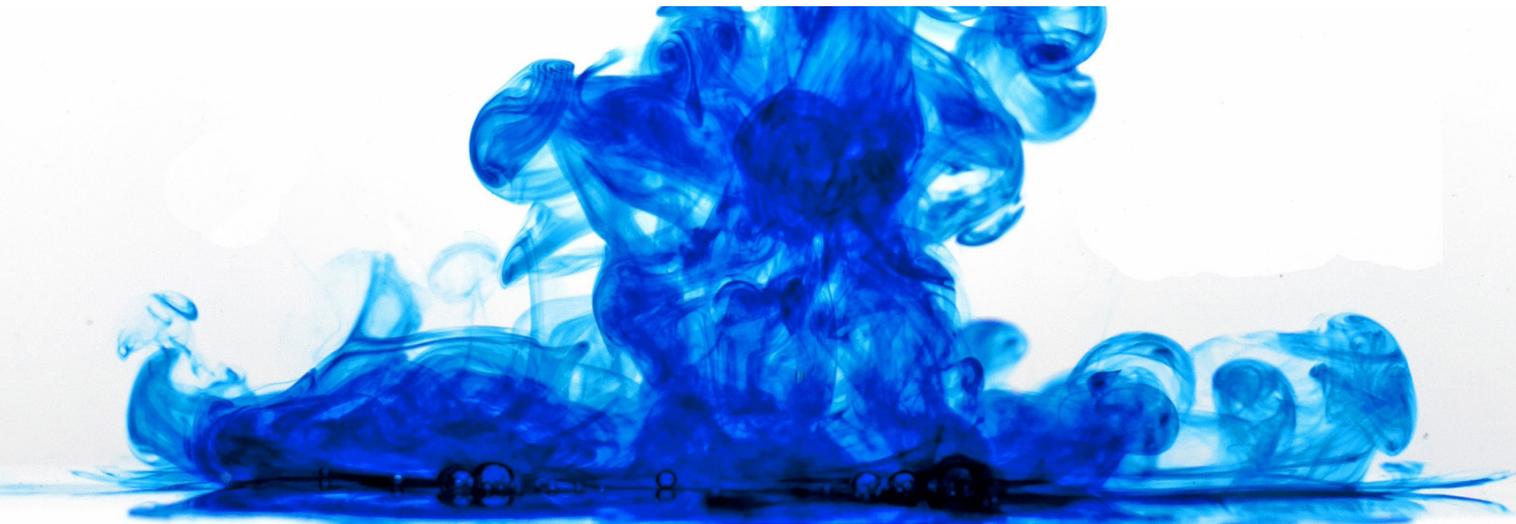


# Tailoring computational fluid dynamics software



Hartree Centre  
Science & Technology Facilities Council



**Mass spectrometer manufacturer Waters is capitalising on a Knowledge Transfer Partnership (KTP) with the STFC Hartree® Centre to add a new dimension to its computing capabilities, enhance product offerings and boost its market share.**

## Challenge

Waters designs and manufactures state-of-the-art mass spectrometry systems, widely used in the pharma, chemical, food and other industries to measure substances' unique chemical 'fingerprints'. In this fiercely competitive market, the key to success is to add new types of functionality to the systems – a complex, time-consuming process that can require years to develop a sales-ready product upgrade. Even using powerful simulation software, the company has only been able to model potential system improvements in isolation from each other. To integrate new components simultaneously and seamlessly into its products and cut time to market, Waters needs to achieve a step change in the speed, sophistication and versatility of its modelling and simulation capabilities.

## Solution

Waters recognised the potential to achieve this goal by tapping into the Hartree Centre's exceptional suite of software skills and hardware facilities. With 50% funding from Innovate UK, a 3-year KTP is providing full-time support for a Hartree Centre expert to tailor ANSYS Fluent software – a widely used computational fluid dynamics (CFD) tool – to the company's specific needs. The KTP is also enabling Waters to run simulations on multiple compute cores at the Hartree Centre (running simulations of the required scale in-house would simply not be viable) as well as providing access to a range of supporting specialist expertise (e.g. in Monte Carlo simulations used to model molecular gas interactions with ions).

## Benefits

The Hartree Centre's input is equipping Waters to layer a variety of user-designed functions onto the basic Fluent software package. This makes it possible, for example, to integrate the effects of key parameters (e.g. electrostatic field, space charge and flow field) on ion motion into its mass spectrometry systems, resulting in improved electrospray source models. Waters is confident that the KTP will enhance the performance of its product offerings and increase its share of key instrument markets.

*"Our work with the Hartree Centre has, in particular, enhanced our ability to predict the behaviour of ion populations in atmospheric pressure ion sources."*

– Dr Steve Bajic, Senior Research Scientist, Waters

## Work with us

We collaborate with industrial clients and research partners on projects that create insights and value using high performance computing, big data analytics, simulation and modelling.

By combining our world-class facilities with access to our specialists and computational scientists, we can enable your organisation to produce better outcomes, products and services more quickly and cost-effectively than through conventional R&D workflows.

With our partners we are developing the next generation of supercomputing architectures and software, combining existing best practice with innovation to deliver faster, cooler and more sustainable solutions capable of meeting the challenges of data intensive computing.

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