

HPC Is Brain Surgery: Cray® XC30™ Supercomputer Shows Future Clinical Benefits as Development Tools Partner Helps Application Reach Petascale

Organizations



Leading HPC users turn to Allinea Software for extremely scalable, capable and intuitive tools to improve the efficiency and value of their HPC investment by reducing development time and increasing application performance.

www.allinea.com



CRESTA (Collaborative Research into Exascale Systemware, Tools & Applications) is a collaborative research effort funded by the European Union exploring how to meet the exaflop challenge.

www.cresta-project.eu



The University of Edinburgh is one of Europe's leading research universities. It is the project coordinator of the CRESTA proposal and is represented in this project by its supercomputing center, EPCC.

www.epcc.ed.ac.uk



The CCS is concerned with many aspects of theoretical and computational science, from chemistry and physics to materials, life and biomedical sciences as well as informatics.

ccs.chem.ucl.ac.uk

Cray Inc.
901 Fifth Avenue, Suite 1000
Seattle, WA 98164
Tel: 206.701.2000
Fax: 206.701.2500
www.cray.com

Situation

The HemeLB research group at University College London (UCL) has an exciting vision, one that will change the way neurosurgeons operate in the future and improve outcomes for patients.

The group develops software to model intracranial blood flow – and a collaboration with Cray and Allinea Software, a Cray development tools partner, is helping them address the challenges of application development at high scale.

UCL's HemeLB software applies computational fluid dynamics to model blood flow around cerebral vessels and simulate pressure at points of weakness, such as aneurysms. Using data from MRI scans of a patient's blood vessels, the group anticipates that simulations will one day help them decide the best clinical option for individual patients.

Challenge

Presently, MRI scans are small, reduced models. But as large-scale supercomputing grows in affordability and capability, simulations will be of clinical value – helping caregivers determine the best course of action within the right time frame for the patient.

Today, the UCL team use ARCHER, the U.K.'s flagship Cray® XC30™ system. ARCHER is managed by the Edinburgh Parallel Computing Centre (EPCC) on behalf of EPSRC and other U.K. research councils.

ARCHER's 3,008 nodes each hold two Intel ES-2697 Ivy Bridge CPUs with 12 cores, making a system total of 72,192 cores. It is one of the world's Top 25 machines by capability.

The Cray XC30 supercomputer enables UCL to accelerate its science – but in their effort to run the application at this extreme scale, the developers found new challenges that required software-driven solutions.

Many of today's large supercomputers have around 100,000 CPU cores or more – and yet, of all the parallel applications that can run on the machines, precious few can use even close to that number of cores simultaneously. Without development, codes will run slower or may not run at all and crash.

The HemeLB application crashed when using 50,000 processor cores. The crash stopped the team in their tracks.

"The crash was totally unexpected," says post-doctoral researcher Derek Groen. "I didn't know how I would diagnose or fix it at that scale – it was beyond anything I had tried to do before."

Solving bugs at scale

Allinea Software, one of Cray's solution partners, provides a suite of scalable debugging and performance profiling tools that are designed to help developers address those challenges. Tools from Allinea Software are integral to the user environment provided by ARCHER.

The UCL team and Allinea Software were brought together by the EU CRESTA project – which is preparing applications for future extreme-scale computing.

Allinea DDT is the only parallel debugger that handles applications running at those ARCHER levels of process counts – and higher. Even at 100,000 cores, it is as fast and interactive on a Cray XC30 system as debugging a single workstation application. Its user interface simplifies the vast concurrency so developers can spot problems easily.

In Groen's case, debugging all 50,000 application processes simultaneously soon identified the point of the crash and its root cause.

"Getting HemeLB to scale to 50,000 ARCHER cores is a real achievement," says Professor Peter Coveney, Director, Centre for Computational Science, UCL. "We are thankful for the productive collaborations we enjoy with Allinea Software that have allowed us to reach these intoxicating heights, which are enabling us to study hemodynamics within the Circle of Willis [a cerebral arterial circle] for the first time."

Increasing performance

With all the bugs resolved, the UCL team were eager to improve the code's overall performance, too.

Allinea Software's profiling tool, Allinea MAP, explained the performance at a glance. A simple adjustment avoided an I/O bottleneck, enabling the application to scale successfully – and improving performance on those cases by over 25 percent.

"We'd never been able to look at this many cores – and get a clear view of how the time was being used. We were keen to see it in Allinea MAP," Groen adds.

A rich environment

"Seeing HemeLB used at this scale on ARCHER is very impressive and highlights the success of the co-design approach used by UCL and Allinea Software on the CRESTA project," says Dr Lorna Smith, CRESTA project manager and deputy director of the ARCHER CSE team.

"This achievement with Allinea Software is a great example of the importance of providing a rich tooling environment for our users on ARCHER."



CRAY XC30 SUPERCOMPUTER:

The Cray XC30 series is an adaptive supercomputing architecture that provides both extreme scalability and sustained performance, with offerings across the supercomputing performance and price spectrum.

allinea

Allinea Software Inc.
2033 Gateway Pl Ste. 500, San Jose,
CA. 95110 USA
Tel: +1 (408) 884 0282

www.allinea.com • info@allinea.com

Allinea Software Ltd.
The Innovation Centre, Warwick Technology Park,
Gallows Hill, Warwick CV34 6UW UK
Tel: +44 (0)1926 623 231 Fax: +44 (0)1926 623 232

For more information about Allinea Software tools, to request a quote or a demo, visit www.allinea.com