Designing Materials with High-Performance Computing

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Guido Chiarotti, MaX CoE, Scientist, Entrepreneur, Manager

Suppose you are in your kitchen and decide to ask your mother for a recipe that you intend to prepare for your dinner party. You and your mother live on different continents, so you decide to send her an email. You take your smartphone out of your pocket and start typing. By doing such a simple action you are actually using a number of new materials: the glass of the touch screen, a certain number of silicon-based electronic devices, the reinforced titanium plate the case is made of, etc. The same holds true if you go to a hospital for a test or switch on the engine of your new car: new materials are ubiquitous around you and are at the basis of most of your actions. It was always so: from the bronze or iron ages, i.e., from the moment in which humankind has decided to forge matter according to their needs, any innovation was accompanied by the discovery (whether intentional or not) of new materials, that are now crucial to scientific or technological change and industrial competitiveness, as well as to tackle key societal challenges - from energy and the environment to healthcare, information and communications, industrial processes and manufacturing, safety and transportation.

The creative process around new materials has changed in the course of time: in the past it was basically mostly serendipitous, i.e., once discovered a new material by chance, as casually mixing some known elements, you then tried to figure out how to use it. Nowadays, it mostly goes the other way round: starting from a need (e.g., the touchscreen), you embark on a search process to identify the material (existing or not) that better complies with requirements (including production constraints) and allows you to answer your need. This process is by no mean unidirectional: as in any strategic decision process, you start from an idea in order to satisfy what you then perceive to be a need, but you might end up finding something slightly different and therefore modify your original plan (and probably also your perception of the need). So on and so forth, you can have at the end something completely different from what you were initially looking for. The development of the Post-it Notes at 3M Corporation is probably the most famous case history. A researcher wo was trying to produce a very strong glue, by chance, and by mixing some chemical components, found a very weak one. It was a bad glue in fact, but left no halo on the paper when removed. A brilliant team involving researchers, marketing experts, and, at a certain point, even the company's CEO came up with the idea of post-its the way we know them. Crucial to this idea's success was the free - non focussed - discovery process and the open mindset of researchers and innovators.

Today, the new material search process, which is mostly experimentally-based, could be speeded up by efficiently searching for new materials through computer simulations. This would bring down the time-to-market, and cut the developments costs. The increasingly-higher accuracy and predictive power of computer simulations, combined with growing levels of computing power and large amounts of storage capacity of High-Performance Computing (HPC) technologies, enable a paradigm shift in material design and discovery, in which every increasingly complex material behaviour will be addressed by easily-accessible, interdisciplinary, easy-to-use computational experiments. The focus must again be on the search process. In order to find new materials the search process should be open, multidirectional (as in the case of 3M), with the possibility of

adjusting the target according to the search process itself and of ending up with something different from what expected by innovators at the beginning.

> **MaX (Materials design at the eXascale)** has been conceived and established to significantly speed up the material innovation cycle. **MaX** is a user-driven European Centre of Excellence supporting developers and end-users in materials simulations, design and discovery. It focuses on enabling the best use and evolution of HPC technologies by creating an open ecosystem of knowledge, capabilities, open software applications, data workflows, analytic tools and user-oriented services.

At the same time, **MaX** enables the exascale transition in the materials domain by developing advanced programming models and novel algorithms, as well as new business and delivering models suitable for HPC technology, to make the search of new material easily available to researchers and innovators.
MaX is designed and managed to support the needs and the visions of a number of players: *end-users in research and innovation* (both in industry and academia) who explore materials discovery and rely on computer experiments; *domain scientists* who develop new methods, algorithms and tools in materials simulations; *software engineers and vendors*, who optimise hardware and software performance and usability along with analytical tools for increasingly efficient computer-assisted materials design; *HPC centres and industry* that are interested in empowering the most advanced solutions and in hardware-software co-design.
The **MaX implementation strategy** consists in developing a new ecosystem to serve industrial and academic community through end-user oriented actions, which include: implementing a sustainable programming platform designed to develop new software functionalities; building a Dynamic Data Framework (DDF) to manage the automation of workflows interchange where data provenance, preservation and reproducibility are guaranteed - incidentally, DDF is crucial to implement both a material search open process, where data and workflows can easily be shared and reused among innovators, as well as to efficiently perform combinatorial (High Throughput Computing) search for new materials; promoting the exascale transition through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design; establishing the user needs and solutions integrating protocol by aligning the technological offer with leading end-users requirements; developing a catalogue of services accommodating end-users support, communities' integration, industrial outreach, and custom development; contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of training and education programs combining HPC and material science.
MaX acts as a central service hub providing project management, coordination and dissemination for each project partner, shifting and reducing costs by sharing resources and effort. To guarantee the quality of the provided services, **MaX** maintains toolsets, templates, and documentation of best practices, procedures, and techniques.
A number of pilot cases are currently being developed in **MaX**, in connection with leading industrial partners (for the search of innovating materials in the production of food, batteries, lubricants and energy). These will constitute the basis for a 'market-place' where solutions developed for a given problem will be made available and tailored to other end-users: such a process is expected to enable rapid response to short-term issues, and is particularly interesting for SMEs.

MaX Partners include five research institutions (CNR Modena, SISSA Trieste, ICN2 Barcelona, FZ Jülich, EPFL Lausanne) and five supercomputing centres (CINECA Bologna, ETH/CSCS Zürich/Lugano, FZ Jülich, KTH Stockholm, BSC Barcelona) plus one global research & education institution (ICTP Trieste). Two business partners specialised in hardware solutions and open source technologies are also involved: E4 Computer Engineering (Italy) and CloudWeavers (UK).
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