processor	1x Intel Xeon W-3400 Series
GPU	Supports 4x NVIDIA RTX 6000 Ada or 2x RTX 4090/4080 GPUs
Memory	Up to 2TB DDR5 ECC Memory
<i>MedeA</i>	Version 3.x (most recent)

Rackmountable GPU Workstation

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

Property/Device	Value
CPU processor	Intel Xeon W-3400
GPU	Up to 4x Double-Wide GPUs: RTX 6000 Ada, A800, etc.
Memory	8 DDR5 ECC DIMMs (up to 2TB)
Storage	2x 3.5" and 4x 2.5" Internal Drives
Interconnect	1GBASE-T + 10GBASE-T
<i>MedeA</i>	Version 3.x (most recent)

HPC GPU Server

An HPC server in a 4U rack mount chassis with 64 to 128 cores.

Property/Device	Value
CPU processor	2x AMD EPYC 7003/7003X CPUs
GPU	Up to 8x Double Wide GPU: H100, RTX 6000/5000 Ada, and more
Memory	16 DDR4 ECC DIMM Slots (Up to 4TB)
Storage	8x 3.5" Hot-swap (4x SATA, 4x NVMe)
<i>MedeA</i>	Version 3.x (most recent)

HPC Cluster

Call for additional specs and recommendations.

Performance and Scaling

To be completed

Required Modules

- *MedeA Environment*

Supported Modules

- All *MedeA* components

Recommended Modules

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

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.**