Science and Technology Facilities Council

Hartree Centre

Accelerating elastomer innovation through digital-first materials design

STFC Hartree® Centre and IBM collaborated with Falcon Project Ltd through the Hartree National Centre for Digital Innovation (HNCDI) to develop digital workflows that support faster, safer exploration of advanced elastomer materials using computer simulation.

Challenge

Elastomeric binders are a key component in high-performance applications such as composite rocket propellants. Their performance depends on a complex combination of factors, including polymer structure, how additives are dispersed, and how the material responds to mechanical stresses. Recent advances in energetic polymers offer opportunities to improve performance, but testing new formulations is difficult. Traditional experimental approaches are slow, costly and can pose safety risks due to the energetic nature of the materials involved. Specialist facilities are often required, limiting how many candidates can be explored. Falcon Project Ltd needed a safer, faster way to assess and refine new material formulations without relying solely on physical testing.

Approach

We developed automated digital workflows that enable polymer materials to be built, tested and analysed virtually. These workflows use computer simulations to model material behaviour at a molecular level, providing insight into properties such as strength, flexibility, compatibility between components, and surface adhesion. The project delivered reusable tools to generate realistic digital representations of polymer systems and simulate how they behave under different conditions. By running these virtual experiments, the team was able to explore how changes in material composition affect performance without producing physical samples. Although developed to meet The Falcon Project Ltd's specific needs, the workflows were designed to be modular and have already been applied in other HNCDI projects.

> **"We are in an exciting time where computer simulations are capable of leading R&D experiments and the highly skilled team at the Hartree Centre have enabled Falcon to further this journey by creating future options and possibilities for the UK."**

Professor, Ken Lewtas
The Falcon Project Ltd.

Credit: Adobe Stock

Benefits

The project established a digital-first approach to materials development that reduces cost, time and risk in early-stage research. The Falcon Project Ltd can now screen more material candidates safely and focus physical testing on the most promising options. The tools developed have wider relevance across sectors such as aerospace, automotive and advanced manufacturing, where performance, safety and sustainability are critical. By enabling earlier insight into material behaviour, the project supports better decision-making and accelerates innovation.

At a glance

- Faster, safer exploration of elastomer materials
- Automated digital workflows that enable polymer materials to be built, tested and analysed virtually
- Digital-first approach reduces cost, time and risk in early-stage research
- Work has wider relevance across sectors like aerospace, automotive and advanced manufacturing

The programme

The Hartree National Centre for Digital Innovation is a collaboration between the Hartree Centre and IBM which offers a safe and supportive environment for UK organisations to explore the latest digital technologies and skills, develop proofs-of-concept and apply them to industry and public sector challenges.

Who we are

The Hartree Centre was created by UK Government to help businesses and public sector organisations accelerate the adoption of high performance computing (HPC), big data analytics, artificial intelligence (AI) and quantum technologies. We play a key role in realising UK Government's Industrial Strategy by stimulating applied digital research and innovation, creating value for the organisations we work with and generating economic and societal impact for the UK. We are proud to be part of UK Research and Innovation.

What we do

- Boost productivity and innovation for industry
- Offer training and skills development
- Provide insights into future technologies
- Give tailored business development support