

	<h2 style="text-align: center;">Tutorial Scientific Report</h2>
	<p>Please do not repeat the program (unless there were last-minute changes) or the initial description - we already have this material.</p>
Title	<p style="text-align: center;">Electronic structure at the cutting edge with Elk</p>
Dates	<p style="text-align: center;">15 July - 19 July 2013</p>
Location	<p style="text-align: center;">CECAM-HQ-EPFL, Lausanne, Switzerland</p>
Organizers	<p>Sangeeta Sharma, John Kay Dewhurst and E. K. U. Gross</p> <p>Max Planck Institute of Microstructure Physics, Halle Germany</p>
<p>Aim(s) of the Tutorial (maximum 200 words)</p> <p>The Elk LAPW code is an electronic structure code based on the state-of-the-art full-potential linearized augmented plane-wave (LAPW) method. It was designed from the start to be a user- and developer-friendly code, allowing PhD students and post-docs to both use the code for their research as well as implement new ideas in the field of electronic structure.</p> <p>The present Elk-LAPW CECAM tutorial was second in the series of tutorials. The previous tutorial, which was held in 2011, was aimed at basic introduction to the ELK code. The aim of the latest tutorial was to introduce to students with the cutting edge science and implementations in the field of electronic structure methods.</p> <p>The tutorial was divided into two parts:</p> <ol style="list-style-type: none"> 1. Morning sessions which were aimed at bringing together experts in the field of electronic structure methods, density functional theory (DFT), the LAPW method, superconductivity and time-dependent DFT. The talks given by the speakers were to teach the attendees the physics behind various implementations in the Elk code. This session was also aimed at introducing the cutting edge topics. 2. Evening sessions were aimed at (a) teaching attendees the most efficient method of using the Elk code and (b) discussing implementational as well as advanced level problems with running of the code. 	

Outcomes:

What were the most important learning objectives of the tutorial? Were these achieved? What could have been improved? (maximum 200 words)

This year the main objective of the tutorial was not just to teach attendees to use the code, but also to introduce the cutting edge physics issues and progress in this direction in terms on implementation. This objective was certainly reached. Owing to this, a few students, who were not physicists but rather chemists, found the morning sessions too advanced. This is one area where the tutorial could be improved-- to have some invited lectures by chemists and not just physicists. In 2015 we plan to do this and have already made a list of potential invited speakers in the field of chemistry, who are heavily using the code (Claudia Felser (Dresden), Markus Meinert (Bielefeld) and Frank Wagner (Dresden)).

The aims of the hands on part of the tutorial was to

- (1) introduce the basic code
- (2) allow trouble-shooting for advanced users and
- (3) introduction of the cutting edge features.

All the objectives were met. In fact the trouble shooting part of the tutorial was especially appreciated by many students. Several of these students have explicitly requested recordings of the lectures. This time we tried a new strategy for doing the tutorials-- we requested all participants to bring a laptop if possible. We did the tutorials without the CECAM local machines. For this we went to the length of opening accounts for all participants on our computer cluster in Halle. The reason for this was to simulate a realistic environment for running a code on any supercomputer in the world. Several students found it chaotic in the beginning but were able to learn this very quickly. We feel this is very important aspect of running codes and should be a part of tutorials.

On the last day we had a special session asking people for "wish-list". We were given a six point wish-list by the students and we believe this will help us in taking the code to the next level of sophistication.

Report on the feedback from the “students” (one paragraph at least)

The students showed great interest in fundamental talks given by experts as well as in learning the code. Some of the students have shown interest in not just using but also implementing new features in the code (Lukas Wllmann, Olga Kremenetskaya and Manuel Geisler).

Not just the students, but also some of the invited speakers (D. Singh, S. Pittalis and Carsten Ullrich) actually attended the hands on session to get to know the more sophisticated features of the code. In this regard the CECAM workshop has been useful not just for attendees but also for developers, by having experts working on the code.

Some of the students attending the workshop were experienced users of the Elk code and were able to discuss advanced level problems with the developers during the evening sessions (one whole session was devoted to this). They also provided a list of changes made and features added to the code. This has further helped the developers in improving the code.

For students we will, as in the case of 2011 tutorial, set up a web-page with all the talks as pdf files. We also filmed all the lectures and have obtained permission from each speaker to put these movies on the Elk web-site. This will be an invaluable resource for researchers using electronic structure methods.

Do you have suggestions for new related tutorials?

We have a few suggestions for future such tutorials:

1. The size of the lecture hall is too small. Also the lecture hall should be layered such that the speakers can maintain eye contact with all students
2. The tutorials should be done on peoples personal laptops and not on local machines because
 - (a) this helps simulate a realistic environment and
 - (b) the local computers are not at representative of the computers on which people work these days.