Jacobian Study

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Comparison of RELAP5-3D Jacobian matrix against a numerical approximation provides clues for improvement.

Background

Improvement projects for many aspects of RELAP5-3D are underway. Past issues, conference papers, and journal articles have reported an automated code verification technique that ensures, to 34 decimal places, that unintended changes do not occur between base and modified source code. Another ongoing effort provides verification of the RELAP5-3D code as compared to the RELAP5-3D manuals Vols. I, II, and IV. A third effort to find and reduce sources of mass error is reported here.

The first step is to examine the Jacobian of the governing equations. The governing equations for mass, energy, and noncondensable quality are:

$$\frac{\partial(\alpha_g\rho_g X_n)}{\partial t}+\frac{1}{A}\frac{\partial}{\partial x}(\alpha_g\rho_g X_n v_g A)=0. \tag{1}$$

$$\frac{\partial(\alpha_g\rho_g U_g)}{\partial t}+\frac{1}{A}\frac{\partial\alpha_g\rho_g U_g v_g A}{\partial x}=-P\frac{\partial\alpha_g}{\partial t}-\frac{P}{A}\frac{\partial(\alpha_g v_g A)}{\partial x}+Q_{wg}+Q_{ig}-Q_{gf}+\Gamma_{ig}h_g^*+\Gamma_w h_g'+DISS_g \tag{2}$$

$$\frac{\partial(\alpha_f\rho_f U_f)}{\partial t}+\frac{1}{A}\frac{\partial\alpha_f\rho_f U_f v_f A}{\partial x}=-P\frac{\partial\alpha_f}{\partial t}-\frac{P}{A}\frac{\partial(\alpha_f v_f A)}{\partial x}+Q_{wf}+Q_{if}+Q_{gf}-\Gamma_{ig}h_f^*-\Gamma_w h_f'+DISS_f \tag{3}$$

$$\frac{\partial(\alpha_g\rho_g)}{\partial t}-\frac{\partial(\alpha_f\rho_f)}{\partial t}+\frac{1}{A}\frac{\partial(\alpha_g\rho_g v_g A-\alpha_f\rho_f v_f A)}{\partial x}=2\Gamma_g=2(\Gamma_{ig}+\Gamma_w) \tag{4}$$

$$\frac{\partial(\alpha_g\rho_g)}{\partial t}+\frac{\partial(\alpha_f\rho_f)}{\partial t}+\frac{1}{A}\frac{\partial(\alpha_g\rho_g v_g A+\alpha_f\rho_f v_f A)}{\partial x}=0 \tag{5}$$

Eqns. (1)-(5) are given in Vol. 1[1] as Eqns. (3.1-39), (3.1-11,), 3.1(12), (3.1-2), and (3.1-3). The primary dependent variables are X_n, U_g, U_f, α_g, P, denoting respectively: noncondensable quality, gas and liquid specific internal energy, volume fraction of the gas, and pressure. Expansion of derivatives, closure laws, simplifications, and auxiliary equations reduce PDEs (1)-(5) to the discrete system given in Eqns (6)-(7).

$$\bar{\bar{A}}_{JL}\bar{x}_L=\bar{b}_L+\bar{g}_L^1 v_{g,j+1}^{n+1}+\bar{g}_L^2 v_{g,j}^{n+1}+\bar{g}_L^3 v_{f,j+1}^{n+1}+\bar{g}_L^4 v_{f,j}^{n+1} \tag{6}$$

$$\bar{x}=\begin{bmatrix}\tilde{\Delta}^{n+1}X_{n,L}\\ \tilde{\Delta}^{n+1}U_{g,L}\\ \tilde{\Delta}^{n+1}U_{f,L}\\ \tilde{\Delta}^{n+1}\alpha_{g,L}\\ \Delta^{n+1}P_L\end{bmatrix},\ \bar{b}_L=\begin{bmatrix}0\\ b_2\\ b_3\\ b_4\\ 0\end{bmatrix},\ \bar{g}_L^1=\begin{bmatrix}g_1^1\\ g_2^1\\ 0\\ g_4^1\\ g_5^1\end{bmatrix},\ \bar{g}_L^2=\begin{bmatrix}g_1^2\\ g_2^2\\ 0\\ g_4^2\\ g_5^2\end{bmatrix},\ \bar{g}_L^3=\begin{bmatrix}0\\ 0\\ g_3^3\\ g_4^3\\ g_5^3\end{bmatrix},\ \bar{g}_L^4=\begin{bmatrix}0\\ 0\\ g_3^4\\ g_4^4\\ g_5^4\end{bmatrix}. \tag{7}$$

In Eqns. (6) and (7), n+1 is the new time level, L is the control volume, j is the junction on the left of volume L, j+1 is on the right of volume L, $\bar{g}_L^1$ through $\bar{g}_L^4$ are vectors of old time values, and $\tilde{\Delta}^{n+1}$ denotes the forward difference in time. The liquid and gas velocity, v_f, v_g, are primary variables in the momentum equations, which are part of the governing equations as well, but due to the ingenious multi-stage solution method, contribute to the right hand side of the final discrete system, as shown in Eqn. (6), and are solved for in a different stage of the method.

Overall, the solution method seeks to solve for the conserved quantities, which occur in the first terms of each equations, namely $\alpha_g\rho_g X_n$, $\alpha_g\rho_g U_g$, $\alpha_f\rho_f U_f$, $\alpha_g\rho_g$, $\alpha_f\rho_f$. It does so by first solving for the primary dependent variables then combining them to form approximations of the conserved quantities.

The mass error is estimated by solving a second set of equations, one that does not expand the partial derivatives via the product rule, for the conserved quantities through a separate set of approximations and simplifications. The masses from each process are compared to find mass error.

Discussion

The method used in RELAP5-3D is referred to as the analytical method because it relies on calculus and physical laws for much of the simplification. For instance, Taylor polynomials eliminate many non-primary variables such as temperature from the equation set. However, these polynomials require partial derivatives of temperature supplied by differentiating state relations. The coefficient matrix of Eqn. (6) is named the analytical Jacobian matrix, A_{ana}.

A simple numerical analysis approach to solving the conservation equations applies a first order finite difference to the temporal derivative of the conserved quantities. It also recasts the other terms of the equations, using the multi-variate chain rule, so they are products where one factor is the temporal derivative of a primary variable. The result is named the numerical Jacobian matrix, A_{num}.

The elements of A_{ana} and A_{num} can be compared to find improvements. This can be done for a variety of fluid states. Due to the complexity of RELAP5-3D, this is not a simple process.

Initial analysis shows reasonably good agreement between the temporal terms, but some of the mass and energy terms appear to have room to improve. Another observation is that the Jacobian matrices, both analytical and numerical, are generally ill-conditions. Preconditioning may also reduce mass error. Also, use of Gaussian Elimination with partial pivoting may reduce round-off error and even run faster.

References

1. The RELAP5-3D Code Development Team, “RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods,” INL-EXT-98-00834-V1, Revision 4.1, June, 2013.