Parallel Calculation of Uncertainty Propagation in CFD Using Adjoint Equations

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The present report addresses to the uncertainty estimation for the set of flow-field parameter ε_j using sensitivity coefficients $\partial\varepsilon_j / \partial f_i$ calculated via adjoint equations. If we need to get uncertainties for m parameters (density, temperature etc) in k checkpoints, we should simultaneously solve n=m*k practically identical adjoint problems. The uncertainty propagation by adjoint equations can be efficiently calculated by parallel approach. At first step we compute the flow-field, at the second we may parallelly run n adjoint tasks having approximately the same time of computation. The fields of adjoint "temperature", adjoint "density" etc. depend on flow-field, estimated parameter, checkpoint location and do not depend on the set of input data, which have an uncertainty. So, they are universal and permit the calculation of considered checkpoint uncertainty caused by any parameter of the system of equations.

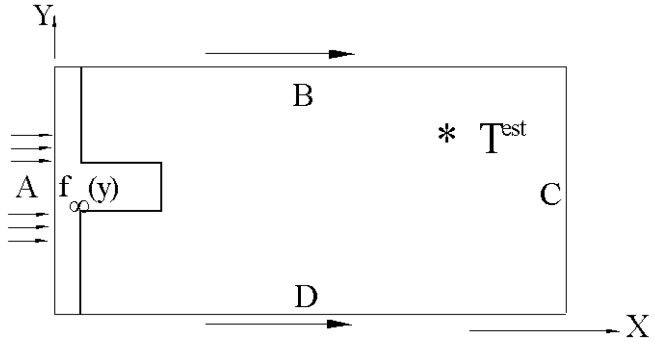

Fig. 1.

We consider the uncertainty estimation in supersonic viscous flow (Fig. 1). The flow parameters are calculated by the finite-difference approximation of parabolized Navier-Stokes [2]. The march along *X* coordinate was used.

$$\frac{\partial(\rho U)}{\partial X} + \frac{\partial(\rho V)}{\partial Y} = 0 \tag{1}$$

$$U\frac{\partial U}{\partial X} + V\frac{\partial U}{\partial Y} + \frac{1}{\rho}\frac{\partial P}{\partial X} = \frac{1}{\mathrm{Re}\,\rho}\frac{\partial^2 U}{\partial Y^2} \tag{2}$$

$$U\frac{\partial V}{\partial X} + V\frac{\partial V}{\partial Y} + \frac{1}{\rho}\frac{\partial P}{\partial Y} = \frac{4}{3\rho\,\mathrm{Re}}\frac{\partial^2 V}{\partial Y^2} \tag{3}$$

$$U\frac{\partial e}{\partial X} + V\frac{\partial e}{\partial Y} + (\kappa-1)e\left(\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y}\right) = \frac{1}{\rho}\left(\frac{\kappa}{\mathrm{Re}\,\mathrm{Pr}}\frac{\partial^2 e}{\partial Y^2} + \frac{4}{3\,\mathrm{Re}}\left(\frac{\partial U}{\partial Y}\right)^2\right) \tag{4}$$

$P=\rho RT$; $e=C_v T$; $(X,Y)\in\Omega=(0<X<X_{max};\ 0<Y<1)$;

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The entrance boundary (($X=0$)) conditions follow:

$e(0,Y)=e_\infty(Y);\ \rho(0,Y)=\rho_\infty(Y));\ U(0,Y)=U_\infty(Y);\ V(0,Y)=V_\infty(Y);$ (5)

the outflow conditions $\partial f/\partial Y=0$ are used on $Y=0,\ Y=1$.

Let the inflow parameters to contain the uncertainty. We assume the discrete analogues of these parameters to contain a normally distributed statistically independent error with standard deviations $\sigma_\rho, \sigma_U, \sigma_V, \sigma_e$.

Let we seek for total flow-field and the accuracy of certain parameter (let it be temperature) in some check point $T(t_{est}, x_{est})$, more precisely: a dependence of the temperature standard deviation from the input data deviations $\sigma_T = f(\sigma_\rho, \sigma_U, \sigma_V ...)$.

Note $\boldsymbol{T}(X^{est}, Y^{est})$ as $\varepsilon(f_\infty(Y), \mathrm{Re})$. If the estimated parameter is located on the outflow boundary we may express it as

$$\varepsilon(\boldsymbol{f}_\infty(Y)) = \int \boldsymbol{T}(X_{\max}, Y)\delta(Y - Y^{est})dy \tag{6}$$

If $\boldsymbol{T}(X^{est}, Y^{est})$ is located within the field we write

$$\varepsilon(\boldsymbol{f}_\infty(Y)) = \int\limits_\Omega \boldsymbol{T}(X, Y)\delta(Y - Y^{est})\delta(X - X^{est})dxdy \tag{7}$$

The input data dispersion is transformed to the result dispersion by gradients [1], in our case:

$$\sigma_\varepsilon^2 = \sum_{i=1}^{NY}\left(\frac{\partial\varepsilon}{\partial T_\infty^i}\sigma_{T_i}\right)^2 + \sum_{i=1}^{NY}\left(\frac{\partial\varepsilon}{\partial\rho_\infty^i}\sigma_{\rho_i}\right)^2 + \sum_{i=1}^{NY}\left(\frac{\partial\varepsilon}{\partial U_\infty^i}\sigma_{U_i}\right)^2 + \sum_{i=1}^{NY}\left(\frac{\partial\varepsilon}{\partial V_\infty^i}\sigma_{V_i}\right)^2 + \left(\frac{\partial\varepsilon}{\partial(1/\mathrm{Re})}\sigma_{(1/\mathrm{Re})}\right)^2 \tag{8}$$

The most efficient way for gradient calculation is based on adjoint equations. For these equations inference we introduce the Lagrangian $L(f_\infty(Y), \Psi)$, composed of the estimated value and weak statement of problem (1-5). Consider the influence of inflow data variation $\Delta f_\infty(X)$ and coefficient variation $\Delta(1/\mathrm{Re})$. By subtracting the undisturbed solution we get the linear tangent model. Integrating Lagrangian variation by parts with the account of linear tangent model allows estimating the variation of target parameter in dependence on the disturbed parameters.

$$\Delta L(\boldsymbol{f}_\infty(Y), \boldsymbol{f}, \Psi) = \Delta\varepsilon(f_\infty(Y)) = \int\limits_Y \left(\left(\Psi_e U + (\kappa-1)\Psi_U\right)\Delta e_\infty(Y)\right)\Big|_{X=0} dY +$$

$$+\int\limits_Y \left(\left(\Psi_\rho U + (\kappa-1)\Psi_U e/\rho\right)\Delta\rho_\infty(Y)\right)\Big|_{X=0} dY +$$

$$+\int\limits_Y \left(\left(\Psi_U U + \rho\Psi_\rho + (\kappa-1)\Psi_e e\right)\Delta U_\infty(Y)\right)\Big|_{X=0} dY + \int\limits_Y \left(\Psi_V U \Delta V_\infty(Y)\right)\Big|_{X=0} dY - \tag{9}$$

$$-\Delta(1/\mathrm{Re})\int\limits_\Omega \left(\frac{1}{\rho}\frac{\partial^2 U}{\partial Y^2}\Psi_U + \frac{4}{3\rho}\frac{\partial^2 V}{\partial Y^2}\Psi_V + \frac{\kappa}{\rho\,\mathrm{Pr}}\frac{\partial^2 e}{\partial Y^2}\Psi_e + \frac{4}{3\rho}\left(\frac{\partial U}{\partial Y}\right)^2\Psi_e\right)dXdY$$

Eq. (9) is valid if the remaining terms of $\Delta L(\boldsymbol{f}_\infty(Y), \boldsymbol{f}, \Psi)$ equal zero, i.e. on the solution of the adjoint problem (10-15).

Adjoint problem

$$U\frac{\partial\Psi_\rho}{\partial X} + V\frac{\partial\Psi_\rho}{\partial Y} + (\kappa-1)\frac{\partial(\Psi_V e/\rho)}{\partial Y} + (\kappa-1)\frac{\partial(\Psi_U e/\rho)}{\partial X} -$$

$$-\frac{\kappa-1}{\rho}\left(\frac{\partial e}{\partial Y}\Psi_V + \frac{\partial e}{\partial X}\Psi_U\right) + \left(\frac{1}{\rho^2}\frac{\partial P}{\partial X} - \frac{1}{\rho^2\,\mathrm{Re}}\frac{\partial^2 U}{\partial Y^2}\right)\Psi_U + \frac{1}{\rho^2}\left(\frac{\partial P}{\partial Y} - \frac{4}{3\,\mathrm{Re}}\frac{\partial^2 V}{\partial Y^2}\right)\Psi_V -$$

$$-\frac{1}{\rho^2}\left(\frac{\kappa}{\mathrm{RePr}}\frac{\partial^2 e}{\partial Y^2} + \frac{4}{3\mathrm{Re}}\left(\frac{\partial U}{\partial Y}\right)^2\right)\Psi_e = 0 \tag{10}$$

$$U\frac{\partial \Psi_U}{\partial X}+\frac{\partial(\Psi_U V)}{\partial Y}+\rho\frac{\partial \Psi_\rho}{\partial X}-\left(\frac{\partial V}{\partial X}\Psi_V+\frac{\partial e}{\partial X}\Psi_e\right)+\frac{\partial}{\partial X}\left(\frac{P}{\rho}\Psi_e\right)+$$
$$+\frac{\partial^2}{\partial Y^2}\left(\frac{1}{\rho\ \mathrm{Re}}\Psi_U\right)-\frac{\partial}{\partial Y}\left(\frac{8}{3\ \mathrm{Re}}\frac{\partial U}{\partial Y}\Psi_e\right)=0 \qquad (11)$$
$$\frac{\partial(U\Psi_V)}{\partial X}+V\frac{\partial \Psi_V}{\partial Y}-\left(\frac{\partial U}{\partial Y}\Psi_U+\frac{\partial e}{\partial Y}\Psi_e\right)+$$
$$+\rho\frac{\partial \Psi_\rho}{\partial Y}+\frac{\partial}{\partial Y}\left(\frac{P}{\rho}\Psi_e\right)+\frac{4}{3\ \mathrm{Re}}\frac{\partial^2}{\partial Y^2}\left(\frac{\Psi_V}{\rho}\right)=0 \qquad (12)$$
$$\frac{\partial(U\Psi_e)}{\partial X}+\frac{\partial(V\Psi_e)}{\partial Y}-\frac{\kappa-1}{\rho}\left(\frac{\partial\rho}{\partial Y}\Psi_V+\frac{\partial\rho}{\partial X}\Psi_U\right)-(\kappa-1)\left(\frac{\partial U}{\partial X}+\frac{\partial V}{\partial Y}\right)\Psi_e+$$
$$+(\kappa-1)\frac{\partial\Psi_V}{\partial Y}+(\kappa-1)\frac{\partial\Psi_U}{\partial X}+\frac{\kappa}{\mathrm{Re\ Pr}}\frac{\partial^2}{\partial Y^2}\left(\frac{\Psi_e}{\rho}\right)-\delta(X-X^{est})\delta(Y-Y^{est})=0 \qquad (13)$$

The source term in equation describing Ψ_e (13) corresponds the checkpoint location within the flow-field. Initial conditions are

$$C\ (X{=}X_{max}):\ \Psi_{\rho,U,V}\Big|^{X=X_{\max}}=0;\ \ U\Psi_e+(\kappa-1)\Psi_U+\delta(Y-Y^{est})=0; \qquad (14)$$

Expression for Ψ_e in (14) corresponds the checkpoint location on the inflow boundary X_{max}.. Boundary conditions are

$$B,D\ (Y{=}0;\ Y{=}1):\frac{\partial\Psi_f}{\partial Y}=0; \qquad (15)$$

The statement (10-15) differs from the adjoint equations used in Inverse CFD problems by the form of the target functional and, respectively, by the source term form in (13,14). The adjoint problem is solved in the reverse direction along *X*. It's statement is determined by the forward problem, check point position, and the choice of the estimated parameter. The adjoint problem does not depend on the choice of parameters containing the uncertainty. So, the same field of adjoint parameters may be used for the calculation of uncertainty propagation from any parameters (initial, boundary conditions, coefficients, sources). The gradients used for the uncertainty propagation have the following form:

$$\partial\varepsilon/\partial e_\infty(Y)=\Psi_e U+(\kappa-1)\Psi_U,\ \ \partial\varepsilon/\partial\rho_\infty(Y)=\Psi_\rho U+(\kappa-1)\Psi_U e/\rho,$$
$$\partial\varepsilon/\partial U_\infty(Y)=\Psi_U U+\rho\Psi_\rho+(\kappa-1)\Psi_e e,\ \ \partial\varepsilon/\partial V_\infty(Y)=\Psi_V U,$$
$$\nabla\varepsilon_{1/\mathrm{Re}}=-\int_\Omega\left(\frac{1}{\rho}\frac{\partial^2 U}{\partial Y^2}\Psi_U+\frac{4}{3\rho}\frac{\partial^2 V}{\partial Y^2}\Psi_V+\frac{\kappa}{\rho\,\mathrm{Pr}}\frac{\partial^2 e}{\partial Y^2}\Psi_e+\frac{4}{3\rho}\left(\frac{\partial U}{\partial Y}\right)^2\Psi_e\right)dXdY \qquad (16)$$

The calculation of the gradient implies the consequent solution of the direct and adjoint problems. So, the time for uncertainty calculation of the single parameter in the single checkpoint equals approximately two times of the flow-field calculation. The uncertainty estimation of every additional parameter needs the solution of additional adjoint equation.

The singular source in (13) is integrated over the cell and thus transformed to the finite source term $\delta_{ij}/(\Delta X\Delta Y)$, if check point is located within flow-field, and $\delta_{ij}/\Delta Y$ if the check point is on the boundary (14), where δ_{ij} is the unit matrix.

The flow-field parameters and their gradients form sources and coefficients of adjoint equations. So, the tests are conducted for non-uniform flow corresponding to underexpanded jet with the temperature ratio *Tj/T=3* (density isolines are provided in Fig. 2). Adjoint "temperature" field is presented in Figure 3. The uncertainty propagation is calculated by the adjoint equations and Monte-Carlo method (averaged over 100 trials) for the comparison. The inflow parameters contain the normally distributed error with the standard deviation in the range of 0.01-0.1.

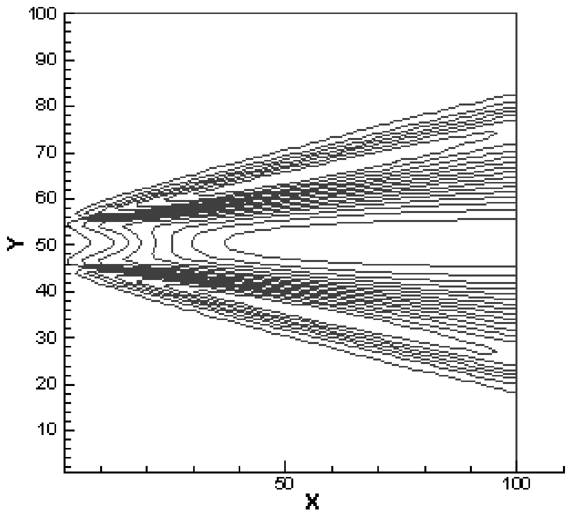

Fig. 2.

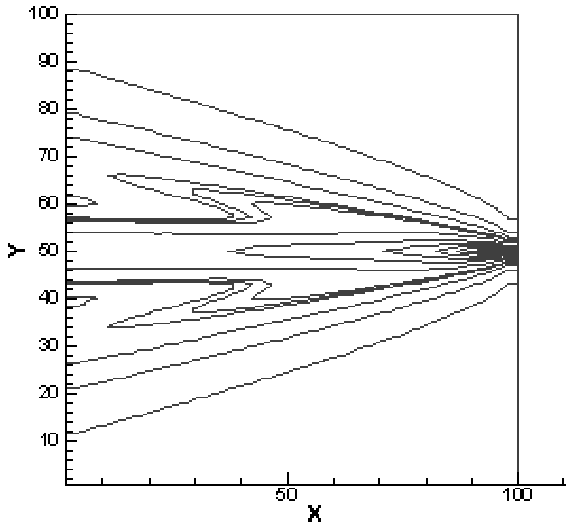

Fig. 3.

Generally, the results of both approaches (Monte-Carlo and adjoint) correlate, while the consumed computer time differs by two orders of magnitude for these tests.

Conclusion

The computation of the uncertainty of single parameter at the single checkpoint needs calculation of the flow-field and the adjoint field. The estimation of the uncertainty of another parameter (or the same in another check point) needs calculation of the new adjoint field for the same flow-field. The calculation of the uncertainty of *n* flow parameters needs the calculation of *n+1* fields (flow-field + *n* adjoint fields). All the adjoint fields are calculated by the same algorithm with the slightest differences in form of sources and their location.

We should run *n* independent samples of adjoint codes when calculating the uncertainty of *n* parameters. The adjoint problem is similar to flow-field calculation problem as to computer memory and the time of computation.

References

1. Putko M.M., Newmann P.A., Taylor III A.C., and Green L.L., Approach for Uncertainty Propagation and Robust Design in CFD Using Sensitivity Derivatives, AIAA paper, 2001-2528, 2001, pp. 1-14.
2. A.K. Alekseev, I.M. Navon, The analysis of an ill-posed problem using multiscale resolution and second order adjoint techniques, Computer Methods in Appl. Mech. and Eng., v.190, issue 15-17, pp. 1937-1953, 2001