Chapter 2
Mathematical Models

As it has already been stated in the introduction, the developments which have been made in the scope of this work aim at a generic framework for numerical simulations on unstructured grids. The vast majority of applications at the Institut für Verbrennung und Gasdynamik, however, deal with compressible gas flow. Thus the compressible Navier-Stokes Equations will be described in detail in this chapter.

2.1 Generic Form of Partial Differential Equations

Consider the following general system of $N_{eq}$ time dependent equations in integral form

$$\sum_m \left( \int_V \frac{\partial^m \mathbf{q}}{\partial t^m} \, dV \right) + \int_V \mathbf{H} \cdot \mathbf{n} \, dA = \int_V \mathbf{s} \, dV, \quad (2.1)$$

which contains time-derivatives of different orders (the exponent $m$ denotes the order of the time-derivative). For the unknowns of a system of partial differential equations, $\mathbf{q}$ has been generally used in the scope of this work. The appendix A describes the symbols and notation which has been used in this text. Many problems can be described by an equation of this form. Furthermore many problems do only have a first derivative in time. Thus (2.1) becomes a conservation law:

$$\int_V \frac{\partial q}{\partial t} \, dV + \int_V \mathbf{H} \cdot \mathbf{n} \, dA = \int_V \mathbf{s} \, dV \quad (2.2)$$

Now, $\mathbf{q}$ denotes the vector of conservative properties and $\mathbf{H}$ is a general flux describing a possible transport of the conservative properties. For a fluid dynamics problem $\mathbf{q}$ would contain the mass, momentum and energy. Possible source terms are summarized in the vector $\mathbf{s}$. $V$ denotes the control volume and $A$ its boundary, with the local normal vector $\mathbf{n}$. Many time dependant physical problems can be described using an equation of this type. Steady state problems can quite often be tackled with a similar approach, using the originally physical time $t$ as an iteration index. Difficulties might arise if integral terms
have to be included into the model. An example for this is radiative heat transfer. An example for an equation with a second derivative in time is the linear wave equation (see also 7.3.1).

### 2.2 Compressible Navier-Stokes Equations

The compressible Navier-Stokes Equations form a set of equations with only first derivatives in time:

\[
\int_V \frac{\partial \mathbf{q}}{\partial t} \, dV + \int_{\partial V} \mathbf{H} n \, dA = \int_V f \, dV. \tag{2.3}
\]

With the conservative variables defined as following:

\[
\mathbf{q} = \begin{bmatrix}
\rho \\
\rho \mathbf{v} \\
\rho E
\end{bmatrix}. \tag{2.4}
\]

Where \( \mathbf{v} \) is the fluid velocity:

\[
\mathbf{v} = \begin{bmatrix}
u \\
v \\
w
\end{bmatrix}. \tag{2.5}
\]

\( E \) is the sum of inner and kinetic energy:

\[
E = e + \rho \mathbf{v}^2. \tag{2.6}
\]

Thus there are five equations in case of a three dimensional compressible flow problem. The vector \( \mathbf{f} \) from (2.3) describes external forces and other source terms (e.g. gravity, heat sources). If free convection has to be simulated, the gravity can not be neglected, as it is usually for aerodynamical applications.

#### 2.2.1 Fluxes

For the Navier-Stokes equations the flux vector becomes

\[
\mathbf{H} = \begin{bmatrix}
\rho \mathbf{v} \\
\rho \mathbf{v} \cdot \mathbf{v} + \mathbf{\sigma} \\
\rho (\mathbf{v} \cdot \mathbf{v}) + \mathbf{\sigma} + h_{\text{heat}}
\end{bmatrix}, \tag{2.7}
\]

the conductive heat transfer is defined as

\[
h_{\text{heat}} = \lambda \nabla T \tag{2.8}
\]

and the stress tensor, with \( p \) as the local pressure can be written as

\[
\mathbf{\sigma} = \begin{bmatrix}
\tau_{xx} + p & \tau_{xy} & \tau_{xz} \\
\tau_{yx} & \tau_{yy} + p & \tau_{yz} \\
\tau_{zx} & \tau_{zy} & \tau_{zz} + p
\end{bmatrix}. \tag{2.9}
\]
The other components of the stress tensor are functions of the spatial derivatives of the velocity components, with \( \mu \) as the dynamic viscosity of the gas:

\[
\tau_{xx} = -2/3\mu \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right)
\]
\[
\tau_{yy} = -2/3\mu \left( -\frac{\partial u}{\partial x} + 2\frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right)
\]
\[
\tau_{zz} = -2/3\mu \left( -\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} + 2\frac{\partial w}{\partial z} \right)
\]
\[
\tau_{xy} = \tau_{yx} = -\mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right)
\]
\[
\tau_{yz} = \tau_{zy} = -\mu \left( \frac{\partial u}{\partial z} + \frac{\partial v}{\partial z} \right)
\]
\[
\tau_{zx} = \tau_{xz} = -\mu \left( \frac{\partial w}{\partial y} + \frac{\partial w}{\partial y} \right).
\] (2.10)

Additional closures are necessary to compute the pressure and the temperature out of the conservative variables \((\rho, \rho \mathbf{v}, \rho E)\) and vice versa. Assuming a perfect gas the ideal gas law can be applied:

\[
p = \rho RT.
\] (2.11)

\( R \) is the gas constant and it can also be expressed as the difference of the specific heat at constant pressure and the specific heat at constant density:

\[
R = c_p - c_v.
\] (2.12)

Inner energy and temperature can be related using the following formula for an ideal gas:

\[
e = c_v T.
\] (2.13)

With the specific heat ratio \( \gamma \)

\[
\gamma = \frac{c_p}{c_v}.
\] (2.14)

pressure and temperature can be computed from the conservative properties:

\[
p = (\gamma - 1) \left( \rho E - \frac{1}{2} \frac{(\rho \mathbf{v})^2}{\rho} \right)
\] (2.15)

\[
T = \frac{p}{\rho R} = \frac{\gamma - 1}{\rho R} \left( \rho E - \frac{1}{2} \frac{(\rho \mathbf{v})^2}{\rho} \right).
\] (2.16)

The flux \( H \) can be into an inviscid and a viscous part:

\[
H = H_{\text{inv}} + H_{\text{vis}},
\] (2.17)

with

\[
H_{\text{inv}} = \begin{bmatrix}
\rho \mathbf{v} \\
\rho \mathbf{v} \mathbf{v} + \rho \mathbf{I} \\
\rho \mathbf{v} E + \mathbf{v} \rho
\end{bmatrix}
\] (2.18)
and

\[
\mathbf{h}_{\text{vis}} = \begin{bmatrix}
0 \\
\sigma - p \mathbf{I} \\
(\sigma - p \mathbf{I})\mathbf{v} + \mathbf{h}_{\text{heat}}
\end{bmatrix}.
\]  

(2.19)

This is useful due to the very different nature of these. \( \mathbf{I} \) denotes a unit matrix with the same dimension as the spatial dimension of the problem to be solved. Both fluxes are usually treated very differently. In the scope of this work \( \mathbf{h}_{\text{lev}} \) and \( \mathbf{h}_{\text{vis}} \) have been implemented as individual building blocks. Thus it is possible to compute without a viscous flux, in order to solve the Euler equations. Furthermore it is possible to combine different discretizations for both parts of the Navier-Stokes flux.