Analytical Sensitivity Methods for ODEs
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These notes introduce a few of the ideas and concepts associated with sensitivity analysis for algebraic and ordinary differential equations. By sensitivity I mean what are the effects of changes in the numerical values of the parameters in a system of equations relative to a response function of interest. The response function can take any mathematical form, but I will focus on the values of the dependent variables of the equation system.

Summary

Mathematical methods for identification of, and quantifying the importance of, parameters in complex mathematical models of physical phenomena and processes are discussed. These methods are useful for calculating the sensitivity of the models and numerical solution methods embedded into computer software to the parameters associated with the application areas for the computer codes. Sensitivity investigations, a form of 'what if' analysis, are an integral part of the application of computer software. Generally we are almost always asking a question like, what is the effect on the calculated result (a system response) of changes in the parameters of the model equations and application. The mathematical methods discussed here are designed to provide an answer and additionally are also useful in uncertainly, parameter estimation, and optimization analyses.

Of the several methods available for calculating the sensitivity, the discrete adjoint sensitivity method (DASM) is the one that is most applicable, from both theoretical and practical aspects, to models and solution methods already coded into software. From the theoretical view, the DASM methodology is based on exactly the model equations and solutions methods used in the software, which are generally finite difference equation (FDE) approximations to the continuous equations. The adjoint approach also allows efficient investigations into alternative response functions and in particular very efficient investigations of many parameters for a given response. From the practical viewpoint, especially when implicit numerical solution methods are used, the amount of additional coding needed for the sensitivity methodology is relatively small. Finally, the solutions for the sensitivities are very low-cost calculations.

Some of the benefits expected from applications of analytical sensitivity analysis methods to models and software are as follows. Analytical sensitivity analysis, especially the discrete adjoint method applied to finite-difference equations, can be used to achieve a significant reduction in the number of computer runs needed to complete application analyses. Analytical sensitivity analysis is also useful for the case of determination and optimization of model and correlation parameters from experimental data when models embedded into computer codes are used as the method of finding the parameters. Application of sensitivity analyses will significantly improve the objectivity and efficiency of model and correlation development.

Introduction and Background

Identification of, and quantifying the importance of, parameters in complex mathematical models of physical phenomena and processes is an integral part of the application of computer software. Two kinds of parameters are introduced into almost all mathematical models of physical phenomena and engineering equipment: those that are well-based theory, and those of a more empirical, or heuristic nature. The former kind of parameter includes equation-of-state and thermophysical and transport properties of materials, for examples. And although these are well-founded in theory, the exact value might be uncertain for a variety of reasons. The second kind of parameter is associated with engineering models and empirical correlations of physical processes. The numerical value of parameters in the correlations, or even the form of the correlating functions, might be uncertain due to the nature of engineering models and correlations.

Additional parameters of interest are introduced by the use of software in analyses. The geometry of the equipment and systems that are the object of applications of the software is generally well-established. Sometimes, however, the effects of changes in the geometry on the results of an analysis might be of interest. Finally, the continuous equations are usually not solved by the software. Approximate solutions to discrete finite-difference approximations to the continuous equations are usually solved in the software. The effects of changes in parameters associated with finite-difference methods on the solution are usually of interest. The effects of changes in the numerical values of the discrete temporal and spatial increments, and stopping criteria for iterative methods, for examples, are generally investigated.

Questions almost always arise concerning which of the many parameters in the models and methods are the most important and what are the effects of the uncertainty of the numerical values of the important parameters relative to some calculated response of interest. The responses of interest range for the local-instantaneous values of the principal dependent variables, to auxiliary calculations of quantities of interest, to integral functionals of the dependent variables, to global functionals of all the models and methods in the code and an entire calculations. A general notion of a response function will be given below in these notes.

Some examples of local-instantaneous values of the principal dependent variables are the velocity components, pressure, and temperature at specific points in the phase space for the problem. Some examples of integral functionals of the dependent variables are the mass flow rate through and pressure drop across a section of flow channel and the total deposition of a solid onto the wall of the channel an example of an auxiliary calculation is a critical heat flux model or correlation which uses information based on the dependent variables. engineering software generally has many such auxiliary algebraic calculations that depend on the solution of the basic model equations. A supra-global functional might be simply the value of the temperature alone independent of its location in phase space. Other examples of responses are associated with each different model, method, and code and the application areas for the software.

In the practice of everyday application of software to analyses of systems and processes, only a single run of the code is almost never sufficient because of the issues of uncertainty of numerical values of the parameters and their importance relative to a response of interest. Various methods have been developed to try to simplify the determination of the sensitivity of the response of models and methods to the parameters. Response surface methodology is a classic example. More likely, however, the usual practice is to execute the code with several different values of the parameters in order to cover the expected range of values. that is, direct re-calculation of the application. This approach must be carried out for each individual application and associated response in order to both identify the important parameters and then to quantify the effects of changes in these on the response. For even the most straightforward physical processes, limited number of responses, and a reasonable number of parameters, the number of direct re-calculations can seem to grow without bounds. The number of re-calculations seems to get to be very large for the case of finding the parameters of a model and correlation from experimental data and for optimization problems.

Analytical sensitivity analysis (ASA), the nomenclature for a general approach to the problem, has been developed to significantly improve of the state of affairs outlined above. Citations in the literature to original development of ASA usually cite [6-1., 6-2., and 6-3.] The methodology was probably first known as differential sensitivity analysis (DSA), a method in which ordinary differential equations for the sensitivity of the response to changes in parameters were derived. Within DSA a few variations have been developed primarily to increase the efficiency of ASA relative to computer utilization because the number of equations that must be solved, for each response, is generally many times the number of equations in the original model.

Much of the early development of ASA was associated with models based on ordinary differential equations. A resurgence of interest in DSA in the 1970s and 1980s was lead by Cacuci, Oblow and colleagues at the Oak Ridge National Laboratory (ORNL); [6-7. through 6-19.]. A significant generalization of the theoretical foundation of the methodology was an important result for the ORNL work, the relationship between sensitivity and optimization being developed in [6-20]. A large number of applications in many application areas are discussed in the reports and papers listed in [6.21. through 6-41.] in Section 6.0 References.

Recently the focus has been on development of analytical sensitivity analysis methods for discrete finite-difference approximations to the continuous equations. For a variety of reasons the finite-difference equations, and the associated numerical solution do not always accurately reflect the exact nature of the continuous equations for which they are approximations. Application of ASA directly to the actual discrete equations in the code provides more nearly accurate representations of the sensitivity properties of the mathematical models.

Applications of ASA to algebraic finite-difference equations which are a part of the entire model-equation system have been implemented into a version of the RELAP5 [6-42., 6-43.] code. Sensitivity coefficients for the equation-of-state representation was investigated in RELAP5. ASA was applied to the finite-difference representations of the continuous equations in the CATHARE [6-44., through 6-48.] thermal-hydraulic code. the discrete adjoint sensitivity method (DASM) is used in CATHARE.

The remainder of these notes is organized as follows. A first specification of the sensitivity problem is given in next Section, and some of the methods that have been used to implement solutions to the problem are introduced. Following that introduction, some simple example problems are used to introduce and illustrate ASA.

A few words about the list of references. I have not updated this list for several years. For development of theoretical aspects a Google Scholar search for D. G. Cacuci (or Dan Cacuci) should prove fruitful. Cacuci and colleagues have also been heavily involved in large-scale applications of the theoretical aspects. Google Scholar searches for L. Petzold (or Linda Petzold) will likewise yield significant results. You can also check her Web site at the University of California at Santa Barbara. Professor has many of here papers and reports available for download. She and her colleagues also provide software in which the methods have been implemented.

A Definition Of The Sensitivity Problem

Various notations are used in the literature for the sensitivity problem, some arising from different mathematical basis, ODEs, DAEs, PDEs, and FDEs, and different application areas. A straightforward nomenclature is associated with DAEs and ODEs, the latter being a special case of the former, for which the response is taken to be the dependent variables themselves. Pure PDEs, such as encountered in continuum-mechanic type applications (pure CFD and elastic displacements in solids) [6-39., 6-40], in which the response is again usually the dependent variables, is the next level of development. Most engineering models and computer codes and applications, however, present a more general setting, being comprised of complex basic equations, almost all of which have algebraic modeling in them, and several analysis objectives.

The sensitivity problem for the ODE case, the setting for almost all the original developments in the field, will be briefly outlined first. The underlying methodology, however, can be applied to any equations; algebraic, differential, either linear or non-linear. The discrete adjoint sensitivity method which is the focus of the notes, for example, is applied to very large systems of the non-linear algebraic equations.

Ordinary Differential Equations (ODEs)

A system of first-order ODEs can be represented by

$$\frac{d}{dt}\underset{\sim}{\mathbf{Y}}\left(t,\underset{\sim}{\mathbf{P}}\right)=\underset{\sim}{\Im}\left(\underset{\sim}{\mathbf{Y}},t;\underset{\sim}{\mathbf{P}}\right) \tag{1.1}$$

where $\underset{\sim}{\mathbf{Y}}\left(t,\underset{\sim}{\mathbf{P}}\right)$ is the vector of an NY-dimension vector of dependent variables

$$\underset{\sim}{\mathbf{Y}}=\left(Y_1,Y_2,\ldots,Y_{NY}\right) \tag{1.2}$$

with initial conditions

$$\underset{\sim}{\mathbf{Y}}\left(0,\underset{\sim}{\mathbf{P}}\right)=\underset{\sim}{\mathbf{Y}}^0\left(\underset{\sim}{\mathbf{P}}^{\mathbf{0}}\right) \tag{1.3}$$

and $\underset{\sim}{\mathbf{P}}$ is an NP-dimension constant vector of specified model parameters for the problem

$$\underset{\sim}{\mathbf{P}} = \left(P_1, P_2, \ldots, P_{NP}\right) \tag{1.4}$$

and the left-hand side of Eq. (1.1) has been written to indicate that the solutions for the system are functions of the parameters. A first-order system has been used for convenience only, any system of ODEs can be handled.

The sensitivity of the j^{th} dependent variable with respect to changes in the i^{th} parameter is

$$S_{ij} = \frac{\partial Y_j}{\partial P_i} \tag{1.5}$$

Frequently the sensitivity coefficients are normalized in the form

$$\overline{S}_{ij} = \frac{P_i^0}{Y_j^0} \frac{\partial Y_j}{\partial P_i} \tag{1.6}$$

where P_i^0 and Y_j^0 are appropriate values for the parameter and dependent variable, respectively, such as steady-state or boundary initial values.

Applying the definition of the sensitivity coefficient Eq. (1.5), to the ODEs of Eq. (1.1) gives the system of equations

$$\frac{d}{dt} \frac{\partial Y_j}{\partial P_i} = \left(\frac{\partial \Im_i}{\partial Y_j} \right) \frac{\partial Y_j}{\partial P_i} + \frac{\partial \Im_j}{\partial P_i} \tag{1.7}$$

or

$$\frac{d}{dt} \underset{\sim}{\mathbf{S}} = \underset{\sim}{\mathbf{J}} \underset{\sim}{\mathbf{S}} + \frac{\partial}{\partial \underset{\sim}{P}} \underset{\sim}{\Im} \tag{1.8}$$

The Jacobian, $\underset{\sim}{\mathbf{J}}$, will play an important role in the discrete adjoint sensitivity analysis method, especially for computer codes based on implicit numerical solution methods. The initial conditions for the sensitivity equations are

$$\underset{\sim}{\mathbf{S}}(0) = 0 \tag{1.9}$$

Equation (1.8) represents *NY* x *NP* equations that must be solved in addition to the *NY* dependent variables for the original system, giving a total of *NY* (*NP* +1) ODEs. Note that the number of equations can easily out-number those for the original system.

Some important properties of Eqs. (1.8) for the sensitivity coefficients are, (1) the equations are linear, (2) the equations for the sensitivity coefficients do not feed back into the original equations system, and (3) the Jacobian on the right-hand side of the equations is the same as for implicit solution methods applied to the original system.

In the above development, the sensitivity coefficients for the original dependent variables to changes in the problem parameters were obtained. Sensitivity coefficients for other quantities associated with the original problem can be equally used. Such calculated responses, also called objective functions in other applications, can be any integral, differential, or algebraic function (linear or nonlinear), or solution functional for the problem.

The solution methodology chosen for the sensitivity problem is influenced greatly by the number of responses associated with an application and the number of important parameters for the response and the problem. Analytical sensitivity analysis can be used to both identify the important parameters and determine the effects of changes in all parameters on the responses of interest.

The objective of sensitivity analysis is to determine the changes in a system response of interest for the problem to changes in the parameters. Almost all results calculated by computer codes can be represented in the integral form

$$R\left(\left(\underset{\sim}{\mathbf{Y}}(\underset{\sim}{\chi}\right),\underset{\sim}{\mathbf{P}}\left(\underset{\sim}{\chi}\right)\right)=\int_{\Omega} F\left[\left(\underset{\sim}{\mathbf{Y}}(\underset{\sim}{\chi}\right),\underset{\sim}{\mathbf{P}}\left(\underset{\sim}{\chi}\right)\right]d\omega \tag{1.10}$$

where Ω represents integration over phase space for the problem. Equation (1.10) can be used to represent either instantaneous or time-averaged values of the dependent variables. Taking the case of phase space comprised of time and one space dimension, x,

$$F\left[\left(\underset{\sim}{\mathbf{Y}}(\underset{\sim}{\chi}\right),\underset{\sim}{\mathbf{P}}\left(\underset{\sim}{\chi}\right)\right]=\delta_{ij}\delta\left(s-s_1\right)\delta\left(\tau-\tau_1\right)Y_k\left(s,\tau\right) \tag{1.11}$$

in Eq. (1.10) for example, where δ_{ij} represents the Kronecker-delta function and $\delta\left(s-s_1\right)$ and $\delta\left(\tau-\tau_1\right)$ are the Dirac-delta function gives the instantaneous value of the k^{th} dependent variable at location x_1 and time t_1 in phase space as the response.

$$R=Y_k\left(s_1,t_1\right) \tag{1.12}$$

Space-time averages of the dependent variables are handled in the same way. For applications to systems of non-linear algebraic equations which arise from finite-difference approximations to continuous equations, the response of interest might be the local-instantaneous value of a dependent variable and the parameters might be quantities associated with the numerical methods such as the discrete increments in the phase-space independent variables.

3.3 Nomenclature for Implementation of ASA

Several methods for implementing ASA methodology into computer software have been developed and these have specific names attached to them. A brief review of the names is given here.

Direct Re-calculation. The classic method for performing sensitivity studies has been to change the parameter of interest and re-do the entire calculation. The effects of every parameter of interest for every response of interest must be determined by re-calculating the entire original problem several times. This method is very computer-time and labor intensive because of the very large number of parameters and somewhat large number of system-responses that generally arise in most engineering problems. The direct re-calculation method is the least efficient of all methods. If the original problem is non-linear, as very frequently the case for engineering analyses, computer CPU costs can be quite large.

For a single response and few important parameters this method can be effective relative to the costs of putting a formal methodology into a computer code. Generally because of the evolutionary nature of engineering software, in which new applications and analyses are identified as a function of time, we frequently find that implementing a formal methodology into the software might have proven to be cost effective in the long run.

The vast majority of sensitivity analyses for large complex engineering problems continue to use the direct re-calculation method.

Direct Analytical Sensitivity Analysis (Forward Method). For only a few responses and a few parameters the direct method is a good choice. the solution methodology is basically to solve the sensitivity equations, such as Eqs. (3-8), at the same time that the original system is solved. Almost all the original methods, especially for systems of ODEs, involved variations on this approach. Recently the focus for ODEs has been on efficient direct methods. Many of the large number of convenient, user-friendly, off-the-shelf software packages for ODE solvers have been modified to incorporate this approach to the sensitivity problem. For many of the implementations into standard ODE packages the original dependent variables are taken as the response of interest.

Additionally, the direct method was an initial focus method for large, complex engineering software. The enormous problem facing implementation into such computer codes, especially for legacy codes, was the lack of the Jacobian, see Eq. (3-8), in the codes. A small cottage industry evolved around devising a methodology to obtain the Jacobian from the (awful) fortran coding in existing software through automated differentiation of the model equations as coded into fortran; [6-50.] through [6-55.]. For system-analysis codes such as we deal, and live with, little success has been attained. Recently, the focus has shifted to re-engineering the legacy software to prepare it for automated differentiation with software.

Leap Frog Analytical Sensitivity Analysis (A Direct Method). This is an implementation of the direct method in which the solution for the sensitivities is interlaced with the solution for the original state variables. Frequently seen in off-the-shelf solvers for systems of ODEs and differential-algebraic equations (DAEs). The ODESSL code [6-32. and 6-33.] was an early implementation of the method. Recent work on these systems has been given by Petzold and her colleagues [6-56. through 6-65.], including modifications of the DASSL and DASPK codes to handle the sensitivity analysis in an efficient manner. Some of these standard packages have also been modified to handle the case of a response function that is more general than simply the original dependent variables.

Adjoint Analytical Sensitivity Analysis (Backward Method). For a few responses and a large number of parameters, generally the class on analyses of interest in many engineering calculations, the adjoint method is a good choice. additionally, frequently in engineering calculations the response is a solution functional or global or supra-global functionals, so that the number of truly important parameters is usually greatly reduced. the adjoint approach is somewhat easily implemented because the equation system for the sensitivity coefficients is linear. The base computer code in which the original problem is solved, however, must be modified.

Following the calculation of the adjoint functions, additional parameters for a given response can be very easily, and cheaply, investigated. In particular, the original model equations do not need to be solved over again so long as the response does not change. Additional responses having different functional dependencies, however, require additional calculations.

Discrete Adjoint Sensitivity Analysis Method. The discrete adjoint sensitivity analysis method is especially suited for large and complex computer models and codes that have already been developed and in use. Additionally, the discrete adjoint method has all the advantages of the continuous adjoint method for investigations of large equation systems with large numbers of parameters. The analytical sensitivity analysis methodology for systems of continuous equations can be applied also to the systems of algebraic equations which arise from finite-difference approximations used for numerical solution methods. This subject is discussed in the following paragraphs.

The sensitivity of dependent variables to changes in the parameters in the discrete finite-difference space of numerical solution methods is discussed in the following paragraphs. An objective is to demonstrate that if numerical solution methods are used to get solutions, the sensitivity analysis must be conducted with the discrete finite-difference equations.

For any number of reasons the finite difference equations are not exactly equal to the original continuous equations. The donor-cell approximation applied to convective flux terms is one good example. Additionally, really accurate resolution of the local-instantaneous values of the dependent variables in phase space is not always an objective in engineering applications. Instead, engineering applications usually focus on solution functionals and global functionals in contrast to local -instantaneous values of the basic dependent variables. A solution functional can be represented by an integration over some part of the phase space for the problem.

A global functional might be the maximum or minimum value of a state variable without regard to its location in phase space. Calculation of the sensitivity of the response within the framework of discrete finite difference equations is not exactly equal to that for the continuous equations, even if the latter could be carried out successfully.

Application of analytical sensitivity analysis to the discrete finite difference equations leads to the adjoint formulation for the sensitivity problem. Having the adjoint functions allows straightforward evaluation of both different responses and different parameters for the responses. An important consideration is that the Jacobian associated with implicit numerical methods, which is already calculated in may computer codes, is an integral part of the sensitivity analysis of the discrete equations.

Finally, and maybe the most important, note the following properties of the adjoint analytical sensitivity analysis methodology.

1. The equations for the sensitivity of the response function are linear and are thus very cheap to solve relative to CPU time, and many well-established, proved-to-work solution methods are available.

2. The sensitivity of the response function needs the solution of the discrete equations, but the discrete equations for the original problem are not coupled to the sensitivity equations.

3. Once the coefficient matrix for the sensitivity of the response function is determined, the sensitivity of the response function to changes in other parameters is only a matter of substituting additional right-hand sides into the solution.

4. The solution for the sensitivity of the response function can be done all at once at the end of a calculations using stored coefficient matrices and solution vectors for the dependent variables for the original problem.

A few Simple Examples

A couple of introductory examples are discussed in the following just to show the basics of the theory and application process for analytical sensitivity analysis methodology. three examples are given; (1) a single equation with a single parameter, (2) a single equation with several parameters, and (3) a system of two coupled equations with several parameters. The first two examples are used to illustrate that the theory outlined above produces correct results. The third example is more closely related to engineering applications than the first two. Each is discussed in turn below, starting with the most simple.

Startup of Fluid Motion

The first example is a single equation with a single parameter. The equation and parameter are chosen so that a complete analytical solution is possible and complete understanding of the results is achieved.

The model equation is

$$\frac{dy}{dt} = 1 - \tau y \tag{1.13}$$

with the initial condition

$$y(0) = 0 \tag{1.14}$$

Equation (41.13) represents a simplified model of the startup of motion of a fluid in a pipe, or an object falling under the action of gravity, for which the motion is opposed by forces proportional to the speed of the fluid or object. In the early stages of the motion, the speed is dominated by the inertia, and as the final equilibrium state is approached the forces and the driving potential are in balance.

We want to determine how the solution for the dependent variable, the speed, is a function of the changes in the parameter, τ, which has all the physical properties contained in it. The sensitivity for this problem can be defined

$$S = \frac{dy}{d\tau} \tag{1.15}$$

That is, for this simple example the response function is the dependent variable itself. More general cases will be considered later in these notes.

The analytical solution for Eq. (1.13) with boundary condition (1.14) is

$$y(t;\tau) = \frac{1}{\tau}\left(1 - e^{-\tau t}\right) \tag{1.16}$$

A plot of this solution for two values of the parameter is shown in Figure 1 nearby which shows that as τ increases the final equilibrium value for y decreases.

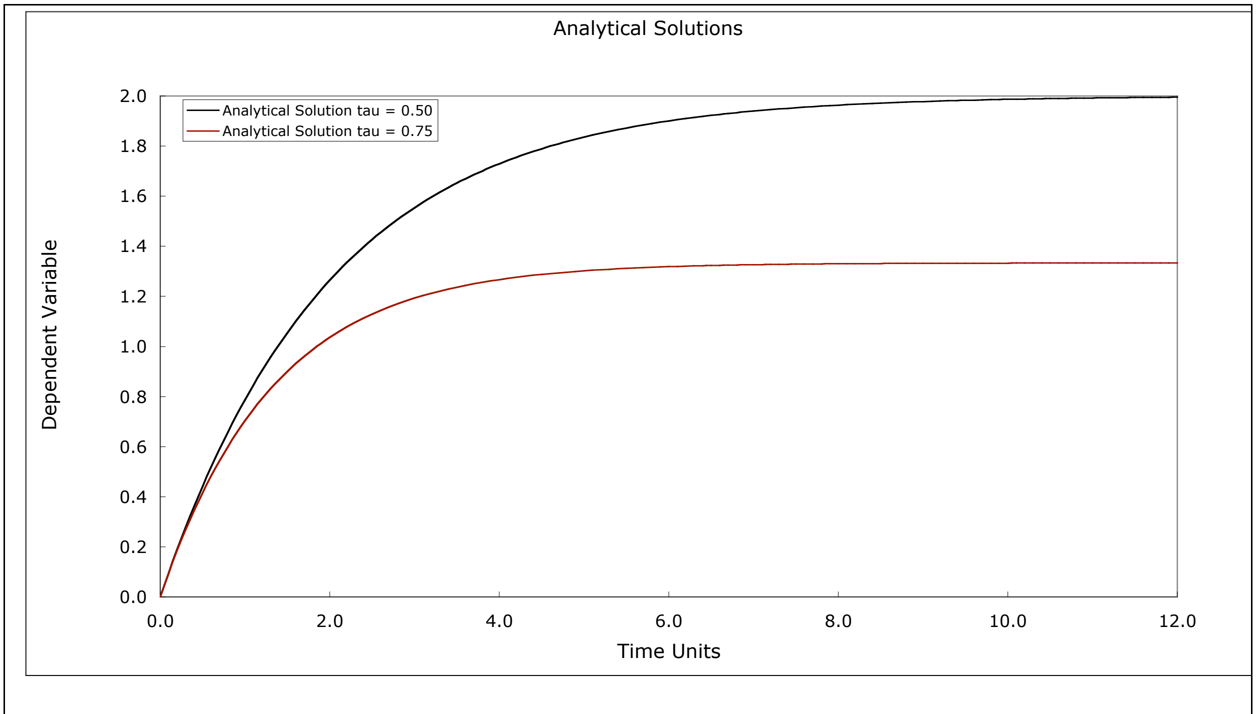

Figure 1. Analytical solution for fluid startup for two values of the time constant.

The steady state final equilibrium for y is

$$y_{ss} = 1/\tau \tag{1.17}$$

The sensitivity of Eq. (1.15) can be normalized to the final equilibrium value of the dependent variable as

$$\hat{S} = \frac{\tau}{y_{ss}} \frac{dy}{d\tau} \tag{1.18}$$

which, using Eq. (1.17), gives

$$\hat{S} = \tau^2 \frac{dy}{d\tau} \tag{1.19}$$

The analytical solution for the sensitivity coefficient of Eq. (1.19) is obtained by use of the solution given by Eq. (1.16). Taking the derivative of the latter equation and putting the results into the former gives

$$\hat{S} = \tau^2 \left(\frac{t}{\tau} e^{-\tau t} - \frac{1}{\tau^2} \left(1 - e^{-\tau t} \right) \right) \tag{1.20}$$

or

$$\hat{S} = \left(e^{-\tau t} - 1 + \tau t e^{-\tau t}\right) = e^{-\tau t}\left(1 + \tau t\right) - 1 \tag{1.21}$$

A plot of Eq. (1.21) is given in Figure 2 nearby

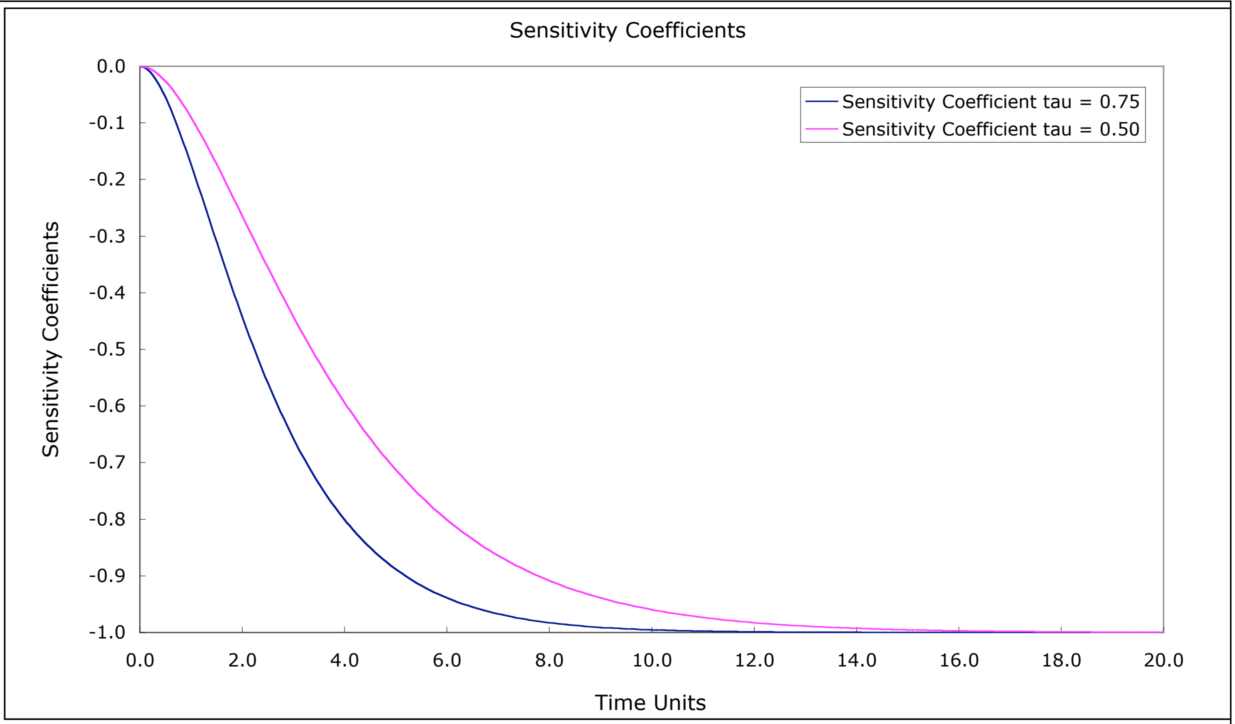

Figure 2. Sensitivity coefficients for the fluid start-up problem.

Equation (1.21) and the plot in Figure 2 show that at small values of the independent variable, the sensitivity coefficient is small and at large values the sensitivity coefficient approaches

$$\hat{S} \cong -1 \tag{1.22}$$

When the parameter is increased, the dependent variable decreases.

These results indicate that at small values of the time the solution for the dependent variable is not a strong function of the parameter and that at larger values the solution is inversely proportional to the value of the parameter. The latter result is in complete agreement with the analytical solution of Eq. (1.17). The former result can be illustrated by the approximate form of Eq. (1.13) for small values of y

$$\frac{dy}{dt} = 1 \tag{1.23}$$

for which the solution is $y = t$ and is the early-time responses shown in the first figure, Figure 1, above.
Physically, the early-time response is controlled by the inertia and the later time response is controlled by the resistance to motion.

Another Simple Example
The Lorenz system from 1963 will be used to further illustrate the concepts. The Lorenz system is

$$\frac{dX}{dt} = -PrX + PrY$$
$$\frac{dY}{dt} = -Y + RaX - XZ \tag{1.24}$$
and
$$\frac{dZ}{dt} = -bZ + XY$$

Analytical sensitivity methods are based on recognizing that the dependent variables *X*, *Y*, and *Z* are functions of the parameters in addition to the independent variable, t. The parameters are the Prandtl number, *Pr*, the Rayleigh number ratio, *Ra*, and the geometric factor, *b*. Thus we can write

$$\begin{aligned} X &= X(t : Pr, Ra, b) \\ Y &= Y(t : Pr, Ra, b) \\ Z &= Z(t : Pr, Ra, b) \end{aligned} \tag{1.25}$$

where the distinction between the value of the function and the function itself has been ignored; not a very sound practice, but used almost universally.

If the instantaneous values of the dependent variables are taken to be the response functions of interest, its variation as the parameters are varied, the sensitivity with respect to changes in the parameters, can be written, for example for *X* as

$$S_{X,\mathrm{Pr}} = \frac{\partial X}{\partial Pr} \tag{1.26}$$

and likewise for the other parameters and other dependent variables. Applying the definition to the equation for *X*, for example gives

$$\frac{dS_{X,Pr}}{dt} = -Pr\frac{\partial X}{\partial Pr} - X + Pr\frac{\partial Y}{\partial Pr} + Y \tag{1.27}$$

or

$$\frac{dS_{X,Pr}}{dt} = -PrS_{X,Pr} - X + PrS_{Y,Pr} + Y \tag{1.28}$$

This straight-forward process is applied to each equation for each parameter and the system of nine additional equations is obtained. I'm not going to repeat all the additional equations in these notes. Maybe they will be in an appendix to appear later.

We get a bunch of them, and the new equations are coupled to the original system, but the new equations will always be linear in the sensitivities, and there is no coupling back to the equations of the original system. The many variations in analytical sensitivity analysis arise from consideration of how best to solve the new equation system. The present example is not too bad in this regard; 12 ODEs with today's desk-top computers do not present computational limitations. This would not be the case if the original system was comprised of a large number of equations, say finite-difference approximations, and many parameters. The new complete system would be quite large. But even for large original systems, if only the sensitivity of a single response function with respect to a small number of parameters was of interest, the new system would not be too large.

For these notes, the new equations are simply appended to the original system and solved by the same method at the same time that the solution for the original system is calculated; a direct analytical sensitivity method

Because the sensitivities all have different units, direct comparisons cannot be carried out. The sensitivities are usually normalized in order to avoid this problem. Then, Eq. (1.26) is written

$$\hat{S}_{X,\mathrm{Pr}} = \frac{Pr_0}{X_0}\frac{\partial X}{\partial Pr} \tag{1.29}$$

where Pr_0 and X_0 are reference values for the parameter and dependent variable, respectively. For the present system, we look at the steady-state form and solution for reference values for the dependent variables. A trivial solution is (*X*, *Y*, *Z*) = (0, 0, 0). The non-trivial steady-state solutions are

$$\begin{aligned} X &= \sqrt{b(Ra-1)} \\ Y &= \sqrt{b(Ra-1)} \\ Z &= Ra - 1 \end{aligned} \tag{1.30}$$

The case of *Ra*=1 is a special case because *Ra* is the ratio of the Rayleigh number to the critical Rayleigh number. Note that the solutions are not functions of *Pr*. These solutions, and the values of the parameters used for each case, will be used to normalize the sensitivity coefficients.

The steady-state sensitivities are obtained by straight-forward application of the definition to the steady-state solutions of Eqs. (1.30). This procedure gives

$$\frac{\partial X}{\partial Pr} = 0$$
$$\frac{\partial X}{\partial Ra} = \frac{b}{2\sqrt{b(Ra-1)}} \qquad (1.31)$$
$$\frac{\partial X}{\partial b} = \frac{\sqrt{b(Ra-1)}}{2b}$$

for the X dependent variable,

$$\frac{\partial Y}{\partial Pr} = 0$$
$$\frac{\partial Y}{\partial Ra} = \frac{b}{2\sqrt{b(Ra-1)}} \qquad (1.32)$$
$$\frac{\partial Y}{\partial b} = \frac{\sqrt{b(Ra-1)}}{2b}$$

for the Y dependent variable, and

$$\frac{\partial Z}{\partial Pr} = 0$$
$$\frac{\partial Z}{\partial Ra} = 1 \qquad (1.33)$$
$$\frac{\partial Z}{\partial b} = 0$$

for the Z dependent variable.

These sensitivities are easily normalized with the steady-state solutions of Eq. (1.30). As an example, the second of Eqs. (1.31) becomes

$$\frac{Ra_0}{X_0}\frac{\partial X}{\partial Ra} = \frac{\partial \overline{X}}{\partial \overline{Ra}} = \frac{\sqrt{b}}{2\sqrt{Ra-1}}\frac{\sqrt{b}}{\sqrt{b}}\frac{Ra_0}{\sqrt{b(Ra-1)}}$$
or $\qquad (1.34)$
$$\left(\overline{\frac{\partial X}{\partial Ra}}\right)_0 = \frac{Ra_0}{2(Ra_0-1)}$$

where the notation on the left-hand side of the last equation is the dimensionless sensitivity of X with Ra; a short-hand notation that will save lots o equation processing. The last of Eq. (1.31) becomes

$$\left(\frac{\partial X}{\partial b}\right)_0 = \frac{1}{2} \qquad (1.35)$$

The same procedure can be applied to the other sensitivities of Eqs. (1.32) and (1.33). The results are not reported here, but they might appear in an Appendix at a later time.

Some Calculated Results

If the values of the parameters in the Lorenz system are such that the solution of the original system does not enter the chaotic regime, then the solutions of the sensitivity equations should give the analytical results of Eqs. (1.31), (1.32), and (1.33). Verification of the coding of all the equations and numerical solution method can be obtained by use of this exercise. The fourth-order Runge-Kutta method is used for the numerical integrations.

With $Pr = 1.0$, $Ra = 2.0$, and $b = 8.0/3.0$, and starting with the steady-state solution of Eqs. (1.30), the numerical solution results in a null transient in that the dependent variables maintain the specified initial values. I could plots these here, but it's a boring plot. The sensitivity results are shown in Figure 3 nearby

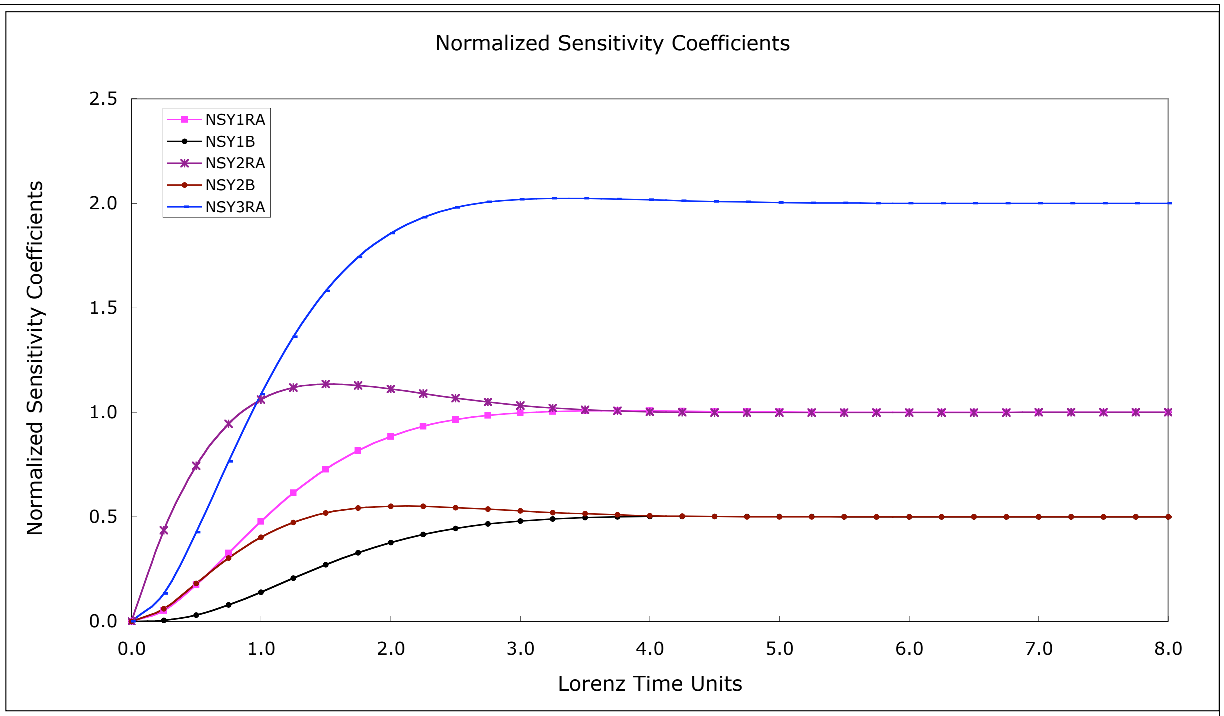

Figure 3. Normalized sensitivity coefficients for the Lorenz system null transient.

The calculation was carried out to 50.0 Lorenz Time Units. Only the first 8.0 LTU are shown as the numbers remain rock solid and don't change beyond this time.

The nomenclature is as follows, for an example; NSY1RA means the Normalized Sensitivity of the Y1 dependent variable (*X*) with respect to the Rayleigh Number; Eq. (1.34) above and Eq.(1.46) in Appendix B.

The coefficients that are zero, sensitivity with respect to *Pr*, have not been plotted. These all remained null throughout the transient. The sensitivity of the *Z* variable with the parameter *b*, Eq. (1.33) above, rapidly approached zero and also is not plotted.

As shown in Figure 3, the numerical solutions are in agreement with the analytical solutions. NSY1B, for example, should have the numerical value given by Eq. (1.35). And likewise for NSY2B, of Eq. (1.49) in Appendix B. Note that the sensitivity of *X* with respect to the Rayleigh number is the dominant sensitivity, and that the sensitivity for all three dependent variables is also dominated by the Rayleigh number. The analytical values are accurately calculated by the sensitivity equations.

One very important aspect of this exercise is that the equations and the coding of the equations and numerical solution method have been Verified. I actually found two bugs; one in the documentation of the equations and another in the coding.

A Couple of Chaotic Response Examples

Now that the equations and coding have been Verified, let's look at a couple of cases that exhibit chaotic response. For the first case the parameters are set to the classic values for the Lorenz system; $Pr = 10.0$, $Ra = 28.0$. and $b = 8.0/3.0$. The initial conditions are the analytical solutions of Eqs. (1.30) plus a small perturbation of plus or minus $1.0\text{x}10^{-6}$. The integration is carried out to 50.0 LTU.

A typical result for the sensitivity coefficients for the *Y* dependent variable with the Rayleigh Number is shown in Figure 4 nearby. The normalized sensitivity coefficient is plotted.

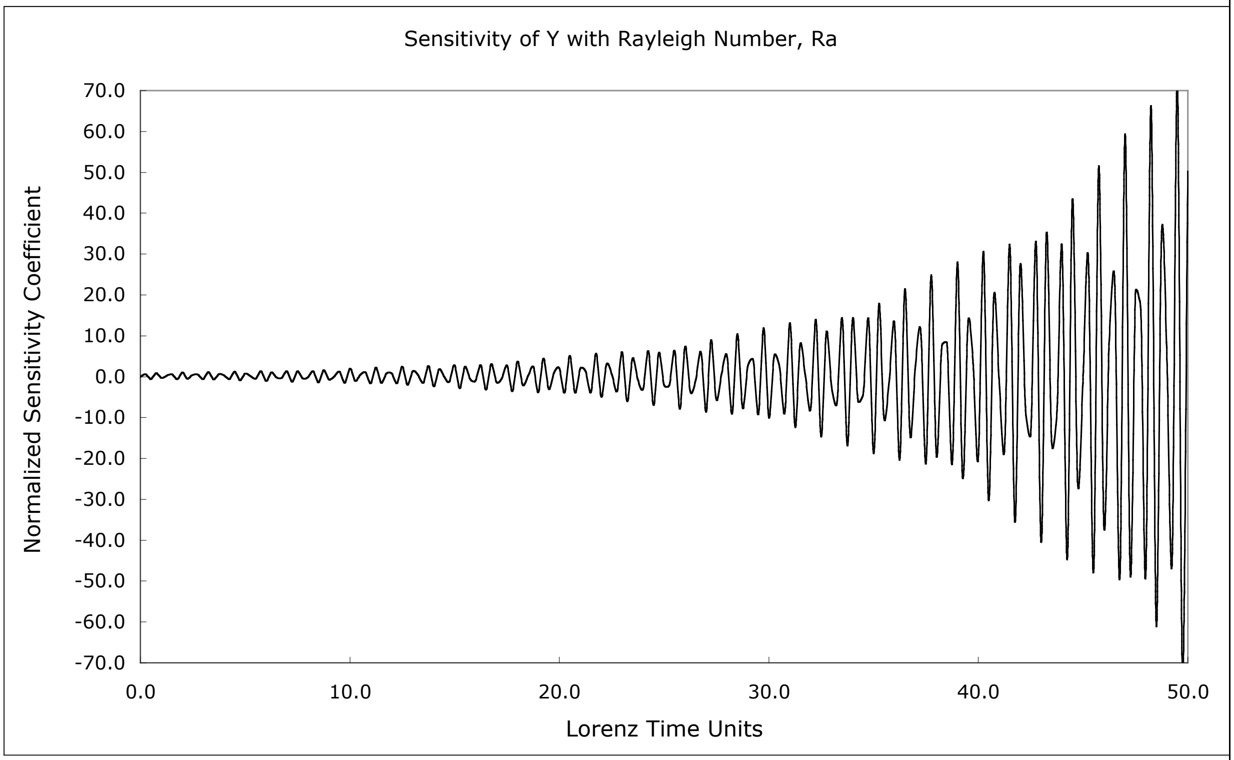

Figure 4. Normalized sensitivity coefficient for *Y* with Rayleigh Number *Ra*.

The sensitivity with the geometric factor, *b*, is given in Figure 5 below. The sensitivity coefficients for the other dependent variables have the same general response. The sensitivity for the Prandtl number is very small for all three dependent variables and shows slow increases in the amplitude and is not plotted.

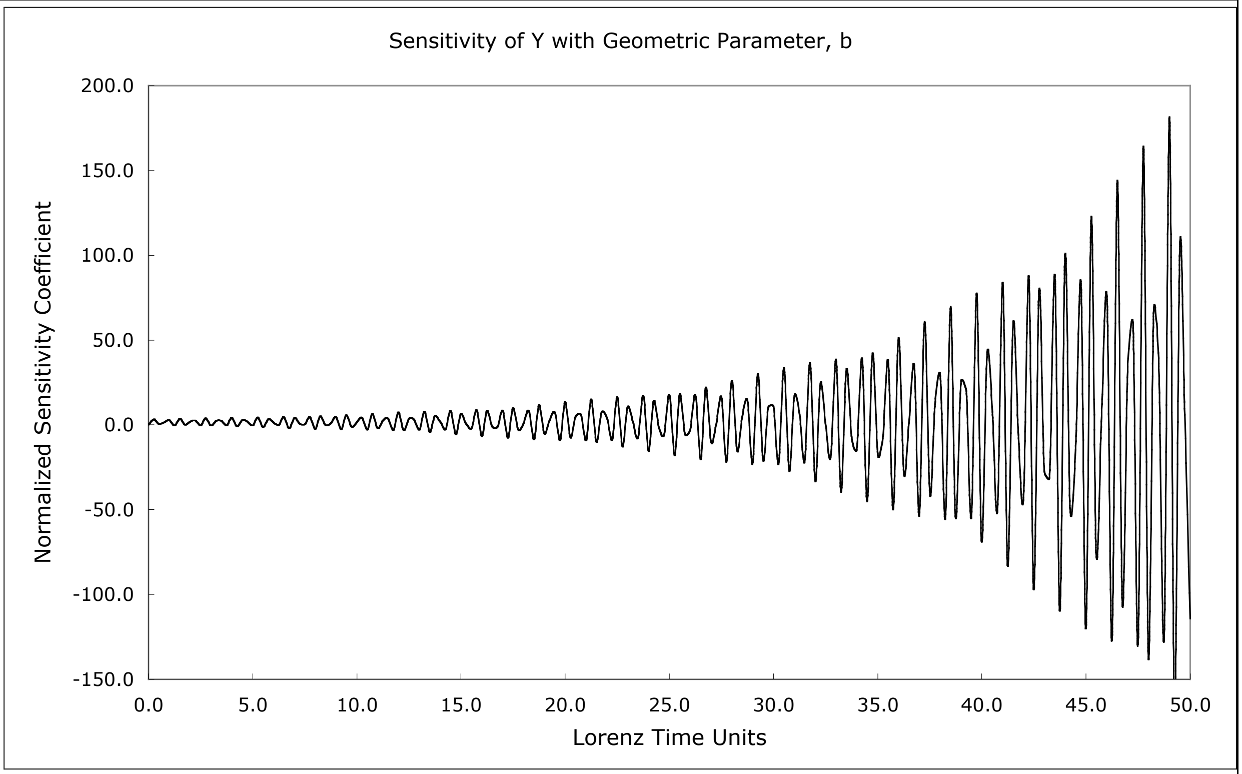

Figure 5. Normalized sensitivity coefficient for Y with geometric parameter b.

One interesting result is that the sensitivity for the geometric parameter, b, given in Figure 5, is quite large. With the Prandtl and Rayleigh numbers at the original values, I set $b = 4.0$ and carried the calculation out to 120.0 LTUs. The initial conditions were the analytical solutions of Eqs. (1.30) plus small perturbations.

All the dependent variables remain unchanged from the initial values and all the sensitivity coefficients reached the analytical values. Another case of non-chaotic response.

Appendix A: The Complete Equation System

The original equation system and the sensitivity equations are summarized in this appendix.

The original system is

$$\frac{dX}{dt} = -PrX + PrY$$
$$\frac{dY}{dt} = -Y + RaX - XZ \tag{1.36}$$
and
$$\frac{dZ}{dt} = -bZ + XY$$

To save the equation-processing effort, the following notation will be used. The sensitivities will be denoted simply as S_1 through S_9 with S_1 being Eq. (1.26) in the main text. This notation is summarized in the following table

Variables Derivative of	Parameters With respect to		
	Pr	***Ra***	***b***
X	S_1	S_2	S_3
Y	S_4	S_5	S_6
Z	S_7	S_8	S_9

The equation for the sensitivity of *X* with respect to *Pr* is

$$\frac{dS_1}{dt} = -PrS_1 - X + PrS_4 + Y \tag{1.37}$$

X with respect to *Ra*

$$\frac{dS_2}{dt} = -PrS_2 + PrS_5 \tag{1.38}$$

and *X* with respect to *b*

$$\frac{dS_3}{dt} = -PrS_3 + PrS_6 \tag{1.39}$$

The sensitivity of *Y* with respect to *Pr* is

$$\frac{dS_4}{dt} = -S_4 + RaS_1 - XS_7 - ZS_1 \tag{1.40}$$

Y with respect to Ra

$$\frac{dS_5}{dt} = -S_5 + X + RaS_2 - XS_9 - ZS_2 \tag{1.41}$$

and Y with respect to b

$$\frac{dS_6}{dt} = -S_6 + RaS_3 - XS_9 - ZS_3 \tag{1.42}$$

The sensitivity of Z with respect to Pr is

$$\frac{dS_7}{dt} = -bS_7 + XS_4 + YS_1 \tag{1.43}$$

Z with respect to Ra

$$\frac{dS_8}{dt} = -bS_8 + XS_5 + YS_2 \tag{1.44}$$

and Y with respect to b

$$\frac{dS_9}{dt} = -Z - bS_9 + XS_6 + YS_3 \tag{1.45}$$

The sensitivities on the left-hand sides could be normalized in these, or the easier approach is to normalize in the coding. Saves lots o equation processing.

Appendix B: All the Normalized Steady-State Sensitivities

The non-trivial solutions of Eqs. (1.30) are used to normalize the steady-state sensitivities of Eqs. (1.31), (1.32), and (1.33). The result for the second of Eqs. (1.31) has been given by Eq. (1.34) in the main text and the results for the third by Eq. (1.35). These and all the others follow here.

The normalized sensitivity of X with respect to the parameter Ra is

$$\left(\frac{\overline{\partial X}}{\partial Ra}\right)_0 = \frac{Ra_0}{2(Ra_0 - 1)} \tag{1.46}$$

the normalized sensitivity of X with respect to the parameter b is

$$\left(\overline{\frac{\partial X}{\partial b}}\right)_0 = \frac{1}{2} \tag{1.47}$$

The normalized sensitivity of Y with respect to the parameter Ra is

$$\left(\overline{\frac{\partial Y}{\partial Ra}}\right)_0 = \frac{Ra_0}{2(Ra_0 - 1)} \tag{1.48}$$

the normalized sensitivity of Y with respect to the parameter b is

$$\left(\overline{\frac{\partial Y}{\partial b}}\right)_0 = \frac{1}{2} \tag{1.49}$$

The normalized sensitivity of Z with respect to the parameter Ra is

$$\left(\overline{\frac{\partial Z}{\partial Ra}}\right)_0 = \frac{Ra_0}{(Ra_0 - 1)} \tag{1.50}$$

These results are Verified by the calculations given in the main text.

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