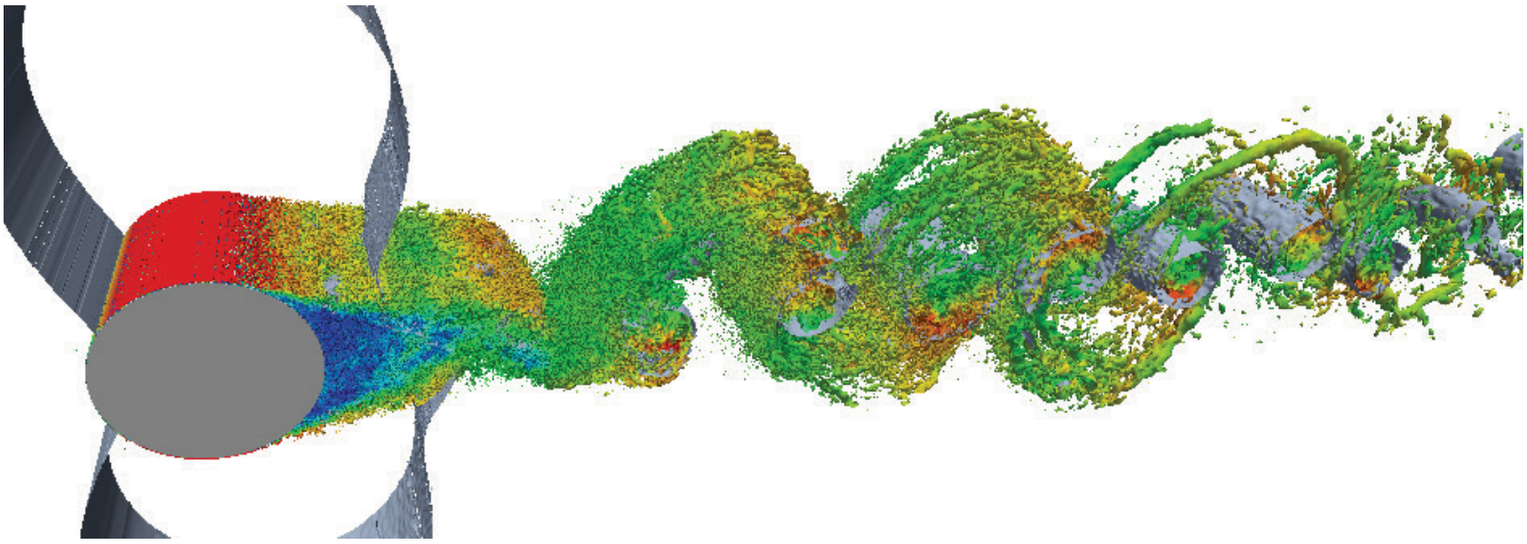
CASE STUDY Enabling new frontiers in CFD research at Argonne with the Mira supercomputer

arm DDT



Argonne NATIONAL LABORATORY

CTTC UPC

Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

CHALLENGE

Demands of more complex CFD projects require massive scale that only leadership facilities provide

PROBLEM

Software defects that only occur on running with tens of thousands of cores must be debugged

SOLUTION

Arm DDT enables fast straightforward interactive debugging at scale

RESULTS

Massive CFD simulations have become possible at over 131,000 cores - a 20x increase in capability

Fluid dynamics researchers using Argonne's supercomputer, Mira, are simulating more complex physics as a result of collaboration between Argonne and Arm on scalable development tools

Scientists at the Heat and Mass Transfer Technological Center (CTTC) at the Technical University of Catalonia in Spain are developing software to simulate projects that range from the design of efficient wind turbines and 3D printer technology, to the solution of thermal problems in electronic devices.

Their main area of activity involves numerical simulations performed with an in-house multi-physics CFD code known as TermoFluids.

Using the capabilities of simulation software to tackle larger and more complex simulations is no easy task. Algorithms and code must change to fully utilize the performance of high-performance computing (HPC) systems.

PREPARING CFD FOR SCALE

'This is not a trivial undertaking,' Ricard Borrell, the research manager behind TermoFluids, explained. 'To provide CFD at the highest level, generally computing requirements grow faster than the complexity of the simulation under consideration. The better we can take advantage of the power of the newest HPC systems, the more complex systems we can understand - more accurately and in less time.'

Borrell had the opportunity to participate at the Argonne Training Program for Extreme Scale Computing (ATPESC). This intensive training programme is offered by the Argonne Leadership Computing Facility (ALCF) with an emphasis on core skills and approaches for the execution of applications on leadership-class computing systems.

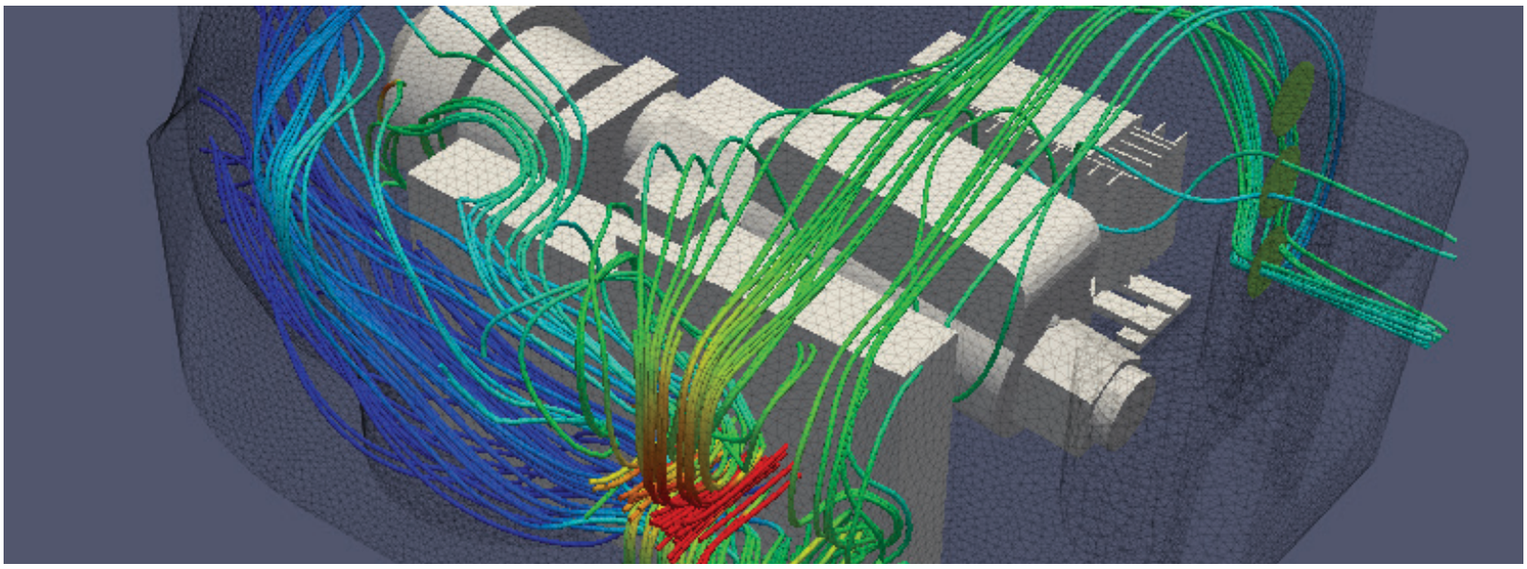
ONE OF THE WORLD'S FASTEST SUPERCOMPUTERS

Any researcher in the world can apply for time on ALCF's supercomputer, Mira; a 10-petaflops IBM Blue Gene/Q supercomputer equipped with 786,432 processors. Not only is Mira one of the fastest supercomputers in the world, as ranked by the Top500 list, but it is backed by a team of computational scientists, performance engineers, and hardware experts devoted to helping users get the most out of the system.

SCALING TO 20X AND BEYOND

Borrell was able to use Mira to test the performance and scalability of its

arm



"Extracting full performance is critical if you want to handle more complex problems, finer resolutions and achieve new frontiers – and you'll need DDT to do it."

code at the first level of parallelization based on a distributed memory model and MPI communications. 'Before accessing Mira, TermoFluids had been used on production simulations up to around 5,000 CPU cores and scalability tests up to 10,000 CPU cores,' he commented.

'On Mira we have increased this figure by an order of magnitude and have now run the code up to 131,072 CPU cores. Not only did this include the most time-consuming part of the simulations, i.e. the time-integration, but other aspects that can become critical overheads such as the pre-processing, the simulation set-up, and IO operations for check pointing as well.'

THE UNEXPECTED HAPPENS AT SCALE

Through Mira, the code could be run on much larger problems up to billions of unknowns. This required some changes, such as avoiding integer overflows errors. When achieving this order of magnitude leap in the size of the problem and number of parallel processors being used, Borrell encountered new problems in the code that only appeared at this larger scale. Given that the issues couldn't be reproduced on a smaller scale in order to find the bugs, the team turned to a powerful debugger, Arm DDT.

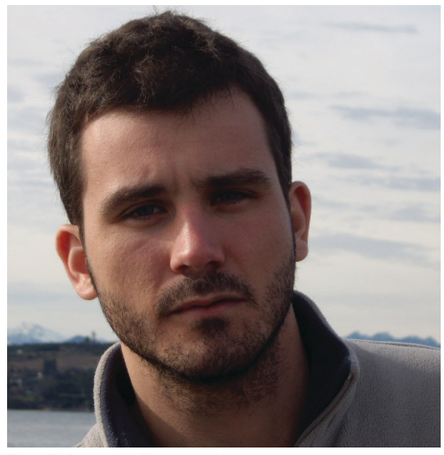
AN ESSENTIAL TOOL OF SCIENCE

'Debuggers are essential tools for our users as they scale their application on Mira. There have been several instances where users have leaned on a debugger to find issues as they have scaled on the system.' Kalyan Kumaran, Manager, Performance Engineering at ALCF, explained.

'Arm scaled their debugger to perform well on leadership class systems like ours. This helped us to choose this tool as we were looking for a debugger that would scale to the entire Mira system.' He added that as most ALCF users access the systems remotely, a remote connection client such as Arm's is important for ease of use.

Every year, ACLF holds the Mira Performance Boot Camp to help users improve and scale their codes for the supercomputer. At the workshop, tools developers like Arm work with attendees individually to show them how the tools can benefit their applications.

'The training allowed us to see the what DDT could do for us,' Borrell remarked. 'The most important aspect for us was that the tool provides visibility of what precisely is happening on large simulations and where the problems are appearing. We saved a lot of time by not only locating bugs and errors incredibly quickly, but by being able to go directly to them in order to solve the issues.



Dr Ricard Borrell

ACHIEVING NEW FRONTIERS

'I recommend that everyone start using DDT as it's invaluable for delivering guidance to errors, as well as a better understanding of your code. Without this tool there to reveal those gaps in your code, you could be missing out on a lot of performance.'

Borrell concluded by adding: 'High-performance computing resources like Mira give developers like us the power to go further. Extracting that full performance is critical if you want to handle more complex problems, finer resolutions and achieve new frontiers – and you'll need DDT to do it.'

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Contact Details: www.arm.com/hpc-tools
UK +44(0)1926 355 280 US +1(408) 576-1500
email: sales-hpc-sw@arm.com