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# IMPROVING VIRTUALLY GUIDED PRODUCT CERTIFICATION WITH IMPLICIT FINITE ELEMENT ANALYSIS AT SCALE

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## EXECUTIVE SUMMARY

We continue advancing the state-of-the-art in implicit finite element analysis (FEA) by studying real-world models and identifying and removing scaling barriers. We study large-scale representative gas turbine engine models used in virtually guided certification to support physical engine testing, and for post-test validation of modeling and simulation techniques. Blue Waters is an enabling platform where massively parallel solver technology can be tested and advanced. Using it, we were the first to solve, in-core, an implicit LS–DYNA model with over 100 million finite element equations. While some of the challenges were known in the abstract, their details were only discovered by actually running at scale. Given the popularity of implicit finite element methods, the results of this effort will further expand the impact of high-fidelity multiphysics modeling of complex structures.

## RESEARCH CHALLENGE

Modeling and simulation have become increasingly important in both product design and support. Model complexity and size have increased accordingly, leading to longer runtimes for simulation software. The increase in runtime is not linear, but exponential. Research and development of modeling and simulation software are needed to improve its parallel scalability so that larger, more sophisticated models can be run with faster time-to-solution, informing and shortening the design cycle. Without improvements in scalability, high-fidelity analysis will remain a postdesign or pretest analysis without being integrated into the design cycle. The effort of scaling up is motivated by three broad industrial goals: improving product design, developing high-fidelity digital twins, and allowing for virtual certification for original equipment manufacturers.

## METHODS & CODES

LS–DYNA is an FEA software package used by a wide range of industries, including aerospace, automotive, biomedical, construction, and consumer products. It is used to analyze a diverse set of manufacturing problems such as the simulation of automotive collisions, explosions, manufacturing, and problems with large deformations. Commercially supported multipurpose codes are preferred by industry for product design and analysis. These codes provide important features, such as a rich library of elements, contact capabilities, nonlinear material constitutive models, mesh adaptivity, and flexible coupling.

Our work follows a measure–analyze–improve cycle using a large-scale real-life model. It is a continuation of the implicit analysis work started on Blue Waters in 2017 and builds on an even earlier examination of explicit analysis with LS–DYNA. Our cross-disciplinary research team involves members from NCSA, Rolls-Royce, Livermore Software Technology Corporation (LSTC), and Cray. Rolls-Royce, NCSA's Industry partner, provides large-scale, whole-engine FEA models (Fig. 1) having as many as 200 million degrees of freedom. These are representative of gas turbine engine problems used in virtually guided certification for risk mitigation, for supporting physical engine testing, and for post-test validation of modeling and simulation techniques.

## RESULTS & IMPACT

Multifrontal direct solvers are commonly the default solver technology in implicit FEM codes due to their generality and robustness. Their scaling has been investigated for decades. Solution of a sparse linear system by factoring is generally performed in four stages: reordering to reduce the required storage and number of operations in numeric factorization; symbolic factorization, in which the elimination tree is created; numeric factorization; and forward elimination and backward substitution. Previous work has usually ignored the reordering and symbolic factorization stages, which were often sequential.

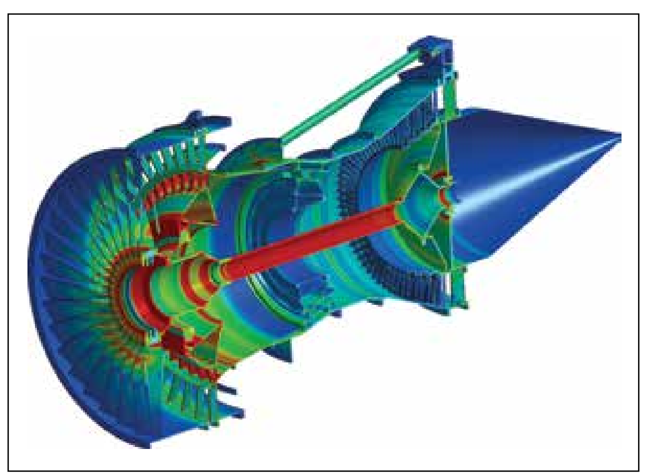

Figure 1: A cross-section of the jet engine model.

Scaling studies on Blue Waters show that the reordering and symbolic factorization stages are sequential bottlenecks, consuming a large and increasing fraction of the wall-clock time as the processor count grows. We have developed a new graph partitioning algorithm (LS–GPart) to replace Metis for sparse matrix reordering. Metis has been the default option for many years and was a sequential bottleneck in both time and memory. LS–GPart uses heuristics that aim to maintain the same quality regardless of the number of MPI ranks. Reordering scales well (Fig. 2a) and will do even better once OpenMP directives are added. The reordering stage has a significant impact on memory requirements and the number of floating-point operations of the factorization. The plot of the memory footprint and computation rate for factorization (Fig. 2b) shows scaling to 16,000 threads with hybrid (MPI and OpenMP) parallelization. We are continuing performance optimizations of the LS–GPart reordering and are also working toward eliminating the symbolic factorization sequential bottleneck.

We also discovered another scaling bottleneck in LS–DYNA that was unknown to its authors. Even a small Blue Waters configuration of 256 nodes exceeds that available to developers at LSTC or similar U.S. independent software vendors. By increasing to 2,048 Blue Waters nodes, the code was stressed in new ways, and a constraint processing function whose timing was heretofore insignificant suddenly emerged as a sequential bottleneck, growing with the number of processors. This too is now being addressed.

## WHY BLUE WATERS

Sparse direct solver algorithms in implicit FEM analysis are both computation- and memory-bound, as well as being communication-bound at large scales. While some of these challenges were known in the abstract, their details were only discovered when we tried to scale. Processing and memory bottlenecks revealed themselves as the number of processors increased by an order of magnitude beyond that familiar to today's developers and users. Many other scientific and engineering codes intended to run on high-performance computing platforms will have similar challenges. Blue Waters is an enabling platform where massively parallel sparse solver technology can be tested and advanced by taking full advantage of large amounts of distributed memory, thousands of multicore processors, and the low latencies and increased bandwidth of advanced interconnect technologies.

## PUBLICATIONS & DATA SETS

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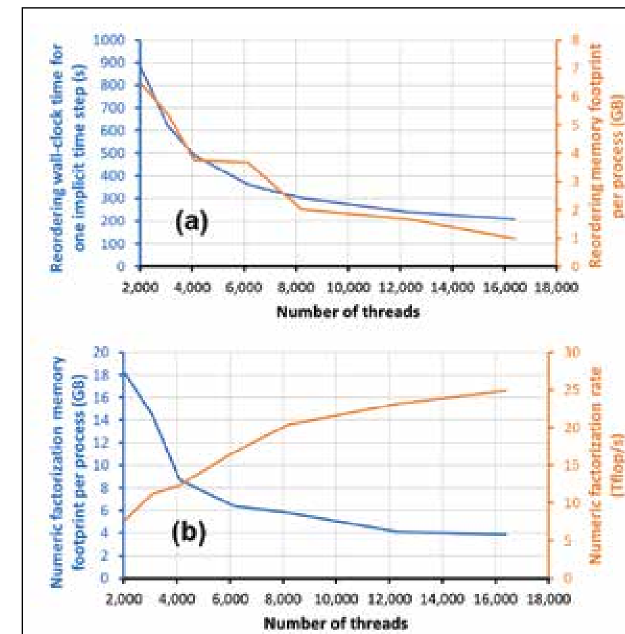


Figure 2: Scaling of sparse matrix reordering—(a) Scaling of numeric factorization, (b) A hybrid (MPI and OpenMP) parallelization model using eight threads per MPI rank. The finite element model has 105 million degrees of freedom.