

Discussion of the NAS Parallel Benchmark for CFD

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14 December 1994

Abstract

The Numerical Aerodynamics Simulation (NAS) group at NASA Ames has developed a "pencil and paper" benchmark for Computational Fluid Dynamics (CFD) Applications. A set of synthetic Partial Differential Equations (PDE's) and the solution methodology, embodying many salient features of a typical application code, are specified. In the benchmark specification, the derivation of the discretized equations and the solution algorithm are not considered. Here, these equations are derived beginning with the differential form of the Navier-Stokes equations. Discrepancies between the resulting equations developed here and those specified in the NAS benchmark are delineated, and the correspondence of the synthetic set of PDE's to those in a "real" CFD code is discussed. This report is targeted to an audience that has an interest in establishing the physical significance of various variables that appear in the set of synthetic PDE's in the NAS benchmark.

1 The Compressible Navier-Stokes Equations

The compressible Navier-Stokes equations in conservative form are given by

$$\begin{aligned}
\partial_t^* \rho^* + \partial_j^* (\rho^* u_j^*) &= 0 , \\
\partial_t^* (\rho^* u_i^*) + \partial_j^* [\rho^* u_i^* u_j^* + p^* \delta_{ij} - \tau_{ij}^*] &= \rho^* F_i^* , \\
\partial_t^* (\rho^* E^*) + \partial_j^* [\rho^* u_j^* H^* - u_i^* \tau_{ij}^* - k^* \partial_j^* T^*] &= \rho^* u_i^* F_i^* + \dot{q}^* , \quad (1)
\end{aligned}$$

where the superscript ‘*’ denotes dimensional quantities and

$$\tau_{ij}^* = \mu^* [\partial_j^* u_i^* + \partial_i^* u_j^*] + \lambda^* \delta_{ij} \partial_k^* u_k^* , \quad (2)$$

ρ^* : density

u_i^* : i^{th} velocity component, $i = 1, 3$

p^* : pressure

F_i^* : i^{th} component of the external force

E^* : total internal energy = $e^* + \frac{u_i^* u_i^*}{2}$, where e^* is the specific internal energy

H^* : total enthalpy = $h^* + \frac{u_i^* u_i^*}{2}$, where h^* is the specific enthalpy

T^* : temperature

k^* : thermal conductivity

μ^* : absolute (or dynamic) viscosity

λ^* : second coefficient of viscosity (= $-\frac{2}{3}\mu^*$ upon invoking Stokes assumption)

\dot{q}^* : volumetric heat generation

The specific enthalpy is related to the specific internal energy by

$$h^* = e^* + \frac{p^*}{\rho^*} \Rightarrow H^* = E^* + \frac{p^*}{\rho^*} . \quad (3)$$

A perfect gas is assumed, in which case,

$$e^* = E^* - \frac{u_i^* u_i^*}{2} = C_v^* T^* \Rightarrow T^* = \frac{1}{C_v^*} \left[E^* - \frac{u_i^* u_i^*}{2} \right]. \quad (4)$$

Furthermore, for a perfect gas, $p^* = \rho^* R^* T^*$. Hence,

$$p^* = \rho^* \frac{R^*}{C_v^*} \left[E^* - \frac{u_i^* u_i^*}{2} \right] = (\gamma - 1) \rho^* \left[E^* - \frac{u_i^* u_i^*}{2} \right], \quad (5)$$

where

C_v^* : specific heat at constant volume

R^* : gas constant

γ : ratio of specific heats = $\frac{C_p^*}{C_v^*}$

C_p^* : specific heat at constant pressure

2 Nondimensional Form of the Equations

We non-dimensionalize the equations by defining the following reference values:

U_∞^* : reference velocity

L_∞^* : reference length scale

ρ_∞^* : reference density

μ_∞^* : reference absolute viscosity

k_∞^* : reference thermal conductivity

$C_{v\infty}^*$: reference specific heat

All non-dimensional quantities are denoted without the superscript ‘*’. Hence,

$$\begin{aligned} u_i &= \frac{u_i^*}{u_\infty^*} ; & x_i &= \frac{x_i^*}{L_\infty^*} ; & \rho &= \frac{\rho^*}{\rho_\infty^*} ; \\ \mu &= \frac{\mu^*}{\mu_\infty^*} ; & \lambda &= \frac{\lambda^*}{\mu_\infty^*} ; & k &= \frac{k^*}{k_\infty^*} ; & C_v &= \frac{C_v^*}{C_{v\infty}^*} . \end{aligned} \quad (6)$$

In addition, we non-dimensionalize the other quantities in equations (1)–(4) as follows:

$$\begin{aligned} t &= \frac{t^* U_\infty^*}{L^*} ; & p &= \frac{p^*}{\rho_\infty^* U_\infty^{*2}} ; & F_i &= \frac{F_i^*}{U_\infty^{*2} / L_\infty^*} ; & E &= \frac{E^*}{U_\infty^{*2}} ; \\ H &= \frac{H^*}{U_\infty^{*2}} ; & \dot{q} &= \frac{\dot{q}^*}{\rho_\infty^* U_\infty^{*3} / L_\infty^*} ; & \tau_{ij} &= \frac{\tau_{ij}^*}{(U_\infty^* \mu_\infty^*) / L_\infty^*} . \end{aligned} \quad (7)$$

Upon substituting equations (6) and (7) into equations (1)–(2) and using equation (4), it may be easily shown that

$$\begin{aligned} \partial_t \rho + \partial_j (\rho u_j) &= 0 , \\ \partial_t (\rho u_i) + \partial_j \left[\rho u_i u_j + p \delta_{ij} - \frac{1}{\text{Re}} \tau_{ij} \right] &= \rho F_i , \\ \partial_t (\rho E) + \partial_j \left[\rho u_j H - \frac{1}{\text{Re}} u_i \tau_{ij} - \right. \\ \left. \frac{\gamma}{\text{Re Pr}} k \partial_j \left\{ \frac{1}{C_v} \left(E - \frac{u_i u_i}{2} \right) \right\} \right] &= \rho u_i F_i + \dot{q} , \end{aligned} \quad (8)$$

where

$$\tau_{ij} = \mu (\partial_j u_i + \partial_i u_j) - \frac{2}{3} \mu \delta_{ij} \partial_k u_k , \quad (9)$$

and

$$\text{Re} = \frac{\rho_\infty^* u_\infty^* L_\infty^*}{\mu_\infty^*} ,$$

$$\text{Pr} = \frac{\mu_{\infty}^* C_{p\infty}^*}{k_{\infty}^*} = \frac{\mu_{\infty}^* C_{v\infty}^* \gamma}{k_{\infty}^*}.$$

Here, Re and Pr denote the Reynolds and Prandtl numbers, respectively. Finally, the non-dimensional form of equations (3) and (4) are given by

$$H = E + \frac{p}{\rho}, \quad (10)$$

$$p = (\gamma - 1)\rho \left[E - \frac{u_i u_i}{2} \right]. \quad (11)$$

Note: The Stokes' assumption has been invoked in equation (9).

3 Comparison with the NAS Benchmark

Let the system of equations (8) be written as

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x_1} + \frac{\partial \mathbf{F}}{\partial x_2} + \frac{\partial \mathbf{G}}{\partial x_3} = \frac{\partial \mathbf{U}}{\partial x_1} + \frac{\partial \mathbf{V}}{\partial x_2} + \frac{\partial \mathbf{W}}{\partial x_3} + \mathbf{H}, \quad (12)$$

where

$$\mathbf{q} = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{bmatrix};$$

$$\mathbf{E} = \begin{bmatrix} \rho u_1 \\ \rho u_1^2 + p \\ \rho u_1 u_2 \\ \rho u_1 u_3 \\ u_1(\rho E + p) \end{bmatrix}; \quad \mathbf{F} = \begin{bmatrix} \rho u_2 \\ \rho u_1 u_2 \\ \rho u_2^2 + p \\ \rho u_2 u_3 \\ u_2(\rho E + p) \end{bmatrix}; \quad \mathbf{G} = \begin{bmatrix} \rho u_3 \\ \rho u_1 u_3 \\ \rho u_2 u_3 \\ \rho u_3^2 + p \\ u_3(\rho E + p) \end{bmatrix};$$

$$\mathbf{U} = \text{Re}^{-1} \begin{bmatrix} 0 \\ \tau_{11} \\ \tau_{21} \\ \tau_{31} \\ \alpha_1 \end{bmatrix}; \quad \mathbf{V} = \text{Re}^{-1} \begin{bmatrix} 0 \\ \tau_{12} \\ \tau_{22} \\ \tau_{32} \\ \alpha_2 \end{bmatrix}; \quad \mathbf{W} = \text{Re}^{-1} \begin{bmatrix} 0 \\ \tau_{13} \\ \tau_{23} \\ \tau_{33} \\ \alpha_3 \end{bmatrix};$$

and

$$\mathbf{H} = \begin{bmatrix} 0 \\ \rho F_1 \\ \rho F_2 \\ \rho F_3 \\ \rho u_k F_k + \dot{q} \end{bmatrix}.$$

The quantities α_i , $i = 1, 3$ are given by

$$\begin{aligned} \alpha_1 &= u_k \tau_{k1} + \frac{\gamma^k}{\text{Pr}} \partial_1 \left\{ \frac{1}{C_v} \left(E - \frac{u_i u_i}{2} \right) \right\}, \\ \alpha_2 &= u_k \tau_{k2} + \frac{\gamma^k}{\text{Pr}} \partial_2 \left\{ \frac{1}{C_v} \left(E - \frac{u_i u_i}{2} \right) \right\}, \\ \alpha_3 &= u_k \tau_{k3} + \frac{\gamma^k}{\text{Pr}} \partial_3 \left\{ \frac{1}{C_v} \left(E - \frac{u_i u_i}{2} \right) \right\}. \end{aligned}$$

Let

$$\mathbf{U} = \mathbf{U}_I + \mathbf{U}_E,$$

$$\mathbf{V} = \mathbf{V}_I + \mathbf{V}_E,$$

$$\mathbf{W} = \mathbf{W}_I + \mathbf{W}_E,$$

so that $\frac{\partial \mathbf{U}_I}{\partial x_1}$, $\frac{\partial \mathbf{V}_I}{\partial x_2}$, and $\frac{\partial \mathbf{W}_I}{\partial x_3}$ involve no cross derivatives, and $\frac{\partial \mathbf{U}_E}{\partial x_1}$, $\frac{\partial \mathbf{V}_E}{\partial x_2}$, $\frac{\partial \mathbf{W}_E}{\partial x_3}$ do involve cross derivatives.

As demonstrated in the development of the Beam and Warming algorithm, only those terms which do not involve cross-derivatives are handled implicitly. Cross-derivative terms are handled explicitly. The focus of the NAS benchmark is on the implicit solution algorithm, and not on the evaluation of the right-hand side. Therefore, in effect, a solution of the following equation is sought:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x_1} + \frac{\partial \mathbf{F}}{\partial x_2} + \frac{\partial \mathbf{G}}{\partial x_3} - \frac{\partial \mathbf{U}_I}{\partial x_1} - \frac{\partial \mathbf{V}_I}{\partial x_2} - \frac{\partial \mathbf{W}_I}{\partial x_3} = \mathbf{H}^*, \quad (13)$$

where

$$\mathbf{H}^* = \mathbf{H} + \frac{\partial \mathbf{U}_E}{\partial x_1} + \frac{\partial \mathbf{V}_E}{\partial x_2} + \frac{\partial \mathbf{W}_E}{\partial x_3} . \quad (14)$$

In a real CFD application, equation (4) would be evaluated at each time step (for reference, see equation (22) of BW). However, in the NAS benchmark, the individual contributions to \mathbf{H}^* are ignored, but in order to guarantee the existence of a steady-state solution, the function \mathbf{H}^* is specified in the following manner. Let \mathbf{q}^* denote the steady-state solution (which, for the NAS benchmark, is given). Then at steady state,

$$\mathbf{H}^* = \frac{\partial \mathbf{E}^*}{\partial x_1} + \frac{\partial \mathbf{F}^*}{\partial x_2} + \frac{\partial \mathbf{G}^*}{\partial x_3} - \frac{\partial \mathbf{U}_I^*}{\partial x_1} - \frac{\partial \mathbf{V}_I^*}{\partial x_2} - \frac{\partial \mathbf{W}_I^*}{\partial x_3} . \quad (15)$$

If \mathbf{H}^* is specified according to the above identity, a steady-state solution of equation (13) exists. Thus, for the NAS benchmark, we need to consider only those terms that do not involve cross-derivatives.

First consider the solution \mathbf{q} and the inviscid fluxes (for reference, see page 46 of NAS benchmark).

Present Notation

NAS Benchmark Notation

$$\mathbf{q} = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{bmatrix}$$

\equiv

$$\mathbf{U} = \begin{bmatrix} u^{(1)} \\ u^{(2)} \\ u^{(3)} \\ u^{(4)} \\ u^{(5)} \end{bmatrix}$$

$$\mathbf{E} = \begin{bmatrix} \rho u_1 \\ \rho u_1^2 + p \\ \rho u_1 u_2 \\ \rho u_1 u_3 \\ u_1(\rho E + p) \end{bmatrix}$$

\equiv

$$-\mathbf{E} = \begin{bmatrix} u^{(2)} \\ [u^{(2)}]^2 / [u^{(1)}] + \phi \\ u^{(2)}u^{(3)} / u^{(1)} \\ u^{(2)}u^{(4)} / u^{(1)} \\ u^{(2)} / u^{(1)} [u^{(5)} + \phi] \end{bmatrix}$$

$$\mathbf{F} = \begin{bmatrix} \rho u_2 \\ \rho u_1 u_2 \\ \rho u_2^2 + p \\ \rho u_2 u_3 \\ u_2(\rho E + p) \end{bmatrix}$$

\equiv

$$-\mathbf{F} = \begin{bmatrix} u^{(3)} \\ u^{(2)}u^{(3)} / u^{(1)} \\ [u^{(3)}]^2 / [u^{(1)}] + \phi \\ u^{(3)}u^{(4)} / u^{(1)} \\ u^{(3)} / u^{(1)} [u^{(5)} + \phi] \end{bmatrix}$$

$$\mathbf{G} = \begin{bmatrix} \rho u_3 \\ \rho u_1 u_3 \\ \rho u_2 u_3 \\ \rho u_3^2 + p \\ u_3(\rho E + p) \end{bmatrix}$$

\equiv

$$-\mathbf{G} = \begin{bmatrix} u^{(4)} \\ u^{(2)}u^{(4)} / u^{(1)} \\ u^{(3)}u^{(4)} / u^{(1)} \\ [u^{(4)}]^2 / [u^{(1)}] + \phi \\ u^{(4)} / u^{(1)} [u^{(5)} + \phi] \end{bmatrix}$$

$$p = (\gamma - 1) \left[\rho E - \frac{\rho u_i u_i}{2} \right] \equiv$$

$$\phi = k_2 \left[u^{(5)} - \frac{1}{2} \left\{ \frac{[u^{(2)}]^2 + [u^{(3)}]^2 + [u^{(4)}]^2}{u^{(1)}} \right\} \right],$$

$$\Rightarrow k_2 = \gamma - 1 .$$

(16)

Next, consider the momentum equations. It follows from equation (9) that

$$\partial_j \tau_{ij} = \begin{bmatrix} \partial_1 \left(\frac{4}{3} \mu \partial_1 u_1 \right) + \partial_2 (\mu \partial_2 u_1) + \partial_3 (\mu \partial_3 u_1) + \text{c.d.} \\ \partial_1 (\mu \partial_1 u_2) + \partial_2 \left(\frac{4}{3} \mu \partial_2 u_2 \right) + \partial_3 (\mu \partial_3 u_2) + \text{c.d.} \\ \partial_1 (\mu \partial_1 u_3) + \partial_2 (\mu \partial_2 u_3) + \partial_3 \left(\frac{4}{3} \mu \partial_3 u_3 \right) + \text{c.d.} \end{bmatrix}, \quad (17)$$

where ‘c.d.’ denotes cross-derivative terms. Next, consider the energy equation. Upon substituting for τ_{ij} from equation (9), it may be shown that

$$\begin{aligned} & \partial_j \left[u_i \tau_{ij} + \frac{\gamma^k}{\text{Pr}} \partial_j \left\{ \frac{1}{C_v} \left(E - \frac{u_i u_i}{2} \right) \right\} \right] \\ = & \partial_1 \left[\frac{\mu}{2} \left(1 - \frac{\gamma^k}{\text{Pr} \mu C_v} \right) \partial_1 (u_1^2 + u_2^2 + u_3^2) + \frac{\mu}{6} \partial_1 (u_1^2) + \frac{\gamma^k}{\text{Pr} C_v} \partial_1 E \right] \\ + & \partial_2 \left[\frac{\mu}{2} \left(1 - \frac{\gamma^k}{\text{Pr} \mu C_v} \right) \partial_2 (u_1^2 + u_2^2 + u_3^2) + \frac{\mu}{6} \partial_2 (u_2^2) + \frac{\gamma^k}{\text{Pr} C_v} \partial_2 E \right] \\ + & \partial_3 \left[\frac{\mu}{2} \left(1 - \frac{\gamma^k}{\text{Pr} \mu C_v} \right) \partial_3 (u_1^2 + u_2^2 + u_3^2) + \frac{\mu}{6} \partial_3 (u_3^2) + \frac{\gamma^k}{\text{Pr} C_v} \partial_3 E \right] + \text{c.d.}, \end{aligned} \quad (18)$$

where C_v is assumed const.

Now we can construct the functions \mathbf{U}_I , \mathbf{V}_I , and \mathbf{W}_I using equations (17) and (18).

Present Notation

NAS Benchmark Notation

$$\mathbf{U}_I = \text{Re}^{-1} = \begin{bmatrix} 0 \\ \frac{4}{3}\mu\partial_1 u_1 \\ \mu\partial_1 u_2 \\ \mu\partial_1 u_3 \\ u_I^5 \end{bmatrix} \equiv T = \begin{bmatrix} 0 \\ \frac{4}{3}k_3k_4\frac{\partial}{\partial\xi}\left(\frac{u^{(2)}}{u^{(1)}}\right) \\ k_3k_4\frac{\partial}{\partial\xi}\left(\frac{u^{(3)}}{u^{(1)}}\right) \\ k_3k_4\frac{\partial}{\partial\xi}\left(\frac{u^{(4)}}{u^{(1)}}\right) \\ t^{(5)} \end{bmatrix} \quad \text{where}$$

$$u_I^5 = \frac{\mu}{2} \left(1 - \frac{\gamma k}{\text{Pr}\mu C_v}\right) \partial_1 (u_1^2 + u_2^2 + u_3^2) + \frac{\mu}{6} \partial_1 (u_1^2) + \frac{\gamma k}{\text{Pr}C_v} \partial_1 E ,$$

and

$$\begin{aligned} t^{(5)} &= \frac{1}{2} (1 - k_1 k_5) \frac{\partial}{\partial\xi} \left[\frac{[u^{(2)}]^2 + [u^{(3)}]^2 + [u^{(4)}]^2}{[u^{(1)}]^2} \right] \\ &+ \frac{1}{6} \frac{\partial}{\partial\xi} \left[\frac{[u^{(2)}]^2}{[u^{(1)}]^2} \right] + k_1 k_5 \frac{\partial}{\partial\xi} \left[\frac{u^{(5)}}{u^{(1)}} \right] . \end{aligned}$$

Similarly, the correspondence between \mathbf{V}_I and \mathbf{V} , and, \mathbf{W}_I and \mathbf{W} , may be constructed.

4 Discussion of the Discrepancies

4.1 Physical Properties

- Comparison of elements 2–4 (i.e., the momentum equations) indicates that

$$k_3 k_4 = \text{Re}^{-1} \mu . \quad (19)$$

- Comparison of the energy equation indicates inconsistencies. The two forms may be reconciled if $t^{(5)}$ is correctly rewritten as

$$t^{(5)} = k_3 k_4 \left\{ \frac{1}{2} (1 - k_1 k_5) \frac{\partial}{\partial \xi} \left[\frac{[u^{(2)}]^2 + [u^{(3)}]^2 + [u^{(4)}]^2}{[u^{(1)}]^2} \right] + \frac{1}{6} \frac{\partial}{\partial \xi} \left[\frac{[u^{(2)}]^2}{[u^{(1)}]^2} \right] + k_1 k_5 \frac{\partial}{\partial \xi} \left[\frac{u^{(5)}}{u^{(1)}} \right] \right\},$$

where

$$k_1 k_5 = \frac{\gamma k}{\text{Pr} \mu C_v}. \quad (20)$$

Note: Although the above factor of $k_3 k_4$ is missing in the definitions of $t^{(5)}$, $v^{(5)}$, and $w^{(5)}$ (c.f. see pages 47–48 NAS-BM), it is correctly taken into account subsequently in the analytical evaluation of the various Jacobian matrices (c.f., see $n_{51} \dots n_{55}$; $q_{51} \dots q_{55}$; $s_{51} \dots s_{55}$ on pages 55–56 NAS-BM).

4.2 Discussion of the values of k_i , $i = 1, 5$

Although the values of k_i are immaterial insofar as the parallel implementation of the computational algorithm is concerned, we discuss here how well these values correspond to those encountered in a “real” CFD application code.

The suggested values in the NAS benchmark are as follows:

$$k_1 = 1.4, \quad k_2 = 0.4, \quad k_3 = 0.1, \quad k_4 = 1.0, \quad k_5 = 1.4.$$

However, the above appear in only three groups, viz., k_2 , $(k_1 k_5)$ and $(k_3 k_4)$. The first constant k_2 was found to be $k_2 = \gamma - 1$ (c.f. equation (16)). Since the ratio of specific heats, γ , for a diatomic gas is 1.4 (such as air which is composed mainly of $\text{N}_2 + \text{O}_2$), the above value for k_2 is appropriate.

Next, consider $k_1 k_5$ which is given by equation (20). Recall that $\text{Pr} = \frac{\mu_\infty^* C_{p\infty}^*}{k_\infty^*}$, and, hence,

$$k_1 k_5 = \frac{\gamma}{\text{Pr}_{\text{local}}},$$

where

$$\text{Pr}_{\text{local}} = \frac{\mu^* C_p^*}{k^*}.$$

For a very wide range of temperatures, $\text{Pr} \simeq 0.72$ (for air). Since $\text{Pr}^{-1} \simeq 1.4$, then the values of k_1 and k_5 specified by the NAS benchmark are appropriate.

On the other hand, for most flows of interest, $\text{Re} \sim \text{O}(10^6)$ or higher. Hence, the relatively high values of $k_3 k_4$ does not correspond well to the values in a typical “real” CFD code. However, since second-order central differences are used to discretize the governing equations, a low value of $k_3 k_4$ would produce non-physical oscillatory solutions. Therefore, a relatively high value of $k_3 k_4$ is chosen to circumvent such numerical difficulties in the solution of the synthetic PDE’s.

4.3 Discussion of Additional terms in the NAS benchmark

All such terms are associated with the constants $d_\xi^{(m)}$, $d_\eta^{(m)}$ and $d_\zeta^{(m)}$, $m = 1, 5$. An exact correspondence with the original N-S equations would be possible if the above constants are all zero; however, they are $\text{O}(1)$ in the NAS benchmark. Upon inspection of these terms, it is clear that they all represent an added second-order dissipation although this has not been explicitly stated in the text of the NAS-BM. In practice, a blend of second and fourth-order dissipation functions are usually incorporated into the discretized equations to suppress high-frequency, non-physical oscillations. However, such a second-order dissipation function with constants of $\text{O}(1)$ would produce incorrect (excessively diffused) solutions in a real CFD application. Note, however, that the inclusion of these terms does not alter the computational algorithm to solve these equations nor does it alter the communication pattern.

5 References

1. Bailey, D., Barszcz, E., Barton, J., Browning, D., Carter, R., Dagum, L., Fatoohi, R., Fineberg, S., Frederickson, P., Lasinski, T., Schreiber,

R., Simon, H., Venkatakrisnan, V. and Weeratunga, S., (1994) "The NAS Parallel Benchmarks," *RNR Technical Report RNR-94-007*.

2. Degani, A. T. and Fox, G. C., (1994) "Derivation of the Beam and Warming Algorithm for Compressible Navier-Stokes Equations," *SCCS-675*.