



Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

Proposal Title: Electronic structure at the cutting edge with the Elk code.

Application Reference N°: 5701

1) Summary (up to one page)

The Elk LAPW code is an electronic structure code based on the state-of-the-art fullpotential 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.

The present Elk-LAPW CECAM tutorial was third in the series of tutorials. The previous tutorial were held in 2011 and 2013. The aim of the latest tutorial was two fold: introduction to the ELK code and to introduce the cutting edge science and implementations in the field of electronic structure methods.

The tutorial was divided into two parts:

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, many-body theory 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.

2) **Description of the scientific content of and discussions at the event (up to four pages)**

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 of implementation. This objective was certainly reached.

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 as always especially appreciated by the students. Several of these students have explicitly requested the pdf of the lectures.

We did the tutorials without the CECAM local machines for computations. They were only used as login servers. We went to the length of opening accounts for all participants on our computer cluster in Halle and a large part of the cluster was reserved for the tutorial. 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 sent mails by several students requesting specific features in the code. This we believe will help in taking the code to the next level of sophistication.

3) **Assessment of the results and impact of the event on the future directions of the field (up to two pages)**

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 (Markus Gruner, Eli Kraisler). Not just the students, but also some of the invited speakers also 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. They also provided a list of changes made and features added to the code. This has further helped the developers in improving the code.

We also will put all the lectures on the Elk web-site.

In future we plan to continue with this series of Elk workshops. These workshops take place every 2 years and that gives us chance to add new features to the code. With each passing year, we are able to introduce new scientific results and implementation to the attendees.

Thanks to such events the user base of the Elk code is now above 1000 users across the world.

After the workshop some of the students sent mails to us. To just give an example we attach a copy of one of the mails here

"Dear Dr. Sangeeta Sharma,

I just wanted to thank you once more for organizing such a great workshop and giving me the opportunity to take part in it. During those 5 days everyone was really nice and warm so that I had the feeling that I am in a big family. This gives me a huge amount of energy and motivation for my future work.

Regarding your requested suggestion, I dont think I have any. This is probably because I was thrilled during the days so that i didn't notice any bad things. If something comes up to my mind, I will let you know.

With warm wishes to your and your family,

Aleksandar(azivkovic@fizika.unios.hr)"

- 4) **Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants**

Annex 4a: Programme of the meeting

Day 1 - August, 10th 2015 Density functional theory and LAPW

- 09:00 to 09:20 - Welcome
- 09:20 to 10:20 - ABC of DFT (K. Burke)
- 10:20 to 11:20 - The linearized augmented plane wave method (Dewhurst)
- 11:20 to 12:00 - Coffee Break
- 12:00 to 13:00 - EFG of DFT (K. Burke)
- 13:00 to 15:00 - Lunch
- 15:00 to 16:00 - Functionals: New and old (S. Pittalis)
- 16:00 to 16:30 - Coffee Break
- 16:30 to 17:00 - Introduction to Elk (Dewhurst)
- 17:00 to 18:30 Exercises: Compiling the code, setting up the input and performing ground-state calculations (Jose Livas Flores, Dewhurst)

Day 2 - August, 11th 2015 Magnetism

- 09:00 to 09:30 Magnetism: collinear and non-collinear (L. Nordstroem)
- 09:30 to 10:30 DFT+U method and tensor moments (L. Nordstroem)
- 10:30 to 11:00 - Coffee Break
- 11:00 to 12:30 - TDDFT: Introduction (E.K.U. Gross)
- 12:30 to 14:30 - Lunch
- 14:30 to 16:30 - Exercises: Magnetism (Jose Livas Flores, Dewhurst)
- 16:30 to 18:30 - Poster Session and poster prize

Day 3 - August, 12th 2015 Many body perturbation theory:

- 09:00 to 10:00 - Introction to MBPT (L. Rening)
- 10:00 to 11:00 - Hedin equations and GW method (P. Rinke)
- 11:00 to 11:30 - Coffee Break
- 11:30 to 12:30 - MBPT: Excitations and BSE (Lucia Rening)
- 12:30 to 14:30 - Lunch
- 14:30 to 15:30 - Organic solar cells (S. Botti)
- 16:30 to 17:00 - Coffee Break
- 17:00 to 18:30 - Exercises: Linear response TDDFT (Sharma, Shinohara)

Day 4 - August, 13th 2015 Linear response

- 9:00- 10:00 Phonons and electron-phonon coupling (Dewhurst)
- 10:00 to 11:00 - Superconductivity an overview (A. Sanna)
- 11:00 to 11:30 - Coffee Break
- 11:30 to 12:30 - Super conducting density functional theory (A. Sanna)
- 12:30 to 14:30 - Lunch
- 14:30 to 15:30 - Materials prediction (M. A. L. Marques)
- 15:30 to 17:30 - Exercises: Phonons and superconductivity (Davydov, Sanna)
- 17:30 to 21:00 - Dinner

Day 5 - August, 14th 2015

- 09:30 to 10:30 - Dynamical mean field theory (D. Jacob)
- 10:30 to 11:00 - Coffee Break
- 11:00 to 12:00 - Machine learning (R-. K. Mueller)
- 12:00 to 13:30 - Lunch
- 13:00 to 14:00 - Quantum electro dynamics (W. Tarantino)
- 14:00 to 15:00 - Summary (E. K. U. Gross and K. Burke)
- 15:00 to 16:00 - Coffee Break
- 16:00 to 17:00 - Trouble shooting (Dewhurst and Sharma)

Annex 4b: Full list of speakers and participants

Organizers

John Kay DEWHURST	Germany	Organiser
E.K.U. GROSS	Germany	Organiser
Sangeeta SHARMA	Germany	Organiser

Participants

Arijan ALEKSIÆ	Croatia	Attendee
Tomás ALONSO-LANZA	Spain	Attendee
Lugovskoy ANDREY	Russian Federation	Attendee
SAAD BINOMRAN	Saudi Arabia	Attendee
Silvana BOTTI	Germany	Speaker
Felix BROCKHERDE	Germany	Attendee
Kieron BURKE	USA	Speaker
Arkadiy DAVYDOV	Germany	Tutor
José A. FLORES LIVAS	Switzerland	Tutor
Anastasia GAZHULINA	Russian Federation	Attendee
Jhon Wilfer GONZALEZ SALAZAR	Spain	Attendee
Migle GRAUZINYTE	Switzerland	Attendee
Markus GRUNER	Germany	Attendee
Thijs HOLLEBOOM	Sweden	Attendee
David JACOB	Germany	Speaker
Eli KRAISLER	Israel	Attendee
Sohan LAL	India	Attendee
Kai LECKRON	Germany	Attendee
Hyungjun LEE	Switzerland	Attendee
Adilmo LIMA	Brazil	Attendee
Alexander LINDMAA	Sweden	Ateendee
Galya MADZHAROVA	Germany	Ateendee
Hamza MAIZ HADJ AHMED	Algeria	Attendee
Miguel M. MARQUES	France	Speaker
Yu-ichiro MATSUSHITA	Germany	Tutor

Thomas MILLICHAMP	United Kingdom	Attendee
Klaus-Robert MUELLER	Germany	Speaker
Ayoub NASSOUR	France	Attendee
Dennis NENNO	Germany	Attendee
Lars NORDSTRÖM	Sweden	Speaker
Luciano ORTENZI	Italy	Attendee
Stefano PITTALIS	Italy	Speaker
Lucia REINING	France	Speaker
Patrick RINKE	Finland	Speaker
Antonio SANNA	Germany	Speaker
Sebastian SCHWALBE	Germany	Attendee
Dongbin SHIN	South Korea	Attendee
Yasushi SHINOHARA	Germany	Tutor
Walter TARANTINO	France	Speaker
Sami VASALA	Switzerland	Attendee
Cecilia VONA	United Kingdom	Attendee
Angelica ZACARIAS	Germany	Attendee
Aleksandar ZIVKOVIC	Croatia	Attendee