

Scalable codes on the Blue Gene @ 11/11/07

Segment	Area	Institution / Owner	Code	Availability	Algorithm	URL
01 Classified Defense & Scientific Research						
	011 Physics					
		Argonne National Lab	QMC (Quantum Monte Carlo)	02 Proprietary	nuclear physics - uses monte-carlo simulaiton for quantum mechanics	
		Argonne National Laboratory	GFMC	01 Open Source	Bob Wiringa and Steven Pieper of Argonne, Joe Carlson of LANL, and Vijay Pandharipande of UIUC attempted an accurate calculation of the distribution of the two protons in the nucleus of 6He. They use realistic two- and three-nucleon forces	http://www.alcf.anl.gov/accomp_phys.html
		General Atomics, Wisconsin, CU-Boulder, UCLA	Nimrod	04 Community	A non-Ideal magnetohydrodynamic code. It uses finite element method. Fusion using toroidal geometry.	https://nimrodteam.org/ , http://www-unix.mcs.anl.gov/~siegela/peta-apps.htm
		IBM	QCD-IBM	02 Proprietary	developed by IBM BG/L team based on Columbia code. Using conjugate gradient method to invert Dirac matrices.	
		IPP	GENE	04 Community	Plasma physics turbulence code. Both ORB5 and GENE solve the nonlinear gyrokinetic equations pertinent to the study of transport-related instabilities and turbulence in the tokamak geometry.	
		LLNL	SPHOT	01 Open Source	Monte Carlo Photon Transport	http://www.llnl.gov/asci/purple/benchmarks/limited/sphot/
		Princeton Plasma Physics Lab	GTC (Gyrokinetic Toroidal Code)	02 Proprietary	For plasma microturbulence study, magnetic fusion code - uses particle in cell approach to solve nonlinear gyrophase-averaged Vlasov-Poisson (i.e., gyro-kinetic) equations. The code solves Vlasov 5D or 6D formulation using particle mesh m	http://w3.pppl.gov/theory/GPSC.html , http://www-unix.mcs.anl.gov/~siegela/applications.html
		USC	RXMD	02 Proprietary	Dynamics of chemically reacting mixtures	
	012 AstroPhysics					
		ASTRON	Capreole	N/A	Astrophysical hydrodynamics code. Works in one / two/ three spatial dimensions. Parallelized with MPI. Relies upon REM solver.	
		CITA	CubePM	02 Proprietary	A cubic decomposition 2-level particle mesh gravitational N-body solver that is used to simulate cosmological dark matter structure formation	www.cita.utoronto.ca , http://www.cita.utoronto.ca/~merz/
		U Chicago / ANL	Flash	04 Community	Parallel adaptive-mesh multi-physics simulation, nuclear astrophysical problems in exploding stars. Code solves the Euler equations for compressible flow and the Poisson equation for self-gravity.	http://flash.uchicago.edu/website/home/
		UCSD/SDSC	Enzo	02 Proprietary	Simulation of evolution of the early universe. This code uses hydrodynamics to simulate ordinary matter. The gravity is provided by dark matter, however.	

	013 High Res. Atmospheric/Ocean Weather & Climate					
		European Project	XHIRLAM	04 Community	weather forecasting - mesoscale	http://www.knmi.nl/onderzk/applied/am/en/am_xhr.html
		LANL/ANL/NCAR	POP (Parallel Ocean Program)	04 Community	Ocean Circulation model Solves 3d primitive equations for fluid motions on the sphere under hydrostatic and Boussinesq approximations	http://climate.lanl.gov/Models/POP/index.htm
		NCAR	HOMME (High Order Multiscale Modeling Environment)	04 Community	Climate code, part of CCSM package.	http://www.homme.ucar.edu/
		NCAR	WRF (Weather Research and Forecasting)	04 Community	A mesoscale numerical weather prediction system that features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility	http://www.wrf-model.org/
	014 Material Science					
		IBM	FDTD Nanophotonics	02 Proprietary	Finite Difference Time Domain (FDTD) nanoscience simulation, models light propagation by discretizing Maxwell's equation in time and space coordinates.	http://sunoptics.caltech.edu/~goffbo/papers/Burr_PECs_poster.pdf , http://www-unix.mcs.anl.gov/~siegela/peta-apps.htm
		LLNL	ParaDis	02 Proprietary	Parallel Dislocation Simulator, direct computation of plastic strength of materials. It tracks simultaneous motion of millions of dislocation lines.	http://www.llnl.gov/str/November05/Bulatov.html
		ORNL	LSMS (Locally Self-consistent Multiple Scattering)	01 Open Source	Solves Kohn Sham equation using weak scaling. Involves complex number matrix manipulation. It studies interaction of electrons with atoms in magnetic materials, i.e., spin polarized magnetic alloys with potential use in high capacity magnets	http://www.ccs.ornl.gov/mri/repository/LSMS/index.html
02 BioSciences						
	021 Classical Molecular Dynamics					
		CCLRC (Council for the Central Laboratory of the Research Councils)	DL-POLY	03 Commercial (ISV)	A general purpose serial and parallel Molecular Dynamics simulation package.	http://www.cse.clrc.ac.uk/msi/software/DL_POLY/
		IBM	Blue Matter	02 Proprietary	Classical Molecular dynamics code written specifically for BG by IBM Research - simulates protein folding and lipids. Study the G protein coupled receptor rhodopsin.	
		LANL	SPaSM (Scalable Parallel Short-range Molecular Dynamics)	02 Proprietary	Scalable Parallel Short-range Molecular dynamics simulation. A variety of finite-range empirical potentials are implemented including EAM & MEAM for metals, Stillinger-Weber Si/Ge, & a reactive empirical bond-order (REBO) potential for de	http://bifrost.lanl.gov/MD/MD.html , http://www-unix.mcs.anl.gov/~beckman/bluegene/SSW-Utah-2005/BGL-SSW22-LLNL-Apps.pdf
		LLNL	ddcMD (domain decomposition classical Molecular Dynamics)	02 Proprietary	Scalable, General Purpose code for Classical Molecular Dynamics simulations using highly accurate MGPT potentials. Applies to Classical Molecular Dynamics simulations, classical metals, actinides under extreme conditions.	www.llnl.gov

		LLNL	MDCASK	02 Proprietary	Atomic dynamics with Newtonian Mechanics and Electrostatics. It uses classical molecular dynamics to calculate the trajectories of atoms.	http://www.llnl.gov/asci/platforms/purple/rfp/benchmarks/limited/mdcask/
		SNL	Grasp	N/A	A scalable, general purpose code for performing classical molecular dynamics (MD) simulations. Supports a wide range of different force fields: twobody, threobody, Tersoff, EAM, REaxFF, electrostatics, charge equilibration.	http://www-unix.mcs.anl.gov/~beckman/bluegene/SSW-Utah-2005/BGL-SSW22-LLNL-Apps.pdf
		SNL	LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)	02 Proprietary	LAMMPS is a classical molecular dynamics code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, metallic, or granular, systems using a variety of force fields and bounda	http://www.cs.sandia.gov/~sjlrimp/lammmps.html ; http://www.cs.sandia.gov/~sjlrimp/lammmps/doc/Manual.html
		UCSF	Amber8 (Assisted Model Building through Energy Refinement)	03 Commercial (ISV)	Molecular mechanics simulation.	http://amber.scripps.edu
		UCSF	AMBER9	N/A	Molecular Dynamics simulation	http://amber.scripps.edu/
		UIUC/NCSA University of Washington	NAMD	01 Open Source	A parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects.	http://www.ks.uiuc.edu/Research/namd/
	022 Quantum Chemistry		Rosetta	04 Community	protein structure prediction	
		Accelrys/Castep.org	CASTEP	03 Commercial (ISV)	Quantum Mechanics-Density Functional Theory - software package which uses density functional theory to provide a good atomic-level description of materials and molecules. CASTEP can give information about total energies, forces and stresses	http://www.accelrys.com/ceius2/castep.html , http://www.tcm.phy.cam.ac.uk/castep/
		Ames/Iowa State	GAMESS (General Atomic and Molecular Electronic Structure System)-US	01 Open Source	A general ab initio quantum chemistry package.	http://www.msg.ameslab.gov/GAMESS/GAMESS.html
		IBM	CPMD (Car-Parrinello Molecular Dynamics)	01 Open Source	Ab-initio quantum molecular dynamics. A well-parallelized, plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics.	http://www.cpm.org/
		LLNL	FEQMD	02 Proprietary	First principle (quantum mechanical) molecular dynamics.	
		LLNL	Qbox	02 Proprietary	Simulations of condensed matter subject to extreme conditions. Plane wave, pseudopotential, ab-initio molecular dynamics method with Density Functional Theory (DFT).	http://www.llnl.gov/str/JanFeb06/Schwegler.html
		PWscf	CPV	01 Open Source	Part of the Quantum Espresso package - ab-initio Molecular Dynamics in the plane wave ultrasoft pseudopotential scheme.	www.pwscf.org
		QuantumBIO	Divcon Discovery Suite	03 Commercial (ISV)	Scoring application	http://www.quantumbioinc.com/

		University of Vienna & Duisburg	VASP (Vienna ab initio Simulation Package)	03 Commercial (ISV)	Ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set	http://cms.mpi.univie.ac.at/vasp/
	024 Bio Informatics					
		Boston University	GibTigs	02 Proprietary	Gibbs sampling Monte Carlo Markov chains.	
		Iowa State U	PaCE (Parallel Clustering of ESTs)	N/A	PaCE is recently developed software to cluster EST sequences on parallel or cluster computers.	www.iastate.edu
		MPI	mpiBlast-PIO	01 Open Source	A freely available open source parallelization of NCBI BLAST that segments the BLAST database and distributes it across cluster nodes, permitting BLAST queries to be processed on many nodes simultaneously.	http://mpiblast.org/
		University of Virginia	FASTA / Smith-Waterman	01 Open Source	Part of FASTA package. Compares a protein sequence to another protein sequence or to a protein database, or a DNA sequence to another DNA sequence or a DNA library.	http://fasta.bioch.virginia.edu/fasta_www2/fasta_list2.shtml
		WSTL-OS, Various-C	HMMER	01 Open Source	Sequence analysis using profile Hidden Markov Models. HMMER is a freely distributable implementation of profile HMM software for protein sequence analysis.	http://hmmerr.wustl.edu/
	025 Medical					
		ANL	PNEO Blue Brain Project	N/A	Simulation of Epiform Activity in the Neocortex to understand and fix seizures. Hodgkin-Huxley Model.	http://www-unix.mcs.anl.gov/~siegela/Presentations/Jan19_03.1.ppt
		EPFL		02 Proprietary	Neocortical Column model	
		Gene Network Sciences (GNS)	GNS	03 Commercial (ISV)	N/A	www.gnsbiotech.com
		Immunetrics	Immunetrics	03 Commercial (ISV)	N/A	Immunetrics.com
		KTH	SPLIT	02 Proprietary	Research Code for Cortex simulations.	
03 MCAD/CAE						
	031 CFD					
		ANL	PETSc-FUN3D	01 Open Source	PETSc-FUN3D is a well tuned CFD code intended to allow comparisons between the strengths and weaknesses of high-performance scientific computers and to provide insight into the performance implications of coding practices, for multicomponent	http://www-fp.mcs.anl.gov/petsc-fun3d/
		ANL	PPanel	N/A	Fluid Mechanics using boundary element method.	http://www-unix.mcs.anl.gov/~siegela/peta-apps.htm
		CERFACS	AVBP	03 Commercial (ISV)	Turbulent combustion in gas turbines, fully explicit implementation. AVBP solves the reacting Navier Stokes equations on hybrid meshes using Large Eddy Simulation.	http://www.cerfacs.fr/cfd/avbp_code.php , http://www.cerfacs.fr/cfd/
		EDF	Code_Saturne	01 Open Source	Fluid dynamics code for non compressible fluids. It is a home grown code, but the underlying mathematic algorithm is similar to StarCD.	
		Fluent / ANL	NEKTON	03 Commercial (ISV)	Fluid dynamics computer modeling tool for simulation and analysis of a wide range of coating flows - developed originally for NASA, commercialized by FLUENT. Navier Stokes solver using spectral element method.	http://www-unix.mcs.anl.gov/appliedmath/Flow/cfd.html

		Georgia Tech	DNS (Direct Numerical Simulation)	02 Proprietary	Turbulence simulation using Lagrangian method. It is Fourier pseudospectral in space and explicit, second order in time.	
		LANL/SAIC	SAGE (SAIC's Adaptive Grid Eulerian Code)	02 Proprietary	SAGE (SAIC's Adaptive Grid Eulerian) for tsunami simulation. Models for the atmosphere, seawater and ocean crust. Hydrodynamics, heat and radiation transport with adaptive mesh refinement.	www.llnl.gov
		LLNL	Miranda	02 Proprietary	Research hydrodynamics code ideal for simulating Rayleigh-Taylor and Richtmyer-Meshkov instability growth. Studies the behavior of instabilities that evolve when materials of different densities are accelerated. Can run as either a direct	www.llnl.gov
		LLNL	Raptor	02 Proprietary	Part of AMRh code development project. Multi-physics Eulerian Adaptive Mesh Refinement (AMR) code used for Astrophysics, Inertial Confinement Fusion (ICF), shock-driven instabilities and turbulence.	http://www.llnl.gov/asci/platforms/bluegene/papers/22greenough.pdf
		NASA	Overflow-2	01 Open Source	Computational fluid dynamics code developed and maintained by NASA. solves the time-dependent, Reynolds-averaged, Navier-Stokes equations (RANS) using multiple overset structured grids. It provides an alternative, cost-effective means of	http://ad-www.larc.nasa.gov/~buning/codes.html
		NASA Langley	FUN3D	04 Community	A tetrahedral vertex-centered unstructured Euler and Navier-Stokes solver for compressible and incompressible fluids. It uses pseudo-transient Newton-Krylov-Schwarz method. For turbulence, it uses the Spalart-Allamras model. Algorithms de	
		National Univ of Ireland / Galway	Ludwig	02 Proprietary	A simulator of many complex fluid based on lattice Boltzmann method.	
		NCAR/ANL	NEK5000	02 Proprietary	Solves incompressible fluid using Navier Stokes equation with spectral element method. Uses hexagonal mesh with domain decomposition. It also can solve thermal problems, thus useful for nuclear reactor core thermal hydraulics simulation.	http://www-unix.mcs.anl.gov/~siegela/peta-apps.htm
		Stanford Univ.	CDP	02 Proprietary	CFD Combustion. Unstructured Large Eddy Simulation (LES) code, designed to integrate with the block-structured TFLO code and support the centers overarching goal of full engine simulations. CDP can also be run as a standalone LES code.	http://www.stanford.edu/group/cits/research/combustor/cdp.html
		University of Wyoming/NASA, Prof D. Mavriplis	NSU3D	02 Proprietary	Mixed Element Unstructured Grid Solver with Edge-Based Data-Structure, Roe-Rieman Solver (Matrix Dissipation). Solution Technique: Agglomeration Multigrid, Line / Point(Jacobi) Preconditioning, Optional Low Mach Number Preconditioning.	
	032 CAE/Crash					

		Allied Engineering Corporation	ADVC	N/A	An implicit based structural FEA system developed for parallel computation. They developed the CGCG (Coarse Grid based Conjugate Gradient) method.	http://www.alde.co.jp/english/
	034 CAE/EDA					
		Petersen Advanced Lithography	EMF3	03 Commercial (ISV)	Semiconductor lithography simulation tool that allows modeling semiconductor mask effects. EMF3 is a large area full Maxwell Equation solver.	www.advlitho.com
04 Petroleum						
	041 Reservoir Simulation					
		University of TX at Austin	IPARS (Integrated Parallel Accurate Reservoir Simulator)	04 Community	IPARS models multiphase, multiphysics flow in porous media.	http://www.ticam.utexas.edu/Groups/SubSurfMod/ACT1/ipars.html
	042 Seismic					
		SDSC	AWM	N/A	Finite difference method for Earthquake simulation.	
		Tsunami Development	PSTM / PSDM / Ray Tracer	03 Commercial (ISV)	Pre-Stack Time and Depth Migration (PSTM and PSDM)	www.tsunamidevelopment.com
		U Houston	MOSRP (Mission-Oriented Seismic Research Program)	04 Community	Mission-Oriented Seismic Research Program: multiple projects univ in collaboration w/ industrial partners	www.mosrp.uh.edu
		N/A	Hercules	02 Proprietary	The overall goal of Hercules is to assess seismic hazard by computer simulation of earthquake scenarios. It has multiple spatial scales, multiple temporal scales, highly irregular basin geometry, highly heterogeneous soils material proper	
06 Other						
	061 Other					
		SmartOps	MIPO (Multistage Inventory Planning & Optimization)	03 Commercial (ISV)	Supply chain optimization software. Multistage Inventory Planning & Optimization software solution for dynamic network design	www.smartops.com
07 Libraries and Tools						
	071 Libraries					
		ANL	PETSc (The Portable, Extensible Toolkit for Scientific Computation)	01 Open Source	PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled with partial differential equations. MPI-based.	http://www-unix.mcs.anl.gov/petsc/petsc-2/ http://www-unix.mcs.anl.gov/petsc/petsc-as/developers/index.html
		Free Math Libraries	ATLAS,BLAS,LAPACK	01 Open Source	ATLAS: Automatically Tuned Linear Algebra Software. Provides C and Fortran77 interfaces to a portably efficient BLAS implementation, as well as a few routines from LAPACK. BLAS: Basic Linear Algebra Subprograms. For performing basic vector	http://directory.fsf.org/atlas.html http://www.netlib.org/blas/ http://www.netlib.org/lapack/
		IBM	ESSL	03 Commercial (ISV)		
		OakRidge/U Tenn	ScaLAPACK	01 Open Source	ScaLAPACK is a library of high-performance linear algebra routines for distributed-memory message-passing MIMD computers and networks of workstations. The ScaLAPACK routines are based on block-partitioned algorithms in order to minimize th	http://www.netlib.org/scalapack/

		Pacific Northwest Libraries	Global Arrays	N/A	Parallel APIs for matrix operations	http://www.emsl.pnl.gov/docs/global/ga.html
		University of Vienna	FFTW	01 Open Source	FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data (as well as of even/odd data, i.e. the discrete cosine/sine transforms	www.fftw.org
	072 Tools					
		Altair	PBSPro	03 Commercial (ISV)	Job Scheduler	http://www.altair.com/software/pbspro.htm
		ASPEED Software	ACCELERANT	03 Commercial (ISV)	Parallelization SW and (multiprocessor) porting services	www.aspeed.com
		Cluster File Systems Inc.	LUSTRE	03 Commercial (ISV)	global parallel file system	http://www.clusterfs.com/
		Condor Project - U Wisconsin	Condor-HTC	01 Open Source	Open source Cluster, Grid and Workflow schedulers, part of the Condor Project from U Wisconsin. Will support both High Throughput Computing (HTC) and High Performance Computing (HPC w/ MPI) modes on the BG.	http://www.cs.wisc.edu/condor/
		IBM	GPFS	03 Commercial (ISV)	IBM's Global Parallel File System	
		IBM	HPC Toolkit	N/A	performance monitor	
		IBM	LoadLeveler	03 Commercial (ISV)	Job Scheduler	http://www-03.ibm.com/systems/clusters/software/loadleveler/
		NIC, Juelich, Germany	KOJAK (Kit for Objective Judgment and Automatic Knowledge)	01 Open Source	A Kit for Objective Judgment and Automatic Knowledge-based detection of bottlenecks. A performance analyzer.	http://www.fz-juelich.de/zam/kojak/
		Platform Computing	LSF	03 Commercial (ISV)	Job Scheduler	www.platform.com
		TotalView Technologies	Total View	03 Commercial (ISV)	parallel debugger	http://www.etnus.com/TotalView/
		University of Oregon	TAU / KTAU	N/A	TAU (Tuning and Analysis Utilities) is a portable profiling and tracing toolkit for performance analysis of parallel programs written in Fortran, C, C++, Java, Python. KTAU: Kernel Tuning and Analysis Utilities is a toolkit for profiling	http://www.cs.uoregon.edu/research/ktau/home.php
	08 Benchmarks					
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		Benchmark	GUPS (HPC Challenge)	01 Open Source	HPC Challenge benchmark, tests random memory access.	http://icl.cs.utk.edu/projectsfiles/hpcc/RandomAccess/
		Benchmark	HPL - LINPACK	01 Open Source	Industry Standard Benchmark	http://www.netlib.org/benchmark/hpl/
		DARPA	HPC Challenge	01 Open Source	Industry Standard Benchmark suite	http://icl.cs.utk.edu/hpcc/
		LANL	Sweep3D	01 Open Source	ASCI benchmark: 3D Discrete Ordinates Neutron Transport. It solves a 1-group time-independent discrete ordinates (Sn) 3D cartesian (XYZ) geometry neutron transport problem. The XYZ geometry is represented by an IJK logically rectangular grid	http://www.llnl.gov/asci_benchmarks/asci/limited/sweep3d/asci_sweep3d.html
		LLNL	SPPM (Simplified Piecewise-Parabolic Method)	01 Open Source	CFD benchmark - The SPPM benchmark solves a 3D gas dynamics problem on a uniform Cartesian mesh, using a simplified version of the PPM (Piecewise Parabolic Method) code -- hence the "s" for simplified. The code is written to simultaneously	www.llnl.gov, http://www.llnl.gov/asci_benchmarks/asci/limited/ppm/asci_sppm.html
		LLNL	UMT2K	01 Open Source	Benchmark - 3D deterministic multigroup photon transport code for unstructured meshes.	http://www.llnl.gov/asci/purple/benchmarks/limited/umt/umt1.2.readme.bm.html