NUMERICAL EVALUATION OF MASS-DIFFUSIVE COMPRESSIBLE 
FLUIDS FLOWS MODELS

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Abstract
This contribution presents first numerical tests of some recently published alternative models for solution of viscous compressible and nearly incompressible models. All models are solved by high resolution compact finite difference scheme with strong stability preserving Runge-Kutta time stepping. The two simple but challenging computational test cases are presented, based on the double-periodic shear layer and the Kelvin-Helmholtz instability. The obtained time-dependent flow fields are showing pronounced shear and vorticity layers being resolved by the standard as well as by the new mass-diffusive modified models. The preliminary results show that the new models are viable alternative to the well established classical models.

Keywords: compressible Navier-Stokes, nearly incompressible flow, mass diffusion, compact finite-difference

1 Introduction
Theoretical analysis and numerical solution of various fluids flows problems poses a challenging problem. The widely used mathematical models describing the compressible fluids flows and incompressible fluids flows are the Navier-Stokes-Fourier and the Incompressible Navier-Stokes systems respectively. These are mixed type systems of non-linear strongly coupled partial differential equations of hyperbolic, parabolic and elliptic type. Their mathematical analysis as well as numerical solution remains one of the most difficult problems of contemporary science.

Recently there have been attempts to revise and possibly improve the traditional mathematical models describing the fluids flows. The works of Brennen [5] and Svärd [16] are example of such possible model updates. In these new models, the basic physical principles (conservation/balance laws) are still being used, but the interpretation of certain physical variables and processes brings other options for into the mathematical formulations of such revised models. These changes are bringing some interesting results from the point of view of mathematical analysis [8] of the corresponding models as well as possible increase in the efficiency of numerical methods [6], [11].

The aim of this paper is to present the initial results of a computational study based on the mass-diffusive compressible and nearly-incompressible fluids flows models based on the works of Svärd [16] extended by Kajzer & Pozorski in [11]. The new alternative models are first presented, side by side with the standard systems for both compressible and incompressible fluids flows. The new, mass-diffusive models are then solved by high-resolution compact finite-difference methods. The model results are mutually compared for two test cases, documenting the agreement and comparative advantages of the newly formulated models.

2 Mathematical model
The full system of Navier-Stokes-Fourier (NSF) equations describing the flow of a compressible heat conducting fluid can be written as

\[
\frac{\partial t}{\partial t} \rho + \nabla \cdot (\rho v) = 0 \\
\frac{\partial t}{\partial t} (\rho v) + \nabla \cdot (\rho v \otimes v + p I) = \nabla \cdot \mathbb{S} \\
\frac{\partial t}{\partial t} E + \nabla \cdot ((E + p) v) = \nabla \cdot (\mathbb{S} \cdot v + \kappa \nabla T)
\]
Here the $\mathbf{v}$ is the fluid velocity, $\rho$ density, $p$ pressure. The fluid total energy $E$ is defined as

$$E = \frac{1}{2} \rho |\mathbf{v}|^2 + \frac{p}{\gamma - 1}, \quad \text{where} \quad \gamma = \frac{c_p}{c_v} \tag{4}$$

for the perfect gas obeying the state equation $p = \rho R T$ with the gas constant $R = c_p - c_v$ being linked to heat capacities $c_p, c_v$ at constant pressure and volume respectively. The stress tensor $\mathbf{S}$ for Newtonian fluid is then defined as

$$\mathbf{S} = \mu \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T - \frac{2}{3} (\nabla \cdot \mathbf{v}) I \right). \tag{5}$$

The dynamic viscosity $\mu$ and heat conductivity $\kappa$ depend on the fluid considered.

The standard NSF system (1)–(3) was reformulated by Svärd [16] who replaced it by a modified Navier-Stokes-Fourier (M-NSF) system, having similar form, but different right-hand sides in all equations.

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = \nabla \cdot (\nu \nabla \rho) \tag{6}$$
$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + \rho \mathbf{I}) = \nabla \cdot (\nu (\nabla \mathbf{v})) \tag{7}$$
$$\partial_t E + \nabla \cdot \left((E + p) \mathbf{v}\right) = \nabla \cdot (\nu E) \tag{8}$$

The most notable change, probably, is the added mass-diffusive term in the equation for density (6). But the right-hand sides in the momentum and energy equations (7) and (8) have changed as well, consisting now just from the divergence of the gradient of the conserved quantity (in the same form as in the modified mass conservation (6)). The diffusion coefficient $\nu = \mu/\rho$ has now the same value in all the considered equations of the modified M-NSF system.

In the case of incompressible fluid flow, where the density and temperature are considered constant, pressure looses its thermodynamical role and becomes purely kinematic variable, assuring that the velocity field becomes divergence-free. In such a case the NSF system reduces to the well known system of Incompressible Navier-Stokes (INS) equations:

$$\nabla \cdot \mathbf{v} = 0 \tag{9}$$
$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + \rho \mathbf{I}) = \mu \nabla^2 \mathbf{v}, \tag{10}$$

where the viscous stress tensor $\mathbf{S}$ given by (5) reduced to

$$\mathbf{S} = \mu \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) = 2\mu \mathbb{D} \quad \text{div} \mathbf{v} = 0 \quad \Rightarrow \quad \nabla \cdot \mathbf{S} = \mu \nabla^2 \mathbf{v}. \tag{11}$$

with $\mathbb{D}$ being the symmetric part of the velocity gradient (rate of deformation tensor).

Instead of solving the INS system (9)-(10), in the paper [11], the authors suggest to reduce the full NSF and M-NSF systems into their nearly incompressible counterparts. This is done considering an isothermal flow where the pressure and density are linked by an artificial equation of state, containing an artificial speed of sound parameter $c_a$:

$$p(\rho) = c_a^2 \rho. \tag{12}$$

Using these assumptions, the nearly Incompressible Navier-Stokes (nINS) model can be written as

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{13}$$
$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + c_a^2 \rho \mathbb{I}) = \nabla \cdot (\mu \nabla \mathbf{v}) \tag{14}$$

and the (mass-diffusive) modified nearly Incompressible Navier-Stokes (M-nINS) system

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = \nabla \cdot (\nu \nabla \rho) \tag{15}$$
$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + c_a^2 \rho \mathbb{I}) = \nabla \cdot (\nu (\nabla \mathbf{v})) \tag{16}$$
3 Numerical Simulations

The models were solved by high-resolution methods on simple orthogonal equispaced grids. Special care was taken to avoid any discretization artifacts emanating either from spatial or temporal discretization. The test cases were chosen to represent low velocity (low Mach number) flows, with important solution gradients, evolving in time. The question to be answered by these simulations is whether the solutions of the simplified models closely mimic the evolution of their corresponding classical counterparts. Special focus is on the mass-diffusion effects on the sharpness of gradients at interfaces.

3.1 Numerical methods

To achieve sufficiently high accuracy of numerical approximation of the governing system, the compact finite-difference approximation [12], [10], [17] of spatial derivatives was adopted, together with high-order compact filters for stabilizing the purely central (upwinding free) scheme [1], [2], [13]. The spatial derivatives of all quantities are being discretized by the same compact scheme, with high-order compact filters for stabilizing the purely central (upwinding free) scheme [1], [2], [13]. The spatial derivatives of all quantities are being discretized by the same compact scheme, requiring the solution of three-diagonal system on a five point stencil (in one dimension), so the approximation of the derivative \( \phi' \) of a certain quantity \( \phi \) on equidistant grid with spacing \( h \) can be written as:

\[
a \phi'_{i-1} + \phi'_i + a \phi'_{i+1} = \frac{\alpha_1}{2h} (\phi_{i+1} - \phi_{i-1}) + \frac{\alpha_2}{4h} (\phi_{i+2} - \phi_{i-2}) .
\]  

(17)

The specific scheme is obtained by choosing the coefficient \( a \), together with \( \alpha_1 = \frac{2}{3} (a + 2) \) and \( \alpha_2 = \frac{2}{3} (a - 1) \). In simulations presented hereafter, the choice \( a = 1/3 \) was made, leading to a sixth order accurate discretization in space. In the same manner a compact low-pass filter is constructed, see for example [10], [4]. Here the eighth order filter [3] with \( b = 0.49 \) was used. The temporal discretisation was carried out using explicit Runge-Kutta multistage scheme in the Strong Stability Preserving (SSP) form proposed in [14], [15]. The third order, three stage SSP(3,3) time integration scheme [3] was adopted for the simulations presented in this paper. The results presented here were obtained on uniform grid with 400 cells in each direction, leading to spatial resolution \( \Delta x = 1/400 = 2.5 \cdot 10^{-3} \) and constant time step \( \Delta t = 10^{-4} \).

3.2 Test cases

Numerical tests were performed on simple two-dimensional cases, demonstrating the spatial and temporal evolution of the corresponding solutions. In both cases presented here, the unit square geometry was used and periodic boundary conditions adopted for the numerical simulations. This allows to get the highest possible accuracy from the numerical methods and avoid issues associated with specific implementation of boundary conditions.

Double-Periodic Shear Layer (DPSL)

The double periodic shear layer test case is adopted based on the setup used in [11], where the initial flow field \( u(x, y, t) = (u, v) \) of the form

\[
\begin{align*}
    u(x, y, 0) &= \begin{cases} 
    U \tanh \left( b(y - L/4) \right) & \text{for } y \leq L/2 \\
    U \tanh \left( b(3L/4 - y) \right) & \text{for } y > L/2
    \end{cases} \\
    v(x, y, 0) &= 0.05 U \sin \left( 2\pi(x + L/4) \right),
\end{align*}
\]  

(18)

where \( L = 1, b = 80, U = 1 \). The computational domain is a square \( \Omega = [0; L] \times [0; L] \), where periodic boundary conditions are prescribed on all boundaries. The remaining parameters are \( \rho = 1.0, \mu = 10^{-4} \), leading to Reynolds number \( Re = \frac{UL}{\mu} = 10^4 \). For the nearly incompressible Navier-Stokes models the artificial speed of sound was set to \( c_a^2 = 100 \), leading to artificial Mach number \( Ma = 1/10 \).

The DPSL test case was used for all four considered models, i.e. compressible NSF, M-NSF and nearly incompressible nINS, M-nINS, to document the mutual differences between the resulting solutions and their evolution in time.
Kelvin-Helmholtz Instability (KHI)

In this case the flow field initialized by

\[
\begin{align*}
    u(x, y, 0) &= \begin{cases} 
        -0.5 + 0.01 \sin(4\pi x), & \rho = 2 \quad \text{for} \quad 0.25 < y < 0.75 \\
        +0.5 + 0.01 \sin(4\pi x), & \rho = 1 \quad \text{for} \quad y \leq 0.25 \text{ and } y \geq 0.75
    \end{cases} \\
    v(x, y, 0) &= 0.01 \sin(4\pi y) \\
    p(x, y, 0) &= 2.5
\end{align*}
\]

Similarly to the previous test case, the computational domain is a unit square \( \Omega = [0; 1] \times [0; 1] \), with periodic boundary conditions prescribed on all boundaries. Exactly as in [16], the other parameters are set to \( \mu = 2.0 \cdot 10^{-4}, \ c_p = 1005, \ Pr = 0.72, \ k = \frac{\mu c_p}{Pr}, \ \gamma = 1.4 \). In contrast to the DPSL test case, the initial density is piecewise constant, with a jump at the shearing interfaces, where the fluid velocity changes its sign. This is why the KHI test case is only suitable for the comparison of fully compressible NFS and M-NFS models. The spatio-temporal evolution of the interfaces (shear layers) is of primary interest here.

4 Numerical Results

The DPSL case is characterized by strong vorticity concentrated in shear layers, which is tricky to capture numerically. Here the solution is well captured, due to high resolution, non-diffusive discretization being used.

The difference between the fully compressible and the simplified nearly incompressible models is in this flow regime just marginal, showing-up mainly in the velocity divergence fields in Figs. 1b, 1d and 1f, 1h respectively. The larger divergence in the nearly incompressible models can be reduced by choosing higher artificial speed of sound \( c_a \).

![Figure 1: Flow variables at \( T = 1.5 \) for the Double Periodic Shear Layer.](image)

The side-by-side comparison of the vorticity evolution for all four considered models (compressible NSF, M-NSF and nearly incompressible nINS, M-nINS) shown in Fig. 2 reveals that there virtually no differences between the obtained solutions.
For the Kelvin-Helmholtz Instability (KHI) case the density field evolution shows (see Fig. 3) the creation of larger vortices from the original flow perturbations, which contribute to the mixing. The sharp density interfaces rolls-up due to shear and create fine scale patterns in the field. These features are resolved by both the NSF and M-NSF models and only small differences can be observed at larger times, where the density gradients seem to be a bit sharper in the modified (mass-diffusive) M-NSF model. The closer look at the final results KHI solution shown in Fig. 4 at time $T = 3.0$ reveals that the velocity magnitude and vorticity fields look virtually the same for the NSF and M-NSF models. The only true differences can be seen from comparing the divergence of the velocity fields in Figs 4b and 4c, where the divergence pattern is more pronounced in the shear layers resolved by the original NSF in comparison with the modified M-NSF model.

## Discussion and Conclusions

The numerical simulations of the alternative compressible as well as nearly incompressible flows models shown their potential in solving problems of practical interest. Although the presented new models offer certain advantages over their classical counterparts (better analytical properties, easier and more efficient numerical implementation), there are numerous issues to be addressed.
Figure 3: Density evolution for the Kelvin-Helmoltz Instability.
One of the possible troubles may come from the formulation of the (stress tensor on the) right hand side of the mass-diffusive M-NSF model (7). The principle of material frame indifference and the conservation of moment of momentum require the stress tensor to be symmetric (depending just on the symmetric part of velocity gradient) [7], [9]. This and many other properties will be in the focus of our future investigation.

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