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Utility of Coupling Nonlinear Optimization Methods with Numerical Modeling Software

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Utility of Coupling Nonlinear Optimization Methods with Numerical Modeling Software [1]

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Abstract

The utility of coupling nonlinear optimization methods with numerical modeling software is described in this paper. The results of using GLO (Global Local Optimizer), a general purpose nonlinear optimization software package for investigating multi-parameter problems in science and engineering is discussed. The software package consists of the modular optimization control system (GLO), a graphical user interface (GLO-GUI), a pre-processor (GLO-PUT), a post-processor (GLO-GET), and nonlinear optimization software modules, GLOBAL & LOCAL GLO is designed for controlling and easy coupling to any scientific software application. GLO runs the optimization module and scientific software application in an iterative loop. At each iteration, the optimization module defines new values for the set of parameters that are being optimized. GLO-PUT inserts the new parameter values into the input file of the scientific application. GLO runs the application with the new parameter values. GLO-GET determines the value of the objective function by extracting the results of the analysis and comparing to the desired result. GLO continues to run the scientific application over and over until it finds the "best" set of parameters by minimizing (or maximizing) the objective function. An example problem showing the optimization of material model is presented.

Introduction

The automated optimization of design configurations using GLO (Global Local Optimizer) [1], is a viable design methodology for the scientist and engineer. We expect this new optimization methodology to result in a significant improvement in designs as well as to provide an advancement in the methodology used for design. The GLO software package is based on the coupling of the variable metric nonlinear optimization code, NLQPEB [2], with sophisticated hydrocodes [3,4]. The nonlinear optimization software package has been demonstrated for a variety of applications including EFP problems [5-8] and high explosive ignition and growth of reaction problems [9,10].

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The optimization software package consists of the controller, GLO, the optimization code, NLQPEB, and a user-supplied hydrocode or other scientific applications software. GLO runs the optimization code and hydrocode in an iterative loop to minimize an objective function (or figure of merit, FOM -- also known as goodness, cost, or fitness). For software model calibration, the FOM might be the difference between the analysis result and the known experimental result. NLQPEB uses a Broyden, Fletcher Goldfarb, & Shanno variable metric sequential quadric programming methodology with a modified Powell merit function [11,12]. It treats the hydrocode as an objective function, supplying it with new parameter values for optimization. The result of the hydrocode analysis is used to determine a figure of merit, FOM, which in the above described example is the squared error difference between the experimental result and the calculated result. GLO runs NLQPEB and the hydrocode in a loop until it finds the "best" set of parameters by minimizing or maximizing the FOM.

The analysis methodology of running a hydrocode over and over to improve a design is not new. It has been done done by every scientist using hydrocodes since the first hydrocode was written. Typically, a user first calibrates the hydrocode model and material model parameters by matching the calculated result to an experiment or known solution. He then uses the calibrated hydrocode and material models to improve an existing design or to create a new design. With GLO, the overall methodology of iterating the hydrocode runs is still being used; however, the user is not responsible for the task of running the hydrocode. This task is done by GLO. Figure 1 shows how the scientist or engineer is more effective concentrating on the optimization strategy while GLO performs the iterative task of running the scientific software application.

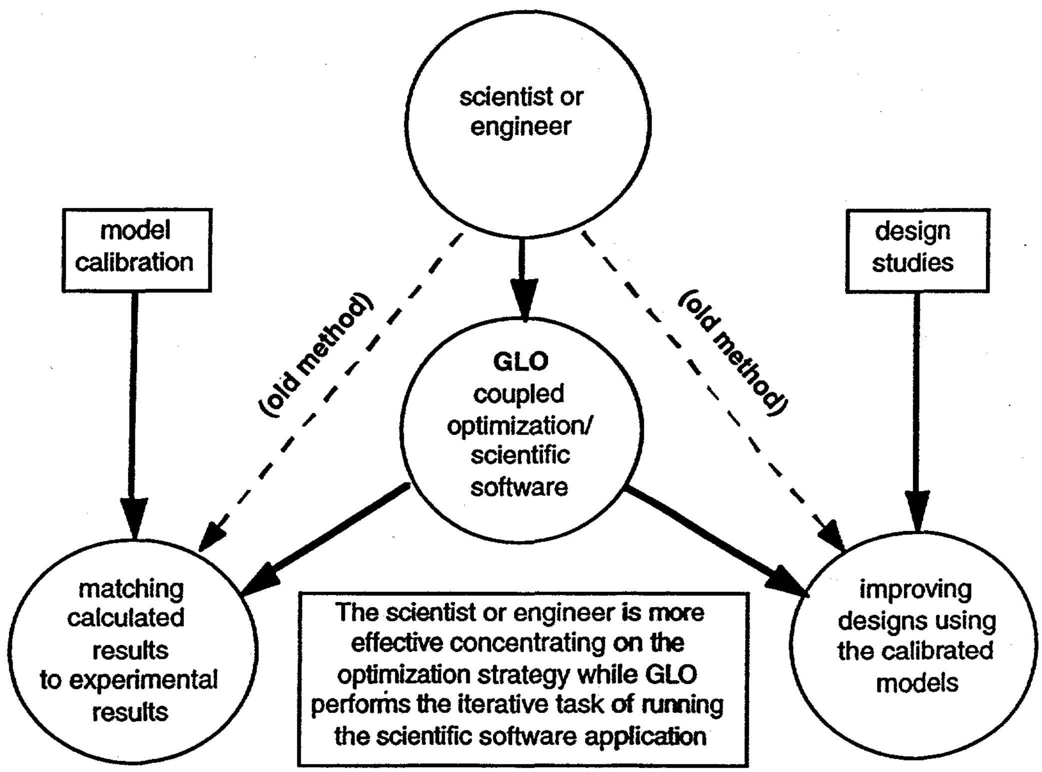

Figure 1 The scientist or engineer is more effective concentrating on the optimization strategy while GLO runs the scientific software application.

Hydrocode Modeling Background

Lawrence Livermore National Laboratory and the other U.S Department of Energy National Laboratories have historically relied on hydrocode modeling and simulation combined with a few key tests to:

- better understand the chemistry and physics of what we are doing (i.e. if we can't model it we don't completely understand it),
- minimize the number of experiments required to create a design,
- shorten the overall design process, and
- to minimize costs.

The next generation of scientists in this community will not have the same luxuries as previous generations due to cost reductions and testing constraints. However, we expect that improved hydrocode simulation tools coupled to modern nonlinear optimization methods will help ease the burden. Additionally, cheap/fast workstations and multi-processor systems will combine to make nonlinear optimization a viable methodology for coupled hydrocode design as shown graphically in Figure 2. We have had good/stable hydrocodes in use for many years, as well as modelers and designers that have spent their careers running them. With cheap/fast workstations and multi-CPU systems now available, the coupling of nonlinear optimization to the hydrocodes will revolutionize the overall design process.

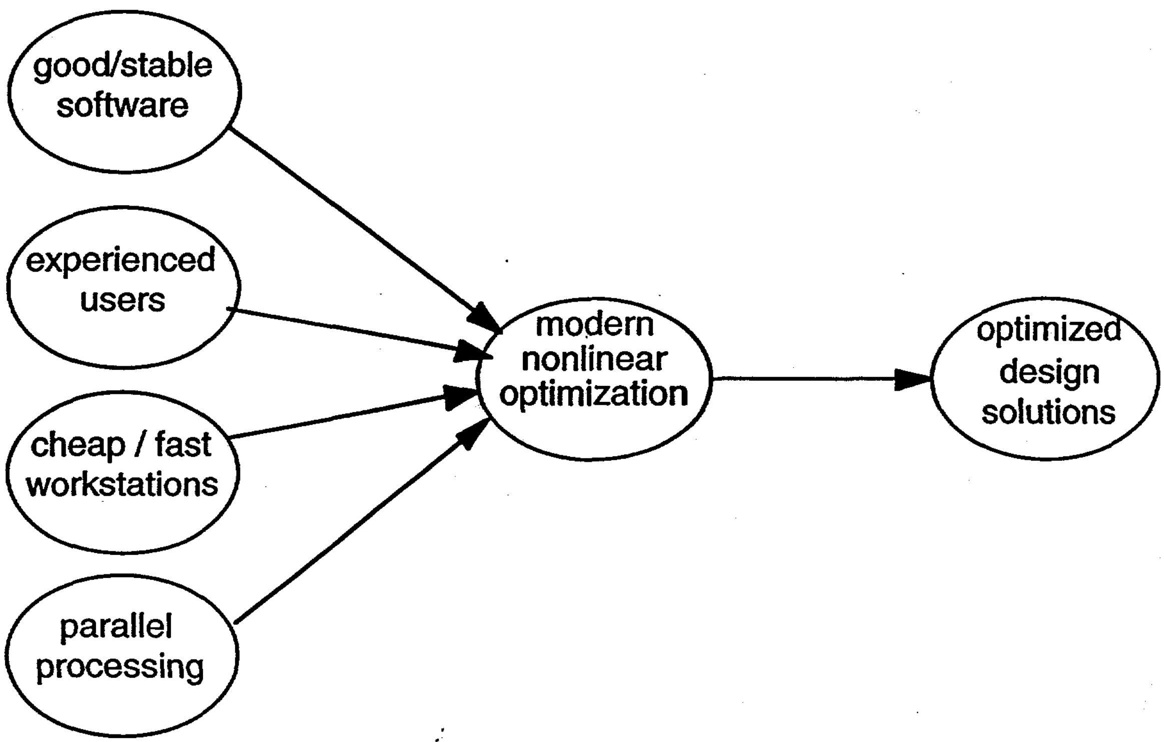

Figure 2. Nonlinear optimization has now become a viable design methodology because of several important factor: good software, experienced users, fast workstations, and parallel processing.

Optimization Approach

GLO is a modular optimization control system developed for optimization problems where the objective function calculation requires a lot of CPU time. It consists of the modular optimization control system GLO, a graphical user interface GLO-GUI, a pre-processor, GLO-PUT, a post-processor GLO-GET, the local nonlinear optimization software module, LOCAL (NLQPEB), and the global optimization software package, GLOBAL. The GLO software package can be coupled to any hydrocode. GLO runs the optimization code and hydrocode in an iterative loop as shown in Figure 3. At each iteration, the optimization module supplies the hydrocode with a set of parameters. The hydrocode runs the problem and determines the value of the objective function by comparing the results of the analysis to the desired result. GLO runs the optimization module and the hydrocode in a loop until it finds the "best" set of parameters by minimizing (or maximizing) the objective function.

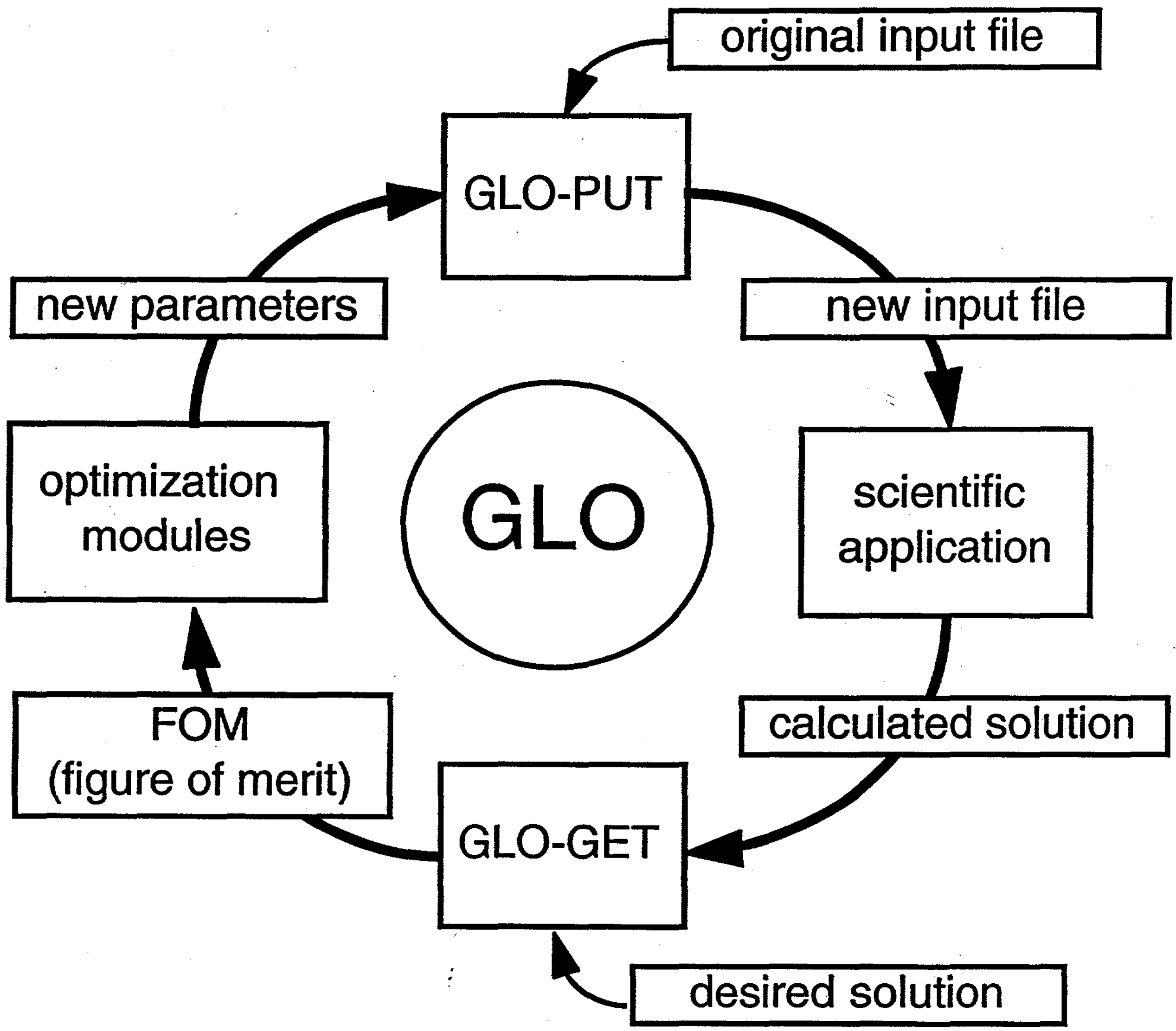

Figure 3. Description of GLO (Global Local Optimizer) methodology

Nonlinear Optimization

Nonlinear optimization problems occur in all areas of science and engineering, arising whenever there is a need to minimize (or maximize) an objective function that depends on a set of variables while satisfying some constraints [13].

Objective function: The coupling of the nonlinear optimization code with the hydrocode allows us to treat the results of the hydrocode as the objective function of the nonlinear optimization problem. Thus, the objective function of a particular problem might be to minimize the difference between the result of the hydrocode analysis and experimental results. In another problem, the objective function might be the maximizing an effect as predicted by the hydrocode.

Set of variables: Any of the input parameters to the hydrocode can be considered as the "set of variables" for the optimization problem. We have successfully worked with constitutive material properties and the design geometry as variables for optimization. Any set of the input parameters can be treated as the "set of variables"

Constraints: Constraints can be placed on the optimization problem to force it match a desired condition while maximizing or minimizing the objective function. A typical example of constraints are a range of acceptable material properties from lab experiment.

Example GLO Analysis

We have analyzed the classic Taylor cylinder impact test for determining material model flow stress parameters as an example of the utility of GLO. The cylinder impact test was introduced by Taylor [14] in 1945. It has been used over the last few decades by researchers to estimate the dynamic flow stresses for various materials [15, 16]. In this example problem we have used GLO to determine the best values of three material property constants in the Zerilli-Armstrong [17] dislocation mechanics based material model. The equation describing this flow stress model is given below.

$$\mathbf{Y = C0 + C2\sqrt{ep} \cdot (exp)\left[-C3T + C4T \cdot \ln\left(\dot{e}\right)\right] + k\sqrt{l}}$$

The Taylor cylinder impact test consists of a right circular cylinder of material that impacts a non-deforming, surface which remains rigid during the deceleration of the impacting material specimen. The resulting deformation of the cylindrical material specimen at various impact velocities is used to calibrate the flow stress model. A description of the finite element mesh used to analyze this test is shown in Figure 4. The calculated deformed geometry of the material specimen is shown in Figure 5.

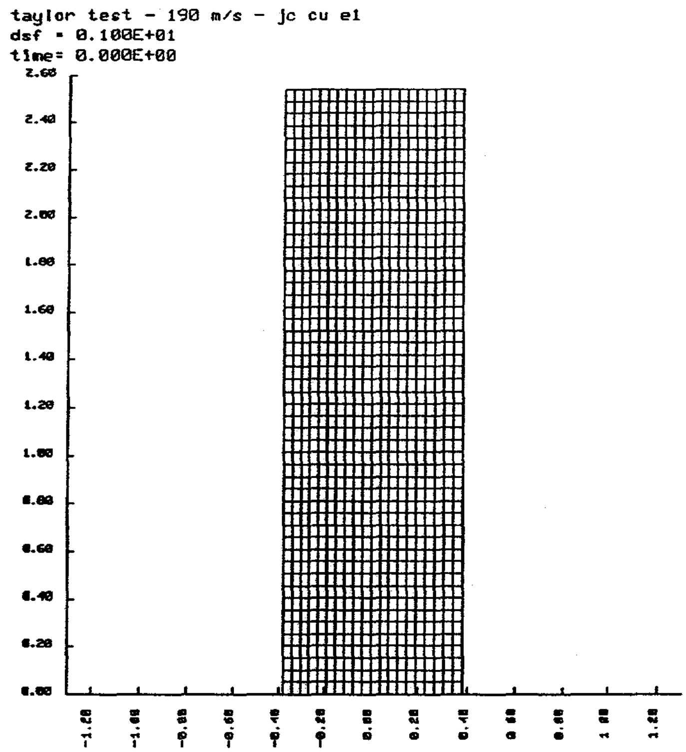

Figure 4. A description of the Taylor cylinder impact test finite element mesh.

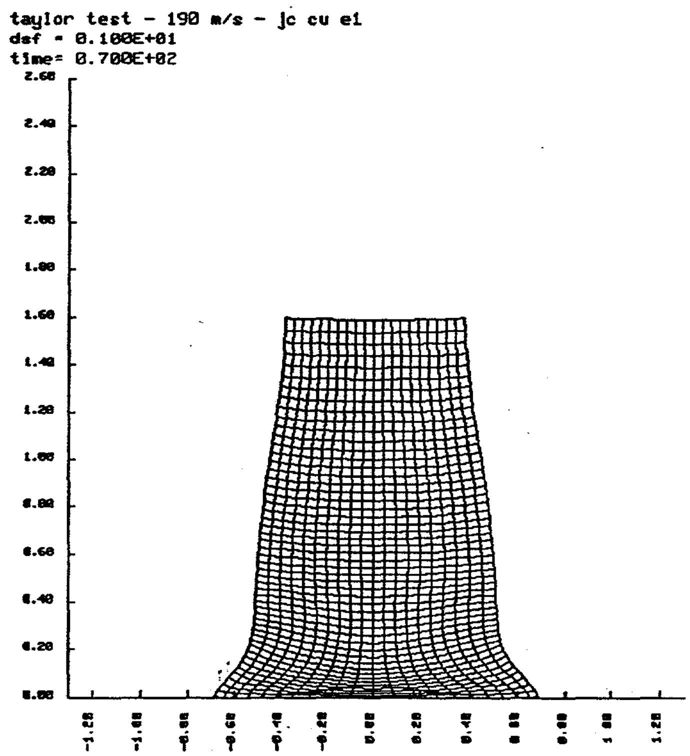

Figure 5. Calculated deformed geometry of the material specimen.

In this example problem, we first calculated the deformation of the impacting cylinder using published material property values. We then determined the deformed geometry and used this result as our goal (or experimental result) for the GLO analysis. Three of the published material property values in the flow stress equation, C2, C3, & C4, were change. GLO was then used to re-determine these values by iterating the hydrocode runs until a match the original deformed geometry was obtained.

A figure of merit, FOM, for each iteration of the hydrocode analysis was calculated by taking the squared difference between the original calculated projectile diameter and the new calculated projectile diameter for each iteration. The squared difference at several positions along the length of the projectile was summed to determine the FOM for that iteration. GLO then varied the material property parameters until the FOM was reduced to zero (i.e. no difference between the original and final deformed geometry). A plot showing the FOM as a function of hydrocode iteration is given in Figure 6. This figure shows GLO conducting the gradient calculations for each parameter as well as the Newton steps where all parameter values are improved. **A key point to note is that the gradient calculations can be done simultaneously on a multi-processor computer.**

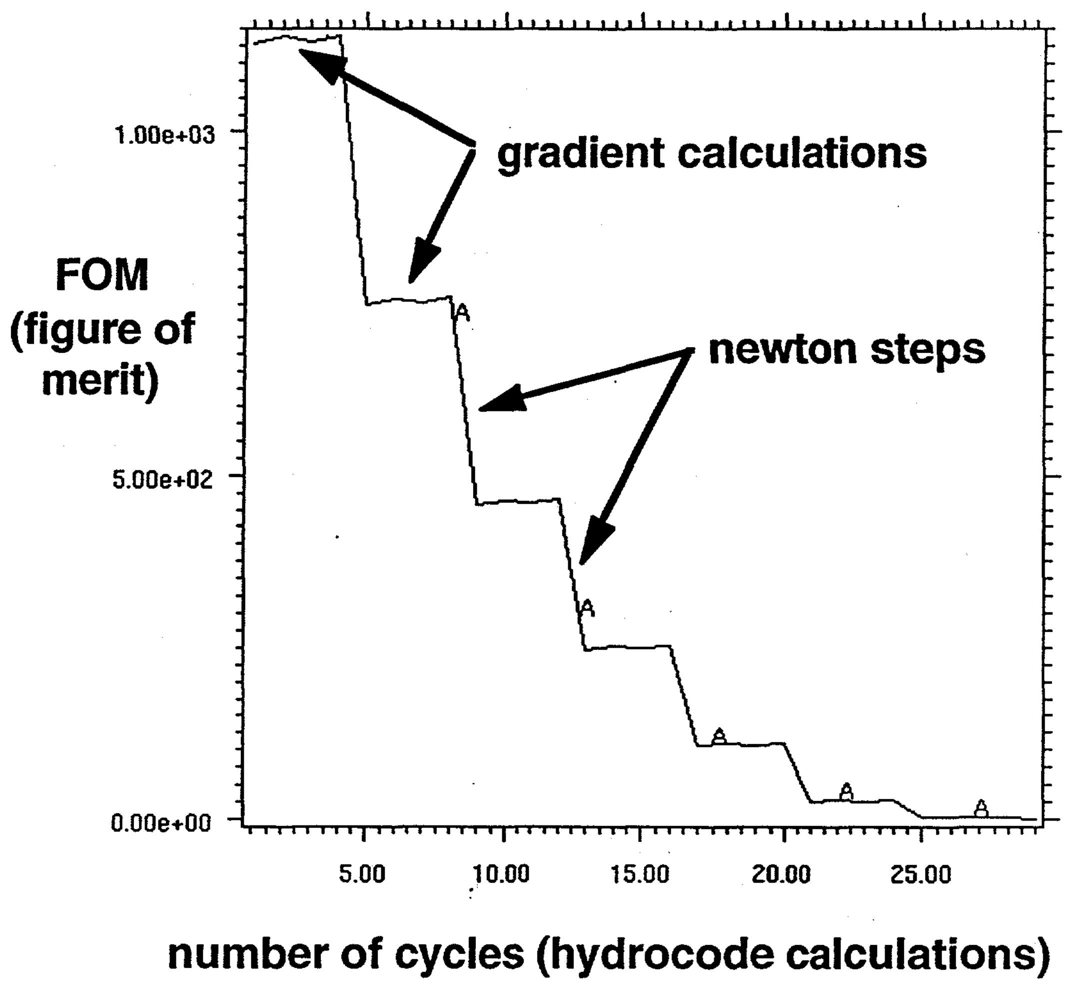

Figure 6. GLO calculated figure of merit versus hydrocode iteration

Conclusions

Modern nonlinear optimization technology is fast, accurate, and useful for automated ptimization in hydrocode model calibration and for developing new designs. It is important to note that the hydrocode model must be robust and treat the salient features of the optimization problem. In addition, the accuracy of the "optimized" set of parameters produced by GLO is primarily limited by the accuracy of the hydrocode numerical solution (not the optimization code). We have demonstrated the utility of this technology for material property parameter value determination by correlating to test results as well as for optimal design geometries.

Our conclusion is that modern nonlinear optimization technology coupled with state-of-the-art finite element codes is the future. It has resulted in a significant improvement in design capability and it is revolutionizing the design process. This methodology allows the user to be more effective concentrating on the optimization strategy while GLO performs the iterative task of running the scientific applications software..

Acknowledgments

The GLO development project has been a team effort and would not be possible without the hard work of several individuals. Dr. Ernest L. Baker has spent many years developing and perfecting the NLQPEB optimization module, the backbone of GLO. Robb Matzke did a superb job developing the GLO controller which is written in Perl. Bob Corey and Kristen Buxton developed the X11 graphical user interface (GUI) that will make this a software package that can be easily picked up and used by anyone experienced at running hydrocodes. I would also like to acknowledge Al Holt and Suzanne Lake for seeing the vast potential of this technology and for obtaining the funding that allowed us to fast track the development.

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