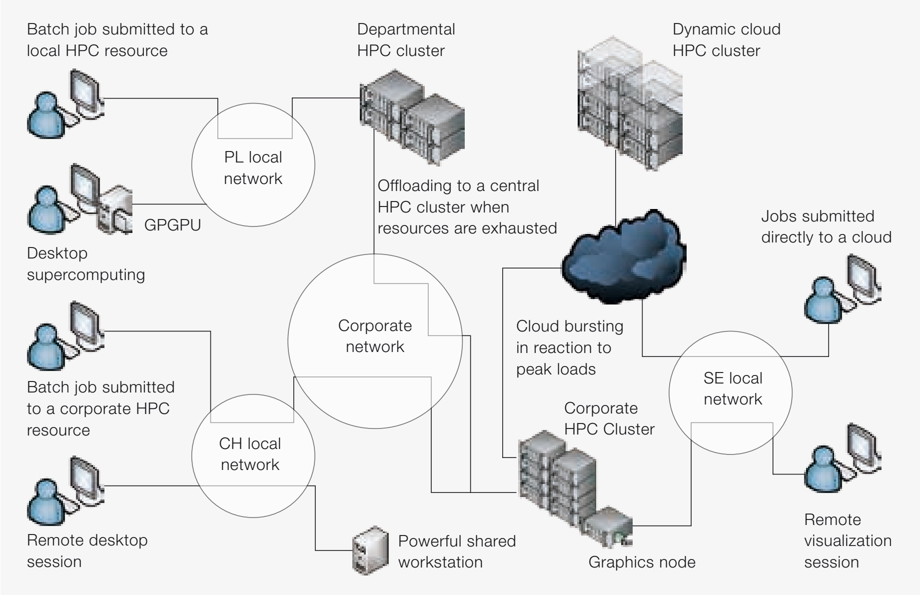
Resisting obsolescence

The changing face of engineering simulation

BARTOSZ DOBRZELECKI, OLIVER FRITZ, PETER LOFGREN, JOERG OSTROWSKI, OLA WIDLUND – One of the many benefits of computer simulation is the ability to solve complex industrial problems quickly and relatively cheaply. Computer simulation is an evolving field, and the interplay between research in numerical methods and developments in computer architecture is ensuring progress. Recent changes in the landscape of information-processing technology have been characterized by increasing parallelism in this regard. Many simulation tools are now able to utilize tens of computing cores to solve bigger and more complex problems with increased accuracy in practical timescales. In addition to commercial simulation packages and customized ABB proprietary tools that are developed in-house, there is also a growing number of tools developed by open-source communities. What are the forces influencing such changes in simulation in engineering applications?

1 Future landscape of computational infrastructure for simulations



Infrastructure diagram mixing the current state with possible future directions

Simulation is an important element of product development at ABB – compared with physical prototyping, it is often faster, less expensive, more detailed and better able to provide innovative ways of solving complex industrial problems. So how is this achieved?

Clusters, clouds and desktop supercomputing

The key to simulation is, quite simply, high-performance computing (HPC). With this in mind, ABB has invested in its own computational clusters over the years. Today the company has a number of dedicated HPC resources available internally. While large HPC systems allow simulation of the most complex products, they are not the only computational resources used by simulation experts.

Commoditization of high-end computing, together with the multicore revolution, brought parallel scalability to the desktop. Many simulations are being performed locally on fat workstations (ie, one computer does all the computation). For a while it seemed that a desktop simulation approach – ie, bringing supercomputing to the desktop – would become prevalent with the emergence of GPU (graphics processing unit) accelerators dedicated to number crunching, but this disruptive technology has yet to deliver on the front of engineering simulations.

Another emerging force with the potential to reshape the simulation infrastructure is the rapid development of publicly available data centers, which provide computational power on demand using a pay-per-use charging model. This new model of outsourcing infrastructure is widely known as cloud computing.

General-purpose clouds are poorly suited for simulation workloads, which often require specialized networking solutions characterized by high bandwidth and low latency. However, some cloud providers design parts of their data centers with HPC requirements in mind. Initial cloud benchmarking experiments performed by ABB indicate that distributed-memory parallel applications with a moderate amount of message exchanges achieve satisfactory performance. Simulated cost projections based on historical usage data extracted from ABB's current HPC system suggest that moving suitable workloads to the cloud could halve the total cost of ownership for supporting infrastructure. The biggest hurdle with respect to corporate use of cloud computing is information security. Much work needs to be done in this area before engineering companies and their clients will be willing to store and process their data on an infrastructure that is outside corporate control.

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In the short term, a centralized HPC resource will likely be the most cost-effective solution. Such a resource may be augmented by smaller, localized departmental clusters. The potential landscape of the future computational infrastructure for simulations is presented in → 1. In the future, in addition to GPGPU (general-purpose GPU) powered workstations, there may be a more dynamic setup where peaks of activity are dealt with by transferring some of the load among corporate resources and using cloud bursting (ie, utilizing a public cloud) in cases where internal resources are exhausted.

Title picture
As information-processing capabilities evolve, so too do the simulation tools used to engineer new products.

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With the infrastructure in place, suitable processes need to be developed to ensure efficient use of available hardware and software resources.

Ensuring efficient resource utilization

The cost of investing in and maintaining HPC hardware is usually lower than the cost of licensing the simulation software. In order to dimension and use these limited resources efficiently, a balance must be reached among several factors: the number of available CPU cores, the hardware topology (shared or distributed memory), the cluster interconnect (communication speed), the number of available licenses and the configuration of queue systems (eg, to maximize throughput of batch simulations, but still have licenses available for daytime interactive use).

The weighting of these factors is influenced by the licensing model used by the software vendor. Usually one costly single-core license is consumed for each job, while each additional CPU (central processing unit) core consumes a cheaper HPC license. Most vendors have a degressive pricing for the HPC licenses, so that the cost per HPC license decreases with the number of licenses acquired. The pricing is usually such that it is desirable to run each simulation on as many cores as possible, for as short a time as possible, so that the costly single-core licenses are used as efficiently as possible.

Over the past eight years, an extensive collaboration has evolved within ABB for coordinating and sharing both hardware and software resources. This effort started rather informally with some of the larger simulation teams, but is now supported by the global IS/IT organization. The main objective is to be cost conscious, but sharing resources is also advantageous in other ways. For teams with low-volume usage, or for new users, it is possible to share the resources of other teams for a limited amount of time. This simplifies testing and evaluation of simulation tools and limits the initial investment. Especially for the corporate research centers, the ability to easily share hardware and licenses with business unit partners is very important for technology transfer within projects; users in the business units can easily get early access to the tools and models developed. Most software vendors have also recognized the benefits to them; eg, giving new users easy access to their products and gaining a better overview of customer needs.

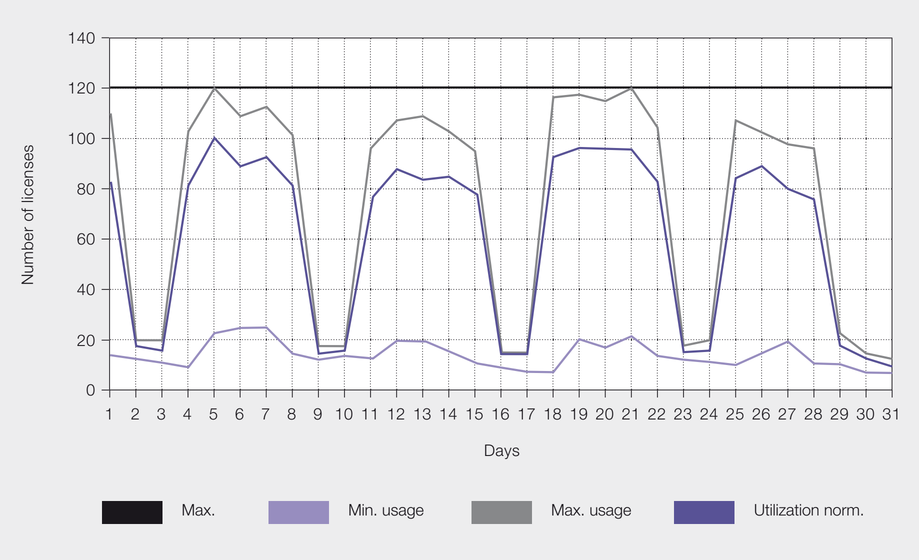
The ability to share software licenses across units and geographical locations usually involves special global-level contractual agreements with the software vendors. The advantage then is that ABB becomes a more visible customer. Today ABB has global contracts and license pools in place for several large simulation-software suites.

A good example of sharing of HPC hardware resources is the new Linux cluster ”leo” hosted by one of ABB’s corporate research centers. This cluster is used mainly for complex fluid mechanics simulations and molecular dynamics simulations. Leo is jointly financed by two corporate research centers, and is used by several teams in multiple countries. Another cluster, ”krak,” is financed and maintained by a third corporate research center, but for practical reasons is co-located with the leo cluster. Krak serves as a computational backend for the ABB Simulation Toolbox, a distributed system that provides the company’s worldwide business unit partners with transparent access to HPC resources.

Sharing of resources of course has its challenges. Some are of a technical nature and are usually easy to resolve, but there are many more difficult “soft” issues that must be addressed, eg:

- How to resolve conflicts
- How to accommodate for different usage patterns
- Determining who should pay for new resources when there is a shortage
- How to interpret license statistics

2 ABB's eLicense tool



The tool allows for optimal license utilization by giving invaluable input to the license purchase processes.

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As for sharing of software licenses, the key to success is to implement a well-defined process for the governance of the license pool; that is, to define common policies and rules for resource usage, anticipate potential problems and propose solutions. This could entail telephone conferences with representatives from all teams contributing to the pool, but there could also be a smaller group of people handling day-to-day issues. To ensure fairness and smooth conflict resolution, when needed, it is extremely important to collect and monitor usage statistics, and to make the information available to all users. For this purpose, ABB has developed a Web-based tool called eLicense for managing license pools and monitoring license usage ➔ 2.

Physical models and numerical methods

A starting point for any simulation tool is a mathematical model that describes the physical phenomena of the process. Once it is developed, a numerical algorithm that carries out the calculation of the model can be implemented.

Mathematical models and numerical algorithms are as important as the computer itself. For example, it would be impossible to compute the electromagnetic field in a transformer by choosing an atomistic model even on the fastest supercomputer. Instead, a model is created by averaging the behavior of atoms and electrons and deriving bulk material properties. This bulk description combined with the fundamental electromagnetic field equations (Maxwell's equations) results in a model that is suitable for the simulation of the electromagnetic fields in a transformer.

Still, this is not enough. After choosing a suitable model on an adequate level of simplification, the computer must be told how to calculate the model. This means an algorithm for solving the constitutive mathematical equations of the physical model on the computer must be chosen and implemented. This is called a numerical method. The finite element method is an example. The numerical method has to be chosen such that the computation is precise, fast and robust. A good computational method is a problem-dependent, well-coordinated combination of physical model, numerical method and hardware.

Classical simulation tasks in engineering include structural mechanics problems, fluid dynamics problems and electromagnetic field calculations. Good computational methods for these standard tasks are often available as commercial or open-source software products. Nonstandard simulation, however, requires the development of customized computational methods on all three levels – modeling, algorithms and hardware.

Complications can result from nonstandard material properties or from special geometrical settings. Nonstandard types of simulations include multiphysics computations, in which several physical domains have to be

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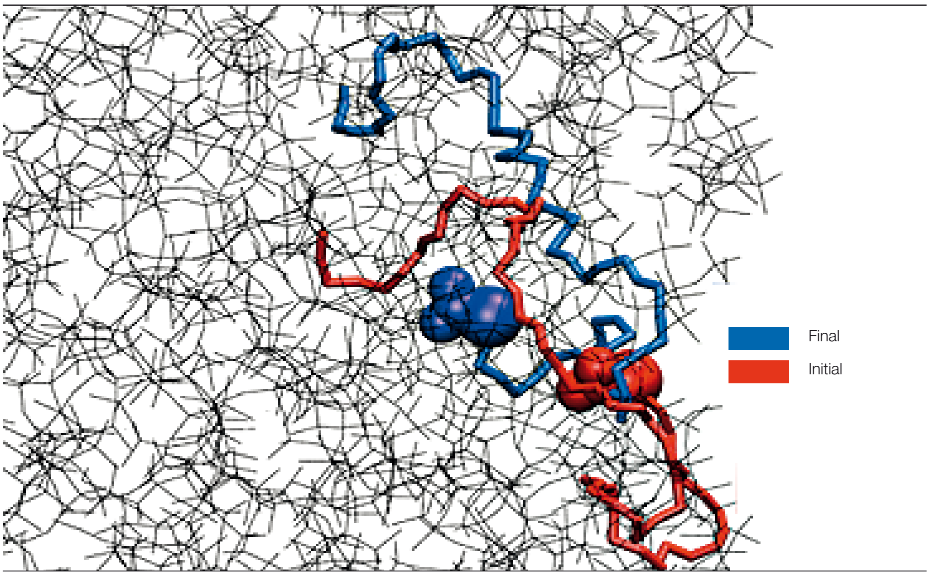
3 Molecular dynamics simulation



An initial and final orientation of a charged molecule near the surface of a PDMS insulator are shown. In the final configuration, the charged group is buried more deeply in the bulk.

coupled. The growing interest in these calculations forced commercial vendors to introduce this coupling into their products. However, for some combinations of physical phenomena there are no off-the-shelf solutions available or the existing ones are inefficient. An example of phenomena important in ABB products that are poorly supported by existing tools are arc processes, where fluid dynamics and electromagnetism have to be coupled.

Beyond the classical domains tractable with mesh-based methods, such as finite elements, are elaborate computational methods for molecular or even atomistic processes. The best known ones are the density functional theory (DFT) and molecular dynamics (MD). Although these highly advanced computational methods are not expected to become as important for ABB as they already are in the pharmaceutical industry, there is increasing ambition to apply these methods to resolve important material science questions. In the field of insulation for high-voltage AC and DC transmission systems, eg, they improve the microscopic picture of electric transport and other dynamic processes. A concrete application of the molecular dynamics method was recently developed in collaboration with IBM Research. Diffusion of lightweight molecules in silicone-rubber polymers (PDMS) was calculated to explain an important surface-hydrophobicity restoration process crucial for the long-term stability of HV outdoor cable insulation. As shown in → 3, a net orientation and polarization of molecules with methyl groups on the surface could be simulated. This result offers an explanation for the loss of surface hydrophobicity in the case of oxidation. It also explains the restoration of hydrophobicity through a particular interaction between cyclomethicone molecules, oxidized methyl groups, and Na+ ions.

ABB's path in a changing landscape

The breakthrough of cloud computing and GPU technology with respect to numerical simulation technology may be a long time coming, but parallel simulations on multicore computers and clusters are already essential.

By sharing hardware and software resources, different teams within a company can obtain easy and cost-efficient access to the latest simulation technology and hardware resources. At ABB this means R&D results and best practices can be efficiently transferred between its research centers and business units.

Market research reports invariably show that the most successful industrial companies are those that make use of modern numerical simulation tools in their product development. ABB engineers employ the most efficient tools and the most powerful models to give its customers the best possible products. When it comes to advanced customized simulation tools, the wheel will not be reinvented when there are already good tools available, but ABB's scientists will never hesitate to break new ground in areas where ABB has technology leadership.

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