The build system of Abinit 6: on the road again

Yann Pouillon

Nano-Bio Spectroscopy Group

Facultad de Químicas, Universidad del País Vasco UPV/EHU

Donostia-San Sebastián, Spain

Han-sur-Lesse, Belgium — 2011/04/11

Summary of previous episodes

Abinit 5 $\longrightarrow$ Abinit 6

"Do not let what you are stay in the way of what you want to become."

- Break backward-compatibility with Abinit 4
- Modularize build system (subsystems)
- Create build-system test suite
- Properly document build-system UI
- Take packagers into account

Build-system test suite

- Condition: all tests runnable before the build

- 01–09: check status of source tree
- 10–19: basic build-system consistency
- 20–29: enforce good maintenance practices

- 01: Bazaar conflict markers
- 02: source line lengths
- 03: one include of config.h in each source file
- 10: consistency of configuration
  $\longrightarrow$ environment.conf + options.conf + build-config.ac
- 11: consistency of build examples (test farm)
- 12: consistency of CPP options
- 20: forbidden flags in build examples (test farm)
  $\longrightarrow$ e.g. no optimizations in FCFLAGS_EXTRA

Current issues

TODO

1. Slow down source package size growth (Fatboy Abinit^{TM})
2. Accept more external non-integrable dependencies
3. Handle more complex plugins (libraries, binaries, data)
4. Permit more complete use of plugin capabilities
5. Improve detection of external dependencies for packaging
6. Integrate continuously with test farm
7. Address evolving programming practices & requirements

From plugins to connectors/fallbacks

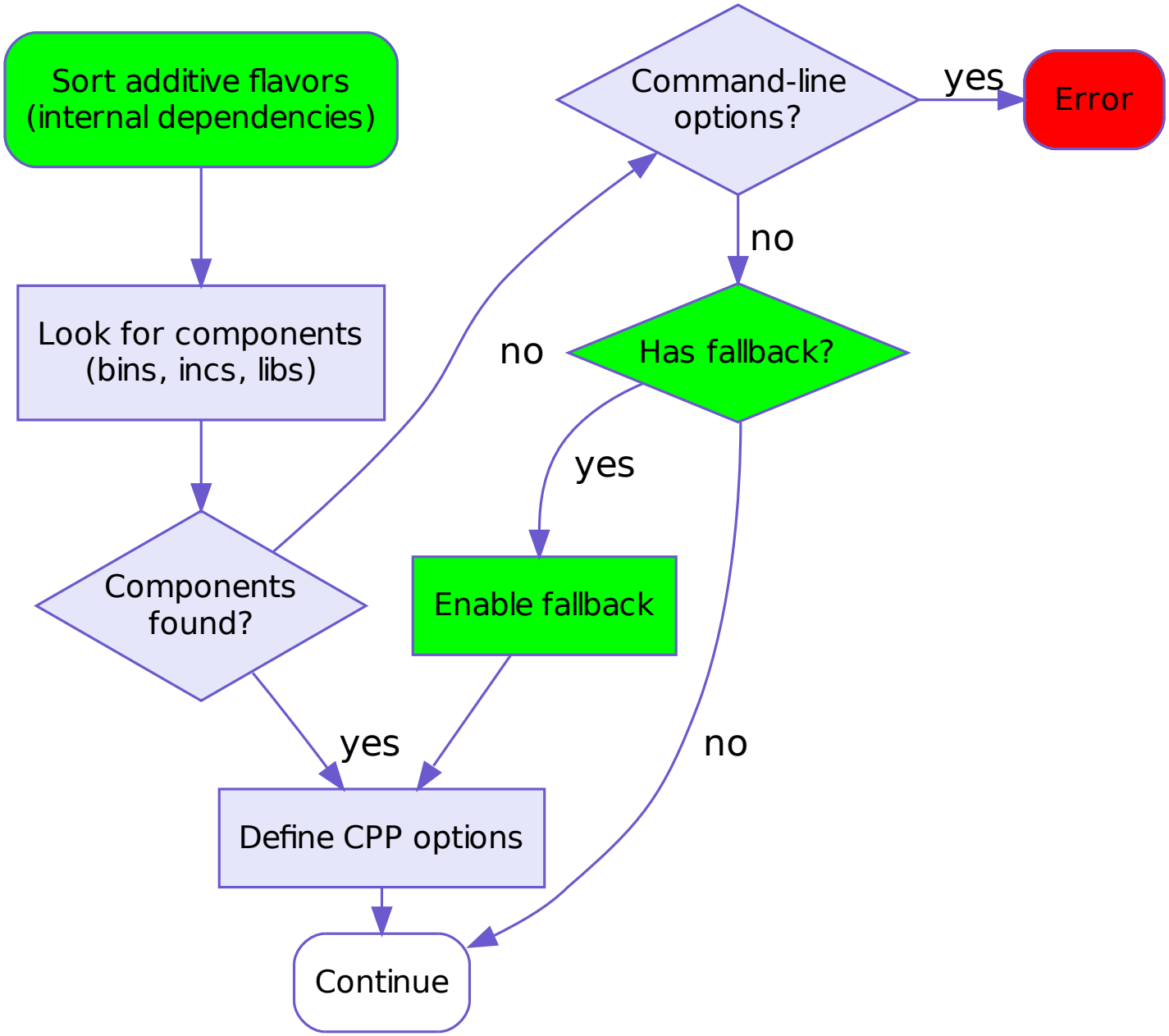
- Plugins
  - flat structure (manual interdependency checking)
  - poor detection of external dependencies
  - preemptive interpretation of user requests
  - non-transparent overriding of options
  - optimized for home-built Abinit versions

- Connectors/Fallbacks
  - hierarchical structure (automatic interdependency checking)
  - advanced detection of external dependencies
  - strict respect of user requests
  - rigorous connector $\longrightarrow$ fallback $\longrightarrow$ error behavior
  - can seamlessly handle home-built and packaged versions

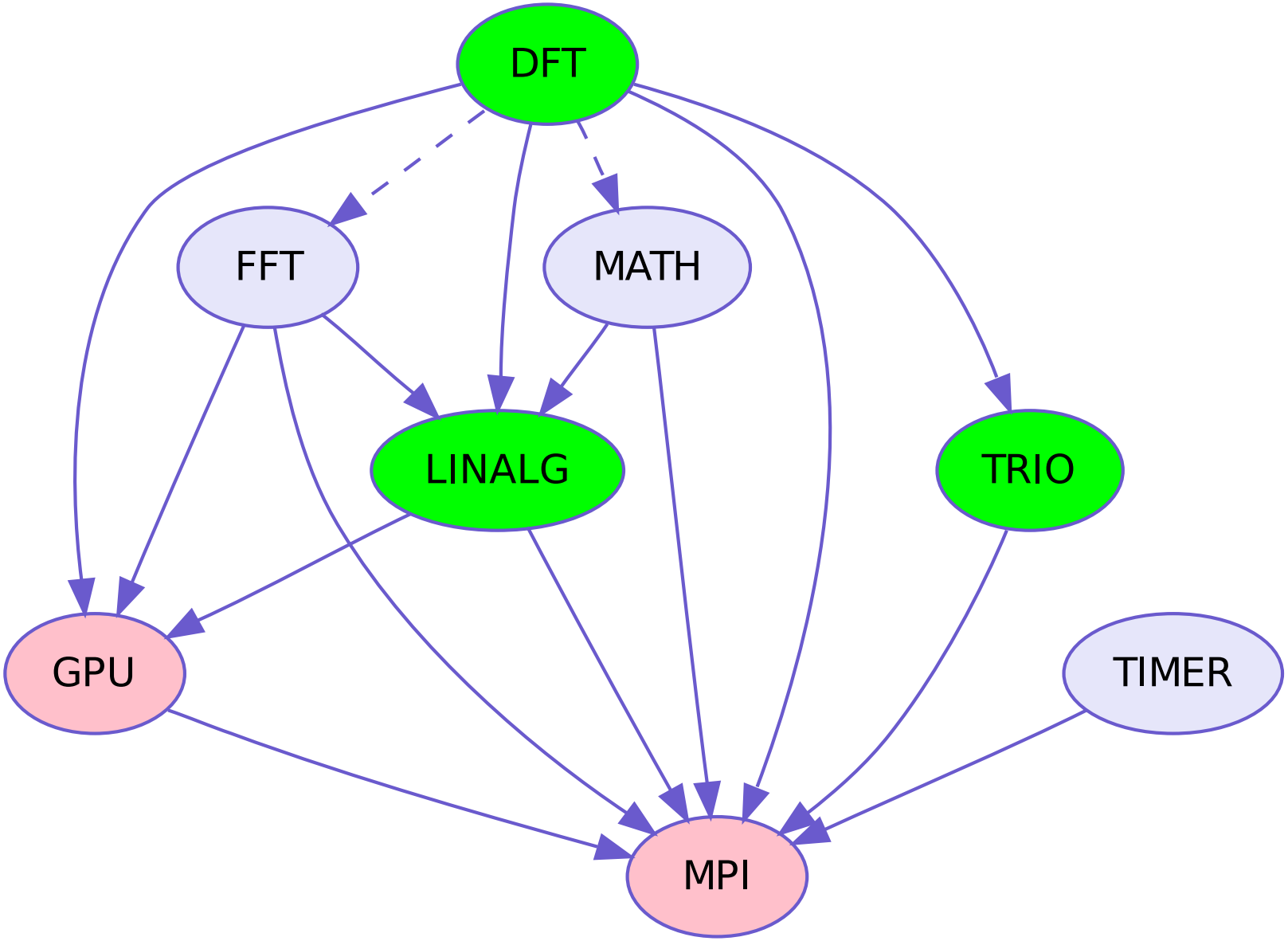
From plugins to connectors/fallbacks

- Plugins
  - flat structure (manual interdependency checking)
  - poor detection of external dependencies
  - preemptive interpretation of user requests
  - non-transparent overriding of options
  - optimized for home-built Abinit versions
- Connectors/Fallbacks
  - hierarchical structure (automatic interdependency checking)
  - advanced detection of external dependencies
  - strict respect of user requests
  - rigorous connector $\longrightarrow$ fallback $\longrightarrow$ error behavior
  - can seamlessly handle home-built and packaged versions

Internals of a connector (Abinit 6.6)



Structure of the connectors (Abinit 6.6)



Flavors of the connectors (Abinit 6.6)

Connector	Flavor
MPI	*with_mpi_prefix* or CC=..., CXX=..., FC=...
GPU	***cuda-single***, cuda-double
TIMER	***abinit***, gptl, none, papi
TRIO	***etsf_io***, fox, ***netcdf***
LINALG	acml, asl, atlas, custom, cxml, essl, goto, goto-mpi, mkl, mkl-mpi, mlib, ***netlib***, netlib-mpi, none, sgimath, sunperf
FFT	asl, custom, fftw2, fftw2-threads, fftw3, fftw3-mkl, fftw3-threads, ***none***, sgimath
MATH	gsl, mlib, ***none***
DFT	***atompaw***, ***bigdft***, ***libxc***, ***wannier90***

- ScaLAPACK: goto-mpi, mkl-mpi, netlib-mpi
- Custom flavors: bypass build-system checks
- TRIO, DFT: additive flavors (e.g. “etsf_io+fox”)

Connector-related options (Abinit 6.6)

- Philosophy: priority on precision
- 2 kinds of flavors: exclusive or additive
- `--with-*-flavor="(<value>|custom|none)"`
  ex: --with-fft-flavor="fftw3"
  ex: --with-trio-flavor="etsf_io+fox+netcdf"
  ex: --with-dft-flavor="atompaw+bigdft+libxc+wannier90"
- `--with-*-bins="..."`
- `--with-*-incs="..."`
- `--with-*-libs="..."`
- `--enable-connectors`: for maintenance
- `--enable-fallbacks`: force external libs if disabled
- See `~abinit/doc/config/build-config.ac` for details

Structure of the fallbacks

- Grouping: package-wise $\longrightarrow$ task-wise
  (uncompress, patch, config, build, install, clean)

- Refactored subtree
  - makefiles
  - patches
  - sources
  - install

- One include path, one library path, one binary path
- Simplified & fully automatic cleaning procedure
- Can select versions to build
- Profiles (e.g. abinit-6.4, abinit-6.6)
- Can be detached from Abinit & used by other projects

Modularization of the build system

Objective

Allow teams to work asynchronously on different Abinit components
$\Longrightarrow$ independent fine-tuning of different blocks
$\Longrightarrow$ easier debugging of individual components

- Different parts $\longleftrightarrow$ different tasks

- Core + bindings: set build parameters
- Fallbacks: delegate builds
- Test suite: set runtime parameters
- Documentation: set publishing parameters
- Data: ensure completeness and consistency

Modularization of the build system

Objective

Allow teams to work asynchronously on different Abinit components
$\Longrightarrow$ independent fine-tuning of different blocks
$\Longrightarrow$ easier debugging of individual components

- Different parts $\longleftrightarrow$ different tasks

- Core + bindings: set build parameters
- Fallbacks: delegate builds
- Test suite: set runtime parameters
- Documentation: set publishing parameters
- Data: ensure completeness and consistency

Coming soon ...

- New freeze of the build-system UI
  $\Longrightarrow$ submit feature requests **NOW!**
- Comprehensive documentation of the build-system UI
  $\Longrightarrow$ improved ease of use
- Activation of subsystems
  $\Longrightarrow$ asynchronous fine-grained tuning
- Complete rewrite of the build-system internals
  $\Longrightarrow$ optimization for speed & efficiency
- Libtool support
  $\Longrightarrow$ export of dynamic shared objects

Acknowledgments

- Whole Abinit community
- Special thanks: Xavier, Jean-Michel, Alain, Damien, Marc, Matthieu, Josef
- Build-system crash test award: Matteo Giantomassi

Special requests

Service evaluation: acknowledgments in papers

« We thank Yann Pouillon for valuable help/support/whatever... »
Send a copy of final paper to `mailto:yann.pouillon@ehu.es`

Looking for a position

Research engineer profile: research + services
Service part focused on software (hardware $< 10\%$)
Starting before Spring 2012 if possible
Forward proposals to `mailto:yann.pouillon@ehu.es`

Special requests

Service evaluation: acknowledgments in papers

« We thank Yann Pouillon for valuable help/support/whatever. . . »
Send a copy of final paper to `mailto:yann.pouillon@ehu.es`

Looking for a position

Research engineer profile: research + services
Service part focused on software (hardware $<$ 10%)
Starting before Spring 2012 if possible
Forward proposals to `mailto:yann.pouillon@ehu.es`