Building and installing ABINIT A matter of collaborations

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- Make DFT software usable by industry
- Contribute directly to open-source packages
- Train researchers & engineers in atomistic simulations
- Create synergies between universities and companies

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We hire!

Simune is looking for a developer, If interested please contact:

careers@simuneatomistics.com



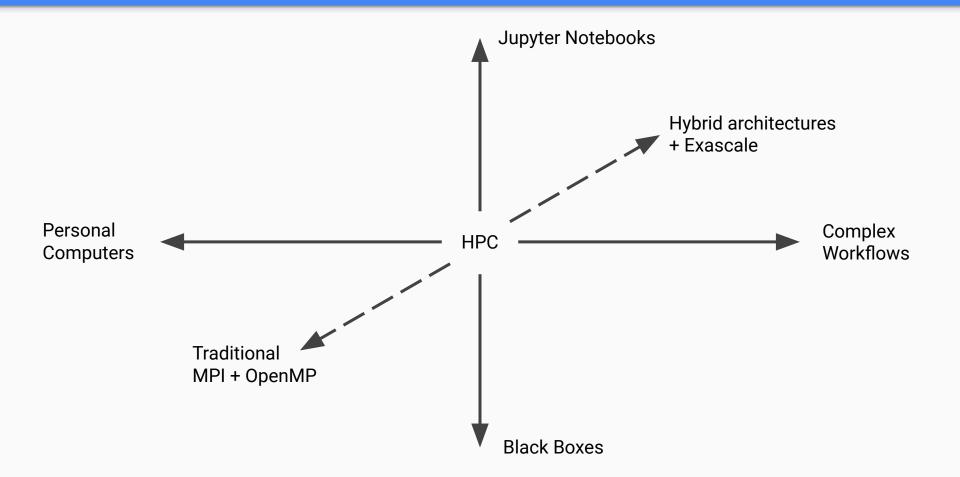


ABINIT over time, seen from the build system



Focus on compilers, automation, portability

2013-Now: Multidimensional polarisation



Impact on the build system

Requirements: support at the same time ...

- Beginner end-users with laptops and highly-automated frameworks with server farms
- Sliced calculations with high verbosity and wrapped highly-optimised black-box runs
- Traditional parallelism and mixes of OpenMP, MPI, GPUs, FPGAs, ..., on new architectures

- + A myriad of intermediate cases
- + Remember the developers!

Addressing the combinatorial explosion

- Minimum number of generic user interfaces for build systems
- Architectural layering: low-level and shareable vs. high-level and specific
- Higher modularity: libraries, source code, data flow
- Comprehensive automation strategies
- Multiple paths to multiple solutions: fallbacks, ESL Bundle, EasyBuild, Spack, ...

Common denominator

Must be based on multilateral

COLLABORATIONS

Let's build ABINIT!

Who builds ABINIT?

Profiles

- End users
- Developers
- Maintainers & Testers
- Scripts & automated frameworks

Sectors

- Education (Students & Teachers)
- HPC
- Academic Research
- Industrial Research + R&D

Workflow

- Autotools trilogy: configure, make, make install
- Optionally: make check before make install
- Most critical step: configure
 - Adapt the build to the user's computer
 - Help beginners without hindering experts
 - Provide hints when something goes wrong
 - Communication through command-line options
 - Quick-and-dirty help with dependencies: ABINIT Fallbacks

Configure options (details on Friday)

• Conventions

- --enable-feature: internal switches of ABINIT, only yes or no
- --with-package: external dependencies and their behaviors, can be yes, no, or a path

• Linear algebra

- --with-linalg: where to look for libraries, or let the build system decide if omitted
- --with-linalg-flavor: what kind of libraries to look for, e.g. Netlib or MKL
- If not sufficient, can be overridden by e.g. LINALG_LIBS="..."
- Interacts with --with-mpi option (automated): decide whether to look for ScaLAPACK
- Influences which values --with-fft-flavor can take
- Internally: complex heuristic to cover as many configurations as possible

Collaboration between expertise levels

• Beginner

- Run configure without command-line option
- Gather hints for missing dependencies
- Get help from more expert users (direct, forum, documentation)
- Use documented configuration template: ~abinit/doc/build/config-template.ac9

• Intermediate

- Use command-line options to tune *configure*
- Fine-tune config file with experts (direct, forum, documentation)
- Help beginners (direct, forum, documentation)

• Expert

- Use environment variables to tune *configure*
- Help intermediate users/developers and beginners (direct, forum, documentation)

All:

Report problems, at least on Forum!

Beyond the build system

Collaborations within the community

Electronic Structure library: https://esl.cecam.org/

- On Gitlab: <u>https://gitlab.com/ElectronicStructureLibrary</u>
- ESL Bundle: Python-based meta-build system
- ESL Demonstrator: understand code needs
- ESCDF: exchange data between DFT codes

🦊 GitLab Projects ~ G	roups 🗸 More 🖌			
esi-bundle	🥏 Electronic Structure Library > 💮 esl-bundle > Releases			
Project overview				
Details	0.6.1-1			
Activity				
Releases	✓ Assets 4			
Repository	 Source code (zip) Source code (tar.gz) Source code (tar.bz2) 			
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Packages & Registries				

HPC-oriented collaborations

- Build frameworks
 - EasyBuild 0
 - Spack 0
- Containerised builds
 - Docker (CI, CD, distribution)
 - Singularity (HPC) 0
- Collaborations
 - **ESL & EasyBuilders** 0
 - FSL & MOLSSI \bigcirc
 - CoEs: E-CAM, MaX, POP, ... 0



EasyBuild docs EasyBuild @ PyPi EasyBuild EasyBuild @ GitHub @ YouTub

EasyBuild is a software build and installation framework that allows you to manage (scientific) software on High Performance Computing (HPC) systems in an efficient way.

A full list of supported software packages is available here.

Latest news

- 20210409 EasyBuild v4.3.4 is available; see also the release notes
- 20210129 Recordings of all talks at the 6th EasyBuild User Meeting are now available
- 20210125 EasyBuild has been selected as the primary software installation tool for LUMI!

EasyBuild Tech Talks

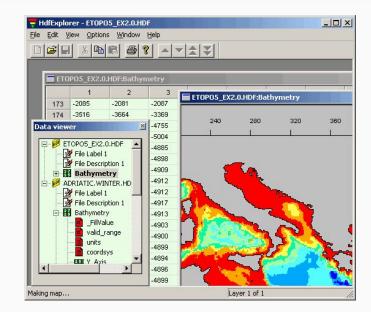
- (Mon Mar 29th 2021) FlexiBLAS
- Martin Köhler, Max Planck Institute Magdeburg
- (Wed Sept 30th 2020) Yes! You Can Run Your Software on Arm Chris Edsall, Univ. of Bristol
- (Jun-Aug 2020) The ABCs of Open MPI Jeff Squyres (Cisco, Open MPI) & Ralph Castain (Intel, Open MPI, PMIx)

Documentation

Read the fine manual (RTFM!) at https://docs.easybuild.io.

Data-oriented collaborations

- Text-based files
 - Input files: $FDF \Rightarrow LibFDF$
 - NC pseudos \Rightarrow PSML, XMLF90, LibPSML
 - PAW datasets \Rightarrow PAW-XML, LibPAW
 - JSON, YAML \Rightarrow Python, BigDFT
- Binary files
 - HDF5, NetCDF
 - ESCDF, LibESCDF (under development)



Current plans

- Improve error messages and hints provided by configure
- Improve support for Intel OneAPI + FFTW side effects
- Improve HDF5 and NetCDF detection
- Unify build-system UIs of libraries, utilities & generators (AtomPAW upcoming)
- Develop a testing & templating framework for build systems
- Get rid of the circular dependency between BigDFT & ABINIT?

Thank you for your time!