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The Yambo code: a comprehensive tool to perform ab-initio simulations of equilibrium and out-of-equilibrium properties[1]

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Density functional theory and many-body perturbation theory methods (such as GW and Bethe-Selpether equation) are standard approaches to the equilibrium ground and excited state properties of condensed matter systems, surfaces, molecules and other several kind of materials. At the same time ultra-fast optical spectroscopy is becoming a widely used and powerful tool for the observation of the out-of-equilibrium dynamical processes. In this case the theoretical tools (such as the Baym-Kadanoff equation) are well known but, only recently, have been merged with the ab-Initio approach. And, for this reason, highly parallel and efficient codes are lacking. Nevertheless, the combination of these two areas of research represents, for the ab-initio community, a challenging prespective as it requires the development of advanced theoretical, methodological and numerical tools. Yambo is a popular community software implementing the above methods using plane-waves and pseudo-potentials. Yambo is available to the community as open-source software, and oriented to high-performance computing. The Yambo project aims at making the simulation of these equilibrium and out-of-equilibrium complex processes available to a wide community of users. Indeed the code is used, in practice, in many countries and well beyond the European borders. Yambo is a member of the suite of codes of the MAX European Center of Excellence (Materials design at the exascale) . It is also used by the user facilities of the European Spectroscopy Facility and of the NFFA European Center (nanoscience foundries fine analysis). In this talk I will discuss some recent numerical and methodological developments that have been implemented in Yambo towards to exploitation of next generation HPC supercomputers. In particular, I will present the hybrid MPI+OpenMP parallelization and the specific case of the response function calculation. I will also discuss the future plans of the Yambo project and its potential use as tool for science dissemination, also in third world countries.

[1]ETSF, MAX European Center of Excellence and NFFA European Center