

Project title: List of HPC applications (DRAFT 08/27/2019)

Word count: 1700

Type: standard, will add sources to function field

Keywords: applications, High performing applications, FlexApp, FlexLM, Flex license server

Jay A. Etchings – Splunk 08/26/2019 v1.2

## Life Sciences, Bio Tech, and Genomics

Program	Function
LAMMPS Large-scale Atomic/ Molecular Massively Parallel Simulator.	This is a molecular dynamics program that makes use of MPI for parallel communication. LAMMPS is distributed by Sandia National Laboratories, a US Department of Energy laboratory. <a href="https://lammps.sandia.gov/">https://lammps.sandia.gov/</a> Source: The file “log.lammps” is the default log file for a LAMMPS run.
SOAPdenovo Short Oliganucleotide Analysis Package	This is a bioinformatics package used for assembly and analysis of DNA sequence. Ultra-fast single-node solution for large and complex metagenomics assembly. <a href="https://github.com/aquaskyline/SOAPdenovo2">https://github.com/aquaskyline/SOAPdenovo2</a> Source: Plain text logs
ABYSS Assembly By Short Sequence.	A de novo, parallel, paired-end sequence assembler that is designed for short readers. <a href="http://www.bcgsc.ca/platform/bioinfo/software/abyss">http://www.bcgsc.ca/platform/bioinfo/software/abyss</a> Source:
Bowtie	Bowtie is an ultrafast, memory-efficient short read aligner for short DNA sequences. Bowtie 2 is an ultrafast and memory-efficient tool for aligning sequencing reads to long reference sequences built for Hadoop. <a href="http://bowtie-bio.sourceforge.net/news.shtml">http://bowtie-bio.sourceforge.net/news.shtml</a> <a href="http://bowtie-bio.sourceforge.net/bowtie2/index.shtml">http://bowtie-bio.sourceforge.net/bowtie2/index.shtml</a> Source:
Burrows- Wheel Aligner	BWA is a software package for mapping low-divergent sequences against a large reference genome, such as the human genome. <a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2705234/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2705234/</a> <a href="http://bio-bwa.sourceforge.net/">http://bio-bwa.sourceforge.net/</a>
Celera Assembler	This is a de novo whole-genome shotgun (WGS) DNA sequence assembler. <a href="http://wgs-assembler.sourceforge.net/wiki/index.php?title=Main_Page">http://wgs-assembler.sourceforge.net/wiki/index.php?title=Main_Page</a>
GATK- Genome Analysis Toolkit	This is a software package developed at the Broad Institute to analyze next-generation sequencing data. <a href="https://www.intel.com/content/www/us/en/healthcare-it/solutions/genomicscode-gatk.html">https://www.intel.com/content/www/us/en/healthcare-it/solutions/genomicscode-gatk.html</a>
HMMR	It is used for searching sequence database for homologs of protein sequences, and for making protein sequence alignments. It implements methods using probabilistic models called profile is hidden Markov models (profile HMMs) <a href="http://hmmer.org/">http://hmmer.org/</a>
BLAST-Basic Local Alignment Search Tool.	In informatics, BLAST is an algorithm for comparing primary biological sequence information, such as the amino-acid sequence of different proteins or the nucleotides of DNA sequences. A BLAST search enables a researcher to compare a query sequence with a library or database of sequences and identify library sequences that resemble the query

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	sequence above a certain threshold. <a href="https://www.nature.com/scitable/topicpage/basic-local-alignment-search-tool-blast-29096/">https://www.nature.com/scitable/topicpage/basic-local-alignment-search-tool-blast-29096/</a>
mpiBLAST	mpiBLAST is a freely available, open-source, parallel implementation of NCBI BLAST. <a href="https://www.sharcnet.ca/help/index.php/MPIBLAST#Introduction">https://www.sharcnet.ca/help/index.php/MPIBLAST#Introduction</a>
NAMD	This is a parallel molecular dynamics code designed for high-performance simulation of large bio molecular systems. <a href="http://www.ks.uiuc.edu/Research/namd/">http://www.ks.uiuc.edu/Research/namd/</a>
Picard	Picard comprises Java-based command-line utilities that manipulate SAM files and a Java API (SAM-JDK) for creating new programs that read and write SAM files. Both SAM text format and SAM binary (BAM) format are supported. <a href="https://github.com/broadinstitute/picard">https://github.com/broadinstitute/picard</a>
SAMtools- Sequence Alignment Map	SAM is a generic format for storing large nucleotide sequence alignments. <a href="https://academic.oup.com/bioinformatics/article/25/16/2078/204688">https://academic.oup.com/bioinformatics/article/25/16/2078/204688</a> <a href="http://samtools.sourceforge.net/">http://samtools.sourceforge.net/</a>
Velvet	Is a sequence assembler for very short reads. <a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2952100/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2952100/</a>
VMD	Is a molecular visualization program for displaying, animating, and analyzing large bimolecular systems using 3-D graphics and built-in scripting. <a href="https://www.ks.uiuc.edu/Research/vmd/">https://www.ks.uiuc.edu/Research/vmd/</a>

## General Science Applications and Libraries

Program	Function
CLHELP( physics) Class Library for High Energy Physics	This is a C++ library that provides utility classes for general numerical programming, vector arithmetic, geometry, pseudorandom number generation, and linear algebra, specifically targeted for high energy physics simulation and analysis software. <a href="http://proj-clhep.web.cern.ch/proj-clhep/">http://proj-clhep.web.cern.ch/proj-clhep/</a>
FDS-SMV( Fire Dynamics Simulator)	<b>FDS</b> is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires. Smoke View (SMV) is

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	<p>a visualization program used to display the output of FDS and CFAST simulations.</p> <p><a href="https://www.softpedia.com/get/Programming/Other-Programming-Files/Fire-Dynamics-Simulator.shtml">https://www.softpedia.com/get/Programming/Other-Programming-Files/Fire-Dynamics-Simulator.shtml</a></p>
Geant4 ( physics)	<p>Geant4 is a toolkit for the simulation of passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science.</p> <p><a href="https://geant4.web.cern.ch/node/155">https://geant4.web.cern.ch/node/155</a></p>
GSL( GNU) scientific Library	<p>GSL is a numerical library for C and C++ programmers.</p> <p><a href="https://www.gnu.org/software/gsl/">https://www.gnu.org/software/gsl/</a></p>
SciPy	<p>SciPy (pronounced “Sigh Pie” is a Python-based ecosystem of open-source software for mathematics, science, and engineering.</p> <p><a href="https://pypi.org/project/scipy/">https://pypi.org/project/scipy/</a></p>
NCAR	<p>NCAR Graphics is a Fortran and C based software package for scientific visualization.</p> <p><a href="http://ngwww.ucar.edu/">http://ngwww.ucar.edu/</a></p>
netCDF and NCO	<p>NCO (netCDF operators) is a suite of programs designed to facilitate manipulation and analysis of self- describing data stored in the netCDF format.</p> <p><a href="http://nco.sourceforge.net/">http://nco.sourceforge.net/</a></p>
OpenCV –Open Source Computer Vision Library	<p>This is a library of programming functions mainly aimed at real-time computer vision.</p> <p><a href="https://opencv.org/about/">https://opencv.org/about/</a></p>
PETSc – Hierarchical Data Format	<p>HDF, HDF4 or HDF5 is the name of a set of file formats and libraries designed to store and organize large amounts of numerical data.</p> <p><a href="https://damask.mpie.de/Installation/HDF5">https://damask.mpie.de/Installation/HDF5</a></p>
Trilinos	<p>This is a collection of open-source software libraries intended to be used as building blocks for the development of scientific applications.</p> <p><a href="https://trilinos.github.io/about.html">https://trilinos.github.io/about.html</a></p>
NWChem	<p>Open-source High- performance computational chemistry package.</p> <p><a href="http://www.nwchem-sw.org/index.php/Main_Page">http://www.nwchem-sw.org/index.php/Main_Page</a></p>
GAMESS- General	<p>GAMESS is a general ab initio quantum chemistry package.</p>

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Atomic and Molecular Electronic Structure System	<a href="https://www.its.hku.hk/services/research/hpc/software/gamess">https://www.its.hku.hk/services/research/hpc/software/gamess</a>
PSI4	Is an open-source suite of ab initio quantum chemistry programs. <a href="http://www.psicode.org/">http://www.psicode.org/</a>

## Mathematics, statistics Application and Libraries

Program	Function
R and Rmpi	R is language and environment for statistical computing and graphics. <a href="https://wiki.rc.usf.edu/index.php/R_and_Rmpi">https://wiki.rc.usf.edu/index.php/R_and_Rmpi</a>
MATLAB	MATLAB is a high-level language and interactive environment for numerical computation, visualization, and programming. <a href="https://cimss.ssec.wisc.edu/wxwise/class/aos340/spr00/whatismatlab.htm">https://cimss.ssec.wisc.edu/wxwise/class/aos340/spr00/whatismatlab.htm</a> <a href="https://www.mathworks.com/products/matlab.html">https://www.mathworks.com/products/matlab.html</a>
NumPy	Is the fundamental package for scientific computing with python <a href="https://www.numpy.org/">https://www.numpy.org/</a>
ATLAS – Automatically Tuned Linear Algebra Software.	This provides C and Fortran interface to an efficient BLAS implementation, as well as a few routines from LAPACK. <a href="http://math-atlas.sourceforge.net/">http://math-atlas.sourceforge.net/</a>
BLAS- Basic Linear Algebra Subroutine.	BLAS is a de facto application programming interface standard for publishing libraries to perform basic linear algebra operations such as vector and matrix multiplication. <a href="http://zone.ni.com/reference/en-XX/help/371361R-01/ivanlsconcepts/basic_linear_algebra_subroutines/">http://zone.ni.com/reference/en-XX/help/371361R-01/ivanlsconcepts/basic_linear_algebra_subroutines/</a>
Boost	Is a set of libraries for the C++ programming language that provides support for tasks and structures such as linear algebra, pseudorandom number generation, multithreading, image processing, regular expressions, and unit testing. <a href="https://www.boost.org/">https://www.boost.org/</a>

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Intel Math Kernel libraries	This includes a wealth of routines to accelerate application performance and reduce development time. <a href="https://software.intel.com/en-us/mkl">https://software.intel.com/en-us/mkl</a>
FFTW – Fastest Fourier Transform in the West.	This is a software library for computing discrete Fourier transforms (DFTs) <a href="http://www.fftw.org/">http://www.fftw.org/</a>
UDUNITS	UDUNITS support conversion of unit specifications between formatted and binary forms, arithmetic manipulation of units, and conversion of values between compatible scales of measurement. <a href="https://www.unidata.ucar.edu/software/udunits/">https://www.unidata.ucar.edu/software/udunits/</a>

## Rendering, Remote Visualization and Image Manipulation

Program	Functions
RealityServer	This is a software platform for the development and deployment of 3D web services and 3D applications. <a href="https://www.migenius.com/products/onshape">https://www.migenius.com/products/onshape</a> <a href="https://www.nvidia.com/object/nvision08-RealityServer.html">https://www.nvidia.com/object/nvision08-RealityServer.html</a>
ImageMagick	This is an open-source software suite for displaying, converting, and editing raster image files. It can read and write over 200 image file formats. <a href="https://imagemagick.org/index.php">https://imagemagick.org/index.php</a>
Blender	This is a free and open-source 3D computer graphics software product used for creating animated films, visual effects, art, 3D printed models, interactive 3D applications and video games. Blender's features included 3D modeling, UV unwrapping, texturing, rigging, and skinning, fluid, and smoke simulation, particle simulation, soft body simulation, animating, match moving, camera tracking, rendering, video editing, and compositing. <a href="https://www.blender.org/">https://www.blender.org/</a>

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## Compilers and Language Tools

Program	Function
Intel C/C++ and Fortran Compilers	Intel compiler suites include C compiler, C++ Compiler, and Fortran compiler, including optimization features and multithreading capabilities: highly optimized performance libraries, and error-checking, security, and profiling tools, allowing developers to create multithreaded applications and maximize application performance, security, and reliability. <a href="https://software.intel.com/en-us/fortran-compilers">https://software.intel.com/en-us/fortran-compilers</a>
Portland Group C/C++ and Fortran Compilers	PGI compilers incorporate global optimization, vectorization, software pipelining, and shared-memory parallelization capabilities. <a href="https://pace.gatech.edu/portland-group-ccfortran-compiler">https://pace.gatech.edu/portland-group-ccfortran-compiler</a>
NVIDIA CUDA compiler	Nvidia CUDA compiler is Nvidia's CUDA compiler. NVCC separates these two parts and sends host code (the part of code which will be run on the CPU) to a C compiler, and sends the device code (the part which will run on the GPU) to the GPU. The device code is further compiled by NVCC. <a href="https://developer.nvidia.com/cuda-llvm-compiler">https://developer.nvidia.com/cuda-llvm-compiler</a>
ANTLR – Another Tool for Language Recognition.	This is a parser generator that uses LL(*) parsing. <a href="https://www.antlr.org/">https://www.antlr.org/</a>
FLTK – Fast Light Toolkit	This is a GUI library made to accommodate 3D graphics programming. <a href="https://www.fltk.org/">https://www.fltk.org/</a>
Gengetopt	This is a tool used to write command-line option parsing code for C programs. <a href="https://www.gnu.org/software/gengetopt/">https://www.gnu.org/software/gengetopt/</a>
SWIG	A tool that easily allows a developer to wrap C/C++ functions for use with scripting. <a href="http://www.swig.org/">http://www.swig.org/</a>

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## Weather Modeling and Cartographic Projections

Program	Functions
WRF –Weather Research and Forecasting	WRF model is a numerical weather prediction system. <a href="https://www.mmm.ucar.edu/weather-research-and-forecasting-model">https://www.mmm.ucar.edu/weather-research-and-forecasting-model</a>
COAMPS	The Coupled Ocean/Atmosphere Mesoscale Prediction System Developed and run by the Naval Research Laboratory in Monterey, CA, is the numerical model used for wind nowcasts and forecasts. <a href="https://www.cencoos.org/data/models/coamps">https://www.cencoos.org/data/models/coamps</a>
GRIB2 -	GRIB(GRIdded Binary or General Regularly-distributed information in Binary form) <a href="https://gdal.org/drivers/raster/grib.html">https://gdal.org/drivers/raster/grib.html</a>
PROJ	A Cartographic Projections library. <a href="https://proj.org/">https://proj.org/</a>

## Finite Element Analysis FEA, computational fluid dynamics CFD, and finite-difference time-domain FDTD Modeling

Program	Function
LS-DYNA/LS-PrePost	LS-DYNA is an advanced general-purpose multiphysics simulation software package. Its competency lies in highly nonlinear transient dynamic finite element analysis (FEA) using explicit time integration. LS-PrePost is an advanced pre and post-processor that is delivered free with LS-DYNA. <a href="https://www.lstc.com/products/ls-dyna">https://www.lstc.com/products/ls-dyna</a> <a href="http://www.lstc.com/lsp/">http://www.lstc.com/lsp/</a>
LS-OPT	LS-OPT is an optimization and probabilistic analysis program that can interface with LS-DYNA. <a href="https://www.lsoptsupport.com/">https://www.lsoptsupport.com/</a>
OpenForm -Open	OpenFOAM is a C++ toolbox for the development of customized

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Source Field Operation and Manipulation.	numerical solvers, and pre-/post-processing utilities for the solution of continuum mechanics problems, including computational fluid dynamics (CFD). <a href="https://www.openfoam.com/">https://www.openfoam.com/</a>
ANSYS HFSS	ANSYS HFSS software is the industry standard for simulating 3-D full-wave electromagnetic fields. Its gold-standard accuracy, advanced solver and computer technology have made it an essential tool for engineers designing high-frequency and high-speed electromagnetic components. <a href="https://www.ansys.com/products/electronics/ansys-hfss">https://www.ansys.com/products/electronics/ansys-hfss</a> <a href="https://www.rfglobalnet.com/doc/ansys-hfss-simulation-software-0001">https://www.rfglobalnet.com/doc/ansys-hfss-simulation-software-0001</a>
Star-CD and Star-CCM+	Star-CCM+ is CD-adapco's newest CFD software product. It uses the well-established CFD solver technologies available in STAR-CD, and it employs a new client-server architecture and object-oriented user interface to provide a highly integrated and powerful CFD analysis environment to users. <a href="https://mdx.plm.automation.siemens.com/star-ccm-plus">https://mdx.plm.automation.siemens.com/star-ccm-plus</a>
Lumerical	This is a simulation tool that implements the FDTD algorithm. <a href="https://www.lumerical.com/about-lumerical/">https://www.lumerical.com/about-lumerical/</a>
SU2	The SU2 suite is an open-source collection of C++ based software tools for performing Partial Differential Equation (PDE) analysis and solving PDE constrained optimization problems. <a href="https://su2code.github.io/docs/home/">https://su2code.github.io/docs/home/</a>
AVL FIRE	AVL FIRE is a powerful multi-purpose thermo-fluid software representing the latest generation of 3D CFD
Abaqus	DSS SIMULIA Abaqus Unified FEA product suite offers powerful and complete solutions for both routine and sophisticated engineering problems covering a vast spectrum of industrial applications. <a href="https://www.3ds.com/products-services/simulia/products/abacus/multiphysics/">https://www.3ds.com/products-services/simulia/products/abacus/multiphysics/</a>