Deterministic and stochastic computations of mysterious internal flows: based on a nonlinear local correction method with global conservativity

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Abstract. The present paper shows a new approach for solving two types of fluid problems, which has recently emerged and has been an unsolved mysteriously for over 100 years. The first problem emerged recently is a very small amount of numerical errors comparable to pollutant emissions such as unburned hydrocarbon fuel (HC) and NOx at order of ppm or less. A new nonlinear numerical method of global and local corrections for the deterministic compressible Navier-Stokes equation for multi-components of gases is proposed and tested to overcome this first problem, while accurately evaluating fluid-dynamic instability related to turbulence and thermal efficiency as result of spatially-integrated thermodynamic quantities, related to total amount of CO2 exhausted, in power systems including combustion engines. It is stressed that the present nonlinear correction method applied for the stochastic Navier-Stokes equation is also effective for the second mysterious problem which has been unsolved for over 100 years, which is the spatial transition point from laminar to turbulent flows in pipes.

Keywords: Nonlinear local correction, Global mass conservation, Deterministic and stochastic, Computational Fluid Dynamics, Gas fuel, Engine.

1. Introduction

Convection terms in various fluid flows are nonlinear. Thus, people have been trying to numerically solve fluid flows by proposing approximate discretization methods for improving accuracy. [1,2,3,4,5,6] An important point is that we should physically reduce errors, not only mathematically with principles of truncation and round-off errors. For example, while spatial mathematical discontinuity such as shock wave and contact surface between components having different densities leads to numerical oscillation phenomenon on local physical density and unrealistic errors on divergence of velocity, spatial summation of mathematical errors appearing while solving large matrices, i.e., global integration in the total analytical domain, is deeply related to physical values such as thermal efficiency and power in energy systems.
Today, thermal efficiency should be improved for various power systems including combustion engines for usage on the ground as well as aerospace. Therefore, thermodynamic quantities must be evaluated accurately by computer simulations because numerical errors of a few percent regarding thermal efficiency as spatially-integral value \[11,16\] are often comparable to the target values set for improvement of energy systems \[27,28\]. However, there is a problem that most of traditional computational fluid dynamics for the deterministic compressible Navier-Stokes equation \[1,2,3,4,5,6,7,8\] does not aim to accurately evaluate the effects of both thermodynamic quantities including thermal efficiency, and fluid-dynamic quantities such as high-speed turbulent jets in power systems including engines, power plants, and fuel cells. This is because efforts are mainly devoted for accurately obtaining local accuracy on spatial variations of fluid-dynamic quantities such as turbulence and shock wave, i.e., for proposing new spatial numerical discretization methods. Each type of spatial numerical discretization method invariably generates some numerical errors on spatial variations of physical quantities, which lead to numerical errors of spatially-integrated thermal efficiency as result of cumulation.

Although finite element methods \[29\] may be expected to precisely evaluate thermodynamic quantities including thermal efficiency, a relatively small number of studies have been done for capturing phenomena such as fluid dynamic instability like turbulence with small numbers of grids. This is because finite element methods may need more computation time (CPU time) for less numerical errors, and also because we empirically know that numerical errors that are too small may relatively lead to more difficulty for capturing unstable phenomena such as that of transition to turbulence.\[9,21,22\] The present paper also shows a clue for solving the mysterious problems shown above.

2. Linear and nonlinear correction methods

In order to overcome the problem on numerical errors of spatially-integrated thermal efficiency, a previous numerical method of linear correction of the form like

\[ f^* = f + \Delta f, \]

where the correction amounts for conservations of physical quantities \( f \) of density, pressure, velocity, and temperature are denoted as \( \Delta f \) with \( f^* \) as the corrected ones, for single components, \[10,11\] show a better possibility to compute both thermodynamic quantity and fluid-dynamic quantity, for low Mach numbers in a subsonic regime, because spatial variations of the fluid dynamic pressure are relatively small in comparison with the space-averaged thermodynamic pressure. However, the linear correction method has not been tested for transonic and supersonic flows.

Then, the linear correction method for problems with multi-species is not useful for accurately evaluating small amount of densities such as fuel, which will be equivalent to emissions including unburned hydrocarbon, because the linear correction due to addition of \( \Delta \rho \) as a base up for density at each computational grid point may logically produce unrealistic error of small densities at each grid point, comparable to the small amount of emissions such as unburned hydrocarbon fuel (HC) and NOx at order of ppm or less.

There are other types of correction methods including the level set methods \[7,8\], which is useful to resolve discontinuous phenomena including contact surfaces. However, these do not aim to reduce numerical errors on global quantities such as thermodynamic quantities like
thermal efficiency.

Thus, in this present paper, we will propose a new nonlinear correction method having the form of

\[ f^* = f \cdot (1 + \Delta f), \]

for fluid dynamic problems with multi-species, which has a possibility to overcome both of the above problems: unrealistic “local” error of small densities at each grid point due to the linear correction method, and also “global” numerical errors of thermodynamic quantities such as thermal efficiency, which could not be considered in traditional correction methods.

In Section 3 of this paper, to check whether or not the nonlinear correction method (globally-conserved and nonlinear local correction method) is useful, we examine two types of internal flow problems with two species, by solving the deterministic Navier-Stokes equation. The first problem is a one-dimensional flow in a shock-tube with a closed domain, while the second one is a three-dimensional high-speed gas jet entering from a narrow straight nozzle into a large chamber.

Moreover, in Section 4, we will show further computation results on the transition point inside a straight nozzle (pipe) from laminar to turbulent flows, which varies according to disturbance at the inlet of the nozzle. Although this is a mysterious problem which has been unsolved for over 100 years since Reynolds first experimentally found it, the nonlinear correction method applied to the stochastic Navier-Stokes equation, with a stochasticity (indeterminacy) theoretically determined in our previous papers [9,21,22], solves the mystery, and also gives an insight to reveal the reason why asymmetric flows including jets and the Karman vortex streets appear in symmetric analytical domains.

3. Computations corrected for the derministic Navier-Stokes equation

3.1. The deterministic compressible Navier-Stokes equation and basic numerical algorithms

Equations (1)-(4) for quantities of \( u_i, T, \rho, \) and \( p \) denoting velocity vector, temperature, density, and pressure are momentum, energy, and mass conservation laws of all species and only fuel, with Eq. (5) as the equation of state, for the large eddy simulation (LES), while \( t \) denotes time, and physical quantity \( F_{i,j} \) implies \( \partial F_i/\partial x_j \) with space \( x_j \) (when \( F_i \) such as velocity vector for example) [25,26] with subscripts \( \text{mix} \) and \( \text{fuel} \) referring to all of the components in the flow field, and only fuel, respectively. [10,11,12]

\[
\frac{Du_{i,j}}{Dt} = -\frac{1}{\rho_{\text{mix}}} p_{\text{mix},j} + \nu_{\text{mix}} \left( u_{i,j} + u_{j,i} - \frac{2}{3} u_{k,k} \delta_{ij} \right)
\]

\[
\frac{DT_{\text{mix}}}{Dt} = -\frac{1}{C_{\text{p,mix}} - R_{\text{mix}}} \frac{p_{\text{mix}}}{\rho_{\text{mix}}} \frac{1}{D} + \frac{1}{C_{\text{p,mix}} - R_{\text{mix}}} \frac{1}{\rho_{\text{mix}}} \left\{ -k_{T,j} T_{j} + \nu_{\text{mix}} \times \rho_{\text{mix}} \left( u_{i,j} + u_{j,i} - \frac{2}{3} u_{k,k} \delta_{ij} \right) u_{i,j} \right\}
\]

\[
\overline{D} = -\frac{C_{\text{p,mix}} - R_{\text{mix}}}{C_{\text{p,mix}}} \frac{1}{p_{\text{mix}}} \frac{Dp_{\text{mix}}}{Dt} + \frac{1}{\rho_{\text{mix}} C_{\text{p,mix}}} \frac{T_{\text{mix}}}{Dt} \left\{ -k_{T,j} T_{j} + \nu_{\text{mix}} \times \rho_{\text{mix}} \left( u_{i,j} + u_{j,i} - \frac{2}{3} u_{k,k} \delta_{ij} \right) u_{i,j} \right\}
\]
\[ \frac{D\rho_{\text{tot}}}{Dt} = -\rho_{\text{tot}}u_i + D_i \rho_{\text{tot},i} \]  
(4)

\[ \rho_{\text{mix}} = \rho_{\text{mix}} R \frac{T_{\text{mix}}}{T} \]  
(5)

In Eq. (3), quantity \( \bar{D} \) is defined as the divergence of velocity [10,11], i.e.,

\[ \bar{D} \equiv u_{,i} = \frac{\partial u_i}{\partial x_i} \]

Quantity \( \delta_{ij} \) denotes the Kronecker delta (\( \delta_{ij}=1 \) for \( i=j \), otherwise \( \delta_{ij}=0 \)), while \( C_p \) is the specific heat at constant pressure dependent to temperature, and \( R \) is the gas constant of mixed gas. [12] In the present paper, we use the equation of state for perfect gas because the real gas effect ascribable to hydrogen gas at nearly atmospheric temperature is fairly small.

For Eqs. (1)-(5), the spatial averaging (filtering) for computational grid size is also performed, due to LES.

Heat flux \( k_{TT} \) is calculated with the turbulent thermal diffusion constant \( k_T \), while \( \nu_T \) and \( D_T \) is the turbulent eddy viscosity and turbulent diffusion coefficient. [The turbulent coefficient of kinematic viscosity according to filtering between the scale for doing continuum assumption and grid size is the Yakhot-Orszag subgrid turbulence model [13].]

Turbulent thermal- and mass-diffusion coefficients are also calculated by using the Schmidt number of 0.7 [14] and Prandtl number of 0.71 [13]. The influence of constants in the subgrid turbulence models for LES on the mass diffusion process is not large [14]. Thus, we use this value for the Schmidt number, which is often used.

In order to numerically solve Eqs. (1)-(5), we use a computational method identical to that of the C-CUP method [6]. This algorithm, which mathematically matches well the governing equation systems in Eqs. (1)-(5) shown above, makes it possible to uniformly handle both compressible and incompressible flows in the same calculation domain. Equation (3) is important to explicitly reduce numerical errors of divergence of velocity, i.e., that of local density.

This C-CUP method includes the CIP method for the convection terms in Eqs. (1) and (2), which is with a higher order of accuracy [5], because the CIP method uses a cubic interpolation function with less numerical diffusion. Then, the wave-Poisson equation of pressure appearing in the C-CUP method [6] can be done by an inverse matrix calculation of the successive over-relaxation (SOR) method [15]. Here, the iterations in the SOR method are stopped when numerical variation of pressure during two iteration timings, which is divided by the initial pressure value at the inlet, become less than \( 3.0 \times 10^{-6} \), i.e., the criterion that we have employed for various problems [11,16]. An interpolation check is also added during this calculation to control nonphysical oscillation and to maintain monotonicity [17].

In Section 3, two types of problems are analyzed: one-dimensional flow in a shock-tube with a closed domain (Fig. 1(a)) and a three-dimensional jet injected from a narrow nozzle into a large chamber (Fig. 1(b)). Boundary and initial conditions are given in each sub-section.
3.2. The linear and nonlinear correction methods for computations of flows in a multi-component system

For energy systems such as engines or closed reactors, thermodynamic quantities must be evaluated accurately by computer simulations because numerical errors of a few percent concerning performance such as efficiency [11,16] are often comparable to the target values set for improvement of energy systems [27,28], and also because emissions such as unburned hydrocarbon fuel (HC), soot, and NOx are of the order of ppm, much smaller than percent.

(a) Linear correction method:
By using the linear correction method described in our previous papers [10,11], spatially averaged values of density, temperature, and pressure, in the total domain $V_{all}$ for an analysis such as combustion chamber in engine, are evaluated accurately. The linear correction method of mass conservation of the form of $\rho^* = \rho + \Delta \rho$, where $\rho^*$ denotes the density after correction with $\Delta \rho$ as the additional correction term, is shown in Eq. (6).

$$
\rho^*_g(t,x_i) = \rho_g(t,x_i) + C_{ex} \times \left( \int_{V_{all}} \rho_g(t=0,x) dV + \int_{t=0}^{t} \int_{V_{all}} \rho_g t dV dtdx \right) \int_{V_{all}} dV
$$

$$
\rho^*_g(t,x_i) = \rho_g(t,x_i) + C_{ex} \times \left( \int_{V_{all}} \rho_g(t=0,x) dV + \int_{t=0}^{t} \int_{V_{all}} \rho_g t dV dtdx \right) \int_{V_{all}} dV \tag{6}
$$

(b) A jet flow injected from a narrow nozzle into a large chamber such as those in engines. The electric valve installed in the nozzle is shown in red.

Figure 1: Computational domains.
The subscript $g$ means either mixed gas (total density obtained by summation of all component species in the flow field), or only fuel, while the superscript $* \text{ indicates the value after correction}$, $\dot{m}$ denotes the fuel mass injected per time entering from the outer region of the analytical domain, $C_{\text{cor}}$ is an arbitrary constant between 0 and 1, and $t$ and $x_i$ denote time and space. [Although $\dot{m}$ has a certain value in cases which the flow enters from an inlet boundary such as the valve in the injection nozzle shown in Fig. 1(b), $\dot{m} = 0$ for Fig. 1(a).]

The numerator in the second term of the right hand side of Eq. (6),

$$
\left( \int_{V_{\text{all}}} \rho_g(t = 0, x_i) dV + \int_{t>0} \dot{m} dt \right) - \int_{V_{\text{all}}} \rho_g(t, x_i) dV
$$

implies the difference between total mass “entering” into the domain (overall mass “entering” evaluated by using velocity and density at the inlet of analytical domain, plus initial mass in the domain) and mass actually “existing” in the domain (total mass “existing” at time $t$ in the total domain volume $V_{\text{all}}$ such as combustion chamber in an engine). Thus, if there is no numerical error, this second term is 0.0. However, generally in numerical computations, the second term is slightly larger or smaller than 0.0. For example, if the second term is slightly larger than 0.0, mass “entering” at the inlet is more than mass existing (entered). It is stressed that the linear correction of density based on the second term in the right hand side of Eq. (6) is performed with the form of addition at each point in the total analytical domain. Equation (6) locally corrects the densities, while overall mass in the total domain $V_{\text{all}}$ for analysis such as combustion chamber in an engine is completely conserved.

Let us think about a jet flow injected from a narrow nozzle into a large chamber such as those in engines, shown in Fig. 1(b). Emphasis is placed on the fact that, for multi-component systems, this correction method of linear addition shown in Eq. (6) may often result in unrealistic non-zero density in the chamber far from the injection point of the jet, although the actual density of the fuel gas injected from the nozzle is zero in the chamber during a certain period from the onset of injection. This non-zero density in the region without fuel appears because the linear correction based on Eq. (6) is performed with the form of addition at each point in the analytical domain of the chamber and nozzle, having an effect like a “base-up”. This may result in a miscalculation of the penetration length of the jet.

(b) Nonlinear correction method:
Here, we propose a new nonlinear numerical method of correction (globally-conserved and nonlinear local correction method), shown as Eq. (7), for a wide range of Mach numbers including transonic and supersonic flows.

While the subscript $g$ means either mixed gas (total amount of all component species), or only fuel, Eq. (7) used for correcting $\rho_{\text{mix}}$ as density of air-fuel mixture brings precise values of thermal quantities such as total mass inside chamber, which also leads to accurate temperature and thermal efficiency, while Eq. (7) for $\rho_{\text{fuel}}$ maintains the fuel density to be zero at grid points where injected gas does not actually exist, which leads to accurate evaluations of penetration length and fuel vapor distribution.

$$
\rho_g^* (t, x_i) = \rho_g(t, x_i) \times \frac{\int_{V_{\text{all}}} \rho_g(t = 0, x_i) dV + \int_{t>0} \dot{m} dt}{\int_{V_{\text{all}}} \rho_g(t, x_i) dV}
$$

(7)
The superscript * indicates the value after correction, and $\dot{m}$ denotes the fuel mass injected per time entering from the outer region of the analytical domain, such as the valve in the injection nozzle shown in Fig. 1 (b), while $t$ and $x$ denote time and space.

For both the densities of the mixture and fuel, corrections based on Eq. (7) are done by multiplying the correction form of

$$
\int_{V_{all}} \rho_g (t=0,x_i) dV + \int_{t>0} \dot{m} dt

\int_{V_{all}} \rho_g (t,x_i) dV.

$$

(8)

When total mass existing in the chamber,

$$
\int_{V_{all}} \rho_g (t,x_i) dV,
$$

is different from the mass entering,

$$
\int_{V_{all}} \rho_g (t=0,x_i) dV + \int_{t>0} \dot{m} dt,
$$

due to some numerical errors, densities are corrected.

It is logically emphasized that the nonlinear correction method, i.e., multiplication of the nonlinear correction term in Eq. (7), essentially differs from that of the linear correction method, i.e., Eq. (6). Equation (7) is important, because usage of Eq. (6), or without usage of any correction, may often lead to non-zero density in regions without fuel, due to numerical oscillations around contact surface between gas fuel and oxygen, even though numerical schemes with a higher-order of accuracy such as the CIP methods, TVD methods, or compact schemes [1,2,3,4,5,6] are employed for convection terms. Even a small amount of false non-zero density will result in unrealistic unburned fuel (HC) at level of ppm.

In this paper, to check whether or not the nonlinear correction method (globally-conserved and nonlinear local correction method) is useful, we examine two types of jet flow problems with two-species. The first problem is for only a straight pipe, which is completely closed, such as a shock tube, shown in Fig. 1(a). The second problem is for the whole domain shown in Fig. 1(b).

### 3.3. Application to one-dimensional flow in a straight pipe

The first problem analyzed is for only a straight pipe, which has a completely closed domain, such as a shock tube [18,19]. (Fig. 2) After a partition (diaphragm) lying between two initial regions of high pressure fuel (hydrogen) at upstream, and low pressure oxygen at downstream is broken (Fig. 2 (a)), a flow having a shock wave is produced (Fig.2 (b)).

Figure 3 shows an example of the computational results of the spatial distribution of pressure, density of mixed gas, and hydrogen gas density for a closed straight pipe, obtained without any correction (Case A), with the previous linear correction method shown in Eq. (6) (Case B), and with the new nonlinear correction method shown in Eq. (7) (Case C). [Pressure and density of mixed gas are demonstrated in Fig. 3(a), while hydrogen gas density is shown in Fig. 3(b).]
The region with high pressure at the upstream region (0 < x < 2.5 m at t = 0 ms) expands to the downstream region, while there is a flow having shock wave. (Fig. 3, pressure distribution) The traveling speed of shock front for the three cases are 675 m/s (Case A), 681 m/s (Case B), and 681 m/s (Case C), while the theoretical speed is 680 m/s [19]. The numerical errors between the three cases on the traveling speed of shock front can not clearly be observed in Fig. 3, because the numerical error is only about 1.0 %. However, computation results obtained with the linear and nonlinear corrections agree well with the theoretical value. Also, the ratio between the pressures after and before the shock wave (4.89 for Case A, 4.75 for Case B, and 4.75 for Case C) is close to the theoretical value obtained by the Rankine-Hugoniot equation, 4.80 [12,19].

Computational results obtained by the linear and nonlinear correction methods accurately compute the total mass inside the straight pipe for both mixed gas and hydrogen gas, although computations without corrections result in some numerical errors. (Tables 1 and 2) It is noted that the nonlinear correction method gives the best result.

Next, Table 3 shows another important point, that the previous linear correction method with Eq. (6) often miscalculates with unrealistic gas fuel of the order of 0.1% (against the initial gas fuel density in the high pressure region, 0.2512 kg/m$^3$) in the right hand side (x > 4 m), although there is initially no fuel, and also there shoud be no fuel in the right hand side (x > 4 m) of the straight pipe at t = 1.5 ms. This problem of very small amount of unrealistic fuel shown in Table 3 comes from numerical error related to numerical instability around discontinuous physical quantities. On the other hand, the nonlinear shape of Eq. (7) maintains the fuel density to be zero at grid points where injected gas does not exist. (Table 3)

Figure 2: Flow in a shock tube. (a) The initial pressure distribution. (b) Pressure distribution after breaking of the diaphragm.
Figure 3: Time evolution of the spatial distribution of (a) Pressure and density of mixed gas, and (b) Density of hydrogen gas, for the three cases: (Case A) Without correction method, (Case B) With linear correction method \((C_e=0.1)\), and (Case C) With nonlinear correction method. Initial condition for the high pressure region filled with hydrogen \((0<\text{x}<2.5 \text{ m})\) is pressure of 0.31 MPa and density of 0.252 kg/m\(^3\), while low pressure region filled with oxygen \((2.5<\text{x}<6.0 \text{ m})\) is pressure of 0.04 MPa and density of 0.516 kg/m\(^3\). The initial temperature and velocity is 298 K and 0 m/s, respectively, for the whole computation domain \(V_{\text{all}}\) \((0<\text{x}<6 \text{ m})\). Grid size \(\Delta x=6.0 \text{ mm}\), with total of 1000 grid points. The time step \(\Delta t=5.0\times10^{-7} \text{ s}\), while the Courant number \(\approx 0.036\) when evaluated with the velocity of hot gas after the shock front, 433 m/s. As the analytical domain is closed, the boundary condition for velocity is zero at both ends of the shock tube, while the Neumann condition is given for pressure and temperature, i.e., zero gradient for the direction normal to the boundary wall.
Table 1: Error of the total mass of mixed gas at $t=1.5$ ms against initial value (2.444 kg)

| Without correction method (Case A) kg | With linear correction method (Case B) kg | With nonlinear correction method (Case C) kg |
|--------------------------------------|------------------------------------------|------------------------------------------|
| -9.002\times10^{-4}                 | 1.074\times10^{-6}                       | 6.617\times10^{-14}                       |

Table 2: Error of the total mass of hydrogen gas at $t=1.5$ ms against initial value (0.6248 kg)

| Without correction method (Case A) kg | With linear correction method (Case B) kg | With nonlinear correction method (Case C) kg |
|--------------------------------------|------------------------------------------|------------------------------------------|
| -1.108\times10^{-3}                 | -4.958\times10^{-6}                      | 0.000                                   |

Table 3: Hydrogen gas density at each point of analytical domain at $t=1.5$ ms

| Distance m | Without correction method (Case A) kg/m$^3$ | With linear correction method (Case B) kg/m$^3$ | With nonlinear correction method (Case C) kg/m$^3$ |
|------------|---------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| 0.0        | 0.2521                                       | 0.2523                                        | 0.2522                                        |
| 1.0        | 0.2050                                       | 0.2052                                        | 0.2052                                        |
| 2.0        | 0.1793                                       | 0.1794                                        | 0.1794                                        |
| 3.0        | 0.1793                                       | 0.1794                                        | 0.1794                                        |
| 4.0        | 0.0000                                       | 2.300\times10^{-4}                           | 0.0000                                        |
| 5.0        | 0.0000                                       | 2.300\times10^{-4}                           | 0.0000                                        |
| 6.0        | 0.0000                                       | 2.300\times10^{-4}                           | 0.0000                                        |

3.4. Application to a three-dimensional jet flow injected into a large chamber

Next, Figs. 4 and 5 show examples of the three-dimensional computational results of a hydrogen-fuel jet flow injected into the large constant-volume chamber initially filled with only air in Fig. 1(b), which are obtained with the previous linear correction method shown in Eq. (6) and the new nonlinear correction method shown in Eq. (7), respectively.

We confirmed that the computational results obtained by the linear and nonlinear correction methods accurately compute the total mass inside the straight pipe, although computations without corrections result in some numerical errors for total mass, i.e., less conservativity.

However, application of the linear correction method of Eq. (6) to the jet flow in this multi-component system resulted in unrealistic non-zero density, i.e., a small amount of false fuel density of the order of 1% (against density of the high pressure fuel tank), as in Fig. 4(b), whereas there is no fuel density around the solid chamber wall in Fig. 5(b) obtained with the nonlinear correction method. This implies that the gas jet has already reached the right wall (at the right end in Fig. 4), although actually the jet has only reached about halfway across the chamber, i.e., although the density of the injected fuel gas inside the chamber is zero during a certain period from the onset of injection (Fig. 4). This results in the false penetration length of gas jets with unrealistic gas fuel density of the order of 1%.
This unrealistic non-zero density at grid points having no actual gas fuel appears because the linear correction is performed with the form of addition at each point in the analytical domain of the chamber and nozzle, i.e., having an effect like a “base-up”, although the addition is very small. This prediction failure of penetration length will also lead to small amounts of unrealistic emissions including hydrocarbon (HC), i.e., unburned fuel.

Of course, traditional computational fluid dynamics without linear corrections may also lead to certain amount of unrealistic non-zero gas fuel, which is related to numerical oscillation around the contact surface between gas fuel and oxidant or around shock wave. This problem, shown in Fig. 4, is also related to a very small amount of gas fuel caused by numerical error resulting from numerical instability around discontinuous physical quantities.

Emphasis is placed on the fact that the nonlinear correction method of Eq. (7) maintains the fuel density to be zero at grid points where injected gas does not exist, because multiplication of zero by no fuel is zero (Eq. (7) and Fig. 5).

Figure 4: Three-dimensional LES of a high-speed gas jet flow done with the linear correction method. (a) Spatial distributions of hydrogen gas density (top) and pressure (bottom) at 0.895 ms at the cross section at the chamber center. Computed with initial tank pressure of 10 MPa (density of 8.27 kg/m$^3$) and initial chamber pressure of 3.5 MPa for initial atmospheric temperature. (b) Scale-up figure of hydrogen gas density distribution inside the chamber with magnified scale (top) and hydrogen density along the center jet axis (bottom) at 0.895 ms. For the solid walls in analytical domain except for the inlet, the boundary condition for velocity is zero, while the Neumann condition is given for pressure and temperature, i.e., zero gradient for the direction normal to the boundary wall. At the inlet lying at the upstream end of the nozzle, constant conditions of pressure, temperature, and density in the fuel tank are employed. Grid size $\Delta x=\Delta y=\Delta z=0.21$ mm, with total of 5,100,000 (472×104×104) grid points. The Courant number is set to be 0.1, while the time step $\Delta t \approx 0.14 \times 10^{-7}$ s, when evaluated with the largest velocity of hydrogen gas, nearly 1500 m/s.
Figure 5: Three-dimensional LES of a high-speed gas jet flow done with the nonlinear correction method. (a) Spatial distributions of hydrogen gas density (top) and pressure (bottom) at 0.895 ms at the cross section at the chamber center. Computed with initial tank pressure of 10 MPa (density of 8.27 kg/m³) and initial chamber pressure of 3.5 MPa for initial atmospheric temperature. (b) Scale-up figure of hydrogen gas density distribution inside the chamber with magnified scale (top) and hydrogen density along the center jet axis (bottom) at 0.895 ms. The boundary conditions and other conditions of computation are the same as those of Fig. 4.

In addition, if we compulsorily neglect the region with the unrealistic non-zero fuel density due to the linear correction in Fig. 4(b) (about 55 mm<x<70 mm), the compulsorily shortened penetration length coincides with that obtained with the nonlinear correction, shown in Fig. 5(b). However, because the threshold value for compulsory neglection will change for various conditions such as jet speeds, initial pressure ratios, and chamber geometries, the nonlinear correction method considering physics is much better.

Moreover, on the penetration length, computation results with the nonlinear correction method is similar to computation results without corrections, which agrees with experiment results on the penetration length of the hydrogen jet [20].

4. Corrected computations for the stochastic Navier-Stokes equation: Trial to reveal the transition point from laminar to turbulent flows in a nozzle (pipe)

The above results for jet flows with the new nonlinear correction method, which indicate improvement on local and global numerical errors, lead to and recall two new and old mysteries in computational fluid dynamics.

First is that lots of traditional computations for jet flows injected from straight nozzles reported for over 30 years do not examine the influence of disturbance at nozzle inlet on transition to turbulence in nozzle, i.e., whether or not movement of spatial transition point from laminar to turbulent flows in a nozzle (pipe) according to increasing inlet disturbance varies jet flow expanding after entering into a large chamber. This problem in a straight nozzle (pipe) is a very old problem unsolved for over 100 years, after Reynolds first revealed it
experimentally, whereas transition to turbulence in open regions such as that on flat plates or airfoils are explained theoretically and computationally.

Just to be sure, computations for jet flows in the above section are with Reynolds number \( Re = 2.6 \times 10^6 \), so that transition to turbulence in a nozzle will occur at a very early stage around the fuel tank. Thus, the relation between inlet disturbance and transition point is not very important in the above section. However, we should consider further in cases with lower Reynolds numbers, i.e., as the next step in the near future.

Second is the reason why turbulent flows expanding in a large chamber can become asymmetric in computations, even though traditional boundary conditions and our boundary conditions for computations used in Section 3 are deterministic without any disturbance at the inlet, i.e., we use symmetric boundary condition at the inlet. (To be sure, even the Reynolds-averaged Navier-Stokes equation (RANS) and its boundary condition are deterministic without any disturbance such as that due to random number.) In experiments for a straight nozzle (pipe), disturbance at the inlet, i.e., indeterminacy in the outer upstream region, leads to asymmetric flow, i.e., turbulence.

We should further think about these two mysteries, by including numerical errors, because there should be no asymmetric flows in computations of the jet flow in Section 3, if without any numerical errors.

Therefore, we try to analyze these problems by using the nonlinear correction method shown above, while the other type of approach is also included, which is a stochastic Navier-Stokes equation with a new type of boundary condition. (“Stochastic” or “stochasticity” is a mathematical term, while “indeterminant” or “indeterminacy” is a physical term.)

4.1. Indeterminacy, stochasticity, disturbance, and numerical errors on the divergence of velocity

Although we use the deterministic Navier-Stokes equation [12] in Section 3, we here employ the stochastic Navier-Stokes equation obtained by averaging clusters of molecules in a little smaller volume than that for the continuum assumption. [9,21,22]

The basic idea, shown in Fig. 6, is that physical quantities such as velocity, pressure, temperature, and density are intentionally averaged in a mesoscopic window (MW) being a spatial window on a scale smaller than that for continuum mechanics, in order to resolve the minimum scale (Lms) dominating the phenomenon, which is between molecular mean free path (Lmfp) and the fluid particle size (Dc) [12] (as continuum like the Kolmogorov scale), which is also mesoscopic window size for averaging (Dmw). For some cases, this will be important because spatial variations of physical quantities smaller than the fluid particle may give influence on the flow field, i.e., for example, that in the boundary layer thickness around the inlet of nozzle (pipe) much thinner than the Kolmogorov scale, although the number of molecules inside the window Dmw varies, and also the physical quantities are a little vague, i.e., indeterminant, when the smaller spatial window for averaging, including a small number of molecules, moves to the right and left a little. (The number of molecules in Fig. 6b, less than that in Fig. 6a, leads to more indeterminacy.)

As a result, a mesoscopic equation in the form of a stochastic partial differential equation for the field, for example, stochastic Navier-Stokes equation, is obtained with stochastic fluctuations with indeterminacy, in which stochasticity comes from the discontinuity of molecules. [9,21,22]
The stochastic partial differential equation obtained by averaging in a smaller averaging window (mesoscopic window size: Dmw), for the physical quantity \( f(t, x_i) \) such as density, fluid velocities, pressure, and temperature defined in four-dimensional space of time \( t \) and space \( x_i \), can be written as

\[
L f(t, x_i) = q(t, x_i) + \varepsilon(t, x_i)
\]

with a partial difference operator \( L \) on time and Euclid space, a source term \( q \), and stochastic fluctuation \( \varepsilon \) implying the indeterminacy due to the mesoscopic window size (Dmw).

Figure 6: Indeterminacy \( \varepsilon \) generated by a mesoscopic window size smaller than that of continuum mechanics. a: Weak stochasticity in density averaged in a larger window. b: Stronger stochasticity in density averaged in a smaller window. [Size of mean free path: Lmfp; Mesoscopic window size for averaging: Dmw; Minimum scale dominating the phenomenon: Lms; Continuum assumption window: Dc] It should be stressed that indeterminacy \( \varepsilon \) exists even for zero kelvin of temperature, i.e., even when there is no molecular motion. c: Diagram of the flow inside a straight pipe. Diagrams a and b are enlarged views of the turbulent flow inside the straight pipe. (For a fluid particle, the size of the circle in Fig. 6a should actually be much larger than the molecular mean free path.)

Next, we must determine the strength of stochastic fluctuation with indeterminacy \( \varepsilon \). Then, the size volume for averaging (Dmw), which is also the minimum scale (Lms) dominating the phenomenon, can be chosen so that the level of “indeterminacy” at inlet \( \delta \) is identical to “indeterminacy” \( \varepsilon \) in the analytical domain, because both of \( \delta \) and \( \varepsilon \) are indeterminant. (Fig. 6c) [9,21,22]

As a result, the relation between \( \varepsilon \), i.e., stochasticity in a nozzle (pipe) approximated by a random number, and inlet disturbance \( \delta \), which is also approximated by a random number, is described by Eq. (9).
Stronger inlet disturbance $\delta$ results in early transition to turbulence, because stronger inlet disturbance leads to more inhomogeneous velocity distributions at the starting point of instability inside the laminar boundary layer, i.e., smaller mesoscopic window ($D_{mw} = L_{ms}$) and larger $\varepsilon$. Thus, Eq. (9) is used in this study,

$$\sum_{n=1}^{N} |\varepsilon| / N = C_\varepsilon |\delta|$$

with an arbitrary constant $C_\varepsilon$ and the number of grid points $N$. In this paper, $C_\varepsilon$ is set to be of the order of 1.0.

In our previous papers [9,21,22], we intuitionistically consider that disturbances remain at each computational grid point, as numerical errors of divergence of velocity, may be similar to random disturbance in mathematics, or random number generators in computer programs. Thus, we can use numerical errors of divergence of velocity instead of random number generators. However, we here use random numbers for stochasticity (indeterminacy) of $\varepsilon$ and $\delta$ because numerical errors of divergence of velocity are extremely reduced by employing a staggered grid system.

### 4.2. The stochastic Navier-Stokes equation and basic numerical algorithm

Here, we analyze the spatial transition point from laminar to turbulent flows in a nozzle (pipe), which is related to disturbance level at the inlet. There are less experimental data at high Mach numbers on this theme, because it is difficult to perform quantitative experiments. Thus, we here examine incompressible flows of $Re = 20,000$ in a straight nozzle (pipe). Temporal and spatial derivatives of density in Eqs. (1)-(4) are eliminated and simplified to the stochastic Navier-Stokes equation of Eq. (10), [9,21,22]

$$F = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} \bar{D} \\ \frac{Du_i}{Dt} + \frac{\partial p}{\partial x_i} - \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j^2} \end{bmatrix} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \end{bmatrix}$$

with indeterminacy $\varepsilon_1$ and $\varepsilon_2$ for mass and momentum conservation laws, respectively.

The numerical algorithm is basically the Marker and Cell (MAC) method [15]. As the numerical discretization for the convection term, an upwind scheme having a third-order of accuracy proposed by Kawamura and Kuwahara is employed. [10,11].

Here, the Poisson equation of pressure, obtained by taking the spatial derivation of the second one among Eq. (10), is additionally computed for improving accuracy, which can be done by an inverse matrix calculation of the successive over-relaxation (SOR) method [15].

In Section 4, three-dimensional computations inside a straight pipe are performed in order to examine the relation between the spatial transition point from laminar to turbulent flows and inlet disturbance level. As the initial condition, a potential flow for velocity and pressure is given. As the boundary condition on the pipe wall, we set the Neumann condition for pressure (zero pressure gradient at the direction normal to wall) with zero velocity on wall, with a homogeneous velocity profile at the pipe inlet, and the Neumann condition for velocity (zero gradient along the direction of the main flow) at the outlet.
4.3. Nonlinear correction method for velocity

In this section, we examine an incompressible flow in a straight nozzle (pipe). Thus, by using Eq. (11), the nonlinear correction is performed for velocity, for only $u_1$ in the direction of the main flow $x_1$,

$$u_1^* = u_1 \times \frac{Q_{in}}{Q_{out}}$$  \hspace{1cm} (11)

where $Q_{in}$ and $Q_{out}$ denote masses at inlet and outlet of the straight nozzle (pipe), respectively. (In the present paper, Eq. (11) is deterministic. However, formulation including indeterminacy of $Q_{in}$ and $Q_{out}$ may also be possible.)

4.4. Application to the transition to turbulence in a straight nozzle (pipe)

Table 4 shows the computational conditions including disturbance level at the inlet. Figure 7 demonstrates an example of time-dependent computational velocity distributions, in which velocity fluctuation, the transition to turbulence, occurs around the middle of the straight nozzle (pipe), at dimensionless distance $x/D=10$, in case of the inlet disturbance $\delta=3.8\%$, whereas computational results of dimensionless transition distance is $x/D=8$, in case of the inlet disturbance $\delta=5.5\%$. The present distances from the inlet to the transition point agree with experimental data [23] well. Figure 8 shows that the computational turbulence intensity also agrees with the experimental one [24] well. Thus, it is noted that the present nonlinear correction method is also effective for low Mach numbers.

| Table 4: Computational conditions |
|----------------------------------|
| Reynolds number                  | Re= 20,000                      |
| Grid type                        | Staggered                       |
| The number of grid points        | $2500 \times 50 \times 300$ (about 37,500,000) |
| Grid size                        | $\Delta x_1 = \Delta x_2 = \Delta x_3 = 0.02$ |
| Time increment                   | $\Delta t=0.001$                |
| Dimensionless time               | $t=0-100$ (0-100000step)        |
| Courant number                   | $c=U_0/\Delta t/\Delta x_1 = 0.05$ |
| Inlet disturbance level against main flow speed $U_0$ | $\delta/U_0 = 5.5, 3.8\%$ |
Figure 7: Velocity distribution computed on the center surface of a straight nozzle (pipe) \((t=0-100)\). Inlet disturbance \(\delta=3.8\%\), solved with the nonlinear correction method for velocity.

Figure 8: Distribution of turbulence intensity. Inlet disturbance \(\delta=3.8\%\)  
(a) Computation with the nonlinear correction method for velocity at \(x/D=40.0, x_3/D=0.5\) (b) Experiment taken by Laufer, 1950 [24].
5. Conclusions

The present nonlinear correction method based on Eq. (7) can reduce both global numerical errors on total and component masses such as fuel, as well as local numerical errors on the small amount of components such as fuel, while this correction method is simple. Thus, it is very important and necessary for evaluating performance such as thermal efficiency and emissions of engines and power systems. It is also stressed that the nonlinear correction method is effective even for transonic and supersonic flows, whereas the linear correction may be unsuitable for transonic and supersonic regimes, where density, pressure, and temperature all vary in space and time, resulting in strongly nonlinear tendencies.

Others who have written research papers might forcefully eliminate the small amount of numerical errors by using built-in mathematical functions such as MIN or MAX. However, artificial corrections using these functions are not versatile, because the cut-off level for MIN and MAX varies according to each problem. Although there are more accurate discretization schemes now and in the future, approaches based on discretization cannot guarantee “zero” on error for global quantities in principle.

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