

Outline

- Current state of test farm (update since 2022)
- abinit-fallbacks 10.0 : last versions of all fallbacks
- Benchmarks
- Build systems : autotools and cmake

Finally, we have successfully migrated to buildbot version 3 !

<https://buildbot.abinit.org/#/builders>

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Builder Name		Builds	Tags Workers
__Janitor			4
abiref_gnu_9.5_sdebug		766 765 764 763 762 761 760 759 758 757 756 755 754 753 752	night openblas gnu fast ref 7
abiref_intel_19.1_mpic		446 445 444 443 442 441 440 439 438 437 436	mkl intel night mpich 7
alps_gnu_9.3_openmpi		729 728 727 726 725 724 723 722 721 720 719 718 717 716	openmpi night openblas gnu fast 10
alps_gnu_9.3_serial		615 614 613 612 611 610 609 608 607 606 605 604 603	openmpi night openblas gnu fast 10
alps_intel_21.4_elpa		455 454 453 452 451 450 449 448 447	mkl intel night mpich fast 10
alps_nag_7.1_openmpi		441 440 439 438 437 436 435 434 433	openmpi night slow nag 10
atlas_intel_18.0_openmpi		450 449 448 447 446 445 444 443 442	openmpi mkl intel night fast 6
atlas_intel_19.1_bdir		434 433 432 431 430 429 428 427 426	mkl intel night mpich 6
bob_gnu_13.2_openmp		316 315 314 313 312 311 310 309 308	night gnu serial atlas 3
buda2_gnu_8.5_cuda			openmpi mkl gnu fast oonly check 2
eos_gnu_13.2_openmpi			openmpi gnu newbot scalapack 1
eos_nvhp_23.11_elpa			openmpi fast nvhp newbot elpa cuda12.3 gpu 1
eos_nvhp_23.1_elpa		370 369 368 367 366 365 364 363 362	openmpi night fast nvhp elpa gpu 1
eos_nvhp_23.9_elpa		387 386 385 384 383 382 381 380 379 378 377	openmpi night fast nvhp elpa cuda12.2 gpu 1
eos_nvhp_23.9_hpc			openmpi fast nvhp newbot cuda12.2 hpc gpu 1

Name	Brand	CPU / Freq (Ghz)	# cores (#TH)	RAM Gb	OS
abiref	HP DL360 G9	Xeon E5-2670v3 / 2.3	2 x 12 (48)	32	CentOS 7.9
alps	HP DL360 G10	Xeon Gold 6230 / 2.1	2 x 20 (80)	64	CentOS 8.3
atlas	Supermicro	Xeon E5-2623v4 / 2.6	2 x 4 (16)	64	CentOS 7.9
bob	Dell R430	Xeon E5-2603v3 / 1.60	2 x 6 (12)	8	Fedora 39
buda2*	Supermicro	Xeon Silver 4110 / 2.7	2 x 8 (32)	16	CentOS 7.8
eos*	Dell R7525	AMD EPYC 7643 / 2.3	2 x 48 (192)	256	Ubuntu 22.04
higgs	HP DL 360 G8	Xeon E5-2440 / 2.4	2 x 6 (24)	32	Ubuntu 18.04
minimac	Apple Mac Studio	M1 Ultra / 3.23	20 (16+4)	64	macOS 14.5
scope	HP DL385 G10	AMD EPYC 7502 / 2.5	2 x 32 (128)	96	Ubuntu 18.04
ubu	HP DL360 G9	Xeon E5-2670v3 / 2.3	2 x 12 (48)	32	Ubuntu 16.10

* buda2 is equipped with 3 GPU cards : 2 x K40c and TITAN V

* eos is equipped with 2 GPU cards : 2 x Nvidia A30

Name	Compiler	MPI	MATH	misc
abiref_gnu_9.5_debug	GNU 9.5	OpenMPI 4.0.3	OpenBLAS 0.3.7	many services
abiref_intel_19.1_mpich	intel 19.1	MPICH 3.3.1	mkl 2020	scalapack
alps_gnu_9.3_openmpi	GNU 9.3	Open MPI 4.0.4	OpenBLAS 0.3.10	Reference
alps_gnu_9.3_serial	GNU 9.3		OpenBLAS 0.3.10	Ref for serial
alps_intel_21.4_elpa	oneAPI 21.4	intel mpi	mkl 2021.4	elpa 2020.11
alps_nag_7.1_openmpi	NAG 7.1	Open MPI 4.1.2	NetLib 3.9	
atlas_intel_18.0_openmpi	INTEL 18.0	Open MPI 3.0.1	mkl 2018	
atlas_intel_19.1_bdir	INTEL 19.1	Open MPI 3.3.2	mkl 2019	build/ dir
bob_gnu_13.2_openmp	GNU 13.2		atlas 3.10	OpenMP n=2
eos_nvhpc_23.1_elpa	nvhpc 23.1	Open MPI 3.0.5		cuda 12.2
eos_nvhpc_23.9_elpa	nvhpc 23.9	Open MPI 4.1.2		cuda 12.2
higgs_intel_19.0_serial	INTEL 19.0		mkl 2019	
scope_gnu_12.2_mpich	GNU 12.2	MPICH 4.0.3	OpenBLAS	memory leak
scope_gnu_10.2_parallel	GNU 10.2	MPICH 3.3.2	OpenBLAS	Ref for tparallel_24
scope_gnu_13.2_dep	GNU 13.2	MPICH 4.1.2	OpenBLAS	check dependency
scope_gnu_12.2_abipy	GNU 12.2	MPICH 4.0.3	OpenBLAS	check abipy
ubu_gnu_9.2_openmpi	GNU 9.2	Open MPI 4.0.2	mkl 11.3	
ubu_intel_16.0_mpich	INTEL 16.0	MPICH 3.3.2	mkl 11.3	BigDFT
ubu_intel_16.0_openmp	INTEL 16.0		mkl 11.3	OpenMP n=2

nightly			
Name	Compiler	MPI	MATH
abiref_gnu_9.5_debug	GNU 9.5	OpenMPI 4.0.3	OpenBLAS 0.3.9
<ul style="list-style-type: none"> ○ checks build system with less used options (e.g. openmp, exports, cclock) ○ checks doc in sources (ROBODoc) ○ tests “make distcheck” (tarball creation) ○ checks 15 abirules (rules for developers) (for ex: “Unused variable”, “Unused dummy argument”, “Nonstandard type declaration”, ...) ○ checks 10 buildsys (“check-build-examples”, “check-cpp-options”, “check-libpaw”, ...) ○ checks to find the broken links in docs with linkchecker 			

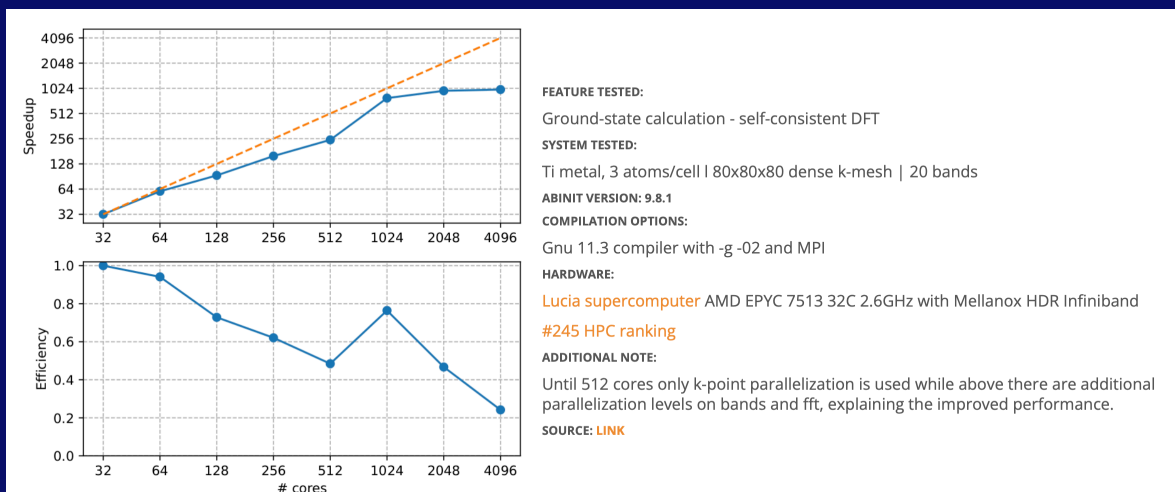
odonly				
Name	Compiler	MPI	MATH	misc
higgs_gnu_12.3_cov	GNU 12.3	MPICH 4.1.2	MKL2019/FFTW3	coverage + BigDFT
scope_gnu_10.2_s64	GNU 10.2	MPICH 3.3.2	OpenBLAS 0.3.10	tutoparal with np=64
buda2_gnu_8.5_cuda	GNU 8.5	Open MPI 3.1.4	mkl 2017/magma	

- GNU <= 7 is no longer supported

current versions	next versions*
[9.8] atompaw = 4.2.0.2 bigdft = abinit-1.7.1.30 hdf5 = 1.10.8 libpsml = 1.1.12 libxc = 6.0.0 lapack = abinit_6.10 netcdf4 = 4.9.0 netcdf4_fortran = 4.6.0 wannier90 = 3.1.0 xmlf90 = 1.5.6	[10.0] atompaw = 4.2.0.3 bigdft = abinit-1.7.1.30 hdf5 = 1.14.4-2 libpsml = 2.0.1 libxc = 6.2.2 lapack = abinit_6.10 netcdf4 = 4.9.2 netcdf4_fortran = 4.6.1 wannier90 = 3.1.0 xmlf90 = 1.6.3

* tested with beuken/develop/4252a3da with eos_gnu_13.2_openmpi

<https://www.abinit.org/benchmarks>



SOURCE : [LINK](https://github.com/abinit/abinit_assets/tree/main/abinit_web_site/benchmarks) -> https://github.com/abinit/abinit_assets/tree/main/abinit_web_site/benchmarks

abinit / abinit_assets Public

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Files

main

Go to file

- abinit_build
- abinit_package
- abinit_web_site
 - benchmarks
 - Abinit-GPU2023.png
 - GPU-Jun2023.png
 - README.md

















abinit_assets / abinit_web_site / benchmarks

jmbeuken Add files via upload 8b148ba · 3 weeks ago History

Name	Last commit message	Last commit date
..		
benchmark_GPU_CPU_gfortran11.2.tar	Add files via upload	3 weeks ago
benchmark_GPU_CPU_nvhpc22.11.tar	Add files via upload	3 weeks ago
benchmark_Ti_dense_kmesh.tar	Introduce a structure for this abinit_asset repo.	last year
benchmark_defect_supercell.tar	Introduce a structure for this abinit_asset repo.	last year

abinit_assets/abinit_web_site/benchmarks/benchmark_Ti_dense_kmesh.tar

content of the tar file :

Name	Kind	^
▼  n_cpus_32	Folder	
 run.abi	Document	
 run.abo	Document	
 run.log	Log File	
>  n_cpus_64	Folder	
>  n_cpus_128	Folder	
>  n_cpus_256	Folder	
>  n_cpus_512	Folder	
>  n_cpus_1024	Folder	
>  n_cpus_2048	Folder	
>  n_cpus_4096	Folder	
>  pseudos	Folder	
 Results.ipynb	Document	
 structure.cif	Document	
 Scaling.pdf	PDF Document	
 README	Plain Text	

-> can rerun tests to compare

autotools and cmake

AUTOCONF

- improved the build system :
 - better detection of compiler : consequently, simplification and even, deletion of the ac9 file
 - > for examples, on lucia with cray compiler and on lemaitre4 with gnu
 - improved OpenMP management (MT)
 - better management of FCFLAGS, FCFLAGS_EXTRA and FCFLAGS_OPENMP (MT, MV, YP)
- Autoconf 2.69 -> update to 2.71 : remove "Obsolete Macros"
(done on eos with beuken/develop branch)
not yet in prod : need to update Autoconf on all builders

CMAKE

- <https://docs.abinit.org/installation/#how-to-build-abinit-with-cmake>

```
cd $(ABINIT_TOPLEVEL_SOURCE)
# step 1: cmake configure
cmake -S . -B _build/cmake
# step 2: cmake build using 6 threads
cmake --build _build/cmake -j 6
```

no success yet compiling with cmake