Understanding Jacobian Algebra for my paper: <u>77 New Thermodynamic Identities among Crystalline Material Properties Leading to a Shear Constitutive Law in Isotropic Solids</u>. The thermodynamics has 7 independent variables: all 6 stresses and temperature. The system is a free energy with iso-piezo mechanics. In that sense, the system is a Gibbs like free energy. What is given below can be used to evaluate any of the Jacobian tables in the *Journal of Applied Physics* paper.

Consider the following 8 equations:

$$
\begin{aligned}
y_1 &= y_1(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_2 &= y_2(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_3 &= y_3(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_4 &= y_4(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_5 &= y_5(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_6 &= y_6(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_7 &= y_7(x_1, x_2, x_3, x_4, x_5, x_6, x_7) \\
y_8 &= y_8(x_1, x_2, x_3, x_4, x_5, x_6, x_7)
\end{aligned}
$$

Their chain rule derivatives are

$$
\begin{aligned}
dy_1 &= \frac{\partial y_1}{\partial x_1}dx_1 + \frac{\partial y_1}{\partial x_2}dx_2 + \dots\dots\dots\dots \frac{\partial y_1}{\partial x_7}dx_7 \\
dy_2 &= \frac{\partial y_2}{\partial x_1}dx_1 + \frac{\partial y_2}{\partial x_2}dx_2 + \dots\dots\dots\dots \frac{\partial y_2}{\partial x_7}dx_7 \\
&\vdots \\
dy_8 &= \frac{\partial y_8}{\partial x_1}dx_1 + \frac{\partial y_8}{\partial x_2}dx_2 + \dots\dots\dots\dots \frac{\partial y_8}{\partial x_7}dx_7
\end{aligned}
$$

Let y_1 and y_2 vary while holding $y_3, y_4, ..., y_8$ constant. The following 8 homogeneous equations are found:

$$0 = -dy_1 + \frac{\partial y_1}{\partial x_1} dx_1 + \frac{\partial y_1}{\partial x_2} dx_2 + \ldots\ldots\ldots\ldots \frac{\partial y_1}{\partial x_7} dx_7$$

$$0 = -dy_2 + \frac{\partial y_2}{\partial x_1} dx_1 + \frac{\partial y_2}{\partial x_2} dx_2 + \ldots\ldots\ldots\ldots \frac{\partial y_2}{\partial x_7} dx_7$$

$$0 = \quad 0 \quad + \frac{\partial y_3}{\partial x_1} dx_1 + \frac{\partial y_3}{\partial x_2} dx_2 + \ldots\ldots\ldots\ldots \frac{\partial y_3}{\partial x_7} dx_7$$

$$\vdots$$

$$0 = \quad 0 \quad + \frac{\partial y_8}{\partial x_1} dx_1 + \frac{\partial y_8}{\partial x_2} dx_2 + \ldots\ldots\ldots\ldots \frac{\partial y_8}{\partial x_7} dx_7$$

or

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -dy_1 & \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_1}{\partial x_7} \\ -dy_2 & \frac{\partial y_2}{\partial x_{1\ 1}} & \frac{\partial y_2}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_2}{\partial x_7} \\ 0 & \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_3}{\partial x_7} \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \frac{\partial y_8}{\partial x_1} & \frac{\partial y_8}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_8}{\partial x_7} \end{pmatrix} \bullet \begin{pmatrix} 1 \\ dx_1 \\ dx_2 \\ dx_3 \\ dx_4 \\ dx_5 \\ dx_6 \\ dx_6 \\ dx_7 \end{pmatrix}$$

The determinate of the matrix must be zero for a solution

$$0 = \det \begin{vmatrix} -dy_1 & \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_1}{\partial x_7} \\ -dy_2 & \frac{\partial y_2}{\partial x_{1\ 1}} & \frac{\partial y_2}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_2}{\partial x_7} \\ 0 & \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_3}{\partial x_7} \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ 0 & \frac{\partial y_8}{\partial x_1} & \frac{\partial y_8}{\partial x_2} & \ldots\ldots\ldots\ldots & \frac{\partial y_8}{\partial x_7} \end{vmatrix}$$

Evaluating the determinate using Cramer's Rule gives

$$0 = -dy_1 \left(\det \begin{vmatrix} \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_2}{\partial x_7} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_3}{\partial x_7} \\ & & & \\ \frac{\partial y_8}{\partial x_1} & \frac{\partial y_8}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_8}{\partial x_7} \end{vmatrix} \right) + dy_2 \left(\det \begin{vmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_1}{\partial x_7} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_3}{\partial x_7} \\ & & & \\ \frac{\partial y_8}{\partial x_1} & \frac{\partial y_8}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_8}{\partial x_7} \end{vmatrix} \right) \text{ so}$$

$$\left.\frac{\partial y_1}{\partial y_2}\right|_{y_3, y_4, \ldots\ldots y_8} = \frac{\det \begin{vmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_1}{\partial x_7} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_3}{\partial x_7} \\ & & & \\ \frac{\partial y_8}{\partial x_1} & \frac{\partial y_8}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_8}{\partial x_7} \end{vmatrix}}{\det \begin{vmatrix} \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_2}{\partial x_7} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_3}{\partial x_7} \\ & & & \\ \frac{\partial y_8}{\partial x_1} & \frac{\partial y_8}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial y_8}{\partial x_7} \end{vmatrix}}$$

or

$$\left.\frac{\partial y_1}{\partial y_2}\right|_{y_3, y_4, \ldots\ldots y_8} = \frac{J(y_1, y_3, y_4, y_5, y_6, y_7, y_8)}{J(y_2, y_3, y_4, y_5, y_6, y_7, y_8)}$$

Tables 1-5 in the text are all written to be in Jacobian format so any partial derivative can be found. For example

$$\left.\frac{\partial y_1}{\partial y_2}\right|_{y_3, y_4, \ldots\ldots y_8}$$

is formed by reading the rows in the tables. MatLab works well in evaluating the 7X7 determinates. For example:

```
%% Evaluation of determinates from Jacobians in Strain Volume Thermodynamics
%% c is constant stress heat capacity; T is absolute temperature;
%% betai are crystallographic thermal expansion coefficients; v is volume
%% per unit mass; sij are elastic compliances.

syms c T v beta1 beta2 beta3 beta4 beta5 beta6 s11 s12 s13 s14 s15 s16
M1=[c/T, v*beta1, v*beta2, v*beta3, v*beta4, v*beta5, v*beta6;
    1, 0, 0, 0, 0, 0, 0;
    0, 0, 1, 0, 0, 0, 0;
    0, 0, 0, 1, 0, 0, 0;
    0, 0, 0, 0, 1, 0, 0;
    0, 0, 0, 0, 0, 1, 0;
    0, 0, 0, 0, 0, 0, 1]
det(M1)

M2= [ v*beta1, v*s11, v*s12, v*s13, v*s14, v*s15, v*s16;
    1, 0, 0, 0, 0, 0, 0;
    0, 0, 1, 0, 0, 0, 0;
    0, 0, 0, 1, 0, 0, 0;
    0, 0, 0, 0, 1, 0, 0;
    0, 0, 0, 0, 0, 1, 0;
    0, 0, 0, 0, 0, 0, 1]

det(M2)

det(M1)/det(M2)
```

Which has a MatLab evaluation as:

```
M1 =
[ c/T, beta1*v, beta2*v, beta3*v, beta4*v, beta5*v, beta6*v]
[   1,       0,       0,       0,       0,       0,       0]
[   0,       0,       1,       0,       0,       0,       0]
[   0,       0,       0,       1,       0,       0,       0]
[   0,       0,       0,       0,       1,       0,       0]
[   0,       0,       0,       0,       0,       1,       0]
[   0,       0,       0,       0,       0,       0,       1]
ans =
-beta1*v

M2 =
[ beta1*v, s11*v, s12*v, s13*v, s14*v, s15*v, s16*v]
[       1,     0,     0,     0,     0,     0,     0]
[       0,     0,     1,     0,     0,     0,     0]
[       0,     0,     0,     1,     0,     0,     0]
[       0,     0,     0,     0,     1,     0,     0]
[       0,     0,     0,     0,     0,     1,     0]
[       0,     0,     0,     0,     0,     0,     1]
ans =
-s11*v
```

ans =
beta1/s11

so the above expression used in equation (17) is evaluated as

$$\left.\frac{\partial s}{\partial \Omega_1}\right|_{\mathrm{T},\sigma_2,\ldots\ldots\sigma_6} = \frac{J(s,\mathrm{T},\sigma_2,\sigma_3,\sigma_4,\sigma_5,\sigma_6)}{J(\Omega_1,\mathrm{T},\sigma_2,\sigma_3,\sigma_4,\sigma_5,\sigma_6)} = \frac{\beta_1}{S_{11}}$$