LIFE & MATERIALS SCIENCES APPLICATIONS CATALOG

Application	Description	Supported Features	Expected Speed Up*	Multi-GPU Support	Release Status
Bioinformatics					
BarraCUDA	Sequence mapping software	Alignment of short sequencing reads	6-10x	Yes	Available now Version 0.6.2
CUDASW++	Open source software for Smith-Waterman protein database searches on GPUs	Parallel search of Smith-Waterman database	10-50x	Yes	Available now Version 2.0.8
CUSHAW	Parallelized short read aligner	Parallel, accurate long read aligner - gapped alignments to large genomes	10x	Yes	Available now Version 1.0.40
GPU-BLAST	Local search with fast k-tuple heuristic	Protein alignment according to blastp, multi cpu threads	3-4x	Single Only	Available now Version 2.2.26
GPU-HMMER	Parallelized local and global search with profile Hidden Markov models	Parallel local and global search of Hidden Markov Models	60-100x	Yes	Available now Version 2.3.2
mCUDA-MEME	Ultrafast scalable motif discovery algorithm based on MEME	Scalable motif discovery algorithm based on MEME	4-10x	Yes	Available now Version 3.0.12
MUMmerGPU	A high-throughput DNA sequence alignment program	Aligns multiple query sequences against reference sequence in parallel	3-10x	Yes	Available now Version 2
SeqNFind	A GPU Accelerated Sequence Analysis Toolset	HW & SW for reference assembly, blast, SW, HMM, de novo assembly	400x	Yes	Available now
UGENE	Opensource Smith-Waterman for SSE/CUDA, Suffix array based repeats finder & dotplot	Fast short read alignment	6-8x	Yes	Available now Version 1.11
WideLM	Fits numerous linear models to a fixed design and response	Parallel linear regression on multiple similarly-shaped models	150x	Yes	Available now Version 0.1-1
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	GPU Simulation of molecular mechanics force fields, implicit & explicit solvent	Written for use on GPUs	160 ns/day Requires GPU	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 Version12
DL-POLY	Simulate macromolecules, polymers, ionic systems, etc on a distributed memory parallel computer	Two-body forces, Link-cell pairs, Ewald SPME forces, Shake VV	4x	Yes	Available now, Version4.0 Source only
GROMACS	Simulation of biochemical molecules with complicated bond interactions	Implicit (5x), Explicit(2x) solvent	165 ns/Day DHFR	Single Only	Available now Version 4.5
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, Version 2.9
OpenMM	Library and application for molecular dynamics on high-performance	Implicit and explicit solvent, custom forces	Implicit: 127-213 ns/day; Explicit: 18-55 ns/day DHFR	Yes	Available now Version 4.0

NVIDIA® GPUs are enabling tremendous performance speedups for a number of packaged applications spanning a variety of disciplines. For additional information on GPU-accelerated applications and to view most current version of this Application Catalog, please visit **www.nvidia.com/teslaapps**

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Quantum Chemistry					
Abinit	Allows to find total energy, charge density & electronic structure of systems made of electrons and nuclei within DFT	Local Hamiltonian, non-local Hamiltonian, LOBPCG algorithm, diagonalization / orthogonalization	1.3-2.7x	Yes	Available now Since version 6.1
ACES III	Takes best features of parallel implementations of quantum chemistry methods for electronic structure	Integrating scheduling GPU into SIAL programming language and SIP runtime environment	10x Kernels	Yes	In development
ADF	Density Functional Theory (DFT) software package that enables first-principles electronic structure calculations	Fock Matrix, Hessians	TBD	Yes	In development
BigDFT	Implements density functional theory by solving the Kohn-Sham equations describing the electrons in a material	DFT; Daubechies wavelets, part of Abinit	5-25x	Yes	Available now Version 1.6.x
Casino	Code for performing quantum Monte Carlo (QMC) electronic structure calculations for finite and periodic systems	TBD	TBD	Yes	In development
CP2K	Program to perform atomistic and molecular simulations of solid state, liquid, molecular and biological systems	DBCSR (space matrix multiply library)	2-7x	Yes	In development
GAMESS-UK	Is the general purpose ab initio molecular electronic structure program for performing SCF-, DFT- and MCSCF-gradient calculations	(ss|ss) type integrals within calculations using Hartree Fock ab initio methods and density functional theory. Supports organics & inorganics.	8x	Yes	In development
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	Yes	Available now
Gaussian	Joint NVIDIA, PGI & Gaussian collaboration. Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems	TBD	TBD	Yes	In development
GPAW	Real-space grid DFT code written in C and Python	Electrostatic poisson equation, orthonormalizing of vectors, residual minimization method (rmm-diis)	8x	Yes	Available now
MOLCAS	Methods for calculating general electronic structures in molecular systems in both ground and excited states	CU_BLAS	1.1x	Yes	In development
MOLPRO	Used for accurate ab initio quantum chemistry calculations	Density-fitted MP2 (DF-MP2), density fitted local correlation methods (DF-RHF, DF-KS), DFT	1.7-2.3x	Yes	In development
NWChem	Computational chemistry package designed for HPC clusters	Triples part of Reg-CCSD(T), CCSD & EOMCCSD task schedulers	3-10x	Yes	In development
Q-CHEM	Computational chemistry package designed for HPC clusters	Various features including R1-MP2	8x-14x	Yes	Available Version4.0
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 1.5

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Materials Science					
LSMS	Materials code for investigating the effects of temperature on magnetism	Generalized Wang-Landau method	3x 2 GPUs vs 128 CPU cores	Yes	In development
PEtot	First principles materials code that computes the behavior of the electron structures of materials	Density functional theory (DFT) plane wave pseudopotential calculations	6-10x	Yes	Available now
QMCPACK	Solves the many-body Schrodinger equation for electronic structures using a quantum Monte Carlo method	Main features	3-4x 512 GPUs vs. 512 (16-core) CPUs	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 (matix multiply), explicit computational kernels, 3D FFTs	2.5-3.5x	Yes	Available now Version 5.0
VASP	First principles materials code that computes the behavior of electronic structures based on quantum theory	Hybrid Hartree-Fock DFT functionals including exact exchange	2x 2 GPUs vs. 128 CPU cores	Yes	Available on request
Visualization & Docking Software					
Amira 5	A multifaceted software platform for visualizing, manipulating, and understanding Life Science and bio-medical data.	3D visualization of volumetric data and surfaces	70x	Yes	Available now Version 5.5
Core Hopping	Rapid screening of novel cores to improve drug properties	GPU accelerated application	10x	Yes	Available now
FastROCS	Molecule shape comparison application	All features are GPU-enabled	800-3000x	Yes	Available now
Molegro Virtual Docker 5	Method for performing high accuracy flexible molecular docking	Energy grid computation, pose evaluation and guided differential evolution	25-30x	Single only	Available now
PyMol	User-sponsored molecular visualization system on an open-source foundation	Lines: 460% increase, Cartoons: 1246% increase, Surface: 1746% increase, Spheres: 753% increase, Ribbon: 426% increase	17x	Single only	Available now Version 1.5
VMD	Visualization and analyzing large bio-molecular systems in 3-D graphics	GPU acceleration for computationally demanding analysis and visualization tasks	100-125x Kernels	Yes	Available now Version 1.9.x

* Expected speedups are highly dependent on system configuration. Unless noted otherwise, speedup is for entire code. Speedup data based on NVIDIA in house testing or ISV's documentation. 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. For configuration details, please view the application website. To view the complete list of GPU-accelerated applications in other disciplines and industries, visit **www.nvidia.com/teslaapps**

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