COVID 19: The crisis and high-energy physics

Mar 30 2020

CERN COVID-19 Particle Physics Computing high-energy physics

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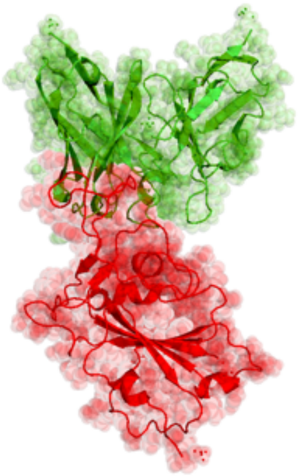
As the new coronavirus has infected hundreds of thousands of people around the world and continues to spread, leading the WHO to declare a pandemic, scientists and public health officials are racing to understand the virus and tackle the growing public health crisis. In this rapidly evolving situation, many unknowns remain about the new properties of the virus.

Perhaps two of the most crucial questions occupying virologists and drug developers in the fight against COVID-19 are: what makes the new virus so good at infecting people? and how does it reproduce so quickly? Understanding its biochemical and structural makeup is crucial for diagnosing infections, for developing and testing drugs and tremendously helpful for designing efficient vaccines.

These questions and the scale of the challenge has mobilized the high-energy physics community to spring into action. This is not surprising for a dynamic fast-moving field like particle physics with a long record of successes based on the interaction of calculation, inspiration, engineering, and tinkering. As Tedros Adhanom Ghebreyesus, the president of the WHO commented: “This is not just a public health crisis, it is a crisis that will touch every sector — so every sector and every individual must be involved in the fight” **[1]**.

Researchers have been working around the clock since the COVID-19 outbreak came to light to characterize the virus, and understand why it is so infectious. First reports of an unknown pneumonia were reported on the 31st December 2019 and by 11th January six virus sequences were made available to researchers. A few weeks later, on the 5th of February, a research team at ShanghaiTech University in China uploaded the structure of the virus’s main protease to the Protein Data Bank (DOI:10.2210/pdb6lu7/pdb), having obtained the dataset using X-ray crystallography at the Shanghai Synchrotron Radiation Facility. The above timescale is impressive given that just a decade ago we would need more than three months would have been required as was the case for the SARS coronavirus in 2003, and perhaps even a year for previous viruses like HIV.



A model of the SARS-COV-2 RBD (Receptor-Binding Domain) bound to a human antibody simulated thanks to the Folding@home project. (Image: Folding@home, CC BY-SA 4.0).

Acquiring such high-quality data within a short timescale was made possible thanks to advances in

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accelerator techniques and the development of new-generation synchrotron facilities and free-electron laser facilities around the globe. The combination of intensity and tunability makes synchrotron facilities a powerful all-purpose tool to get detailed information on the structure of the virus, providing unprecedented precision. Fundamental research for high performance future colliders have significantly reduced the costs for building and operating such facilities and boosted their performance, offering higher resolution and in parallel reducing the required running times. The role of experienced accelerator operators and experts in control systems should not be neglected, that maximize the reliability and availability of these infrastructures.

The role of accelerator physics in current efforts to tackle the COVID-19 outbreak are discussed in two recent articles in Physics World **[2]** by Jon Cartwright and in the CERN Courier **[3]** by Tessa Charles, an accelerator physicist at the University of Melbourne. The latter tells in some detail the story of the UK's DIAMOND synchrotron facility, one of the first to set up experimental trials for generating protein crystals and determine the atomic structure of the new virus. "With the huge numbers of data sets, they could pin down the parameters of the viral protease with a high degree of confidence. And with the synchrotron light source they were able to create and analyse the diffraction patterns rapidly. The same amount of data collected with a lab-based X-ray source would have taken approximately 10 years. At Diamond, they were able to collect the data in a few days of accumulated beamtime."

As of today, several synchrotron facilities contribute in mapping molecules that could work against the virus, and the community has published calls enabling researchers working on these studies to gain rapid access to beamtime. The website www.lightsources.org offers a rich repository of access policies and open calls for proposals. Structures of the CoV-2 spike protein, the primary target of most medical approaches, have already been solved by crystallography or electron cryo-microscopy (cryo-EM) techniques by groups at facilities in Europe, United States and China.

Researchers are sequencing both the novel coronavirus, by focusing on several tell-tale features of the virus, and the genomes of people with COVID-19 to understand, among other things, the spread of the disease and who is most vulnerable. Efforts are ongoing to analyse the genetic template for spike proteins, armatures on the outside of the virus that it uses to penetrate the outer walls of human cells and reproduce in our body.

Protein structure simulations are a computationally intensive effort that requires large computing resources. Citizen science projects like Folding@Home and Rosetta@Home use numerical calculations to resolve the 3D structure of such proteins. Folding@home **[4]** provides a distributed computing network that allows people to donate their idle PCs running at homes and offices for globally distributed processing. There has been a roughly 1200% increase in contributors according to Folding@Home with 400,000 new members since the middle of March. The distributed computing project is now working with about 470 petaflops in its quest to fold proteins, enough to eclipse the world's top seven supercomputers combined. HEP people are collaborating with them and other initiatives, bringing in their expertise in tackling large scale high performance computing problems and computing centres, including CERN, are offering specific resources where needed.

Fast data sharing and analysis are key for tackling the current COVID-19 outbreak. Scientists around the world are using platforms like ZENODO at CERN to effectively share open data and information. Initiatives like Science-Responds.org take advantage of the internationally linked high-energy physics community to exchange information about ideas and projects, to establish contacts with experts, in an effort to help fight the disease. People are engaging themselves in public hackathons like the upcoming versusvirus.ch to develop community solutions for a broad spectrum of questions, from strategies and tools to prevent spreading the virus, to using data to fight fake news.

Data scientists from within our community work are reaching out to epidemiologists and medical experts, to help them in their data analysis and modelling efforts. However, when turning our attention to healthcare data we need to remember how crucial it is to ensure that information is interpreted and visualised appropriately. Amanda Makulec **[5]**, an expert in healthcare visualisation reminds us that "the stakes are high around how we communicate about this epidemic to the wider public" and stresses the necessity of "always understand the context of the data you're working with, but is essential when creating and sharing visualizations during an epidemic where those visualizations have the potential to incite panic just as much as they have the potential to inform."

In the face of this global crisis, the global high-energy physics community - a community with a long-standing tradition of international collaboration - is offering resources, technologies and useful expertise to fight the pandemic. CERN as a global centre of excellence in scientific research has established a dedicated task force "CERN against COVID-19" to draw from the numerous proposals of the community and to help turning them into well-coordinated projects to maximise their impact profiting of the large network of CERN collaborations with laboratories, universities and industries. Among the many proposals received the ones concerning rapidly manufactured ventilator systems, availability of CERN computing resources for protein search for fighting the virus and manufacturing of full or parts of 3D printed masks are the ones that have been already addressed, while educational proposals and many others are being worked on very actively in this moment.

Stay home. Be safe.

References:

[1] WHO DG's Opening Remarks at a Media Briefing on COVID-19 on the 11th of March 2020:

https://www.who.int/dg/speeches/detail/who-director-general-s-opening-remarks-at-the-media-briefing-on-covid-19---11-march-2020

[2] "How Physics is helping fight the pandemics" by Jon Cartwright (Physics World, April 2020 issue): https://physicsworld.com/a/covid-19-how-physics-is-helping-the-fight-against-the-pandemic/

[3] "Synchrotrons on the coronavirus frontline" by Tessa Charles (CERN Courier, April-May 2020 issue): https://cerncourier.com/a/synchrotrons-on-the-coronavirus-frontline/

[4] "Coronavirus - What we're doing and how you can help in simple terms) by Greg Bowman: https://foldingathome.org/2020/03/15/coronavirus-what-were-doing-and-how-you-can-help-in-simple-terms/

[5] "Ten Considerations Before You Create Another Chart About COVID-19" by Amanda Makulec (The Medium, 11 March 2020): https://medium.com/nightingale/ten-considerations-before-you-create-another-chart-about-covid-19-27d3bd691be8