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

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Blue Waters Symposium 2019, June 5th

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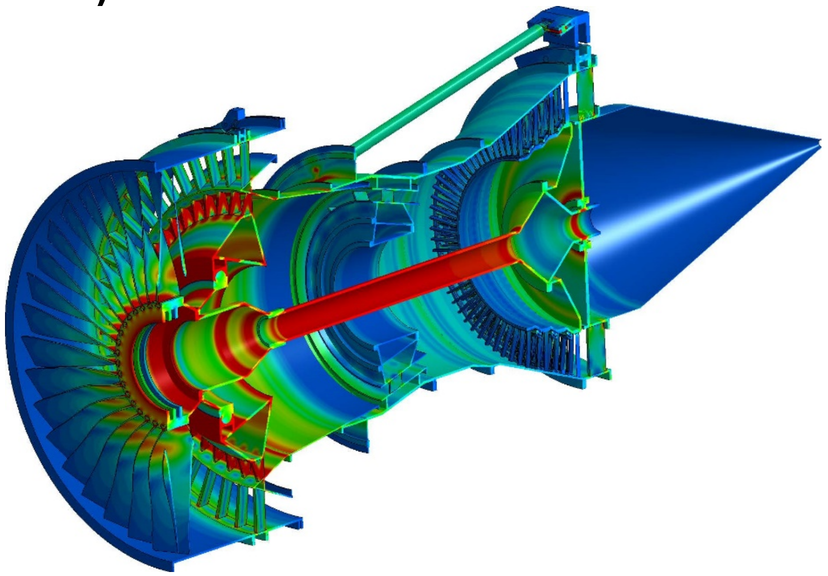
Rolls-Royce — Todd Simons, James Ong

LSTC Livermore Software Technology Corp. — Robert Lucas, Roger Grimes, Francois-Henry Rouet

CRAY — 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

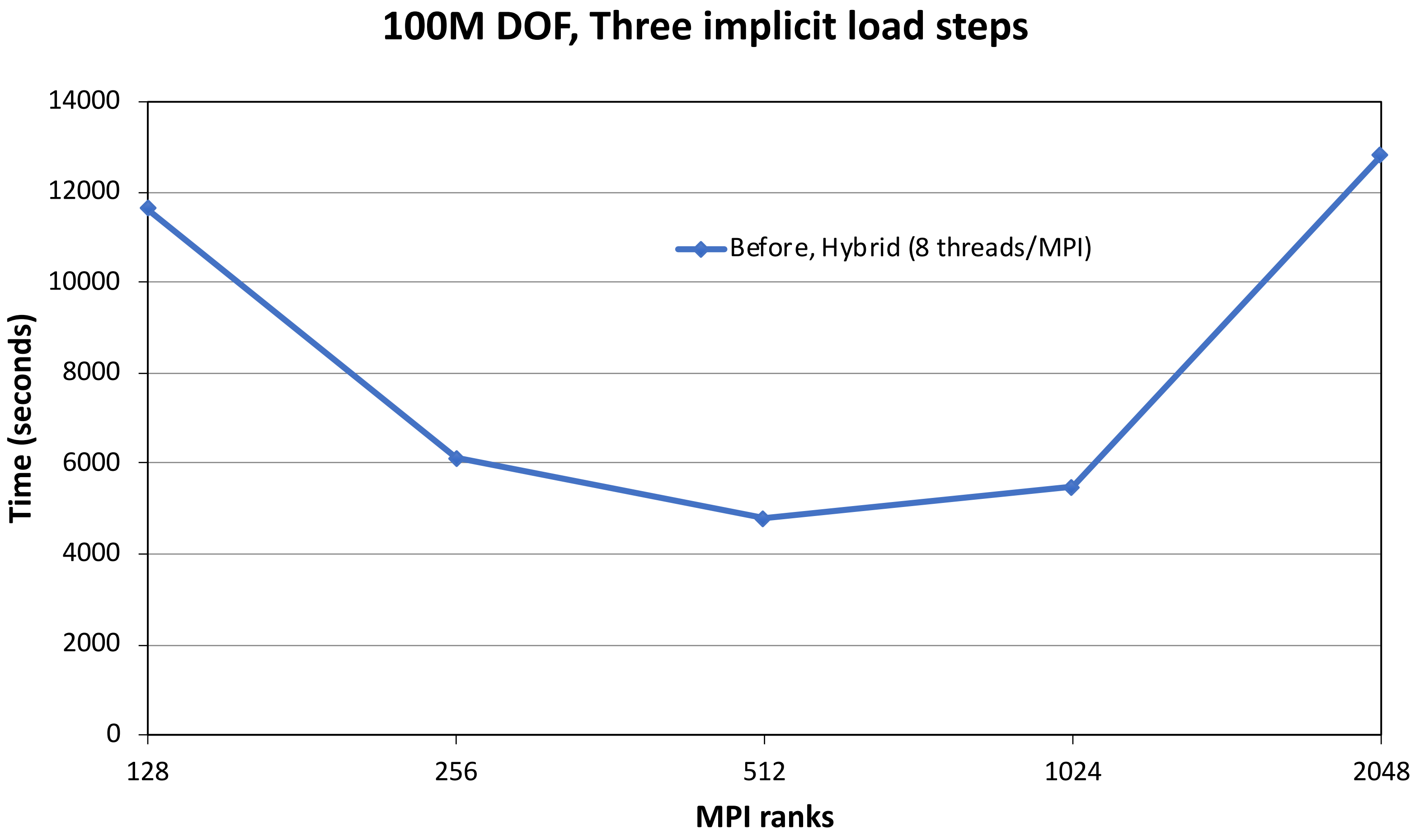


Rolls-Royce Representative Engine Model

Overview of challenges

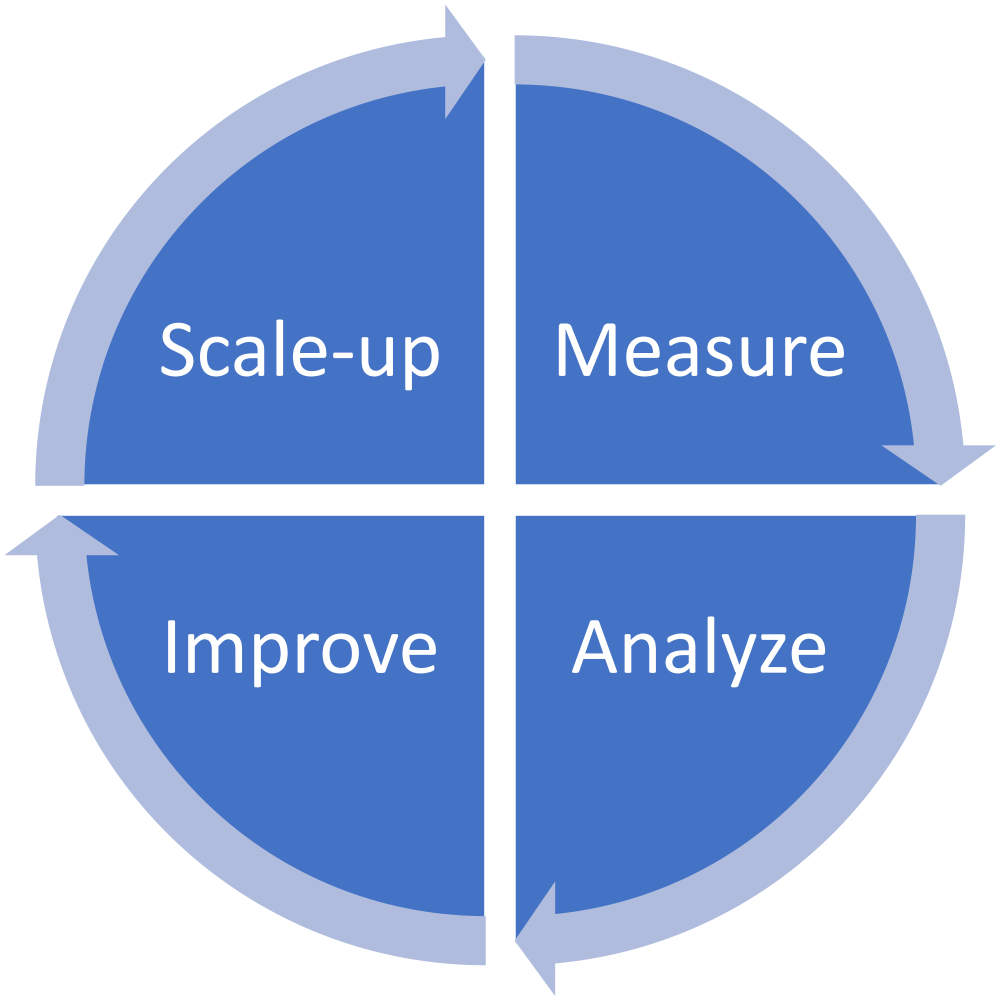
- **More specific:** These apply to LS-DYNA, and any other significant MCAE ISVs
  - Large legacy code, cannot start from scratch, must gracefully evolve
  - General-purpose code, cannot optimize for narrow class of problems
  - Key algorithms are NP-complete/hard, need to depend on heuristics
- **More 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

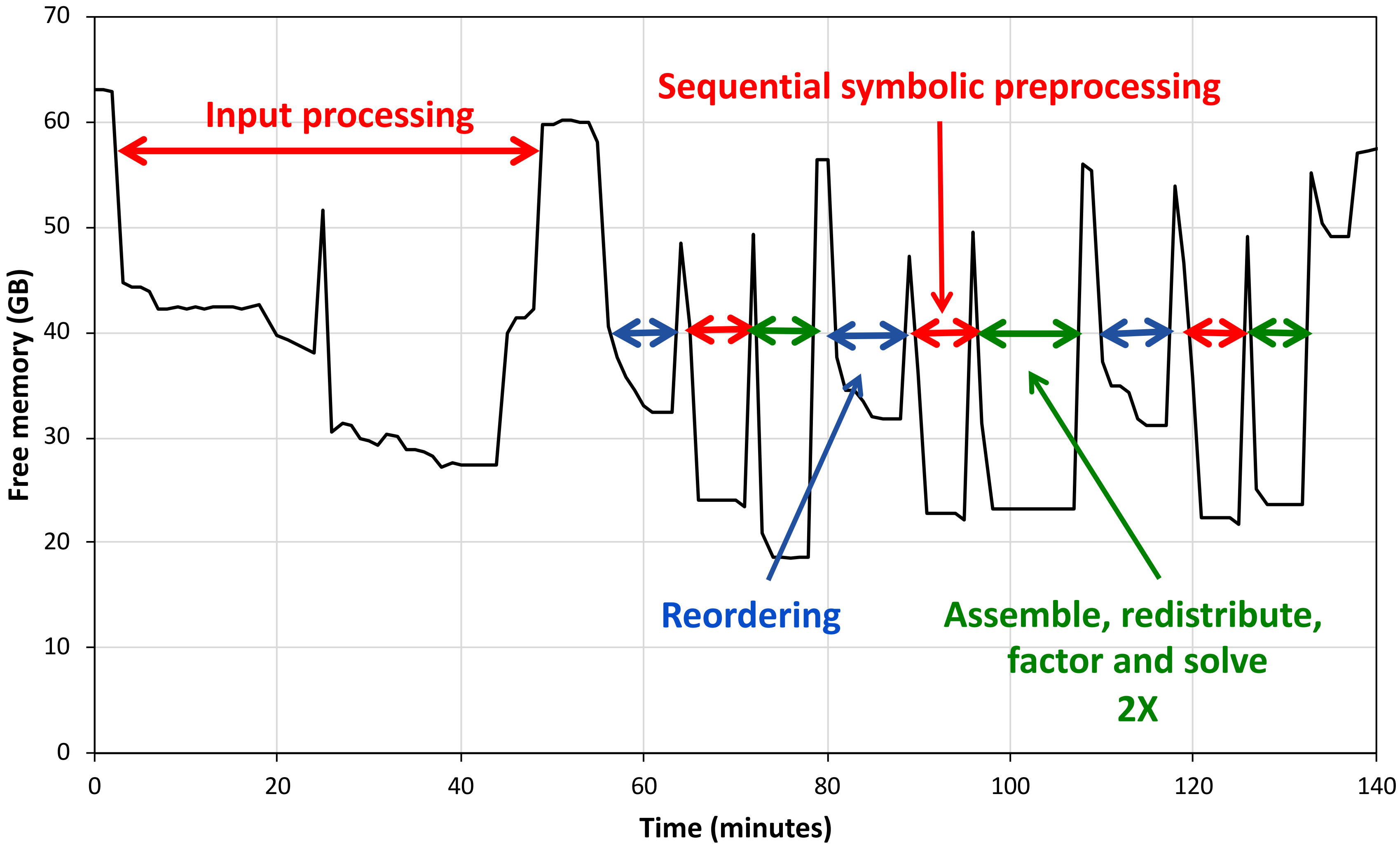


Improvement framework and progress highlights

- ❑ 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

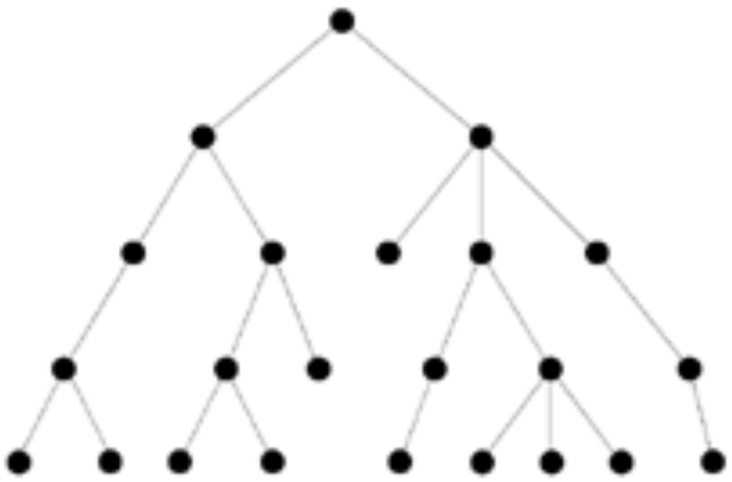


105M DOF model, 256 MPI ranks, 8 threads each
Free memory on MPI rank zero's node

Multifrontal sparse linear solver

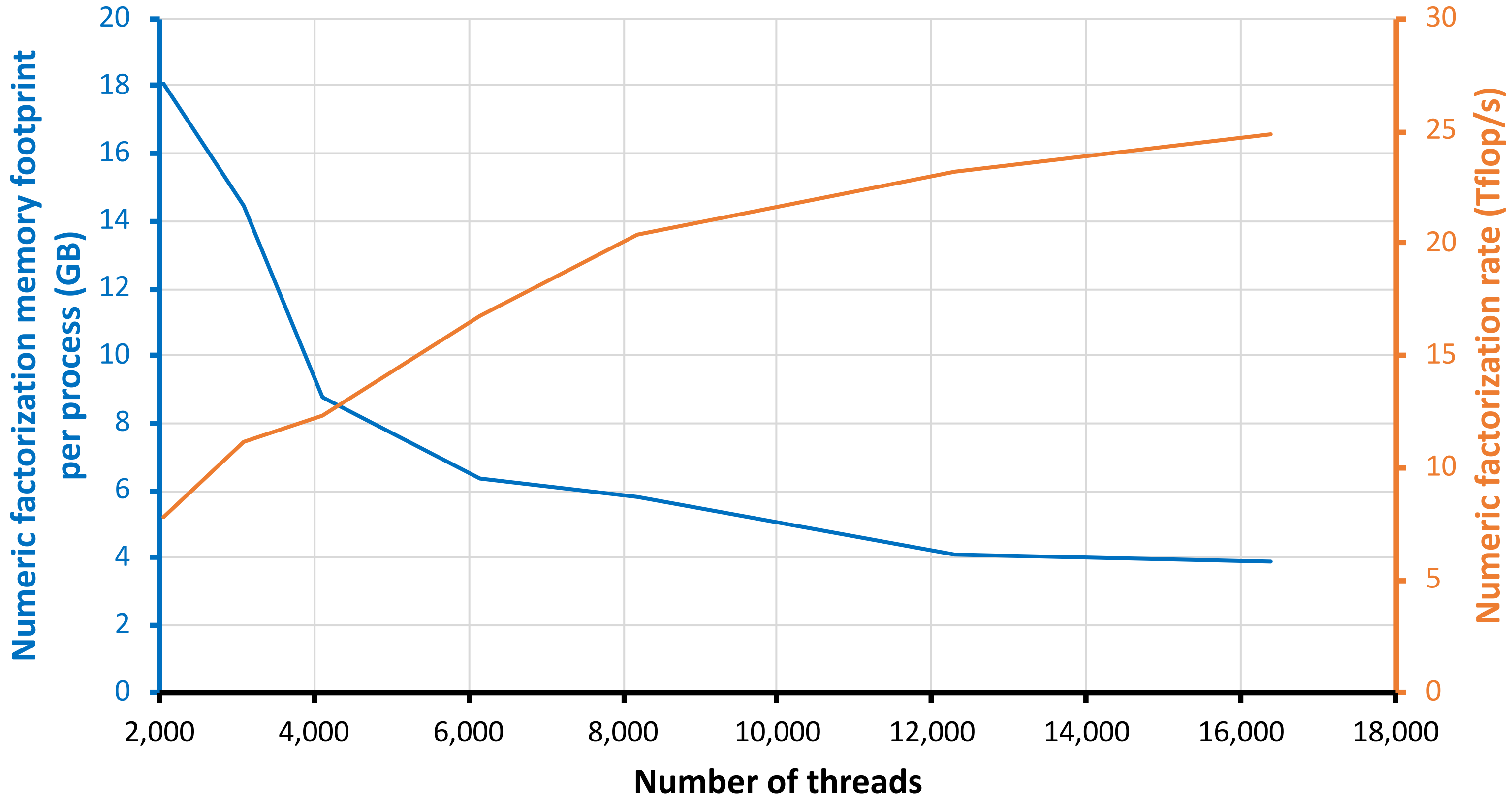
$$\left[K_{i-1}^{t+\Delta t}\right]\left\{\Delta u_{i-1}^{t+\Delta t}\right\}=\left\{R_{i-1}^{t+\Delta t}\right\}$$

Sparse linear system



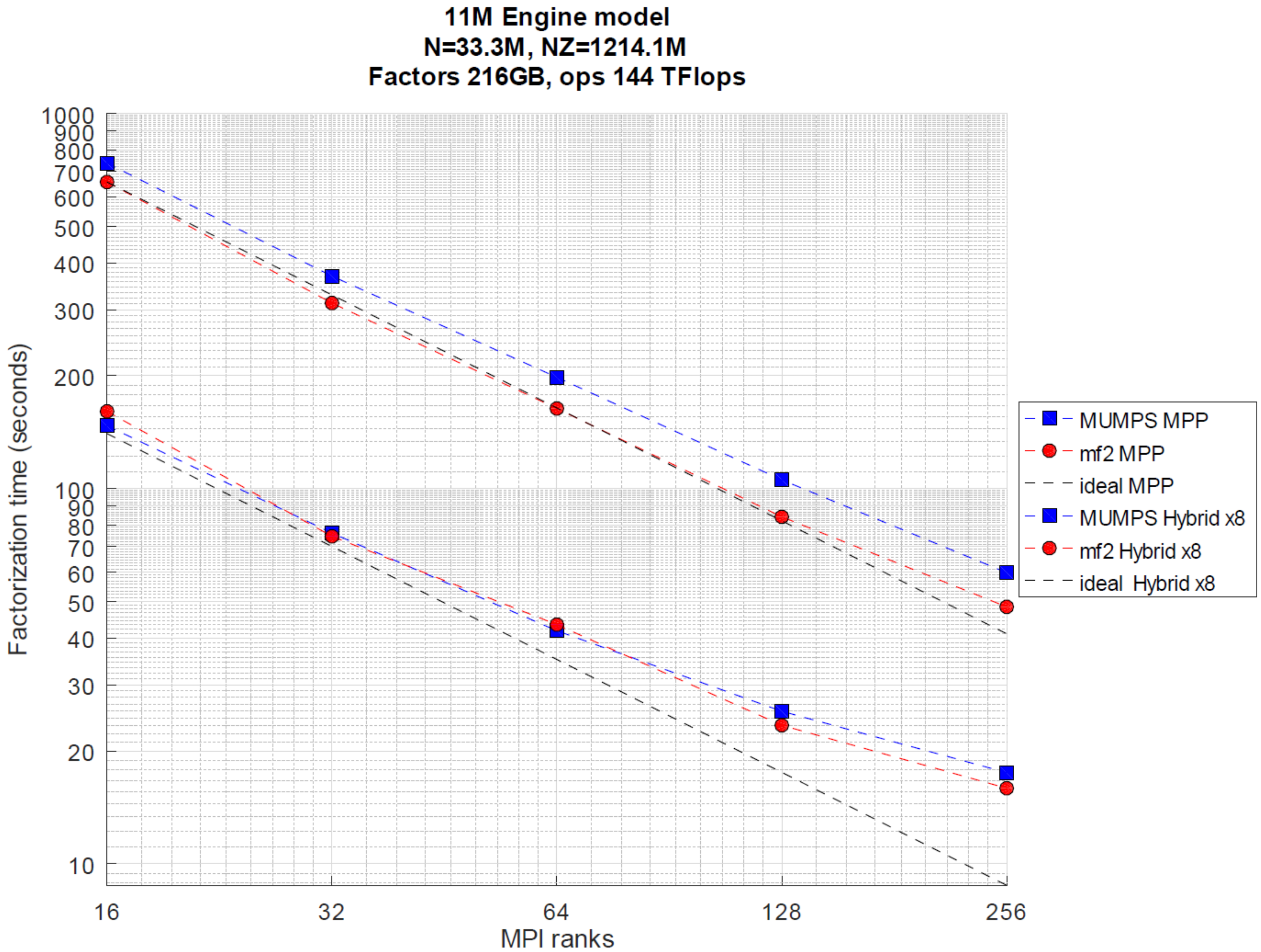
Assembly tree of submatrices

Multifrontal factorization parallel scaling



Multifrontal method: Input processing **>** Matrix reordering **>** Symbolic factorization **>** Numeric factorization **>** Triangular solution

Results – Comparison with MUMPS factorization



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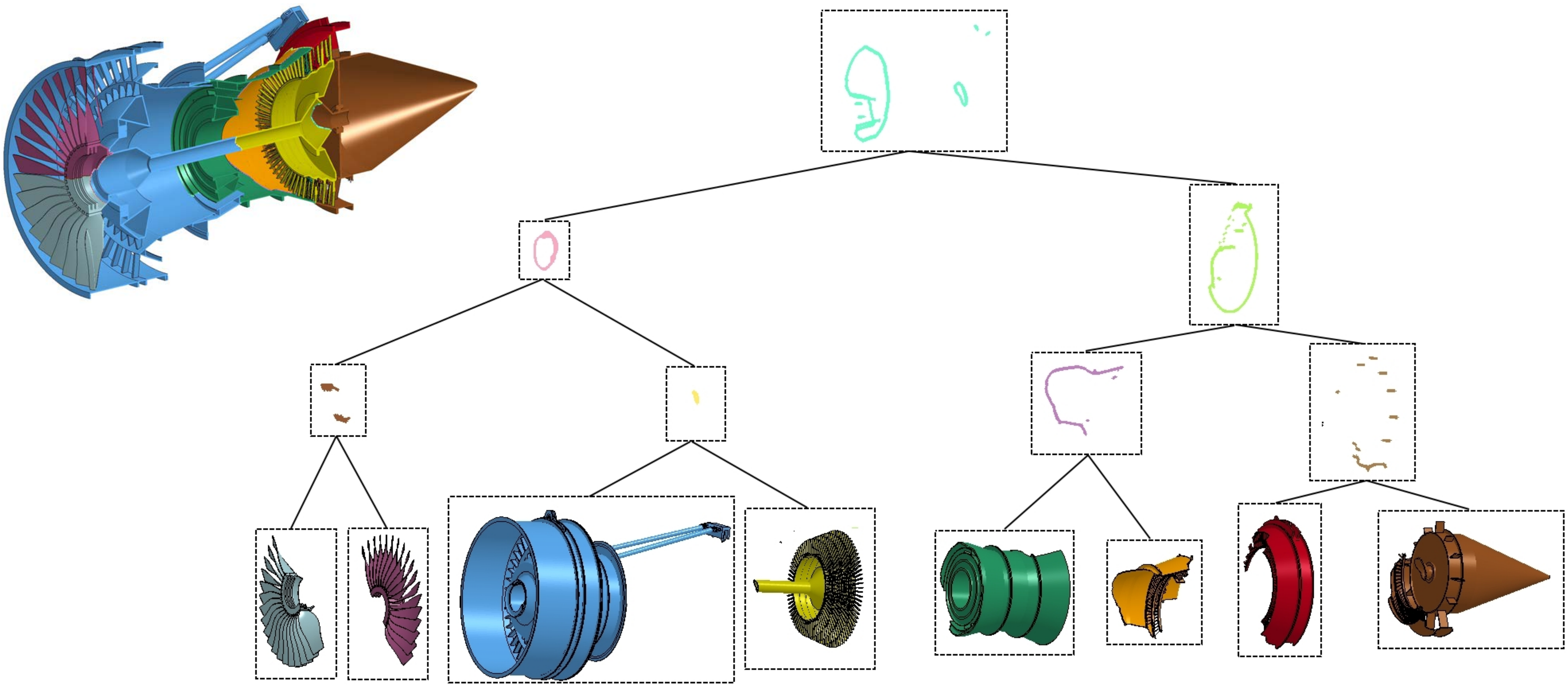
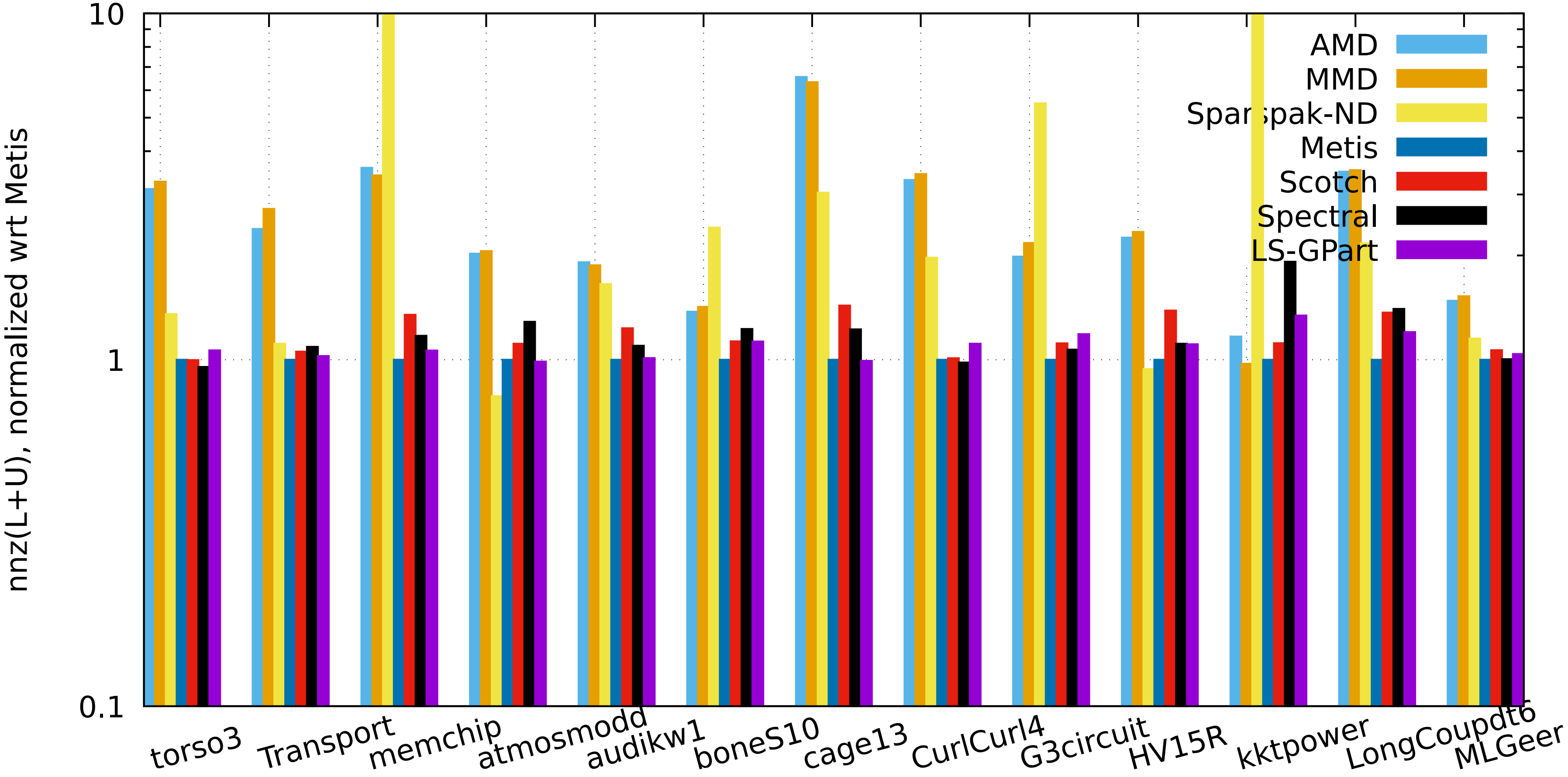
LS-GPart nested dissection for eight processors

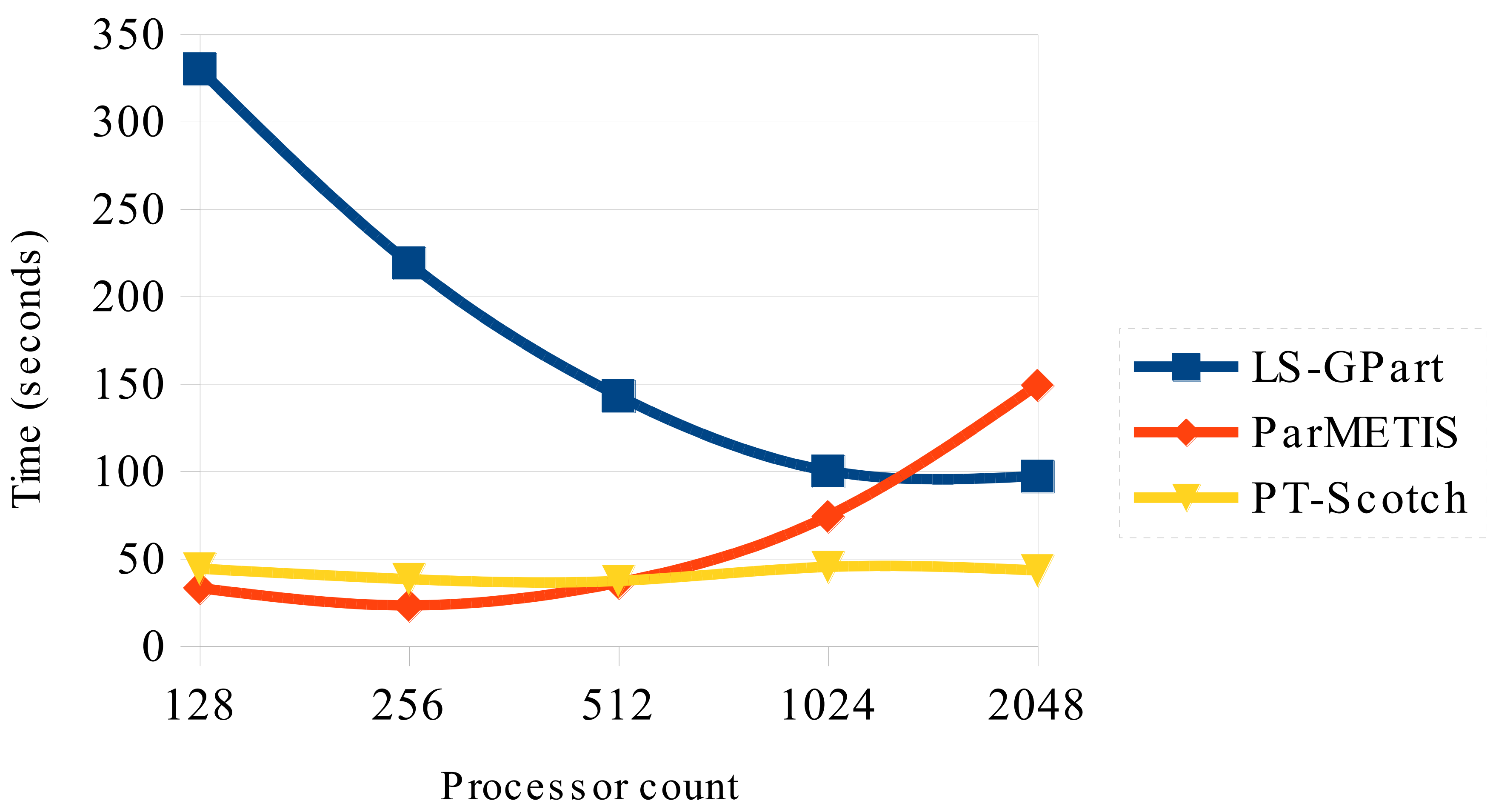


Results – LS-GPart matrix reordering quality

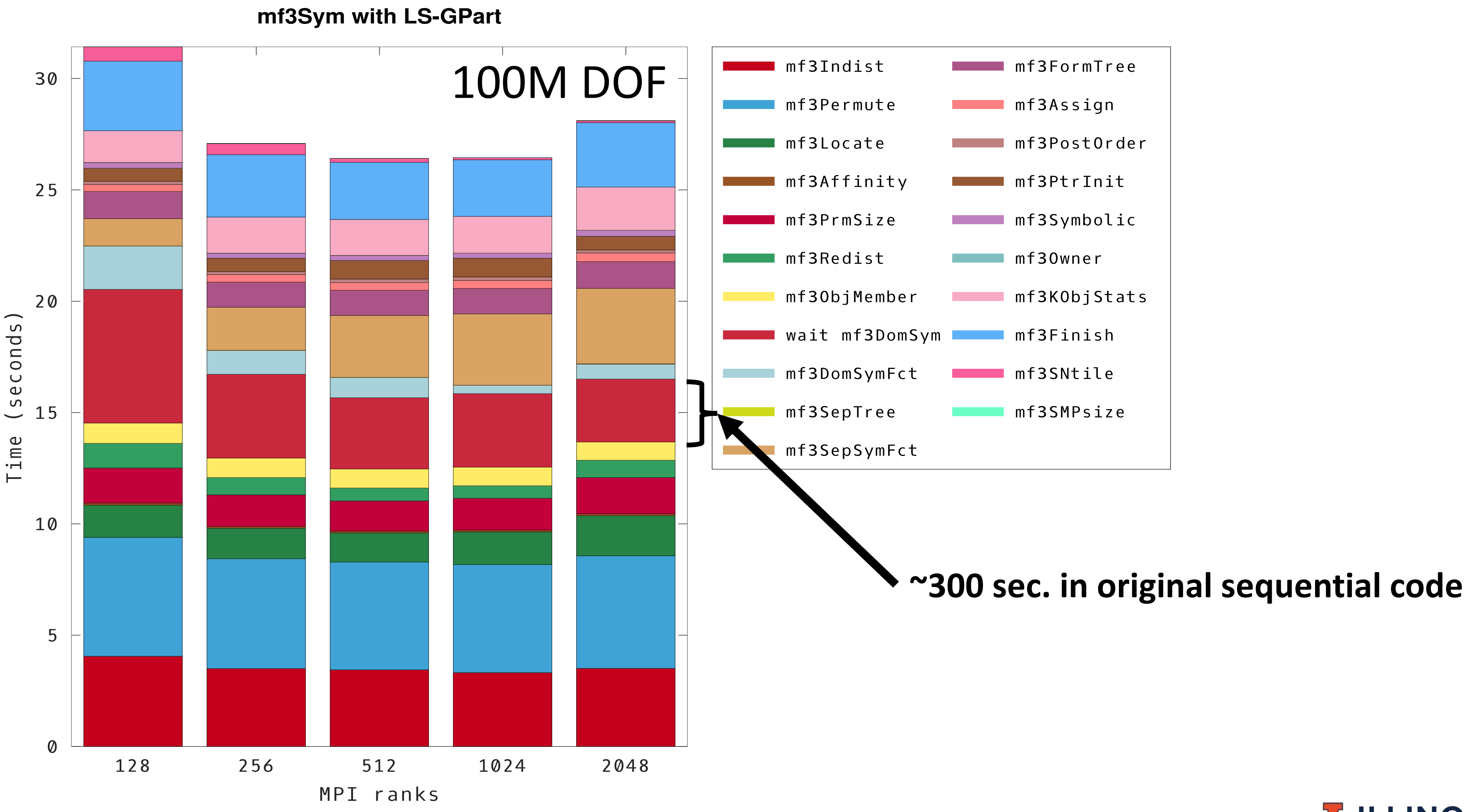


LS-GPart added to reordering comparison presented in "Preconditioning using Rank-structured Sparse Matrix Factorization", Ghysels, et.al., SIAM PP 2018

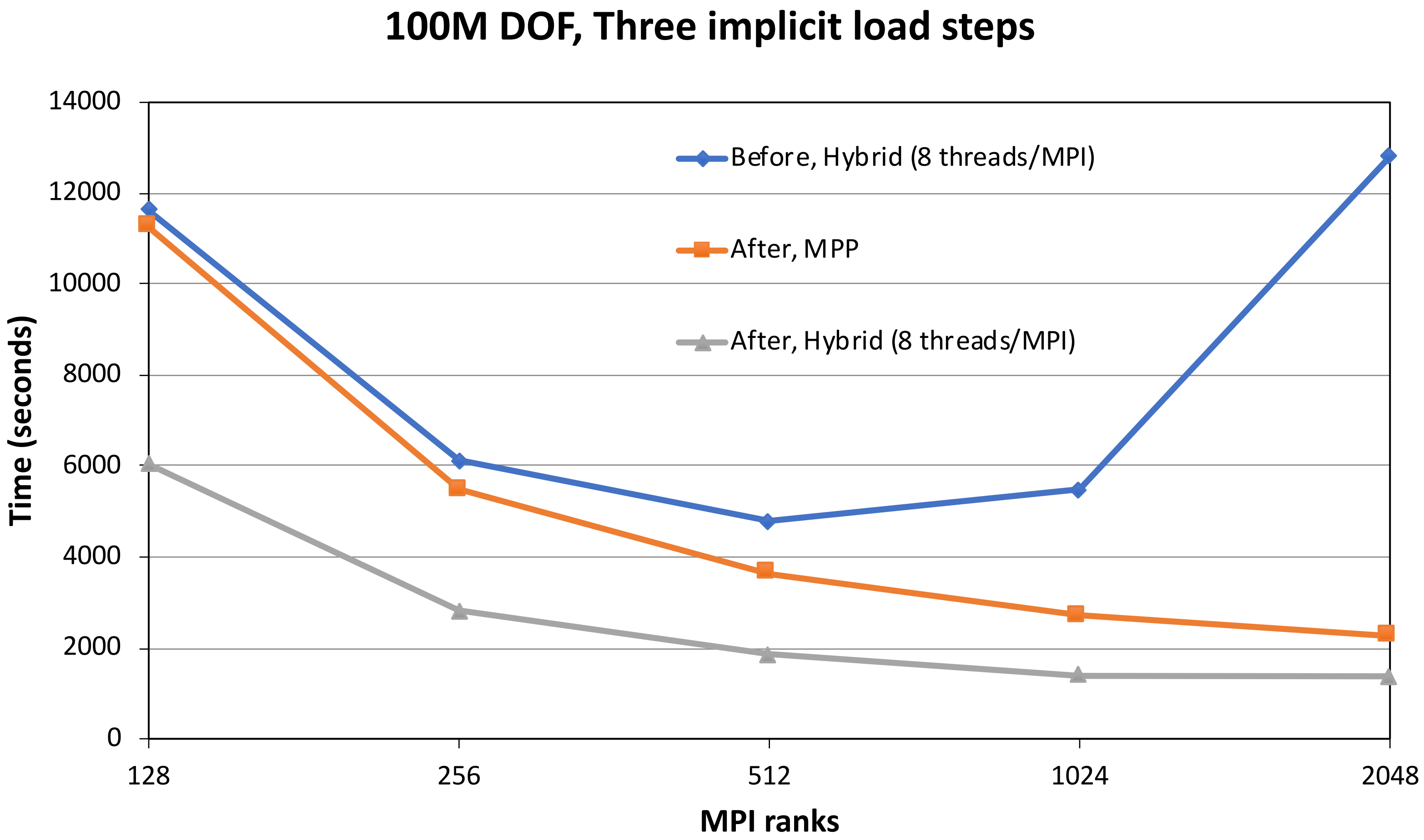
Results - LS-GPart performance



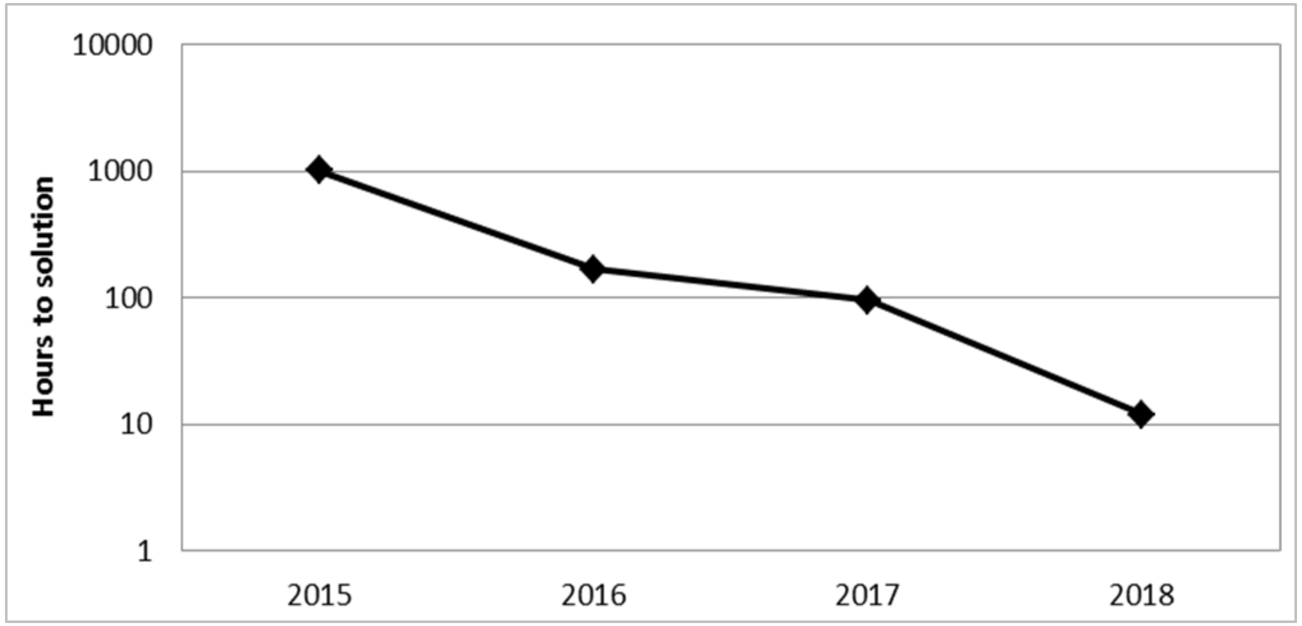
Results – New symbolic factorization performance scaling

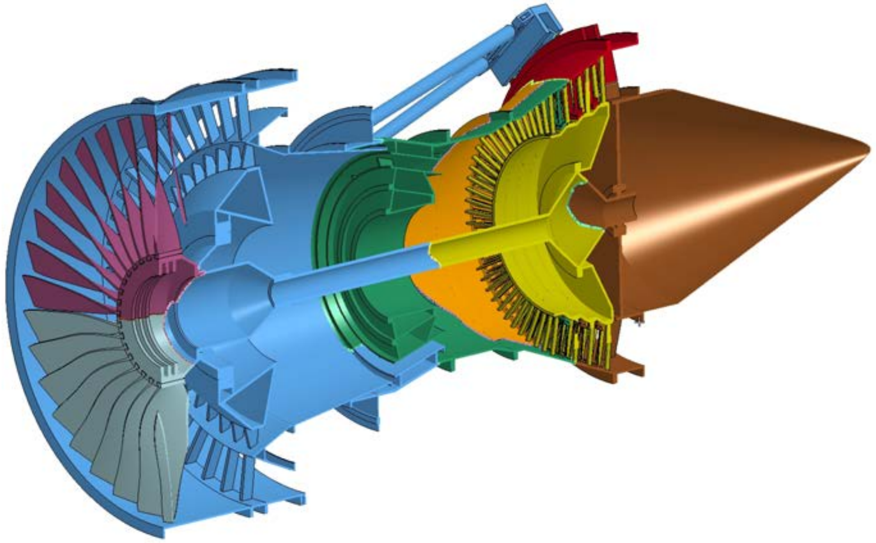


Results – Before and after Blue Waters engagement



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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