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RELFIT: A Program for Determining Prony Series Fits to Measured Relaxation Data

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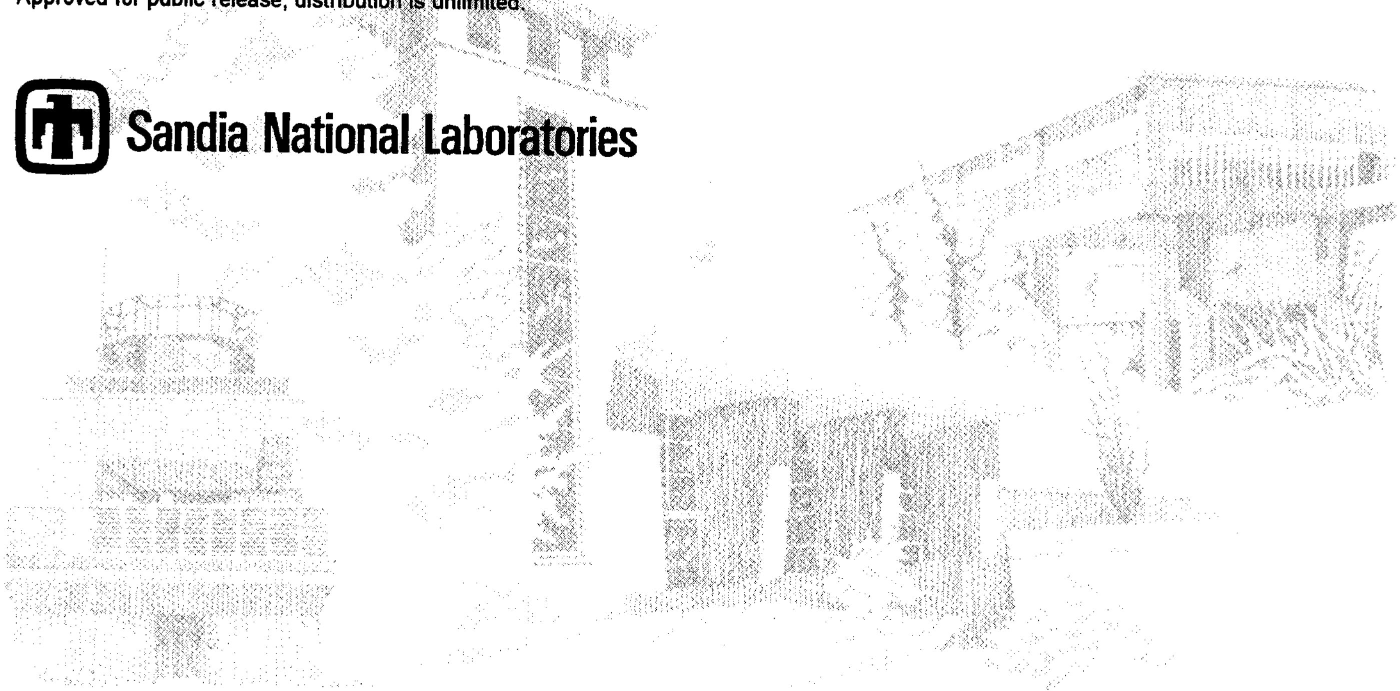

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Abstract

Viscoelastic materials are often characterized in terms of stress relaxation moduli which decay in time. Finite element programs which model viscoelastic materials frequently require that these relaxation functions be defined as an exponential series (i.e., Prony Series) to exploit the numerical advantages of developing recursive equations for evaluating hereditary integrals. Obtaining these data fits can be extremely difficult when the data is spread over many decades in the logarithm of time. RELFIT is a nonlinear optimization program that iteratively determines the Prony series coefficients and relaxation times so as to minimize the least squares error in the data fit. An overview of the code, a description of the required inputs (i.e., users's instructions), and a demonstration problem are presented.

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Relaxation Fits

Viscoelastic materials are often characterized by stress relaxation moduli which decay in time. Finite element programs which contain models of viscoelastic materials frequently require that these relaxation functions be specified as an exponential series of the following form:

$$E(t) = E_\infty + \sum_{i=1}^{N} E_i e^{-t/\tau_i} \tag{1}$$

where N is the number of terms in the Prony series, E_∞ is the rubbery modulus, and E_i and τ_i are the coefficients and relaxation times in the series expansion. The computer program RELFIT is an optimization code that employs an iterative technique to fit the relaxation function defined by Equation 1 to a set of user supplied data points. Since the code was developed for stress relaxation functions, it is tailored to fit the data collected from a classical stress relaxation experiment where a strain is imposed on a sample and the subsequent decay in stress is measured as a function of time. Strains are assumed to be imposed by a constant strain rate ramp (see Figure 1). The stress history following imposition of the strain is com-

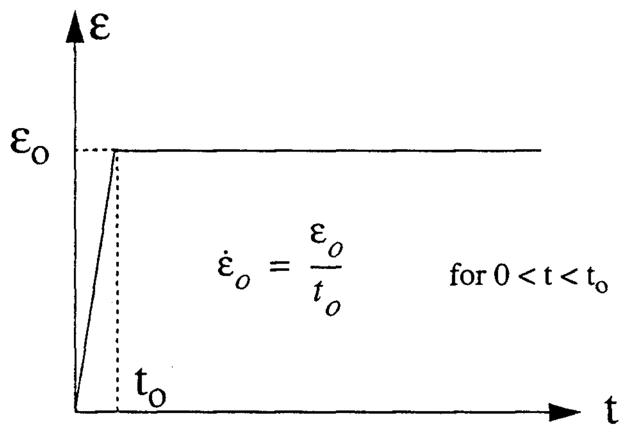

Figure 1. Strain History Applied in Stress Relaxation Experiment

puted from the integral constitutive equation:

$$\sigma(t) = \int_0^t E(t-s)\frac{d\varepsilon}{dt}ds \tag{2}$$

Substituting Equation 1 into Equation 2 and adopting the strain history defined in Figure 1, the resulting stress is

$$\sigma(t) = E_{\infty}\varepsilon(t_o) + \sum_{i=1}^{N} E_i \tau_i \dot{\varepsilon}_o e^{-t/\tau_i}\left\{e^{t_o/\tau_i} - 1\right\} \text{ for } t \geq t_o \tag{3}$$

Optimization

Predictions from Equation 3 are compared to the measured data, and the values of E_i and τ_i are determined by minimizing the least squares error, F, defined by:

$$F = \sum_{p=1}^{P} \{\sigma(t_p) - \sigma_p\}^2 \tag{4}$$

where P is the number of data points, σ_p is the value of the stress measured at time t_p, and $\sigma(t_p)$ is Equation 3 evaluated at time t_p. The iterative process that is employed to minimize the least squares error requires the user to provide a "first guess" for the Prony series coefficients and relaxation times. Optimization then proceeds on two levels:

1. the Prony series coefficients are directly optimized for the specific set of relaxation times provided by the user, and
2. each pair of Prony coefficients and relaxation times in the series is optimized successively.

Because this is a nonlinear iterative process, the user must specify a limit on the maximum number of iterations to be performed. Convergence is achieved when the relative change of all parameters is less than a user specified tolerance. The convergence criterion then becomes:

$$\frac{|\Delta X|}{X} < Tolerance \tag{5}$$

where X is the parameter being optimized (i.e., coefficient or relaxation time).

Helpful Hints

The code performance improves with the quality of the initial guess for the Prony series coefficients. A good strategy is to begin with just a few Prony terms where it is easier to make a reasonable estimate. It is then possible to build on this optimization by adding terms one or two at a time until the desired quality of the fit is obtained. Note that convergence may not be fully attained with one execution of the code. You may need to run it more than once to get enough iterations to do the job. If many terms are being requested, it is strongly recommended that you execute the software on a machine that uses a 64-bit word (i.e., about 15 decimal places of accuracy). Otherwise, the code should probably be rewritten for double precision.

Input Format

The code is structured to receive 8 types of input from the user. Most input definitions are obvious from the material that has been previously presented. The input format is summarized below. Items in italics identify the actual parameter values or inputs which must be specified by the user. The regular text found on some input lines (expressed in capital letters) provides readable definitions for the user and the code and must be reproduced just as shown below. Input 3 is an optional input line that is added to tell the code that the data is not to be read as time/stress pairs. Instead, time and force values are read where the area is defined on this line and stress is computed from the inputs by dividing the force by the area. If the data is to be read as time/stress pairs simply do not specify this input line.

Input 1	*Title*	
Input 2	TIMO, t_o, EPS0, ε_o	(This is time of ramp & magnitude of strain)
Input 3	TIME FORCE AREA, A	(This line is optional)
Input 4	t_1, $\sigma(t_1)$	
	t_2, $\sigma(t_2)$	
	t_3, $\sigma(t_3)$	(These are data points that are to be fit)
	.. ..	
	t_P, $\sigma(t_P)$	
	END	(Data points must terminate with an END card)
Input 5	N	(This is the number of terms in Prony series)
Input 6	E_∞	
Input 7	E_1, τ_1	
	E_2, τ_2	
	.. ..	(This is a 1st guess for Prony Series)
	E_N, τ_N	
Input 8	ITERATIONS, *iter*, RELATIVE ERROR, *relerr*	

Example Problem

Consider a Prony series fit of the power law function defined by

$$G(t) = t^{-0.1} \tag{6}$$

over the interval [0.01, 1.0E+7]. The input deck for a 3-term optimization is shown in Figure 2. The data to be fit were computed from the power law equation by evaluating the function at five equally spaced points (in log time) per decade. Notice that the strain ramp was assumed to be a unit strain applied over a relatively short period of 1.0E-6 time units. A unit strain was imposed to make the input "stress" be identically equal to the "modulus" (employing the terminology of the previous discussions). Although three Prony terms are not expected to fit the data very well over a range of 9 decades in time, this fit provides a good "seed" on which to build better estimates. A reasonable fitting strategy is to obtain the 3-term optimized fit, then add two new terms to make a 5-term guess and compute a 5-term optimization. The same procedure can be repeated to obtain a 7-term optimization from the 5-term fit, and so on

```
Prony Series Fit of Power Law Function (1/t)**0.1
 TIMO 1.0E-6   EPSO 1.00
  1.00000E-02   1.58489E+00
  1.58489E-02   1.51356E+00
  2.51189E-02   1.44544E+00
  3.98107E-02   1.38038E+00
  6.30957E-02   1.31826E+00
  1.00000E-01   1.25893E+00
  1.58489E-01   1.20226E+00
  2.51189E-01   1.14815E+00
  3.98107E-01   1.09648E+00
  6.30957E-01   1.04713E+00
  1.00000E+00   1.00000E+00
  1.58489E+00   9.54993E-01
  2.51189E+00   9.12011E-01
  3.98107E+00   8.70964E-01
  6.30957E+00   8.31764E-01
  1.00000E+01   7.94328E-01
  1.58489E+01   7.58578E-01
  2.51189E+01   7.24436E-01
  3.98107E+01   6.91831E-01
  6.30957E+01   6.60693E-01
  1.00000E+02   6.30957E-01
  1.58489E+02   6.02560E-01
  2.51189E+02   5.75440E-01
  3.98107E+02   5.49541E-01
  6.30958E+02   5.24807E-01
  1.00000E+03   5.01187E-01
  1.58489E+03   4.78630E-01
  2.51189E+03   4.57088E-01
  3.98107E+03   4.36516E-01
  6.30958E+03   4.16869E-01
  1.00000E+04   3.98107E-01
  1.58489E+04   3.80189E-01
  2.51189E+04   3.63078E-01
  3.98107E+04   3.46737E-01
  6.30958E+04   3.31131E-01
  1.00000E+05   3.16228E-01
  1.58489E+05   3.01995E-01
  2.51189E+05   2.88403E-01
  3.98108E+05   2.75423E-01
  6.30958E+05   2.63027E-01
  1.00000E+06   2.51189E-01
  1.58489E+06   2.39883E-01
  2.51189E+06   2.29087E-01
  3.98108E+06   2.18776E-01
  6.30958E+06   2.08930E-01
  1.00000E+07   1.99526E-01
END
3
  0.0
  5.00000E-01   1.00000E-02
  5.00000E-01   1.00000E+03
  5.00000E-01   1.00000E+07
ITERATIONS 1000  RELATIVE ERROR 1.0E-10
END
EXIT
```

Figure 2. Code Input (2 Column Format) for 3-Term Prony Series Fit of Specified Data

Table 1: Results From 3 Term Prony Series Fit

Initial Guess			Least	Optimized			Least
Prony Series Coefficients			Squares	Prony Series Coefficients			Squares
i	E_i	τ_i	Error	i	E_i	τ_i	Error
1	5.000E-1	1.000E-2	2.188E+0	1	6.218E-1	4.132E-1	2.080E-1
2	5.000E-1	1.000E+3		2	4.699E-1	2.101E+2	
3	5.000E-1	1.000E+7		3	3.809E-1	7.426E+6	

until the desired accuracy is obtained. If the "initial guess" for the rubbery modulus is identically zero, then the code assumes that the rubbery modulus is not to be fit (i.e., it is zero).

Tables 1-3 show the initial guess and optimized sets of Prony coefficients for the 3, 5, and 7 term Prony fits respectively. The least squares errors for each data set, both before optimization and after optimization, also is provided. The optimized results are readily seen to be an order of magnitude (or more) better than the initial estimate. Notice that the initial estimate for the Prony series coefficients can readily be built by adding terms to "fill-in the gaps" in the spectrum of relaxation times. A plot of the 3, 5, and 7 term fits is shown in Figure 3 along with the original power law function data points.

Table 2: Results From 5 Term Prony Series Fit

Initial Guess			Least	Optimized			Least
Prony Series Coefficients			Squares	Prony Series Coefficients			Squares
i	E_i	τ_i	Error	i	E_i	τ_i	Error
1	6.218E-1	4.132E-2	7.672E-1	1	4.609E-1	6.710E-2	2.086E-2
2	1.000E-1	1.000E+1		2	3.549E-1	2.221E+0	
3	4.699E-1	2.101E+2		3	2.848E-1	1.117E+2	
4	1.000E-1	1.000E+4		4	2.195E-1	1.526E+4	
5	3.809E-1	7.425E+6		5	2.967E-1	1.587E+7	

Table 3: Results From 7 Term Prony Series Fit

Initial Guess			Least	Optimized			Least
Prony Series Coefficients			Squares	Prony Series Coefficients			Squares
i	E_i	τ_i	Error	i	E_i	τ_i	Error
1	4.609E-1	6.710E-2	1.093E+0	1	4.348E-1	5.119E-2	5.079E-3
2	3.549E-1	2.221E+0		2	3.410E-1	1.243E+0	
3	2.848E-1	1.117E+2		3	2.559E-1	3.829E+1	
4	1.000E-1	1.000E+3		4	1.596E-1	1.155E+3	
5	2.195E-1	1.526E+4		5	1.068E-1	1.651E+4	
6	1.000E-1	1.000E+6		6	9.657E-2	3.715E+5	
7	2.967E-1	1.587E+7		7	2.462E-1	4.076E+7	

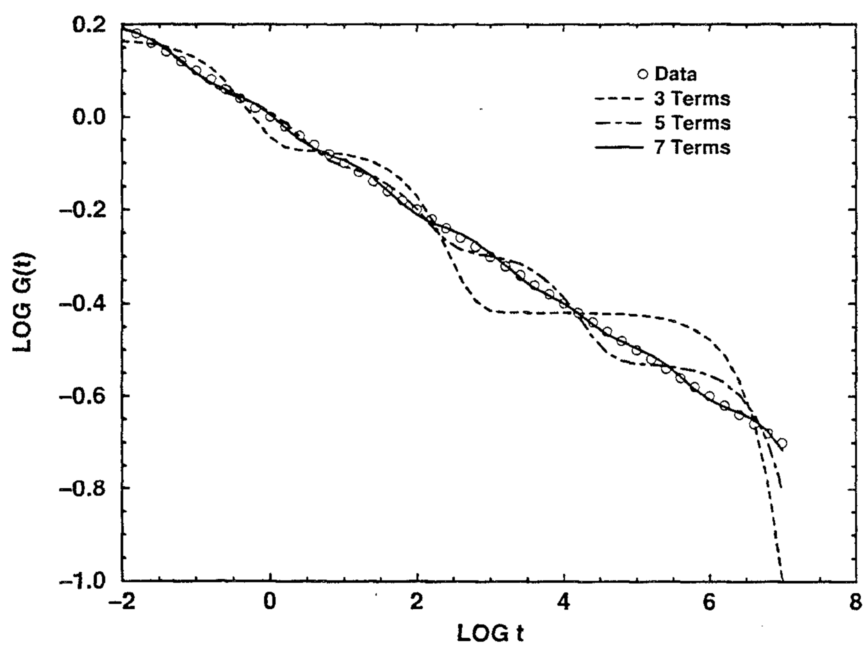

Figure 3. Prony Series Fits to Power Law Function Data

Program Notes

The RELFIT computer program is written in FORTRAN. It uses routines from the SUPES[1] library to open and assign files and to acquire the capability for free-field inputs. Hence, the binary code must be linked with the SUPES library to satisfy unresolved external references. The UNIX[2] script that is currently being used to execute the code is:

```
echo $1
setenv FOR005 $1'.input'
setenv FOR006 $1'.output'
setenv FOR030 $1'.data'
echo $FOR005 $FOR006 $FOR030
relfit.out
```

The script assumes that the input file has the form, *filename.input*, where the file name is provided by the user and the "input" extension is mandatory. Two files are created during the code execution: *filename.output* and *filename.data*. The output file echoes the data read by the code and provides information on the code execution as well as the definition of the optimized Prony coefficients. The data file prints the data along with the comparable results of the fit. This is provided so that the user may readily plot these results for a visual assessment of the quality of the fit. On a UNIX operating system, the code is executed by entering a command line:

relfit.script *filename*

where relfit.script is the name of the file containing the above script and relfit.out is the executable.

The script, compilation, linking, and execution are functions of the operating system where the code is being executed. The above information is provided only as an example based on Sandia's current environment.

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1. Red-Horse, John R., Mills-Curran, William C., and Dennis P. Flanagan, SUPES Version 2.1 A Software Utilities Package for the Engineering Sciences, SAND90-0247, Sandia National Laboratories, Albuquerque, NM, June 1992.
2. UNIX is a trademark of Bell Laboratories

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