TOWARD ROBUST AND HIGH-FIDELITY MULTIPHYSICS MODELING ON PETASCALE ARCHITECTURE

Allocation: Exploratory/50 Knh
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EXECUTIVE SUMMARY

Demonstrating the exceptional level of parallel scalability of the massively parallel multiphysics finite element code Alya from the Barcelona Supercomputing Center (BSC) on the petascale architecture of Blue Waters was one of the major global high-performance computing (HPC) breakthroughs in 2015. The next step in this joint international work is to provide Alya with a fast and efficient direct solver to deal with solid mechanics simulations in which using an iterative solver together with preconditioning techniques is either too expensive or it does not converge to the desired solution. Research teams from the National Center for Supercomputing Applications, BSC, and IBM–Watson have been working jointly integrating the solver from IBM–Watson into Alya's multiphysics code. A numerically challenging problem of the buckling of thin structures was chosen to test the implementation of solvers from the Watson Sparse Matrix Package (WSMP) into Alya.

RESEARCH CHALLENGE

Complex physical problems for both applied fields and basic research, such as fluid dynamics, heat transfer problems, solid mechanics, or general transport equations, are often represented by partial differential equations that have to be discretized and solved numerically. This takes the continuum formulations of physics to systems of algebraic equations, and in order to obtain good approximations to the real-life solutions of such problems it is necessary to solve linear systems, such as Ax=b, with a large number of unknowns. The resulting matrices obtained from this discretization are very sparse (few nonzero matrix elements), ill-conditioned, and frequently are unsolvable by iterative solution methods.

METHODS & CODES

The WSMP [1] solver, developed by Dr. Anshul Gupta of IBM–Watson, is the first direct solver showing good scalability and robustness in dealing with problem sizes of millions of ill-conditioned equations on tens of thousands of processor cores on Blue Waters. This work, published by Drs. Korić and Gupta [2], was named by *HPCwire* as a top supercomputing achievement [3] at SC17.

Alya is the multiphysics code developed at the Computer Applications in Science and Engineering (CASE) department of the BSC. The code was built from the ground up to run efficiently in parallel, solve many different problems, and maintain programmatic ease. We used Blue Waters to evaluate the parallel performance of Alya for several coupled multiphysics applications such as airflow in the human body, contraction of the heart, and combustion in a kiln furnace. Alya showed good scalability up to 100,000 cores [4].

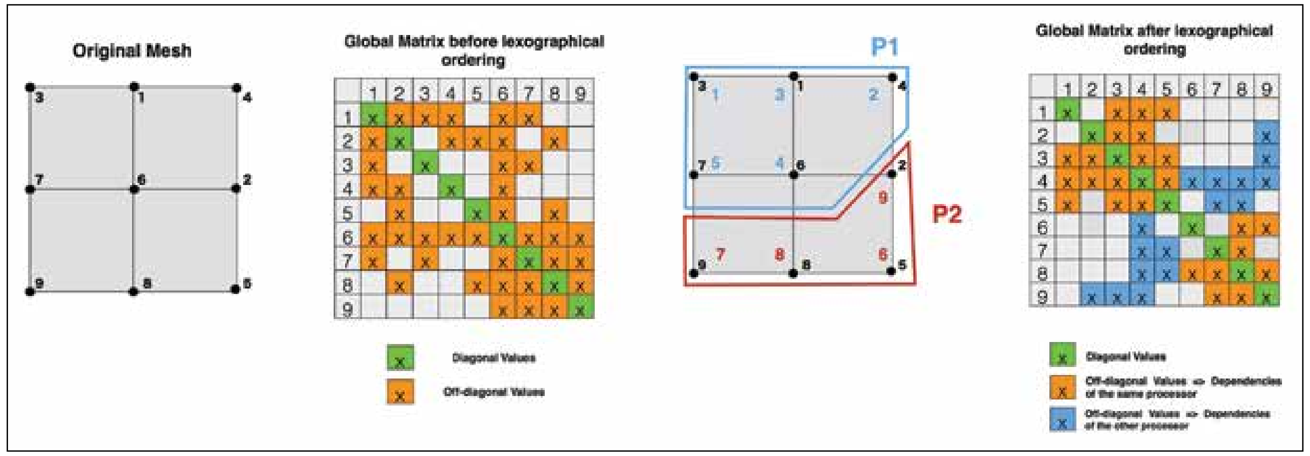

Figure 1: Global matrix structure before and after the lexicographical reordering

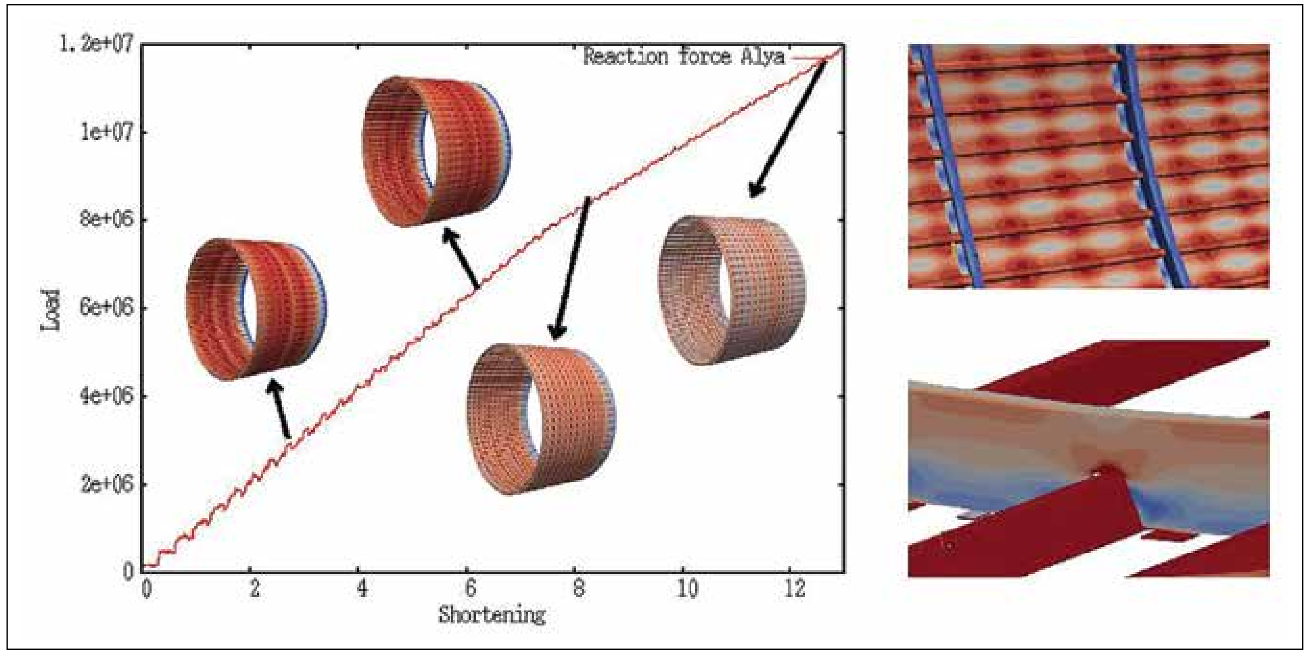

Figure 2: Fuselage barrel 4M mesh and results

Alya did not originally provide full and consecutive rows on interface nodes as required by WSMP. To achieve this, sequential processes must contain consecutive portions of the matrix, which we achieved by a lexicographical ordering. An example is shown in Fig. 1. Then, Alya's block compressed sparse row matrix format was modified to match WSMP's format. Finally, we integrated WSMP into Alya's workflow for symbolic and numerical factorizations as well as solution steps

RESULTS & IMPACT

We have validated the WSMP implementation in Alya while solving a challenging large ill-conditioned structural problem of great practical importance for society inside the Alya's Solidz module.

One of the main objectives in the structural analysis of thin structures such as fuselages has been to determine a panel's buckling and postbuckling capacity, trying to assure the structural integrity up to the ultimate load. Postbuckling determination for thin, curved panels in aero-structures becomes a critical factor in certification and generally requires very fine meshes to model the phenomenon. This is often beyond the regular finite element analysis software and HPC hardware resources.

We conducted a buckling and postbuckling analysis of a full fuselage barrel loaded in uniaxial compression (Fig. 2). The problem has been validated within the European project SHERLOC (CS2-AIR-GAM-2014-2015-01). The analysis is highly dynamic and nonlinear. In previous work, we generated a mesh of four million 3D solid elements with a high-aspect ratio to perform the finite element analysis using Alya [5]. The direct solver in Alya has provided a more efficient and robust solution than the iterative solvers.

WHY BLUE WATERS

Blue Waters is the only resource where massively parallel multiphysics codes such as Alya with the WSMP solver can be tested by taking full advantage of large amounts of distributed memory, hundreds of thousands of computing cores, and the low latencies and increased bandwidth of leading interconnect network technologies.

PUBLICATIONS & DATA SETS

Córdoba, P., et al., Petascale Level Multiphysics Modeling. *Workshop on Materials Computation* (University of Illinois, Urbana-Champaign, Ill., August 14–15, 2017).

Borrell, R., et al., Parallel mesh partitioning based on space filling curves. *Computers & Fluids*, 173 (2018), pp. 264–272.

Lu, Q., et al., Convergence Analyses for Fluid Structure Interaction Simulation in a Thin Hyper-Elastic Pipe. *International Conference on Computational Fluid Dynamics-ICCFD10* (Barcelona, Spain, July 9–10, 2018).