Improving Virtual Prototyping and Certification with Implicit Finite Element Method at Scale

Seid Koric\textsuperscript{1,2}, Robert F. Lucas\textsuperscript{3}, Erman Guleryuz\textsuperscript{1}

\textsuperscript{1}National Center for Supercomputing Applications
\textsuperscript{2}Mechanical Science and Engineering Department, University of Illinois
\textsuperscript{3}Livermore Software Technology Corporation

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Seid Koric, Erman Guleryuz

Todd Simons, James Ong

Robert Lucas, Roger Grimes, Francois-Henry Rouet

Jef Dawson, Ting-Ting Zhu
Overview of the project

- **Today:** Virtual prototypes supplement physical tests in design and certification
- **Vision:** Further reduce cost & risk (Supplement → Replacement)
- **Immediate goal:** Increase impact of simulation technology
- **Impact of simulation** = \( f \) (speed, scale, fidelity)
- **Performance scaling** = \( f \) (code, input, machine)
- **FEM:** Partial differential equations → Sparse linear system
- **HPC strategy:** Sparse linear algebra → Dense linear algebra
- **Overall approach:** Scale-analyze-improve with real-life models

Rolls-Royce Representative Engine Model
Overview of challenges

More specific: These apply to LS-DYNA, and any other significant MCAE ISVs

- Large legacy code, cannot start from scratch, must gracefully evolve
- General-purpose code, cannot optimize for narrow class of problems
- Key algorithms are NP-complete/hard, need to depend on heuristics

More universal: These probably apply to any significant scientific or engineering code

- Limited number of software development tools, especially for performance engineering
- Increasing complexity of hardware architectures, combined with frequent design updates
- Performance portability constraints for codes used on many systems
- Limited HPC access, especially true for ISVs
Parallel scaling at the beginning of the Blue Waters project

100M DOF, Three implicit load steps

Time (seconds)

MPI ranks

Before, Hybrid (8 threads/MPI)
Improvement framework and progress highlights

- Memory management improvements
  - Dynamic allocation
- Existing algorithm improvements
  - Inter-node communication
- Previously unknown bottlenecks
  - Constraint processing
- Entirely new algorithms
  - Parallel matrix reordering
  - Parallel symbolic factorization
- Computation workflow modifications
  - Offline parsing and decomposition of the model
NCSA OVIS view of LS-DYNA execution

Free memory (GB) vs. Time (minutes)

- Input processing
- Sequential symbolic preprocessing
- Reordering
- Assemble, redistribute, factor and solve (2X)

105M DOF model, 256 MPI ranks, 8 threads each
Free memory on MPI rank zero’s node
Multifrontal sparse linear solver

\[
\begin{bmatrix}
K_{i-1}^{t+\Delta t}
\end{bmatrix}
\begin{bmatrix}
\Delta u_{i-1}^{t+\Delta t}
\end{bmatrix} =
\begin{bmatrix}
R_{i-1}^{t+\Delta t}
\end{bmatrix}
\]

Sparse linear system

Assembly tree of submatrices

**Multifrontal method:** Input processing > Matrix reordering > Symbolic factorization > Numeric factorization > Triangular solution
Results – Comparison with MUMPS factorization

11M Engine model
N=33.3M, NZ=1214.1M
Factors 216GB, ops 144 TFlops
LS-GPart nested dissection for eight processors
Results – LS-GPart matrix reordering quality

LS-GPart added to reordering comparison presented in “Preconditioning using Rank-structured Sparse Matrix Factorization”, Ghysels, et.al., SIAM PP 2018
Results - LS-GPart performance

Time (seconds)

Processor count

LS-GPart
ParMETIS
PT-Scotch
Results – New symbolic factorization performance scaling

~300 sec. in original sequential code
Results – Before and after Blue Waters engagement

100M DOF, Three implicit load steps

- Before, Hybrid (8 threads/MPI)
- After, MPP
- After, Hybrid (8 threads/MPI)
Results – Overall practical impact

- Finite element model with 200 million degrees of freedom
- Cumulative effect of better code and more compute resources
- Two orders of magnitude reduction in time-to-solution
- Work in progress for more practical impact
Future work and concluding remarks

- Industrial challenges are beyond the capabilities of today’s H/W and S/W!
- New design decisions based on finer grain analyses and more benchmarks!
- More scale will also couple with more physics!
- The right collaboration model accelerates progress!
- HPC access is critical in advancing the state of the art!
- Project benefits much broader community and sectors!
- Special thanks to Blue Waters SEAS team for technical support!
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