Case Study: Laboratoire J.A. Dieudonné

"Using vSMP Foundation from ScaleMP, we were able to grant our researchers access to a computing resource capable of running any type of code: multi-threaded, MPI-parallel, or using large memory, at a lower cost and with better performance than any of the alternatives we reviewed."

Jean-Marc Lacroix, Network and System Administrator, HPC, Laboratoire J.A. Dieudonné

The J.A. Dieudonné Laboratory use-case

A single, cost-effective HPC solution for a wide and diverse group of researchers using a variety of HPC application profiles

BACKGROUND

Located in the beautiful city of Nice in the south of France, the J.A. Dieudonné laboratory is a mixed research unit supported by two organizations:

- The National Center for Scientific Research (CNRS)
- The University of Nice Sophia Antipolis (UNS)

The research at the laboratory spans from fundamental mathematics to applied mathematics. Most of the researchers use computers intensively for their simulations.

The laboratory focuses on the following research domains:

- Algebra, geometry and topology
- Geometric analysis and dynamics
- EDP and numerical analysis
- Numerical modelling and fluid dynamics
- Probability and statistics
- Interfaces of mathematics and complex systems

The laboratory's research teams are the key users of the lab's HPC infrastructure for computer simulations.

The laboratory implements a policy seeking to promote and support the interaction of mathematics with other disciplines. It hosts many non-mathematician teachers and researchers, and has partnered with INRIA, CEA and EDSFA. (http://math.unice.fr/laboratoire/equipes-de-recherche)

A shared SMP resource with 140 cores and 448GB shared memory, capable of running workloads ranging from thread-parallel OpenMP programs to MPI cluster jobs and large memory jobs. A single, cost-effective resource, fitting all application profiles

"Forklift upgrades are history. We were able to upgrade part of the underlying hardware, reuse other parts, and continue to use the same versatile SMP license. The same functionality remained, performance was increased and the savings were great!"

THE CHALLENGE

The laboratory caters to a variety of researcher computing needs, while operating on a very tight HPC infrastructure budget. The computing needs are driven by the variety of applications in use, for which the underlying software architectures and operational models include:

- Serial codes simulations that need a lot of memory
- MPI distributed codes
- OpenMP thread-parallel codes
- Other multi-threaded codes

The laboratory could not afford to set up a separate computing system per each class of workload, so a single, cost-effective system that could handle all HPC challenges was needed.

THE SOLUTION

In order to meet requirements of the research community supported in the laboratory, the team surveyed the available technologies and solutions, and selected a solution comprising of ScaleMP's vSMP Foundation and Dell servers. This solution covers any and all classes of simulations scenarios for an attractive cost/performance ratio. Additionally, the researchers highly appreciate the simplification of parallel code development on a single SMP machine.

The laboratory deployed its first generation of ScaleMP's versatile SMP system in 2009. It upgraded the underlying Dell servers in 2014 for its second-generation versatile SMP system, boasting 140 cores running at 2.80GHz, and 448GB shared memory (essentially, seven Dell servers, 14 x Intel Xeon E5-2680 v2, and Mellanox 40Gb/s InfiniBand). This is yet another unique feature of vSMP Foundation: No longer does one need to "forklift upgrade" an SMP resource. You can simply upgrade the underlying cluster hardware, and continue using the existing interconnect and software, further extending the life of your IT investments.

SUMMARY

The J.A. Dieudonné laboratory selected vSMP Foundation for its HPC infrastructure to enable its researchers to run any type of scientific application — distributed, thread-parallel and large memory — utilizing a cost-effective cluster solution from Dell, and transformed it into an SMP system by ScaleMP's technology.

As a long-time ScaleMP client, an additional benefit was the ability to upgrade the underlying Dell servers, while maintaining the software and interconnect stacks, thus further extending the life of investments made in scientific IT equipment to serve researchers for many years.

Scientific Results Obtained With the Versatile SMP

Below is a non-exhaustive list of publications, conferences, theses and contracts that have extensively used the computer resources of the vSMP Foundation-based SMP of the J.A. Dieudonné laboratory.

These works mainly concern fluid mechanic, plasma physics and numerical methods development for scientific computing. These codes are mainly serial codes using very large memory or distributed codes based on MPI, except Quantum Chemistry where OpenMP is used.

Fluid Mechanic / Plasmas / Numerical Methods

Publications

R. Pasquetti, Comparison of some isoparametric mappings for curved triangular spectral elements, J. of Comput. Phys., 316, 573-577, 2016.

R. Pasquetti, J.L. Guermond, B. Popov, stabilized spectral element approximation of the Saint Venant system using the entropy viscosity technique, in Lecture Notes in computational Science and Engineering: Spectral and High Order Methods Partial Differential Equations - ICOSAHOM 2014, R.M. Kirby, M. Berzins and J.S. Hesthaven Eds, Springer,397-404, 2015.

R. Pasquetti, N. Peres, A penalty model of synthetic micro-jet actuator with application to the control of wake flows, Computers & Fluids, 114, 203-217, 2015.

S. Minjeaud, R. Pasquetti, High order approximation of a tokamak edge plasma transport minimal model with Bohm boundary conditions, J. of Comput. Phys., 285, 84-87, 2015.

N. Peres, R. Pasquetti, SVV-LES and active control of flow around the square back Ahmed body, in ERCOFTAC Series: Direct and Large-Eddy Simulation IX, Jochen Fröhlich, Hans Kuerten, Bernard J. Geurts and Vincenzo Armenio Eds, Springer, 73-79, 2015.

A. Bonnement, S. Minjeaud, R. Pasquetti, Towards a Fourier-SEM solver of fluid models in tokamaks, Lecture Notes in Computational Science and Engineering: Spectral and High Order Methods for partial Differential Equations - ICOSAHOM 2012, 95, Springer, 169-178, 2014.

R. Pasquetti, F. Rapetti, Spectral element methods on simplicial meshes, Lecture Notes in computational Science and Engineering: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM 2012, 95, Springer, 37-55, 2014.

E. Serre, M. Minguez, R. Pasquetti, E. Guilmineau, G.B. Deng, M. Kornhaas, M. Schaefer, J. Froehlich, C. Hinterberger, W. Rodi, On simulating the turbulent flow around the Ahmed body: a French-German collaborative evaluation of LES and DES, Computers & Fluids, 78, 10-23, 2013.

L. Lazar, R. Pasquetti, F. Rapetti, Fekete-Gauss spectral elements for incompressible Navier-Stokes flows: The two-dimensional case, Comm. in Comput. Phys., 13, 1309-1329, 2013.
J.L. Guermond, R. Pasquetti, A correction technique for the dispersive effects of mass lumping for transport problems, Comput. Methods Appl. Math. Engrg., 253, 186-198, 2012.
L. Biancofiore, F. Gallaire, R. Pasquetti, Influence of confinement on obstacle free turbulent wakes, Computers & Fluids, 58, 27-44, 2012.

Scientific Symposiums

R. Pasquetti, S. Minjeaud, Fourier-spectral element approximation of the ion-electron Braginskii system with application to tokamak edge plasma in divertor configuration, 2nd frontiers in Computational Physics: Energy sciences, Zurich, June 3-5, 2015.
N. Peres, R. Pasquetti, Large-eddy simulations of controlled wake flows using a penalty model of synthetic micro-jets, GAMM 86th Annual Scientific Conference, Lecce (Italy), March 23-25, 2015.
R. Pasquetti, Entropy viscosity stabilized spectral element approximation of the shallow water equations with dry-wet transitions, ICCP 9, Singapore, January 7-11, 2015.
R. Pasquetti, J.L. Guermond, B. Popov, stabilized spectral element approximation of the Saint Venant system using the entropy viscosity technique, ICOSAHOM 2014, Salt Lake City, June 23-27, 2014.
N. Peres, R. Pasquetti, Numerical investigations on wake control using synthetic micro jets, Aero vehicle 1, Bordeaux, June 23-25, 2014.
R. Pasquetti, High order finite elements for partial differential equations: The Fekete-Gauss approach, workshop “Challenges in medical imaging: Numeric, High Performance Computing, Inverse Problems”, Univ. of Strathclyde, Glasgow, May 21-23, 2014 (Invited lecture).
N. Peres, R. Pasquetti, Micro-jets synthétiques et contrôle de sillages : Modélisation et Simulation, Workshop CNRT - R2A, Recherche en Aérodynamique et Aéroacoustique des Véhicules Terrestres, Paris, Janvier 22, 2014.
S. Minjeaud, R. Pasquetti, A Fourier-SEM solver of fluid models in tokamaks, 15th European Fusion Theory Conference, Merton College, Oxford, September 23-26, 2013.
N. Peres, R. Pasquetti, Numerical study of drag reduction of a car model by active control using micro-jets, CFM 2013, Bordeaux, August 26-30, 2013.
N. Peres, R. Pasquetti, SVV-LES and active control of flow around the square back Ahmed body, DLES 9 workshop, Dresden, April 3-5, 2013.
S. Minjeaud, R. Pasquetti, Fourier-SEM solver of fluid models in tokamaks, HONOM 2013 workshop, Bordeaux, March 18-23, 2013.
R. Pasquetti, L. Lazar, F. Rapetti, Fekete-Gauss TSEM and application to incompressible flows, Int. Conf. on Mathematical Modeling, Analysis and Computation (ICM2AC), Xiamen, China, July 21-25, 2012 (Invited lecture).
R. Pasquetti, A. Bonnement, S. Minjeaud, Towards a Fourier-SEM solver of fluid models in tokamaks, ICOSAHOM 2012, Gammarth (Tunisie), June 21-25, 2012.
A. Bonnement, H. Guillard, B. N’Konga, R. Pasquetti, Modèle de type fluide volumes / éléments finis pour la simulation du plasma de bord des tokamaks, CANUM 2012, SuperBesse, 21-25 mai 2012.

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Thesis

A. Bonnement, Modélisation numérique fluide du plasma de bord des tokamaks (projet ITER), UNS, co-directeur H. Guillard (03-07-2012).

Post-Docs / ANR project

N. Peres, 2 years long (2012-2014), in the frame of the ANR project LIVECAMS devoted to the use of synthetic micro jets to decrease the drag coefficient of vehicles.

Quantum Chemistry

Publications

P. Cassam-Chenaï, Y. Bouret, M. Rey, S. A. Tashkun, A. V. Nikitin, VL. G. Tyuterev, Ab initio effective rotational Hamiltonians: A comparative study, International Journal of Quantum Chemistry, 112, p.2201-2220, (2012).

P. Cassam-Chenaï, A. Ilmane, Frequently Asked Questions on the mean field configuration interaction method. I- Distinguishable degrees of freedom, Journal of Mathematical Chemistry, 50, p.652-667, (2012).

P. Cassam-Chenaï, J. Liévin, Ab initio calculation of the rotational spectrum of methane vibrational ground state, The Journal of Chemical Physics, 136, p.174309 (15 pages), (2012) and supplementary material.

P. Cassam-Chenaï, D. Jayatilaka, Contributions of the electronic spin and orbital current to the CoCl magnetic field probed in polarised neutron diffraction experiments, The Journal of Chemical Physics, 137, p.064107 (10 pages), (2012) and supplementary material.

P. Cassam-Chenaï, J. Liévin, An improved third order dipole moment surface for methane, Journal of Molecular Spectroscopy, 291, p.77-84, (2013) and supplementary material.

P. Cassam-Chenaï, G. Rousseau, A. Ilmane, Y. Bouret, M. Rey, Application of quasi-degenerate perturbation theory to the calculation of rotational energy levels of methane vibrational polyads, The Journal of Chemical Physics, 143, p.034107 (15 pages), (2015).

P. Cassam-Chenaï, B. Suo, W. Liu, Decoupling electrons and nuclei without the Born-Oppenheimer approximation: The Electron-Nuclei Mean-Field Configuration Interaction Method, Physical Review A, 92, p.012502 (15 pages), (2015).

Thesis

Thèse d'Amine ILMANE : Développements autour de la méthode de d'interactions de configurations en champ moyen. (Huge Quantum Chemistry computations using the CONVIV Code, with OpenMP; https://svn.oca.eu/trac/conviv).

ANR

ANR Cocoriso (demandée en 2016 toujours en course pour le 2ème tour): calculs de chimie quantique des spectres rovibronique de NH2 et ses isotopologues

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Dynamics / Particles

Publications

Approximated center-of-mass motion for systems of interacting particles with space and velocity dependent friction and anharmonic potential. A. Olivetti, G. Labeyrie, R. Kaiser, . Phys. Rev. E 89, 052120 (2014)

Long-range gravitational-like interaction in a neutral atomic cold gas (pdf) M. Chalony, J. Barre, B. Marcos, A. Olivetti, D. Wilkowski. Phys. Rev. A 87, 013401 (2013)

Algebraic damping in the one-dimensional Vlasov equation (pdf) J. Barré, A. Olivetti, Y. Y. Yamaguchi J. Phys. A: Math. Theor. 44 405502 (2011); preprint: math-ph. / 1104.1890

Breathing dynamics for systems of interacting particles in the micro-canonical and canonical descriptions A. Olivetti, J. Barré, B. Marcos, F. Bouchet, R. Kaiser Transport Theory and Statistical Physics (2011)

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