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A UNIFIED FRAMEWORK FOR ACCELERATING THE CONVERGENCE OF ITERATIVE SUBSTRUCTURING METHODS WITH LAGRANGE MULTIPLIERS

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ABSTRACT

The FETI algorithms are a family of numerically scalable substructuring methods with Lagrange multipliers that have been designed for solving iteratively large-scale systems of equations arising from the finite element discretization of structural engineering, solid mechanics, and structural dynamics problems. In this paper, we present a unified framework that simplifies the interpretation of several of the previously presented FETI concepts. This framework has enabled the improvement of the robustness and performance of the transient FETI method, and the design of a new family of coarse operators for iterative substructuring algorithms with Lagrange multipliers. We report on both of these new developments, discuss their impact on the iterative solution of large-scale finite element systems of equations by the FETI method, and illustrate them with a few static and dynamic structural analyses on an IBM SP2 parallel processor. © 1998 John Wiley & Sons, Ltd.

KEY WORDS: parallel computing; finite elements; substructures

1. INTRODUCTION

With the advent of parallel processing, domain decomposition (DD) or substructure-based iterative algorithms have become increasingly popular for the solution of systems of equations arising from the finite element discretization of solid and structural mechanics problems. Indeed, domain decomposition provides a higher level of concurrency than global algebraic approaches, and is simpler to implement on most parallel computational platforms.[1] Many DD-based iterative methods are also interesting as serial solution algorithms, because they have been shown to be more memory efficient and faster than direct solution methods for sufficiently large problems. In general, the substructure equations are solved by a direct skyline or sparse factorization-based algorithm,

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and the interface problem is solved iteratively—usually, by a preconditioned conjugate gradient (PCG) method. The success of a DD-based iterative algorithm hinges on two important properties: *numerical* scalability with respect to the mesh size h and the substructure size H, and *parallel* scalability. The first property, often referred to in the mathematical literature as optimality or quasi-optimality, characterizes the class of DD-based iterative solvers whose convergence rate deteriorates only weakly with the size of the problem (for example, the number of elements in the mesh), and the size of the mesh partition (for example, the number of substructures). The second property characterizes those DD methods which are amenable to parallel processing, and whose parallel implementation can deliver larger speedups when larger number of processors are used. It follows that numerical scalability with respect to the substructure size is a necessary condition for parallel scalability.

The FETI method[2–11] is among the first DD methods that have demonstrated both numerical and parallel scalability for the solution of second-order elasticity as well as fourth-order plate and shell problems. Its ability to outperform several popular direct and iterative algorithms on both sequential and parallel computers has been extensively demonstrated, and has earned it a place in commercial finite element structural mechanics and multibody dynamics software (see, for example, References 12 and 13). Essentially, the FETI method can be viewed as a two-step PCG-based iterative procedure where substructure problems with Dirichlet boundary conditions are solved in the preconditioning step, and related substructure problems with Neumann boundary conditions are solved in a second step. It is also known as the dual Schur complement method because on the outset, it constructs a dual Schur complement operator.[1] When the FETI method is equipped with the so-called Dirichlet preconditioner,[6] and with the optional corner Lagrange multipliers for plate[9, 10] and shell[11] problems, the condition number of its interface problem grows asymptotically only as

$$\kappa = O\left(1 + \log^m\left(\frac{H}{h}\right)\right), \quad m \leqslant 3 \tag{1}$$

The above conditioning result (1) holds for second-order elasticity problems as well as fourth-order plate and shell problems; it establishes the numerical scalability of the FETI method with respect to both the mesh size h and the substructure size H. The parallel scalability of this DD method has also been demonstrated on many massively parallel processors and for several realistic structural problems.[1, 8, 11]

The FETI method has been successfully extended to component mode synthesis,[14] transient response analysis,[8] heterogeneous problems,[15] and systems with multiple and/or repeated right-hand sides.[16] These developments have always been guided by mechanical reasonings, often justified with rigorous mathematical proofs,[6–9] and always evaluated with the solution of complex structural mechanics and structural dynamics problems. All pieces of this integrated work have shared the concept of substructuring with Lagrange multipliers, and have addressed the efficient implementation of the resulting algorithms on massively parallel processors. However, depending on the class of problems to be solved, different approaches have been followed in the past to construct the different coarse problems needed for ensuring numerical scalability. We remind the reader that domain decomposition theory[17, 18] suggests augmenting any DD-based iterative solver with a 'coarse grid' problem that is large enough to disseminate significant information globally and therefore accelerate convergence, and yet small enough to keep the corresponding additional computations and interprocessor communications affordable. With the growing interest in FETI methods and their variants,[19–23, 34] the need for a simple and general framework for designing and

understanding such coarse problems has become urgent. The main objective of this paper is to describe such a framework, and highlight its impact on improving the performance of existing FETI methods as well as other DD algorithms with Lagrange multipliers,[24] and on constructing new ones. We note that this framework is equally applicable to non-overlapping DD methods without Lagrange multipliers such as the so-called Neumann–Neumann preconditioned Schur complement method,[25, 26] and the balancing method.[27] For this purpose, the remainder of this paper is organized as follows.

In Section 2, the concept of substructuring with Lagrange multipliers is overviewed, and in Section 3, the basic FETI methodology is summarized. Section 4 focuses on the notion of a FETI coarse problem, and Section 5 describes a unified framework for interpreting previously developed FETI coarse problems and designing new ones. Finally, the impact on the performance of the FETI method of two new coarse problems described in Section 5 is assessed in Section 6. Section 7 concludes this paper.

2. ITERATIVE SUBSTRUCTURING WITH LAGRANGE MULTIPLIERS

In order to keep this paper self-contained as much as possible, we begin with an overview of the original FETI method.[2–5]

The problem to be solved is

$$Au = f \tag{2}$$

where A is an $n \times n$ symmetric positive semi-definite sparse matrix arising from the finite element discretization of a second- or fourth-order elastostatic (or elastodynamic) problem defined over a region Ω, and f is a right-hand side n-long vector representing some generalized forces. If Ω is partitioned into a set of N_s *disconnected* substructures $\Omega^{(s)}$, the FETI method consists in replacing equation (2) with the equivalent system of substructure equations

$$\begin{aligned} A^{(s)}u^{(s)} &= f^{(s)} - B^{(s)^{\mathrm{T}}}\lambda \quad s = 1, \ldots, N_s \\ \Delta &= \sum_{s=1}^{s=N_s} B^{(s)}u^{(s)} = 0 \end{aligned} \tag{3}$$

where $A^{(s)}$ and $f^{(s)}$ are the unassembled restrictions of A and f to substructure $\Omega^{(s)}$, λ is a vector of Lagrange multipliers introduced for enforcing the constraint $\Delta = 0$ and represents the normal derivatives of the 'primal' variable of the problem on the substructure interface boundary $\Gamma_{\mathrm{I}}^{(s)}$, and $B^{(s)}$ is a signed Boolean matrix that describes the interconnectivity of the substructures. From a physical viewpoint, the first of equations (3) expresses the substructure equations of equilibrium with Neumann boundary conditions, λ represents the 'gluing' surface forces (tractions) between the disconnected substructures (Figure 1), and the second of equations (3) expresses the compatibility of the substructure solutions $u^{(s)}$ on the substructure interfaces $\Gamma_{\mathrm{I}} = \bigcup_{s=1}^{s=N_s} \Gamma_{\mathrm{I}}^{(s)}$. A more elaborate derivation of equations (3) can be found in References 1 and 6.

In general, a mesh partition may contain $N_f \leqslant N_s$ floating substructures—that is, substructures without enough essential boundary conditions to prevent the substructure matrices $A^{(s)}$ from being singular—in which case N_f of the local Neumann problems

$$A^{(s)}u^{(s)} = f^{(s)} - B^{(s)^{\mathrm{T}}}\lambda \quad s = 1, \ldots, N_f \tag{4}$$

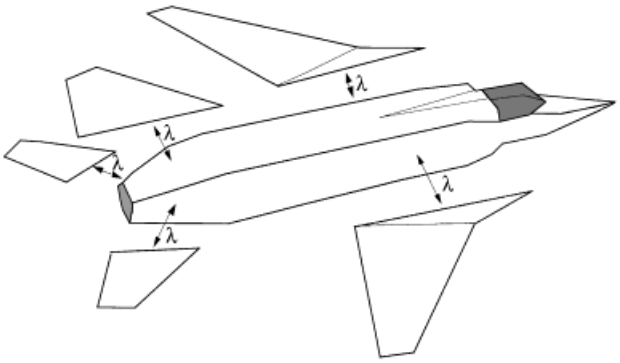

Figure 1. Assembling the substructures with Lagrange multipliers

are ill-posed. To guarantee the solvability of these problems, we require that

$$(f^{(s)} - B^{(s)^{\mathrm{T}}}\lambda) \perp \mathrm{Ker}(A^{(s)}) \quad s = 1, \ldots, N_f \tag{5}$$

and compute the solution of equation (4) as

$$u^{(s)} = A^{(s)^{+}}(f^{(s)} - B^{(s)^{\mathrm{T}}}\lambda) + R^{(s)}\alpha^{(s)} \tag{6}$$

where $A^{(s)^{+}}$ is a generalized inverse of $A^{(s)}$ that need not be explicitly computed,[4] $R^{(s)} = \mathrm{Ker}(A^{(s)})$ is the null space of $A^{(s)}$, and $\alpha^{(s)}$ is a vector of six or fewer constants (in the absence of mechanisms, there are at most six rigid body modes in a three-dimensional structural mechanics problem). The introduction of the few additional unknowns $\alpha^{(s)}$ is compensated by the additional equations resulting from (5)

$$R^{(s)^{\mathrm{T}}}(f^{(s)} - B^{(s)^{\mathrm{T}}}\lambda) = 0 \quad s = 1, \ldots, N_f \tag{7}$$

Substituting equation (6) into the second of equations (3) and using equation (7) leads after some algebraic manipulations to the following FETI interface problem:

$$\begin{bmatrix} F_{\mathrm{I}} & -G_{\mathrm{I}} \\ -G_{\mathrm{I}}^{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \alpha \end{bmatrix} = \begin{bmatrix} d \\ -e \end{bmatrix} \tag{8}$$

where

$$F_{\mathrm{I}} = \sum_{s=1}^{s=N_s} B^{(s)} A^{(s)^{+}} B^{(s)^{\mathrm{T}}}, \quad G_{\mathrm{I}} = [B^{(1)} R^{(1)} \ldots B^{(N_f)} R^{(N_f)}]$$

$$\alpha = [\alpha^{(1)^{\mathrm{T}}} \ldots \alpha^{(N_f)^{\mathrm{T}}}]^{\mathrm{T}}, \quad d = \sum_{s=1}^{s=N_s} B^{(s)} A^{(s)^{+}} f^{(s)}$$

$$e = [f^{(1)^{\mathrm{T}}} R^{(1)} \ldots f^{(N_s)^{\mathrm{T}}} R^{(N_f)}]^{\mathrm{T}}$$

$$A^{(s)^{+}} = A^{(s)^{-1}} \quad \text{if } \Omega^{(s)} \text{ is not a floating substructure}$$

$$A^{(s)^{+}} = \text{a generalized inverse of } A^{(s)} \text{ if } \Omega^{(s)} \text{ is a floating substructure}$$

For structural mechanics and structural dynamics problems, F_{I} is symmetric because the substructure matrices $A^{(s)}$ are symmetric. The objective is to solve by a PCG algorithm the interface

problem (8) instead of the original problem (1). In the sequel, we denote by N_I the total number of active interface degrees of freedom (d.o.f.), and by λ^k the approximate solution at iteration k of problem (8).

3. THE BASIC FETI METHODOLOGY

3.1. Alternative interface problems

First, we note that F_I is the sum of independent substructure operators, which makes a matrix–vector product of the form $F_I\lambda^k$ trivial to parallelize. In References 1 and 6, it is shown that away from the crosspoints—that is, points that are connected to more than two substructures—F_I is the sum of the inverses of the substructure Schur complements, which justifies the labelling of the FETI method as the dual Schur complement method. This dual method has interesting spectral properties that trigger a superconvergent behaviour of a PCG algorithm applied to the solution of equation (8).[1, 6]

Next, we point out that any iterate λ^k can be decomposed as follows:

$$\begin{aligned} &\lambda^k = \lambda_1^k + \lambda_2^k \\ &\lambda_1^k \in \mathrm{Ker}(G_I^T) \Rightarrow G_I^T\lambda_1^k = 0 \\ &\lambda_2^k \in \mathrm{Range}(G_I) \Rightarrow \exists \alpha^k / \lambda_2^k = G_I\alpha^k \end{aligned} \tag{9}$$

In other words, given an initial value λ^0 that satisfies the constraint $G_I^T\lambda^0 = e$, each iterate λ^k generated by a PCG algorithm applied to the solution of the interface problem (8) can be decomposed as the sum of a component λ_1^k that satisfies the constraint $G_I^T\lambda_1^k = 0$, and a component λ_2^k that does not satisfy this constraint ($G_I^T\lambda_2^k \neq 0$). In the sequel, we call λ_1^k an admissible Lagrange multiplier.

If P is defined as

$$P = I - G_I(G_I^T G_I)^{-1} G_I^T \tag{10}$$

the reader can check that P satisfies

$$\begin{aligned} P^2 &= P \\ P^T &= P \\ P\lambda^k &= \lambda_1^k \\ PG_I &= 0 \\ G_I^T P &= 0 \end{aligned} \tag{11}$$

Hence, P is an orthogonal projector onto $\mathrm{Ker}\,(G_I^T)$. Premultiplying the first of equations (8) by P transforms the DD interface problem in

$$\begin{aligned} PF_I\lambda &= Pd \\ G_I^T\lambda &= e \end{aligned} \tag{12}$$

Given an initial value λ^0 that satisfies

$$G_I^T\lambda^0 = e \tag{13}$$

a solution of problem (12) can be obtained iteratively by applying any variable step length algorithm to the homogeneous problem

$$\begin{aligned} PF_{\mathrm{I}}\lambda &= Pd \\ G_{\mathrm{I}}^{\mathrm{T}}\lambda &= 0 \end{aligned} \tag{14}$$

where λ should be interpreted in the sequel as an 'increment' Lagrange multiplier. From equations (11), it follows that

$$\forall(\eta,\delta)/G_{\mathrm{I}}^{\mathrm{T}}\delta = G_{\mathrm{I}}^{\mathrm{T}}\eta = 0, \quad \delta^{\mathrm{T}}PF_{\mathrm{I}}\eta = \delta^{\mathrm{T}}P^{\mathrm{T}}F_{\mathrm{I}}\eta = (P\delta)^{\mathrm{T}}F_{\mathrm{I}}\delta = \delta^{\mathrm{T}}F_{\mathrm{I}}\eta \tag{15}$$

which shows that PF_{I} is symmetric on the space of Lagrange multipliers λ satisfying the constraint $G_{\mathrm{I}}^{\mathrm{T}}\lambda = 0$. Hence, the interface problem (14), which is equivalent to the interface problem (8), can be solved in particular by a PCG algorithm.

The initial residual associated with λ^0 is

$$w^0 = Pd - PF_{\mathrm{I}}\lambda^0 = P(d - F_{\mathrm{I}}\lambda^0) \tag{16}$$

From the last of equations (11), it follows that this residual satisfies

$$G_{\mathrm{I}}^{\mathrm{T}}w^0 = G_{\mathrm{I}}^{\mathrm{T}}P(d - F_{\mathrm{I}}\lambda^0) = 0 \tag{17}$$

Let $\{p_1, \ldots, p_k\}$ denote the set of search directions generated during the first k iterations by a PCG algorithm applied to the solution of the interface problem (14). It is well known that

$$\lambda^k \in \mathrm{span}\{p_1, \ldots, p_k\} = \mathrm{span}\{w_0, PF_{\mathrm{I}}w_0, \ldots, (PF_{\mathrm{I}})^{k-1}w_0\} \tag{18}$$

which, in view of equations (11)–(18), leads to the final conclusion

$$\begin{aligned} \text{if } \lambda^k \text{ is generated by PCG applied to } PF_{\mathrm{I}}\lambda = Pd &\Rightarrow G_{\mathrm{I}}^{\mathrm{T}}\lambda^k = 0 \\ &\Rightarrow \lambda^k \text{ is admissible} \end{aligned} \tag{19}$$

In summary, the analysis presented above shows that the DD interface problem (8) can be solved iteratively by computing an initial value λ^0 that satisfies the constraint (13), and applying PCG to the simpler interface problem

$$PF_{\mathrm{I}}\lambda = Pd \tag{20}$$

Such a strategy can also be viewed as solving the interface problem (8) by a preconditioned conjugate projected gradient algorithm.[28]

3.2. Preconditioning

Two preconditioners have been previously developed for the FETI method: (a) a mathematically optimal (see the Introduction) Dirichlet preconditioner that can be written as

$$\overline{F}_{\mathrm{I}}^{D^{-1}} = \sum_{s=1}^{s=N_s} B^{(s)} \begin{bmatrix} 0 & 0 \\ 0 & A_{\mathrm{bb}}^{(s)} - A_{\mathrm{ib}}^{(s)^{\mathrm{T}}} A_{\mathrm{ii}}^{(s)^{-1}} A_{\mathrm{ib}}^{(s)} \end{bmatrix} \quad B^{(s)^{\mathrm{T}}} = \sum_{s=1}^{s=N_s} B^{(s)} \begin{bmatrix} 0 & 0 \\ 0 & S_{\mathrm{bb}}^{(s)} \end{bmatrix} B^{(s)^{\mathrm{T}}} \tag{21}$$

where the subscripts i and b designate the internal and interface boundary unknowns, respectively, and $S_{\mathrm{bb}}^{(s)} = A_{\mathrm{bb}}^{(s)} - A_{\mathrm{ib}}^{(s)^{\mathrm{T}}} A_{\mathrm{ii}}^{(s)^{-1}} A_{\mathrm{ib}}^{(s)}$ denotes the primal Schur complement of substructure $\Omega^{(s)}$;

and (b) a 'lumped' preconditioner that lumps the Dirichlet operator on the substructure interface unknowns

$$\overline{F}_{\mathrm{I}}^{L^{-1}} = \sum_{s=1}^{s=N_s} B^{(s)} \begin{bmatrix} 0 & 0 \\ 0 & A_{\mathrm{bb}}^{(s)} \end{bmatrix} B^{(s)^{\mathrm{T}}} \tag{22}$$

The mathematical justification and mechanical interpretation of these two preconditioners can be found in References 1 and 6.

Unlike $\overline{F}_{\mathrm{I}}^{D^{-1}}$, the preconditioner $\overline{F}_{\mathrm{I}}^{L^{-1}}$ is not mathematically optimal. However, it is more computationally economical than $\overline{F}_{\mathrm{I}}^{D^{-1}}$, and has often proved to be more efficient for second-order elasticity problems.[1, 6] For fourth-order plate and shell problems, the Dirichlet preconditioner is preferred.

Both the Dirichlet and lumped preconditioners are substructure based, and therefore incur embarrassingly parallel computations. Their computer implementation requires only standard finite element data structures.

3.3. The natural coarse problem

Solving the alternative interface problem (20) by a PCG algorithm requires performing at each iteration k the matrix–vector product

$$(PF_{\mathrm{I}})\lambda^k = (I - G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}})F_{\mathrm{I}}\lambda^k \tag{23}$$

The application of the projector P to the vector $F_{\mathrm{I}}\lambda^k$ means that an auxiliary problem of the form $(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})x^* = b^*$ must be solved in each FETI iteration. This auxiliary problem is a coarse one because its size is less than $6\times N_s$. It was shown in Reference 6 that this coarse problem is small enough to keep the corresponding overhead affordable, and yet efficient enough to propagate the error globally and make it possible to bound the condition number of the interface problem (20) by a logarithmic function of the number of elements per substructure. This coarse problem is called 'natural' because it derives from the solvability conditions (5), independently from convergence rate issues.

3.4. The basic FETI solver

In the absence of floating substructures, the interface problem (20) can be interpreted as the result of preconditioning the system of equations

$$F_{\mathrm{I}}\lambda = d \tag{24}$$

with a projector P.[30] Since in a PCG algorithm the residual is usually defined in terms of the unpreconditioned system, we adopt in the sequel the following nomenclature and notation:

$$\begin{aligned} \text{residual } r^k &= d - F_{\mathrm{I}}\lambda^k \\ \text{Projected residual } w^k &= Pd - PF_{\mathrm{I}}\lambda^k = P(d - F_{\mathrm{I}}\lambda^k) = Pr^k \end{aligned} \tag{25}$$

Using the above notation, the basic iterative FETI solver for second-order elasticity problems can be written as

1. Initialize

$$\lambda^0 = G_I (G_I^T G_I)^{-1} e$$
$$r^0 = d - F_I \lambda^0$$

2. Iterate $k = 1, 2, \ldots$ until convergence

$$\begin{aligned}
\text{Project} \quad & w^{k-1} = P^T r^{k-1} \\
\text{Scale} \quad & \bar{w}^{k-1} = W^{-1} w^{k-1} \\
\text{Precondition} \quad & z^{k-1} = \overline{F_I^{-1}} \bar{w}^{k-1} \\
\text{Re-scale} \quad & \bar{z}^{k-1} = W^{-1} z^{k-1} \\
\text{Re-project} \quad & y^{k-1} = P \bar{z}^{k-1} \\
& \zeta^k = y^{k-1^T} w^{k-1} / y^{k-2^T} w^{k-2} \quad (\zeta^1 = 0) \\
& p^k = y^{k-1} + \zeta^k p^{k-1} \quad (p^1 = y^0) \\
& v^k = y^{k-1^T} w^{k-1} / p^{k^T} F_I p^k \\
& \lambda^k = \lambda^{k-1} + v^k p^k \\
& r^k = r^{k-1} - v^k F_I p^k
\end{aligned} \tag{26}$$

Remark 1. Scaling is employed to redistribute the projected residuals according to the valence of the interface d.o.f.—that is, the number of substructures they belong to—and the relative stiffnesses of the substructures. In its most primitive form, W is a diagonal matrix that stores for each interface d.o.f. its valence (geometrical scaling). More sophisticated scaling procedures that account for both material and geometrical heterogeneities are described in Reference 29.

Remark 2. The reader can verify that because of the presence of the second projection step, the iterates are independent of the particular choice of the generalized inverse introduced in equation (6).

Remark 3. The project, scale, precondition, re-scale, and re-project steps can be interpreted as a single preconditioning step using the *symmetric* product $P^T W^{-1} \overline{F_I^{-1}} W^{-1} P$ as a preconditioner. Hence, the re-project step is introduced to preserve symmetry.

Remark 4. The FETI algorithm is always used with a reorthogonalization procedure to accelerate convergence. In Reference 1, it was shown that such a strategy is cost effective for substructure problems because reorthogonalization is applied only to the interface Lagrange multiplier unknowns.

4. THE FETI COARSE PROBLEMS

4.1. Mechanical interpretation of $G_I\alpha$ and $P(d - F_I\lambda^k)$

At the highest level, equations (3) govern the mechanics of the FETI solver. The first of these equations expresses the equilibrium of the substructures, and the second the continuity of the displacement solution u along the substructure interfaces.

At each iteration k of the FETI solver, a new traction λ^k is computed. Because the corresponding substructure displacements $u^{(s)^k}$ are obtained from the solution of the first of equations (3), equilibrium is satisfied in each substructure. However, only at convergence the substructure solutions $u^{(s)^k}$ are continuous along Γ_I; at each iteration k, their jump is evaluated by the second of equations (3)

$$\Delta^k = \sum_{s=1}^{s=N_s} B^{(s)} u^{(s)^k} \tag{27}$$

Using equation (6) and the notation introduced after equation (8), this jump can be re-written as

$$\begin{aligned} \Delta^k &= \sum_{s=1}^{s=N_s} B^{(s)} A^{(s)^+} f^{(s)} - B^{(s)} A^{(s)^+} B^{(s)^T} \lambda^k + B^{(s)} R^{(s)} \alpha^{(s)^k} \\ &= d - F_I\lambda^k + G_I\alpha^k \end{aligned} \tag{28}$$

Hence, Δ^k can be decomposed as the sum of two components

$$\begin{aligned} \Delta^k &= \Delta_1^k + \Delta_2^k \\ \Delta_1^k &= d - F_I\lambda^k = r^k \\ \Delta_2^k &= G_I\alpha^k \end{aligned} \tag{29}$$

which shows that at each iteration k, two separate but related entities contribute to the jump of the displacement solution at the substructure interfaces

(1) the non-converged iterate α^k that specifies the contributions of the substructure rigid body modes to the substructure displacement solutions,
(2) and the non-converged tractions λ^k.

Equations (29) reveal that $d - F_I\lambda^k$ and $G_I\alpha^k$ have the physical meaning of the jump of the displacement field across the substructure interfaces due to the non-converged tractions λ^k, and that caused by the non-converged values of the contributions of the substructure rigid body modes, respectively.

On the other hand, equation (19) establishes that the role of the projector P is to ensure that every iterate λ^k generated by PCG is an admissible Lagrange multiplier ($G_I^T\lambda^k = 0$). However, solving the projected problem (19) is equivalent to solving the interface problem (8) from which we deduce after using equation (25)

$$\begin{aligned} G_I\alpha^k &= -r^k \\ \Rightarrow \alpha^k &= -(G_I^T G_I)^{-1} G_I^T r^k \end{aligned} \tag{30}$$

Hence, using equations (29) and (30), it follows that at each iteration k the projector P ensures that

$$G_I^T\Delta^k = G_I^T r^k + G_I^T G_I\alpha^k = G_I^T r^k - (G_I^T G_I)(G_I^T G_I)^{-1} G_I^T r^k = 0 \tag{31}$$

In other words, the effect of the coarse problem generated by the projector P can alternatively be understood as that of enforcing throughout the PCG iterations a weak form $G_I^T \Delta^k = 0$ of the continuity along Γ_I of the substructure displacement solutions ($\Delta^k = 0$).

Furthermore, from equations (11) and (29) we have

$$P\Delta^k = P\Delta_1^k + P\Delta_2^k = Pr^k + PG_I\alpha^k = Pr^k = w^k \tag{32}$$

which also shows that the projected residual w^k has the physical meaning of the value of the jump of the displacement solution across the substructure interfaces *after* the contributions of the substructure rigid body modes have been adjusted to satisfy equation (31)—or after the Lagrange multiplier iterate λ^k has been made admissible.

4.2. Previously developed auxiliary coarse problems

For problems where a substructure matrix $A^{(s)}$ can be singular—for example, for a structural mechanics statics problem and a mesh partition with floating substructures—the projector $P = I - G_I(G_I^T G_I)^{-1} G_I^T$, and therefore the auxiliary coarse problem of the form $(G_I^T G_I)x^* = b^*$, are non-optional ingredients of the FETI method. They are required by the solvability conditions (5), independently from any convergence rate consideration. The fact that this coarse problem accelerates the PCG iterations and ensures the scalability of the FETI method with respect to the substructure size H are positive *consequences*. Indeed, the natural and effective coarse problem associated with the projector P is what distinguishes the FETI method from other DD-based iterative algorithms.

For structural dynamics problems, an implicit time integrator leads to a system of equations whose governing substructure matrix is usually given by

$$A^{(s)} = M^{(s)} + \zeta \Delta t^2 K^{(s)} \tag{33}$$

where $M^{(s)}$ and $K^{(s)}$ are, respectively, the substructure mass and stiffness matrices, Δt is a given time step, and ζ is a constant that depends on the algorithm chosen for time-integrating the finite element equations of dynamic equilibrium. In general, $M^{(s)}$ is positive definite, and therefore $\mathrm{Ker}(A^{(s)})$ is empty whether $\Omega^{(s)}$ is floating or restrained. In that case, the local Neumann problems associated with the FETI method do not require any solvability condition because they are well posed. Hence, a straightforward extension of the FETI method to structural dynamics problems does not involve any projector similar to P. Unfortunately, losing the projector in the FETI method is losing the natural mechanism for propagating the error globally during the PCG iterations, and therefore, losing scalability with respect to the substructure size H. For this reason, a different projector was proposed in Reference 8 for solving by the FETI method finite element systems of equations arising from structural dynamics problems. This new projector is optional but essential to the numerical scalability of the FETI method with respect to the number of substructures. It was derived in Reference 8 using multilevel principles.

The basic FETI algorithm displayed in box (26) is numerically scalable when applied to the solution of systems of equations arising from the finite element discretization of second-order partial differential equations. In References 10 and 11, the G matrix and the coarsening operator $G_I^T G_I$ were expanded to include the so-called substructure corner modes in addition to the substructure rigid body modes, and the resulting FETI method was shown to be numerically scalable for fourth-order plate and shell problems as well. The derivation of this new coarse problem was motivated

by plate theory and numerical experiments, and did not follow explicitly the same principles as those used for designing the coarse problem of the FETI method for elastodynamics.

Next, we present a unified framework for constructing the various coarse problems needed for ensuring the numerical scalability of the FETI method for different classes of problems. This framework has the merit of simplifying the derivation and understanding of previously developed FETI coarse problems,[8, 10, 11] and inspiring new ones.

5. A SIMPLE AND UNIFIED FRAMEWORK FOR DESIGNING FETI COARSE PROBLEMS

5.1. Optional admissible displacement constraints

Recall that at each PCG iteration k, the substructures are in equilibrium, but their local displacement iterates $u^{(s)^k}$ are not necessarily continuous along the substructure interface boundaries. The objective of each FETI iteration is to reduce the jump $\Delta^k = r^k + G_I\alpha^k$ of the displacement solution of equation (3) across $\Gamma_I^{(s)}$. At convergence, this jump vanishes in the usual numerical sense. At each PCG iteration, the basic FETI algorithm employs the projector P to enforce the solvability conditions (5). In Section 4.1, we have shown that the role of this projector—and its corresponding coarse problem—can also be interpreted as that of enforcing at each PCG iteration the displacement constraint

$$\mathscr{C}(u^{(s)^k}) = G_I^T\Delta^k = 0 \tag{34}$$

Here, we exploit this interpretation to develop a simple but general framework for designing a rich family of coarse problems for the FETI method.

Let $\mathscr{C}(u^{(s)^k}) = 0$ denote a constraint on the substructure displacement iterates $u^{(s)^k}$. We call $\mathscr{C}$ an admissible constraint if (a) it is linear, and (b) $\mathscr{C}(u^{(s)}) = 0$—that is, this linear constraint is verified by the exact solutions $u^{(s)}$ of the substructure problems. We also refer to $\mathscr{C}$ as an optional displacement constraint if it is not required by a solvability condition of the FETI formulation.

First, we note that the PCG algorithm applied to the solution of the interface problem (8) can be modified to enforce at each iteration any optional admissible displacement constraint, and will still recover the exact solution of the governing equations (3).

Next, we also note that if $\mathscr{C}$ is chosen as

$$\mathscr{C}(u^{(s)^k}) = Q^T\Delta^k = Q^T(r^k + G_I\alpha^k) = 0 \tag{35}$$

where Q is an $N_I \times m$ matrix with $m \leqslant N_I$, then $\mathscr{C}$ is admissible and its enforcement at each PCG iteration can only accelerate the convergence of the FETI method. Indeed, $Q^T\Delta^k = 0$ is a weighted-residual weak form of $\Delta^k = 0$, and therefore, its effect at each iteration k is to reduce the error in the compatibility of the substructure solutions $u^{(s)^k}$ at the interface Γ_I. For example, if $m = N_I$ and Q is non-singular, then the FETI method equipped with the optional admissible constraint $Q^T\Delta^k = 0$ is guaranteed to converge in one iteration. However, m must be chosen small enough to keep the corresponding additional computations and interprocessor communications affordable.

A straightforward approach for enforcing at each PCG iteration an optional admissible displacement constraint of the form $Q^T\Delta^k = 0$ is to introduce an additional Lagrange multiplier of the form $\mu = Q\gamma$ in the FETI formulation, where γ is an m long vector of additional unknowns. More

specifically, the PCG algorithm is modified so that each iterate λ^k is transformed into an iterate $\tilde{\lambda}^k$ as follows:

$$\tilde{\lambda}^k = \lambda^k + \mu^k = \lambda^k + Q\gamma^k \tag{36}$$

where as before, the role of λ^k is to enforce at convergence $\Delta = \sum_{s=1}^{s=N_s} B^{(s)}u^{(s)} = 0$, and the role of the correction term $\mu^k = Q\gamma^k$ is to enforce exactly at each iteration k the optional admissible displacement constraint $Q^{\mathrm{T}}\Delta^k = 0$. Furthermore, if the FETI formulation requires the solvability conditions (5), $\tilde{\lambda}^k$ must in turn be transformed into an admissible Lagrange multiplier iterate—that is, an iterate $\bar{\lambda}^k$ that satisfies the non-optional constraint $G_{\mathrm{I}}^{\mathrm{T}}\bar{\lambda}^k = 0$. This latter condition can be enforced by introducing yet another Lagrange multiplier v of the form $v = G_{\mathrm{I}}\beta$ and requiring that

$$\bar{\lambda}^k = \tilde{\lambda}^k + G_{\mathrm{I}}\beta^k = \lambda^k + Q\gamma^k + G_{\mathrm{I}}\beta^k \tag{37}$$

However, if $\bar{\lambda}^k$ is forced to be an admissible Lagrange multiplier, then the corresponding displacement jump Δ^k will satisfy $G_{\mathrm{I}}^{\mathrm{T}}\Delta^k = 0$ as demonstrated in equation (31). Hence, the unknowns γ^k, β^k and α^k are determined from the solution of the constraint equations

$$\begin{aligned} Q^{\mathrm{T}}\Delta^k &= 0 \Rightarrow Q^{\mathrm{T}}(d - F_{\mathrm{I}}\bar{\lambda}^k + G_{\mathrm{I}}\alpha^k) = 0 \\ G_{\mathrm{I}}^{\mathrm{T}}\Delta^k &= 0 \Rightarrow G_{\mathrm{I}}^{\mathrm{T}}(d - F_{\mathrm{I}}\bar{\lambda}^k + G_{\mathrm{I}}\alpha^k) = 0 \\ G_{\mathrm{I}}^{\mathrm{T}}\bar{\lambda}^k &= 0 \end{aligned} \tag{38}$$

After substituting equation (37) into equation (38) and using the first of equation (25), the above system of equations can be re-written in matrix form as

$$\begin{bmatrix} T^{\mathrm{T}}F_{\mathrm{I}}T & -T^{\mathrm{T}}G_{\mathrm{I}} \\ -G_{\mathrm{I}}^{\mathrm{T}}T & 0 \end{bmatrix} \begin{bmatrix} \delta^k \\ \alpha^k \end{bmatrix} = \begin{bmatrix} T^{\mathrm{T}}r^k \\ G_{\mathrm{I}}^{\mathrm{T}}\lambda^k \end{bmatrix}$$

where

$$T = [Q \quad G_{\mathrm{I}}], \qquad \delta^k = \begin{bmatrix} \gamma^k \\ \beta^k \end{bmatrix} \tag{39}$$

In summary, the convergence of the FETI method can be accelerated by enforcing at each PCG iteration an optional admissible displacement constraint of the form $Q^{\mathrm{T}}\Delta^k = 0$. This requires transforming each iterate λ^k into the iterate $\tilde{\lambda}^k$ as described in equation (36), which in turn requires solving the auxiliary problem (39). If the number of columns m of Q is kept sufficiently small, this auxiliary problem becomes a coarse problem. It couples all the substructure computations, and therefore provides a mechanism for propagating the error globally, and ensuring the numerical scalability of the FETI method with respect to the number of substructures.

A general projector associated with the general coarse problem (39) can be derived as follows. From equations (39), δ^k can be computed as

$$\begin{aligned}\delta^k = &-(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}(T^{\mathrm{T}}F_{\mathrm{I}} + T^{\mathrm{T}}G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}G_{\mathrm{I}})^{-1}\\ &\times(G_{\mathrm{I}}^{\mathrm{T}} - G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}F_{\mathrm{I}}))\lambda^k\\ &+(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}(I - T^{\mathrm{T}}G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1})T^{\mathrm{T}}d\end{aligned} \tag{40}$$

Substituting equation (40) into equation (37) and using the notation of equation (39) leads to

$$\begin{aligned}\bar{\lambda}^k = \lambda^k &- T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}(T^{\mathrm{T}}F_{\mathrm{I}} + T^{\mathrm{T}}G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}G_{\mathrm{I}})^{-1}\\ &\times(G_{\mathrm{I}}^{\mathrm{T}} - G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}F_{\mathrm{I}}))\lambda^k + \lambda^0\end{aligned} \tag{41}$$

where

$$\lambda^0 = T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}(I - T^{\mathrm{T}}G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1})T^{\mathrm{T}}d$$

If $\bar{P}$ is defined as

$$\bar{P}: \lambda^k \to \bar{\lambda}^k - \lambda^0 \tag{42}$$

it follows from equation (41) that

$$\boxed{\begin{aligned}\bar{P} = I &- T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}(T^{\mathrm{T}}F_{\mathrm{I}} + T^{\mathrm{T}}G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}G_{\mathrm{I}})^{-1}\\ &\times(G_{\mathrm{I}}^{\mathrm{T}} - G_{\mathrm{I}}^{\mathrm{T}}T(T^{\mathrm{T}}F_{\mathrm{I}}T)^{-1}T^{\mathrm{T}}F_{\mathrm{I}}))\end{aligned}} \tag{43}$$

The reader can check that

$$\begin{aligned}\bar{P}^2 &= \bar{P}\\ \bar{P}T &= 0\end{aligned} \tag{44}$$

which shows that $\bar{P}$ is a projector onto $\mathrm{Ker}(T^{\mathrm{T}})$.

Hence, enforcing at each PCG iteration an optional admissible displacement constraint of the form $Q^{\mathrm{T}}\Delta^k = 0$ provides a general framework for devising effective coarse problems and their corresponding projectors for the FETI method. Note that if Q is set to zero, T simplifies to $T = G_{\mathrm{I}}$, and the projector $\bar{P}$ becomes

$$\begin{aligned}\bar{P} &= I - G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}G_{\mathrm{I}})^{-1}(G_{\mathrm{I}}F_{\mathrm{I}} + (G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})^{-1}(G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}G_{\mathrm{I}})(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})^{-1}\\ &\quad\times(G_{\mathrm{I}}^{\mathrm{T}} - G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}))\\ &= I - G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}G_{\mathrm{I}})^{-1}(G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}} + (G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}G_{\mathrm{I}})(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}} - G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}})\\ &= I - G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}}\\ &= P\end{aligned} \tag{45}$$

which shows that the basic FETI method for statics problems is a particular case of the FETI method equipped with the general projector $\bar{P}$. Next, we show that all previously developed FETI coarse problems are particular instances of the methodology described here.

Remark 6. The reader familiar with the Neumann–Neumann preconditioned Schur complement method[25, 26] and the balancing method[27] can check that the concept of optional admissible constraints can also be used to construct coarse problems for these DD methods.

Remark 7. The expression (43) of the projector $\bar{P}$ is derived here for academic purposes. In practice, it is computationally more efficient to compute the effect of $\bar{P}$ by solving the corresponding coarse problem (39).

5.2. *Elastodynamics*

For finite element structural dynamics problems discretized by an implicit time integrator, the FETI formulation does not require any solvability condition because the local matrices $A^{(s)} = M^{(s)} + \zeta \Delta t^2 K^{(s)}$ are never singular, even when they are associated with floating substructures. Therefore, for this class of problems, the basic FETI formulation loses the non-optional constraint $G_{\mathrm{I}}^{\mathrm{T}} \lambda^k = 0$ and the corresponding natural coarse problem. However, an 'artificial' coarse problem whose objective is to propagate the error globally to accelerate the convergence of the FETI method can be restored by enforcing at each PCG iteration an optional admissible constraint of the form $Q^{\mathrm{T}} \Delta^k = 0$.

Since the basic FETI formulation applied to a structural dynamics problem does not require a solvability condition, the jump of the displacement solution Δ^k across Γ_{I} is given by

$$\Delta^k = d - F_{\mathrm{I}} \lambda^k = r^k \tag{46}$$

and there is no need to transform $\tilde{\lambda}^k$ (equation (36)) into $\bar{\lambda}^k$ (equation (37)). In that case, γ^k can be computed directly from

$$\begin{aligned} Q^{\mathrm{T}} \Delta^k = 0 &\Rightarrow Q^{\mathrm{T}} (d - F_{\mathrm{I}} \tilde{\lambda}^k) = 0 \\ &\Rightarrow \gamma^k = -(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} F_{\mathrm{I}} \lambda^k + (Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} d \end{aligned} \tag{47}$$

Substituting equation (47) into equation (36) gives

$$\begin{aligned} \tilde{\lambda}^k &= \lambda^k - Q(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} F_{\mathrm{I}} \lambda^k + Q(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} d \\ &= (I - Q(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} F_{\mathrm{I}}) \lambda^k + \lambda^0 \end{aligned} \tag{48}$$

where

$$\lambda^0 = Q(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} d$$

From equation (48), it follows that the general projector $\bar{P}$ of the FETI method for transient dynamics problems is

$$\boxed{\bar{P} = I - Q(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} F_{\mathrm{I}}} \tag{49}$$

Note that setting G_{I} to zero in equation (43) leads to the above projector, which illustrates the consistency between our static and dynamic formulations.

If Q is set to

$$\begin{aligned} Q &= G_{\mathrm{I}} \\ G_{\mathrm{I}} &= [B^{(1)}R^{(1)} \quad \ldots \quad B^{(N_f)}R^{(N_f)}] \\ R^{(s)} &= \mathrm{Ker}(K^{(s)}) \text{ for a floating substructure } \Omega^{(s)} \end{aligned}$$

then $Q \neq 0$, and $\bar{P}$ becomes

$$\bar{P} = \bar{P}_G = I - G(G^{\mathrm{T}}F_{\mathrm{I}}G)^{-1}G^{\mathrm{T}}F_{\mathrm{I}} \tag{50}$$

This projector was first proposed in Reference 8 and derived using multilevel principles. Recall that F_{I} depends on $A^{(s)}$, and that for structural dynamics problems $A^{(s)} = M^{(s)} + \zeta \Delta t^2 K^{(s)}$ depends on the time step Δt. In Reference 8, it was shown that

$$\lim_{\Delta t \to \infty} I - G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}}F_{\mathrm{I}} = I - G_{\mathrm{I}}(G_{\mathrm{I}}^{\mathrm{T}}G_{\mathrm{I}})^{-1}G_{\mathrm{I}}^{\mathrm{T}} = P \tag{51}$$

and this result was used to show that the FETI method equipped with the projector (50) is numerically scalable for elastodynamics problems.

Both P and $\bar{P}_G$ require the *fast* evaluation of the substructure zero-energy modes. In this context, emphasis on computational speed is justified by the fact that these zero-energy modes are required for constructing a fast iterative FETI solver. When the mesh partitioning process does not generate any mechanism in any substructure, and each substructure has either zero or six (three in two-dimensional problems) rigid body modes, $R^{(s)} = \mathrm{Ker}(K^{(s)})$ is either empty or has six columns that can be easily computed by a geometric procedure.[31, 32] This was first recognized in Reference 8. However, for arbitrary mesh partitions and arbitrary substructure displacement boundary conditions, extracting the rigid body modes of a floating substructure is a more challenging task that seems to require factoring $K^{(s)}$.[32] For elastostatics problems, this is a rather efficient approach because, in any case, each substructure stiffness matrix is factored in order to solve the substructure problem (6) by a direct method. For elastodynamics problems, the direct solution of the substructure problems requires storing and factoring $A^{(s)} \neq K^{(s)}$, so that computing the rigid body modes of $\Omega^{(s)}$ by factoring $K^{(s)}$ entails additional storage and computational costs. Previously, we have justified this overhead by arguing that for a fixed size problem, the computational costs and storage requirements associated with factoring $K^{(s)}$ decrease when the number of substructures increases, and become relatively insignificant for problems with a large number of substructures. However, for fixed size problems with a small number of substructures, say $N_s \leqslant 16$, and/or for large fixed substructure size problems, factoring both $A^{(s)}$ and $K^{(s)}$ can become problematic, especially if storing $K^{(s)}$ in addition to $A^{(s)}$ causes memory swapping.

While the asymptotic result (51) justifies the usage of the correct number of exact rigid body modes in each substructure, the concept of optional admissible constraints presented in this paper suggests that any properly chosen matrix Q with linearly independent columns would accelerate the convergence of the FETI method for elastodynamics. In particular, if Q is set to

$$\begin{aligned} Q &= \hat{G}_{\mathrm{I}} \\ \hat{G}_{\mathrm{I}} &= [B^{(1)}\hat{R}^{(1)} \ldots B^{(N_f)}\hat{R}^{(N_f)}] \\ \hat{R}^{(s)} &= \mathrm{Ker}(\hat{K}^{(s)}) \\ \hat{K}^{(s)} &= \text{ stiffness matrix of } \hat{\Omega}^{(s)} \\ \hat{\Omega}^{(s)} &= \Omega^{(s)} \text{ after removing all specified displacement boundary conditions} \end{aligned}$$

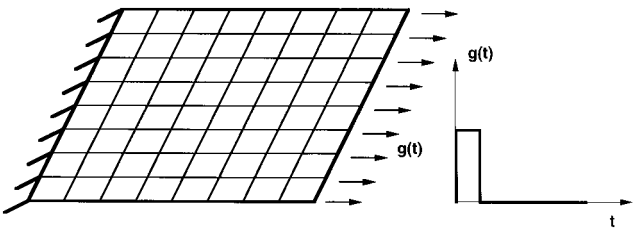

Figure 2. Finite element discretization of a membrane problem

then Q can be easily generated by (a) assuming that all $\Omega^{(s)}$ are floating substructures—even if some of them are partially or fully restrained—and (b) computing all six rigid body modes of each substructure from kinematics (three canonical displacements and three canonical rotations).[31, 32] Hence, computing $\hat{Q} = G_{\mathrm{I}}$ is more economical than computing $Q = G_{\mathrm{I}}$ and leads to the projector

$$\bar{P}_{\hat{G}} = I - \hat{G}(\hat{G}^{\mathrm{T}} F_{\mathrm{I}} \hat{G})^{-1} \hat{G}^{\mathrm{T}} F_{\mathrm{I}} \tag{52}$$

Given that the FETI method equipped with $\bar{P}_G$ is numerically scalable for elastodynamics problems, that $\bar{P}_{\hat{G}}$ differs from $\bar{P}_G$ only in those substructures that are either partially or fully restrained, and that $Q = \hat{G}_{\mathrm{I}}$ is essentially used to enforce at each PCG iteration a weighted residual weak form $Q^{\mathrm{T}} \Delta^k = 0$ of $\Delta^k = 0$, we argue here that the FETI method equipped with the alternative projector $\bar{P}_{\hat{G}}$ is also numerically scalable for transient dynamics problems. We have not attempted to mathematically prove this result. Nevertheless, we have conducted extensive numerical experiments that confirm our conjecture. A sample of these numerical experiments is reported below.

As an example, we consider the implicit transient analysis of a square membrane subjected to a planar impulse load (Figure 2). We construct three different finite element uniform discretizations using, respectively, $N_{\mathrm{e}} = 6400$ $(h = \frac{1}{80})$, $N_{\mathrm{e}} = 25\,600$ $(h = \frac{1}{160})$, and $N_{\mathrm{e}} = 102\,400$ $(h = \frac{1}{320})$ four-node plane stress/strain elements with two d.o.f. per node. These meshes generate, respectively, $N_{\mathrm{eq}} = 12\,800$, $N_{\mathrm{eq}} = 51\,200$, and $N_{\mathrm{eq}} = 204\,800$ equations to be solved at each time step. The coarsest mesh is partitioned into four square substructures $(H = \frac{1}{2})$, the intermediate one into 16 square substructures $(H = \frac{1}{4})$, and the finest mesh is partitioned into 64 square substructures $(H = \frac{1}{8})$. Note that for these three meshes and their decompositions, the substructure problem size H/h is kept constant. For each problem, Table I reports the number of iterations for convergence of the FETI method equipped with the projector $\bar{P}_G$ and with the alternative projector $\bar{P}_{\hat{G}}$. In all cases, the following stopping criterion is used:[1]

$$\frac{\|\bar{z}^k\|_2}{\|f\|_2} \leqslant \varepsilon \leqslant 10^{-6} \tag{53}$$

where $\bar{z}^k$ is the scaled and preconditioned residual case (see equation (26)). The convergence results are reported for the first time-step of the implicit dynamic analysis and for both the lumped and Dirichlet preconditioners.

The performance results reported in Table I show that for both preconditioners, the convergence rate of the FETI method equipped with the modified projector $\bar{P}_{\hat{G}}$ is identical to that of the FETI method with the original projector $\bar{P}_G$. These results also show that using any of these two projectors, the convergence rate of the FETI method equipped with either the lumped or Dirichlet preconditioner grows asymptotically only weakly with the number of substructures. The comparison

Table I. Transient response analysis of a membrane structure FETI with $\bar{P}_G$ vs. FETI with $\bar{P}_{\hat{G}}$, performance results form first time-step analysis

H	h	H/h	N_s	FETI + $\bar{P}_{\hat{G}}$ FETI + $\bar{P}_G$	FETI + $\bar{P}_G$ lumped	FETI + $\bar{P}_{\hat{G}}$ lumped	Dirichlet
$\frac{1}{2}$	$\frac{1}{80}$	40	4	17 itr.	17 itr.	13 itr.	13 itr.
$\frac{1}{4}$	$\frac{1}{160}$	40	16	29 itr.	29 itr.	25 itr.	25 itr.
$\frac{1}{8}$	$\frac{1}{320}$	40	64	30 itr.	30 itr.	27 itr.	27 itr.

between the CPU requirements of the FETI method with $\bar{P}_G$ or $\bar{P}_{\hat{G}}$ as a projector is discussed in Section 6.

5.3. *Plates and shells*

For fourth-order plate and shell statics problems, the condition number of the interface problem associated with the basic FETI method—that is, the FETI method equipped with the projector P—and preconditioned with $\bar{F}_{\mathrm{I}}^{D^{-1}}$ was observed to grow fast with the number of elements per substructure.[6] Plate theory and numerical experiments have suggested a two-level FETI method[10, 11] for which the condition number of the interface problem preconditioned with $\bar{F}_{\mathrm{I}}^{D^{-1}}$ is bounded by a logarithmic function of the number of elements per substructure[9] (see equation (1)). Here, we show that the two-level FETI method for fourth-order problems is a particular case of the FETI method equipped with the general projector $\bar{P}$.

The main idea behind the two-level FETI method for plates (shells) is to enforce exactly the continuity of the transverse (all three components) displacement field at the substructure corners throughout the PCG iterations. We remind the reader that in this context, a corner is defined as a point belonging to more than two substructures. Clearly, such a constraint is an optional admissible displacement constraint that can be written as

$$\mathscr{C} = X^{\mathrm{T}} \left(\sum_{s=1}^{s=N_s} B^{(s)} u^{(s)^k} \right) = X^{\mathrm{T}} \Delta^k = 0 \tag{54}$$

where X is an $N_{\mathrm{I}} \times N_{\mathrm{c}}$ rectangular matrix, N_{c} is the number of interface 'corner' (or crosspoint) d.o.f. that are enforced to be continuous throughout the PCG iterations, $X_{ij} = 1$ at each jth interface corner d.o.f., and $X_{ij} = 0$ elsewhere. In other words, X^{T} extracts from the continuity equations $\Delta = \sum_{s=1}^{s=N_s} B^{(s)} u^{(s)} = 0$ those equations that are associated with substructure corner d.o.f.

Setting $Q = X$ in equation (39) leads to

$$\begin{bmatrix} X^{\mathrm{T}} F_{\mathrm{I}} X & X^{\mathrm{T}} F_{\mathrm{I}} G_{\mathrm{I}} & -X^{\mathrm{T}} G_{\mathrm{I}} \\ G_{\mathrm{I}}^{\mathrm{T}} F_{\mathrm{I}} X & G_{\mathrm{I}}^{\mathrm{T}} F_{\mathrm{I}} G_{\mathrm{I}} & -G_{\mathrm{I}}^{\mathrm{T}} G_{\mathrm{I}} \\ -G_{\mathrm{I}}^{\mathrm{T}} X & -G_{\mathrm{I}}^{\mathrm{T}} G_{\mathrm{I}} & 0 \end{bmatrix} \begin{bmatrix} \gamma^k \\ \beta^k \\ \alpha^k \end{bmatrix} = \begin{bmatrix} X^{\mathrm{T}} r^k \\ G_{\mathrm{I}}^{\mathrm{T}} r^k \\ G_{\mathrm{I}}^{\mathrm{T}} \lambda^k \end{bmatrix} \tag{55}$$

which is the same coarse problem as that proposed in References 9–11.

We have shown in Section 5.2 that for transient dynamics problems, the general projector to be used with the FETI method is $\bar{P} = I - Q(Q^{\mathrm{T}} F_{\mathrm{I}} Q)^{-1} Q^{\mathrm{T}} F_{\mathrm{I}}$. From the above discussion and the

results of Sections 5.1 and 5.2, it follows that the appropriate choice of Q for dynamics plate and shell problems is

$$Q = X_G = [X \;\; G_I] \tag{56}$$

Substituting equation (56) into equation (49) leads to the projector

$$\bar{P} = I - X_G (X_G^T F_I X_G)^{-1} X_G^T F_I \tag{57}$$

which is the same as the optimal FETI projector previously derived in Reference 11.

5.4. The general case

A general approach for constructing a T matrix for statics problems and a Q matrix for dynamics ones, and building the corresponding coarse problem or projector $\bar{P}$ is to combine the effects of multiple optional admissible displacement constraints that are deemed essential for accelerating the convergence of the FETI method for a certain class of problems. If $\mathscr{C}_i$ and C_i denote a generic optional admissible displacement constraint and its corresponding matrix ($C_i^T \Delta^k = 0$), enforcing $N_{\mathscr{C}}$ such constraints throughout the PCG iterations can be done, as discussed earlier, by introducing $N_{\mathscr{C}}$ additional Lagrange multipliers of the form $\mu_i = C_i \gamma_i$. More specifically for statics problems, the PCG algorithm is modified to transform each iterate λ^k into an iterate $\bar{\lambda}^k$ of the form

$$\bar{\lambda}^k = \lambda^k + \sum_{i=1}^{i=N_{\mathscr{C}}} C_i \gamma_i^k + G_I \beta^k \tag{58}$$

where, as before, the role of the term $G_I \beta^k$ is to ensure that the modified Lagrange multiplier $\bar{\lambda}^k$ is admissible. This approach leads to the same coarse problem as in equation (39) with T given by

$$\boxed{T = [C_1 \;\; C_2 \;\; \ldots \;\; C_{N_{\mathscr{C}}} \;\; G_I]} \tag{59}$$

Similarly for dynamics problems, the general projector is that given in (49) with

$$Q = [C_1 \;\; C_2 \;\; \ldots \;\; C_{N_{\mathscr{C}}}] \tag{60}$$

Since $Q = G_I$ was shown in Reference 8 to produce an optimal projector for elastodynamics, and since $Q = \hat{G}_I$ is simpler to implement than $Q = G_I$ and retains its numerical scalability properties, we recommend that the constraint $\hat{G}_I r^k = 0$ be always enforced throughout the PCG iterations, and therefore recommend that $\hat{G}_I$ be always included in the definition of Q for dynamics problems

$$\boxed{Q = [C_1 \;\; C_2 \;\; \ldots \;\; C_{N_{\mathscr{C}}} \;\; \hat{G}_I]} \tag{61}$$

In summary, for structural mechanics statics problems, the general FETI method is the FETI method equipped with projector (43) where $T = [C_1 \;\; C_2 \;\; \ldots \;\; C_{N_{\mathscr{C}}} \;\; G_I]$. This projector generates the general coarse problem given in equation (39). For structural dynamics problems, the general FETI method is the FETI method equipped with the projector (49) with $Q = [C_1 \;\; C_2 \;\; \cdots \;\; C_{N_{\mathscr{C}}} \;\; \hat{G}_I]$.

Previously, only the substructure rigid body and corner modes have been considered for constructing the T and Q matrices and their corresponding coarse problems. The resulting FETI

methods have been proved mathematically to be numerically scalable with respect to both the mesh size h and the substructure size H. Hence, in order to be interesting, a new coarse problem for the FETI method for structural problems would have to

(1) lower the logarithmic power m of the optimal asymptotic condition number (1) achievable with the substructure rigid body and corner modes at a feasible computational price,
(2) or lower the constant of the optimal asymptotic condition number (1) achievable with the substructure rigid body and corner modes at a feasible computational price,
(3) or maintain the numerical scalability properties of the currently available FETI methods at a lower computational price.

Next, we apply the computational framework described in the previous sections to construct a new FETI coarse problem, and use the guidelines outlined above to assess its impact on the convergence of the FETI method. The CPU benchmarking of the FETI method equipped with this new coarse problem is discussed in Section 6.

Remark 8. The reader should keep in mind that a substructure-by-substructure formulation of the Q and T matrices simplifies the parallel implementation of the FETI method on distributed memory systems, and offers a great potential for high-performance execution time because it provides data locality. Furthermore, one should note that $Q^{\mathrm{T}}\Delta^k = 0$ can always be written as $\sum_{s=1}^{s=N_s} Q^{(s)^{\mathrm{T}}} B^{(s)^{\mathrm{T}}} \Delta^{(s)^k} = 0$, and therefore Q can be constructed in a similar manner as G_1: $Q = Q_1 = [B^{(1)}Q^{(1)} \ \ldots \ B^{(N_s)}Q^{(N_s)}]$.

5.5. A new coarse problem

Let $\Gamma_{\mathrm{I}}^{(s,q)} = \Omega^{(s)} \cap \Omega^{(q)}$ and $E^{(s,q)}$ denote, respectively, the interface between two substructures $\Omega^{(s)}$ and $\Omega^{(q)}$, and the signed Boolean matrix that localizes the interface d.o.f. attached to $\Gamma_{\mathrm{I}}^{(s,q)}$. In the sequel, we call $\Gamma_{\mathrm{I}}^{(s,q)}$ an ith *edge*, and rename $E^{(s,q)}$ as E_i.

The matrix–vector product

$$E_i^{\mathrm{T}}\Delta = 0 \tag{62}$$

extracts from the continuity equations $\Delta = \sum_{s=1}^{s=N_s} B^{(s)}u^{(s)} = 0$ those equations that are associated with the d.o.f. attached to the ith edge of the given mesh partition. If N_E is the total number of edges of the decomposed domain, we define

$$E = [E_1 \ E_2 \ \ldots \ E_{N_E}] \tag{63}$$

A simple weak form of the equations of continuity of the substructure displacement iterates is the continuity in an *average* sense of the substructure solutions $u^{(s)^k}$ along the substructure edges $\Gamma_{\mathrm{I}}^{(s,q)}$. This weak form can be written as

$$V_i^{\mathrm{T}}(E_i^{\mathrm{T}}\Delta^k) = 0, \quad i = 1, \ldots, N_E \tag{64}$$

where V_i^{T} is an 'averaging mode' associated with an averaging operator for the d.o.f. of the ith edge. For example, a straightforward *discrete* averaging of the substructure displacement continuity equations along $\Gamma_{\mathrm{I}}^{(s,q)}$ can be expressed as

$$\sum_{j\in\Gamma_{\mathrm{I}}}^{(s,q)} (u_j^{(s)} - u_j^{(q)}) = 0 \tag{65}$$

where u_j denotes the value of the displacement field at the jth d.o.f., and the corresponding mode V_i is given by

$$V_i = [1 \;\; 1 \;\; \ldots \;\; 1]^{\mathrm{T}} \tag{66}$$

A more general discrete averaging procedure can be implemented using the mode

$$V_i = [w_1 \;\; w_2 \;\; \ldots \;\; w_{N_i}]^{\mathrm{T}} \quad \sum_{k=1}^{k=N_i} w_k = 1 \tag{67}$$

where N_i denotes the number of d.o.f. attached to $\Gamma_{\mathrm{I}}^{(s,q)}$, and $\{w_k\}_{k=1}^{k=N_i}$ are weights that can be used to account for a potentially irregular distribution of the jump of the substructure displacement fields across the ith edge, or an irregular spacing between the grid points of a given edge.

Alternatively, a non-discrete averaging procedure of the form

$$\int_{\Gamma_{\mathrm{I}}^{(s,q)}} \mu(u_j^{(s)} - u_j^{(q)})\, \mathrm{d}s = 0 \tag{68}$$

can be employed, where μ is a specified polynomial, or piece-wise polynomial, or mortar Lagrange multiplier.[33, 34]

If the matrix of averaging modes V is defined as follows:

$$V = \begin{bmatrix} V_1 & 0 & \ldots & \ldots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & V_i & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & V_{N_E} \end{bmatrix} \tag{69}$$

then, the idea expressed in equation (64) leads to the new optional admissible displacement constraint

$$(EV)^{\mathrm{T}} \Delta^k = 0 \tag{70}$$

In order to assess the effect of the coarse problem associated with the optional admissible constraint (70) on the convergence rate of the FETI method, we consider the solution by an implicit time integrator of a dynamics plate bending problem. More specifically, we consider four different Q matrices and their corresponding projectors $\bar{P}$ (49)

$$\begin{aligned} Q_1 &= [\hat{G}_{\mathrm{I}}] \\ Q_2 &= [(EV)_z \;\; \hat{G}_{\mathrm{I}}] \\ Q_3 &= [(EV)_3 \;\; \hat{G}_{\mathrm{I}}] \\ Q_4 &= [X_z \;\; \hat{G}_{\mathrm{I}}] \\ Q_5 &= [X_z \;\; (EV)_z \;\; \hat{G}_{\mathrm{I}}] \\ Q_6 &= [X_z \;\; (EV)_3 \;\; \hat{G}_{\mathrm{I}}] \end{aligned} \tag{71}$$

As in Section 5.3, X denotes here the matrix of the substructure corner modes. The z and 3 subscripts are used to indicate that the corner and/or averaging modes are defined only for the transverse displacement d.o.f. or all 3 displacement d.o.f. at a node, respectively. Note that only

Table II. Implicit dynamic analysis of a square plate subjected to a uniform bending load 450 elements per substructure. FETI method with the Dirichlet preconditioner and various projectors—*exact* coarse solver,performance results for the first time-step analysis

h	N_e	N_s	$\bar{P}(Q_1)$	$\bar{P}(Q_2)$	$\bar{P}(Q_3)$	$\bar{P}(Q_4)$	$\bar{P}(Q_5)$	$\bar{P}(Q_6)$
$\frac{1}{60}$	7200	16	60 itr.	49 itr.	33 itr.	22 itr.	20 itr.	18 itr.
$\frac{1}{75}$	11 250	25	87 itr.	63 itr.	34 itr.	25 itr.	21 itr.	18 itr.
$\frac{1}{90}$	16 200	36	116 itr.	79 itr.	47 itr.	26 itr.	24 itr.	21 itr.
$\frac{1}{120}$	28 800	64	168 itr.	92 itr.	81 itr.	30 itr.	27 itr.	23 itr.

X_z is employed here because for plate problems, it was shown in References 9 and 10 that only the continuity of the transverse displacement d.o.f. is needed to accelerate the convergence of the PCG iterations. All weights $\{w_k\}_{k=1}^{k=N_i}$ are set to 1. The plate is assumed to have a square shape of unit length and a thickness equal to 2×10^{-3}. Its Young modulus is $E = 6{\cdot}9 \times 10^{10}$ and its Poisson coefficient is $v = 0{\cdot}3$. It is discretized by three-noded triangular DKT elements and subjected to a uniform pressure load amplified by a Heavy-side function. The mid-point rule is selected for time integration, and the implicit time step is set to $\Delta t = \mathscr{T}_6/15 = 2 \times 10^{-3}$, where $\mathscr{T}_6$ is the period of the sixth natural mode of vibration of the plate. A series of discretizations where the size of each substructure is fixed to 450 elements are performed. The number of substructures is varied between 16 and 64, and therefore the total number of elements in the mesh is varied between 7200 and 28 800. In all cases, the Dirichlet preconditioner is employed, and the stopping criterion (53) is used. Both direct and iterative methods are considered for the solution of the coarse problems associated with the projector $\bar{P}$ (49). The iterative method is a CG algorithm equipped with a reorthogonalization procedure for accelerating the iterative solution of systems with repeated right-hand sides.[16] Solving the coarse problem by a CG algorithm is attractive because it simplifies the implementation of the coarse operator on massively parallel processors, and because the CG computations are more amenable to massively parallel processing than any computations based on Gaussian elimination. We refer to the direct method as an *exact* coarse problem solver, and to the iterative method as an *inexact* coarse problem solver because the solution it computes depends on the tolerance used in the stopping criterion for the coarse problem.

The convergence rates achieved by the FETI method equipped with the Dirichlet preconditioners and the various projectors $\bar{P}$ (49) based on the Q_1 to Q_6 matrices defined in (71) are reported in Table II for the exact coarse problem solver, and in Table III for the inexact one. These results are those obtained during the first time-step analysis.

The first three columns of Tables II and III show that for fourth-order plate problems, neither the coarse problem based on the substructure rigid body modes nor that based on the substructure rigid body and edge averaging modes ensure the numerical scalability of the FETI method. The averaging modes computed for all 3 d.o.f. at the edge nodes are reported to improve the convergence rate of the FETI method by a factor 2, but do not achieve numerical scalability with respect to the number of substructures.

On the other hand, the fourth columns of Tables II and III show that the FETI method equipped with the coarse problem based on the substructure corner modes is numerically scalable, which is consistent with the theories presented in References 9 and 10. Superposing the averaging modes computed for all 3 d.o.f. at the edge nodes to the substructure corner modes improves the

Table III. Implicit dynamic analysis of a square plate subjected to a uniform bending load 450 elements per substructure, FETI method with the Dirichlet preconditioner and various projectors—*inexact* coarse solver, performance results for the first time-step analysis

h	N_e	N_s	$\bar{P}(Q_1)$	$\bar{P}(Q_2)$	$\bar{P}(Q_3)$	$\bar{P}(Q_4)$	$\bar{P}(Q_5)$	$\bar{P}(Q_6)$
$\frac{1}{60}$	7200	16	60 itr.	54 itr.	36 itr.	24 itr.	23 itr.	20 itr.
$\frac{1}{75}$	11 250	25	87 itr.	71 itr.	38 itr.	28 itr.	25 itr.	20 itr.
$\frac{1}{90}$	16 200	36	116 itr.	88 itr.	52 itr.	29 itr.	26 itr.	23 itr.
$\frac{1}{120}$	28 800	64	168 itr.	104 itr.	92 itr.	34 itr.	30 itr.	25 itr.

convergence rate of the FETI method by almost 25 per cent whether the coarse problem is solved exactly or inexactly (see the sixth columns of Tables II and III). For this dynamics plate bending problem, the inexact coarse problem solver is reported to slow down the convergence rate of the FETI method by less than 12 per cent.

5.6. Computational complexity analysis

Because the iteration count by itself is not sufficient to characterize an iterative algorithm, we discuss here the computational complexity of the FETI methods presented in this paper. We focus exclusively on the solution of the chosen coarse problem, because the other steps of the FETI methodology are identical for all FETI algorithms. We consider the case where the coarse problem is constructed substructure-by-substructure (see Remark 8) using the rigid body and a combination of the corner and averaging modes, and solved iteratively by an accelerated CG method for the reasons outlined in the previous section. In that case, computational efficiency requires precomputing $W = F_I T$ or $W = F_I Q$ (see Reference 11 for details). For statics problems, we assume that equations (39) are solved for transforming each iterate λ^k into an improved iterate $\bar{\lambda}^k$ of the form given in equation (58). For dynamics problems, we assume that the projector $\bar{P}$ given in equation (49) is directly used for that purpose.

More specifically, we discuss how the *parallel computational* cost—that is, the computational cost using N_p processors—associated with precomputing W and solving the coarse problem by a CG method grows with the global size of the given problem and/or the number of substructures and processors. For simplicity, we assume that $N_p = N_s$, and that each substructure is assigned to one processor. Let r_c denote the rank of $T^T F_I T$ for statics problems, and that of $Q^T F_I Q$ for dynamics problems. We note that, usually, a CG algorithm equipped with the reorthogonalization technique described in Reference 16 solves a FETI coarse problem in r_c iterations during the first FETI PCG iteration, and in a single iteration afterwards. Hence, the parallel computational cost entailed by the iterative solution of a given coarse problem is dominated by the cost of r_c pairs of matrix-vector multiplications of the form ($x^{(s)} = W^{(s)} \delta^{(s)}$, $y^{(s)} = T^{T^{(s)}} x^{(s)}$ (or $y^{(s)} = Q^{T^{(s)}} x^{(s)}$)). The parallel computational cost of precomputing W is dominated by the cost of $N_M^{(s)}$ pairs of forward and backward substitutions of the form $A^{(s)^+} p^{(s)}$, where $N_M^{(s)}$ is the total number of modes that form the coarse problem and have a non-zero trace on substructure $\Omega^{(s)}$.

For simplicity, we consider a two-and-a-half dimensional uniform discretization characterized by a mesh size h, and a checker-board mesh partition characterized by a substructure size H (Figure 3). The number of substructures N_s, the number of corners N_X, the number of edges N_E,

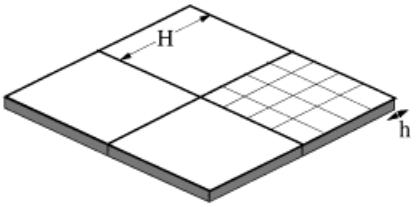

Figure 3. Uniform discretization and checker-board partition. Definition of the h and H parameters for a two-and-a-half-dimensional problem

Table IV. Parallel complexity analysis of three coarse problems

	G_{I} and X modes	G_{I} and EV modes	G_{I}, X, and EV modes
r_{c}	$O((6+d_X)\frac{1}{H^2})$	$O((6+2d_{EV})\frac{1}{H^2})$	$O((6+d_X+2d_{EV})\frac{1}{H^2})$
W	$O((54+12d_X)(\frac{H}{h})^3)$	$O((54+4d_{EV})(\frac{H}{h})^3)$	$O((54+12d_X+4d_{EV})(\frac{H}{h})^3)$
Coarse	$O(2(54+24d_X)4(\frac{6+d_X}{hH}))$	$O(2(54+8d_{EV})4(\frac{6+2d_{EV}}{hH}))$	$O(2(54+24d_X+8d_{EV})4(\frac{6+d_X+2d_{EV}}{hH}))$

the substructure interface size $N_{\mathrm{I}}^{(s)}$, the total interface size N_{I}, and the size $n^{(s)}$ and bandwidth $b^{(s)}$ of a substructure problem are given by

$$\begin{aligned} N_s &= \frac{1}{H^2} \\ N_X &= \left(\frac{1}{H}-1\right)^2 = O(N_s) \\ N_{\mathrm{E}} &= 2\times\frac{1}{H}\times\left(\frac{1}{H}-1\right) = O(2N_s) \\ N_{\mathrm{I}}^{(s)} &= O\left(4\frac{H}{h}\right) \\ N_{\mathrm{I}} &= 2\times\frac{1}{h}\times\left(\frac{1}{H}-1\right) = O\left(\frac{2}{hH}\right) \\ n^{(s)} &= O\left(\left(\frac{H}{h}\right)^2\right) \\ b^{(s)} &= O\left(\frac{H}{h}\right) \end{aligned} \tag{72}$$

From equations (72), it follows that the computational complexity of a pair of local forward and backward substitutions of the form $A^{(s)^+}p^{(s)}$ grows asymptotically as $O((\frac{H}{h})^3)$.

Furthermore, we assume that each substructure has 6 rigid body modes, and denote by d_X and d_{EV} the number of degrees of freedom per node for which corner and averaging modes are defined, respectively. We give in Table IV the asymptotic upper bound of r_{c} and the parallel computation cost associated with precomputing W and solving a FETI coarse problem for three different cases. The values reported in Table IV are upper bounds because any combination of rigid body, corner, and averaging modes is not necessarily linearly independent, and therefore r_{c} is often smaller than the sum of all the modes that form the coarse problem.

Table V. Parallel computational complexity analysis for a two-and-a-half-dimensional problem and an increasing number of substructures

Case	Precomp. W	Sol. coarse pb.
$h = c_1$	$O(N_s^{-3/2})$	$O(\sqrt{N_s}) = O(N_I)$
$\frac{H}{h} = c_2$	$O(1)$	$O(N_s) = O(N_I)$

From the results reported in Table IV, it follows that if the mesh size h is fixed ($h = c_1$) and the number of substructures $N_s = 1/H^2$ is increased, for each coarse problem, the parallel computational cost associated with precomputing W grows asymptotically as $O(H^3) = O(N_s^{-3/2})$. In other words, this parallel computational cost decreases when the number of substructures and processors increases. It also follows that the parallel computational cost associated with the iterative solution of each of the three coarse problems grows as $O(\frac{1}{H}) = O(N_I) = O(\sqrt{N_s})$. This means that, for a fixed-size problem, the computational overhead entailed by the parallel iterative solution of each of the three coarse problems analysed in Table IV increases as the square root of the number of substructures and processors.

On the other hand, if the mesh size h is decreased—that is, the size of the global problem is increased—while the number of substructures $N_s = 1/H^2$ is increased and the ratio $H/h = c_2$ is kept constant—that is, the size of the substructure problem is kept constant—for all three coarse problems, the parallel computational cost associated with precomputing W varies as $O(c_2^3) = O(1)$ and therefore remains constant, and the parallel computational cost associated with solving the coarse problem by CG grows as $O(\frac{1}{H^2}) = O(N_s) = O(N_I)$. In other words, if the global problem size is increased with the number of substructures and processors while the substructure problem size is maintained constant, the computational overhead entailed by the parallel iterative solution of each coarse problem grows as the size of the interface problem.

From the computational complexity analyses presented above and summarized in Table V, it follows that the precomputation of W does not challenge either the numerical efficiency or the parallel scalability of the FETI solvers described in this paper. However, when the number of substructures and processors is increased, whether the problem size is kept constant or increased, the parallel computational cost associated with the solution by CG of the coarse problem grows as the size of the interface problem. This can potentially reduce the numerical efficiency and parallel scalability of the FETI solvers discussed herein, when the size of the coarse problem is no longer a small fraction of the size of the local substructure problem—that is, when a relatively small problem is solved by a FETI method using a large number of substructures and processors. In such cases, the basic FETI method may be faster CPU-wise when only the rigid body modes are used to construct the coarse problem, even if such a strategy is not mathematically optimal for plate and shell problems.

The performance results gathered in Tables II and III indicate that for plate problems ($d_X = d_{EV} = 1$), the FETI method converges three times faster when equipped with the coarse problem based on the substructure rigid body and corner modes than when equipped with that based on the substructure rigid body and averaging modes. These results also suggest that for shell problems ($d_X = d_{EV} = 3$), adding the averaging modes to the coarse problem based on the rigid body and corner modes reduces the number of iterations for convergence of the FETI method by 25 per cent. On the other hand, the complexity analysis results summarized in Table V show

that for $d_X = d_{EV} = 1$, the evaluation of W and solution of the coarse problem are only 1.1 times more expensive when the substructure corner rather than averaging modes are combined with the substructure rigid body modes. These results also indicate that for $d_X = d_{EV} = 3$, superposing the substructure averaging modes to the combined substructure rigid body and corner modes increases the cost of precomputing W and solving iteratively the coarse problem by 20 per cent only. Therefore, we conclude that the substructure averaging modes cannot compete with the substructure corner modes for the solution of plate and shell problems by the FETI method. However, enriching the coarse problem based on the substructure rigid body and corner modes with the substructure averaging modes can potentially improve the performance of the FETI method.

6. APPLICATIONS

Here, we assess the impact of the two new coarse problems presented in Section 5 on the parallel performance of the FETI method, and highlight its scalability properties for the solution of realistic problems. For this purpose, we consider transient analyses of the FUSE diffraction grating system and the ONERA M6 wing, and a static analysis of a stiffened composite shell structure on an IBM SP2 parallel system with 64 Mbytes per processor. We note that our parallel FETI software uses the MPI library for message passing on the IBM SP2 machine, and solves all coarse problems by a CG algorithm equipped with the reorthogonalization procedure proposed in Reference 16 for accelerating the solution of systems with repeated right-hand sides. We use the Greedy algorithm[1] and the substructure aspect ratio optimizer described in Reference 36 for generating all the mesh partitions.

6.1. The FUSE diffraction grating system

We consider the dynamic analysis of a proposed design[35] for the FUSE diffraction grating system that is part of a satellite borne telescope spectrograph. The grating material is fused silica. When mounted, it must have face surface deflections below the micron level in 1 G acceleration for accurate pre-launch alignment with the rest of the spectrograph. It must also be able to withstand accelerations up to 15 G laterally and axially during launch. The grating structure is 263 mm $\times$ 265 mm with a 165 m spherical radius cut into the face. For this structure, we consider a refined version of the three-dimensional finite element model described in Reference 35 that contains 35328 8-noded brick elements and 120 987 d.o.f. (Figure 4). We partition this mesh in 16, 32, and 64 substructures for parallel processing. In all cases, we set the time step to $\Delta t = \mathscr{T}_3/15$, where $\mathscr{T}_3$ is the period of the third mode of the structure. This time step ensures an appropriate representation of the first few low modes of the structure in the computed solution, which is often sufficient for the simulation of low frequency dynamics problems.

We perform several transient analyses of the diffraction grating system using as a solver the FETI method equipped with the lumped preconditioner (22) and the projectors based on $Q = [G_1]$ and $Q = [EV_3 \;\; \hat{G}_1]$. We note that for topologically three-dimensional mesh partitions with brick elements, using the substructure corner modes in the coarse problem cannot be computationally effective, not only because these modes have been motivated by fourth-order plate and shell theory, but most importantly because three-dimensional mesh partitions generate too many corners. The selection of the lumped preconditioner is justified by its well-established superior overall computational efficiency for brick problems.[1, 6] We use Equation (53) as a stopping criterion, and report the performance results obtained during the first time-step analysis in Table VI. The results

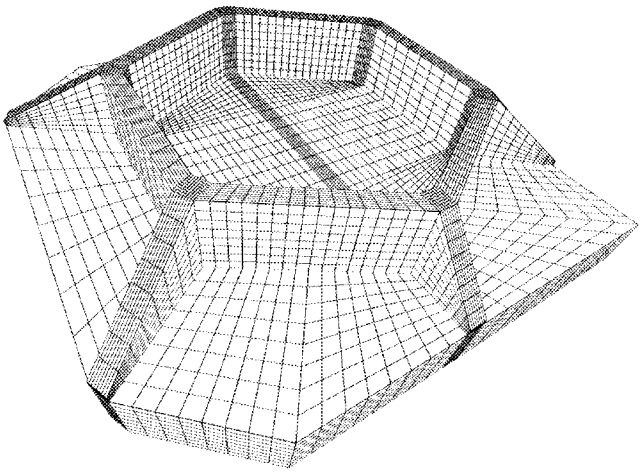

Figure 4. Finite element discretization of a diffraction grating system

Table VI. Implicit dynamic analysis of a structural model of the FUSE diffraction grating system with 120 987 d.o.f., FETI with lumped preconditioner, performance results on an IBM SP2 parallel processor for the first time-step analysis

N_s / N_p	# of iterations	CPU time basic FETI (s)	CPU time W (s)	CPU time coarse problem (s)	CPU time total (s)
16	53 (47)	90·5 (82·0)	58·4 (92·3)	7·0 (10·7)	155·9 (185·0)
32	53 (43)	36·0 (34·0)	10·6 (13·5)	5·0 (19·1)	51·6 (66·6)
64	72 (44)	22·7 (17·6)	4·3 (5·9)	10·1 (42·6)	37·1 (66·1)

reported between parenthesis are for the case where the FETI method is equipped with the projector $\tilde{P}(Q = [EV_3 \;\; \hat{G}_I)]$. The other results correspond to the case where the projector $\tilde{P}(Q = [\hat{G}_I])$ is employed.

Several observations are worthy noting:

(1) whether only the substructure rigid body or the combined substructure rigid body and averaging modes are used to construct the coarse problem, the parallel computational cost of precomputing W is shown to decrease and that of solving the coarse problem to increase when the number of substructure and processors is increased. This is consistent with the complexity analysis presented in Section 5.6. The specific rates of computational cost decrease and increase are different from those given in Table V because the diffraction grating system analysed here is a three-dimensional problem.

(2) enriching the basic coarse problem with the substructure averaging modes is shown to reduce the iteration count of the FETI method by up to 39 per cent. However, this enrichment increases the cost of precomputing W by 30 per cent, and that of solving the coarse problem by the CG method by up to 400 per cent. The majority of this cost increase is due to interprocessor communication.

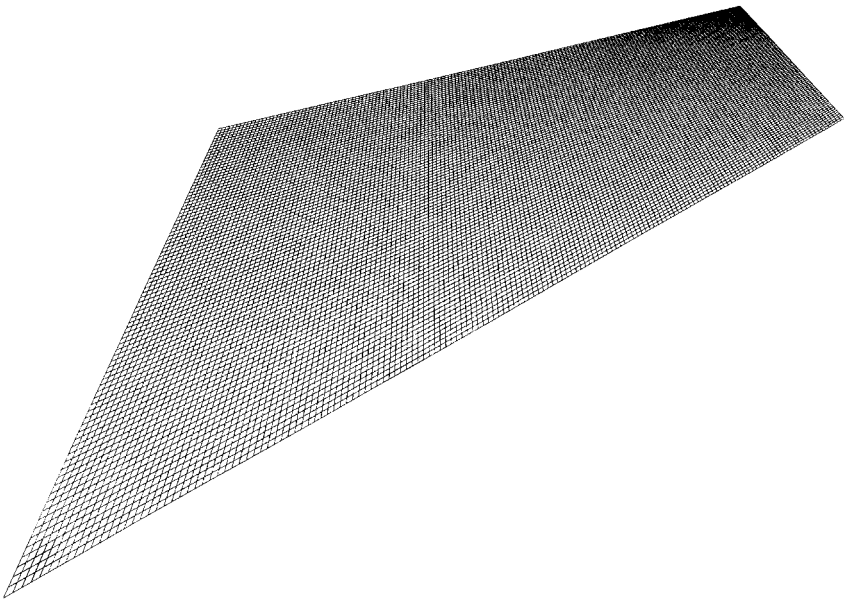

Figure 5. Discretization of an ONERA M6 wing equivalent plate model

(3) for a fixed size problem and an increasing number of substructures and processors, enriching the basic coarse problem with the substructure averaging modes increases sufficiently its size to reach a point where the solution by a CG method of the coarse problem dominates the total solution time. For this diffraction grating structure and 64 processors, the solution of the enriched coarse problem consumes 64 per cent of the total solution CPU time.
(4) at least for this three-dimensional second-order elasticity problem, the averaging modes are not shown to improve the computational performance of the basic FETI method. The fifth column of Table V demonstrates that this is due to the inefficiency of our parallel coarse iterative method at solving larger coarse problems.

6.2. The ONERA M6 wing

The ONERA M6 wing considered here is clamped at one end, loaded by an aerodynamic unsteady pressure field, and represented by an equivalent flat plate structural model with 413451 d.o.f. (Figure 5). The corresponding finite element mesh is partitioned into 30, 40, 60, 80, and 100 substructures.

Several transient analyses of the ONERA plate model are performed using the FETI method equipped with the Dirichlet preconditioner and the projectors based on $Q = [X_z \;\; G_I]$ and $Q = [X_z \;\; \hat{G}_I]$, and the stopping criterion (53). The performance results obtained for the first time-step analysis are summarized in Table VII.

For this almost half-a-million d.o.f. fixed size problem, the FETI method equipped with the Dirichlet preconditioner and either projector $\bar{P}([X_z \;\; G_I])$ or $\bar{P}([X_z \;\; \hat{G}_I])$ is numerically scalable even for 100 substructures and processors. Furthermore, it delivers impressive parallel speedups. For the case of 30 substructures, the memory requirements per substructure of the FETI method equipped with the projector $\bar{P}([X_z \;\; G_I])$ exceed the amount of memory available per processor of

Table VII. Implicit dynamic analysis of an ONERA wing equivalent flat plate structural model with 413 452 d.o.f., FETI with Dirichlet preconditioner and substructure rigid body and corner modes performance results on an IBM SP2 parallel processor for the first time-step analysis

N_s / N_p	$\bar{P}([X_z \quad G_I])$ # of iterations	$\bar{P}([X_z \quad \hat{G}_I])$ # of iterations	$\bar{P}([X_z \quad G_I])$ Total CPU time (s)	$\bar{P}([X_z \quad \hat{G}_I])$ Total CPU time (s)
30	45 itr.	45 itr.	187·6	102·1
40	47 itr.	47 itr.	91·3	86·4
60	55 itr.	55 itr.	39·7	38·0
80	58 itr.	58 itr.	32·9	32·0
100	59 itr.	59 itr.	28·6	28·1

the IBM SP2 machine, which causes memory swaps and a performance degradation. On the other hand, for this same case, the memory requirements per substructure of the FETI method equipped with the projector $\bar{P}([X_z \ \hat{G}_I])$ are less than the amount of memory available per processor, which illustrates the advantages of using $\hat{G}_I$ instead of G_I. Note also that as expected, when the problem size is fixed and the number of substructures is increased, using $\hat{G}_I$ instead of G_I improves the total CPU time of the FETI method only by a modest amount.

6.3. The NASA water tank shell problem

Here, we focus on the static analysis of the NASA water tank[37] shown in Figure 6. This tank is made of a composite material. It is discretized by 47 936 three-noded ANDES shell elements, which generates 145 092 d.o.f. The corresponding finite element mesh is partitioned into 8 and 16 substructures. The tank is clamped at one end, and a uniform displacement is applied at the other. This uniform displacement field has zero components at all d.o.f. except those corresponding to the displacement along the longitudinal axis of the cylinder. The FETI method with the Dirichlet preconditioner is applied twice as a solver: first with the projector based on the substructure rigid body and corner modes, and then with the projector based on the substructure rigid body and corner modes as well as the edge averaging modes. We do not consider using a coarse problem constructed with the substructure rigid body and averaging modes only because of the conclusion made in Section 5.6. Because the tank is a shell and not a plate, the corner modes are generated for all 3 displacement d.o.f. of every substructure corner node.[11] The averaging modes are also generated for all 3 displacement d.o.f. of an edge node. The performance results obtained on an IBM SP2 machine using the stopping criterion (53) are reported in Table VIII.

Here again, the FETI method equipped with either projector $\bar{P}(T = [X_3 \ G_I])$ or $\bar{P}(T = [X_3 \ (EV)_3 \ G_I])$ demonstrates both numerical and parallel scalability. Enriching the basic shell coarse problem with the edge-averaging modes is shown to reduce the number of iterations by roughly 25 per cent, which is consistent with the results reported in Section 5.5 for the model plate problem. However, the averaging modes improve the solution CPU time of the FETI method based on the substructure rigid body and corner modes by only 5 per cent in the case of 8 substructures, and unfortunately increases this solution CPU time by 24 per cent in the case of 16 substructures. The main reason for this computational inefficiency of the edge-based averaging modes is related to the iterative nature of the method implemented for solving the coarse problems on a parallel processor. Indeed, as discussed earlier in this paper, the CG algorithm equipped with the reorthogonalization

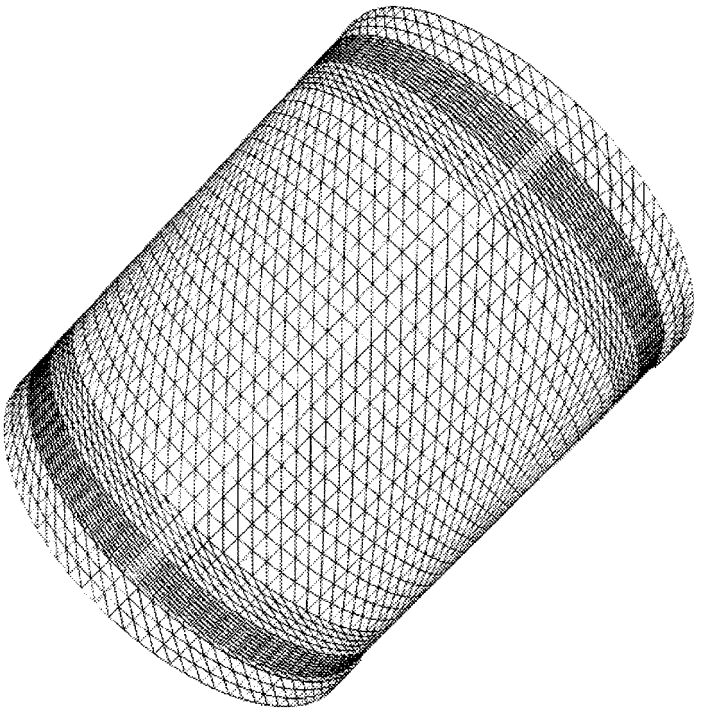

Figure 6. The NASA water tank composite shell structure

Table VIII. Static analysis of the NASA water tank composite shell structure with 145092 d.o.f. FETI with Dirichlet preconditioner, impact of the edge averaging modes performance results on an IBM SP2 system

N_s N_p	$\bar{P}([X_3\ G_1])$ # of iterations	$\bar{P}([X_3\ (EV)_3\ G_1])$ # of iterations	$\bar{P}([X_3\ G_1])$ Total CPU time (s)	$\bar{P}([X_3\ (EV)_3\ G_1])$ Total CPU time (s)
8	32	25	57·2	54·9
16	29	21	27·4	34·4

procedure discussed in Reference 16 solves a FETI coarse problem in r_c iterations during the first FETI PCG iteration, and in a single iteration during each other FETI PCG iteration. When the coarse problem size exceeds a certain limit that depends on the global problem size and the hardware characteristics of a parallel processor, the overhead induced by the computations and communications associated with the first r_c CG iterations offsets the reduction of the number of FETI PCG iterations. For this tank problem and 16 substructures, the size of the coarse problem associated with $T = [X_3\ (EV)_3\ G_1]$ is roughly 1·7 times larger than that associated with $T = [X_3\ G_1]$, and its computational complexity is twice as large (see first and third rows of Table IV). Furthermore, the size of this enriched coarse problem appears to exceed the critical limit of feasibility for parallel computations on an IBM SP2 system. However, it should be noted that a different solution method for the coarse problem—for example, a direct method—and/or a different computational

platform changes the critical limit and therefore could have produced better CPU results for the FETI method equipped with $T = [X_3 \;\; (EV)_3 \;\; G_1]$.

7. CONCLUSIONS

Iterative substructuring methods with Lagrange multipliers are gaining acceptance and popularity for the parallel solution of large-scale systems of equations. In these methods, the computational domain of the target problem is decomposed into substructures, and a set of Lagrange multipliers is introduced at the substructure interfaces to enforce the compatibility of the substructure displacement solutions. The original problem is transformed into a dual interface problem, and this interface problem is solved by a preconditioned conjugate gradient (PCG) method to find first the values of the Lagrange multipliers, and then compute the substructure displacement solutions. In this paper, we have presented a general framework for accelerating the convergence of such a solution methodology. This framework, which is based on the concept of enforcing at each PCG iteration applied to the solution of the interface problem a weak form of the substructure displacement compatibility equations, allows the formulation and design of a large family of iterative substructuring algorithms with a coarse problem. This family includes the various FETI methods previously published in the literature. We have applied this framework to modify the coarse problem of the FETI method for transient dynamics, in order to reduce its memory and computational requirements without affecting its numerical and parallel scalability properties. We have also used it to upgrade existing FETI coarse problems with edge-based displacement averaging modes. Such an upgrade appears to reduce the iteration count of the FETI method that is mathematically optimal for second-order elasticity problems by up to 39 per cent, and the iteration count of the FETI method that is mathematically optimal for fourth-order plate and shell problems by 25 per cent. However, such an upgrade also increases the size of the coarse problem to be solved at each PCG iteration. Previously, we have advocated the solution of the coarse problem by a CG algorithm because it simplifies the implementation of the coarse operator on massive parallel processors, and because the CG computations are more amenable to massive parallel processing than any computations based on Gaussian elimination. Such a strategy is also computationally efficient when the size of the coarse problem is relatively small, for example, when it is limited to those ingredients that suffice to ensure the mathematical optimality of the iterative substructuring method with Lagrange multipliers. When the coarse problem is enriched beyond that point—for example, when the averaging modes developed in this paper are added to the optimal coarse problem—the iterative solution of the coarse problem by CG becomes inefficient and its cost offsets any reduction in the iteration count due to the enlargement of the coarse problem. Hence, more sophisticated parallel iterative solvers are needed for solving the coarse problem, and a direct solution method may even prove to be useful for some coarse problems. Finally, for a plate problem with almost half-a-million degree of freedom, we have shown that the FETI method equipped with the suitable coarse problem scales both numerically and parallel-wise up to at least 100 substructures and 100 IBM SP2 processors.

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