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1. Introduction:

The 22x direct coupled-field elements (PLANE223, SOLID226-227) provide a wide array of material behavior for multiphysics applications. This memo hopes to introduce some of the pertinent features of these elements.

2. Background on Coupled-Field Analyses:

The ability to solve multiphysics problems has been a feature of ANSYS for many years. Typically, the physics are solved in such a manner that the results of one analysis become input for the other, such as the pressure field calculated in a CFD analysis applied as loading to a structural model. If tightly coupled, the results of the second physics become input for the first, such as the deformation affecting the flow domain in the same example. These types of coupled-field analyses can be solved in an automated fashion with the ANSYS Multi-field solvers.[1] The models are typically set up independently (but solved together) with the possibility of having different meshes for each physics to satisfy the specific meshing requirements that may arise.

There are some cases, however, which do not lend themselves to this segregated approach. Specifically, when multiple physics are coupled via material response, such as in the case of piezoelectricity, the physics need to be solved simultaneously. This is a typical application of the use of 22x coupled-field elements, which have multiple DOF and can support various types of coupled constitutive laws.

3. Overview of 22x Coupled-Field Elements:

The 22x coupled-field elements support piezoelectric, piezoresistive, thermoelastic (piezocaloric), and thermoelectric materials. In fact, many of these behaviors can be combined, such as structural-thermoelectric or thermal-piezoelectric applications, and the physics are specified via KEYOPT(1) for PLANE223, SOLID226, and SOLID227.

The 17x contact elements (CONTA171-175) support multiphysics applications, and the contact elements' DOF set is also controlled by KEYOPT(1). Since 22x coupled-field elements support large-deflection analyses, they are ideally suited for use with multiphysics contact.

For analyses including electrical effects, the 22x elements can be combined with circuit elements – either CIRCU94 for piezoelectricity or CIRCU124 otherwise.[2]

Although multiple physics are solved simultaneously, the coefficients for different DOF may vary by orders of magnitude in the assembled [K] matrix. Because of the resulting ill-conditioning of the matrix, the sparse direct solver is often preferred for most applications. Thermoelasticity and thermoelectricity may also result in unsymmetric matrices, another situation where the use of the sparse direct solver may be advised.

[1] Two ANSYS Multi-field solvers exist: the MFS solver allows multiple ANSYS fields (physics) to be solved together while the MFX solver allows users to couple ANSYS and CFX together to solve coupled-field problems.

[2] Although electric elements have VOLT DOF, the 'reaction force' must be the same for elements to be compatible. See Chapter 12 "Electric Field Analysis" in the *ANSYS Low-Frequency Electromagnetic Analysis Guide* for details

4. Introduction to Piezoelectricity:

In piezoelectric materials, the structural and electric fields are coupled in such a manner that an applied voltage generates a strain (and vice versa). Consequently, piezoelectric ceramics are used as transducers to convert electrical energy to a mechanical response or as sensors to convert mechanical energy to an electrical signal.

The mechanical stress {T} and strain {S} are related to the electric displacement {D} and electric field {E} via the following constitutive equations:

$$\{S\} = [s^E]\{T\} + [d]\{E\}$$
$$\{D\} = [d]^T\{T\} + [\varepsilon^T]\{E\}$$

Here, $[s^E]$ is the compliance matrix evaluated at constant electric field, $[\varepsilon^T]$ is the permittivity matrix evaluated at constant stress, and [d] is the piezoelectric matrix relating strain to electric field.

The above relationship provides a basis for the FEA piezoelectric matrix equations:

$$\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{Bmatrix} \ddot{u} \\ \ddot{V} \end{Bmatrix} + \begin{bmatrix} C^u & 0 \\ 0 & C^V \end{bmatrix}\begin{Bmatrix} \dot{u} \\ \dot{V} \end{Bmatrix} + \begin{bmatrix} K^u & K^Z \\ K^{Z^T} & K^V \end{bmatrix}\begin{Bmatrix} u \\ V \end{Bmatrix} = \begin{Bmatrix} F \\ L \end{Bmatrix}$$

Description of the terms:

- $[K^Z]$ contains the piezoelectric effect, and the piezoelectric constants can be input as either [d] form (strain/electric field) or [e] form (stress/electric field)
- $[K^u]$ contains the (anisotropic) stiffness coefficients, and these are either compliance $[s^E]$ or stiffness $[c^E]$ coefficients evaluated at constant electric field
- $[K^V]$ is the (anisotropic) permittivity matrix with permittivity values evaluated at constant strain $[\varepsilon^S]$ or constant stress $[\varepsilon^T]$
- $[C^u]$ is the structural damping matrix whereas $[C^V]$ represents dielectric losses

It is useful to understand the relationship between the various coefficients discussed above. They are simply presented here for brevity but the derivation is a trivial exercise:[3]

$$[\varepsilon^S] = [\varepsilon^T] - [d]^T[s^E]^{-1}[d]$$
$$[e] = [s^E][d]$$

If a user inputs $[\varepsilon^T]$ or [d], this conversion is performed automatically internally, so it is transparent to the user, and the user is given flexibility on the input of the coefficients.

Some points of consideration when solving piezoelectric problems:

- Since the coupling is via the coefficient matrix, a single iteration is required for calculating coupled effects.
- These elements support nonlinear static, modal, harmonic response, and transient analyses
- The dielectric loss tangent $tan\delta$ can be input via MP,LSST. This effect will then be included in $[C^V]$, typically useful for harmonic analyses. (The dielectric quality factor Q_E is the inverse of the loss tangent.)
- The mechanical quality factor Q_M is the inverse of twice the damping ratio ξ. The damping ratio can be input as a material-dependent or a constant value for $[C^u]$.

[3] See author's memo on "Conversion of Piezoelectric Material Data", STI45:000509C for details.

- Manufacturers' data typically have mechanical vectors in the form {x, y, z, yz, xz, xy} whereas ANSYS requires the input to be {x, y, z, xy, yz, xz}, so the 4/5/6 terms need to be rearranged.
- If only the piezoelectric voltage constants [g] are available, these can be related to the piezoelectric coefficients [d] via $d_{ij} = g_{ij}\varepsilon^{T}_{ii}$
- If only the electromechanical coupling factors [k] are available, the piezoelectric coefficients [d] can be approximated at low frequencies by $d_{ij} = k_{ij}\sqrt{(s^{E}_{jj}\varepsilon^{T}_{ii})}$
- Generally speaking, because of the difficulty of obtaining all of the coefficients, the stiffness and dielectric constants of most piezoelectric materials are treated as orthotropic. The piezoelectric constants d_{31}, d_{33}, d_{15} are often supplied.
- Because of the directional-dependence, the user must ensure that an appropriate element coordinate system is defined for each element, with the poling direction consistent between the element coordinate system and material definition.
- The location of electrodes represent constant electric potential, so the nodes at those locations would usually be coupled together with the VOLT DOF only.

5. Introduction to Piezoresistivity:

For piezoresistive materials, an applied mechanical stress or strain causes a change in the material's resistivity. This makes piezoresistive materials useful as sensors where a mechanical load affects the electrical signal.

The electrical resistivity [ρ] is related to the stress as follows:

$$[\rho] = [\rho_o]([I] + [\pi][\sigma])$$

where $[\rho_o]$ is the input (nominal) resistivity and $[\pi]$ is the piezoresistive stress matrix. Alternatively, the piezoresistive strain matrix [m] may be input instead, relating relative change in resistivity to strains.

The resulting matrix equations are shown below:

$$\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} \ddot{u} \\ \ddot{V} \end{Bmatrix} + \begin{bmatrix} C^u & 0 \\ 0 & C^V \end{bmatrix} \begin{Bmatrix} \dot{u} \\ \dot{V} \end{Bmatrix} + \begin{bmatrix} K^u & 0 \\ 0 & K^V \end{bmatrix} \begin{Bmatrix} u \\ V \end{Bmatrix} = \begin{Bmatrix} F \\ I \end{Bmatrix}$$

Description of terms:

- $[K^V]$ is the (orthotropic) electrical conductivity matrix, which includes piezoresistive effects as described above.
- $[K^u]$ contains the (anisotropic) stiffness coefficients
- $[C^u]$ is the structural damping matrix whereas $[C^V]$ represents dielectric effects

Some points of consideration when solving piezoresistive problems:

- The coupling is in the coefficient matrix, but the resistivity is based on the calculated stress or strain. Consequently, multiple iterations are required for calculating coupled effects.
- These elements support nonlinear static and full transient analyses. (Because of the iterative nature of the calculations, piezoresistive materials are currently not used with linear dynamic analyses.)

- Usually, piezoresistive materials are defined in such a pattern to form a Wheatstone bridge configuration. The change in resistivities can be measured in this manner, such as for strain gauge or sensor applications.
- To make measurements of the voltage easier, the VOLT DOF may be coupled at the ends (and optionally connected to CIRCU124).
- For non-piezoresistive regions, omission of the piezoresistive material will still allow for non-coupled structural and electric current calculations. On the other hand, PLANE183, SOLID186-187 may represent structural-only parts while PLANE230, SOLID231-232 may represent electric conduction-only regions connected to piezoresistive elements.
- Input of permittivity allows for definition of $[C^V]$ to account for dielectric effects.
- The structural and electrical properties of piezoresistive materials are typically treated as isotropic or orthotropic. The piezoresistive constants π_{11}, π_{12}, π_{44} are often supplied. The element coordinate system must be defined appropriately.

6. Introduction to Thermoelectricity:

In thermal-electric applications, two types of coupling are present. *Joule heating* is an irreversible process that occurs when current flows through material with electrical resistance, proportional to the current squared, and independent of the current direction:

$$Q^j = I^2 R$$

Thermoelectricity consists of the reversible *Seebeck*, *Peltier*, and *Thomson* effects.

The Seebeck effect, defined by the coefficient α, relates a temperature gradient with a potential difference. This is useful, for example, in MEMS power generation to convert wasted heat or combustion into electrical power.

$$\alpha = \frac{\Delta V}{\Delta T}$$

The Peltier effect, noted by π, is the reverse of this where a current can cause a heat differential, and the direction of the current determines whether heat is removed or input into the system. Typical examples are thermoelectric coolers or other devices which control temperatures by removing heat through an applied current.

$$Q^p = (\pi_a - \pi_b) I$$

The Thomson effect, described by the coefficient μ, illustrates what occurs when a current flows through a material with a temperature gradient:

$$q^{th} = -\mu I \frac{\Delta T}{\Delta x}$$

The Seebeck, Peltier, and Thomson coefficients are related using absolute temperature T_o as follows:

$$\pi = \alpha T_o$$

$$\mu = -T_o \frac{d\alpha}{dT}$$

This means that only the Seebeck coefficients (and the temperature offset for absolute temperature calculations) need to be defined for thermoelectric materials.

The thermal-electric equations are incorporated into the FE matrices as follows:

$$\begin{bmatrix} C^T & 0 \\ 0 & C^V \end{bmatrix}\begin{Bmatrix} \dot{T} \\ \dot{V} \end{Bmatrix} + \begin{bmatrix} K^T & 0 \\ K^{VT} & K^V \end{bmatrix}\begin{Bmatrix} T \\ V \end{Bmatrix} = \begin{Bmatrix} Q + Q^j + Q^p \\ I \end{Bmatrix}$$

Description of terms:

- $[K^{VT}]$ is the Seebeck coefficient coupling matrix.
- Joule heating $\{Q^j\}$ and the Peltier effect $\{Q^p\}$ are included in the load vector
- The Thomson effect is not explicitly included above since it is accounted for when temperature-dependent Seebeck coefficients exist.

Things to keep in mind when solving thermal-electric problems:

- For Joule heating, the coupling is via the load vector $\{Q^j\}$. For thermoelectric effects, the $[K^{VT}]$ term produces an unsymmetric matrix, and the Peltier effect is included via a load vector coupling in $\{Q^p\}$. Moreover, coupling may also exist in temperature-dependent electrical properties. Consequently, thermal-electric analyses are iterative in nature.
- This material behavior supports nonlinear static and transient analyses.
- Absolute temperature needs to be defined via TOFFST in order to properly account for the relationship between the Seebeck and Peltier coefficients.
- Thermal-electric elements PLANE67, LINK68, SOLID69, and SHELL157 only account for Joule heating, but they may be combined with 22x coupled-field elements (especially if line or shell elements are required for modeling purposes).
- The electrical resistivity, thermal conductivity, and Seebeck coefficients can be orthotropic (and temperature-dependent).
- For transient analyses, density and specific heat are required for thermal capacitance while permittivity is required for dielectric losses.

7. Introduction to Thermoelasticity:

Thermal-stress analyses are commonplace, where the temperature field is calculated and imposed as a load vector on the structural model. However, the piezocaloric effect ("thermoelastic damping") can also be modeled with the 22x coupled-field elements for dynamic applications. The constitutive relations are described below:

$$\{\varepsilon\} = [D]^{-1}\{\sigma\} + \{\alpha\}\Delta T$$

$$S = \{\alpha\}^T\{\sigma\} + \frac{\rho C_P}{T_o}\Delta T$$

where $\{\alpha\}$ is the coefficient of thermal expansion, S is entropy density, and T_o is the absolute temperature. For the second equation, entropy and heat can be related using the second law of thermodynamics, and this would be expressed as a rate form. The combined system of equations is expressed in matrix form:

$$\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{Bmatrix} \ddot{u} \\ \ddot{T} \end{Bmatrix} + \begin{bmatrix} C^u & 0 \\ C^{Tu} & C^T \end{bmatrix}\begin{Bmatrix} \dot{u} \\ \dot{T} \end{Bmatrix} + \begin{bmatrix} K^u & K^{uT} \\ 0 & K^T \end{bmatrix}\begin{Bmatrix} u \\ T \end{Bmatrix} = \begin{Bmatrix} F \\ Q \end{Bmatrix}$$

Description of terms:

- $[K^{uT}]$ is the thermoelastic stiffness matrix (thermal expansion term) while $[C^{Tu}]$ is the thermoelastic damping matrix.

- Although [C^T] uses specific heat at constant strain, the user should input specific heat at constant stress, which is automatically converted internally

Things to keep in mind when solving thermoelastic problems:

- The system of equations is unsymmetric, although by having it matrix-coupled, the effects are considered in a single iteration. (Temperature-dependent material properties would make it iterative, however.)
- Nonlinear static, full transient, or harmonic response analyses are available.
- The piezocaloric term is only present for dynamic (harmonic or transient) analyses. Typically, the piezocaloric term is negligible compared to other sources of damping in many general applications, although this becomes an important effect for certain materials or specific MEMS applications, such as resonator beams. Although also known as "thermoelastic damping," because of the coupling of the energy equation, this effect does *not* act like structural or viscous damping by always lowering the resonant frequencies.
- Consistent energy units must be used between the structural and thermal model. (For example, do not use BTUs for energy.)
- The coefficient of thermal expansion (defined by secant ALPX, instantaneous CTEX, or thermal strain THSX) provides the coupling response for both [K^{uT}] and [C^{uT}] terms.
- A temperature offset via TOFFST is required since the thermoelastic damping calculations utilize the absolute temperature. The reference temperature (TREF or MP,REFT) designates the strain-free temperature.
- An important note, however, is that through the selection of KEYOPT(2), a load-vector coupling form can be utilized instead:

$$\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} \ddot{u} \\ \ddot{T} \end{Bmatrix} + \begin{bmatrix} C^u & 0 \\ 0 & C^T \end{bmatrix} \begin{Bmatrix} \dot{u} \\ \dot{T} \end{Bmatrix} + \begin{bmatrix} K^u & 0 \\ 0 & K^T \end{bmatrix} \begin{Bmatrix} u \\ T \end{Bmatrix} = \begin{Bmatrix} F + F^{th} \\ Q + Q^{ted} \end{Bmatrix}$$

  In this situation, the matrices remain symmetric, but because the coupling is defined via load vector terms, it requires an iterative solution. Harmonic response analysis, being linear, is not available for this load vector-coupling form.

7. Conclusion:

The 22x coupled-field elements provide a wealth of features enabling users to solve complex multiphysics phenomena. These elements are continually enhanced, so it is suggested to the user to review the *ANSYS Release Notes* for each new version to see what capabilities have been added to the 22x coupled-field elements.