Date	November 4, 2001	Memo Number	STI:01/07
Subject	**Sheldon's ANSYS Tips and Tricks: Understanding Lagrange Multipliers**		
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1. Introduction:

Lagrange multipliers are a general term used in different areas of ANSYS, specifically contact and element formulation. This memo hopes to provide the user with a simplified introduction to the most important concepts in using elements with Lagrange multipliers, in hopes that some of the element options and solver selection can be better understood.

Currently, at ANSYS 6.0, the node-to-node gap element CONTA178 and the Mixed U-P formulation of the 18x elements (i.e., KEYOPT(6)>0) utilize Lagrange multipliers, so the discussion will focus on these elements.

2. Discussion of Contact Problems:

In contact problems, two important considerations are as follows: (a) contact forces are transferred between bodies and (b) the impenetrability condition states that one body cannot penetrate another body.

Because we deal with displacement-based solutions, we have an equation of the form:

$$[K]\{x\} = \{F\}$$

For contact problems, we can deal with this via a *penalty method* or a *Lagrange multiplier method*. For now, we will limit ourselves to the normal contact forces only, as in the case of frictionless contact.

For the *penalty method*, we assume that contact force is written in a similar manner as below:

$$K_{contact}\Delta x_{penetration} = \Delta F_{contact}$$

$K_{contact}$ is considered to be our "contact stiffness," defined by real constant FKN for the 17x contact elements. The penetration (or gap) $x_{penetration}$ is defined to be the distance between two existing nodes on separate contact bodies. As noted earlier, $x_{penetration}$ should equal to zero to satisfy the impenetrability condition. However, because of this formulation, the amount of penetration will be finite, although as $K_{contact} \rightarrow \infty$, then $x_{penetration} \rightarrow 0$.

This form can easily be added to our existing matrix equation for multiple bodies. Because of the fact that $\Delta x_{penetration}$ describes the distance between existing nodes, $K_{contact}$ is added into the existing stiffness matrix [K]. The size of [K] does not change. The contact force $F_{contact}$ can then be transferred between the two bodies.

Three problems may arise from this method:

- How is the contact stiffness FKN chosen?
- If $K_{contact}$ is too high, the matrix may become *ill-conditioned*
- How much penetration is acceptable?

Regarding the first point, ANSYS automatically chooses the real constant FKN as a scale factor of the stiffness of the underlying elements, providing some convenience to the user (the user only has to think in terms of a scale factor, usually between 0.1 to 10). FKN can also be defined to be an absolute value instead, if it is defined as a negative value.

If the contact stiffness is too high, the matrix will be ill-conditioned – there will be a large variation in the terms of the stiffness matrix [K] if $K_{contact}$ is too big. Consequently, some iterative solvers (e.g., PCG solver) may have difficulties, requiring more solver iterations to solve ill-conditioned matrices. Direct solvers such as the sparse (direct) solver do not have problems solving ill-conditioned matrices.

Penetration ($x_{penetration}$) can be postprocessed via PLESOL,CONT,PENE. If the penetration is small enough, its effect on the response of the system will usually be negligible. For pure penalty-based methods, penetration is something the user must often consider by re-running the analysis with a larger contact stiffness and seeing if the values have changed. Although this method should always be done to ensure that the solution is not dependent on the penetration values, the *augmented Lagrangian method* (described later) helps alleviate some of these problems by being able to control the penetration to a given tolerance, which helps to ensure that penetration values are small.

For the *Lagrange multiplier method*, instead of rewriting the contact force $F_{contact}$ in a displacement-based manner, it is treated as a separate DOF. That means that we solve for contact force (or contact pressure) directly, similar to the equation below:

$$[K]\{x\} = \{F\} + \{F_{contact}\}$$

This has the benefit of being able to satisfy the impenetrability condition without dealing with "contact stiffness" or "penetration." Since we know that the contact force is a finite value, if we tried to satisfy impenetrability (zero penetration) with the penalty method, this means that the contact stiffness should be infinite. Have zero penetration via the penalty method is not something which can be realized on hardware with machine precision. Hence, if we treat that finite contact force/pressure as a separate DOF instead (i.e., Lagrange multiplier), we bypass these problems.

There are some things to keep in mind when using pure Lagragian methods:

- The form of the stiffness matrix will have zero diagonals, resulting in limited solver selection
- (Slightly) larger stiffness matrix due to additional DOF
- Chattering may need to be controlled

The first point leads to the fact that direct solvers such as the sparse or frontal solvers need to be used with Lagrange multipliers because iterative solvers such as the PCG solver often encounter difficulties with zero diagonals which result from Lagrange multipliers.

Chattering is due to abrupt changes in the contact status. This is controlled with the maximum allowable penetration TOLN and maximum allowable tensile force FTOL real constants. Although the pure Lagrange method should theoretically result in zero penetration when closed and zero tensile force when open, these parameters help to control chattering (oscillating changes in contact status) and to provide more efficient solutions.

The *augmented Lagrange method* is actually a penalty method with penetration control. The Newton-Raphson iterations start off similar to the pure penalty method. Similar to the pure Lagrange multiplier method, the real constant TOLN determines the maximum allowable penetration.[1] If the penetration at a given equilibrium iteration exceeds this maximum allowable penetration, the contact stiffness per contact element is augmented with Lagrange multipliers for contact force (pressure). Put in other words, for the contact element stiffness, the force (pressure) is

$$\lambda_{i+1} = \lambda_i + k_{cont} x_{pene}$$

if the penetration is greater than the maximum allowable value. Although the Lagrange multipliers are condensed out at the element level, one can think of this method as the same as a regular penalty method except that the contact stiffness is "updated" per contact element. This is repeated until the penetration is less than the maximum allowable value.

Although there still exists penetration (within TOLN value) and possibly more equilibrium iterations than the pure penalty method, the augmented Lagrangian method has the following advantages:

- Less ill-conditioning due to better "selection" of the contact stiffness per element. Remember that the penalty method uses real constant FKN. Augmented Lagrage method uses FKN but also "updates" the stiffness per element using Lagrange multipliers.
- Because of less degree of ill-conditioning compared with pure penalty method and no zero diagonals compared with pure Lagrange method, the iterative solvers such as PCG can often be used with these type of contact problems.
- User control over allowable penetration TOLN (TOLN is ignored for pure penalty method since there is no penetration control).

The foregoing discussion, of course, is a *very simplified* treatment of pure penalty, pure Lagrange, and augmented Lagrange methods for contact problems. However, the author hopes that some of this may shed light as to the pros and cons of each approach for those unfamiliar with these formulations.

The treatment of friction is done in a similar manner as the normal contact force, which was described above. Note that friction introduces more complexity due to its unsymmetric nature, although ANSYS, by default, employs a symmetrization algorithm to allow users to utilize conventional matrix solving techniques. The ANSYS direct solvers do support unsymmetric matrices for friction-dominated problems.

[1] For surface-to-surface contact elements 171-174, a similar parameter is called FTOLN instead of TOLN, as in the case of 178.

3. Discussion of Incompressible Materials:

Many nonlinear materials are treated as nearly or fully incompressible. For example, inelastic strains[2] are associated with no volume change. For problems exhibiting large inelastic strains, the overall material response will consequently be *nearly incompressible.* Another common material is hyperelasticity, which is treated as *nearly or fully incompressible*.

When a material is nearly or fully incompressible, a numerical difficulty arises. To understand why this is so, one can consider the material response. The material stress state can be separated into a hydrostatic and deviatoric component:

$$\sigma = p + s$$

$$p = \kappa \cdot \varepsilon_v$$

$$s = 2 \cdot G \cdot \varepsilon_d$$

where p is hydrostatic stress (dilatational), s is the deviatoric stress (distortional), κ is the bulk modulus, G is the shear modulus, ε_v is the volumetric strain, and ε_v is the deviatoric strain.

Recall that, as noted above, most nonlinear materials assume *near or full incompressibility*, based on the material characteristics. In other words, there is little or no volumetric (dilatational) change, and only change in element shape (distortional) is assumed to occur. This can be thought of as having an effective Poisson's ratio approaching or equal to 0.5.

A further look at hydrostatic stress p is warranted. The bulk modulus and volumetric strains can be defined as:[3]

$$\kappa = \frac{E}{3(1-2\nu)}$$

$$\varepsilon_v = \frac{1-2\nu}{E}\left(\sigma_x + \sigma_y + \sigma_z\right)$$

If one considers what occurs as the effective Poisson's ratio approaches 0.5, $\varepsilon_v \to 0$ while $\kappa \to \infty$. The extremely large bulk modulus causes numerical difficulties (ill-conditioned matrices), and, moreoever, volumetric locking often occurs with conventional, fully-integrated, displacement-based elements.

Here, the analogy with contact problems may be apparent – as the bulk modulus (contact stiffness) approaches infinity, the volumetric strain (penetration) approaches zero, yet hydrostatic pressure (contact force/pressure) should be a finite value.

Since strains are calculated as derivatives of displacements (DOF), volumetric strains are not as accurate as displacements – any small error in strains will result in large error in hydrostatic pressure, causing mesh locking.[4]

To circumvent this problem, hydrostatic stress can be treated as a separate DOF by introducing Lagrange multipliers. This is called the *Mixed U-P formulation*, which is present in the 18x family of elements and controlled via KEYOPT(6)>0. Here, the name "Mixed U-P" comes from the fact that displacements (U) and hydrostatic pressure (P) are treated as DOF.

As in the case of pure Lagrange contact, there are a few things to consider:

- The added pressure DOF increases the size of [K] matrix and computational cost associated with solving the equations.
- Because of the zero diagonals for fully-incompressible Mixed U-P formulation, only direct solvers can be used. Currently at 6.0, the frontal solver is preferred over the sparse solver for reasons related to robustness

Mixed U-P should only be used in the case of fully-incompressible hyperelastic problems (material compressibility parameter d=0 in TB,HYPER for 18x elements). In most other cases, B-Bar, Enhanced-Strain, or URI should suffice to alleviate volumetric locking in *nearly incompressible plasticity or hyperelasticity problems.*

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[2] Inelastic strains include creep, viscoplasticity, and rate-independent plasticity, with the exception of Drucker-Prager

[3] The equations are only valid for linear elastic materials, but they are presented in the context of nonlinear materials such as hyperelasticity for illustrative purposes only.

[4] A user can view whether or not volumetric locking has occurred in a model by postprocessing hydrostatic pressure via PLESOL,NL,HPRES. If a checkerboard pattern in hydrostatic pressure is present, volumetric locking has occurred.

4. Conclusion:

This memo meant to serve as a very simplified introduction to Lagrange multipliers and its use in contact problems as well as those involving nearly or fully incompressible materials. The author hopes that this may help users understand some of the pros and cons regarding different contact or element formulations. Although a detailed understanding of the numerical theory is probably unnecessary for the end-user, more practical/procedural information on contact and material nonlinearities is covered in the "Advanced Contact and Bolt Pretension" and "Advanced Structural Nonlinearities" seminars which the ANSYS Support Distributors and ANSYS, Inc. offer.

5. References:

- ANSYS 6.0 Theory Manual, Ch. 3.5 "General Element Formulations" and Ch. 14.178 "CONTA178 – 3D Point-to-Point Contact", available in online help
- ANSYS 6.0 Advanced Structural Nonlinearities Seminar notes, Ch. 2 "Element Technology"
- ANSYS 6.0 Advanced Contact and Bolt Pretension Seminar notes

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