PARAMETER ESTIMATION FOR VISCOPLASTIC MATERIAL MODELING*

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Introduction

A key ingredient in the design of engineering components and structures under general thermomechanical loading is the use of mathematical constitutive models (e.g. in finite element analysis) capable of accurate representation of short and long term stress/deformation responses. In addition to the ever-increasing complexity of recent viscoplastic models of this type, they often also require a large number of material constants to describe a host of (anticipated) physical phenomena and complicated deformation mechanisms. In turn, the experimental characterization of these material parameters constitutes the major factor in the successful and effective utilization of any given constitutive model; i.e., the problem of constitutive parameter estimation from experimental measurements.

Traditionally, simple, basically trial-and-error procedures (graphical/mechanistic fitting) have been used for simple models, but these are certainly rather limited in more general situations Fig. 4 . This is particularly true in dealing with very large number of material constants that are often lacking in their direct physical interpretation, where complications due to the vastly different scaling and highly interactive nature of these parameters in a large test matrix under various controls (stress, strain, or mixed) under transient and steady-state conditions Fig. 2.

An urgent need and obvious need therefore exists for a systematic development of a general methodology for constitutive parameter estimation. This provides the main motivation for the present work.

Background and Approach

The problem belongs to the class of inverse problems [1] of mathematical programming and optimization theories. Its solution requires three major and interrelated parts Fig. 4 in its application to the present dynamic (time-variant) case; i.e., (a) primal analysis

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(response functionals) for the differential form of the constitutive model, (b) sensitivity analysis, and (c) optimization of an error/cost function. The optimization algorithms for the last part (c) are presently very well developed [2]. This is not the case, however, regarding work on the other two, intimately related, parts (a) and (b). Mainly due to the greater mathematical complexity and associated intensive computational demands for the present dynamic and nonlinear case, compared to other more traditional optimization problems of linear structures. This renders unsuitable or even inapplicable several of the available solution methods and algorithms for primal and sensitivity analyses, Fig. 5.

For example, using an explicit integration method, with its known material-dependent conditional stability limits, becomes very ineffective for primal analysis, in which essentially thousands of "different materials" are being processed for response predictions (in a typical optimization cycle), thus making any adaptive time-stepping strategy very complicated, if at all possible. Similarly, in addition to several accuracy and numerical instability problems, the use of finite-differencing schemes for sensitivity analysis can easily become computationally prohibitive with the increase in material constants and time windows for fitting with long-duration tests.

The highlights of the mathematical formulations and main features of the present development (Figs. 6 and 7) are summarized as follows. Posed as a least-square, constrained, nonlinear mathematical optimization [2], we use an objective functional of the minimum-deviation-error type, i.e., differences in the predicted and measured responses at varying times. The material constants constitute the design variables, with several (side) constraints to ensure a physically-meaningful model. For the primal response analysis part, we utilize an implicit, unconditionally-stable, integration algorithm. Details and several applications of this scheme are described in a separate presentation in this proceeding; see also [3]. The sensitivity and analysis is of the direct type preformed on the basis of an explicit, recursive, form associated with the above integrator. Finally, the optimizer segment is of the gradient-based type, utilizing a sequential-quadratic programming scheme [4]. It is these three approaches combined that provide for the robustness and computational efficiency.

The overall strategy is summarized in the flow chart of Fig. 8. Its main driver (dubbed COMPARE for COnstitutive Model PARamter Estimator) controls the three solution modules (primal analysis, sensitivity, optimizer), together with the management of data files and results. From the practical standpoint (Fig. 9), the overall strategy is sufficiently general to handle comprehensive test-matrix data, under arbitrary load-control variables, multiaxial stress/strain tests, and transient as well as steady-state response measurements.

Results

All applications given utilize a viscoplastic model of the nonlinear kinematic-hardening type, GVIPS [5], having a total of eight material constants (Fig. 10). The first part of the studies [Figs. 11-15] are performed on a simulated ("exact") model material, for validation and to investigate the issues of parameter sensitivities, accuracy, comparisons, and

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In the second part [Figs. 17-22], we use actual test-matrix results for TIMETAL21S material. This includes three tensile test under different strain rates, creep tests with three different imposed stresses, a relaxation test, as well as a three-step creep test. The "fitting" success in this latter, more realistic application, with vastly different conditions and very large number of data points, clearly points to the potential benefit and practicality of the general methodology.

References

1. Bui, H. D., and Tanaka, M. (editors): Inverse Problems in Engineering, Balkema, Rotterdam, 1994.

2. Luenberger, D. G.: Linear and Nonlinear Programming, second edition, Addison-Wesley, Reading, 1984.

3. Saleeb, A. F. and Li, W.: Robust Implicit Integration Schemes for Generalized Viscoplastic Models - Part I: Theoretical Developments and Applications; Part II: Algorithmic Developments and Implementation, NASA CR-195453, 1995.

4. Schittkowski, K.: The Nonlinear Programming Method of Wilson, Han, and Powell with an Augmented Lagrangian Type Line Search Function, Numerische Mathematik, Vol. 38, No. 1, pp.83-114, 1981.

5. Arnold, S. M., Saleeb, A. F., and Castelli, M. G.: A Fully Associative, Nonlinear Kinematic, Unified Viscoplastic Model for Titanium Based Matrices, Life Prediction Methodology for Titanium Matrix Composites, ASTM STP 1253, W. S. Johnson, J. M. Larsen, and B. N. Cox, Eds. 1996, or NASA TM-106609, 1994.

OUTLINE

- Motivation
- Objectives
- Background
- Mathematical formulation
- Computational algorithms
- Sensitivity analysis
- Applications

Fig. 1

MOTIVATION

Two major obstacles to fully utilizing recent time-dependent/hereditary constitutive models in practical engineering analysis:

- Lack of efficient and robust integration algorithms
- **Difficulties associated with characterizing large number of required material parameters**

    - Most material parameters lack obvious/direct physical interpretations

    - Even under load histories in simple laboratory tests, several parameters will highly interact to affect predicted responses

    - Further complications due to:

    (i) Incompleteness of response measurment in both time and state

    (ii) Vastly different scaling of constitutive parameters

    - Urgent need exists for specific guidelines in the systematic development of general methodology for constitutive- parameter-identification

Fig. 2

OBJECTIVES

General: Systematic development of general methodology for constitutive parameter estimation

Specific:

- Mathematical formulation of a <u>basic</u> optimal material parameter estimation scheme

- Computational <u>algorithms</u> for implementation

- <u>Validation</u> tests and <u>performance</u> studies

- Alternatives for further <u>refinements</u> in fitting;
  that is, variable/cost function scaling, weights, multicriteria optimization theories, etc.

Fig. 3

BACKGROUND

- "Traditional" approaches for constitutive parameter estimations:

  - Essentially <u>trial-and-error</u> in nature

  - Based on several <u>assumptions</u> about test conditions and material behavior that are <u>rarely</u> satisfied in actual tests

  - Difficult to control <u>error propagation</u> in sequential evaluations of parameters

  - Rather <u>limited</u> in applications

- Modern approaches for constiutive parameter estimations based on mathematical programming and <u>optimization</u> theories:

  - More <u>general</u>/systematically derived

  - Three major parts for <u>modular</u> implementations:

    (a) <u>Primal</u> analysis for response functionals
        (integrated history)

    (b) <u>Sensitivity</u> analysis

    (c) <u>Optimization</u> of "cost" function

Fig. 4

BACKGROUND

- Methods and algorithmic details differ greatly for the sensitivity analysis:

    - Finite difference methods (prohibitively expensive; prone to errors)

    - Evolutionary sensitivities approach (expensive two-subproblem integrations; special coding for number of parameters dependent sizes of arrays; stiffness/singularity problems)

    - Adjoint sensitivity approach (regressive computations with large storage requirements; or increased computational cost for terminal adjoint problems)

    - Direct-differentiation sensitivity (most effective and accurate when consistently derived with the underlying implicit integration of the model)

Fig. 5

MATHEMATICAL FORMULATION

- Framework required characteristics:

    - Coupled nonlinear system (internal/external state variables)

    - Transient response with different possible steady-state conditions (time variance)

    - Arbitrary (optional) control variables; i.e., stress-, strain-, mixed-types of loading (general test matrix)

- Approach:

    - A least-square, constrained, nonlinear mathematical optimization problem

    - Material parameters constitute the design variables, with several associated side constraints to ensure physically meaningfull model

    - The technique is of the minimum-deviation-error type, for the integrated multiaxial response (functionals)

Fig. 6

MATHEMATICAL FORMULATION

- Noteworthy aspects:

    (i) Robustness and effectiveness:

    - Unconditionally stable implicit integration for primal analysis (model problem)

    - Direct-differentiation approach for accurate sensitivity analysis

    - State-of-the-art optimizer using sequential quadratic programming (with exact gradient and variable metric/Hessian) for least-squares minimization

    (ii) Computational efficiency:

    - Non-iterative "exact" sensitivities (once after primal analysis time-step convergence)

    - Effective scaling for both the design variables and the objective function in optimization

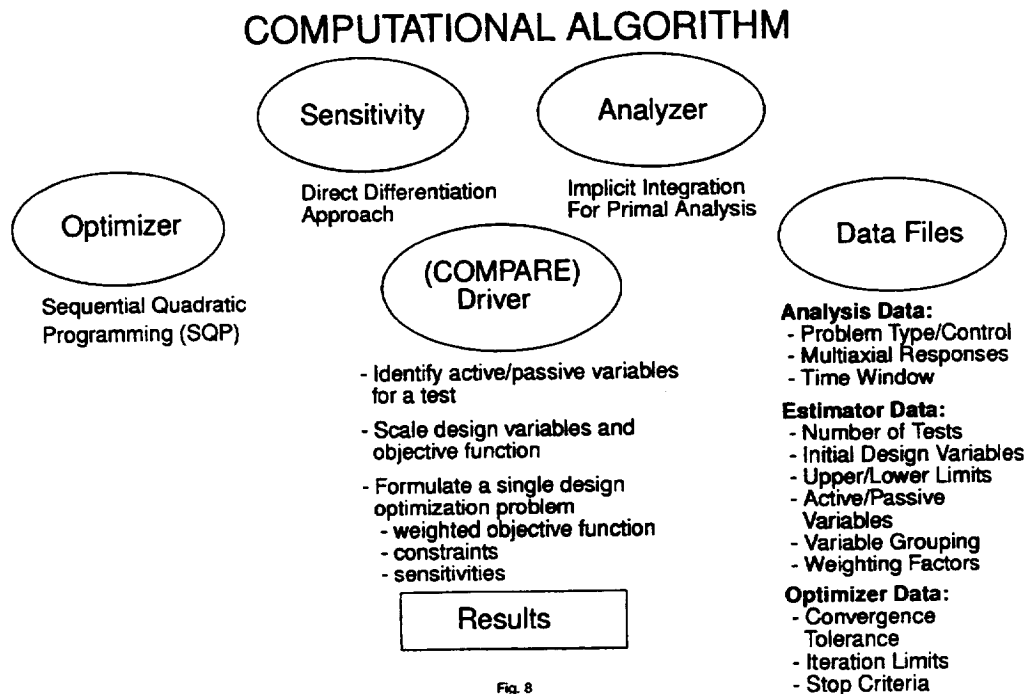   - Enhanced iterations with line searches in implicit integration

Fig. 7

COMPUTATIONAL ALGORITHM

Sensitivity

Analyzer

Optimizer

Direct Differentiation
Approach

Implicit Integration
For Primal Analysis

Data Files

(COMPARE)
Driver

Sequential Quadratic
Programming (SQP)

- Identify active/passive variables
  for a test

- Scale design variables and
  objective function

- Formulate a single design
  optimization problem
    - weighted objective function
    - constraints
    - sensitivities

Analysis Data:
- Problem Type/Control
- Multiaxial Responses
- Time Window

Estimator Data:
- Number of Tests
- Initial Design Variables
- Upper/Lower Limits
- Active/Passive
  Variables
- Variable Grouping
- Weighting Factors

Optimizer Data:
- Convergence
  Tolerance
- Iteration Limits
- Stop Criteria

Results

Fig. 8

COMPUTATIONAL ALGORITHMS

- Features and capabilities:

    - General test matrix with arbitrary control (stress, strain, or mixed) with multiaxial measurements (two normal plus one shear component), e.g.,

Stress-control	Creep
Mixed-control	Relaxation
Stress-control	Tension/constant stress rate
Mixed-control	Tension/torsion test

    - Active/passive design parameter activation (e.g., parametric study)

    - Upper/lower side constraints

    - Arbitrary number of tests and time windows selected for fitting

    - Goodness-of-fit statistical measures

Fig. 9

SENSITIVITY ANALYSIS

- Model problem

    - Unified viscoplasticity with potential GVIPS (nonlinear hardening; static recovery mechanism; isotropic/nonisotropic yielding)

    - Total of seven viscoplastic parameters (design variables)

Flow equation	= 2 (viscosity μ; exponent n)
Evolution equation	= 4 2 (hardening; modulus H, exponent β)
	+ 2 (recovery; modulus R, exponent m)
Yield threshold	= 1 (κ_f)

- Simulated "actual" material (perfect model representation capability)

    - Normalized sensitivity plots

    - "Accuracy" and efficiency comparisons with traditional finite-differencing schemes

    - Creep, relaxation, constant-strain-rate tension as representative tests

Fig. 10

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SENSITIVITY ANALYSIS (SIMULATED TESTS)

DESIGN PARAMETERS	T_1		T_{25}		T_{50}	
	IMPLICIT	F.D.	IMPLICIT	F.D.	IMPLICIT	F.D.
κ_T	1.7899 (10)-1	1.7864 (10)-1	4.5844	4.5816	4.5844	4.5817
n	-1.1361 (10)-1	-1.1384 (10)-1	2.1588 (10)-1	2.1525 (10)-1	2.1588 (10)-1	2.1525 (10)-1
μ	1.4583 (10)-6	1.4570 (10)-6	-1.7294 (10)-6	-1.7291 (10)-6	-1.7295 (10)-6	-1.7291 (10)-6
m	9.2111 (10)-19	0.000	-6.3965 (10)-6	-6.4033 (10)-6	-1.5127 (10)-5	-1.5144 (10)-5
β	4.2054 (10)-3	4.2041 (10)-3	-9.4439 (10)-1	-9.4236 (10)-1	-9.4395 (10)-1	-9.4325 (10)-1
R	-9.1043 (10)-9	0.000	-9293.57	-9293.71	-2.1978 (10)+5	-2.1976 (10)+5
H	1.4634 (10)-7	1.4628 (10)-7	3.6125 (10)-5	3.6085 (10)-5	3.6124 (10)-5	3.6084 (10)-5

Scaling →

Time Evolution →

Fig. 11

SENSITIVITY ANALYSIS (SIMULATED TESTS)
TIME EVOLUTION
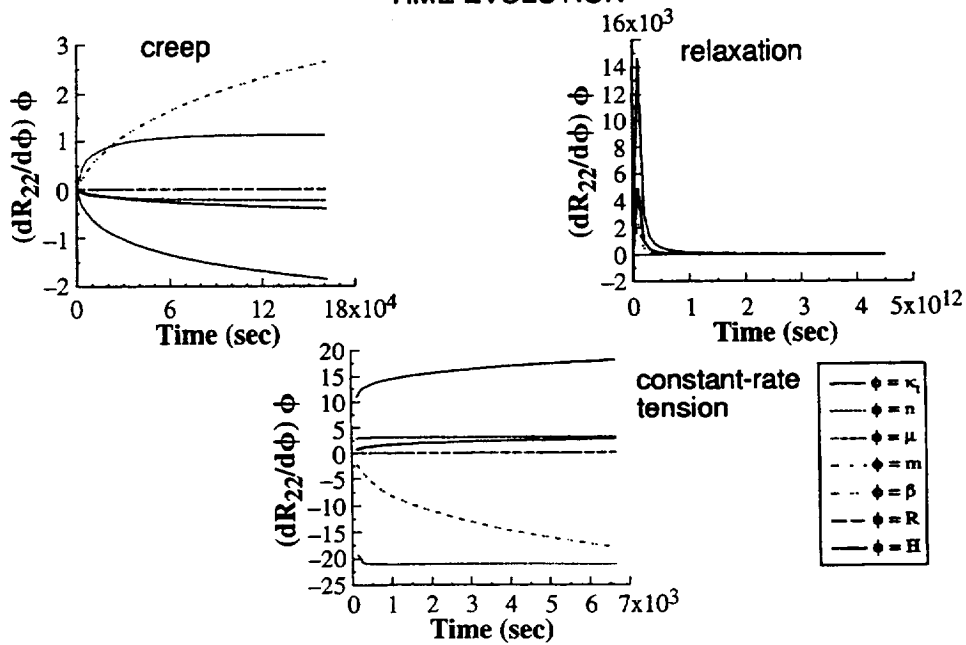
Fig. 12

EFFICIENCY OF IMPLICIT SENSITIVITY SCHEME

		TENSILE	CREEP	RELAXATION
RELATIVE CPU	IMPLICIT	1.0	1.0	1.0
	F.D.	8.004	8.235	7.931

General Estimate:

Relative CPU $\cong 8 \times N_i \times N_w \times N_t \times \eta$

N_i = Number of integration steps per each (equal) optimization interval

N_w = Number of (equal) sampling points (time windows) per test

N_t = Number of total tests

η = Trial-Differencing-Accuracy Factor $\eta = 2 \rightarrow 10 \rightarrow$?

Fig. 13

TYPICAL CONVERGENCE AND FITTING ACCURACY
(SIMULATED MATERIAL FOR TENSILE/CREEP/RELAXATION TEST)

Convergence

Accuracy in Tensile Test

Fig. 14

TYPICAL CONVERGENCE AND FITTING ACCURACY
(SIMULATED MATERIAL FOR TENSILE/CREEP/RELAXATION TEST
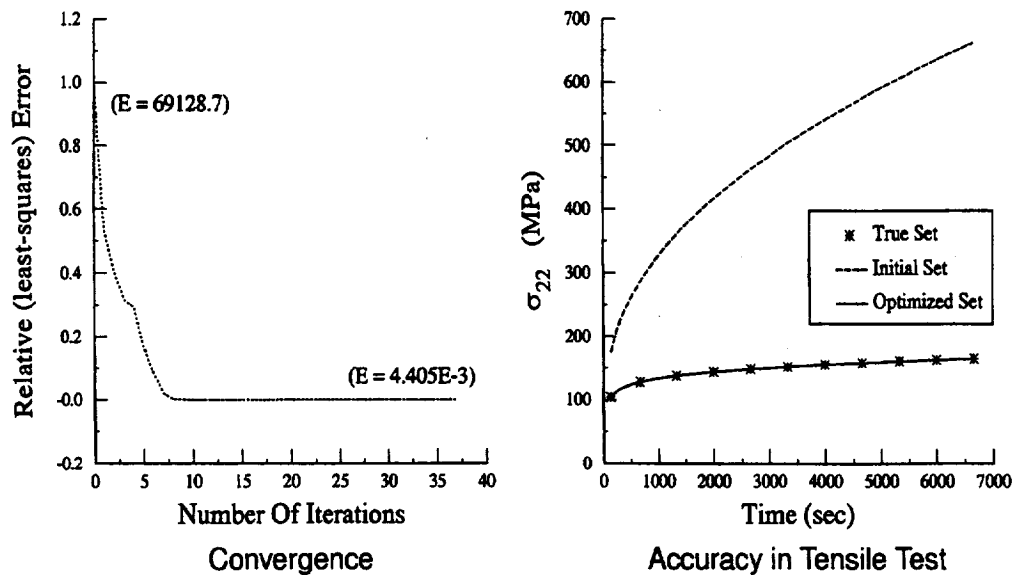
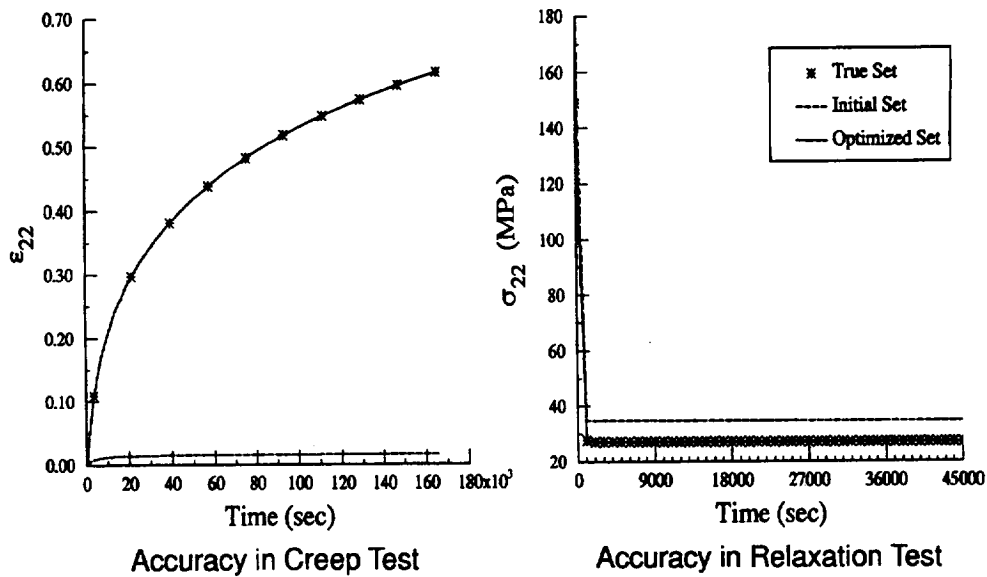Accuracy in Creep Test   Accuracy in Relaxation Test

Fig. 15

APPLICATIONS

- Material: - *TIMETAL 21S*
    - Temperature = 650°C

- Experimental tests available

    (a) 3 tensile tests

    (b) 3 creep test

    (c) 1 relaxation test

    (d) single 3-step creep test

- Results/Studies

    - varied number of tests included in fitting

    - varied sampling-time intervals within each test

    - varied material-parameter bounds and optimization weights

    - comprehensive case: all tests (a)-(d) included in fitting

Fig. 16

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SUMMARY OF COMPREHENSIVE FIT CASE

(*TIMETAL 21S*; 8 TESTS; T=Tensile, C=Creep, R=Relaxation, SC=3-Step Creep)

	T1	T2	T3	C1	C2	C3	R	SC
Number of Fitting Points	93	67	57	96	103	107	72	285
Weight Factors (equal weight)	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125
Weight Factors (variable weight)	0.1193	0.1657	0.1947	0.116	0.1077	0.1037	0.1542	0.0389

a) Fitted Points and Weights

	Number of Iterations	Number of Function Calls	Number of Gradient Calls	Normalized CPU
Estimated (equal)	53	61	54	1.0
Estimated (variable)	49	54	50	0.882

b) Solution Efficiency

Fig. 17

SUMMARY OF COMPREHENSIVE FIT CASE
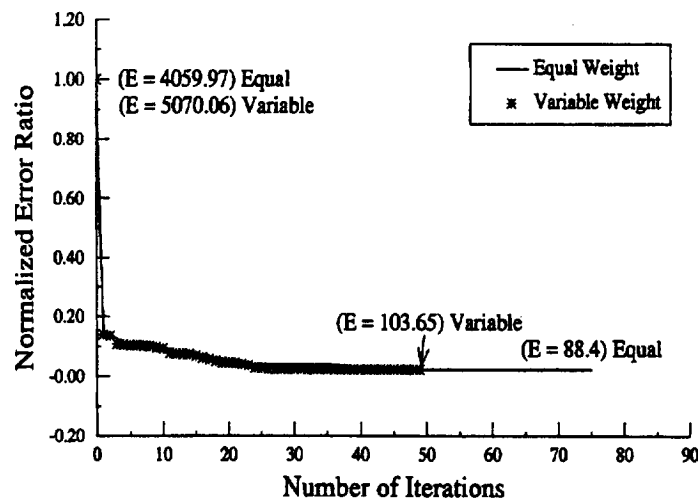
(*TIMETAL 21S*; 8 TESTS)

Fig. 18

TENSILE BEHAVIOR CORRELATION
(COMPREHENSIVE FIT)

Given:
- a "far" initial guess
- with/without bounds on parameters
→ unique "optimal" response

$$\dot{\varepsilon}_0 = 8.333 x 10^{-6}$$

Legend:
- × Experiment
- ---- Initial Set
- —— Optimum Set
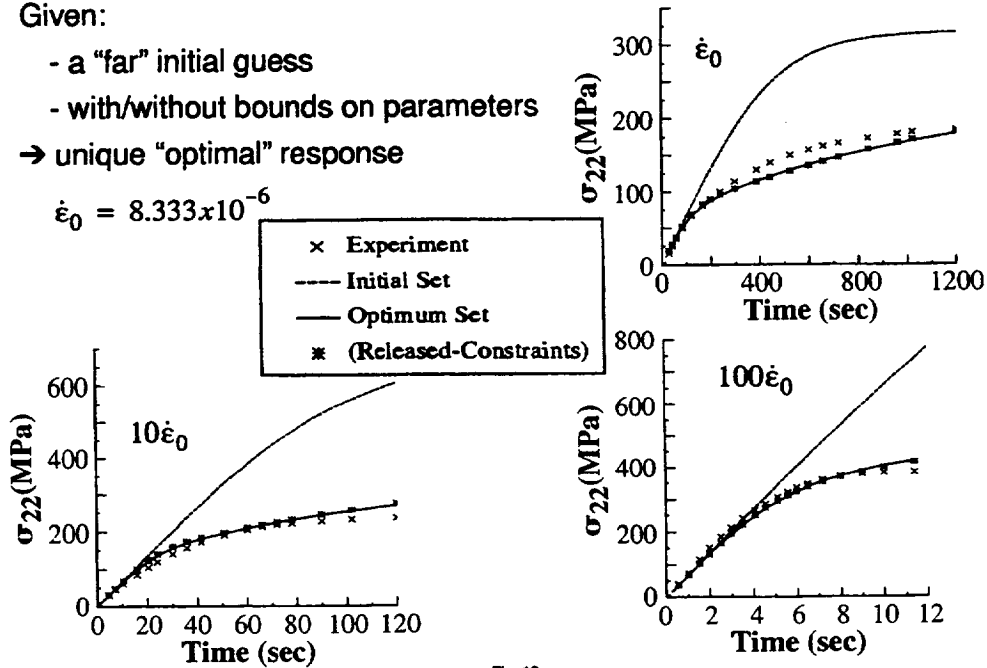- ✳ (Released-Constraints)

Fig. 19

CREEP BEHAVIOR CORRELATION
(COMPREHENSIVE FIT)

Given:
- a "far" initial guess
- varying sample-time intervals
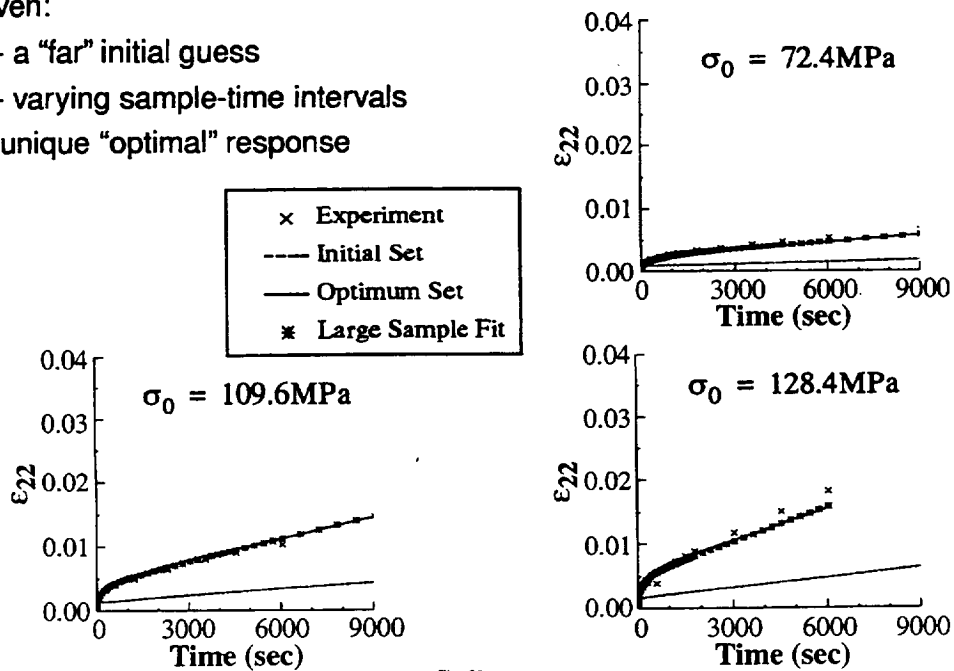→ unique "optimal" response

Legend:
- × Experiment
- ---- Initial Set
- —— Optimum Set
- ✳ Large Sample Fit

Fig. 20

13

RELAXATION BEHAVIOR CORRELATION
(COMPREHENSIVE vs. SINGLE-RELAXATION TEST FIT

Given:

- a "far" initial guess

- <u>variable</u> optimization weights

→ unique optimized response

Comprehensive fit gives better overall predictions with comparable accuracy to the "pure" single-response curve correlation
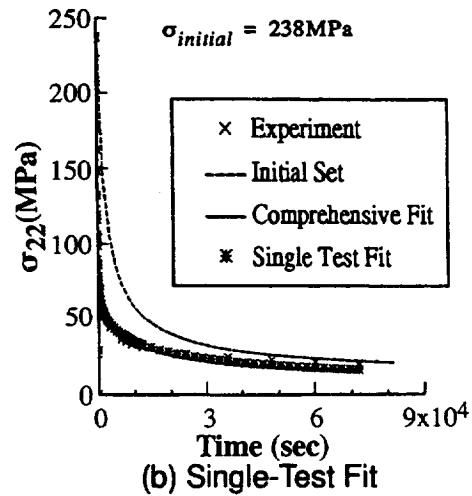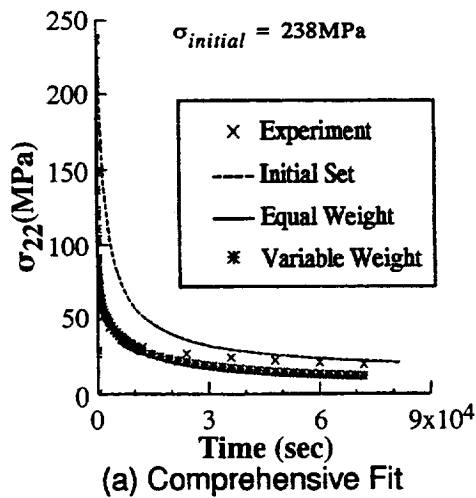

(a) Comprehensive Fit

(b) Single-Test Fit

Fig. 21

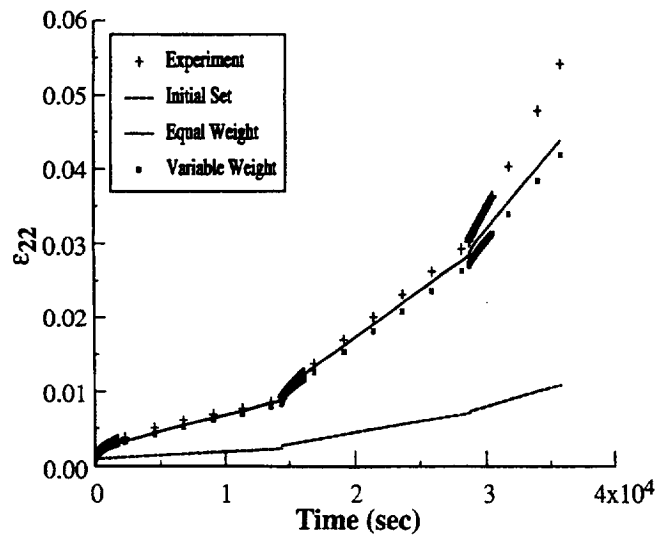# 3-STEP CREEP CORRELATION
(COMPREHENSIVE FIT)

Fig. 22

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SUMMARY/CONCLUSIONS

- Validation with exact (simulated) material
  - Given an accurate constitutive model, exact correlation is achievable by COMPARE
- Assessment with real materials (*TIMETAL 21S*)
  - Automated material parameter estimation enables the model to achieve its "best" correlation
  - Serves as a tool for identifying critical experiments to maximize pertinent "data content" (e.g., one test for tension, creep, cyclic and (initial) relaxation)
  - Requires minimum "user expertise"
  - Gives a measure for model suitability and directions for its further enhancement in realistic range of applications
  - Estimates for effects of model versus experimental (noisy data) deficiencies (COMPARE's knowledge of parameter sensitivities)

Fig. 23

SUMMARY/CONCLUSIONS

  - Including more data points in fitting enhances the optimizer convergence speed
- New model implementation
  - Demands more than just a definition of elementary (differential) flow/evolution equations - integrated form Jacobian

Fig. 24

FUTURE WORK

- Inclusion of new material models in COMPARE library
- Experience in applications with multiaxial test fitting
- "User-friendly" enhancements

Fig. 25

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