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Domain Decomposition Methods for Three-Dimensional Thermoelastic Problems on Parallel Computers

Ralf Quatember and Wolfgang L. Wendland

1 Introduction

For the computation of thermoelastic and thermoelastic-plastic stress distributions in engine parts, boundary element methods are used, for instance by the Mercedes-Benz company. These methods are preferred to FE methods because of the decisively faster mesh generation (presently three instead of twelve months). Moreover, substructuring arising from the geometrical data and different material constants on subdomains can nowadays be realized efficiently on parallel computers. In substructuring, coupling interfaces have to be introduced in the interior of the original domain.

For the computation of complex structures, serial high performance computers as the CRAY C 94 are no longer able to handle the large systems of equations and data. As a result, only rather simple machine parts can currently be simulated with the traditional software.

In this work, we present a domain decomposition algorithm which is suitable also for rather complex problems. A numerical comparison between a sequential, a (data-) parallel, and a domain decomposition boundary element program is presented.

For the practical work, a pure "number crunching" program is not sufficient. Since we have to solve problems in $\mathbb{R}^3$, the visualization of the input data and the computed results is an important part of our work as well. Moreover, it is necessary to generate test meshes for the three-dimensional problems.

Figure 1 shows a typical flow-chart for our project, which is divided into the following tasks:

1. Generation of the mesh and input data (tractions and displacements) or the adaption of meshes and input data given by our partner from industry.
2. Controlling of the mesh and mesh refinement if necessary.

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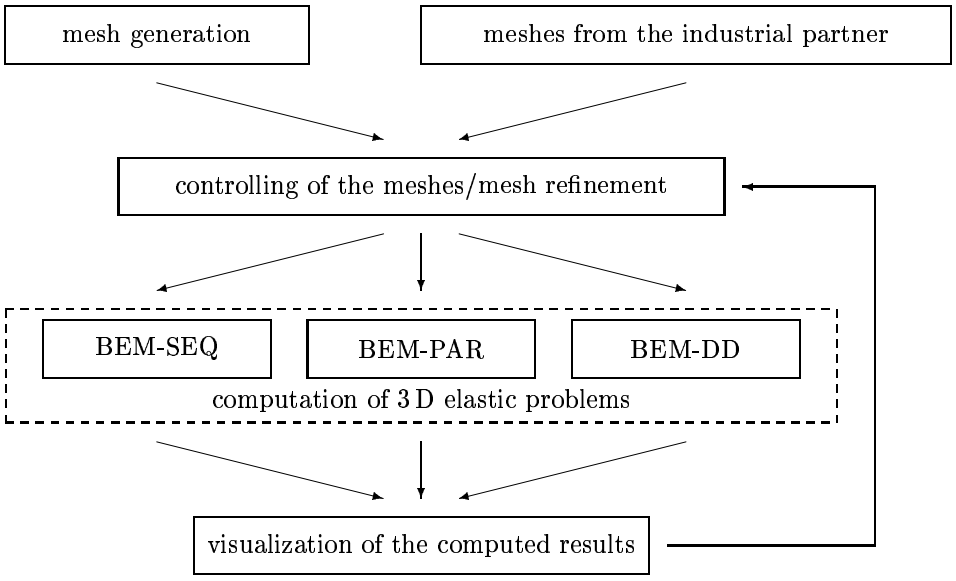
Figure 1 A typical flow-chart of our project



3. Solution of the three-dimensional elasticity problem. Here we can use one of our three boundary element programs:
   (a) BEM-SEQ: sequential boundary element program,
   (b) BEM-PAR: (data-)parallel boundary element program. This means that the system of equations is generated distributedly and solved in parallel on the family of processors, and
   (c) BEM-DD: boundary element program for the solution of the problem by a domain decomposition algorithm on multiple processors.
4. Visualization of the computed results.

In [QSW97] we present a program which handles the visualization and the mesh generation of surface meshes in $\mathbb{R}^3$. This program manages triangles as well as quadrangles on the boundary surface, which are described by linear or quadratic form functions. In section 2 we describe our domain decomposition algorithm and in section 3 we present some numerical results.

2 Domain Decomposition Formulation

Let us consider a three-dimensional thermo-elastic body in the domain $\Omega \subset \mathbb{R}^3$ with given displacements g on the boundary part Γ_D and given boundary stresses h on the remaining boundary part Γ_N.

We further assume that a temperature field $\theta(x)$ is given in Ω. Then the volume

forces $\tilde{f}$ can be split into a thermo-elastic (Duhamel-Neumann material law [Kup79]) and an elastic part:

$$\tilde{f}_i = f_i - \frac{\partial}{\partial x_i}\left[\Big(2\mu(x) + 3\lambda(x)\Big)\,\alpha(x)\,\theta(x)\right] \text{ for } i = 1,\dots,3. \tag{2.1}$$

Here α is the given coefficient of linear heat expansion. For given volume forces we can write the static equilibrium equations as

$$\sigma_{ij,j}(u,x) + \tilde{f}_i(x) = 0 \text{ for } i = 1,\dots,3 \text{ and } x \in \Omega, \tag{2.2}$$

where the stress tensor σ_{ij} is related to the strain tensor e_{ij} by Hooke's law

$$\sigma_{ij}(u,x) = \delta_{ij}\lambda(x)\sum_{k=1}^{3} e_{kk}(u,x) + 2\mu(x)\,e_{ij}(u,x). \tag{2.3}$$

λ and μ are the well-known Lamé constants. The linear strain-displacement relations are given by

$$e_{ij}(x) = \frac{1}{2}\Big(u_{i,j}(x) + u_{j,i}(x)\Big), \tag{2.4}$$

where $u_{\cdot,j}$ denotes the partial derivative with respect to x_j. Assuming a given non-overlapping domain decomposition

$$\overline{\Omega} = \bigcup_{i=1}^{p} \overline{\Omega}_i \text{ with } \Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j, \quad \Gamma_i = \partial\Omega_i, \quad \Gamma_{ij} = \Gamma_i \cap \Gamma_j, \tag{2.5}$$

we call $\Gamma_S = \bigcup_{i=1}^{p} \Gamma_i$ the skeleton. The Lamé constants in (2.3) are assumed to be piecewise constant on each of the subdomains:

$$\mu(x) = \mu_i, \qquad \lambda(x) = \lambda_i \text{ for } x \in \Omega_i \text{ and } i = 1,\dots,p. \tag{2.6}$$

For each subdomain Ω_i, the Kelvin fundamental solution is defined by

$$U^i_{kl}(x,y) = \frac{\lambda_i + \mu_i}{8\pi\mu_i(\lambda_i + 2\mu_i)}\left[\frac{\lambda_i + 3\mu_i}{\lambda_i + \mu_i}\,\frac{1}{|x-y|}\,\delta_{kl} + \frac{(x_k - y_k)(x_l - y_l)}{|x-y|^3}\right]. \tag{2.7}$$

Let $\big((T^i_{kl}(\cdot,\cdot))\big)$ be the corresponding boundary stress of the field of the fundamental solution. Then the solution of the differential equation (2.2) is given by the Somigliana representation formula for $x \in \Omega_i$ in each of the subdomains Ω_i:

$$c_{kl}u^i_k(x) = \int_{\Gamma_i} U^*_{kl}(x,y)\,t^i_k(y)\,ds_y - \int_{\Gamma_i} T^*_{kl}(x,y)\,u^i_k(y)\,ds_y + \int_{\Omega_i} U^*_{kl}(x,y)\,\tilde{f}^i_k(y)\,ds_y. \tag{2.8}$$

The solution u^i satisfy the boundary conditions on the individual parts of the exterior boundary,

$$u^i(x) = g \text{ for } x \in \Gamma_D \text{ and } t^i(x) = h \text{ for } x \in \Gamma_N \tag{2.9}$$

and the coupling conditions on the skeleton,

$$t^i(x) + t^j(x) = 0 \text{ and } u^i(x) - u^j(x) = 0 \text{ for all } x \in \Gamma_{ij}. \tag{2.10}$$

For the computation of the unknown Cauchy data (u_i, t_i) we use the integral equation resulting from (2.8):

$$\left(V_i t^i\right)(x) = \left(\frac{1}{2} I + K_i\right) u^i(x) + \left(N_i \tilde{f}^i\right)(x) \text{ for } x \in \Gamma_i. \tag{2.11}$$

V_i denotes the single layer potential, K_i denotes the double layer potential and N_i denotes the Newton potential. Introducing the Steklov-Poincaré operator by the equation

$$S_i := V_i^{-1} \left(\frac{1}{2} I + K_i\right) \tag{2.12}$$

we obtain from (2.11) the Dirichlet-Neumann mapping

$$t^i = S_i u^i + V_i^{-1} N_i \tilde{f} = S_i u^i + f^i. \tag{2.13}$$

With this mapping, the equivalent variational formulation for the solution of the mixed boundary value problem (2.2) can be written as:

Find $u \in H^{1/2}(\Gamma_S)$ *with* $u|_{\Gamma_D} = g$ *and* $u^i = u|_{\Gamma_i}$ *such that*

$$\sum_{i=1}^{p} \int_{\Gamma_i} S_i u^i(x) v^i(x) ds_x = \int_{\Gamma_N} h(x) v(x) ds_x - \sum_{i=1}^{p} \int_{\Gamma_i} f^i v^i(x) ds_x \tag{2.14}$$

holds for all $v \in H^{1/2}(\Gamma_S)$ *with* $v|_{\Gamma_D} = 0$.

Let Γ_H be a triangulation of the boundary $\Gamma = \partial\Omega$ with maximal mesh size H and

$$u_H(x) = \sum_{k=1}^{N_u} u_k \, {}^{\nu_u}_{k}(x) \in V_H \subset H^{1/2}(\Gamma_S), \tag{2.15}$$

a finite representation of the displacements with respect to a B-spline basis of degree ν_u. On the subspace V_H, the variational problem (2.14) leads to

$$\sum_{i=1}^{p} \int_{\Gamma_i} S_i^h u_H^i(x) v^i(x) ds_x = f(v_H), \tag{2.16}$$

where S_i^h are approximations of the local Steklov-Poincaré operators S^i on an appropriately chosen fine grid boundary element discretization W_h^i on Γ_i,

$$S_i^h v_H := t_h^i \in W_h^i \subset H^{-1/2}(\Gamma_i). \tag{2.17}$$

t_h^i can be found by the solution of the local finite-dimensional variational problem

$$\left\langle V_i \, t_h^i, \tau_h \right\rangle_{L^2(\Gamma_i)} = \left\langle \left(\frac{1}{2} I + K_i\right) u_H^i(x), \tau_h \right\rangle_{L^2(\Gamma_i)} \quad \text{for all } \tau_h \in \widetilde{W}_h \tag{2.18}$$

With appropriate $\widetilde{W}_h$, this formulation is valid for Galerkin methods as well as for collocation methods for the computation of the approximations of the local Steklov-Poincaré operators S_i^h.

The unique solvability of the variational problem (2.14) results from the W_h^i-ellipticity and boundedness of the local Steklov-Poincaré operators S_i^h [HW92].

For a sufficient refinement h with $h < cH$, the positive definiteness of the approximate operators S_i^h follows for the Galerkin scheme by the Strang lemma and therefore implies for $H \to 0$ the convergence of the approximate solutions of (2.16) to the solution of (2.14) and (2.2), respectively [HSW95].

Equation (2.16) together with the constraints 2.18) leads to the following algorithm:

1. Choose for the Dirichlet data along the coupling and Neumann boundaries a start solution $u^0_{|\Gamma_S}$ with $u_{|\Gamma_D} = g$.
2. Solve pure Dirichlet problems for the realization of the local Steklov-Poincaré operators and compute the corresponding local Neumann data t_i^k.
3. Check the compatibility conditions along the coupling and Neumann boundaries. If a given accuracy is reached, stop the algorithm.
4. Otherwise correct the Dirichlet data $u^{k+1}_{|\Gamma_C}$ with a preconditioned iterative method and continue with step 2.

This algorithm leads to a linear system of equations of the form

$$M_h^T V_h^{-1} \left(\frac{1}{2} \tilde{M}_h + K_h \right) \underline{u} = \underline{f} \tag{2.19}$$

with a positive definite stiffness matrix and an unsymmetric perturbation. For the solution of (2.19) one can use the minimal correction method [QSW96, SN89] as well as some generalized methods of conjugate gradients, like BiCGStab [vdV92] or GMRES [SS86].

For the preconditioning of these methods we use a hierarchical splitting of the unknown function $u \in H^{1/2}(\Gamma_S)$ according to (2.15), (2.18). Let ω be the q-dimensional set of all coarse grid nodes of our domain decomposition (2.5). Then there exists a unique splitting

$$u(x) = \sum_{i=1}^{q} u_j \varphi_j^q(x) + \tilde{u}(x) \tag{2.20}$$

with

$$u_j = u(x_j), \qquad \tilde{u}(x_j) = 0 \text{ for } x_j \in \omega \tag{2.21}$$

and with the "harmonic" basis functions $\varphi_j^q(\cdot)$ solving the differential equation (2.2) in the subdomains Ω_i. This leads to the coupled variational formulation:

Find the pair $(u_H, \tilde{u})$ *assuming the given Dirichlet data on the boundary* Γ_D *such that the coarse grid system*

$$\int_\Omega \sigma_{ij}(u_H)\, e_{ij}(v_H) dx + \sum_{i=1}^{p} \left\langle S_i^h \tilde{u}_{|\Gamma_i}, v^H_{|\Gamma_i} \right\rangle_{\Gamma_i} = f_1(v^H) \tag{2.22}$$

and the fine grid compatibility conditions

$$\sum_{i=1}^{p} \left\langle S_i^h (u^H + \tilde{u})_{|\Gamma_i}, \tilde{v}_{|\Gamma_i} \right\rangle_{\Gamma_i} = f_2(\tilde{v}) \tag{2.23}$$

hold for all test functions $(v^H, \tilde{v})$ *which are zero on* Γ_D.

The coarse grid system is nothing more than a finite-element formulation with respect to the given domain decomposition with harmonic basis functions. Due to this property, the global stiffness matrix can be computed with the local Steklov-Poincaré operators. Moreover, the solution on this coarse grid can be interpreted as a mapping $u^H = R\tilde{u}$ of the fine grid function $\tilde{u}$ onto coarse grid functions.

Inserting this mapping into the compatibility conditions, we have to find a fine grid solution which satisfies the modified compatibility conditions

$$\sum_{i=1}^{p} \left\langle S_i (\tilde{u} + R\tilde{u})_{|\Gamma_i}, \tilde{v}_{|\Gamma_i} \right\rangle_{\Gamma_i} = f(\tilde{v}) \tag{2.24}$$

for all test functions $\tilde{v}$.

The solution process includes only one additional step to solve the coarse grid system for any given fine grid solution. Namely, replace in the algorithm at the beginning of this section the function $u_{|\Gamma_C}$ by $\tilde{u}_{|\Gamma_C}$ and insert between steps 1 and 2 the additional procedure

1.5 Solve for the current fine grid solution $\tilde{u}^k_{|\Gamma_C}$ the coarse grid system and compute the momentary complete iterate $u^k_{|\Gamma_C}$.

For the solution of the variational problem (2.24) along the coupling interfaces Γ_{ij} we need appropriate preconditioning. A reasonable choice is the Neumann-Neumann preconditioner [LT94]

$$M^{-1} = \sum_{i=1}^{p} S_i^{-1}, \tag{2.25}$$

which uses the inverse Steklov-Poincaré operators S_i^{-1}, that can be computed by the solution of local mixed Dirichlet-Neumann or pure Neumann problems. The solution of pure Neumann problems needs some more care because one has to incorporate equilibrium equations. Here we use a modified Neumann series [HW72] in an extended algorithm including a coarse grid solver.

3 Numerical Examples

As a practical example we analyze and compute a three-dimensional crank shaft from our industrial partner Mercedes-Benz, discretisized with 872 boundary elements and 438 boundary points. The computation was performed on one hand with our sequential and (data-)parallel programs, and on the other hand with the domain decomposition algorithm presented here, in particular with a decomposition into two subdomains.

Presently we are developing a program which can treat more than two subdomains and a better memory management such that finer discretizations can be handled, too.

All our computations were performed on a SUN SparcStation 20 with a 90 MHz HyperSparc processor and 128 MB main memory; and also on a Parsytec PowerXplorer with eight MPC 601 processors and 32 MB main memory for each processor. The presented computation times are pure processor times or processor plus communication times. For the determination of the efficiencies we compared the computation times (including the communication times) on 2, 4 and 8 processors with the computation time (without communication) on one processor.

Figure 2 Example for a practical computation: crank shaft (Mercedes-Benz)

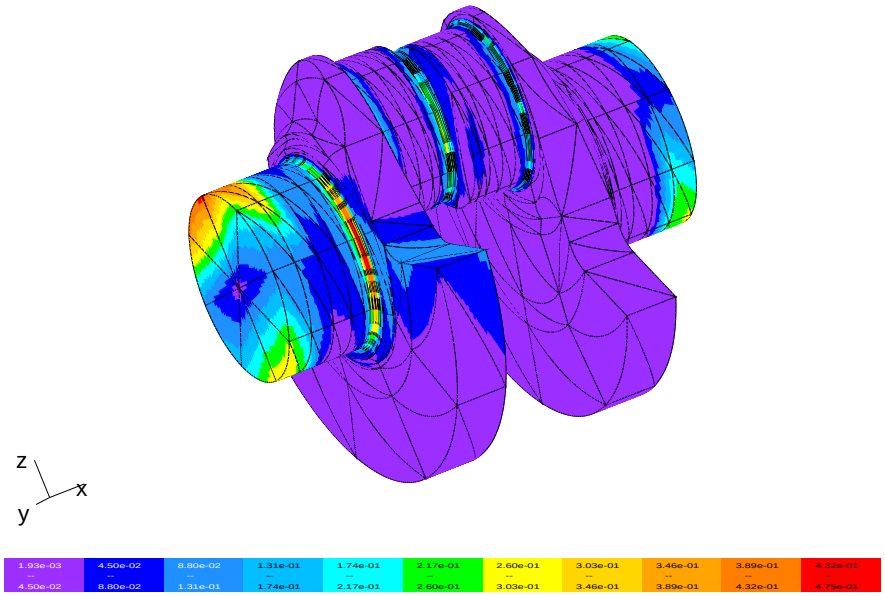


Table 1 Computational times for the numerical computation of the crank shaft discretisized with 872 elements and 438 points (2616 unknowns)

	PowerXplorer BEM-PAR				PowerXplorer BEM-DD	SUN BEM-SEQ
Proc:	1	2	4	8	2	1
time (sec):	249.6	143.0	76.9	44.6	139.3	198.5
efficiency:	100%	87.3%	87.3%	70.0%	89.6%	—

Figure 2 shows the result of these computations. In case of the iterative solution a stopping tolerance of 10^{-4} was chosen. Table 1 shows the computation times needed.

For finer discretizations and subdivisions in more than two subdomains we believe that the comparison between the different algorithms will result even more in favour of the domain decomposition method.

Numerical results for the significantly simpler example of the Laplacian in two dimensions and a subdivision into 16 subdomains obtained by O. Steinbach in [Ste94] show the efficiency of the presented algorithm and we expect similar results for the three-dimensional case.

REFERENCES

[HSW95] Hsiao G. C., Schnack E., and Wendland W. L. (1995) A hybrid coupled finite-boundary element method. Technical Report 95–11, Universität Stuttgart.

[HW72] Haack W. and Wendland W. L. (1972) *Lectures on Partial and Pfaffian Differential Equations.* Pregamon Press, Oxford.

[HW92] Hsiao G. C. and Wendland W. L. (1992) Domain decomposition via boundary element methods. In Alder H. *et al.* (eds) *Numerical Methods in Engineering and Applied Sciences*, pages 198–207. CIMNE, Barcelona.

[Kup79] Kupradze V. D. (1979) *Three-Dimensional Problems of the Mathematical Theory of Elasticity and Thermoelasticity.* North-Holland, Amsterdam.

[LT94] Le Tallec P. (1994) Domain decomposition methods in computational mechanics. *Comput. Mech. Advances* 1: 121–220.

[QSW96] Quatember R., Steinbach O., and Wendland W. L. (1996) Domain decomposition based solvers for industrial stress analysis with boundary elements. In Neunzert H. (ed) *Progress in Industrial Mathematics at ECMI 94.* John Wiley & Sons and B. G. Teubner, Stuttgart.

[QSW97] Quatember R., Steinbach O., and Wendland W. L. (1997) Entwicklung vorkonditionierter Iterationsverfahren für Randelementmethoden der Thermoelastizität auf Parallelrechnern. In Hoffmann K.-H., Jäger W., Lohmann T., and Schunck H. (eds) *Mathematik — Schlüsseltechnologie für die Zukunft*, pages 191–201. Springer, Heidelberg.

[SN89] Samarskij A. A. and Nikolaev E. S. (1989) *Numerical Methods for Grid Equations.* Birkhäuser-Verlag, Basel.

[SS86] Saad Y. and Schultz M. H. (1986) GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.* 7: 856–869.

[Ste94] Steinbach O. (1994) Boundary elements in domain decomposition methods. *Contemp. Math.* 180: 343–348.

[vdV92] van der Vorst H. A. (1992) BI-CGSTAB: A fast and smoothly converging variant of BI-CG for the solution of nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.* 13: 631–644.