SCIENCE IN SOCIETY

MARRIED IN LOCK-DOWN: HOW BEING FORCED TOGETHER HAS TAKEN OUR RESEARCH FURTHER

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COVID-19 hit big science hard. While research across the globe pivoted to SARS-CoV-2 to fight the pandemic, national lockdowns closed most science facilities around the world to other fields of research.

Almost all of the research buildings and laboratories at Europe's flagship neutron source, Institut Laue-Langevin (ILL) in Grenoble, France, were closed – bar preparation for crucial COVID-19 experiments – and while most of my colleagues ended up in isolation from their scientific partners, research teams and essential resources, I found myself in a new environment of scientific collaboration – with my husband, Luigi Genovese.

My research at the ILL focuses on the use of small-angle neutron scattering (SANS) techniques for the study of biological molecules, which helps us to explore biological structures such as enzymes in solution and the impact of proteins on normal cell function. Meanwhile, my husband is a computational physicist at CEA Grenoble, head of the Atomistic Simulation Laboratory.

We had sought to collaborate and bring together our knowledge of theoretical physics with experimental biology, even before the pandemic[1]. Faced with lock-down, we had even more motivation to continue in this direction.

We realised that his work on density functional theory (DFT), a popular and rapidly expanding quantum modelling technique, could be used to complement information coming from the types of neutron experiments I was conducting, on large-scale structures such as enzymes.

And in turn, my research could help him – data from neutron scattering could be used to enhance the realism and accuracy of quantum simulations performed by DFT physicists.

Working as a pair, and remotely with our research teams, we began to explore this melting pot of physics, chemistry, and biology, and adapted what we'd learnt from each other to help study the virus that was keeping us locked in the house. We rapidly shifted our research to simulate crucial components of SARS-CoV-2[2], including the main protease and spike protein, responsible for the infiltration of the virus into human cells.

This attracted a great deal of interest from outside our shared office and even respective scientific communities, and we began a daily collaboration with two new groups, in Oxford and Paris, in addition to our previous co-workers in Boston and Kobe. An interest sparked by discussion in our kitchen over dinner had rapidly become a multi-disciplinary world-wide collaboration, spurred by the incredible response of the scientific community in the face of this global threat.

As scientists, we are always on the hunt for opportunities to collaborate, but until now an obvious collaboration had sat waiting to be put to good use. Now we have helped to forge a path for our two disciplines to collaborate more in future, with plenty of reflections and some big obstacles to overcome, including:

- ***Language*** – researchers from different communities need to commit to understand each other's terminology. A fragment in biological terms might be a far cry from fragmentation in computational physics, as we learned through our numerous misunderstandings. A DFT 'geek', like my husband has a tendency to use plenty of jargon when explaining the concepts of our collaborations. While preparing for interactions with our collaborators, I was often the one who translated his messages such as to be captured by a broader audience.

- ***Accessibility*** – successful collaboration empowers both communities to explore the other's techniques. The DFT calculations needed to be user-friendly for people like me to independently input and process structures coming from neutron crystallography or Small Angle Scattering data, with an output that is easy to understand. Equally, my husband gained an appreciation for the difficulty in setting up and interpreting structural information from neutrons, despite the rewarding evidence at the finish line.

- ***Belief*** – pioneering an alliance between distinct scientific fields is no easy feat. There needs to be dedication to finding scientific parallels and applications of the new approach, despite many communities being set in their way of doing things. Scepticism about our tactics was commonplace, but we believed we could succeed in opening the doors to stimulating new research areas – despite the fact at this early stage we are providing more questions and considerations, not solutions.

Although our access to facilities had been restricted in lockdown, this approach developed over the past months has built the foundations for applying the DFT techniques to many biological systems, not only the coronavirus.

The expansion of these capabilities will be invaluable when the neutron source is back up and running – the ILL has always shown world-class leadership in the community of neutron experiments in biology – and we will be looking to apply these findings to the protein constituents of the coronavirus in order to drive future drug development and vaccine creation through the atomic visualisation of the pathogen.

The COVID-19 pandemic has fuelled some of the most inspiring and innovative research approaches ever seen, with scientists mobilising from far beyond medical and pharmaceutical laboratories. This scientific partnership highlights the opportunities we have to collaborate on discoveries across all aspects of our lives, not just in the lab.

We have the potential to expand our collective techniques to combat this global emergency and create innovative new fields of research in the process.

Questions:

- How can science institutions and journals facilitate more interdisciplinary collaboration in research moving forward?
- How readily do editors of peer-reviewed journals accept new and novel contributions, especially when they have not followed the structure of the accepted scientific paradigm?

Written by Viviana Cristiglio

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[1] https://doi.org/10.1016/j.copbio.2019.09.006

[2] https://doi.org/10.1063/5.0004792

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