

HPC APPLICATION SUPPORT FOR GPU COMPUTING

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EXECUTIVE SUMMARY

In this report, Intersect360 Research has listed the 50 most commonly used high performance computing (HPC) applications, identifying those that currently have GPU acceleration incorporated. According to the latest HPC User Site Census data and additional research, of the 50 most popular application packages mentioned by HPC users, 34 offer GPU support today, with another two currently under development. All 15 of the top 15 applications currently have some form of GPU support. GPU computing has reached a tipping point in the HPC market that will encourage continued increased in application optimization.

The growth of GPU adoption for HPC has been driven almost entirely by NVIDIA, which has invested heavily in building a robust software ecosystem to support its hardware. Specifically, the company has developed a set of parallel programming APIs, libraries, and associated software development tools to support application development on its CUDA (Compute Unified Device Architecture) GPU platform. NVIDIA has also established over 20 GPU centers of excellence around the world, as well as a global network of GPU research and education centers encompassing hundreds of academic institutions. Those efforts have supported the acceleration of software tool development for general-purpose GPU programming, in addition to aiding the porting of open-source HPC codes to GPUs. The company has also collaborated with ISVs to help accelerate commercial HPC applications and libraries.

Today, one of the biggest market dynamics is the advent of AI. Many organizations are looking to deep learning techniques to bring AI advancements to their products, services, or operations. These algorithms often rely on GPUs, to the extent that AI has become a major growth driver for NVIDIA. The rise of AI is reflected in this list with the appearance of TensorFlow, currently tied as the 35th most commonly cited application in the HPC User Site Census survey.

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METHODOLOGY

In the annual HPC User Site Census survey, Intersect360 Research asks end users (among many other questions) to list their top HPC applications, up to five per site. We use this data to determine the most commonly used applications as a proxy for “market share.”¹ Because it is an installed-base survey, we combine previous years’ survey results, taking only the most recent survey entry from any individual HPC site. The data in this report reflects the most recent survey, with data collected in the third calendar quarter of 2017. In total, 534 different applications are counted, with a total of 1,792 total mentions.

The HPC market is by its nature a diverse space, with applications spanning multiple domains. No individual application received as much as 5% of total mentions in the survey; only the top 18 applications received at least 1%. There is a “long tail” of applications usage, with many that are used by only a few sites. Applications that are developed in house, for example, are typically in use only at that one site.

In this report, we focus on the top 50 applications as reported in the HPC User Site Census survey, with the rank order by number of mentions. To limit the list to exactly 50, we selected two applications from the seven tied for the 49th and 50th spots by number of mentions, using appearances in more recent survey iterations as a tiebreaker. With this methodology, we selected Bowtie and VMD, over DOCK (by UCSF), Sequest (Thermo Scientific), Relion (open-source community), and ROMS (open-source community). Mentions of “Schrodinger” were also in this tie, but we eliminated that entry due to the ambiguity as to the actual application, as there are multiple possible applications from that company.

With the top 50 HPC applications identified, Intersect360 Research sought to determine which of the applications currently offer GPU support for at least some functions or modules, and which had support under development. Engineers from NVIDIA contributed significantly to this effort.

RESEARCH AND ANALYSIS

High Performance Computing (HPC) spans a range of application domains in both the technical and business realms. For the purposes of this report, they are organized into major application domains that reflect specific user communities. GPU-accelerated applications are present in the majority of these domains, including chemical research, fluid dynamics analysis, structural analysis, environmental modeling, geophysics, visualization/image processing, and physics. This paper describes how these accelerated codes fit into the application domains and their significance to their respective user communities.

According to the latest HPC User Site Census data and additional research, of the 50 most popular application packages mentioned by HPC users, 34 offer GPU support today, with another two currently under development. All 15 of the top 15 applications currently have some form of GPU support. GPU computing has reached a tipping point in the HPC market that will encourage continued increased in application optimization. The complete distribution is given in Table 1.

¹ In most industry analysis contexts, market share is measured by share of industry revenue, but we find this methodology inadequate for software, where free, open-source software would therefore have 0% revenue share no matter how many people use it. Similarly, share of installations is suboptimal as a measurement, since pre-installed software could get a significant boost even if it is never used. Intersect360 Research finds this survey approach to be the best determinant of true market share of software, as defined by true usage.

Table 1: GPU Support of Top 50 HPC Applications
Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
1	Gromacs.org - GROMACS	79	Yes	Chemistry
2	ANSYS - Fluent	78	Yes	Fluid Dynamics Analysis
3	Gaussian, Inc. - Gaussian	74	Yes	Chemistry
4	U of Vienna - VASP	67	Yes	Chemistry
5	U of Illinois, UC - NAMD	64	Yes	Chemistry
6	Dassault Systemes - Simulia Abaqus	60	Yes	Structural Analysis
7	NCAR - WRF	55	Yes	Weather/Environment Modeling
8	OpenFoam Foundation - OpenFOAM	50	Yes	Fluid Dynamics Analysis
9	ANSYS - ANSYS	43	Yes	Structural Analysis
10	LSTC - LS-DYNA	40	Yes	Structural Analysis
11	NCBI - BLAST	38	Yes	Biosciences
12	Sandia Nat Lab - LAMMPS	33	Yes	Chemistry
13	AmberMD.org - Amber	32	Yes	Chemistry
14	Quantum-espresso.org - Quantum Espresso	30	Yes	Chemistry
15	Iowa State University - GAMESS	29	Yes	Chemistry
16	PNNL - NWChem	27	Yes	Chemistry
17	NCAR - CESM / CCSM	19	No	Weather/Environment Modeling
17	Paraview.org / Kitware - Paraview	19	Yes	Visualization/Image Analysis
19	ANSYS - CFX	17	No	Fluid Dynamics Analysis
20	Harris Geospatial - IDL	16	Yes	Visualization/Image Analysis
20	MSC Software - NASTRAN	16	Yes	Structural Analysis
20	Siemens - CD-adapco Star-CD	16	No	Fluid Dynamics Analysis
23	COMSOL - COMSOL	15	No	Structural Analysis
24	Siemens - CD-adapco Star-CCM+	14	No	Fluid Dynamics Analysis
25	CP2K.org - CP2k	12	Yes	Chemistry
26	ANSYS - ANSYS Mechanical	10	Yes	Structural Analysis
26	LLNL - VisIT	10	Yes	Visualization/Image Analysis
28	Abinit.org - ABINIT	9	Yes	Chemistry
28	Charmm.org - CHARMM	9	Yes	Chemistry
28	SAP AG - SAP	9	In development	Business Intelligence
31	CPMD.org - CPMD	8	Yes	Chemistry
31	Open Source - MrBayes	8	No	Biosciences
31	Q-Chem - Q-Chem	8	Yes	Chemistry
31	SCM - ADF	8	Yes	Chemistry
35	Altair Engineering - HyperWorks	7	Yes	Structural Analysis
35	Dassault Systemes - Accelrys Material Studio	7	No	Chemistry
35	Galaxyproject.org - Galaxy	7	No	Biosciences
35	ICMAB - SIESTA	7	No	Chemistry
35	Illumina - Casava	7	No	Biosciences
35	Oracle - Oracle	7	In development	Business Intelligence
35	Scripps Research Institute - AutoDock	7	No	Biosciences
35	TensorFlow.org - TensorFlow	7	Yes	Pattern Recognition
35	USQCD.org - MILC	7	Yes	Physics
44	Altair Engineering - Optistruct	6	Yes	Structural Analysis
44	Open Source - BWA	6	No	Biosciences
44	STFC - DL_POLY	6	No	Chemistry
44	Tecplot, Inc. - Tecplot	6	Yes	Visualization/Image Analysis
44	U of Vienna - Wien2K	6	No	Chemistry
49	Johns Hopkins School of Medicine - Bowtie	5	Yes	Biosciences
49	U of Illinois, UC - VMD	5	Yes	Chemistry

Chemistry

Chemistry is one of the most common HPC application areas, with organizations employing HPC systems to understand chemical compounds and processes, to design new substances based on this understanding, and to organize this information for future research and product development. This segment includes such applications as computational chemistry, molecular modeling, and software used to analyze mass spectrometry data.

Approximately one-fifth of all application mentions in the Site Census surveys conducted by Intersect360 Research are in the chemistry category, and 20 of the top 50 HPC applications are used in chemistry. The popularity of this software is driven by the interest in biomolecular research and in developing new compounds and materials for industrial use, spanning multiple economic sectors. Products based on better solvents, increased battery performance, advanced construction materials, and more efficient fuels are just a few examples of commercial applications that can be derived from these packages.

As is illustrated in Table 2, GPU support for the top chemistry codes is quite deep, thanks in large part to a preponderance of open-source codes in this application domain and the presence of active developer communities. As a result, 16 of the 20 chemistry applications are currently available with GPU acceleration, including all of the top 15.

Table 2: GPU-Accelerated Applications: Chemical Research
 Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
1	Gromacs.org - GROMACS	79	Yes	Chemistry
3	Gaussian, Inc. - Gaussian	74	Yes	Chemistry
4	U of Vienna - VASP	67	Yes	Chemistry
5	U of Illinois, UC - NAMD	64	Yes	Chemistry
12	Sandia Nat Lab - LAMMPS	33	Yes	Chemistry
13	AmberMD.org - Amber	32	Yes	Chemistry
14	Quantum-espresso.org - Quantum Espresso	30	Yes	Chemistry
15	Iowa State University - GAMESS	29	Yes	Chemistry
16	PNNL - NWChem	27	Yes	Chemistry
25	CP2K.org - CP2k	12	Yes	Chemistry
28	Abinit.org - ABINIT	9	Yes	Chemistry
28	Charmm.org - CHARMM	9	Yes	Chemistry
31	CPMD.org - CPMD	8	Yes	Chemistry
31	Q-Chem - Q-Chem	8	Yes	Chemistry
31	SCM - ADF	8	Yes	Chemistry
35	Dassault Systemes - Accelrys Material Studio	7	No	Chemistry
35	ICMAB - SIESTA	7	No	Chemistry
44	STFC - DL_POLY	6	No	Chemistry
44	U of Vienna - Wien2K	6	No	Chemistry
49	U of Illinois, UC - VMD	5	Yes	Chemistry

Many popular chemistry codes have community sites that talk of the benefits of GPU acceleration for their applications, and there are public citations of GPU support for GROMACS,² GAUSSIAN,³ NAMD,⁴ VASP,⁵

² http://www.gromacs.org/GPU_acceleration

LAMMPS,⁶ AMBER,⁷ Quantum Espresso,⁸ GAMESS,⁹ NWChem,¹⁰ CP2k,¹¹ CHARMM,¹² ABINIT,¹³ CPMD,¹⁴ Q-Chem,¹⁵ ADF,¹⁶ and VMD.¹⁷

Fluid Dynamics Analysis

Solutions based on computational fluid dynamics (CFD) appear across an exceptionally broad range of applications, such as: aircraft design, internal combustion engine design, analysis of airflow around buildings, heart pump design, modeling of protein transport within cells, and so on. Similar to structural analysis, it is an area largely dominated by commercial codes, but with some originally coming from NASA development and open-source efforts. The emergence of OpenFOAM as a top-ten application in HPC is indicative of an industry-wide trend toward increased use of open-source codes.

As seen in Table 3, the two most popular CFD applications, ANSYS Fluent¹⁸ and OpenFOAM,¹⁹ are now available with GPU support.

Table 3: GPU-Accelerated Applications: Fluid Dynamics Analysis
Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
2	ANSYS - Fluent	78	Yes	Fluid Dynamics Analysis
8	OpenFoam Foundation - OpenFOAM	50	Yes	Fluid Dynamics Analysis
19	ANSYS - CFX	17	No	Fluid Dynamics Analysis
20	Siemens - CD-adapco Star-CD	16	No	Fluid Dynamics Analysis
24	Siemens - CD-adapco Star-CCM+	14	No	Fluid Dynamics Analysis

Structural Analysis

Structural analysis includes applications used to analyze a variety of structures, including explicit and implicit finite element analysis (FEA), an important computational tool used for engineering analysis. It is primarily used to determine loads and stresses on structures, including the notable use case of virtual crash testing of automobiles.

Table 4 delineates the eight structural analysis packages that are among the top 50 HPC applications. Seven of the eight have support for GPU computing, including three applications in the top 10 of all HPC applications:

³ <http://gaussian.com/relnotes/?tabid=2>

⁴ <http://www.ks.uiuc.edu/Research/namd/2.9/ug/node88.html>

⁵ <https://www.vasp.at/index.php/news/44-administrative/115-new-release-vasp-5-4-1-with-gpu-support>

⁶ http://lammps.sandia.gov/doc/accelerate_gpu.html

⁷ <http://ambermd.org/gpus/>

⁸ <https://github.com/fspiga/qe-gpu/blob/devel-gpu/README.md>

⁹ <http://www.msg.ameslab.gov/gamess/versions.html>

¹⁰ http://www.nwchem-sw.org/index.php/Release62:TCE#CCSD.28T.29_method_with_CUDA

¹¹ https://www.cp2k.org/howto:compile_with_cuda

¹² <https://www.charmm.org/charmm/documentation/by-version/c40b1/params/doc/gpu/>

¹³ [https://wiki.abinit.org/doku.php?id=build:linear_algebra&s\[\]=gpu](https://wiki.abinit.org/doku.php?id=build:linear_algebra&s[]=gpu)

¹⁴ <http://adsabs.harvard.edu/abs/2010APS..MARP23014M>

¹⁵ https://www.q-chem.com/qchem-website/manual/qchem43_manual/sect-auxRI.html

¹⁶ https://www.scm.com/doc/ADF/Input/Technical_Settings.html

¹⁷ <http://www.ks.uiuc.edu/Research/vmd/current/cuda.html>

¹⁸ <http://www.ansys.com/-/media/ansys/corporate/resourcelibrary/article/accelerationg-ansys-fluent-simulations-with-nvidia-gpus-aa-v9-i1.pdf>

¹⁹ <https://sim-flow.com/rapid-cfd-gpu/>

Simulia Abaqus,²⁰ ANSYS,²¹ and LS-DYNA.²² (In the case of ANSYS, there is ambiguity as to the exact application from the ANSYS suite that is specified. We have left the survey data as is and kept it in this report because it is one of the top ten responses, and because GPU computing is unambiguously supported in the ANSYS structural mechanics suite.) There are also public citations available for NASTRAN,²³ ANSYS Mechanical,²⁴ and both HyperWorks and Optistruct from Altair.²⁵

Table 4: GPU-Accelerated Applications: Structural Analysis
Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
6	Dassault Systemes - Simulia Abaqus	60	Yes	Structural Analysis
9	ANSYS - ANSYS	43	Yes	Structural Analysis
10	LSTC - LS-DYNA	40	Yes	Structural Analysis
20	MSC Software - NASTRAN	16	Yes	Structural Analysis
23	COMSOL - COMSOL	15	No	Structural Analysis
26	ANSYS - ANSYS Mechanical	10	Yes	Structural Analysis
35	Altair Engineering - HyperWorks	7	Yes	Structural Analysis
44	Altair Engineering - Optistruct	6	Yes	Structural Analysis

Visualization/Image Analysis

Visualization is fundamental to many HPC workflows, allowing researchers and engineers to see the results of their simulations in graphical form. There are a large number of visualization packages that users cited in the latest Intersect360 Research survey. Of these, four made it into our top 50 of HPC applications. Visualization software is roughly evenly split between commercial and non-commercial applications.

As can be seen in Table 7, all the top visualization packages are GPU accelerated, which is hardly a surprise considering that graphics processors were originally designed for image and video processing. Pixel analysis algorithms in particular are extremely well-suited to the GPU architecture. In many cases, GPU computing support for these applications comes from plug-ins provided by NVIDIA.²⁶

Table 5: GPU-Accelerated Applications: Visualization/Image Analysis
Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
17	Paraview.org / Kitware - Paraview	19	Yes	Visualization/Image Analysis
20	Harris Geospatial - IDL	16	Yes	Visualization/Image Analysis
26	LLNL - VisIT	10	Yes	Visualization/Image Analysis
44	Tecplot, Inc. - Tecplot	6	Yes	Visualization/Image Analysis

²⁰ <https://www.3ds.com/fileadmin/PRODUCTS/SIMULIA/PDF/scc-papers/multi-gpu-computing-abaqus-benchmarking-scaling-multiphysics-13.pdf>

²¹ <http://www.ansys.com/-/media/ansys/corporate/resourcelibrary/article/aa-v7-i3-accelerating-mechanical-solutions-with-gpus.pdf>

²² <https://www.dynamore.de/de/download/papers/ls-dyna-forum-2012/documents/04-gohner-dynamore.pdf>

²³ <http://pages.mscsoftware.com/rs/mscsoftware/images/GPU%20Computing%20with%20MSC%20Nastran%202013.pdf>

²⁴ <http://www.ansys.com/-/media/ansys/corporate/resourcelibrary/article/aa-v7-i3-accelerating-mechanical-solutions-with-gpus.pdf>

²⁵ http://www.altair.com/NewsDetail.aspx?news_id=10789

²⁶ http://www.harrisgeospatial.com/portals/0/pdfs/idl/uc/GPULib_IDLUG.pdf

Biosciences

Bioscience applications are used to reveal the nature of life and help design medical treatments. They are also used to understand and enhance agricultural production. This segment includes such applications as genomics, proteomics, and drug discovery, among others. We see much of this segment being driven by the genomics revolution, which uses bioinformatics software to analyze the function of genes as it relates to cellular function. This information led to a flowering of applications in biology, pharmacology, and biochemistry/bioengineering. Note that many of the molecular dynamics codes, which were placed in the Chemistry category, have bioscience applications as well.

As Table 6 shows, GPU computing has lagged behind the development for GPUs in the rest of the HPC industry. However, a GPU-enabled version of BLAST, specifically known as GPU-BLAST,²⁷ is now available in the research community, and there is a GPU accelerated version of Bowtie²⁸ as well, available as an NVIDIA Labs project.

Table 6: GPU-Accelerated Applications: Biosciences
Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
11	NCBI - BLAST	38	Yes	Biosciences
31	Open Source - MrBayes	8	No	Biosciences
35	Illumina - Casava	7	No	Biosciences
35	Galaxyproject.org - Galaxy	7	No	Biosciences
35	Scripps Research Institute - AutoDock	7	No	Biosciences
44	Open Source - BWA	6	No	Biosciences
49	Johns Hopkins School of Medicine - Bowtie	5	Yes	Biosciences

Other Top 50 HPC Applications

Table 7 lists the remaining top 50 HPC applications, along with their domains. Two are in business intelligence, two in weather forecasting and environmental modeling, and one each in physics and pattern recognition.

Table 7: GPU-Accelerated Applications: Other Top 50 Applications
Intersect360 Research, 2017

Rank	Supplier - Application	Mentions	GPU Support	Application Category
7	NCAR - WRF	55	Yes	Weather/Environment Modeling
17	NCAR - CESM / CCSM	19	No	Weather/Environment Modeling
28	SAP AG - SAP	9	In development	Business Intelligence
35	Oracle - Oracle	7	In development	Business Intelligence
35	TensorFlow.org - TensorFlow	7	Yes	Pattern Recognition
35	USQCD.org - MILC	7	Yes	Physics

Weather/Environment Modeling

Environmental modeling includes applications used to simulate weather, climate, air quality, and ocean systems. The potential use of weather forecasting ranges from saving lives and property with advanced severe weather alerts, to predicting wildfires, to managing the power grid by predicting energy demands, to estimating

²⁷ <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3018811/>

²⁸ https://nvlabs.github.io/nvbio/nvbowtie_page.html

demand for products at your local supermarket based on weather forecasts. Add in climate modeling research for predicting global climate change and hydrodynamic modeling to predict water movement, and the impact of environmental modeling becomes obvious. Almost all these codes have been developed from non-commercial sources and approximately three-quarters of them are open-source.

Two weather codes are among the top 50 HPC applications. WRF is the most common, one of the top 10 applications overall, and it has been optimized for GPU computing.²⁹

Business Intelligence

SAP and Oracle appear in the list of the top 50 HPC applications. There has always been some crossover between business computing and HPC—even scientific applications use databases—but this is becoming increasingly common thanks to the burgeoning field of analytics. Both SAP and Oracle have GPU-accelerated versions reportedly in development. There is keen interest in this, particularly with respect to AI. Both SAP and Oracle are working toward AI-optimized modules for their enterprise customers, and there is a large affinity for deep learning applications to GPU computing.

Physics

Physics includes applications that are used to model the fundamental principles involved in the behavior of matter and energy. Work in the field ranges from cosmological models of the evolution of the universe to quantum mechanics simulations of matter at the subatomic level. Physicists were among the first users of HPC and continue to have some of the most demanding computational requirements. As might be expected from a research-based domain, the vast majority of these packages are provided by non-commercial organizations as open-source codes. MILC in particular is a commonly used code for quantum physics that has a GPU-accelerated version available.³⁰

Pattern Recognition

Pattern recognition is a fundamental aspect of deep learning. Applications learn from vast quantities of training data in order to be able to make inferences later from similar data. TensorFlow is the most commonly used application for this at present, and to the point where it now appears in the top 50 HPC applications. As noted above, deep learning has a strong affinity to GPU computing, and TensorFlow indeed is offered with GPU acceleration.³¹

²⁹ http://www2.mmm.ucar.edu/wrf/users/workshops/WS2016/oral_presentations/4.4.pdf

³⁰ <http://www.physics.utah.edu/~detar/milc/milcv7.pdf>

³¹ https://www.tensorflow.org/tutorials/using_gpu

INTERSECT360 RESEARCH ANALYSIS

As is evident from the number of GPU-accelerated software packages available across application domains, the use of this accelerator technology has become well-established in the HPC user community. In nearly every domain, GPU-acceleration is now available on one or more of the most commonly used application packages. More significantly, in concert with the expanded use of GPUs reported by HPC users in our latest Site Census surveys, relative to previous years, GPU usage is moving from a test-and-evaluation phase into production work.

In certain areas such as chemistry, structural analysis, and visualization, the availability of GPU acceleration is nearly ubiquitous. In other areas, like biosciences and environmental modeling, penetration remains incomplete. But there is continued progress across all segments, and future trends in AI promise to accelerate the presence of GPUs.

The growth of GPU adoption for HPC has been driven almost entirely by NVIDIA, which has invested heavily in building a robust software ecosystem to support its hardware. Specifically, the company has developed a set of parallel programming APIs, libraries, and associated software development tools to support application development on its CUDA (Compute Unified Device Architecture) GPU platform. Since its introduction, CUDA has been available on platforms running any NVIDIA GPU and was downloadable for free by anyone interested in experimenting with using GPUs as application accelerators. This combination of free software running on existing hardware effectively bootstrapped the accelerator market and positioned NVIDIA as the market leader. Subsequently the company now holds over three quarters of mentions of accelerator implementations in our survey research.

While NVIDIA's efforts have been centered on CUDA-based software tools and middleware, implementations also include support of OpenCL, an open standard framework for developing parallel applications across a variety of processor architectures, and OpenACC, a set of standard compiler directives for high-level languages that can be used for both x86 CPUs and accelerators. NVIDIA has also established over 20 GPU centers of excellence around the world, as well as a global network of GPU research and education centers encompassing hundreds of academic institutions. Those efforts have supported the acceleration of software tool development for general-purpose GPU programming, in addition to aiding the porting of open-source HPC codes to GPUs. The company has also collaborated with ISVs to help accelerate commercial HPC applications and libraries.

The movement from experimentation into production is an outcome of the ecosystem support from NVIDIA and the availability of the application packages described in this report. GPU computing has reached a tipping point, which will encourage GPU support to be incorporated even more broadly into applications that can make use of the architecture's highly parallel features. In fact, this process is well underway. In addition to the 34 top GPU-enabled applications identified here, NVIDIA cites hundreds more on its website. We expect this expansion to continue as the GPU computing user base grows and becomes more comfortable with the technology.