Multi-level FETI-DP for Exa-scale-type Computations

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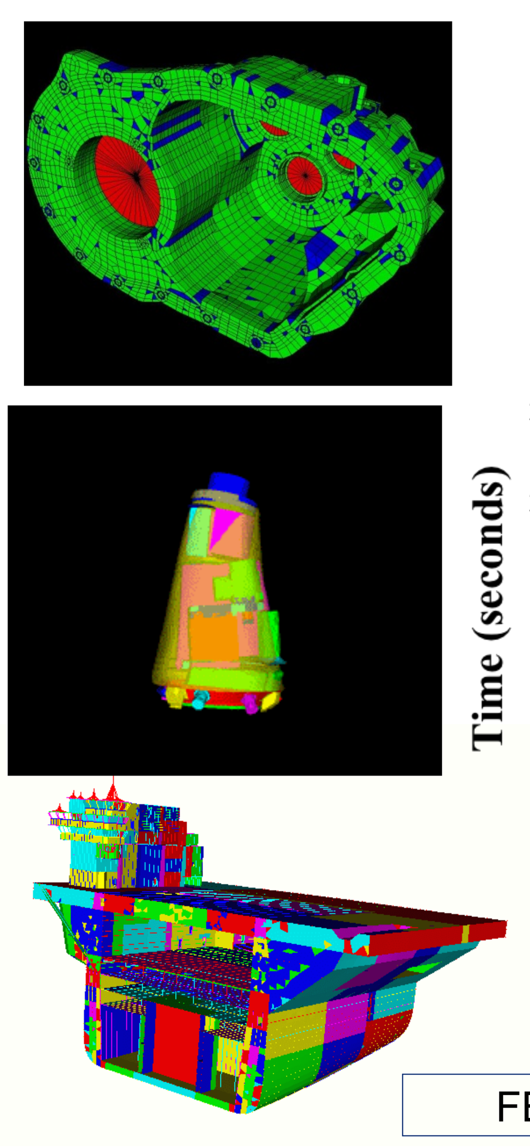
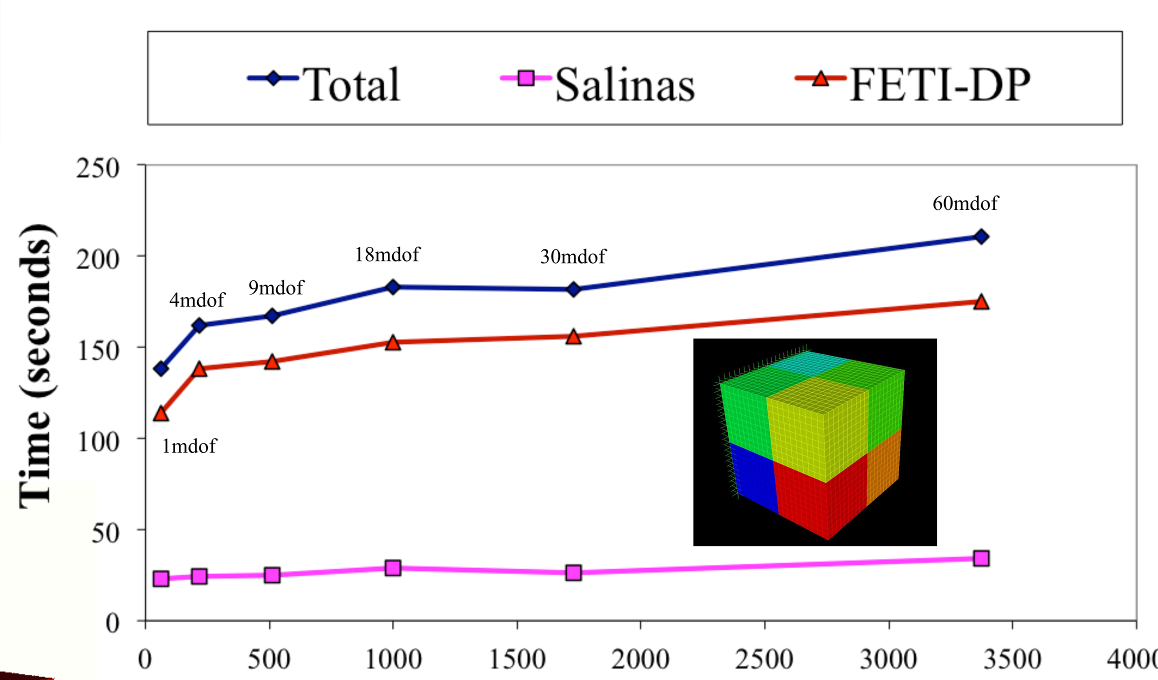
Introduction

- Partial differential equation solvers increasingly require implicit formulations in order to deal with the stiffness associated with large unstructured meshes
- Iterative solvers are often preferred for large-scale systems for both computational complexity and parallel processing reasons
- Large matrices become increasingly ill-conditioned for large problems, leading to slowly converging iterative solvers
- Exa-scale parallel computers will require novel linear solvers whose computational complexity scales linearly with the matrix size, and require a reduced amount of communication between processors
- FETI-DP is chosen here as a starting point for the development of a new, highly scalable (numerical and parallel scalabilities) linear solver for exa-scale machines because of its track record for tera- and peta-scale systems

FETI-DP: The gold standard of scalable solvers



- **Coveted GORDON BELL PRIZE, 2001**
- Implemented in Salinas, Adagio, Andante, Trilinos and many other DOE codes



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FETI-DP enables solution of realistic solid/shell problems

FETI-DP method

- Computes independent discontinuous subdomain solutions in embarrassingly parallel fashion using LU decomposition
- Employs Lagrange multipliers λ to match the solutions on the subdomain interfaces
- The approximate solutions u are formulated to be continuous at the corners of the subdomains

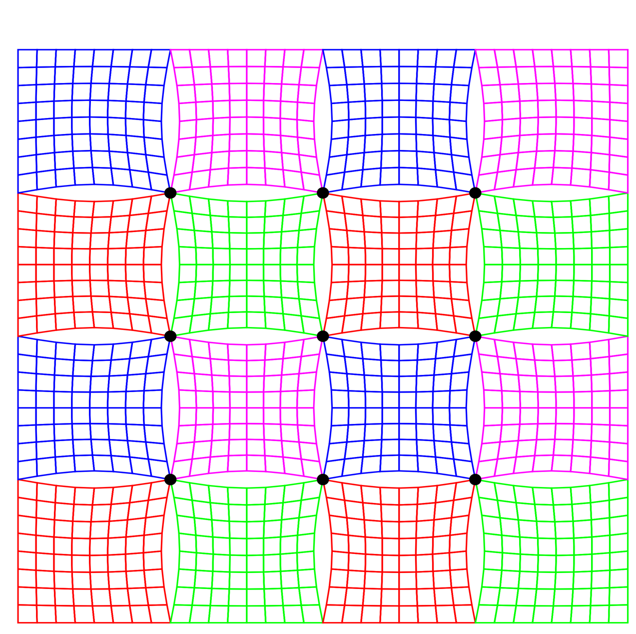
$$\begin{pmatrix} K_{rr} & K_{rc} & B_r^T \\ K_{cr} & K_{cc} & 0 \\ B_r & 0 & 0 \end{pmatrix} \begin{pmatrix} u_r \\ u_c \\ \lambda \end{pmatrix} = \begin{pmatrix} f_r \\ f_c \\ 0 \end{pmatrix}$$

The subscripts c and r denote the corner dofs and the rest of dofs, respectively

Eliminating u leads to the system

$$F\lambda = b$$

for the Lagrange multipliers which is solved iteratively



- For 3D problems continuity constraints for the subdomain edge averages are added
- Forming LU decomposition for 3D domain with n dofs requires $O(n^2)$ flops and solving with it requires $O(n^{4/3})$ flops
- Decomposing the domain into p subdomains reduces the cost of forming the factorizations by $O(p)$ and solving problems with them by $O(p^{1/3})$
- This decomposition makes forming and using the factorizations embarrassingly parallel on p cores
- The number of iterations is $O(1+\log(H/h))$, where H is the diameter of subdomains and h is the diameter of elements → the number of iterations is independent of p and it depends only weakly on the ratio H/h → **numerical scalability**
- For typical problems the number of iterations is order of 10

Coarse problems

- At each iteration the elimination of u requires the solution of the coarse problem

$$S = K_{cc} - K_{cr}K_{rr}^{-1}K_{rc}$$

- This problem couples all corner and edge average dofs
- This coupling is the reason for the numerical scalability, that is, the fact that the number of iterations does not grow with the number of subdomains
- The size of S is proportional to the number of subdomains
- The computational cost of LU limits the number of dofs in subdomains → the number of subdomains and the size of the coarse problem have to grow with the number of dofs in the original problem
- For very large problems the coarse problem can have hundreds of thousands or millions of unknowns
- Such large problems cannot be solved efficiently with LU decomposition

Multi-level formulation

- The idea is to employ FETI-DP method to solve coarse problems with S
- This leads to nested iterations with the inner systems being several orders of magnitude smaller
- Breaks large coarse problems into smaller independent subproblems

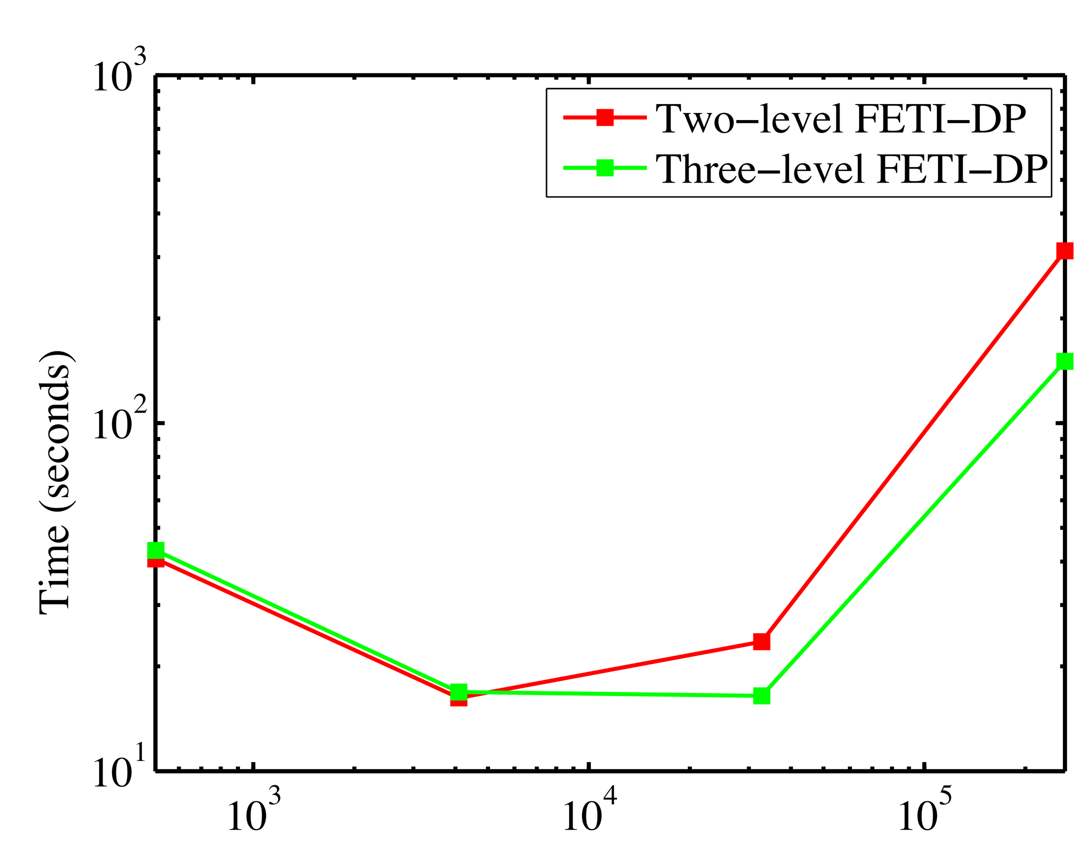
- The traditional Lagrange multiplier treatment of edge averages is not applicable as it leads to indefinite S
- New formulation treating the edge averages in the same way as the corner dofs → positive definite S

- The same analysis of the computational cost applies here as for the first level domain decomposition with the difference that the total number of iterations with S is multiplied by the number of iterations with F
- Each iteration with S requires solution with LU decompositions of the subproblems
- As the number of these subproblems is orders of magnitude smaller than the number of the first level subdomain problems, the nested iteration is computationally affordable

- The multi-level version is obtained by recursively applying the same idea

Scalability for medium size problem

- 3D Poisson problem: 16.58 mdofs
- Solution on 64 cores using 512 to 262,144 subdomains



- Two-level FETI-DP is the standard method
- Three-level method applies two-level FETI-DP method for coarse problems
- With larger problems or more cores the performance difference is much more pronounced

Planned collaborations

- With Eric Darve, AHPCRC, to equip the multilevel FETI-DP with the new generation fast sparse solvers where applicable
- With ARL/CSD to identify codes used by ARL that could benefit from this exa-scale solver when completed