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Mechanical Contact by Constraints and Split-Based Preconditioning

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Mechanical Contact by Constraints and Split-Based Preconditioning

1. Executive summary

An accurate implementation of glued mechanical contact was developed in MOOSE based on its Constraint system. This approach results in a superior convergence of elastic structure problems, in particular in BISON. Adaptation of this technique to frictionless and frictional contact models is under way.

Additionally, the improved convergence of elastic problems results from the application of the split-based preconditioners to constraint-based contact systems. This yields a substantial increase in the robustness of elastic solvers when the number of nodes in contact is increased and/or the mesh is refined.

2. Contact problems in NEAMS

Thermomechanical contact problems are of central importance to many NEAMS applications, most notably, BISON, where they are used to model the pellet-clad interaction in nuclear fuel rods. Taken individually, the elastic and thermal diffusion problems for the fuel pellet and the clad are elliptic and well understood numerically: optimal convergence of iterative linear solvers for these problems can be achieved using multigrid (MG) preconditioners; other robust preconditioners include overlapping domain decomposition methods, such as the Additive Schwarz Method (ASM). PETSc, the solver library underlying MOOSE, provides several scalable approaches to preconditioning elliptic problems, including ASM as well as interfaces to third-party algebraic multigrid preconditioners such as HYPRE.

Once contact between elastic or thermally-conducting structures appears, preconditioning and convergence become increasingly difficult, frequently leading to divergence of thermoelastic solves. To circumvent these problems, we have developed a number of enhancements to MOOSE and PETSc, which we explain here using the simpler example of an elastic contact problem (see Fig. 1).

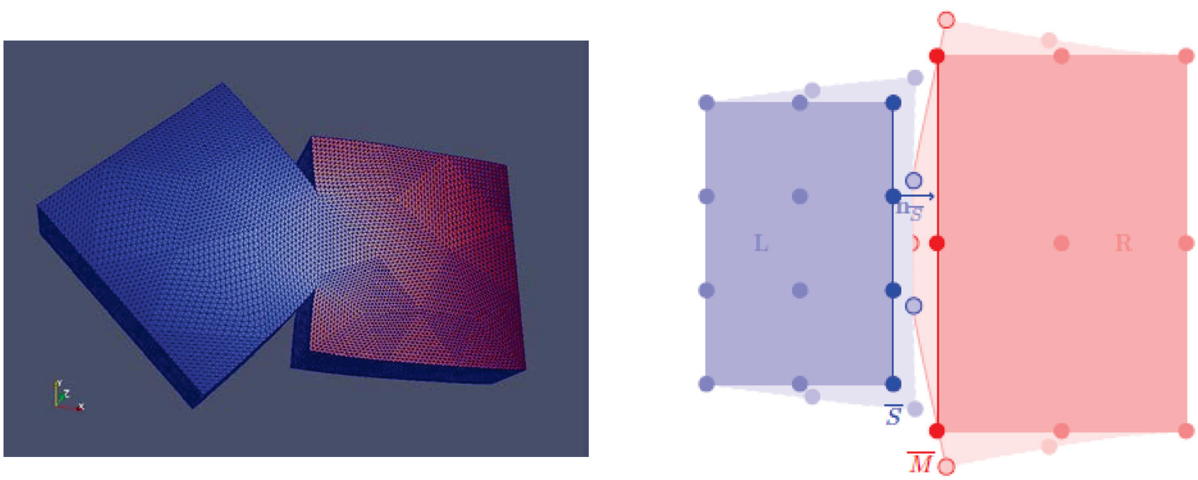

Figure 1: Left: two tetrahedral meshes in contact. Displacement boundary conditions applied on the left and right boundaries squeeze the block, causing elastic deformation. The two meshes are distinct and non-conforming. Right: Slave nodes (S) and master nodes (M) on the corresponding surfaces. Node coordinates are x_S and x_M, respectively, while u_S and u_M are the corresponding displacements. Nodes (S) and (M) are those slave, correspondingly, master, nodes that are in contact. Left (L) and right (R) nodes

only couple to S and M elastically and include the S or, respectively, M nodes not in contact.

3. New code development: MOOSE and PETSc

In order to improve the convergence of contact solvers, three improvements to MOOSE and PETSc were made: (1) the MOOSE Constraint system was used to implement contact, (2) dynamic sparsity modification of the Jacobian constraint rows was added to the Constraint system, and (3) exact matrix elimination and assembly of the reduced system was added to PETSc.

Constrained systems: We have implemented a *constraint-based* formulation of the contact problem in MOOSE that *exactly* enforces the relation between the *slave* and *master* displacements of the elastic material (see Fig. 1(right)). This required a transfer of the slave residual entries and Jacobian rows to the master residual entries and Jacobian rows. Prior to this, the Jacobian row transfer was not done exactly and was replaced by a penalty-based augmentation of the Jacobian rows. Because of this, the linear system did not exactly match the nonlinear residual, resulting in suboptimal convergence.

Dynamic Jacobian sparsity augmentation: The transfer results in an augmentation of the sparsity pattern of the Jacobian, and requires a rebuilding of the preconditioner. PETSc interoperability code for these residual and Jacobian evaluation was added to MOOSE. Beyond contact, it allows for dynamic solver rebuilding by any MOOSE application.

FieldSplit-based preconditioning: The most important contribution to the contact problem was in the enabling of contact-based FieldSplit preconditioner. The idea is to split the system into the slave and non-slave nodes (L, R and M of Fig. 1). PETSc then can easily eliminate the slave nodes, since the corresponding Jacobian block is an identity. Moreover, the eliminated system for the L, R, and M nodes—the Schur preconditioner—can be *assembled* into a regular matrix. This is an important point, since the Schur preconditioner S is typically *dense* and cannot be assembled—it is merely applied to the residual vectors as needed by applying the original blocks of the Jacobian and solving with the eliminated block. The density of the assembled S is due to the density of the eliminated block, but in our case the eliminated block is diagonal and thus the assembled S is actually sparse. Moreover, it is exactly the elasticity operator for the system that would be obtained by gluing the meshes along the slave-master contact. That operator is symmetric positive-definite.

We have made PETSc modifications to enable the general assembly of Schur complements when the eliminated block can be (approximately) inverted using its diagonal or the lumped version. This new PETSc capability is of general utility and can be used, for instance, to eliminate the Dirichlet boundary conditions of elliptic systems, yielding a symmetric positive-definite stiffness matrix. Here we use it in an analogous manner to eliminate the contact slaves. As a result, the usual elliptic preconditioners become much more effective on the Schur complement: we have tested the effectiveness of the approach using the MG (HYPRE) preconditioner and the ASM (PETSc) preconditioner. While ASM exhibited superior performance, even HYPRE's performance was made more robust.

Table 1: Effects of FieldSplit on the solver performance as measured by the total number of linear iterations to convergence. ASM and HYPRE with and without FieldSplit are compared; ∞ indicates divergence. The mesh has 544K elements with 99K nodes; all tests were run on 6 processors; ASM was used with LU on the blocks and overlap of 5; HYPRE was used with 2 smoothing steps and 2 multigrid cycles per preconditioner application. The TensorMechanics linear elasticity material model was used.

ASM	Split-ASM	HYPRE	Split-HYPRE
368	156	∞	557

4. Results

We have tested these improvements on a variety of test problems with the goal of incorporating them into production BISON simulations. For these tests we have used the elastic blocks in Fig. 1(left) with two levels of refinement (the fine mesh is shown in Fig. 1). We have used two types of solvers - HYPRE (BoomerAMG algebraic preconditioner, to be specific) as well as the ASM solver from PETSc, both with and without FieldSplit enabled. The results are presented in Table 1.

5. Summary

There were two major outcomes to this study. First, the constraint-based implementation of the Jacobian substantially improved the nonlinear convergence due to an accurate Jacobian calculation. Second, the use of FieldSplit on the constraint-based Jacobian *substantially* improved the robustness of both HYPRE and ASM: without the splits, HYPRE generally *diverges*, while with FieldSplit the method converges every time. ASM generally converges with or without FieldSplit, but its effectiveness begins to suffer on finer meshes, while with FieldSplit linear convergence is much less sensitive to mesh refinement and increasing the number of contact nodes.