

POPULAR GPU-ACCELERATED APPLICATIONS

Application	Description	Supported Features	Expected Speed Up*	Multi-GPU Support	Release Status
Molecular Dynamics					
Abalone	Models molecular dynamics of biopolymers for simulations of proteins, DNA and ligands	Simulations (on 1060 GPU)	4-29x	Single Only	Available now
ACEMD	Simulation of mechanics force fields, implicit & explicit solvent on CUDA	Written for use on GPUs	160 ns/day	Yes	Available now
AMBER	Suite of programs to simulate molecular dynamics on biomolecules	PMEMD: Explicit and Implicit Solvent	89.44 ns/day JAC NVE	Yes	Available now, V11
DL-POLY	Simulate macromolecules, polymers, ionic systems, etc on a distributed memory parallel computer	Two-body Forces, Link-cell Pairs, Ewald SPME forces, Shake W	4x	Yes	Available now, V4.0 Source only
GROMACS	Simulation of biochemical molecules with complicated bond interactions	Implicit (5x), Explicit(2x) solvent	165 ns/Day DHFR	Single Only	Available now (Multi-GPU in development)
HOOMD-Blue	Particle dynamics package written grounds up for GPUs	Written for GPUs	2x	Yes	Available now
LAMMPS	Classical molecular dynamics package	Lennard-Jones, Gay-Berne	3.5-15x	Yes	Available now
NAMD	Designed for high-performance simulation of large molecular systems	100M atom capable	6.44 ns/days STMV585x 2050s	Yes	Available now, V2.8
Quantum Chemistry					
GAMESS-US	Computational chemistry suite used to simulate atomic and molecular electronic structure	Libqc with Rys Quadrature Algorithm, integral evaluation, closed shell Fock matrix construction	1.3-1.6x	Single only	Available now (Multi-GPU in development)
NWChem	Computational chemistry package designed for HPC clusters	Triples part of Reg-CCSD(T), CCSD & EOMCCSD task schedulers	3-10x	N/A	In Development
Q-CHEM	Computational chemistry package designed for HPC clusters	Various features including R1-MP2	8-14x	N/A	In Development
TeraChem	Quantum chemistry software designed to run on NVIDIA GPU	"Full GPU-based solution". Performance compared to GAMESS CPU version.	44-650x	Yes	Available now, Version 1.45
Materials Science					
LSMS	Materials code for investigating the effects of temperature on magnetism	Wang-Landau method	TBD	Yes	In Development
QMCPACK	Solves the many-body Schrodinger equation for electronic structures using a quantum Monte Carlo method	Solves many-body Schrodinger equation through quantum Monte Carlo method	3-5x	Yes	Available now
Quantum-Espresso/PWscf	An integrated suite of computer codes for electronic structure calculations and materials modeling at the nanoscale	PWscf package: linear algebra (matrix multiply), explicit computational kernels, 3D FFTs	TBD	Single only	Available now
VASP	First principles materials code that computes electronic structures and quantum-mechanical molecular dynamics	Hybrid Hartree-Fock DFT functionals including exact exchange	TBD	Yes	In Development
Visualization & Docking Software					
Amira 5	A multifaceted software platform for visualizing, manipulating, and understanding life sciences and bio-medical data	3D visualization of volumetric data and surfaces	N/A	Yes	Available now Version 5.3.3
Core Hopping	Rapid screening of novel cores to improve drug properties	LIGAND & receptor-based scaffold exploration	3.5-5000x	Yes	Available now
FastROCS	3D molecular shape comparison	All features are GPU enabled	800-3000x	Yes	Available now
VMD	Visualizing and analyzing large bio-molecular systems in 3-D graphics	GPU acceleration for computationally demanding analysis and visualization tasks	100-125x or greater on kernels	Yes	Available now Version 1.9

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Physics					
Chroma	General purpose LQCD application	Wilson-clover fermions, Krylov solvers, Domain-decomposition	5-6x	Yes	Available now
MILC	General purpose LQCD application	Staggered fermions, Krylov solvers, Gauge-link fattening	5-6x	Yes	Available now
Computational Fluid Dynamics					
Altair AcuSolve	General purpose CFD flow solver	Linear equation solver	2x	Yes	Available now
Autodesk Moldflow	Optimize design of plastic parts and injection molds	Linear equation solver	2x	Single Only	Available now
FEFLO (GMU-Lohner)	Navier-Stokes flow solver based on unstructured grids for modeling both compressible and incompressible flows	Explicit solver	10x	Yes	In Development
FluiDyna LBUltra	Computing physical flows in and around solid bodies	LBM, particle CFD	20x	Yes	Available now
FluiDyna Culises-OpenFOAM	Computing physical flows with Culises — a software library with special algorithms for solving systems of equations	Linear equation solvers	3x Solver	Single Only	Available now
Promotech Particleworks	Fluid simulation for free surface flow like Tsunami, material processing and liquids	MPS, Particle CFD	4x-9x	Yes	Available now
S3D (Sandia NL S3D)	Massively parallel direct numerical solver (DNS) for the full compressible Navier-Stokes	Chemistry kernel	8x SP, 5x DP kernel	Yes	In Development
Turbostream	Ultrafast CFD solver for turbomachines	Explicit solver	19x	Yes	Available now
Vratis SpeedIT-OpenFOAM Solver	Set of accelerated solvers for sparse linear systems of equations	Linear equation solvers	3x Solver	Yes	Available now
Computational Structural Mechanics					
Abaqus/Standard	Simulation and analysis tool for structural mechanics	Linear equation solver	1.5-2.5x	Single Only	Available now
ANSYS Mechanical	Simulation and analysis tool for structural mechanics	Linear equation solver	2x	Single Only	Available now
Impetus Afea	Predicts large deformations of structures and components exposed to extreme loading conditions	Linear equation solver, SPH	10x SPH, 2x Total	Yes	Available now
LS-DYNA Implicit	Multiphysics simulation package used	Linear equation solver	3x	Yes	In Development
MSC Nastran	Simulation and analysis tool for structural mechanics	Linear equation solver	1.4-2x	Yes	Available now
Marc	Simulation and analysis tool for structural mechanics	Linear equation solver	1.5x	Yes	In Development
RADIOSS Implicit	Used to maximize durability, NVH, crash, safety, manufacturability and fluid-structure interaction performance	Linear equation solver	2x	Single Only	In Development

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Electronic Design Automation and CEM					
Agilent Technologies ADS	Simulation tool for design of RF, microwave and high speed digital circuits	Signal integrity simulation	4-6x	Single Only	Available now
Agilent Technologies EMPro	Modeling and simulation environment for analyzing 3D EM effects of high speed and RF/Microwave components	FDTD solver	6x	Yes	Available now
ANSYS Nexxim	Circuit simulation engine for RF/analog/mixed-signal IC design; IBIS-AMI analysis speedup with GPU computing	AMI analysis	7-15x	Single Only	Available now
CST Microwave Studio (MWS)	High frequency electromagnetic field simulation	Transient solver	9-20x	Yes	Available now
Gauda OPC, OPV	Collection of several software tools for computational lithography running on Gauda hardware platform	Optical proximity correction & verification	20-100x	Single Only	Available now
Remcom XFDTD	3D EM modeling and simulation	FDTD solver	30-50x	Yes	Available now
Rocketick RocketSim	Verilog simulation	Verilog simulation	10x	Single Only	Available now
SPEAG SEMCAD-X	3D EM modeling and simulation	FDTD solver	100x	Yes	Available now
CAD					
CATIA V6 – Live Rendering	Photorealistic rendering	Interactive. Fully integrated in CATIA V6. Network rendering	3-6x	Yes	Available now
Bunkspeed Pro Suite	Easy to use photorealistic rendering software	Iray based ray-tracing. Animation support. Network rendering	3-6x	Yes	Available now
RTT DeltaGen 10.x	Photorealistic rendering used for design	Interactive ray tracing and global illumination. Integration with Siemens TeamCenter. Cluster support	16x	Yes	Available now
RTT DeltaPix	Photorealistic rendering with integration of TeamCenter and RTT formats	Iray based ray-tracing. Support for JT and csb formats	3-6x	Yes	Available now
Numerical Analysis					
Jacket AccelerEyes	GPU acceleration for MATLAB	CUDA kernels with MATLAB, distributing standalone apps with MATLAB	6-20x	Yes	Available now
Mathematica Wolfram	Symbolic math analysis	Development environment for CUDA and OpenCL kernels	2-10x	Yes	Available now
MATLAB Mathworks	Technical computing language and integrated development environment (MATLAB PCT, MDCS)	CUDA kernels with MATLAB, distributing standalone apps with MATLAB	6-20x	Yes	Available now

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Weather & Climate Forecasting					
ASUCA	Weather forecasting model fully optimized for GPUs	Most routines	12x	Yes	In Development
CAM / SE	Community Atmospheric Model is a global atmosphere model for weather and climate research	Dynamical core	2x Dynamics	Single Only	In Development
GEOS-5	Weather modeling and forecasting application used by NASA	Most routines	10x Models, 3x Dynamics	Yes	In Development
HIRLAM	Weather forecasting model fully optimized for GPUs	Dynamical core	3x Dynamics	Yes	In Development
HOMME	Weather modeling tool for atmospheric scientists	Dynamical core	3x Kernels	Single Only	In Development
HYCOM	Weather forecasting model using icosahedral horizontal grid	Dynamical core	2x Kernels	Single Only	In Development
MITgcm	Numerical model designed for study of the atmosphere, ocean, and climate	Ocean circulation model	3x Solver	Single Only	In Development
NIM	Weather forecasting model using icosahedral horizontal grid	Dynamical core	7x Dynamics	Yes	In Development
WRF	Weather and Ocean modeling application	WSM5, WSM3, Ice Microphysics models	4-6x	Single Only	Available now
Editing and Effects					
Adobe Premiere Pro	Video editing	Mercury Playback Engine; faster video effects	7-14x	Single only	Available now
Avid Media Composer	Video editing	Faster video effects, unique stereo 3D capabilities	2.5-7x	Single Only	Available now
GenArts Sapphire	Effects plug-in for video editing	Faster video effects	10x	Single only	Available now
Sony Vegas Pro	Video editing	Faster video effects and encoding	7x	Single only	Available now
Animation					
Autodesk 3Ds Max	3D modeling, animation, and rendering	iray interactive, photorealistic and physically correct rendering	6-10x	Yes	Available now
Autodesk Maya	3D modeling, animation, and rendering	Increased model complexity, larger scenes	10x	Single Only	Available now
Defense & Intelligence					
DigitalGlobe Advanced Ortho Series	Geospatial Visualization	Image orthorectification	50x	Yes	Available now
Eternix Blaze Terra	Geospatial Visualization	3D visualization of geospatial data	50x	Yes	Available now
Exelis (ITT) ENVI	Geospatial Visualization	Image orthorectification (custom builds only)	70x	Yes	Available now
GeoEye Analytics Signature Analyst	Geospatial Visualization	Terrain analytics	12-15x	Yes	Available now
GeoWeb3d Desktop	Geospatial Visualization	3D visualization of geospatial data	Requires GPU	Yes	Available now
Incogna GIS	Geospatial Visualization	Image processing on Tesla cloud servers object recognition	50x	Yes	Available now
Intergraph Motion Video Analyst	Video filters and mosaic'ing — Geo-fuses FMV analytics with intelligence data	Full motion video ortho mosaic processing	5-7x	No	Available now
Intuvision Panoptes 3.0	Video Analytics	Object recognition and change detection	12x	Yes	Available now
MotionDSP Ikena 2.2	Video Enhancement	Video stabilization, filtering, ortho mosaic, and transcoding	5x	Yes	Available now
Nerve ViD SrX	Video Analytics	Object recognition and tracking	100x	Yes	Available now
PCI Geomatics GXL	Geospatial Visualization	Image orthorectification and additional image processing	20-60x	Yes	Available now

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Oil&Gas					
Acceleware RTM	Seismic Processing	RTM algorithm	14x	Yes	Available now
CGG/Veritas RTM	Seismic Processing	RTM algorithm	3-6x	Yes	Available now
ffA SVI Pro	Seismic Interpretation	Attributes calculations	5-20x	Yes	Available now
Headwave Suite	Seismic Imaging	Attributes calculations	10-100x	Yes	Available now
Geoteric	Seismic Processing/Interpretation	Attributes calculations	11-13x	Yes	Available now
Paradigm EarthStudy360	Reservoir Modeling	Attributes calculations	10-40x	Yes	Available now
Paradigm Echos RTM	Seismic Processing	RTM algorithm	14x	Yes	Available now
Paradigm SKUA	Reservoir Modeling	Faults, Horizons and Flow Simulation Grid	5-40x	Yes	Available now
Paradigm VoxelGeo	Seismic Interpretation	Attributes calculations	10-40x	Yes	Available now
Schlumberger WesterGeco Omega2 RTM	Seismic Processing	RTM algorithm	Non-disclosed	Yes	Available now
Seismic City Prestack Interpretation	Seismic Processing	Attributes calculations	10-40x	Yes	Available now
SpectraSeis	Seismic Processing / Imaging	Full elastic wave-equation imaging and analysis of microseismic fracture data	26x	Yes	Available now
Stoneridge Reservoir Simulation	Reservoir Simulation	Sparse Matrix solver	5-6x	Yes	Available now
Tsunami RTM	Seismic Processing	RTM algorithm	14x	Yes	Available now
Computational Finance					
Hanweck Associates	Real-time options analytical engine (Volera)	Real-time options analytics engine	100x	Yes	Available now
MATLAB Mathworks	Data parallel mathematics (MATLAB PCT, MDCS)	MATLAB operations	3-20x	Yes	Available now
Murex	Risk analytics (MACS)	MACS analytics library	60-400x	Yes	Available now
Numerical Algorithms Group	Random Number Generators	Monte Carlo	50x	Single Only	Available now
SciComp, Inc	Derivative pricing (SciFinance)	Monte Carlo and PDE pricing models	30-50x (MC), 10-35x (PDE)	Single Only	Available now
Wolfram Mathematica	Mathematical Development Environment	CUDA Link Package	3-20x	Yes	Available now

*GPU performance compared against multi-core x86 CPU socket. GPU performance benchmarked on GPU supported features and may be a kernel to kernel performance comparison. Performance results obtained from ISV's documentation and / or NVIDIA benchmarks.

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