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CODE DIFFERENTIATION FOR HYDRODYNAMIC MODEL OPTIMIZATION

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Use of a hydrodynamics code for experimental data fitting purposes (an optimization problem) requires information about how a computed result changes when the model parameters change. These so-called sensitivities provide the gradient that determines the search direction for modifying the parameters to find an optimal result. Here, we apply code-based automatic differentiation (AD) techniques applied in the forward and adjoint modes to two problems with 12 parameters to obtain these gradients and compare the computational efficiency and accuracy of the various methods. We fit the pressure trace from a one-dimensional flyer-plate experiment and examine the accuracy for a two-dimensional jet-formation problem. For the flyer-plate experiment, the adjoint mode requires similar or less computer time than the forward methods. Additional parameters will not change the adjoint mode run time appreciably, which is a distinct advantage for this method. Obtaining "accurate" sensitivities for the jet problem parameters remains problematic.

INTRODUCTION

Use of a hydrodynamics code (hydrocode) for experiment fitting purposes requires information about how some scalar result (or response, R) will change when some code parameter (α) is changed. This so-called sensitivity, $(\partial R / \partial \alpha)$, is the gradient (or Jacobian) that determines the search direction for obtaining an optimum response. Typically, the gradient is obtained by changing parameters one at a time to form a finite-difference derivative. This method, which we call the Direct Method, requires $N+1$ computer runs to determine sensitivities for N problem parameters.

In previous papers (1,2,3) we have described an equation-based sensitivity technique used successfully in the early eighties, which is called Differential Sensitivity Theory (DST) (4). We have seen, however, that this technique does not produce accurate values for all sensitivities and for problems with discontinuities such as material interfaces. We described code-based automatic differentiation (AD) (5) techniques which include ADIFOR (Automatic Differentiation of FORtran)(6) and the TAMC (Tangent-linear and Adjoint Model Compiler)

(7,8). In what follows, we describe results obtained by AD methods for the fitting of data from a uniaxial strain shock physics experiment with MESA1D(9), examine the accuracy of the sensitivities for a two-dimensional copper jet calculation with MESA2D(10), and outline our plans for future work.

UNIAXIAL FLYER PLATE EXPERIMENT

In this subsection we obtain sensitivities for a normal impact copper flyer plate test (11). In this experiment, a 3 mm copper flyer plate at 645 m/s strikes an 18 mm target. The pressure is measured at the center of the target. We use a Mie-Gruneisen EOS (12) and an elastic-perfectly plastic strength model to represent the copper. The values for the EOS and strength parameters are given in Table 1. The response was chosen to be

$$R = C \int_0^{4\mu s} (p_{\text{exp}} - p_{\text{calc}})^2 dt \quad (1)$$

Where C is a constant, p_{exp} is the experimental pressure, and p_{calc} is the calculated pressure. The sensitivities of this response to the initial conditions and the EOS and strength

parameters along with their definitions and nominal values are given in Table 1. We note excellent agreement between the forward and adjoint derivative results with the exception of the strength parameters that have only two to four digit agreement. The accuracy required when using the sensitivities as a gradient for an optimization process has yet to be determined.

The sensitivities listed in Table 1 provide the first gradient in a Polak-Ribiere conjugate-gradient minimization procedure (13). Subsequent gradients for the fitting process were obtained by the adjoint method. Figure 1 shows the experimental pressure trace, the pressure trace produced using the nominal parameters, and the pressure trace produced by the optimized parameters. Obtaining the slightly improved fit

to the experimental data required 16 iterations in the optimization process.

Figure 1. Experimental, nominal-parameter calculated, and optimized-parameter calculated pressure traces for the copper flyer example.

Table 1. Comparison of the copper flyer plate impact cost function (R , Eq. 1) sensitivities.

Parameter Description (Value of α_0)	$\partial R / \partial \alpha$ (ADIFOR & TAMC - Forward) *	$\partial R / \partial \alpha$ (TAMC - Adjoint) *
Initial Density (8.93 g/cm ³)	-1.0941790E-01	-1.0941789E-01
Initial Velocity (0.0645 cm/μs)	-6.9843152E-01	-6.9846815E-01
Initial Internal Energy (0 Mbar-cc/g)	-4.7696492E+00	-4.7696445E+00
Initial Stress Deviator (0 Mbar)	-1.2415942E-01	-1.2360915E-01
Shock Velocity Constant (1.489)	-2.3913351E-02	-2.3913349E-02
Sound Speed (0.3940 cm/μs)	-7.1586681E-01	-7.1586677E-01
Nominal EOS Density (8.93 g/cm ³)	1.0879440E-01	1.0879439E-01
Second Gruneisen Ratio (2.002)	-4.3998139E-04	-4.3998139E-04
Linear Artificial Viscosity Constant (0.2)	-4.9742192E-03	-4.9742184E-03
Quadratic Artificial Viscosity Constant (2.0)	-4.0174342E-04	-4.0174332E-04
Yield Stress (0.0010 Mbar)	1.4882938E-01	1.4919678E-01
Shear Modulus (0.50 Mbar)	2.3197760E-04	2.2725076E-04

* R = cost function, $R_0 = 6.1018943092660E-03$

An important issue when choosing whether to use a forward or adjoint method to determine sensitivities is the amount of computer time that each method requires. As mentioned in previous work (1,2,3), the number of parameters versus

the number of responses plays a key role in this decision. For this problem we have chosen only one response. The run times for the various methods used to obtain the results in Table 1 are listed in Table 2.

Table 2. CRAY YMP run times for a copper flyer plate problem containing 12 parameters.

ADIFOR (CPU sec.)	Direct Method (CPU sec.)	TAMC- Forward (CPU sec.)	TAMC- Adjoint (CPU sec.)
47.1	46.3	27.6	27.8

We see that for this flyer problem TAMC-Forward is the most efficient method for computing 12 sensitivities, with TAMC-Adjoint requiring slightly more time. ADIFOR and the Direct Method require approximately the same amount of computer time. The ratio of TAMC-Adjoint to Direct-Method run times would, of course, improve (decrease) if the number of parameters were increased. These runs have only recently been made and have not been examined in detail to see if further run time improvements can be implemented. We have seen in previous timing comparisons that the adjoint run times are adversely affected by storing required forward results rather than recalculating them, but we have not developed a definitive strategy for obtaining optimal computational efficiency. As we gain experience with these methods, minimization of computational time will be better understood and pursued.

JET APPLICATION

In this section we describe the application of AD techniques to a two-dimensional jet problem in which a copper bar impacts a rigid boundary as is shown in Figure 2. The bar has an initial axial velocity (v_0) of 0.7 km/s and three transverse velocity (u_0) cases: 0.0, -0.1, and -0.7 km/s respectively. For the non-zero transverse velocities a jet is formed that flows along the axis. The response of interest is the jet tip speed that is obtained by following a marker particle that is placed on axis at the right side of the copper bar as shown as a black dot in Figure 2.

Figure 2. Copper bar impacting a rigid boundary subsequently forming a jet when the transverse velocity (u_0) is non-zero; the response is the marker particle (shown as the black dot) velocity at the end of the calculation

For this example the problem parameters are the same as those listed in Table 1. The initial velocity is the axial velocity (v_0). The axial velocity was chosen because the sensitivity of the final velocity to the initial axial velocity is 1.000 for the zero transverse velocity case. This seemingly trivial result provided an excellent test of the advection-scheme adjoint code. Debugging the adjoint code produced by TAMC for the advection routines was difficult. When 1.000 was obtained for the initial velocity sensitivity, the other sensitivities agreed well with the forward results obtained by ADIFOR (which is viewed as the "correct" solution) and the Direct Method. The sensitivities produced by the adjoint code for -0.1 km/s transverse velocity agreed fairly well with ADIFOR for approximately 20 time steps but then diverged from the ADIFOR result as a function of time. It was not possible to produce reasonable sensitivities for times greater than 0.8 μ s by any method for the -0.7 km/s transverse velocity case. Examination of the computed results for this case showed that the sensitivity was proportional to the marker particle acceleration, which became unstable after 0.8 μ s. A different response choice (other than following a marker particle) will be necessary to obtain a numerically smoother characterization of the jet tip speed and stable sensitivities. We intend to explore this issue in future work.

The run times for 800 time steps are given in Table 3. What is clear from the table is that there is considerably more computation for a two-dimensional adjoint calculation. For the adjoint method to become competitive there would have to be a five-fold increase in the number of

parameters or a five-fold decrease in the two-dimensional computational overhead. While some overhead reduction is possible, it appears that problems containing many parameters represent a better application for the adjoint technique.

Table 3. Sun workstation run times for the copper jet problem with 12 parameters.

ADIFOR (CPU sec.)	Direct Method (CPU sec.)	TAMC- Adjoint (CPU sec.)
211	162	902

SUMMARY AND FUTURE WORK

In this paper, we have applied the automatic differentiation tools ADIFOR and TAMC to MESA1D and have obtained accurate sensitivities for use in an optimization (experimental data fitting) process. We have expanded our use of code-based differentiation techniques to two-dimensional problems obtaining sensitivities for a numerically-difficult jet-formation calculation. We remain confident that adjoint-method sensitivities are feasible (although difficult) to obtain and will continue to pursue this methodology in the future.

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Code Differentiation for Hydrodynamic Model Optimization

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The Analysis Exercise

$$\vec{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_N)^T$$

$$\vec{R} = (R_1, R_2, \dots, R_M)^T$$

Would like to know:

- 1. What is the sensitivity of an output Response to the input?*
- 2. To which parameters is the response most sensitive?*
- 3. What is the uncertainty of an output Response to input uncertainties?*
- 4. How can the input be tuned to obtain an optimum output Response?*

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The Sensitivity (Jacobian)

- **The sensitivity ($\frac{\partial \bar{R}}{\partial \alpha}$) can help the analysis process**
- **How is the sensitivity obtained?**
 - Direct Method - [1]
 - Forward Differential Sensitivity (DS), numerical solution of differentiated PDEs or difference equations - [2]
 - Adjoint DS, numerical solution of adjoint PDEs or difference equations - [3]
 - Code-based Manual & Automatic Differentiation (MD & AD) (ADIFOR or TAMC) - [4,5]

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[1] Direct Method

Perform the base case calculation:

Repeat "N" times:

Approximate with finite differences: $\frac{\partial R}{\partial \alpha_i} \approx \frac{(R - R_0)}{\Delta \alpha_i}$

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[4 & 5] AD & MD Basics -Forward Differentiation

- Chain Rule allows determination of R_α (the derivative of R with respect to α) from y_α & z_α
- i.e. $\frac{\partial R}{\partial \alpha_i} = \sum_{j,k} \frac{\partial R}{\partial z_k} \frac{\partial z_k}{\partial y_j} \frac{\partial y_j}{\partial \alpha_i}$ for the i^{th} component of α
- Direction indicates flow of logic for differentiation process; summing over j first, then k , results in forward mode
- The intermediate dimensionality can become very large if α is a vector of large dimension

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[4 & 5] AD & MD Basics -Adjoint Differentiation

- $\frac{\partial R}{\partial \alpha_i} = \sum_{j,k} \frac{\partial R}{\partial z_k} \frac{\partial z_k}{\partial y_j} \frac{\partial y_j}{\partial \alpha_i}$ for the i^{th} component of α
- Direction indicates flow of logic for the code and the differentiation process; summing over k first, then j , results in adjoint mode
- Dimensionality of derivatives similar to those of original code for one response

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[4] AD Tools - ADIFOR

- **ADIFOR (Automatic Differentiation of FORTRAN)**
(Argonne & Rice)
 - *Line-by-line differentiated code produced*
 - *Forward only (ADJIFOR available, but needs work for a time-stepping hydrocode)*
 - *F77 & C (called ADIC)*
 - *Some code modification necessary*
 - *Robust, but conservative dependency analysis produces less efficient code*
 - *"Correct" sensitivities*

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[4] AD Tools - TAMC

- **TAMC (Tangent-linear & Adjoint Model Compiler)**
(Max Planck Inst / MIT / JPL by R. Giering)
 - *Forward & Adjoint*
 - *Line-by-line differentiated code produced*
 - *Backward in time and through routines for adjoint*
 - *F77 (with a few F90 extensions)*
 - *Code modifications necessary (e. g. no "GO TO"s)*
 - *Dependency analysis (which needs some manual help) produces more efficient code*
 - *Check-pointing (storing of time-evolving necessary forward variables) automated*

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Example 2: Cu Flyer Parameter Optimization

Experimental Setup

Cray YMP run time for each set of 17 Sensitivities used as gradients in Optimization

ADIFOR (CPU sec.)	Direct Method (CPU sec.)	TAMC- Forward (CPU sec.)	TAMC- Adjoint (CPU sec.)
47.1	46.3	27.6	27.8

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Example 2: Cu Flyer Parameter Optimization

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Example 3: 2D Jet

Response(R) = jet tip speed

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Example 3: 2D Jet

Response(R) = jet tip speed

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Scorecard (accuracy and computational efficiency)

"2D" Run	2 Mat'l Flyer	1 Mat'l Flyer	Real Cu Flyer	Jet
Run Information				
# Cells in 2D	3 X 50	3 X 40	3 X 216	60 X 100
Timesteps	200	400	800	100
Parameters	10	17	12	17
Sun compiler	g	g	fast	fast
Direct - CPU	28.6	97.2	162.5	151.2
ADIFOR - CPU	39	119	211	197
TAMC-FTL - CPU	42	127		
TAMC-ADJ - CPU	46	109	902	812
Adjoint Results	A	A	C+	D

Grades

A	.GE. 5 digits	All	} $\frac{\partial R}{\partial \alpha_i}$
B	.GE. 3 digits	All	
C	.GE. 2 digits	Some	
D	Ballpark	Some	
F	Out to lunch		

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Summary

- Provided description of sensitivity techniques
- Forward mode better for many responses to single parameter
- Adjoint (reverse) mode better for a single response and many parameters
- Demonstrated accurate adjoint sensitivities for simple multi-material, 1D & 2D problems
- Optimization for multi-material 1D problem
- Goal is to provide a package of methods that can be used for design and evaluation purposes

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