Period 2005-2009

L_Sim section

Inac evaluation by AERES agency
http://www.aeres-evaluation.fr

SP2M E13: Atomistic Simulations L_SIM

This team involves 6 researchers (CEA), 5 PhDs and 5 post-docs.

- Scientific quality and production :

Scientific activity of the group covers a broad range of topics related to numerical simulations: 1) development and promotion of efficient *ab initio* code (BigDFT) which uses wavelets as basis functions; 2) development of atomistic semi-empirical method (TB_Sim), to be used in combination with the *ab initio* one in a multiscale simulation; 3) multi-resolution approach for model treatment of magnetic systems. All these components (in different realisations) are highly demanded in computational materials science community worldwide. While comparable approaches can be found, in a different form, under development elsewhere, the unique situation of L_Sim is that it offers a package with which multiple properties of nanosystems (electronic structure, magnetism, and quantum transport) can be addressed. Moreover, an overlap between the results obtainable on different lengths scales is assured. An about ideal balance must be pointed out in sharing the group's efforts between front-end method development (algorithms), work on numerical efficiency (issues of parallelization, hardware tuning) and practical calculations related to different material science problems.

Each of six permanent staff members of this team has his clear domain of specialisation. Yet multiple joint works emerge in different combinations, an indication of flexibility and vividness of the research atmosphere in the group. The number of publications over the reporting period is impressive (42 articles in 2005-2009, including three PRL and four APL). Moreover each member of the team had at least one invited talk at international conferences (some have much more, up to 10). Two patents were filed, one resulting from cooperation within SP2M and the other a product of internal team work, which is a not self-obvious decoration for a theory group.

The group regularly employs postdocs (whose number roughly equals that of permanent staff members) and about the same number of PhD students. This nearly 1:1:1 structure of working forces seems about ideal and performs well in terms of overall scientific productivity and job perspectives of post-docs and PhD students after leaving the group. Such large proportion of post-docs became possible thanks to an impressive portfolio of contracts, which includes academic as well as more applied national and European ones. Large part of the contracts which kept the group afloat expires in 2009 and 2010; however, in view of existing cooperations and high scientific impact, the chances are good for maintaining the external funding at roughly the same level. International cooperations of the group are not excessively numerous but well established (notably with Basel University) and provide a solid basis for research.

- International recognition and attractivity :

The group is well known in European world of first-principles simulations, and has clearly defined profile and visibility. The quality and contents of the Web site of the team is exemplary in INAC (the decision to restructure the institute's web presentation in the sense of that of L_Sim can be therefore welcomed).

The group is perfectly integrated in the research context of SP2M, offering solutions to numerical simulations on different materials and for different problems.

- Evaluation of the project :

In the ongoing research project, L_Sim participates in five Challenges formulated for the SP2M, offering a good balance between a more secure low-risk work and ambitious daring aims.

Challenge 1 (atomistic study of Si nanowires), with L_Sim as the main player, is, in part, a natural extension of previous activities. A sensitive element is, however, a reasonable combination of approaches - *ab initio* / BigDFT with activation-relaxation technique (ART). In case of success, a novel approach is likely to emerge, able to lead to interesting reality-near simulations of catalysis.

Challenge 3 (atomistic Green's functions for transport properties), purely method development, to be done exclusively by L_Sim. The realisation in the frame as intended (with electron-phonon coupling etc.) is not obvious, but ambitious and certainly interesting for both practical ends and methodological progress.

Challenge 4 (nanostructures for energy conversion) involves three INAC teams and external cooperations. The simulation part assigned to L_Sim is, in view of previous experience, rather routine and does not suggest trouble.

Challenge 10 (confinement effects in nanostructures) is joint project of four teams, of quite applied character (growth conditions, characterisation etc.). The unspecified but obvious problems of simulation are, a priori, well suited for an attack by the tools under development by L_Sim; however the real outcome of joint application of experimental and simulation techniques is difficult to foresee.

Challenge 12 (interpretation of EELS results) is an initiative of LEMMA and L_Sim: the measured spectra are to be compared with predictions from BigDFT, that would allow to decipher structural information. A priori the combination is reasonable. Its implementation would demand certain extensions of BigDFT in order to treat inner-shell ionisations. It looks like a long shot, but certainly a daring and interesting one.

Note that with 6 permanent members only, this is a tough program, yet not unrealistic - provided the external support enabling to hire experienced post-docs will materialize at about the same level as so far.

- Conclusion :

The group delivers a top world-class research and provides valuable theory support for research programs run by many teams of the laboratory. The diversity of tasks and efficiency of performance, given a very compact size of the group, is remarkable.

In view of ambitious research program, the suggestion formulated in the Project of SP2M, to reinforce L_Sim in terms of human resources, seems justified.

- Strengths and opportunities :
  - Good balance between methodological development, optimization of algorithms and applied materials research science.
  - Broad scope of complementary competences within the group, flexibility in adapting to new challenges.
  - Good connectivity to experimental environment.
  - Efficient management of work sharing between permanent staff, post-docs and post-graduates.
- Weaknesses and threats :
  - Relative lack of overseas cooperation.
- Recommendations :
  - When orchestrating a development of essentially open-source software packages of potentially broad interest, more effort could be invested in creating a self-supporting impetus in the users' community. Popularisation efforts for BigDFT and TB_Sim can be done somehow more aggressively.