**Quantum Chemistry.**

The ongoing integration of quantum technologies is one of the most anticipated developments for the armed forces. Yet, how exactly they will modify and disrupt military operations remains blurry. Commercial/economical applications and mainstream use are still years or decades away, but if employed at scale, quantum technologies could show a clear disruptive effect.

But while it’s an almost complete consensus that quantum technologies will show far-reaching effects for armed forces, intelligence communities and law-enforcement agencies, it is unclear how far the traditional balance of power among states (or even between non-state actors) will be altered.

Among the many aspects of quantum technologies, one can be clearly identified as game changing: quantum chemistry.

**Quantum Chemistry**.

*First a bit of definition.*

Quantum chemistry is the application of quantum mechanical principles and equations to the study of molecules. In order to understand matter at its most fundamental level, it’s necessary to use quantum mechanical models and methods.

There are two aspects of quantum mechanics that make it different from previous models of matter. The first is the concept of wave-particle duality; that is, the notion that it’s necessary to think of very small objects (such as electrons) as having characteristics of both particles and waves. Second, quantum mechanical models correctly predict that the energy of atoms and molecules is always quantized, meaning that they may have only specific amounts of energy. Quantum chemical theories allow an explanation of the structure of the periodic table, and quantum chemical calculations allow accurate predictions of the structures of molecules and the spectroscopic behavior of atoms and molecules.

*But why quantum chemistry?*

The ability to predict chemical reactions & processes using computational simulations is seen as a potential major improvement, with great benefits to chemists. Currently, most of the chemical research is done through trial and error processes. It’s long, painful and it doesn’t allow for fast developments. The predictive capabilities of a quantum algorithm would open the door to the study and development of a large panel of new materials, nanomaterials and metamaterials with novel properties.

*So why doing such computational simulations on quantum computers and not on classical hardware?*

Current hardware lacks the exponential scaling required for such simulations. Classical computing isn’t suited for the factorization of large digits and can’t process data both horizontally and vertically. The current generation of quantum technology is not yet ready to tackle such difficulty, of course, but physicists and computer scientists believe it will get there in the near future.

In the meantime, several companies, including Google and IBM, are increasing their investments in research toward the use of quantum computers once they mature. In this new project, a team at Google AI Quantum focused their efforts on a simple chemical process, the Hartree-Fock approximation of a real chemical system. Here, they simulated a diazene molecule undergoing a reaction with hydrogen atoms, resulting in an altered configuration.

*What would be the applications of quantum chemistry?*

Quantum chemistry allows a completely new view on matter and elements. By understanding the quantum mechanics ruling the particle interactions inside elements, it becomes possible to tweak, modify and even alter those elements, creating new versions of existing materials or even brand-new ones. In terms of defense applications, the possibilities are wide, from new stealth materials deviating radio waves to be “radar-invisible” to light bending materials designed by rearranging matter at the nanoscale level. It’s currently impossible to map the entire scope of applications opened by quantum chemistry, but there’s already a good idea of the advantage it might provide.

On a hardware perspective, the simulation of new materials with novel conducting properties and lower cooling threshold could lead to a new generation of electronic, more performant and with low power consumption, which would in turn feed the development of future computing technologies, in a virtuous circle.

Purely military speaking, the ability to simulate materials with desired capabilities instead of resorting to “accidental discoveries” might lead to the development of new capabilities in armor, stealth or aerodynamics. By precisely simulating chemical interactions in order to design a fully tailored material, researchers could create compounds with unknown capabilities (self-repair, complete heat dissipation, cloaking, self-assembly, the list goes on). In terms of military hardware, this would be invaluable, both strategically and economically speaking.

Quantum chemistry might also have an impact on biotechnology, biodefense and pharmaceutical developments. The ability to simulate molecular dynamics gives the opportunity to create new compounds, new medication, with an unprecedented degree of control on the reactions at the atomic and molecular levels. This could lead to an entire new area of medicine, mixing biotechnology, nanotechnology and delivery systems.

*In conclusion*.

In terms of impact and future developments, quantum chemistry is one of the most – if not the most – promising fields among quantum technologies as it doesn’t just improve capabilities and performances, but open the door on new areas of research, widening our understanding of matter and giving chemists a larger control on materials definition. If correctly developed, this field might impact all the strategic technological areas, from soldier enhancement to aerospace innovation and semiconductor design.