Computer Simulation of the Mathematical Modeling Involved in Constitutive Equation Development: Via Symbolic Computations

S.M. Arnold
Lewis Research Center
Cleveland, Ohio

and

H.Q. Tan and X. Dong
The University of Akron
Akron, Ohio

NASA

COMPUTER SIMULATION OF THE MATHEMATICAL MODELING INVOLVED IN CONSTITUTIVE

EQUATION DEVELOPMENT: VIA SYMBOLIC COMPUTATIONS

S.M. Arnold
National Aeronautics and Space Administration
Lewis Research Center
Cleveland, Ohio 44135

H.Q. Tan and X. Dong
Department of Mathematical Sciences
The University of Akron
Akron, Ohio 44325

SUMMARY

Development of new material models for describing the "high temperature" constitutive behavior of real materials represents an important area of research in engineering disciplines. Derivation of mathematical expressions (constitutive equations) which describe this high temperature material behavior can be quite time consuming, involved and error prone; thus intelligent application of symbolic systems to facilitate this tedious process can be of significant benefit. Here a computerized procedure (SDICE) capable of efficiently deriving potential based constitutive models, in analytical form is presented. This package, running under MACSYMA, has the following features: partial differentiation, tensor computations, automatic grouping and labeling of common factors, expression substitution and simplification, back substitution of invariant and tensorial relations and a relational data base. Also limited aspects of invariant theory have been incorporated into SDICE due to the utilization of potentials as a starting point and the desire for these potentials to be frame invariant (objective). Finally not only calculation of flow and/or evolutionary laws have been accomplished but also the determination of history independent nonphysical coefficients in terms of physically measurable parameters, e.g., Young's modulus, has been achieved. The uniqueness of SDICE resides in its ability to manipulate expressions in a general yet predefined order and simplify expressions so as to limit expression growth. Results are displayed when applicable utilizing index notation.

INTRODUCTION

Development of new material models for describing the constitutive behavior of real materials represents an important area of research in engineering disciplines. This is evidenced by research activities, in areas associated, for example, with high temperature composite, reinforced concrete and geotechnical materials (ref. 3). Efforts in constitutive research involve the development of mathematical relationships for predicting nonlinear material response, derivation of material stiffness matrix appropriate for finite element calculations (ref. 2), and finally computer implementation. The entire process requires significant manual algebraic manipulations and computer programming. Hence, the response time for the related efforts is quite long. As a result, it is rather difficult to introduce significant changes or modifications into a constitutive theory. Moreover, the outcome of the research effort may be

affected by human errors which are often difficult to detect. In this regard, symbolic computation can play a major role. Immediate benefits that can be realized are: (1) reduced manual tedium, (2) increased reliability of the derived equations, hence the final analysis results, (3) shortened model development time, and (4) investigation of alternative functional forms. Furthermore, application of symbolic manipulation can provide a significant incentive to the development of new constitutive theories and their finite element applications. However, two major obstacles arise when symbolic manipulation methods are applied for engineering applications; these are the number of steps in the derivation process and the problem of expression growth (refs. 1 and 4 to 7).

Presented here is a problem oriented software package called SDICE (Symbolic Derivation of Constitutive Equations) which is intended to assist in the derivation of potential based constitutive equations (refs. 14 and 18). The major features of SDICE are the automation of the equation derivation steps and its ability to simplify the results so as to alleviate the expression growth problem.

SYSTEM SPECIFICATIONS OF SDICE

In deriving the material constitutive equations and matrices, six types of mathematical manipulations are required, i.e.,

  (1) Partial differentiation
  (2) Tensor computations
  (3) Factorizations of common terms
  (4) Expression simplification
  (5) Back-substitution of invariant and tensorial relations

Also, limited aspects of invariant theory (ref. 13) has been incorporated into SDICE due to the utilization of potentials as a starting point and the desire for these potentials to be frame invariant (objective).

It has been shown that in most cases, the results obtained from direct application of a general purpose symbolic system, such as MACSYMA (ref. 20) are not useful due to the number of steps involved in the derivation process and the problems associated with expression growth. For this reason, resourceful derivation procedures must be developed so that optimal results can be obtained (refs. 14 to 16). The essential features of the approach taken to address the above problems consists of:

  (1) A structured derivation procedure to avoid redundant steps and to minimize expression growth,
  (2) Implementation of special procedures (e.g., procedures for simplification and pattern recognition) to facilitate the derivation process,
  (3) Expression substitution and simplification during the entire derivation process by incorporating several levels of processing,
  (4) Automatic grouping and labeling of common factors,
  (5) Taking advantage of permutation and symmetry relationships of the terms involved in each derivation step, and
  (6) As a rule-based system, intended for constitutive equation research, SDICE will record user defined rules and store them in a relational data base, whereby the information may be retrieved, redefined and restored as required.

2

Some of the above procedures and techniques will be discussed, through application examples, in the next section.

APPLICATION TO CONSTITUTIVE EQUATIONS FOR VISCOPLASTIC MATERIAL MODELS

Constitutive laws provide the link between stress components σ_{ij} and strain components ε_{ij} at any point in a body. These laws may be simple or extremely complex, depending upon the material of the body and the conditions to which it has been subjected. Consider the well known case of a hyperelastic material. Here, the stress and strain components are related through a normality structure utilizing either a strain energy or complementary energy function, i.e.,

$$\sigma_{ij} = \frac{\partial W}{\partial e_{ij}} \tag{1}$$

or

$$e_{ij} = \frac{\partial \Omega}{\partial \sigma_{ij}} \tag{2}$$

For inelastic material behavior the internal state variable potential viewpoint is adopted, i.e.,

$$\Omega = \Omega(\sigma_{ij}, \alpha_\beta, T) \tag{3}$$

with the generalized normality structure (refs. 8 to 10)

$$\dot{\varepsilon}_{ij} = \frac{\partial \Omega}{\partial \sigma_{ij}} \qquad i,j = 1,2,3 \tag{4}$$

and

$$\dot{\alpha}_\beta = -h(\alpha_\gamma) \frac{\partial \Omega}{\partial \alpha_\beta} \qquad \beta = 1,2,\ldots,n \tag{5}$$

Where Ω is the complementary dissipation potential function, $\dot{\varepsilon}_{ij}$ the inelastic strain, and α_β the internal state variables. Equations (4) and (5) are known as the flow and evolutionary equations, respectively.

Frame invariance (objectivity) of the resulting constitutive relations is insured by requiring the potential, Ω, to depend only on certain invariants and invariant products of its respective tensorial arguments, i.e., an integrity basis. Both isotropic and transversely isotropic material symmetries have been considered. Transversely isotropic material symmetry is included in the potentials of equations (1) to (3) by introducing a directional tensor $d_i d_j$, e.g., $\Omega = \Omega(\sigma_{ij}, \alpha_\beta, d_i d_j, T)$ or $W = (e_{ij}, d_i d_j)$. The symmetric tensor $d_i d_j$ is formed by a self product of the unit vector d_i denoting the local preferred direction.

Two viscoplastic theories have been proposed for isotropic materials (refs. 11 and 12). In both theories the existence of a dissipation potential is assumed, and the form is taken to be,

3

$$\Omega = \kappa^2 \left[\frac{1}{2\mu} \int f(F)dF + \frac{R}{H} \int g(G)dG\right] \tag{6}$$

where the dependence of the applied stress and internal stress (cf eq. (3)) enters through the scalar functions $F(\Sigma_{ij})$ and $G(\alpha_{ij})$, respectively.

For a material with transversely isotropic symmetry the dissipation potential is assumed to take the form of equation (6) where now the dependence of the applied stress, internal stress, and preferred direction enters through the scalar functions $F(\Sigma_{ij}, d_i d_j)$ and $G(a_{ij}, d_i d_j)$ respectively. The stress dependence is now given by

$$F = \left[AJ_2 + BJ_5 + CJ_4^2\right] - 1$$

$$G = \left[A\widehat{J}_2 + B\widehat{J}_5 + C\widehat{J}_4^2\right]$$

where

$$J_2 = \frac{1}{2} \Sigma_{ij}\Sigma_{ij}$$

$$J_4 = d_i d_j \Sigma_{ji}$$

$$J_5 = d_i d_j \Sigma_{jk}\Sigma_{ki}$$

$$\widehat{J}_2 = \frac{1}{2} a_{ij}a_{ij}$$

$$\widehat{J}_4 = d_i d_j a_{ji}$$

$$\widehat{J}_5 = d_i d_j a_{jk}a_{ki}$$

$$\Sigma_{ij} = S_{ij} - a_{ij}$$

$$S_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$$

$$a_{ij} = \alpha_{ij} - \frac{1}{3}\alpha_{kk}\delta_{ij}$$

Upon application of equations (4) and (5) the resulting flow and evolutionary laws are:

$$\dot{\varepsilon}_{ij} = \frac{f(F)}{2\mu} \Gamma_{ij} \tag{7}$$

$$\dot{a}_{ij} = h(G)\dot{\varepsilon}_{ij} - \gamma(G)\pi_{ij} \tag{8}$$

4

where

$$\Gamma_{ij} = A\Sigma_{ij} + B[d_k d_i \Sigma_{jk} + d_j d_k \Sigma_{ki} - 2J_4 d_i d_j] + \frac{2}{3} CJ_4 (3d_i d_j - \delta_{ij})$$

$$\pi_{ij} = Aa_{ij} + B[d_k d_i a_{jk} + d_j d_k a_{ki} - 2\hat{J}_4 d_i d_j] + \frac{2}{3} C\hat{J}_4 (3d_i d_j - \delta_{ij})$$

The computations required in the derivation of the above flow and evolutionary equations are partial differentiation and tensorial manipulation of invariant relations. Direct use of a symbolic system, as our tool, in the derivation process is complicated. So, special purpose procedures have to be designed and implemented in order to simplify and expedite the derivation process. Our work thus far has resulted in the development of several strategies, namely:

(1) Store the invariant relations in a relational data base.

(2) Implement procedures to compute tensor expressions according to the rules defined in tensor calculus.

(3) Map a tensor into the domain of a scalar by utilizing a property list to store the variable and its subscript; thereby, allowing all differentiation to be treated in the same way.

(4) Generate subscripts for intermediate tensor variables and store them in the same property list in a predefined order.

(5) Differentiation results are represented by a search tree, starting with the potential function as the root of the tree and its descendants without dependent relations among themselves as leaves. A separate procedure decides whether the function and its variables are tensorial or scalar.

(6) Finally, check the property list and if the function involves tensors, subscripts are added back for the final result according to the predetermined order.

(7) Simplify the result by (a) checking the data base so as to replace any known invariant relation in the final expressions, (b) grouping common terms by factorization, and (c) identifying terms that can be written as a tensor.

For example, when processing the invariant J_2 in the transversely isotropic case, the definition is

$$J_2 = \frac{1}{2} \Sigma_{ij} \Sigma_{ij}$$

the procedure first generates

$$\frac{\partial J_2}{\partial \Sigma_{kl}} = \frac{\partial \frac{1}{2}}{\partial \Sigma_{kl}} \Sigma_{ij} \Sigma_{ij} + \frac{1}{2} \frac{\partial}{\partial \Sigma_{kl}} \Sigma_{ij} \Sigma_{ij}$$

following the chain-rule. Calling the procedure recursively, we have

5

$$\frac{\partial \frac{1}{2}}{\partial \Sigma_{kl}} = 0$$

and

$$\frac{\partial}{\partial \Sigma_{kl}} \Sigma_{ij}\Sigma_{ij} = \frac{\partial \Sigma_{ij}}{\partial \Sigma_{kl}} \Sigma_{ij} + \frac{\partial \Sigma_{ij}}{\partial \Sigma_{kl}} \Sigma_{ij}$$

Then checking the data base for invariant relations and applying the tensor routines, we obtain from above

$$2\Sigma_{ij}\delta_{ik}\delta_{jl}$$

Thus by combining we have,

$$\frac{\partial J_2}{\partial \Sigma_{ij}} = \Sigma_{ij}\delta_{ik}\delta_{jl}$$

Finally, by calling the procedure identifying the rules of tensorial calculus and back-substituting, the result becomes Σ_{kl}.

All the required computational rules for deriving the constitutive equation have been integrated into SDICE along with rules which define tensorial calculus and invariant relations. For example, in deriving the flow law for a transversely isotropic model, we have

$$\dot{\epsilon}_{ij} = \frac{\partial \Omega}{\partial \sigma_{ij}} = \frac{\partial \Omega}{\partial F}\left[\left(\frac{\partial F}{\partial J_2} \frac{\partial J_2}{\partial \Sigma_{kl}} + \frac{\partial F}{\partial J_5} \frac{\partial J_5}{\partial \Sigma_{kl}} + \frac{\partial F}{\partial J_4} \frac{\partial J_4}{\partial \Sigma_{kl}}\right) \frac{\partial \Sigma_{kl}}{\partial S_{rs}} \frac{\partial S_{rs}}{\partial \sigma_{ij}}\right]$$

From equation (6) we know that

$$\frac{\partial \Omega}{\partial F} = \frac{\kappa^2}{2\mu} f(F)$$

and by tensor calculus and indical notation we have

$$\frac{\partial \Sigma_{kl}}{\partial S_{rs}} \frac{\partial S_{rs}}{\partial \sigma_{ij}} = \delta_{kr}\delta_{ls}\left(\delta_{ri}\delta_{sj} - \frac{1}{3} \delta_{ij}\delta_{rs}\right)$$

$$= \left(\delta_{ki}\delta_{lj} - \frac{1}{3} \delta_{ij}\delta_{kl}\right)$$

By introducing constants A, B, and C into the assumed forms of F and G as indicated earlier, requires that

$$\frac{\partial F}{\partial J_2} = A$$

$$\frac{\partial F}{\partial J_4} = 2CJ_4$$

$$\frac{\partial F}{\partial J_5} = B$$

and differentiating invariant relations through the procedures we have just mentioned results in

$$\frac{\partial J_2}{\partial \Sigma_{kl}} = \Sigma_{kl}$$

$$\frac{\partial J_4}{\partial \Sigma_{kl}} = d_p d_q \delta_{qk} \delta_{pl} = d_k d_l$$

and

$$\frac{\partial J_5}{\partial \Sigma_{kl}} = d_p d_q (\delta_{qk} \delta_{lr} \Sigma_{rp} + \Sigma_{qr} \delta_{rk} \delta_{pl})$$

$$= d_p d_q (\delta_{qk} \Sigma_{lp} + \Sigma_{qk} \delta_{pl})$$

$$= d_p d_k \Sigma_{lp} + \Sigma_{qk} d_l d_q$$

Next back substitution is activated,

$$\frac{\partial F}{\partial J_2} \frac{\partial J_2}{\partial \Sigma_{kl}} = A\Sigma_{kl}$$

$$\frac{\partial F}{\partial J_4} \frac{\partial J_4}{\partial \Sigma_{kl}} = 2CJ_4 d_k d_l$$

and

$$\frac{\partial F}{\partial J_5} \frac{\partial J_5}{\partial \Sigma_{kl}} = B(d_p d_k \Sigma_{lp} + d_l d_q \Sigma_{qk})$$

Finally, by checking the data base and substituting back all tensorial as well as invariant relations defined in the table into the original expression, SDICE produced the following form for the flow law

$$ged_{ij} : f(ff)gk^2(bb(3ggtl_{ij} - 2gd_{ij}jj4) + cc(6d_i d_j - 2gd_{ij})jj4 + 3aa\ gss_{ij})/6gm$$

where

$$ggtl_{ij} : d_i d_{il} gss_{jil} + gss_{iil} d_{il} d_j$$

To obtain the associated evolutionary law, equation (5) is applied, i.e., instruct SDICE to take the following action

7

$$\dot{\alpha}_{ij} = -hb \frac{\partial \Omega}{\partial \alpha_{ij}}$$

resulting in

gad_{ij} : hb ged_{ij} - g(gg) gk^2 hb rr (bb(3ggt2$_{ij}$ - 2gd$_{ij}$jja4)

$\qquad\qquad\qquad\qquad$ + cc(6d$_i$d$_j$ - 2gd$_{ij}$)jja4 + 3a a$_{ij}$)/3hh

where

$ggt2_{ij}$: d$_i$d$_{11}$a$_{j11}$ + a$_{i11}$d$_{11}$d$_j$

This agrees completely with equation (7) which was manually obtained. (We have adopted the convention of using double lower case letters for capital letters, and variables starting with "g" mean Greek alphabet).

IMPLEMENTATION OF PROBLEM-ORIENTED COMPUTATION PROCEDURE

Application of symbolic systems for material model development involves the symbolic solutions of systems of simultaneous equations. There are procedures under MACSYMA to solve systems of equations of different type. However, these general-purpose procedures when applied to our application, cause expression growth to become uncontrollable and the results are often not useful.

Under MACSYMA, for example, there are procedures for solving systems of equations, such as solve and linsolve. For certain applications, by setting the parameter backsubst equal to false, the results are simpler and the solution process faster because back substitution is prevented after the system of equations have been triangularized. This may be necessary in very large problems where back substitution would cause the generation of extremely large expressions (readers are referred to MACSYMA Manual for details).

The systems of equations we are dealing with are primarily sparse and the coefficients of their variables are usually not numbers but polynomials. The application of Gaussian elimination which is used in linsolve produces results that are usually lengthy and inefficient.

A new derivation procedure is implemented into SDICE to solve the problem of expression growth and increase the computational efficiency. The underlying concept behind this improved procedure is the identification of the smallest full subsystem contained within the original and then subsequent remaining systems. Gaussian elimination is employed to solve these subsystems independently and sequentially instead of the complete system.

To clarify this procedure, consider the following sparse system of equations:

$$2(u^2 - tu + 3t^2)x2 + 5(u + t)x1 = \frac{11}{2k} \qquad (9)$$

8

$$(2t - 3u)x1 - 2u^2x2 = \frac{7\sqrt{(u + t)}}{8} \tag{10}$$

$$\frac{3u^3x3}{(t - 1)^2} + u^2x2 + x1 = \frac{8(kt - u)^{1/3}}{13} \tag{11}$$

$$7x5 - 4u^4x4 + \frac{71u^3x3}{(t + 1)^3} + \frac{3x2}{7} + ux1 = 9 \tag{12}$$

$$-5u^5x5 + 4u^4x4 + 3u^3x3 + 2u^2x2 + \frac{(u + 2)x1}{t^2} = 10 \tag{13}$$

The procedure first searches for the smallest full subsystem in the system and in our case, chooses (9) and (10). The subsystem is then solved by Gaussian elimination without generation of intermediate variables and we obtain:

$$x1 = \frac{\sqrt{(u + t)}(7ku^2 - 7ktu + 21kt^2) + 44u^2}{16ku^3 + 80ktu^2 - 88kt^2u + 48kt^3}$$

$$x2 = \frac{(24u - 16t)x1 + 7\sqrt{(u + t)}}{16u^2}$$

The symbols x1 and x2 are then stored and treated as constants in the remaining equations. With the remaining 3 x 3 system, the smallest subsystem is 1 x 1. So, an intermediate variable zz1 is generated to represent that part of the equation containing the previously determined variables, that is

$$zz1 = 13u^2x2 + 13x1$$

and x3 can now be solved for immediately.

$$x3 = \frac{(t^2 - 2t + 1)zz1 + (-8t^2 + 16t - 8)(kt - u)^{1/3}}{39u^3}$$

Following the same steps as before, the remaining system of unknowns is a full 2 x 2 system, and two intermediate variables zz2 and zz3 are generated to represent previously obtained variables.

$$zz2 = \frac{71u^3x3}{t^3 + 3t^2 + 3t + 1} + \frac{3x2}{7} + ux1$$

and

$$zz3 = 3u^3x3 + 2u^2x2 + \frac{(u + 2)x1}{t^2}$$

Finally, by applying Gaussian elimination, we have

9

$$x4 = \frac{7zz3 + u^5(5zz2 - 45) - 70}{20u^9 - 28u^4}$$

and

$$x5 = \frac{-zz2 + 4u^4x4 + 9}{7}$$

By comparing with the result obtained from MACSYMA, the expression size is smaller and the computation effort required is less, due to the generation of intermediate variables and the partitioning of the system into smaller subsystems.

CONCLUSION

We have discussed the use of a symbolic computation method to automatically derive constitutive equations. The derivation steps and some of the computational methods used for potential based constitutive model research have been presented. It is hoped that the approach discussed here may find applications in physics as well as other engineering disciplines.

REFERENCES

1. Cecchi, M.M. and Lami, C., "Automatic Generation of Stiffness Matrices for Finite Element Analysis," Int. J. Num. Meth. Engng., 11, 1977, pp. 396-400.

2. Chang, T.Y., "NFAP - A Nonlinear Finite Element Program (Version 85.1)," Department of Civil Engineering, University of Akron, Akron, Ohio, June 30, 1985.

3. Chang, T.Y., Saleeb, A.F., Wang, P.S., and Tan, H.Q., "On the Symbolic Manipulation and Code Generation for Elasto-Plastic Material Matrices," Engineering with Computers--An International Journal for Computer-Aided Mechanical and Structural Engineering, Springer-Verlag, New York, 1986.

4. Golden, J.P., "Differentiation of Unknown Functions in MACSYMA," Bulletin, Vol. 19, No. 2, May 1985, ACM.

5. Korncoff, A.R. and Fenves, S.J., "Symbolic Generation of Finite Element Stiffness Matrices," Comput. Structures, 10, pp. 119-124, 1979.

6. Noor, A.K. and Andersen, C.M., "Computerized Symbolic Manipulation in Non-linear Finite Element Analysis," Comput. Structures, 1, pp. 9-40, 1981.

7. Noor, A.K. and Andersen, C.M. "Computerized Symbolic Manipulation in Structural Mechanics-progress and Potential," Comput. Structures 10, pp. 95-118, 1977.

8. Ponter, A.R.S., "Convexity and Associated Continuum Properties of a Class of Constitutive Relationships," J. Appl. Mech., Vol. 15, No. 4, pp. 527-542, 1976.

9. Ponter, A.R.S., Leckie, F.A., "Constitutive Relationships for Time-Dependent Deformation of Metals," J. Eng. Mech. Technol., Vol. 98, No. 1, pp. 47-57, Jan. 1976.

10. Rice, J.R., "On the Structure of Stress-Strain Relations for Time Dependent Plastic Deformations in Metals," J. Appl. Mech., Vol. 37, No. 3, pp. 728-737, Sept. 1970.

11. Robinson, D.N., "A Unified Creep-Plasticity Model for Structural Metals at High Temperature," ORNL/TM-5969, Oak Ridge National Laboratory, 1978.

12. Robinson, D.N., "A Multiaxial Theory of Viscoplasticity for Isotropic Materials," Turbine Engine Hot Section Technology 1986, NASA CP-2444, 1986, pp. 283-292.

13. Spencer, A.J.M., "Theory of Invariants," in Continuum Physics, A.C. Eringen, ed., Academic Press, Vol. I, 1971, pp. 240-355.

14. Tan H.Q., "Automatic Equation Derivation and Code Generation in Engineering Analysis," Proceedings of IEEE International Computer Science Conference '88 (Artificial Intelligence: Theory and Practice), Hong Kong, 1988.

15. Tan, H.Q., "Symbolic Derivation of Equations for Mixed Formulation in Finite Element Analysis," "Computers and Mathematics," pp. 289-298, Springer-Verlag, New York, 1989.

16. Tan, H.Q., "Integration of Symbolic and Numerical Computations in Finite Element Analysis," Proceedings of 12th IMACS World Congress on Scientific Computation, Paris, France, 1988.

17. Tan. H.Q., "Symbolic Derivation of Material Property Matrices in Finite Element Analysis," Proceedings of ASME Winter Annual Meeting, Chicago, 1988.

18. Tan, H.Q., Dong, X., Arnold, S.M., "Symbolic Derivation of Constitutive Equations," Proceedings of ASME Winter Annual Meeting, Chicago, 1988.

19. Wang, P.S., Tan, H.Q., Saleeb, A.F. and Chang, T.Y., "Code Generation for Hybrid Mixed Mode Formulation in Finite Element Analysis," Proceedings, SYMSAC'86, Toronto, Canada, 1986.

20. "MACSYMA Reference Manual," version 10, The MATHLAB Group, Laboratory for Computer Science, MIT, 1984.

1. Report No. NASA TM-102532	2. Government Accession No.	3. Recipient's Catalog No.
4. Title and Subtitle Computer Simulation of the Mathematical Modeling Involved in Constitutive Equation Development: Via Symbolic Computations		5. Report Date
		6. Performing Organization Code
7. Author(s) S.M. Arnold, H.Q. Tan, and X. Dong		8. Performing Organization Report No. E-5276
		10. Work Unit No. 510-01-0A
9. Performing Organization Name and Address National Aeronautics and Space Administration Lewis Research Center Cleveland, Ohio 44135-3191		11. Contract or Grant No.
		13. Type of Report and Period Covered Technical Memorandum
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D.C. 20546-0001		14. Sponsoring Agency Code

16. Abstract

Development of new material models for describing the "high temperature" constitutive behavior of real materials represents an important area of research in engineering disciplines. Derivation of mathematical expressions (constitutive equations) which describe this high temperature material behavior can be quite time consuming, involved and error prone; thus intelligent application of symbolic systems to facilitate this tedious process can be of significant benefit. Here a computerized procedure (SDICE) capable of efficiently deriving potential based constitutive models, in analytical form is presented. This package, running under MACSYMA, has the following features: partial differentiation, tensor computations, automatic grouping and labeling of common factors, expression substitution and simplification, back substitution of invariant and tensorial relations and a relational data base. Also limited aspects of invariant theory have been incorporated into SDICE due to the utilization of potentials as a starting point and the desire for these potentials to be frame invariant (objective). Finally not only calculation of flow and/or evolutionary laws have been accomplished but also the determination of history independent nonphysical coefficients in terms of physically measurable parameters, e.g., Young's modulus, has been achieved. The uniqueness of SDICE resides in its ability to manipulate expressions in a general yet predefined order and simplify expressions so as to limit expression growth. Results are displayed when applicable utilizing index notation.

17. Key Words (Suggested by Author(s)) Symbolic computations; Constitutive modeling Expert system; MACSYMA	18. Distribution Statement Unclassified – Unlimited Subject Category 39

19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of pages 12	22. Price* A03