The CECAM Electronic Structure Library: Past, Present and Future

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ESL in a nutshell





- Founded in 1969
- 21 member organizations from 12 countries
- HQ at EPFL in Lausanne, Switzerland
- 18 nodes
- Promotes fundamental research on advanced computational methods and their application
- Focus on atomistic and molecular simulations, applied to the physics and chemistry of condensed matter

The "traditional" electronic structure code framework



Duplication of code = Duplication of effort = Wasted time







M. Oliveira

Past

In the beginning

CECAM

Want to move beyond hosting workshops and schools and directly support their computational science community exploiting the new satellite structure of CECAM and the resources provided by this structure.

One suggestion is that they champion an **'Open Innovation'** approach to computational science.

They are currently discussing this with the EC and asking whether there is an opportunity to bid for funds under the FP7 e-Infrastructure Programme

Mike Payne, 2013/14

In the beginning

Open Innovation in Software Engineering



Mike Payne, 2013/14

Kick-off Workshop (July-August 2014)

- Extended software development workshop at CECAM-HQ-EPFL
- Organized by Mike Payne, Emilio Artacho and Dominic Tildesley
- 3 days for discussion + 5 weeks of development
- \sim 10 participants
- Extensive discussions on:
 - coding standards
 - documentation
 - licenses
 - ESL organization
 - etc
- Wiki design and initial content



Start of new projects and inclusion of existing projects into the ESL:

- Libpspio: Parsing and writing of pseudopotentials
- Flexible data format (FDF): Input file parser
- GridXC: Evaluate XC functionals on a grid
- LibOMM: Kohn-Sham equations solver
- MatrixSwitch: matrix storage and manipulation low-level routines

ESL requirements, coding standards, and best practices

ESL modules and libraries should be:

- Easy to maintain
- Easy to use

Recomendations:

- C/Fortran programming languages with bindings to other languages
- Licenses: LGPL, BSD and/or MPL2
- Source code documentation (e.g., Doxygen)
- Version control system
- Use a standard build system type (e.g., Autotools, CMake)
- Provide proper error handling

E-CAM

- European Union H2020 Center of Excellence
- e-infrastructure for software, training and consultancy in simulation and modeling
- 16 CECAM nodes, 3 PRACE Centres, 12 Industrial Partners, and 1 Centre for Industrial Computing



The ESL was a used as a pilot project for E-CAM

Objectives:

- Create over 150 new, robust software modules, directed at industrial and academic users in:
 - electronic structure calculations
 - classical molecular dynamics
 - quantum dynamics
 - mesoscale and multi-scale modelling
- Training of current and future academic and industrial researchers
- Support industrial end-users in their use of simulation and modelling

- Unique opportunity to bring the electronic structure code developers together
- Long workshops (1 week or more)
- 10-20 participants
- Divided into discussion and coding sessions
- Original format for CECAM workshop!

Utilities Toolbox (June 2015)

- Second software development workshop at CECAM-HQ-EPFL
- 1 day for discussion + 4 days of development
- ullet ~ 20 participants (12 for the coding sessions)
- Some of the explored themes:
 - Low-level utilities (memory management, error handling, etc)
 - Further steps towards standardization of coding standards
 - Geometry tools
- More projects added:
 - Flook: Fortran-Lua-hook library
 - MonteCarloLib: general purpose Monte Carlo library
 - Flib: Fortran low level functionalities
 - Libcif: tools to read and manipulate CIF files

Towards a Common Format for Computational Materials Science Data (January 2016)



- Workshop co-organized by ESL and NoMaD
- 3 days of discussion and 8 days of coding
- Objectives:
 - Discuss relevant problems in creating a common data format for materials science
 - Set the specifications for an Electronic Structure Common Data Format (ESCDF)
 - Start the development of a library to read/write ESCDF files

ESL Coding Workshop: Solvers

- Z-CAM, Zaragoza, Spain
- 6-17 June 2016
- 1 day of discussion and 10 days of coding
- 15 participants
- Three themes:
 - Kohn-Sham solvers: ELSI
 - Poisson solvers: PSolver, POKE
 - Atomic solvers: SQARE



ESL Coding Workshop: Drivers

- Trieste, Italy
- 10-21 July 2017
- 1 day of discussion and 10 days of coding
- ${\sim}10$ participants
- Iterative eigensolvers



Present

- CECAM-HQ-EPFL, Lausanne, Switzerland
- 5-16 February 2018
- Write a simple DFT code using the ESL libraries in 10 days
- Create an ESL bundle
- Improve libraries API, documentation, tests, etc

- How to make the ESL into more than a loose collection of libraries?
- How to tackle dependency hell?
- How to make the ESL available to the different types of users:
 - Software developers
 - HPC centers
 - End-users

The ESL bundle

- Includes:
 - Software developed within the ESL
 - Other relevant software distributed with the agreement of the authors
 - Not readily available dependencies
- All modules versions **must** be compatible
- Common installer for easy compilation and installation
- Bindings for different programming languages
- Documentation

https://gitlab.e-cam2020.eu/esl/esl-bundle

- Density Functional Theory code to showcase how ESL components can be used
- A tool to test the ESL modules
- NOT meant for production calculations
- Based on the ESL bundle
- Can use either plane-waves or atomic orbitals

Future

- Sustainability: we need more involvement from the electronic structure community
- Wider integration by community codes: figth the "not invented here syndrome"
- Publicize the work done within the ESL
- Scalability, optimization, and hardware awareness
- Engage more with other projects with similar goals

The ESL bundle

- Include more packages
- Debian and RPM packages (end-users)
- Collection of EasyBuild easyconfigs (HPC)
- Add more configuration files

Release schedule:

- One minor release every 1-2 months
- One major release every 6-12 months

E-CAM Extended Software Development Workshop: Scaling Electronic Structure Applications

- CECAM-IRL, Dublin, Ireland
- 7-18 January 2019
- Parallelization, scalability, performance

E-CAM Extended Software Development Workshop: Integration

- CECAM-HQ, Lausanne, Switzerland
- Dates to be announced
- Integration of ESL modules with electronic structure codes, bindings, etc

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