Summary:

The main objective of the workshop "SYLCA 100" (*Superconductivity 100 Years Later, a Computational Approach*) was to bring together different communities working in the field of superconductivity, to discuss about hot topics and open issues in the field. In fact, the solution of puzzles such as the mechanism of superconductivity and the symmetry of the order parameter in the recently discovered Fe-based superconductors can only come by combining different theoretical methods (computational approaches based on DFT methods and many body approaches that focus on strong correlation and Mott Hubbard physics) and confronting them with up-to-date experimental work in the most significant aspects. The program and location of the workshop was planned to create a friendly atmosphere to boost discussion and new collaborations: besides 23 invited presentations, there were 18 posters, which were shortly presented with 5 minutes oral presentations, and a round table to discuss the most important issues. The total number of participants was 52.

Scientifc content and discussion:

All the talks of the conference have addressed different aspects of superconductivity. Many presentations focused on specific materials, of particular interest because of open problems in the description of the normal and superconducting states (pnictides, cuprates, ruthenates) or because they are relevant to other areas of physics (C-based materials, such as picene, graphene and graphite-intercalation compounds). A few talks concerned methodological advances in density functional theory, relevant to superconductivity, and the illustration of methods that can be used to go beyond first-principles calculations.
The talks on **pnictides**, where there has been a wide consensus on the magnetic origin of the superconducting mechanism, mainly addressed the following points:

(i) the symmetry of the order parameter, and the corresponding implications on the nature of the pairing and on the strength of the pairing and electronic interactions. The topic was introduced already in the first session by Honerkamp, who described how different symmetries of the superconducting gap in the pnictides can be obtained in the functional renormalization group, starting from ab-initio tight-binding models of the band structure, assuming an electronic mechanism for pairing. Other speakers addressed the same problem, discussing the role of impurities in the s+- state of the pnictides (Efremov, who was replacing Dolgov), and Mazin, who discussed the releation between the structure of the order parameter and the Fermi surface topology of several Fe-based superconductors. Two experimental speakers, Gonnelli on point-contact Andreev reflection spectroscopy and S. Borysenko on Angle Resolved Photoemission Spectroscopy (ARPES), presented results on the symmetry and nodes of the superconducting gaps.

(ii) The nature of magnetism, the spin-fluctuation spectra and the relationship between magnetism and superconductivity. This topic was introduced by Antropov on the first day, who showed a comprehensive LDA study of spin fluctuations in the pnictides. David Singh presented an overview of LSDA calculations in magnetic superconductors (such as pnictides and ruthenates), pointing out the similarities and differences, and the signatures of quantum criticality in LSDA calculations. Michelle Johannes presented a model for the magnetism on the pnictides, based on the interpretation of LSDA calculations, which is at the same time

itinerant and localized, and Alessandro Toschi showed that this behavior can be reproduced in Dynamical Mean Field Theory (DMFT), due to the dynamical nature of the self-energy.

(iii) Multiband effects in pnictides: Golubov, Cappelluti and Efremov discussed the consequence of the multiband nature of pnictides on several observables, such as specific heat, optical spectra, etc.

The theoretical talks on other **exotic superconductors** - cuprates and ruthenates - were also concerned with the problems of symmetry of the order parameter, magnetism and superconductivity and correlation (e.g. J. Annett, D. Singh); Mackenzie gave a very broad experimental overview on the field, reviewing phase diagrams of exotic superconductors near the quantum critical point.

A significant part of the meeting has been devoted to **electron-phonon superconductivity** (EPS). Particular attention has been devoted to C-based materials and MgB2 (Profeta, Yildirim, Calandra), to relativistic effects in Pb (Heid). Always within EPS, we mention the presentation of Sanna on the status of the density functional theory applied to the superconducting state (SCDFT). Sanna has shown how from the solution of the Sham–Schlueter equations it is possible to derive the Kohn-Sham superconducting gap, and finally obtain a critical temperature which follows very closely the Eliashberg result in the ideal test case where Coulomb interaction is turned off.

Another topic of discussion, which will have a significant impact on future research, is the **interplay of electron-phonon interaction and strong electronic correlations**. The problem arises in the description of the vibrational properties and electron-phonon coupling in strongly-correlated materials, where the standard DFT approach fails. a very nice example were the time-resolved optical and experiments of F. Carbone on the cuprates. Andrea Floris presented a first and promising attempt to go beyond the standard DFT approach, including the electronic correlations within the DFT+U approach; he presented preliminary results for oxides, which showed a sensible improvement with respect to DFT calculations Finally, we mention two presentations (Bianconi and Peeters) where quantum effects become important at the nanoscale level.

Several topics of discussion emerged during/after the scientific talks at the conference; the most essential ones were summarized in questions, which were then proposed during the round table.
The first question which was discussed was how reliable are estimates based on DFT calculations for standard electron-phonon superconductors. Several speakers raised the issue that for Magnesium diboride (MgB2) the estimates of EP coupling from different groups over the years are quite different. Calandra presented the very recent and highly accurate results, which lead to values of Tc which are too low compared with experiment. This indicates that a quantitative description of superconductivity in this compound requires further studies. Another example was that of intercalated hydrocarbons (picene), in which different groups obtained very different results depending on the approximation used for doping. Also in this case, the discrepancy had important physical implications on the microscopic models for superconductivity. The main outcome for the discussion was that, even in the simple case of phonons, where superconductivity is usually considered to be perfectly understood, there are several open issues before a quantitative description can be achieved.

The second topic was the discussion of the gap symmetry in exotic superconductors. It was pointed out that discussing this issue, in conjunction with the electronic structure of the materials, has important

implications on the microscopic models of the interaction. For this, it was agreed that methods which can treat more or less *ab-initio* both the quasi-particle band structure and the interaction are especially important. For this, both the DFT+fRG calculations presented by Carsten Honerkamp, and the extension of superconducting DFT to spin fluctuations in Hardy Gross's group look extremely promising.

Another topic of discussion was how to read ARPES experiments in superconductors; in particular, how to extract interaction parameters for microscopic models from the quasi-particle dispersions measured by ARPES. This has important consequences in the estimates of electron-boson coupling strength and on the strength of electronic correlations.

Assessment of the results and impact of the event on the future directions of the field:

The major objective of the workshop was to stimulate the discussion among experimentalists and theorists and possibly reach conclusions on the open issues on the most relevant classes of conventional and non-conventional superconducting materials.

In the latter, the issues discussed were (among other) the nature of magnetism, the symmetry of the order parameter and the mechanism in the Fe-based materials. Our discussions reached an agreement on the essential role of the magnetic fluctuations and shed light on the delicacy of the interrelationships between magnetic and superconducting properties. In this respect, in our opinion the workshop was very successful. On the other hand, the discussion is still open on the importance of correlation effects, although most of the participants appear to believe that correlation in pnictides is not an essential ingredient to understand the superconducting pairing, although they affect the magnetism.

The state-of-the-art of new theories and computational technologies has been illustrated for electron-phonon materials. In particular, it has been made clear that coupling in MgB2 is weaker than initially thought, and that new physics has to be invoked to explain the high value of Tc. The point of view had large agreement. Again, this is an important statement which will lead the research of many participants in the next future, and allows us to define the conference as very successful.

Annexes: programme of the meeting and full list of speakers and participants.