Available Software on Altamira Supercomputer

Compilers, Interpreters and Development Utils

Name	Version: Default(Others)	Description
ANT	1.8.4	Apache Ant is a Java library and command-line tool whose mission is to drive processes described in build files as targets and extension points dependent upon each other.
CMAKE	2.8.11(also 3.9.0, 3.3.2, 2.6.0)	Utilidad make
DDD	3.3.12	Data Display Debugger (interfaz a debugger)
gcc	4.6.3 (also 6.1.0, 5.2.0, 5.1.0, 4.9.2, 4.7.2, 4.6.4 y 3.4.6)	Gnu C++, Fortran
GHC	7.4.2	Glasgow Haskell Compiler
GIT	1.9.5 (also 2.6.1)	Version Control System
HASKELL PLATFORM	2012.2.0.0	Glasgow Haskell Compiler + Basic Haskell Libs
INTEL	2018	INTEL Parallel Studio 2018
JAVA	1.6u33(also jdk, 1.7u71, 1.8u91)	
LLVM	3.1	Open Source C/C++ (incl. clang)
PERL	5.16.1	
PYTHON	2.7.3 (also 3.7.4,3.5.4, 3.4.3, 2.7.9, 2.7.5, 2.7.12, 2.7.11, 2.7.10	
RUBY	2.2.1 (4.9.2)	
SWIG	2.0.1 (2.0.4)	Simplified Wrapper and Interface Generator

Development Libraries

Name	Version: Default (Others)	Description
ARGTABLE	2.13	ANSI C library for parsing GNU style command line options with a minimum of fuss
ASTRON	2014	IDL Astronomy Users Library
BEAGLE	r1090	A high-performance library that can perform the core calculations at the heart of most Bayesian and Maximum Likelihood phylogenetics packages. It can make use of highly-parallel processors such as those in graphics cards (GPUs)
BOOST	1.52.0	Boost provides free peer-reviewed portable C++ source libraries
CANTERA	2.2.0(also 2.2.1)	Open-source collection of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and transport processes
CGIS	4.1	
CLASS	Nov2011	
CUDA	4.2.9(also 4.0.17, 7.0.28, 7.5.18)	a parallel computing platform and programming model to exploit the power of graphics processing unit (GPU)
EIGEN	3.8.2	C++ template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms.
GDAL	1.9.2	is a translator library for raster geospatial data formats
GSL	1.15 (1.15 (also 1.15 INTEL, 1.5_ICC, 2.3)	GNU Scientific Library (GSL) is a numerical library for C and C++ programmers
HDF5	1.8.10 (also 1.8.10INTEL, 1.8.16, 1.8.8_ICC)	HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data

IGRAPH	0.7.1	Collection of network analysis tools with the emphasis on efficiency, portability and ease of use. igraph is open source and free. igraph can be programmed in R, Python and C/C++
LAPACK	3.4.1	Linear Algebra PACKage
LIBTOOL	2.4.2	Generic library support script. Libtool hides the complexity of using shared libraries behind a consistent, portable interface.
LUAJIT	2.0	A Just-In-Time Compiler for Lua.
MPFIT	1.3	A MINPACK-1 Least Squares Fitting Library in C
MPICH	3.0.4 (also 3.0.4_ICC)	A high performance and widely portable implementation of MPI standard.
MVAPICH2	2.0 (also 2.1rc1, 2.2)	MPI-3 over OpenFabrics-IB, OpenFabrics-iWARP, PSM, uDAPL and TCP/IP
NETCDF	4.2.1.1 (also 4.1.3, 4.4.0 and fortran 4.4.3)	NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.
OPENBLAS	0.2.15	Optimized BLAS library based on GotoBLAS2 1.13 BSD version
OPENMPI	1.8.3(also 4.0.1, 1.8.4rc1, 1.8.3_ICC,1.6.5,1.6.3_ICC, 1.4.5)	Open source MPI-2 implementation that is developed and maintained by a consortium of academic, research, and industry
PAPI	5.4.0(also 5.0.1)	The Performance API (PAPI) project specifies a standard application programming interface (API) for accessing hardware performance counters available on most modern microprocessors.
PROJ4	4.8.0	Cartographic Projections library
QT4	4.8.5	Cross-platform application development framework for desktop, embedded and mobile

Applications

General

Name	Version: Default (Others)	Description
ANSYS	2019R3	CFD simulation package for internal combustion engines
MATLAB	R2019b	Lenguaje de alto nivel y un entorno interactivo para el cálculo numérico, la visualización y la programación. VERSION EN PARALELO.
SAGE	5.3 (also 6.4.1)	Open source alternative to MATLAB
R	2.15.1 (also 3.2.3, 3.2.1)	Free software environment for statistical computing and graphics. VERSION EN PARALELO

High Energy & Nuclear Physics

Name	Version: Default (Others)	Description
ROOT	5.34.01 (also 5.34.17)	An object oriented framework for large scale data analysis developed at CERN. VERSION EN PARALELO: PROOF
CMS SW		Software setup for the CMS collaboration at CERN

Quantum Models for Atoms and Molecules

Name	Version: Default (Others)	Description
SIESTA	3.1 (also 4.0)	A method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.
CPMD	3.15.1	Car-Parrinello Molecular Dynamics: An ab initio Electronic Structure and Molecular Dynamics Program

DL_POLY	2.20	a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory
LAMMPS	22Feb13	a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.
VASP	**5.4.4_INTEL** 5.3_INTEL	The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

Computing Science

Name	Version: Default (Others)	Description
EXTRAE	2.3	is a dynamic instrumentation package to trace programs compiled and run with the shared memory model (like OpenMP and pthreads), the message passing (MPI) programming model or both programming models (different MPI processes using OpenMP or pthreads within each MPI process)

Bio

Name	Version: Default (Others)	Description
MPIBLAST	1.6.0	open-source, parallel implementation of NCBI BLAST. BLAST finds regions of similarity between biological sequences.
GPU-BLAST	1.1	an accelerated GPU version of the popular NCBI-BLAST.
BLAT	35:: The BLAST-Like Alignment Tool	
MrBayes	3.2.1	a program for Bayesian inference and model choice across a wide range of phylogenetic and evolutionary models
BEAST	1.7.5	cross-platform program for Bayesian MCMC analysis of molecular sequences. Uses BEAGLE.
MIRA	3.4.0.1	whole genome shotgun and EST sequence assembler for Sanger, 454, Solexa (Illumina), IonTorrent data and PacBio (the later at the moment only CCS and error-corrected CLR reads).
BEDTOOLS	2.17.0	allow one to address common genomics tasks such as finding feature overlaps and computing coverage.
BEST	2.3.1	a phylogenetics program to estimate the joint posterior distribution of gene trees and species tree using multilocus molecular data that accounts for deep coalescence but not for other issues such as horizontal transfer or gene duplication
BIOPERL	1.6.1	a community effort to produce Perl code which is useful in biology.
NETLOGO	5.3(also 5.2.1)	
PAML	4.6	package of programs for phylogenetic analyses of DNA or protein sequences using maximum likelihood.
PARTITIONFINDER	1.0.1	Free open source programs for selecting best-fit partitioning schemes and models of molecular evolution for nucleotide and amino acid alignments.
PICARD_TOOLS	1.79	Java-based command-line utilities that manipulate SAM (Sequence Alignment/Map) files, and a Java API (SAM-JDK) for creating new programs that r&w SAM files
PINDEL	0.2.4d	detects breakpoints of large deletions, medium sized insertions, inversions, tandem duplications and other structural variants at single-based resolution from next-gen sequence data.
BOWTIE	2.0.2	an ultrafast, memory-efficient short read aligner. It aligns short DNA sequences (reads) to the human genome at a rate of over 25 million 35-bp reads per hour.
PROTTEST	3.2	bioinformatic tool for the selection of best-fit models of aminoacid replacement for the data at hand.
PhyML	20120412	estimates maximum likelihood phylogenies from alignments of nucleotide or amino acid sequences.

BWA	0.6.2	for aligning sequencing reads against a large reference genome (e.g. human genome).
PhyloBayes	3.3e	is a Bayesian Monte Carlo Markov Chain (MCMC) sampler for phylogenetic reconstruction
RAxML	7.3.1	implements the popular RAxML search algorithm for maximum likelihood based inference of phylogenetic trees. It uses a radically new MPI parallelization approach that yields improved parallel efficiency, in particular on partitioned multi-gene or whole-genome datasets.
FASTQC	0.10.1	A quality control tool for high throughput sequence data.
SAMTOOLS	0.1.18 (also 1.3 and 1.5)	provide various utilities for manipulating alignments in the SAM format, including sorting, merging, indexing and generating alignments in a per-position format.
GATK	2.2-8	The Genome Analysis Toolkit or GATK is a software package developed at the Broad Institute to analyse next-generation resequencing data.
SOAPdenovo	1.05	novel short-read assembly method that can build a de novo draft assembly for the human-sized genomes. The program is specially designed to assemble Illumina GA short reads.
HMMER	3.0 (also 2.3.2-MPI-0.92, GPU-0.92)	is used for searching sequence databases for homologs of protein sequences, and for making protein sequence alignments. It implements methods using probabilistic models called profile hidden Markov models (profile HMMs)
TOPHAT	2.0.6	is a fast splice junction mapper for RNA-Seq reads. It aligns RNA-Seq reads to mammalian-sized genomes using the ultra high-throughput short read aligner Bowtie and then analyzes the mapping results to identify splice junctions between exons.
TRINITY_RNA_SEQ	r2012-06-08	implements a novel method for the efficient and robust de novo reconstruction of transcriptomes from RNA-seq data.
INTERPROSCAN	5-RC4	allows you to scan your sequence for matches against the InterPro collection of protein signature databases.
JMODELTEST	2.1.1	a tool to carry out statistical selection of best-fit models of nucleotide substitution