LA-UR 91-3135

LA-UR--91-3135

DE92 000169

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

Received by OSTI

OCT 04 1991

TITLE: Lagrangian Analysis, Data Covariance, and the Impulse Time Integral

AUTHOR(S): Charles A. Forest

SUBMITTED TO: Proceedings of the APS 1991 Topical Conference

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

Los Alamos **MASTER**
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

LAGRANGIAN ANALYSIS, DATA COVARIANCE, AND THE IMPULSE TIME INTEGRAL

Charles A. FOREST

Reaction Science Group M-9, MS P952, Los Alamos National Laboratory
Los Alamos, New Mexico 87545*

Lagrangian analysis is mathematical analysis of data derived from flow experiments in which embedded gauges move with the material motion (constant Lagrangian mass-point coordinate). With sufficient data, the conservation laws of mass, momentum, and energy are applied to the data in order to construct flow-variable fields, of particle velocity, stress, density, *et cetera*. Toward this end, a new Lagrangian analysis method has been constructed, that is centered upon a function, α , that incorporates conservation of mass and momentum into its definition. Further, the existence of α allows simultaneous, consistent, least-squares fitting of surfaces to all of the flow data. The method also incorporates a novel treatment of the data covariance effects resulting from gauge-to-gauge calibration uncertainty. Analysis of a synthetic data set illustrates the method.

1. INTRODUCTION

Lagrangian analysis is directed to the study of dynamic material properties from flow experiments in which gauges (sensing elements) move with the material at constant Lagrangian (hence the name) mass-point position. The gauges are generally thin, low-mass devices embedded into a subject material and are considered to introduce no significant disturbance to the flow. The gauge response is recorded as a function of time, providing a history of particle velocity, stress, or impulse. Combined experiments or multiple gauges are used to record the material response at a number of Lagrangian positions, which allows analysis of the flow and mechanical variables over a Lagrangian space-time (h, τ) domain. Generally, each gauge is calibrated individually, and each gauge history is therefore a subset of data points with a common calibration error factor (nonzero covariance). Error factors of separate gauges are considered to be independent random variables. Finally, the time sampling is hundreds of times greater than the number of spatial positions, which results in data concentrated on a few constant- h "ribs" in the space-time domain.

The methods of Lagrangian analysis¹⁻⁶ have evolved along with the experiments, the principal change being the kind and quantity of data collected. (For a review of Lagrangian analyses, see the recent paper of Aidun and Gupta.⁶) Certainly the impetus for finding a consistent method of treating a data set of more than one flow variable came from the magnetic-impulse-velocity (MIV) gauge system developed by John Vorthman.⁴ The principal connection between impulse I and particle velocity u is the momentum conservation equation, expressed as $\partial I / \partial h = -\rho_0 u$ (ρ_0 is the initial density); this relation was used by Jerry Wackerle to connect impulse and particle velocity in treating MIV data with a pathline analysis method.⁴ My own first attempts at surface fitting of MIV data were to fit the impulse surface while simultaneously entering the particle velocity data as the partial derivative. Next, I found that the specific volume (and conservation of mass) could be added, and the impulse time-integral function, $\alpha(h, \tau)$, was defined.

As was presented in my prior paper,⁵ it is shown below that $\alpha(h, \tau)$ contains the variables of displacement, impulse, volume, particle velocity and stress as partial

derivatives with respect to h and τ . This imposes the pointwise differential and integral relations of conservation of mass and momentum upon the fitting surface with the various variables all sharing a common set of parameters. This property is particularly important to the analysis of experiments in which more than one physical variable is measured; other methods^{1-4,6} have no means to construct consistent simultaneous fitting of more than one variable. Furthermore, the function α allows the application of elastic boundary values and Rankine-Hugoniot relations to the fitting surface (also discussed below), and enables a statistical treatment of the data covariance. The last feature is a mathematical algorithm for that black art of gauge record "fudging" that is often found necessary in the Lagrangian analysis of imperfect data.

2. IMPULSE TIME INTEGRAL

The following development is taken from Reference 5, in which the function α was first defined and described.

Consider the case of one-dimensional planar flow where a shock enters undisturbed material with initial conditions of pressure = P_0 , density = ρ_0 , and particle velocity = 0. Let the shock position be $\mathcal{H}(\tau)$, with $\mathcal{H}' = U_s$, the shock velocity. Also let $\mathcal{T}(h)$, the shock arrival time, be the inverse of $\mathcal{H}(\tau)$. The conservation equations in Lagrangian coordinates are $\rho_0(\partial u/\partial \tau) = -\partial P/\partial h$, $\partial \eta/\partial \tau = -\partial u/\partial h$, and $\partial E/\partial \tau = v_0 P(\partial \eta/\partial \tau)$, where v = specific volume, $\eta = 1 - v/v_0$ = volume strain, and E = specific internal energy. Define now the function α on the Lagrangian (h, τ) domain,

$$\alpha(h, \tau) = \int_{\mathcal{T}(h)}^{\tau} d\tau' \int_h^{\mathcal{H}(\tau')} u(h', \tau') \rho_0 dh'.$$

(Note that $\rho_0 dh'$ is a mass differential.) By conservation of momentum,

$$\begin{aligned} I(h, \tau) &= \int_{\mathcal{T}(h)}^{\tau} [P(h, \tau') - P_0] d\tau' \\ &= \int_h^{\mathcal{H}(\tau)} u(h', \tau) \rho_0 dh', \end{aligned}$$

et sequentia

FIGURE 1
Impulse time-integral diagram.

where I is the impulse. Then the function α satisfies

$$\alpha(h, \tau) = \int_{\mathcal{T}(h)}^{\tau} I(h, \tau') d\tau',$$

and α is the impulse time integral. By conservation of mass,

$$\begin{aligned} \rho_0 \Delta X &= \rho_0 \int_{\mathcal{T}(h)}^{\tau} u(h, \tau') d\tau' \\ &= \int_h^{\mathcal{H}(\tau)} \eta(h', \tau) \rho_0 dh', \end{aligned}$$

where ΔX is the displacement. Then the function α satisfies

$$\alpha(h, \tau) = \int_h^{\mathcal{H}(\tau)} \Delta X \rho_0 dh',$$

and α is the displacement mass moment. Partial differentiation of α gives $\partial \alpha / \partial \tau = I$, $\partial \alpha / \partial h = -\rho_0 \Delta X$, $\partial^2 \alpha / \partial h^2 = \rho_0 \eta$, $\partial^2 \alpha / \partial h \partial \tau = -\rho_0 u$, and $\partial^2 \alpha / \partial \tau^2 = P - P_0$, as shown in Figure 1. Equality of third crossed partial derivatives yields the conservation of mass and momentum relations.

On the shock line, the integral functions α , I , and ΔX vanish. Note that appropriate differentiation of

$\Delta X(\mathcal{H}(\tau), \tau) = 0$ and $I(\mathcal{H}(\tau), \tau) = 0$ on shock line gives

$$0 = \frac{\partial^2 \alpha}{\partial h^2} U_s + \frac{\partial^2 \alpha}{\partial h \partial \tau} = \rho_0 \eta U_s - \rho_0 u$$

and

$$0 = \frac{\partial^2 \alpha}{\partial \tau \partial h} U_s + \frac{\partial^2 \alpha}{\partial \tau^2} = -\rho_0 u U_s + P - P_0,$$

the familiar Rankine-Hugoniot relations for mass and momentum.

Note here that if a mixture equation of state $P = P(\nu_0 \eta, E, w)$ applies, where w = mass fraction of reactant, then $\alpha_{\tau\tau} = P(\alpha_{hh}, E, w)$ is a partial differential relation for α . (Note: Subscripts of τ and h denote partial differentiation.)

Remark: For those interested in contour derivatives, the line derivatives of displacement and impulse on the shock (a zero contour for both) suggests consideration of general contours. Accordingly, for constant ΔX_0 and I_0 , $\Delta X(h_\Delta(\tau), \tau) = \Delta X_0$ and $I(h_I(\tau), \tau) = I_0$ give, upon differentiation, $-\eta h'_\Delta + u = 0$, and $-\rho_0 u h'_I + P - P_0 = 0$, where h_Δ and h_I are the respective contour functions. The functions ΔX and I of course can be obtained by the time integration of u and P . This represents the low-cost analysis.

3. ELASTIC IMPACT BOUNDARY

For those experiments in which the subject material is struck by a projectile that remains ideally elastic (e.g., Lucalox or Vistal) for some time interval following impact, it is possible to impose an elastic boundary constraint at the impact face. Letting $(\rho_i c_i)$ be the elastic impedance, the elastic relation for the projectile is $P - P_0 = (\rho_i c_i)(u_i - u)$, where u_i is the projectile velocity. By continuity of P and u across the impact face, the same relation applies to (P, u) of the subject material, and is a linear constraint upon $\alpha_{\tau h}$ and $\alpha_{\tau\tau}$. Note that employing an impact-face particle-velocity gauge with an elastic projectile also gives stress data.

4. SHOCK CONDITIONS

The shock line $\mathcal{H}(\tau)$ is perhaps the only curve in the (h, τ) domain that is continuous across the h -extent of the domain upon which data may be obtained. Also, because the function α has special properties on this line, it is important to impose those properties on the fitting surface.

Data for the shock curve $\mathcal{H}(\tau)$ is composed of the few (h, τ) points taken from shock arrivals at gauges, and a derivative $\mathcal{H}'(0)$ obtained by the shock match at the impact face. The result is that fitting $\mathcal{H}(\tau)$ gives fairly accurate shock position but less accurate velocity, $\mathcal{H}'(\tau)$; this situation deters the accurate determination of the shock-line particle velocity from $\mathcal{H}'(\tau) = U_s(u)$ (e.g., $U_s(u) = C + Su$) as "data" on the shock line. However, because $\mathcal{H}'(\tau)$ is at least in the neighborhood of the correct shock velocity, it may be used in the following way.

First, the zeros $\alpha_h = 0$ and $\alpha_\tau = 0$ are used as data for the fitting surface with standard deviations $\rho_0 u \sigma_{\mathcal{H}} / U_s$ and $\rho_0 u \sigma_{\mathcal{H}}$ respectively, where $\sigma_{\mathcal{H}}^2$ is the variance of $\mathcal{H}(\tau)$. Next, for any τ^* , the tangent lines to the Hugoniot functions $P - P_0 = \rho_0 u U_s(u)$ and $\eta = u / U_s(u)$ can be expanded about the particle velocity u^* , where $\mathcal{H}'(\tau^*) = U_s(u^*)$. For example, $\eta - \eta^* = (d\eta/du)^*(u - u^*)$, the differential of η at u^* . These linear expressions are then used as constraints upon α_{hh} , $\alpha_{h\tau}$, and $\alpha_{\tau\tau}$ at a sequence of points on the shock (the number of points depends on the fitting function). The constraints are near the true Hugoniot curves while not prescribing exact values as data, but do impose the Rankine-Hugoniot relations on the fitting surface.

Note that for those cases in which the initial disturbance is not a shock, but rather is a ramp wave, zeros are defined for η , u , and $P - P_0$ with the appropriate variances calculated from the variances of the first disturbance line.

5. DATA COVARIANCE

The data set for an experiment comprises subsets of data measured with various gauges, which are recorded by separate devices. Because each gauge is individually calibrated, each datum (in time) from a gauge record has the same gauge calibration error and thereby the datum error is correlated to the datum error of each in that record; the data errors are not independent. Errors of different gauges are considered independent.

Least-squares fitting of data (without constraints) is the minimization of the merit function ε , the matrix product quadratic form

$$\varepsilon = [y_i - y(x_i)]^T V^{-1} [y_i - y(x_i)],$$

with respect to parameters of $y(x)$, where y_i is the datum and $y(x_i)$ is the true value. The matrix V^{-1} is the inverse of the covariance matrix of data set $\{y_i\}$; for independent data errors, V^{-1} is the diagonal reciprocal-variance matrix, and the merit function is the familiar sum $\Sigma[y_i - y(x_i)]^2/\sigma_i^2$. For the case of gauge data, the matrix V is block diagonal with submatrices V_k where k corresponds to the k 'th gauge. The V_k matrix may be calculated from a data model. For this purpose, consider the data model for the k 'th gauge,

$$y_i = (1 + f_k) y(x_i) + \epsilon,$$

where $x = (h, \tau)$, and where f_k and ϵ are independent random variables with mean and variance $(0, \sigma_f^2)$ and $(0, \sigma_\epsilon^2)$ respectively. The f_k 's are the calibration uncertainty fractions. Then the elements of V_k are $V_k(i, j) = \sigma_\epsilon^2 \delta_{ij} + \sigma_f^2 y(x_i) y(x_j)$, where x_i and x_j are from the k 'th record. The inverse V^{-1} is also block diagonal with submatrices V_k^{-1} . The elements of V_k^{-1} are $V_k^{-1}(i, i) = (D_k - a_i^2)/(\sigma_\epsilon^2 D_k)$ for $i = j$, and $V_k^{-1}(i, j) = (-a_i a_j)/(\sigma_\epsilon^2 D_k)$ for $i \neq j$. Here $a_i = \sigma_f y(x_i)/\sigma_\epsilon$ and $D_k = 1 + \Sigma a_i^2$. This leads to the merit function $\varepsilon = \Sigma \varepsilon_k$, where ε_k is that part due to the k 'th gauge with $\varepsilon_k = \Sigma \Delta_i^2 - (\Sigma a_i \Delta_i)^2/D_k$ and $\Delta_i = (y_i - y(x_i))/\sigma_\epsilon$. Note now that the a_i are functions of the true value $y(x)$ so that the merit function is nonlinear, perhaps requiring an

iterative solution method. Further, library least-squares routines are directed to uncorrelated data, operate on the design matrix, and are not directly applicable here. However, I have found that by expanding the minimization parameter set to include the random variables $\{f_k\}$, an equivalent problem may be posed for which the standard routines that operate on the design matrix can be applied.

Consider once again the data model

$$y_i = (1 + f_k) y(x_i) + \epsilon.$$

Then, $\epsilon = y_i - y(x_i) - f_k y(x_i)$ is a random variable independent of f_k . Define the partial merit function ε_k as $\varepsilon_k = \Sigma(\epsilon/\sigma_\epsilon)^2 + (f_k/\sigma_f)^2$. Then

$$\varepsilon_k = \Sigma[(y_i - y(x_i) - f_k y(x_i))/\sigma_\epsilon]^2 + (f_k/\sigma_f)^2$$

and $\varepsilon = \Sigma \varepsilon_k$ is to be minimized with respect to the parameters of $y(x)$ and the f_k 's. Note that f_k occurs in ε_k only so that $\partial \varepsilon / \partial f_k = \partial \varepsilon_k / \partial f_k$ and that f_k has a solution in terms of $y(x)$, $(f_k/\sigma_f) = (\Sigma \Delta_i a_i)/D_k$. Substitution of this into the merit function to eliminate the f_k 's gives a merit function identical to that obtained from the covariance matrix. Therefore, solution for the f_k along with the parameters of $y(x)$ yields the same minimum and is suitable for application of the standard library routines with iteration of the a_i .

In regard to calibration error, consider an alternative data model

$$y_i = (1 + f_k)(y(x_i) + \epsilon)$$

in which true value and error ϵ are both subject to the calibration uncertainty. For f_k near zero, $1 - f_k \approx 1/(1 + f_k)$ and then $\epsilon \approx y_i - y(x_i) - f_k y_i$. Note that is similar to the first data model with $-f_k y(x_i)$ being replaced by $-f_k y_i$, which is what would be used to start an iterative solution for the first data model. In both cases the covariance effect is correctly taken into account. To scale or not to scale errors may be undecidable. Finally, the variance σ_ϵ^2 and σ_f^2 are required. σ_ϵ can be estimated by least-squares fitting the individual

records prior to fitting the field. However, σ_f must be estimated by the experimenter because it is related to the process of gauge calibration itself.

Remark: The above result is not particular to the Lagrangian analysis only, but is a general result for the given data models.

6. LAGRANGIAN ANALYSIS METHOD

To form a Lagrangian analysis method based on the α function, the properties of α must be imposed on the fitting surface. Largely, this is accomplished by entering the data into the proper derivative of the fitting surface. The functional form of the surface is arbitrary, and need only to satisfy the requirements of the optimization subroutine selected for the purpose. However, linear least squares requires a functional form that is a linear sum of functionally independent basis functions, that is, $y(h, \tau) = \sum c_i g_i(h, \tau)$, where the c_i 's are the parameters and the g_i 's are the basis functions. The basis functions may be defined on the entire domain or be defined on subdomains with continuity constraints at the common boundaries (*e.g.*, splines).

For those cases in which the elastic boundary constraint, or linearized Hugoniot constraints apply, the constraints are used to reduce the optimization parameter set. Finally, if the errors are normally distributed, the full, variance-matrix merit function gives a maximum likelihood estimate of the parameters.

The last task is defining the design matrix for the equivalent least-squares method, using the gauge uncertainty fractions, $\{f_k\}$. Consider again the partial merit function

$$\varepsilon_k = \Sigma [(y_i - y(x_i) - f_k \hat{y}_i) / \sigma_\epsilon]^2 + (f_k / \sigma_f)^2,$$

where $x_i = (h_k, \tau_i)$ and where $\hat{y}_i = y(x_i)$ or $\hat{y}_i = y_i$, depending on the data model discussed above. The sum over the points is entered as the equations

$$\Sigma c_j g_j(x_i) / \sigma_\epsilon + f_k \hat{y}_i / \sigma_\epsilon = y_i / \sigma_\epsilon,$$

where i ranges over the data set. The last term is entered as the single equation $f_k / \sigma_f = 0$. Defining such lines for all gauges thereby creates the design matrix.

After the design matrix and the constraint matrix are defined, the least-squares parameters (including the f_k 's) are solved by standard least-squares routines, which accept such input arrays. If $\hat{y}_i = y(x_i)$, an iteration is required wherein $\hat{y}_i$ is the previous estimate of the true value.

Any data set that is sufficient to define α may be used. Generally, direct data on ΔX or η is lacking. Toward that end, each particle-velocity record is time-integrated to form a corresponding displacement record, which is entered as data having the same error fraction as the velocity record.

7. SYNTHETIC EXAMPLE

A synthetic data set was calculated by James N. Johnson of Los Alamos Group T-1 with his CHARADE 1D fluid dynamics program, using the same reactive flow calculation for PBX 9404 explosive and the JTF decomposition rate model reported in Reference 8. The CHARADE output consisted of time histories of the particle velocity, specific volume, pressure, specific internal energy, and mass fraction of explosive reactant, all at six Lagrangian positions, $h = 0.5, 1.0, 1.5, 2.5, 2.5,$ and 4.5 mm from the impact face. The (Lucalox) impactor was taken as ideally elastic with an elastic impedance of $43.07 \text{ mg}/(\text{mm}^2\text{-}\mu\text{s})$.

The synthetic data for the analysis test were the CHARADE calculations of particle velocity and impulse (obtained by the time integration of the CHARADE pressure), modified to simulate errors such as might arise with experimental data. For this modification, the CHARADE histories were scaled per gauge but no noise in time was added. Scale factors for the six velocity histories were 1.03, 1.03, 1.03, 0.97, 0.97, and 0.97, respectively. The impulse scale factors were 1.02, 0.98, 1.02, 0.98, 1.02, and 1.02, respectively. The particle-velocity scale factors were purposely biased with

FIGURE 2

Impulse histories at the gauge locations. The points are the synthetic data and the solid lines are the least-squares α -function derivative evaluations.

FIGURE 4

Volume strain histories at the gauge locations. The points are the CHARADE calculation (the true function) and the solid lines least-squares α -function derivative evaluations.

FIGURE 3

Particle-velocity histories at the gauge locations. The points are the synthetic data and the solid lines are the least-squares α -function derivative evaluations.

FIGURE 5

Particle-velocity histories at the gauge locations. The symbols and solid lines are as in Figure 4.

the first three high and the second three low; the impulse factors were selected to be ± 2 per cent by coin toss. Tests on the underlying calculation shows it to be a one to two per cent accurate calculation, so the exact error is unknown.

The example is illustrated in Figures 2 and 3. The elastic-impact-boundary and shock-line constructs were used for the analysis. The fitting surface $y(h, \tau)$ was a Taylor polynomial of degree nine on each of two sub-domains, with continuity to the fourth partial derivatives at the common boundary at $h = 2.0$. Also, some smoothing on the derivative $\eta_{hh\tau} = \alpha_{hhhh\tau}$ was imposed throughout the computational domain.

8. RESULTS AND DISCUSSION

The results are shown in Figure 4 through 7, in which the fitted α -surface lines are compared to the underlying true point values—the CHARADE calculation with no rescaling. Most sensitive of these to data error are the volume strain and internal energy, because the volume time rate of change is the particle-velocity gradient. Energy is not one of the α -function partial derivatives, but it may be calculated by integration of $\mathcal{E}_\tau = v_0 P \eta_\tau$ over the time interval $(\tau_s(h), \tau)$, starting at $\tau = \tau_s$ with the shock-jump energy. Two features of the analysis tend to compensate for the gauge-to-gauge error, the shock-line Hugoniot relations and the statistical gauge error fractions; together, they have produced a fitting surface well in agreement with the CHARADE calculation. Omission of either degrades the quality of the fitting surface.

Graphical output from the analyses also includes snapshots, depicting the flow variables plotted against distance- h at fixed times. As shown in Figure 8, these graphs show that the gauge-position data are smoothly connected.

A final point: The fitting surface clearly misses the input data, as seen in Figure 2, but agrees favorably with the true function, the CHARADE calculation. This reminds us that the main purpose of the least-squares

FIGURE 6

Pressure histories at the gauge locations. The symbols and solid lines are as in Figure 4.

FIGURE 7

Internal energy histories at the gauge locations. The points are the CHARADE calculation (the true function) and the solid lines are integrals of $\mathcal{E}_\tau = v_0 P \eta_\tau$, which are evaluated from the α function.

FIGURE 8

Six snapshots of particle velocity over the Lagrangian domain 0.0 to 5.0 mm, at 0.3- μ s time intervals, starting at $\tau = 0.3 \mu$ s.

fitting of data is not to simply conform to the data, but rather is to estimate the true function. In this case, this purpose is aided considerably by the consistency imposed by the α function and by the application of an appropriate data model.

ACKNOWLEDGEMENTS

I wish to thank Jerry Wackerle for his considerable help with the manuscript and for his continued interest and support in Lagrangian analysis over many years. Also, I thank Richard Beckman of Los Alamos Group A-1 for his discussions of statistical matters.

REFERENCES

1. R. Fowles and R. F. Williams, *J. Appl. Phys.* **41** (1970) 360.
2. D. E. Grady, *J. Geophys. Res.* **78** (1973) 1299.
3. L. Seaman, *J. Appl. Phys.* **45** (1974) 4303.
4. J. E. Vorthman and J. D. Wackerle in "Shock Waves in Condensed Matter - 1983," J. R. Asay, R. A. Graham and G. K. Straub, Ed. (North-Holland, 1984)
5. C. A. Forest in "Shock Waves in Condensed Matter - 1989," S. C. Schmidt, J. N. Johnson and L. W. Davison, Ed. (North-Holland, 1990)
6. J. B. Aidun and Y. M. Gupta, *J. Appl. Phys.* **69** (1991) 6998.
7. F. A. Graybill, "An Introduction to Linear Statistical Models," (McGraw-Hill, 1961) pp. 113-117
8. J. N. Johnson, P. K. Tang and C. A. Forest, *J. Appl. Phys.* **57** (1970) 4323.

END

**DATE
FILMED**

10/28/91

11