

# SHOCK

## Structured High-Order Computational Kernel

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April 8, 2015

### 1. Governing equations

SHOCK contains three possible flow configurations:

1. two-dimensional
2. two-dimensional rotational symmetric
3. three-dimensional

The governing equations for unsteady compressible flow are Navier-Stokes equations or Euler equations: conservation equations of mass, momentum and energy closed with the perfect gas law and Sutherland's law for the viscosity. In the following the three-dimensional case is discussed in detail. The Navier-Stokes equations for three-dimensional unsteady, compressible flow in curvilinear coordinates are used in conservative non-dimensional form:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} + \frac{\partial H}{\partial \zeta} = \frac{\partial F^\nu}{\partial \xi} + \frac{\partial G^\nu}{\partial \eta} + \frac{\partial H^\nu}{\partial \zeta} \quad (1)$$

Here, the solution vector  $U$ , the inviscid fluxes  $F$ ,  $G$ ,  $H$  and the viscous fluxes  $F^\nu$ ,  $G^\nu$ ,  $H^\nu$  are defined as

$$U = J \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \end{pmatrix}, \quad F = J \begin{pmatrix} \rho \theta_1 \\ \rho \theta_1 u + \xi_x p \Upsilon \\ \rho \theta_1 v + \xi_y p \Upsilon \\ \rho \theta_1 w + \xi_z p \Upsilon \\ \rho \theta_1 \left( e + \frac{p}{\rho} \Upsilon \right) \end{pmatrix}, \quad G = J \begin{pmatrix} \rho \theta_2 \\ \rho \theta_2 u + \eta_x p \Upsilon \\ \rho \theta_2 v + \eta_y p \Upsilon \\ \rho \theta_2 w + \eta_z p \Upsilon \\ \rho \theta_2 \left( e + \frac{p}{\rho} \Upsilon \right) \end{pmatrix} \quad (2)$$

$$\begin{aligned}
H &= J \begin{pmatrix} \rho\theta_3 \\ \rho\theta_3 u + \zeta_x p \Upsilon \\ \rho\theta_3 v + \zeta_y p \Upsilon \\ \rho\theta_3 w + \zeta_z p \Upsilon \\ \rho\theta_3 \left( e + \frac{p}{\rho} \Upsilon \right) \end{pmatrix}, \quad F^\nu = J \begin{pmatrix} 0 \\ \Psi(\xi_x \tau_{\xi\xi} + \xi_y \tau_{\xi\eta} + \xi_z \tau_{\xi\zeta}) \\ \Psi(\xi_x \tau_{\xi\eta} + \xi_y \tau_{\eta\eta} + \xi_z \tau_{\eta\zeta}) \\ \Psi(\xi_x \tau_{\xi\zeta} + \xi_y \tau_{\eta\zeta} + \xi_z \tau_{\zeta\zeta}) \\ \Psi(u(\xi_x \tau_{\xi\xi} + \xi_y \tau_{\xi\eta} + \xi_z \tau_{\xi\zeta}) + \\ v(\xi_x \tau_{\xi\eta} + \xi_y \tau_{\eta\eta} + \xi_z \tau_{\eta\zeta}) + \\ w(\xi_x \tau_{\xi\zeta} + \xi_y \tau_{\eta\zeta} + \xi_z \tau_{\zeta\zeta})) \\ -\Gamma(\xi_x q_\xi + \xi_y q_\eta + \xi_z q_\zeta) \end{pmatrix} \\
G^\nu &= J \begin{pmatrix} 0 \\ \Psi(\eta_x \tau_{\xi\xi} + \eta_y \tau_{\xi\eta} + \eta_z \tau_{\xi\zeta}) \\ \Psi(\eta_x \tau_{\xi\eta} + \eta_y \tau_{\eta\eta} + \eta_z \tau_{\eta\zeta}) \\ \Psi(\eta_x \tau_{\xi\zeta} + \eta_y \tau_{\eta\zeta} + \eta_z \tau_{\zeta\zeta}) \\ \Psi(u(\eta_x \tau_{\xi\xi} + \eta_y \tau_{\xi\eta} + \eta_z \tau_{\xi\zeta}) + \\ v(\eta_x \tau_{\xi\eta} + \eta_y \tau_{\eta\eta} + \eta_z \tau_{\eta\zeta}) + \\ w(\eta_x \tau_{\xi\zeta} + \eta_y \tau_{\eta\zeta} + \eta_z \tau_{\zeta\zeta})) \\ -\Gamma(\eta_x q_\xi + \eta_y q_\eta + \eta_z q_\zeta) \end{pmatrix}, \quad H^\nu = J \begin{pmatrix} 0 \\ \Psi(\zeta_x \tau_{\xi\xi} + \zeta_y \tau_{\xi\eta} + \zeta_z \tau_{\xi\zeta}) \\ \Psi(\zeta_x \tau_{\xi\eta} + \zeta_y \tau_{\eta\eta} + \zeta_z \tau_{\eta\zeta}) \\ \Psi(\zeta_x \tau_{\xi\zeta} + \zeta_y \tau_{\eta\zeta} + \zeta_z \tau_{\zeta\zeta}) \\ \Psi(u(\zeta_x \tau_{\xi\xi} + \zeta_y \tau_{\xi\eta} + \zeta_z \tau_{\xi\zeta}) + \\ v(\zeta_x \tau_{\xi\eta} + \zeta_y \tau_{\eta\eta} + \zeta_z \tau_{\eta\zeta}) + \\ w(\zeta_x \tau_{\xi\zeta} + \zeta_y \tau_{\eta\zeta} + \zeta_z \tau_{\zeta\zeta})) \\ -\Gamma(\zeta_x q_\xi + \zeta_y q_\eta + \zeta_z q_\zeta) \end{pmatrix} \\
\Theta_1 &= u\xi_x + v\xi_y + w\xi_z, \quad \Theta_2 = u\eta_x + v\eta_y + w\eta_z, \quad \Theta_3 = u\zeta_x + v\zeta_y + w\zeta_z \\
\Upsilon &= \frac{1}{\gamma Ma_{ref}^2}, \quad \Psi = \frac{1}{Re_{ref}}, \quad \Gamma = \frac{1}{(\gamma - 1) Ma_{ref}^2 Pr_{ref}}
\end{aligned}$$

where  $\xi_{x,y,z}$ ,  $\eta_{x,y,z}$ ,  $\zeta_{x,y,z}$  are the metric coefficients and  $J$  is the Jacobian of the transformation of the Cartesian coordinates  $x$ ,  $y$  and  $z$  into the curvilinear coordinates  $\xi(x, y, z)$ ,  $\eta(x, y, z)$  and  $\zeta(x, y, z)$ . The perfect gas law relates the density  $\rho$ , the pressure  $p$  and the temperature  $T$  whereas the viscosity  $\mu$  is calculated by Sutherland's law.

$$p = \rho T \quad (3)$$

$$\mu = \frac{1 + S}{T + S} T^{\frac{3}{2}}, \quad S = \frac{100,4K}{T_{ref}} \quad (4)$$

$\tau$  and  $q$  are the transformed shear stress tensor and heat flux, respectively. The total energy  $e$  is defined as

$$e = \frac{u^2 + v^2 + w^2}{2} + \frac{\Upsilon}{\gamma - 1} \frac{p}{\rho}, \quad (5)$$

Here,  $\gamma$  is the constant ratio of the specific heats and  $Pr$  is the local Prandtl number. Due to a local  $Pr$ , the treatment of isothermal boundary conditions is improved since the heat flux can be adjusted independently from the friction. For the non-dimensionalization of the equations (1)-(5) following reference variables are used:  $u_{ref}$ ,  $T_{ref}$ ,  $p_{ref}$ ,  $\rho_{ref}$ ,  $\mu_{ref}$  and  $L_{ref}$ . The reference Reynolds and Mach numbers are defined as:

$$Re_{ref} = \frac{\rho_{ref} u_{ref} L_{ref}}{\mu_{ref}}, \quad Ma_{ref} = \frac{u_{ref}}{\sqrt{\gamma R_{ref} T_{ref}}} \quad (6)$$

Here,  $R_{ref}$  is the specific gas constant.

## 2. Numerical method

SHOCK contains various capabilities of the numerical method:

1. fifth and ninth order WENO scheme (spatial discretization of first order derivatives)
2. sixth and tenth order central differences (spatial discretization of second order derivatives)
3. third and fourth order Runge-Kutta (temporal discretization)

In the following the fifth order WENO scheme in combination with a tenth order central differences and fourth-order Runge-Kutta scheme is discussed in detail.

### 2.1. WENO scheme

The inviscid fluxes  $F$ ,  $G$  and  $H$  are approximated by using a fifth order Weighted Essentially Non-Oscillatory (WENO5) finite difference scheme corresponding to Jiang and Shu [2]. Exemplary for the flux in  $\xi$ -direction, the WENO5 scheme is explained in following. The derivative of the flux  $F$  at the mesh point  $i$  is defined as

$$\left(\frac{\partial F}{\partial \xi}\right)_i = \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta \xi} \quad (7)$$

where the cell boundary fluxes  $F_{i+\frac{1}{2}}$  are

$$\begin{aligned} F_{i+\frac{1}{2}} &= \sum_{m=0}^{r-1} \omega_m M_m^r \\ M_m^r &= \sum_{l=i+m-r+1}^{i+m} a_{m,l}^r F_l. \end{aligned} \quad (8)$$

$M_m^r$  is the  $m$ -th of  $r$  ( $r = (N+1)/2 = 3$ ) sub-stencil with polynomial coefficients  $a_{m,l}^r$  for  $N = 5$ -th order of approximation. The normalized weights  $\omega_m$ , defined as

$$\begin{aligned} \omega_m &= \frac{\bar{\omega}_m}{\bar{\omega}_0 + \dots + \bar{\omega}_{r-1}} \\ \bar{\omega}_m &= \frac{b_m^r}{(\epsilon + IS_m)^2}, \end{aligned} \quad (9)$$

preserves monotonicity in the vicinity of strong gradients by the means of the smoothness indicators  $IS_m$ . The parameter  $\epsilon$  is added to avoid a division by zero at smooth solutions and is set to  $\epsilon \approx 10^{-150}$  which is close to the minimal floating point value. The coefficients  $b_m^r$  are called optimal coefficients for the 5-th order of accuracy in smooth solution regions.

In order to improve the numerical stability of the scheme, the propagation direction of the characteristics is taken into account resulting in a Lax-Friedrichs flux vector splitting:

$$F_{i+\frac{1}{2}} = F_{i+\frac{1}{2}}^+ + F_{i+\frac{1}{2}}^- \quad (10)$$

where the algebraic sign of the eigenvalue  $\lambda$  of the flux Jacobian  $A = \partial F / \partial U$  determines the propagation direction. Jacobian  $A$  can be transformed into the characteristic form  $A = R\Lambda R^{-1}$  with the diagonal matrix of eigenvalues  $\Lambda$ , the right  $R$  and the left  $R^{-1}$  eigenvectors. Due to the usage of the maximal eigenvalue  $\lambda_{i,max}$  within the stencil, it is called a local Lax-Friedrichs flux-vector splitting. Finally, the inviscid flux yields to

$$F_{i+\frac{1}{2}} = \overbrace{\frac{1}{12} [-F_{i-1} + 7F_i + 7F_{i+1} - F_{i+2}]}^{\text{central term}} + \sum_{s=1}^5 \left[ -\Phi_N \left( R_s^{-1} \Delta F_{i-\frac{3}{2}}^{s,+}, R_s^{-1} \Delta F_{i-\frac{1}{2}}^{s,+}, R_s^{-1} \Delta F_{i+\frac{1}{2}}^{s,+}, R_s^{-1} \Delta F_{i+\frac{3}{2}}^{s,+} \right) \right. \\ \left. + \Phi_N \left( R_s^{-1} \Delta F_{i+\frac{5}{2}}^{s,-}, R_s^{-1} \Delta F_{i+\frac{3}{2}}^{s,-}, R_s^{-1} \Delta F_{i+\frac{1}{2}}^{s,-}, R_s^{-1} \Delta F_{i-\frac{1}{2}}^{s,-} \right) \right] R_s \quad (11)$$

$$\Delta F_{i+\frac{1}{2}}^{s,\pm} = F_{i+1}^{s,\pm} - F_i^{s,\pm} \quad (12)$$

$$F_i^{s,\pm} = \frac{1}{2} \left( F_i^s \pm \lambda_{i,max} \hat{U}_i^s \right) \quad (13)$$

where the function  $\Phi_N$  computes the non-linear corrections added to the central term depending on the weights shown in equation (9), the  $s$ -th component of the flux differences  $\Delta F_{i+\frac{1}{2}}^{s,\pm}$  and the eigenvectors  $R_s$  and  $R_s^{-1}$ . Figure 1 demonstrates the sub-

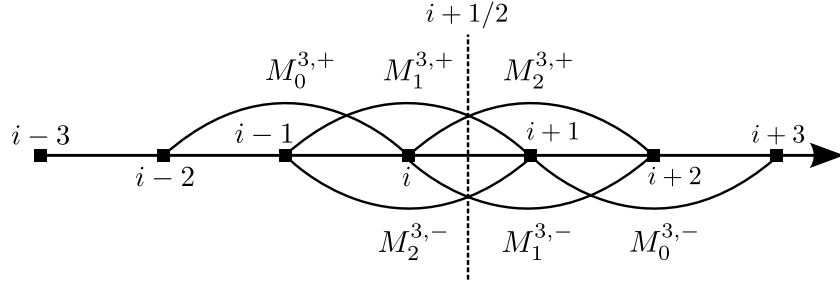


Figure 1: Schematic illustration of flux calculation for the cell boundary flux  $F_{i+\frac{1}{2}}$

stencil configuration for the whole flux calculation including the Lax-Friedrichs flux-vector splitting.

## 2.2. Central difference scheme

The viscous fluxes  $F^\nu$ ,  $G^\nu$  and  $H^\nu$  are approximated by using a sixth order central-difference scheme. The approximation of the derivation is computed corresponding to the Taylor series.

### 2.2.1. Double derivation:

$$\frac{\partial}{\partial \xi} \left( A \frac{\partial u}{\partial \xi} \right)_{i,j} = \frac{\left( A \frac{\partial u}{\partial \xi} \right)_{i+\frac{1}{2},j} - \left( A \frac{\partial u}{\partial \xi} \right)_{i-\frac{1}{2},j}}{\Delta \xi} + \mathcal{O}(\Delta \xi^6) \quad (14)$$

with:

$$\left( A \frac{\partial u}{\partial \xi} \right)_{i+\frac{1}{2},j} = C_{D,0} (u_{i+1} - u_i) + C_{D,1} (u_{i+2} - u_{i-1}) + C_{D,2} (u_{i+3} - u_{i-2}) \quad (15)$$

$$\left( A \frac{\partial u}{\partial \xi} \right)_{i-\frac{1}{2},j} = C_{D,0} (u_i - u_{i-1}) + C_{D,1} (u_{i+1} - u_{i-2}) + C_{D,2} (u_{i+2} - u_{i-3}) \quad (16)$$

$$C_{D,0} = -\frac{1}{90} \quad C_{D,1} = \frac{25}{180} \quad C_{D,2} = -\frac{245}{180} \quad (17)$$

### 2.2.2. Mixed derivation:

$$\frac{\partial}{\partial \xi} \left( A \frac{\partial u}{\partial \eta} \right)_{i,j} = \frac{\left( A \frac{\partial u}{\partial \eta} \right)_{i+\frac{1}{2},j} - \left( A \frac{\partial u}{\partial \eta} \right)_{i-\frac{1}{2},j}}{\Delta \xi} + \mathcal{O}(\Delta \xi^6 + \Delta \eta^6) \quad (18)$$

with interpolation coefficients:

$$\begin{aligned} \left( A \frac{\partial u}{\partial \eta} \right)_{i+\frac{1}{2},j} &= C_{P,0} \left( \left( A \frac{\partial u}{\partial \eta} \right)_{i+1,j} + \left( A \frac{\partial u}{\partial \eta} \right)_{i,j} \right) \\ &+ C_{P,1} \left( \left( A \frac{\partial u}{\partial \eta} \right)_{i+2,j} + \left( A \frac{\partial u}{\partial \eta} \right)_{i-1,j} \right) \\ &+ C_{P,2} \left( \left( A \frac{\partial u}{\partial \eta} \right)_{i+3,j} + \left( A \frac{\partial u}{\partial \eta} \right)_{i-2,j} \right) \end{aligned} \quad (19)$$

The derivations are computed by:

$$\left( \frac{\partial u}{\partial \eta} \right)_{i,j} = \frac{u_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}}}{\Delta \eta} \quad (20)$$

with:

$$\begin{aligned}
u_{i,j+\frac{1}{2}} &= C_{P,0} (u_{i,j+1} + u_{i,j}) \\
&+ C_{P,1} (u_{i,j+2} + u_{i,j-1}) \\
&+ C_{P,2} (u_{i,j+3} + u_{i,j-2})
\end{aligned} \tag{21}$$

$$C_{P,0} = -\frac{1}{60} \quad C_{P,1} = \frac{3}{20} \quad C_{P,2} = -\frac{3}{4} \tag{22}$$

### 2.3. Explicit Runge-Kutta scheme

For time integration an explicit, fourth order, low storage Runge-Kutta scheme is applied.

$$\frac{\partial U}{\partial t} = Q \tag{23}$$

with  $Q$  being the sum of inviscid and viscous fluxes.

$$U^a = U^n + \frac{\Delta t}{2} Q(U^n) \tag{24}$$

$$U^b = U^n + \frac{\Delta t}{2} Q(U^a) \tag{25}$$

$$U^c = U^n + \Delta t Q(U^b) \tag{26}$$

$$U^{n+1} = U^n + \frac{\Delta t}{6} \underbrace{\left[ Q(U^n) + 2Q(U^a) + 2Q(U^b) + Q(U^c) \right]}_{Q_{sum}} \tag{27}$$

## 3. Features

### 3.1. Mesh Topology

SHOCK uses a powerful mesh topology containing subzones with rotated coordinate systems. By using the example of an triangle, this features is explained.

Figure 2 sketches the considered geometry of the isosceles triangle.

By adapting the mesh to the triangle, the number of mesh points for these edges are interdependent. That is why the number of mesh points for all three sides is constant. While using a structured mesh, the generation of a mesh which takes the triangle into account is a challenging task. Immersed boundaries are an easy solution if complex geometries have to be considered in structured meshes. The disadvantage of the immersed boundaries in conjunction with triangles is that the mesh line crossing oblique edges cannot be represented smoothly. Depending on the local mesh resolution the resulting boundaries are more or less serrated. This effect is called sawtooth distortion or aliasing. In order to avoid this disadvantage another solution is presented. The triangle is exactly modeled if it is replaced by three quadrilateral. Now, the mesh lines represent exactly the edges of the triangle improving the smoothness of the solution. Connecting

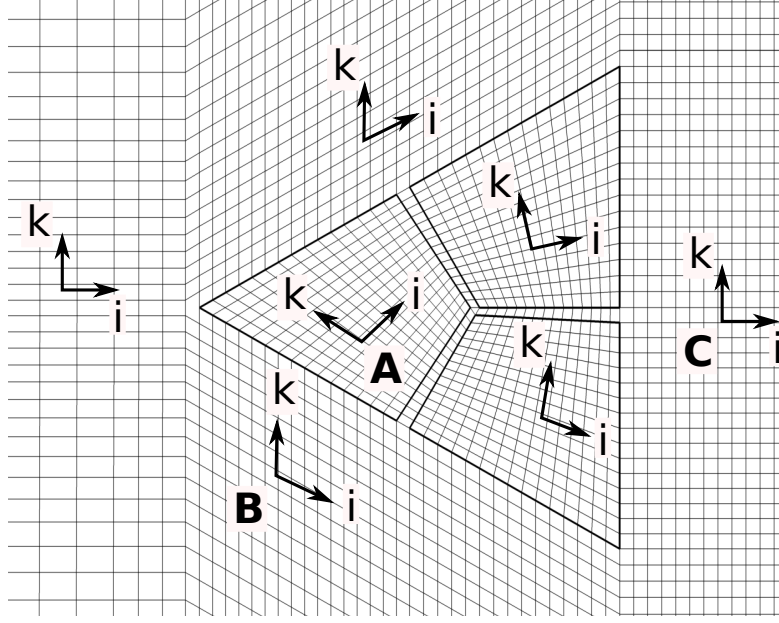


Figure 2: mesh cut through triangle

the different parts of the mesh around the triangle, in Fig. 2 it is apparent, that only *non-easy* mesh topologies are possible. Some adjacent zones, i.e. zone A and B in Fig. 2, use differently oriented coordinate systems. Consequently, to allow rotated coordinate systems, the introduction of a transformation matrix between the zones is necessary. It has to be noted, that besides the advantages of a more generalized mesh topology containing transformation matrices, the Message Passing Interface (MPI)-communication becomes more complex. While a simple rectangular mesh allows the use of a *Cartesian Communicator* and a synchronous MPI-communication (MPI-Sendrecv), the mesh shown in Figure 2 is not compatible, because the identification of the neighbors is no longer unique. Considering the neighbors in the *i*-direction, the zone B is the lower neighbor of the zones A and C. As a consequence, the communication is changed into an asynchronous one (MPI-Isend/MPI-Irecv). Further, instead of a global, *Cartesian Communicator*, now the mesh, or rather the interfaces provide the information about communication partners that are connected via the interfaces.

### 3.2. Memory

In the following, the memory management is considered. First of all, it is important to note, that SHOCK has no master process. Every thread uses nearly the same amount of memory. Considering one mesh point, nearly 300 double precision variables are allocated. This also includes variables for saving instantaneous data. The memory cost besides these variables is negligible.

### 3.3. I/O

The I/O of SHOCK is limited to the start and the end of the simulation. A file format for CFD data (CGNS [CFD General Notation System], using HDF5, [3] ) supports the comfortable handling of big amount of data. In a bachelor thesis [5], the parallel CGNS commands were implemented which enables SHOCK to use one single cgns-file containing the data for all threads instead one file for each thread. This dramatically simplifies the data management since a data post processing is not needed any more. SHOCK's results can be transferred continuously from the production system.

### 3.4. Parallelization & scalability

SHOCK is parallelized with pure MPI (Message Passing Interface), in order to carry out simulations with large numerical costs in a realistic time. A hybrid parallelization was tested but showed no benefit and therefore, it was deactivated. The communication is asynchronous since the mesh topology enables rotated coordinate systems. In such cases, a synchronous communication (i.e. all send to left and receive from right) is not possible. Nevertheless, the general mesh topology has great advantages since it is not limited to simple meshes and the scalability of the code is not significantly worse which is shown in the following.

On JUQUEEN using 32 threads per node (pure MPI code), scalability tests have been performed in order to demonstrate that the code is appropriate to be used for a massive parallelization. On a three dimensional grid consisting of  $16 \cdot 10^6$  grid points ( $256 \times 256 \times 256$ ) a test simulation with 500 time steps was conducted. Figure 3 illustrates the results for five levels of parallelization. Starting with 512 cores while the number of cores was doubled from one level to the next. The highest number of cores that was considered in this scaling test is 8,192. In general, the code can run on further levels of parallelization (recent record (23.11.2014): 262,144 threads), but for the used grid a further decomposition was not meaningful. The relation of the number of ghost points, which define the communicated data, and the number of grid points, where the solution is computed, rises up to a value of 4.06 for the highest level of decomposition. As a result the communication time takes 17.8 % of the absolute time for this level. Assuming a cubic decomposition, the number of ghost points  $GHP$  and grid points  $GRP$  per thread are approximated by  $GRP = 256^3 / no. threads$  and  $GHP = (GRP^{1/3} + 2 \cdot N)^3 - GRP$  with  $N = 3$  for the used spatial order.

## References

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cores	time (s)	comm. time (s)	$GHP/GRP$	speedup
512	1,166	46 [3.9%]	1.89	1.0
1,024	598	36 [6.1%]	2.18	1.9
2,048	316	27 [8.6%]	2.6	3.7
4,096	171	23 [13.5%]	3.2	6.8
8,192	94	17 [17.8%]	4.06	12.4

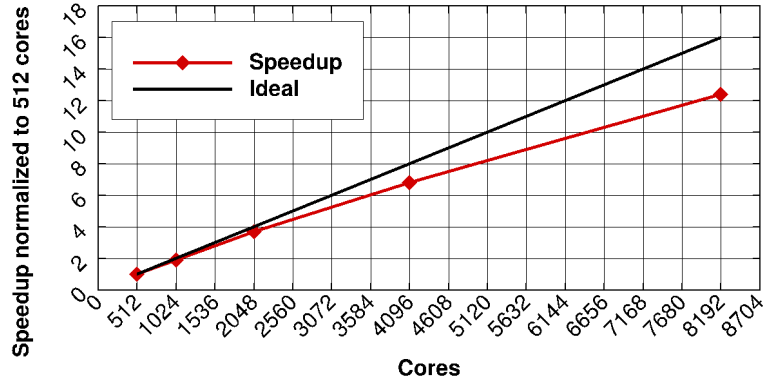


Figure 3: Scaling behaviour of SHOCK (WENO  $5^{th}$  and Runge-Kutta  $3^{rd}$  order) on JUQUEEN (256x256x256 grid points and 500 time steps). Speedup is normalized to 512 cores.

## A. Erhaltungsgleichungen

### A.1. In Vektorschreibweise

$$\frac{\partial \tilde{U}}{\partial \tilde{t}} + \frac{\partial \tilde{F}}{\partial \tilde{x}} + \frac{\partial \tilde{G}}{\partial \tilde{y}} + \frac{\partial \tilde{H}}{\partial \tilde{z}} = \frac{\partial \tilde{F}^\nu}{\partial \tilde{x}} + \frac{\partial \tilde{G}^\nu}{\partial \tilde{y}} + \frac{\partial \tilde{H}^\nu}{\partial \tilde{z}}$$

$$\frac{\partial}{\partial \tilde{t}} \begin{pmatrix} \tilde{\rho} \\ \tilde{\rho} \tilde{u} \\ \tilde{\rho} \tilde{v} \\ \tilde{\rho} \tilde{w} \\ \tilde{\rho} \tilde{e} \end{pmatrix} + \frac{\partial}{\partial \tilde{x}} \begin{pmatrix} \tilde{\rho} \tilde{u} \\ \tilde{\rho} \tilde{u}^2 + \tilde{p} \\ \tilde{\rho} \tilde{u} \tilde{v} \\ \tilde{\rho} \tilde{u} \tilde{w} \\ \tilde{\rho} \tilde{u} \left( \tilde{e} + \frac{\tilde{p}}{\tilde{\rho}} \right) \end{pmatrix} + \frac{\partial}{\partial \tilde{y}} \begin{pmatrix} \tilde{\rho} \tilde{v} \\ \tilde{\rho} \tilde{v}^2 + \tilde{p} \\ \tilde{\rho} \tilde{u} \tilde{v} \\ \tilde{\rho} \tilde{v} \tilde{w} \\ \tilde{\rho} \tilde{v} \left( \tilde{e} + \frac{\tilde{p}}{\tilde{\rho}} \right) \end{pmatrix} + \frac{\partial}{\partial \tilde{z}} \begin{pmatrix} \tilde{\rho} \tilde{w} \\ \tilde{\rho} \tilde{w}^2 + \tilde{p} \\ \tilde{\rho} \tilde{u} \tilde{w} \\ \tilde{\rho} \tilde{v} \tilde{w} \\ \tilde{\rho} \tilde{w} \left( \tilde{e} + \frac{\tilde{p}}{\tilde{\rho}} \right) \end{pmatrix} = \frac{\partial}{\partial \tilde{x}} \begin{pmatrix} 0 \\ \tilde{\tau}_{\tilde{x}\tilde{x}} \\ \tilde{\tau}_{\tilde{x}\tilde{y}} \\ \tilde{\tau}_{\tilde{x}\tilde{z}} \\ \tilde{\tau}_{\tilde{x}\tilde{x}} \tilde{u} + \tilde{\tau}_{\tilde{x}\tilde{y}} \tilde{v} + \tilde{\tau}_{\tilde{x}\tilde{z}} \tilde{w} + \tilde{q}_{\tilde{x}} \end{pmatrix} + \frac{\partial}{\partial \tilde{y}} \begin{pmatrix} 0 \\ \tilde{\tau}_{\tilde{y}\tilde{x}} \\ \tilde{\tau}_{\tilde{y}\tilde{y}} \\ \tilde{\tau}_{\tilde{y}\tilde{z}} \\ \tilde{\tau}_{\tilde{y}\tilde{x}} \tilde{u} + \tilde{\tau}_{\tilde{y}\tilde{y}} \tilde{v} + \tilde{\tau}_{\tilde{y}\tilde{z}} \tilde{w} + \tilde{q}_{\tilde{y}} \end{pmatrix} + \frac{\partial}{\partial \tilde{z}} \begin{pmatrix} 0 \\ \tilde{\tau}_{\tilde{z}\tilde{x}} \\ \tilde{\tau}_{\tilde{z}\tilde{y}} \\ \tilde{\tau}_{\tilde{z}\tilde{z}} \\ \tilde{\tau}_{\tilde{z}\tilde{x}} \tilde{u} + \tilde{\tau}_{\tilde{z}\tilde{y}} \tilde{v} + \tilde{\tau}_{\tilde{z}\tilde{z}} \tilde{w} + \tilde{q}_{\tilde{z}} \end{pmatrix}$$

### A.2. Einführung von dimensionslosen Größen

$$x = \frac{\tilde{x}}{L_{ref}}, \quad y = \frac{\tilde{y}}{L_{ref}}, \quad z = \frac{\tilde{z}}{L_{ref}}, \quad t = \frac{\tilde{t}}{u_{ref} L_{ref}}, \quad u = \frac{\tilde{u}}{u_{ref}}, \quad v = \frac{\tilde{v}}{u_{ref}}, \quad w = \frac{\tilde{w}}{u_{ref}}, \quad \rho = \frac{\tilde{\rho}}{\rho_{ref}}, \quad e = \frac{\tilde{e}}{u_{ref}^2}, \quad p = \frac{\tilde{p}}{p_{ref}}, \quad T = \frac{\tilde{T}}{T_{ref}}, \quad \mu = \frac{\tilde{\mu}}{\mu_{ref}}, \quad \lambda = \frac{\tilde{\lambda}}{\lambda_{ref}},$$

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u^2 + \Upsilon p \\ \rho uv \\ \rho uw \\ u(\rho e + \Upsilon p) \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v^2 + \Upsilon p \\ \rho uv \\ \rho vw \\ v(\rho e + \Upsilon p) \end{pmatrix} + \frac{\partial}{\partial z} \begin{pmatrix} \rho w^2 + \Upsilon p \\ \rho vw \\ w(\rho e + \Upsilon p) \end{pmatrix} = \frac{\partial}{\partial x} \begin{pmatrix} 0 \\ \Psi \tau_{xx} \\ \Psi \tau_{xy} \\ \Psi \tau_{xz} \\ \Psi \tau_{xx} u + \Psi \tau_{xy} v + \Psi \tau_{xz} w - \Gamma q_x \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} 0 \\ \Psi \tau_{yx} \\ \Psi \tau_{yy} \\ \Psi \tau_{yz} \\ \Psi \tau_{yx} u + \Psi \tau_{yy} v + \Psi \tau_{yz} w - \Gamma q_y \end{pmatrix} + \frac{\partial}{\partial z} \begin{pmatrix} 0 \\ \Psi \tau_{zx} \\ \Psi \tau_{zy} \\ \Psi \tau_{zz} \\ \Psi \tau_{zx} u + \Psi \tau_{zy} v + \Psi \tau_{zz} w - \Gamma q_z \end{pmatrix}$$

$$\Upsilon(Upsilon) = \frac{1}{\gamma Ma_{ref}^2} \quad \Psi(Psi) = \frac{1}{Re_{ref}} \quad \Gamma(Gamma) = \frac{1}{(\gamma - 1) Ma_{ref}^2 Re_{ref} Pr_{ref}}$$

$$e = \frac{T}{\gamma(\gamma - 1) Ma_{ref}^2} + \frac{1}{2} (u^2 + v^2 + w^2) \quad p = \rho T \quad \mu = \frac{1 + S}{T + S} T^{\frac{3}{2}}, \quad S = \frac{100, 4K}{T_{ref}} \quad \lambda = \mu$$

$$q_x = -\lambda \frac{\partial T}{\partial x} \quad q_y = -\lambda \frac{\partial T}{\partial y} \quad q_z = -\lambda \frac{\partial T}{\partial z}$$

$$\tau_{xx} = \mu \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial w}{\partial z} \right) \quad \tau_{xy} = \tau_{yx} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)$$

$$\tau_{yy} = \mu \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial w}{\partial z} \right) \quad \tau_{xz} = \tau_{zx} = \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)$$

$$\tau_{zz} = \mu \left( \frac{4}{3} \frac{\partial w}{\partial z} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \quad \tau_{yz} = \tau_{zy} = \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)$$

### A.3. Koordinatentransformation $x, y, z \rightarrow \xi, \eta, \zeta$

Die allgemeine Beziehung der Koordinatentransformation lautet:

$$\frac{\partial f}{\partial x} = \xi_x \frac{\partial f}{\partial \xi} + \eta_x \frac{\partial f}{\partial \eta} + \zeta_x \frac{\partial f}{\partial \zeta} \quad \frac{\partial f}{\partial y} = \xi_y \frac{\partial f}{\partial \xi} + \eta_y \frac{\partial f}{\partial \eta} + \zeta_y \frac{\partial f}{\partial \zeta} \quad \frac{\partial f}{\partial z} = \xi_z \frac{\partial f}{\partial \xi} + \eta_z \frac{\partial f}{\partial \eta} + \zeta_z \frac{\partial f}{\partial \zeta}$$

Mithilfe des strukturierten Gitters lassen sich die Ableitungen  $(x, y, z)_{(\xi, \eta, \zeta)}$  berechnen und die Jakobischen Determinante  $J$  bestimmen:

$$J = x_\xi * y_\eta * z_\zeta + x_\eta * y_\zeta * z_\xi + x_\zeta * y_\xi * z_\eta - x_\zeta * y_\eta * z_\xi - x_\eta * y_\xi * z_\zeta - x_\xi * y_\zeta * z_\eta;$$

Daraus ergeben sich die metrischen Koeffizienten:

$$\begin{aligned} \xi_x &= (y_\eta * z_\zeta - y_\zeta * z_\eta) / J & \xi_y &= (x_\zeta * z_\eta - x_\eta * z_\zeta) / J & \xi_z &= (x_\eta * y_\zeta - x_\zeta * y_\eta) / J \\ \eta_x &= (y_\zeta * z_\xi - y_\xi * z_\zeta) / J & \eta_y &= (x_\xi * z_\zeta - x_\zeta * z_\xi) / J & \eta_z &= (x_\zeta * y_\xi - x_\xi * y_\zeta) / J \\ \zeta_x &= (y_\xi * z_\eta - y_\eta * z_\xi) / J & \zeta_y &= (x_\eta * z_\xi - x_\xi * z_\eta) / J & \zeta_z &= (x_\xi * y_\eta - x_\eta * y_\xi) / J \end{aligned}$$

Angewendet auf die Erhaltungsgleichungen ergibt dies:

$$\frac{\partial U}{\partial t} + \xi_x \frac{\partial F}{\partial \xi} + \eta_x \frac{\partial F}{\partial \eta} + \zeta_x \frac{\partial F}{\partial \zeta} + \xi_y \frac{\partial G}{\partial \xi} + \eta_y \frac{\partial G}{\partial \eta} + \zeta_y \frac{\partial G}{\partial \zeta} + \xi_z \frac{\partial H}{\partial \xi} + \eta_z \frac{\partial H}{\partial \eta} + \zeta_z \frac{\partial H}{\partial \zeta} = \xi_x \frac{\partial F^\nu}{\partial \xi} + \eta_x \frac{\partial F^\nu}{\partial \eta} + \zeta_x \frac{\partial F^\nu}{\partial \zeta} + \xi_y \frac{\partial G^\nu}{\partial \xi} + \eta_y \frac{\partial G^\nu}{\partial \eta} + \zeta_y \frac{\partial G^\nu}{\partial \zeta} + \xi_z \frac{\partial H^\nu}{\partial \xi} + \eta_z \frac{\partial H^\nu}{\partial \eta} + \zeta_z \frac{\partial H^\nu}{\partial \zeta}$$

Auf diese Gleichung wird die Produktregel angewandt

$$\frac{\partial (\xi_x F)}{\partial \xi} = \xi_x \frac{\partial F}{\partial \xi} + F \frac{\partial \xi_x}{\partial \xi} \Leftrightarrow \xi_x \frac{\partial F}{\partial \xi} = F \frac{\partial \xi_x}{\partial \xi} - \frac{\partial (\xi_x F)}{\partial \xi}$$

und mit der Jakobischen J multipliziert um folgende Form zu erhalten

$$\begin{aligned}
& \frac{\partial (JU)}{\partial t} \\
& + F \frac{\partial (J\xi_x)}{\partial \xi} - \frac{\partial (J\xi_x F)}{\partial \xi} + F \frac{\partial (J\eta_x)}{\partial \eta} - \frac{\partial (J\eta_x F)}{\partial \eta} + F \frac{\partial (J\zeta_x)}{\partial \zeta} - \frac{\partial (J\zeta_x F)}{\partial \zeta} \\
& + G \frac{\partial (J\xi_y)}{\partial \xi} - \frac{\partial (J\xi_y G)}{\partial \xi} + G \frac{\partial (J\eta_y)}{\partial \eta} - \frac{\partial (J\eta_y G)}{\partial \eta} + G \frac{\partial (J\zeta_y)}{\partial \zeta} - \frac{\partial (J\zeta_y G)}{\partial \zeta} \\
& + H \frac{\partial (J\xi_z)}{\partial \xi} - \frac{\partial (J\xi_z H)}{\partial \xi} + H \frac{\partial (J\eta_z)}{\partial \eta} - \frac{\partial (J\eta_z H)}{\partial \eta} + H \frac{\partial (J\zeta_z)}{\partial \zeta} - \frac{\partial (J\zeta_z H)}{\partial \zeta} \\
& = \\
& F^\nu \frac{\partial (J\xi_x)}{\partial \xi} - \frac{\partial (J\xi_x F^\nu)}{\partial \xi} + F^\nu \frac{\partial (J\eta_x)}{\partial \eta} - \frac{\partial (J\eta_x F^\nu)}{\partial \eta} + F^\nu \frac{\partial (J\zeta_x)}{\partial \zeta} - \frac{\partial (J\zeta_x F^\nu)}{\partial \zeta} \\
& + G^\nu \frac{\partial (J\xi_y)}{\partial \xi} - \frac{\partial (J\xi_y G^\nu)}{\partial \xi} + G^\nu \frac{\partial (J\eta_y)}{\partial \eta} - \frac{\partial (J\eta_y G^\nu)}{\partial \eta} + G^\nu \frac{\partial (J\zeta_y)}{\partial \zeta} - \frac{\partial (J\zeta_y G^\nu)}{\partial \zeta} \\
& + H^\nu \frac{\partial (J\xi_z)}{\partial \xi} - \frac{\partial (J\xi_z H^\nu)}{\partial \xi} + H^\nu \frac{\partial (J\eta_z)}{\partial \eta} - \frac{\partial (J\eta_z H^\nu)}{\partial \eta} + H^\nu \frac{\partial (J\zeta_z)}{\partial \zeta} - \frac{\partial (J\zeta_z H^\nu)}{\partial \zeta}
\end{aligned}$$

In dieser Gleichung kommen “metrische Invarianten” vor, welche analytisch null sind und daher gestrichen werden können (Ausmultiplizieren von Jakobischer mit metrischen Koeffizienten, im Anschluß kürzen sich die Terme gegeneinander heraus). Hermes beschreibt dies genauer im Anhang seiner Diss und weist darauf hin, dass die Produktregel und damit sämtliche anderen Umformungen bei Finiten Differenzen nicht erfüllt sind. Er zitiert alternative Vorschläge in der Literatur. Verwendet wird aber folgende Form, die:

**Stark Konservative Form**

$$\frac{\partial U}{\partial t} + \frac{\partial (\xi_x JF + \xi_y JG + \xi_z JH)}{\partial \xi} + \frac{\partial (\eta_x JF + \eta_y JG + \eta_z JH)}{\partial \eta} + \frac{\partial (\zeta_x JF + \zeta_y JG + \zeta_z JH)}{\partial \zeta} = \frac{\partial (\xi_x JF^\nu + \xi_y JG^\nu + \xi_z JH^\nu)}{\partial \xi} + \frac{\partial (\eta_x JF^\nu + \eta_y JG^\nu + \eta_z JH^\nu)}{\partial \eta} + \frac{\partial (\zeta_x JF^\nu + \zeta_y JG^\nu + \zeta_z JH^\nu)}{\partial \zeta}$$

#### A.4. Einführung der transformierten Flüsse $\hat{F}, \hat{G}, \hat{H}$

$$\begin{aligned}
& \underbrace{\frac{\partial U}{\partial t}}_{\text{Runge Kutta}} + \underbrace{\frac{\partial \hat{F}}{\partial \xi} + \frac{\partial \hat{G}}{\partial \eta} + \frac{\partial \hat{H}}{\partial \zeta}}_{\text{WENO}} = \underbrace{\frac{\partial \hat{F}^\nu}{\partial \xi} + \frac{\partial \hat{G}^\nu}{\partial \eta} + \frac{\partial \hat{H}^\nu}{\partial \zeta}}_{\text{Zentrale Differenzen}} \\
& \frac{\partial U}{\partial t} = Q \\
& Q = -\frac{\partial \hat{F}}{\partial \xi} - \frac{\partial \hat{F}}{\partial \eta} - \frac{\partial \hat{G}}{\partial \zeta} + \frac{\partial \hat{F}^\nu}{\partial \xi} + \frac{\partial \hat{G}^\nu}{\partial \eta} + \frac{\partial \hat{H}^\nu}{\partial \zeta}
\end{aligned}$$

## A.5. Erhaltungsgrößen

### A.5.1. Erhaltungsvektor $U$

$$U = J \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \end{pmatrix}$$

## A.6. Viskose Flüsse [Zentrale Differenzen]

$$\frac{\partial \hat{F}^\nu}{\partial \xi} = \frac{\partial}{\partial \xi} \begin{pmatrix} 0 \\ \Psi J (\xi_x \tau_{xx} + \xi_y \tau_{xy} + \xi_z \tau_{xz}) \\ \Psi J (\xi_x \tau_{xy} + \xi_y \tau_{yy} + \xi_z \tau_{yz}) \\ \Psi J (\xi_x \tau_{xz} + \xi_y \tau_{yz} + \xi_z \tau_{zz}) \\ J (\Psi (u (\xi_x \tau_{xx} + \xi_y \tau_{xy} + \xi_z \tau_{xz}) + v (\xi_x \tau_{xy} + \xi_y \tau_{yy} + \xi_z \tau_{yz}) + w (\xi_x \tau_{xz} + \xi_y \tau_{yz} + \xi_z \tau_{zz})) - \Gamma (\xi_x q_x + \xi_y q_y + \xi_z q_z)) \end{pmatrix}$$

$$\frac{\partial \hat{G}^\nu}{\partial \eta} = \frac{\partial}{\partial \eta} \begin{pmatrix} 0 \\ \Psi J (\eta_x \tau_{xx} + \eta_y \tau_{xy} + \eta_z \tau_{xz}) \\ \Psi J (\eta_x \tau_{xy} + \eta_y \tau_{yy} + \eta_z \tau_{yz}) \\ \Psi J (\eta_x \tau_{xz} + \eta_y \tau_{yz} + \eta_z \tau_{zz}) \\ J (\Psi (u (\eta_x \tau_{xx} + \eta_y \tau_{xy} + \eta_z \tau_{xz}) + v (\eta_x \tau_{xy} + \eta_y \tau_{yy} + \eta_z \tau_{yz}) + w (\eta_x \tau_{xz} + \eta_y \tau_{yz} + \eta_z \tau_{zz})) - \Gamma (\eta_x q_x + \eta_y q_y + \eta_z q_z)) \end{pmatrix}$$

$$\frac{\partial \hat{H}^\nu}{\partial \zeta} = \frac{\partial}{\partial \zeta} \begin{pmatrix} 0 \\ \Psi J (\zeta_x \tau_{xx} + \zeta_y \tau_{xy} + \zeta_z \tau_{xz}) \\ \Psi J (\zeta_x \tau_{xy} + \zeta_y \tau_{yy} + \zeta_z \tau_{yz}) \\ \Psi J (\zeta_x \tau_{xz} + \zeta_y \tau_{yz} + \zeta_z \tau_{zz}) \\ J (\Psi (u (\zeta_x \tau_{xx} + \zeta_y \tau_{xy} + \zeta_z \tau_{xz}) + v (\zeta_x \tau_{xy} + \zeta_y \tau_{yy} + \zeta_z \tau_{yz}) + w (\zeta_x \tau_{xz} + \zeta_y \tau_{yz} + \zeta_z \tau_{zz})) - \Gamma (\zeta_x q_x + \zeta_y q_y + \zeta_z q_z)) \end{pmatrix}$$

$$q_x = -\lambda \frac{\partial T}{\partial x} = -\lambda \left( \xi_x \frac{\partial T}{\partial \xi} + \eta_x \frac{\partial T}{\partial \eta} + \zeta_x \frac{\partial T}{\partial \zeta} \right)$$

$$q_y = -\lambda \frac{\partial T}{\partial y} = -\lambda \left( \xi_y \frac{\partial T}{\partial \xi} + \eta_y \frac{\partial T}{\partial \eta} + \zeta_y \frac{\partial T}{\partial \zeta} \right)$$

$$q_z = -\lambda \frac{\partial T}{\partial z} = -\lambda \left( \xi_z \frac{\partial T}{\partial \xi} + \eta_z \frac{\partial T}{\partial \eta} + \zeta_z \frac{\partial T}{\partial \zeta} \right)$$







$$\theta_1 = u\xi_x + v\xi_x + w\xi_x$$

$$\theta_2 = u\eta_x + v\eta_x + w\eta_x$$

$$\theta_3 = u\zeta_x + v\zeta_x + w\zeta_x$$

$$\begin{aligned} u &= -\frac{\theta_1\eta_y\zeta_z-\theta_1\eta_z\zeta_y-\theta_2\xi_y\zeta_z+\theta_2\xi_z\zeta_y+\theta_3\xi_y\eta_z-\theta_3\xi_z\eta_y}{-\xi_x\eta_y\zeta_z+\xi_x\eta_z\zeta_y+\xi_y\eta_x\zeta_z-\xi_y\eta_z\zeta_x-\xi_z\eta_x\zeta_y+\xi_z\eta_y\zeta_x} \\ v &= -\frac{-\theta_1\eta_x\zeta_z+\theta_1\eta_z\zeta_x+\theta_2\xi_x\zeta_z-\theta_2\xi_z\zeta_x-\theta_3\xi_x\eta_z+\theta_3\xi_z\eta_x}{-\xi_x\eta_y\zeta_z+\xi_x\eta_z\zeta_y+\xi_y\eta_x\zeta_z-\xi_y\eta_z\zeta_x-\xi_z\eta_x\zeta_y+\xi_z\eta_y\zeta_x} \\ w &= -\frac{-\theta_1\eta_x\zeta_y+\theta_1\eta_y\zeta_x+\theta_2\xi_x\zeta_y-\theta_2\xi_y\zeta_x-\theta_3\xi_x\eta_y+\theta_3\xi_y\eta_x}{\xi_x\eta_y\zeta_z-\xi_x\eta_z\zeta_y-\xi_y\eta_x\zeta_z+\xi_y\eta_z\zeta_x+\xi_z\eta_x\zeta_y-\xi_z\eta_y\zeta_x} \end{aligned}$$

## A.8. 2D-Rotationssymmetrisch

X-Achse ist Symmetrieachse und y entspricht dem Radius r.

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ \rho e\end{pmatrix}+\frac{\partial}{\partial x}\begin{pmatrix}\rho u^2+\Upsilon p\\ \rho uv\\ u\left(\rho e+\Upsilon p\right)\end{pmatrix}+\frac{\partial}{\partial y}\begin{pmatrix}\rho v^2+\Upsilon p\\ \rho uv\\ v\left(\rho e+\Upsilon p\right)\end{pmatrix}+\frac{1}{y}\begin{pmatrix}\rho v\\ \rho uv-\Psi\tau_{xy}\\ \rho v^2-\Psi\tau_{yy}\\ v\left(\rho e+\Upsilon p\right)-\Psi\tau_{xy}u-\Psi\tau_{yy}v-\Gamma q_y\end{pmatrix}=\frac{\partial}{\partial x}\begin{pmatrix}0\\ \Psi\tau_{xx}\\ \Psi\tau_{xy}\\ \Psi\tau_{xx}u+\Psi\tau_{xy}v+\Gamma q_x\end{pmatrix}+\frac{\partial}{\partial y}\begin{pmatrix}0\\ \Psi\tau_{yx}\\ \Psi\tau_{yy}\\ \Psi\tau_{yx}u+\Psi\tau_{yy}v+\Gamma q_y\end{pmatrix}$$

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$$\Upsilon(Upsilonpsilon)=\frac{1}{\gamma Ma_{ref}^2}\qquad \Psi(Psi)=\frac{1}{Re_{ref}}\qquad \Gamma(Gamma)=\frac{1}{(\gamma-1)Ma_{ref}^2Re_{ref}Pr_{ref}}$$

$$e=\frac{T}{\gamma\left(\gamma-1\right)Ma_{ref}^2}+\frac{1}{2}\left(u^2+v^2\right)\qquad p=\rho T\qquad \mu=\frac{1+S}{T+S}T^{\frac{3}{2}},\;S=\frac{100,4K}{T_{ref}}\qquad \lambda=\mu$$

$$q_x=\lambda\frac{\partial T}{\partial x}\qquad q_y=\lambda\frac{\partial T}{\partial y}$$

$$\tau_{xx}=\mu\left(\frac{4}{3}\frac{\partial u}{\partial x}-\frac{2}{3}\left(\frac{\partial v}{\partial y}+\frac{v}{y}\right)\right)\qquad \tau_{yy}=\mu\left(\frac{4}{3}\frac{\partial v}{\partial y}-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{v}{y}\right)\right)\qquad \tau_{xy}=\tau_{yx}=\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)$$

## B. Numerische Methode

### B.1. Approximation der zeitlichen Ableitung [Runge-Kutta]

Folgende Definitionen der Zwischenschritte sind verwendet:

#### B.1.1. TVD 3.Ordnung

$$\begin{aligned}U_A &= U^n + \Delta t Q(U^n) \\U_B &= \frac{3}{4}U^n + \frac{1}{4}U_A + \frac{1}{4}\Delta t Q(U_A) \\U^{n+1} &= \frac{1}{3}U^n + \frac{2}{3}U_B + \frac{2}{3}\Delta t Q(U_B)\end{aligned}$$

#### B.1.2. 4.Ordnung

$$\begin{aligned}U_A &= U^n + \frac{\Delta t}{2}Q(U^n) \\U_B &= U_A + \frac{\Delta t}{2}(-Q(U^n) + Q(U_A)) \\U_C &= U_B + \frac{\Delta t}{2}(-Q(U_A) + 2Q(U_B)) \\U^{n+1} &= U_C + \frac{\Delta t}{6}(Q(U^n) + 2Q(U_A) - 4Q(U_B) + Q(U_C))\end{aligned}$$

Eingesetzt erhält man:

$$\begin{aligned}U_A &= U^n + \frac{\Delta t}{2}Q(U^n) \\U_B &= U^n + \frac{\Delta t}{2}Q(U_A) \\U_C &= U^n + \Delta t Q(U_B) \\U^{n+1} &= U^n + \frac{\Delta t}{6}Q(U_C) + \frac{\Delta t}{6}\overbrace{[Q(U^n) + 2Q(U_A) + 2Q(U_B)]}^{Q_{Summe}}\end{aligned}$$

## B.2. Approximation der viskosen Flüsse - ausmultipliziert [Zentrale Differenzen]

### B.2.1. Doppelte Ableitung: $\frac{\partial^2}{\partial \xi^2}$

Approximation der Ableitung über Taylor-Reihe :

$$\left. \frac{\partial^2 u}{\partial \xi^2} \right|_{i,j} = \frac{A_{i+\frac{1}{2},j} \left( \frac{\partial u}{\partial \xi} \right)_{i+\frac{1}{2},j} - A_{i-\frac{1}{2},j} \left( \frac{\partial u}{\partial \xi} \right)_{i-\frac{1}{2},j}}{\Delta \xi} + \mathcal{O}(\Delta \xi^{10})$$

Mit :

$$\left( A \frac{\partial u}{\partial \xi} \right)_{i+\frac{1}{2},j} = C_{D,0} (u_{i+1} - u_i) - C_{D,1} (u_{i+2} - u_{i-1}) + C_{D,2} (u_{i+3} - u_{i-2}) - C_{D,3} (u_{i+4} - u_{i-3}) + C_{D,4} (u_{i+5} - u_{i-4})$$

$$\left( \frac{\partial u}{\partial \xi} \right)_{i-\frac{1}{2},j} = C_{D,0} (u_i - u_{i-1}) - C_{D,1} (u_{i+1} - u_{i-2}) + C_{D,2} (u_{i+2} - u_{i-3}) - C_{D,3} (u_{i+3} - u_{i-4}) + C_{D,4} (u_{i+4} - u_{i-5})$$

$$C_{D,0} = -\frac{3}{9450} \quad C_{D,1} = \frac{351}{75600} \quad C_{D,2} = -\frac{2649}{75600} \quad C_{D,3} = \frac{15351}{75600} \quad C_{D,4} = -\frac{110649}{75600}$$

### B.2.2. Gemischte Ableitung: $\frac{\partial}{\partial \xi} \left( A \frac{\partial u}{\partial \eta} \right)$

$$\frac{\partial}{\partial \xi} \left( A \frac{\partial u}{\partial \eta} \right) = \frac{A \frac{\partial u}{\partial \eta} \Big|_{i+\frac{1}{2},j} - A \frac{\partial u}{\partial \eta} \Big|_{i-\frac{1}{2},j}}{\Delta \xi} + \mathcal{O}(\Delta \xi^{10} + \Delta \eta^{10})$$

Mittels folgender Interpolation :

$$A \frac{\partial u}{\partial \eta} \Big|_{i+\frac{1}{2},j} = C_{P,0} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+1,j} + A \frac{\partial u}{\partial \eta} \Big|_{i,j} \right) - C_{P,1} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+2,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-1,j} \right) + C_{P,2} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+3,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-2,j} \right) - C_{P,3} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+4,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-3,j} \right) + C_{P,4} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+5,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-4,j} \right)$$

$$A \frac{\partial u}{\partial \eta} \Big|_{i-\frac{1}{2},j} = C_{P,0} \left( A \frac{\partial u}{\partial \eta} \Big|_{i,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-1,j} \right) - C_{P,1} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+1,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-2,j} \right) + C_{P,2} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+2,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-3,j} \right) - C_{P,3} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+3,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-4,j} \right) + C_{P,4} \left( A \frac{\partial u}{\partial \eta} \Big|_{i+4,j} + A \frac{\partial u}{\partial \eta} \Big|_{i-5,j} \right)$$

Dabei werden die Ableitungen so gebildet :

$$\frac{\partial u}{\partial \eta} \Big|_{i,j} = \frac{u_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}}}{\Delta \eta}$$

Mit :

$$u_{i,j+\frac{1}{2}} = C_{P,0} (u_{i,j+1} + u_{i,j}) - C_{P,1} (u_{i,j+2} + u_{i,j-1}) + C_{P,2} (u_{i,j+3} + u_{i,j-2}) - C_{P,3} (u_{i,j+4} + u_{i,j-3}) + C_{P,4} (u_{i,j+5} + u_{i,j-4})$$

$$u_{i,j-\frac{1}{2}} = C_{P,0} (u_{i,j} + u_{i,j-1}) - C_{P,1} (u_{i,j+1} + u_{i,j-2}) + C_{P,2} (u_{i,j+2} + u_{i,j-3}) - C_{P,3} (u_{i,j+3} + u_{i,j-4}) + C_{P,4} (u_{i,j+4} + u_{i,j-5})$$

$$C_{P,0} = \frac{1}{1260} \quad C_{P,1} = -\frac{23}{2520} \quad C_{P,2} = \frac{127}{2520} \quad C_{P,3} = -\frac{473}{2520} \quad C_{P,4} = \frac{1627}{2520}$$

### B.3. Approximation der konvektiven Flüsse inkl. Flux Vector Splitting

#### Flussberechnung mit Hilfe der Stencil

$$\frac{\partial \hat{F}}{\partial \xi} = \frac{\hat{F}_{i+\frac{1}{2},j,k} - \hat{F}_{i-\frac{1}{2},j,k}}{\Delta \xi}$$

$$\hat{F}_{i+\frac{1}{2},j,k} = \sum_{m=0}^{r-1} \omega_m M_m^r$$

$$M_m^r = \sum_{l=i+m-r+1}^{i+m} a_{m,l}^r \hat{F}_{l,j,k}$$

Gewichtskoeffizienten :  $\omega_m = \frac{\bar{\omega}_m}{\bar{\omega}_0 + \dots + \bar{\omega}_{r-1}}$

$$\bar{\omega}_m = \frac{b_m^r}{(\epsilon + IS_m)^p}$$

$$\epsilon = 10^{-6} (schlecht)$$

$$\epsilon = 10 * \sqrt{DBL\_MIN} \approx 10^{-150} (gut)$$

### Flux Vector Splitting

$$\hat{F}_{i,j,k} = \hat{F}_{i,j,k}^+ + \hat{F}_{i,j,k}^-$$

$$\Delta \hat{F}_{i+\frac{1}{2},j,k}^\pm = \hat{F}_{i+1,j,k}^\pm - \hat{F}_{i,j,k}^\pm$$

$$\hat{F}_{i,j,k}^\pm = \frac{1}{2} \left( \hat{F}_{i,j,k} \pm \lambda_{i,j,k}^{max} J \hat{U}_{i,j,k} \right)$$

Es gibt drei Varianten für das J, welches mit dem U in diese Gleichung kommt:  
 Variante 1): Für den gesamten Stencil wird ein mittleres  $\bar{J} = 0.5 / (J_i + J_{i+1})$  berechnet.  
 Variante 2):  $J$  wird über den stencil nicht mehr als konstant angesehen, sondern man nimmt für jeden Punkt den lokalen Wert.  
 Variante 3):  $J$  wird mit in die  $\lambda_{Max}$ -Berechnung genommen und findet sich dann als Faktor in  $\lambda$  wieder.

$$\hat{F}_{i+\frac{1}{2},j,k} = \Theta_{i+\frac{1}{2}} \left( \hat{F}_{i-\frac{N-1}{2}+1,j,k}, \dots, \hat{F}_{i+\frac{N-1}{2},j,k} \right)$$

$$+ \sum_{c=1}^N \left[ \varphi \left( \hat{R}_{i+\frac{1}{2},j,k}^{-1,c} \Delta \hat{F}_{i-\frac{N}{2},j,k}^-, \dots, \hat{R}_{i+\frac{1}{2},j,k}^{-1,c} \Delta \hat{F}_{i+\frac{N}{2}-2,j,k}^- \right) \right.$$

$$\left. - \varphi \left( \hat{R}_{i+\frac{1}{2},j,k}^{-1,c} \Delta \hat{F}_{i-\frac{N}{2}+1,j,k}^+, \dots, \hat{R}_{i+\frac{1}{2},j,k}^{-1,c} \Delta \hat{F}_{i+\frac{N}{2}-1,j,k}^+ \right) \right] \hat{R}_{i+\frac{1}{2},j,k}^c$$

### B.3.1. WENO9 (r=5)

$$\begin{aligned}\Theta_{i+\frac{1}{2}}\left(\hat{F}_{i-3}, \hat{F}_{i-2}, \hat{F}_{i-1}, \hat{F}_i, \hat{F}_{i+1}, \hat{F}_{i+2}, \hat{F}_{i+3}, \hat{F}_{i+4}\right) &= \frac{1}{840}\left[533\left(\hat{F}_{i+1}+\hat{F}_i\right)-139\left(\hat{F}_{i+2}+\hat{F}_{i-1}\right)+29\left(\hat{F}_{i+3}+\hat{F}_{i-2}\right)-3\left(\hat{F}_{i+4}+\hat{F}_{i-3}\right)\right] \\ \varphi\left(F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, F_9\right) &= \frac{1}{5} \omega_0 q_1+\frac{1}{20} \omega_2 q_2+\frac{1}{60} \omega_3\left(3 q_2-2 q_3\right)+\frac{1}{60} \omega_4\left(3 q_2-2 q_3+3 q_4\right)-\frac{1}{840}\left(39 q_2-14 q_3+3 q_4\right) \\ q_1 &= F_1-4 F_2+6 F_3-4 F_4+F_5 \\ q_2 &= F_2-4 F_3+6 F_4-4 F_5+F_6 \\ q_3 &= F_3-4 F_4+6 F_5-4 F_6+F_7 \\ q_4 &= F_4-4 F_5+6 F_6-4 F_7+F_8\end{aligned}$$

$$\begin{aligned}\text{Optimale Gewichtskoeffizienten : } b_0^5 &= \frac{1}{126} \\ b_1^5 &= \frac{10}{63} \\ b_2^5 &= \frac{10}{21} \\ b_3^5 &= \frac{20}{63} \\ b_4^5 &= \frac{5}{126}\end{aligned}$$

$$\begin{aligned}
\text{Glättungsindikatoren : } IS_0^5 = & \hat{F}_{i-4}(22658\hat{F}_{i-4} - 208501\hat{F}_{i-3} + 364863\hat{F}_{i-2} - 288007\hat{F}_{i-1} + 86329\hat{F}_i) \\
& + \hat{F}_{i-3}(482963\hat{F}_{i-3} - 1704396\hat{F}_{i-2} + 1358458\hat{F}_{i-1} - 411487\hat{F}_i) \\
& + \hat{F}_{i-2}(1521393\hat{F}_{i-2} - 2462076\hat{F}_{i-1} + 758823\hat{F}_i) \\
& + \hat{F}_{i-1}(1020563\hat{F}_{i-1} - 649501\hat{F}_i) + 107918\hat{F}_i^2
\end{aligned}$$

$$\begin{aligned}
IS_1^5 = & \hat{F}_{i-3}(6908\hat{F}_{i-3} - 60871\hat{F}_{i-2} + 99213\hat{F}_{i-1} - 70237\hat{F}_i + 18079\hat{F}_{i+1}) \\
& + \hat{F}_{i-2}(138563\hat{F}_{i-2} - 464976\hat{F}_{i-1} + 337018\hat{F}_i - 88297\hat{F}_{i+1}) \\
& + \hat{F}_{i-1}(406293\hat{F}_{i-1} - 611976\hat{F}_i + 165153\hat{F}_{i+1}) \\
& + \hat{F}_i(242723\hat{F}_i - 140251\hat{F}_{i+1}) + 22658\hat{F}_{i+1}^2
\end{aligned}$$

$$\begin{aligned}
IS_2^5 = & \hat{F}_{i-2}(6908\hat{F}_{i-2} - 51001\hat{F}_{i-1} + 67923\hat{F}_i - 38947\hat{F}_{i+1} + 8209\hat{F}_{i+2}) \\
& + \hat{F}_{i-1}(104963\hat{F}_{i-1} - 299076\hat{F}_i + 179098\hat{F}_{i+1} - 38947\hat{F}_{i+2}) \\
& + \hat{F}_i(231153\hat{F}_i - 299076\hat{F}_{i+1} + 67923\hat{F}_{i+2}) \\
& + \hat{F}_{i+1}(104963\hat{F}_{i+1} - 51001\hat{F}_{i+2}) + 6908\hat{F}_{i+2}^2
\end{aligned}$$

$$\begin{aligned}
IS_3^5 = & \hat{F}_{i-1}(22658\hat{F}_{i-1} - 140251\hat{F}_i + 165153\hat{F}_{i+1} - 88297\hat{F}_{i+2} + 18079\hat{F}_{i+3}) \\
& + \hat{F}_i(242723\hat{F}_i - 611976\hat{F}_{i+1} + 337018\hat{F}_{i+2} - 70237\hat{F}_{i+3}) \\
& + \hat{F}_{i+1}(406293\hat{F}_{i+1} - 464976\hat{F}_{i+2} + 99213\hat{F}_{i+3}) \\
& + \hat{F}_{i+2}(138563\hat{F}_{i+2} - 60871\hat{F}_{i+3}) + 6908\hat{F}_{i+3}^2
\end{aligned}$$

$$\begin{aligned}
IS_4^5 = & \hat{F}_i(107918\hat{F}_i - 649501\hat{F}_{i+1} + 758823\hat{F}_{i+2} - 411487\hat{F}_{i+3} + 86329\hat{F}_{i+4}) \\
& + \hat{F}_{i+1}(1020563\hat{F}_{i+1} - 2462076\hat{F}_{i+2} + 1358458\hat{F}_{i+3} - 288007\hat{F}_{i+4}) \\
& + \hat{F}_{i+2}(1521393\hat{F}_{i+2} - 1704396\hat{F}_{i+3} + 364863\hat{F}_{i+4}) \\
& + \hat{F}_{i+3}(482963\hat{F}_{i+3} - 208501\hat{F}_{i+4}) + 22658\hat{F}_{i+4}^2
\end{aligned}$$

### B.3.2. WENO5 (r=3)

$$\begin{aligned}\Theta_{i+\frac{1}{2}}(\hat{F}_{i-1}, \hat{F}_i, \hat{F}_{i+1}, \hat{F}_{i+2}) &= \frac{1}{12} \left[ -(\hat{F}_{i-1} + \hat{F}_{i+2}) + 7(\hat{F}_i + \hat{F}_{i+1}) \right] \\ \varphi(F_1, F_2, F_3, F_4) &= \frac{1}{3} \omega_0 q_1 + \frac{1}{6} \left( \omega_2 - \frac{1}{2} \right) q_2 \\ q_1 &= F_1 - 2F_2 + F_3 \\ q_2 &= F_2 - 2F_3 + F_4\end{aligned}$$

$$\begin{aligned}\text{Optimal Gewichtskoeffizienten : } b_0^3 &= \frac{1}{10} \\ b_1^3 &= \frac{3}{5} \\ b_2^3 &= \frac{3}{10}\end{aligned}$$

$$\begin{aligned}\text{Glättungsindikatoren : } IS_0^3 &= 13 \left( \hat{F}_{i-1} - \hat{F}_i \right)^2 + 3 \left( \hat{F}_{i-1} - 3\hat{F}_i \right)^2 \\ IS_1^3 &= 13 \left( \hat{F}_i - \hat{F}_{i+1} \right)^2 + 3 \left( \hat{F}_i + \hat{F}_{i+1} \right)^2 \\ IS_2^3 &= 13 \left( \hat{F}_{i+1} - \hat{F}_{i+2} \right)^2 + 3 \left( 3\hat{F}_{i+1} - \hat{F}_{i+2} \right)^2\end{aligned}$$

### B.3.3. Eigenvektoren für $\hat{F}$ , $\hat{G}$ und $\hat{H}$

$$\begin{aligned}\hat{\xi}_x &= \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}} & \hat{\xi}_y &= \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}} & \hat{\xi}_z &= \frac{\xi_z}{\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2}} \\ \hat{\eta}_x &= \frac{\eta_x}{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}} & \hat{\eta}_y &= \frac{\eta_y}{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}} & \hat{\eta}_z &= \frac{\eta_z}{\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2}} \\ \hat{\zeta}_x &= \frac{\zeta_x}{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}} & \hat{\zeta}_y &= \frac{\zeta_y}{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}} & \hat{\zeta}_z &= \frac{\zeta_z}{\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2}}\end{aligned}$$



## Eigenvektoren für $\hat{F}$

$$R_1 = \begin{array}{c|c|c|c|c} \hat{\xi}_x & \hat{\xi}_y & \hat{\xi}_z & \frac{1}{\sqrt{2c}} & \frac{1}{\sqrt{2c}} \\ \hline u\hat{\xi}_x & u\hat{\xi}_y - \rho\hat{\xi}_z & u\hat{\xi}_z + \rho\hat{\xi}_y & \frac{1}{\sqrt{2c}}(u + \hat{\xi}_x c) & \frac{1}{\sqrt{2c}}(u - \hat{\xi}_x c) \\ \hline v\hat{\xi}_x + \rho\hat{\xi}_z & v\hat{\xi}_y & v\hat{\xi}_z - \rho\hat{\xi}_x & \frac{1}{\sqrt{2c}}(v + \hat{\xi}_y c) & \frac{1}{\sqrt{2c}}(v - \hat{\xi}_y c) \\ \hline w\hat{\xi}_x - \rho\hat{\xi}_y & w\hat{\xi}_y + \rho\hat{\xi}_x & w\hat{\xi}_z & \frac{1}{\sqrt{2c}}(w + \hat{\xi}_z c) & \frac{1}{\sqrt{2c}}(w - \hat{\xi}_z c) \\ \hline \frac{u^2+v^2+w^2}{2}\hat{\xi}_x + \rho(v\hat{\xi}_z - w\hat{\xi}_y) & \frac{u^2+v^2+w^2}{2}\hat{\xi}_y + \rho(w\hat{\xi}_x - u\hat{\xi}_z) & \frac{u^2+v^2+w^2}{2}\hat{\xi}_z + \rho(u\hat{\xi}_y - v\hat{\xi}_x) & \frac{1}{\sqrt{2c}}\left[\frac{u^2+v^2+w^2}{2} + \frac{c^2}{\gamma-1} + c(u\hat{\xi}_x + v\hat{\xi}_y + w\hat{\xi}_z)\right] & \frac{1}{\sqrt{2c}}\left[\frac{u^2+v^2+w^2}{2} + \frac{c^2}{\gamma-1} - c(u\hat{\xi}_x + v\hat{\xi}_y + w\hat{\xi}_z)\right] \end{array}$$

$$R_1^{-1} = \begin{array}{c|c|c|c|c} \left(1 - \frac{\gamma-1}{2}M^2\right)\hat{\xi}_x - \frac{1}{\rho}(v\hat{\xi}_z - w\hat{\xi}_y) & (\gamma-1)\frac{u}{c^2}\hat{\xi}_x & (\gamma-1)\frac{v}{c^2}\hat{\xi}_x + \frac{\hat{\xi}_z}{\rho} & (\gamma-1)\frac{w}{c^2}\hat{\xi}_x - \frac{\hat{\xi}_y}{\rho} & -\frac{\gamma-1}{c^2}\hat{\xi}_x \\ \hline \left(1 - \frac{\gamma-1}{2}M^2\right)\hat{\xi}_y - \frac{1}{\rho}(w\hat{\xi}_x - u\hat{\xi}_z) & (\gamma-1)\frac{u}{c^2}\hat{\xi}_y - \frac{\hat{\xi}_z}{\rho} & (\gamma-1)\frac{w}{c^2}\hat{\xi}_y & (\gamma-1)\frac{w}{c^2}\hat{\xi}_y + \frac{\hat{\xi}_x}{\rho} & -\frac{\gamma-1}{c^2}\hat{\xi}_y \\ \hline \left(1 - \frac{\gamma-1}{2}M^2\right)\hat{\xi}_z - \frac{1}{\rho}(u\hat{\xi}_y - v\hat{\xi}_x) & (\gamma-1)\frac{u}{c^2}\hat{\xi}_z + \frac{\hat{\xi}_y}{\rho} & (\gamma-1)\frac{w}{c^2}\hat{\xi}_z - \frac{\hat{\xi}_x}{\rho} & (\gamma-1)\frac{w}{c^2}\hat{\xi}_z & -\frac{\gamma-1}{c^2}\hat{\xi}_z \\ \hline \frac{c}{\sqrt{2}}\left[\frac{\gamma-1}{2}M^2 - \frac{1}{c}(u\hat{\xi}_x + v\hat{\xi}_y + w\hat{\xi}_z)\right] & \frac{1}{\sqrt{2}}\left(\hat{\xi}_x - \frac{\gamma-1}{c}u\right) & \frac{1}{\sqrt{2}}\left(\hat{\xi}_y - \frac{\gamma-1}{c}v\right) & \frac{1}{\sqrt{2}}\left(\hat{\xi}_z - \frac{\gamma-1}{c}w\right) & \frac{\gamma-1}{\sqrt{2c}} \\ \hline \frac{c}{\sqrt{2}}\left[\frac{\gamma-1}{2}M^2 + \frac{1}{c}(u\hat{\xi}_x + v\hat{\xi}_y + w\hat{\xi}_z)\right] & -\frac{1}{\sqrt{2}}\left(\hat{\xi}_x + \frac{\gamma-1}{c}u\right) & -\frac{1}{\sqrt{2}}\left(\hat{\xi}_y + \frac{\gamma-1}{c}v\right) & -\frac{1}{\sqrt{2}}\left(\hat{\xi}_z + \frac{\gamma-1}{c}w\right) & \frac{\gamma-1}{\sqrt{2c}} \end{array}$$

## Eigenvektoren für $\hat{G}$

$$R_2 = \begin{array}{c|c|c|c|c} \hat{\eta}_x & \hat{\eta}_y & \hat{\eta}_z & \frac{1}{\sqrt{2c}} & \frac{1}{\sqrt{2c}} \\ \hline u\hat{\eta}_x & u\hat{\eta}_y - \rho\hat{\eta}_z & u\hat{\eta}_z + \rho\hat{\eta}_y & \frac{1}{\sqrt{2c}}(u + \hat{\eta}_x c) & \frac{1}{\sqrt{2c}}(u - \hat{\eta}_x c) \\ \hline v\hat{\eta}_x + \rho\hat{\eta}_z & v\hat{\eta}_y & v\hat{\eta}_z - \rho\hat{\eta}_x & \frac{1}{\sqrt{2c}}(v + \hat{\eta}_y c) & \frac{1}{\sqrt{2c}}(v - \hat{\eta}_y c) \\ \hline w\hat{\eta}_x - \rho\hat{\eta}_y & w\hat{\eta}_y + \rho\hat{\eta}_x & w\hat{\eta}_z & \frac{1}{\sqrt{2c}}(w + \hat{\eta}_z c) & \frac{1}{\sqrt{2c}}(w - \hat{\eta}_z c) \\ \hline \frac{u^2+v^2+w^2}{2}\hat{\eta}_x + \rho(v\hat{\eta}_z - w\hat{\eta}_y) & \frac{u^2+v^2+w^2}{2}\hat{\eta}_y + \rho(w\hat{\eta}_x - u\hat{\eta}_z) & \frac{u^2+v^2+w^2}{2}\hat{\eta}_z + \rho(u\hat{\eta}_y - v\hat{\eta}_x) & \frac{1}{\sqrt{2c}}\left[\frac{u^2+v^2+w^2}{2} + \frac{c^2}{\gamma-1} + c(u\hat{\eta}_x + v\hat{\eta}_y + w\hat{\eta}_z)\right] & \frac{1}{\sqrt{2c}}\left[\frac{u^2+v^2+w^2}{2} + \frac{c^2}{\gamma-1} - c(u\hat{\eta}_x + v\hat{\eta}_y + w\hat{\eta}_z)\right] \end{array}$$

$$R_2^{-1} = \begin{array}{c|c|c|c|c} \left(1 - \frac{\gamma-1}{2}M^2\right)\hat{\eta}_x - \frac{1}{\rho}(v\hat{\eta}_z - w\hat{\eta}_y) & (\gamma-1)\frac{u}{c^2}\hat{\eta}_x & (\gamma-1)\frac{v}{c^2}\hat{\eta}_x + \frac{\hat{\eta}_z}{\rho} & (\gamma-1)\frac{w}{c^2}\hat{\eta}_x - \frac{\hat{\eta}_y}{\rho} & -\frac{\gamma-1}{c^2}\hat{\eta}_x \\ \hline \left(1 - \frac{\gamma-1}{2}M^2\right)\hat{\eta}_y - \frac{1}{\rho}(w\hat{\eta}_x - u\hat{\eta}_z) & (\gamma-1)\frac{u}{c^2}\hat{\eta}_y - \frac{\hat{\eta}_z}{\rho} & (\gamma-1)\frac{v}{c^2}\hat{\eta}_y & (\gamma-1)\frac{w}{c^2}\hat{\eta}_y + \frac{\hat{\eta}_x}{\rho} & -\frac{\gamma-1}{c^2}\hat{\eta}_y \\ \hline \left(1 - \frac{\gamma-1}{2}M^2\right)\hat{\eta}_z - \frac{1}{\rho}(u\hat{\eta}_y - v\hat{\eta}_x) & (\gamma-1)\frac{u}{c^2}\hat{\eta}_z + \frac{\hat{\eta}_y}{\rho} & (\gamma-1)\frac{v}{c^2}\hat{\eta}_z - \frac{\hat{\eta}_x}{\rho} & (\gamma-1)\frac{w}{c^2}\hat{\eta}_z & -\frac{\gamma-1}{c^2}\hat{\eta}_z \\ \hline \frac{c}{\sqrt{2}}\left[\frac{\gamma-1}{2}M^2 - \frac{1}{c}(u\hat{\eta}_x + v\hat{\eta}_y + w\hat{\eta}_z)\right] & \frac{1}{\sqrt{2}}\left(\hat{\eta}_x - \frac{\gamma-1}{c}u\right) & \frac{1}{\sqrt{2}}\left(\hat{\eta}_y - \frac{\gamma-1}{c}v\right) & \frac{1}{\sqrt{2}}\left(\hat{\eta}_z - \frac{\gamma-1}{c}w\right) & \frac{\gamma-1}{\sqrt{2c}} \\ \hline \frac{c}{\sqrt{2}}\left[\frac{\gamma-1}{2}M^2 + \frac{1}{c}(u\hat{\eta}_x + v\hat{\eta}_y + w\hat{\eta}_z)\right] & -\frac{1}{\sqrt{2}}\left(\hat{\eta}_x + \frac{\gamma-1}{c}u\right) & -\frac{1}{\sqrt{2}}\left(\hat{\eta}_y + \frac{\gamma-1}{c}v\right) & -\frac{1}{\sqrt{2}}\left(\hat{\eta}_z + \frac{\gamma-1}{c}w\right) & \frac{\gamma-1}{\sqrt{2c}} \end{array}$$

## Eigenvektoren für $\hat{H}$

$$R_3 = \begin{array}{c|c|c|c|c} \hat{\zeta}_x & \hat{\zeta}_y & \hat{\zeta}_z & \frac{1}{\sqrt{2c}} & \frac{1}{\sqrt{2c}} \\ \hline u\hat{\zeta}_x & u\hat{\zeta}_y - \rho\hat{\zeta}_z & u\hat{\zeta}_z + \rho\hat{\zeta}_y & \frac{1}{\sqrt{2c}} \left( u + \hat{\zeta}_x c \right) & \frac{1}{\sqrt{2c}} \left( u - \hat{\zeta}_x c \right) \\ \hline v\hat{\zeta}_x + \rho\hat{\zeta}_z & v\hat{\zeta}_y & v\hat{\zeta}_z - \rho\hat{\zeta}_x & \frac{1}{\sqrt{2c}} \left( v + \hat{\zeta}_y c \right) & \frac{1}{\sqrt{2c}} \left( v - \hat{\zeta}_y c \right) \\ \hline w\hat{\zeta}_x - \rho\hat{\zeta}_y & w\hat{\zeta}_y + \rho\hat{\zeta}_x & w\hat{\zeta}_z & \frac{1}{\sqrt{2c}} \left( w + \hat{\zeta}_z c \right) & \frac{1}{\sqrt{2c}} \left( w - \hat{\zeta}_z c \right) \\ \hline \frac{u^2+v^2+w^2}{2}\hat{\zeta}_x + \rho \left( v\hat{\zeta}_z - w\hat{\zeta}_y \right) & \frac{u^2+v^2+w^2}{2}\hat{\zeta}_y + \rho \left( w\hat{\zeta}_x - u\hat{\zeta}_z \right) & \frac{u^2+v^2+w^2}{2}\hat{\zeta}_z + \rho \left( u\hat{\zeta}_y - v\hat{\zeta}_x \right) & \frac{1}{\sqrt{2c}} \left[ \frac{u^2+v^2+w^2}{2} + \frac{c^2}{\gamma-1} + c \left( u\hat{\zeta}_x + v\hat{\zeta}_y + w\hat{\zeta}_z \right) \right] & \frac{1}{\sqrt{2c}} \left[ \frac{u^2+v^2+w^2}{2} + \frac{c^2}{\gamma-1} - c \left( u\hat{\zeta}_x + v\hat{\zeta}_y + w\hat{\zeta}_z \right) \right] \end{array}$$

$$R_3^{-1} = \begin{array}{c|c|c|c|c} \left( 1 - \frac{\gamma-1}{2} M^2 \right) \hat{\zeta}_x - \frac{1}{\rho} \left( v\hat{\zeta}_z - w\hat{\zeta}_y \right) & (\gamma-1) \frac{u}{c^2} \hat{\zeta}_x & (\gamma-1) \frac{v}{c^2} \hat{\zeta}_x + \frac{\hat{\zeta}_x}{\rho} & (\gamma-1) \frac{w}{c^2} \hat{\zeta}_x - \frac{\hat{\zeta}_y}{\rho} & -\frac{\gamma-1}{c^2} \hat{\zeta}_x \\ \hline \left( 1 - \frac{\gamma-1}{2} M^2 \right) \hat{\zeta}_y - \frac{1}{\rho} \left( w\hat{\zeta}_x - u\hat{\zeta}_z \right) & (\gamma-1) \frac{u}{c^2} \hat{\zeta}_y - \frac{\hat{\zeta}_x}{\rho} & (\gamma-1) \frac{u}{c^2} \hat{\zeta}_y & (\gamma-1) \frac{w}{c^2} \hat{\zeta}_y + \frac{\hat{\zeta}_x}{\rho} & -\frac{\gamma-1}{c^2} \hat{\zeta}_y \\ \hline \left( 1 - \frac{\gamma-1}{2} M^2 \right) \hat{\zeta}_z - \frac{1}{\rho} \left( u\hat{\zeta}_y - v\hat{\zeta}_x \right) & (\gamma-1) \frac{u}{c^2} \hat{\zeta}_z + \frac{\hat{\zeta}_y}{\rho} & (\gamma-1) \frac{v}{c^2} \hat{\zeta}_z - \frac{\hat{\zeta}_x}{\rho} & (\gamma-1) \frac{w}{c^2} \hat{\zeta}_z & -\frac{\gamma-1}{c^2} \hat{\zeta}_z \\ \hline \frac{c}{\sqrt{2}} \left[ \frac{\gamma-1}{2} M^2 - \frac{1}{c} \left( u\hat{\zeta}_x + v\hat{\zeta}_y + w\hat{\zeta}_z \right) \right] & \frac{1}{\sqrt{2}} \left( \hat{\zeta}_x - \frac{\gamma-1}{c} u \right) & \frac{1}{\sqrt{2}} \left( \hat{\zeta}_y - \frac{\gamma-1}{c} v \right) & \frac{1}{\sqrt{2}} \left( \hat{\zeta}_z - \frac{\gamma-1}{c} w \right) & \frac{\gamma-1}{\sqrt{2}c} \\ \hline \frac{c}{\sqrt{2}} \left[ \frac{\gamma-1}{2} M^2 + \frac{1}{c} \left( u\hat{\zeta}_x + v\hat{\zeta}_y + w\hat{\zeta}_z \right) \right] & -\frac{1}{\sqrt{2}} \left( \hat{\zeta}_x + \frac{\gamma-1}{c} u \right) & -\frac{1}{\sqrt{2}} \left( \hat{\zeta}_y + \frac{\gamma-1}{c} v \right) & -\frac{1}{\sqrt{2}} \left( \hat{\zeta}_z + \frac{\gamma-1}{c} w \right) & \frac{\gamma-1}{\sqrt{2}c} \end{array}$$

### B.3.4. Eigenwertbestimmung $\lambda_{max}$

Innerhalb eines Stencils wird der maximale Eigenwert  $\lambda_{max}$  bestimmt

$$\begin{array}{lll} \Theta_1 = u\xi_x + v\xi_y + w\xi_z & \Theta_2 = u\eta_x + v\eta_y + w\eta_z & \Theta_3 = u\zeta_x + v\zeta_y + w\zeta_z \\ c_1 = c\sqrt{\xi_x^2 + \xi_y^2 + \xi_z^2} & c_2 = c\sqrt{\eta_x^2 + \eta_y^2 + \eta_z^2} & c_3 = c\sqrt{\zeta_x^2 + \zeta_y^2 + \zeta_z^2} \end{array}$$

$$\lambda_{max} = \max(\lambda_k) \\ \lambda_k = (|\Theta_k|, |\Theta_k|, |\Theta_k|, |\Theta_k + c_k|, |\Theta_k - c_k|)$$

### B.3.5. Sonstige Formeln

$$y^+ \approx \frac{20}{Re_{ref}}$$

## C. Randbedingungen

Die Randbedingungen werden bisher mittels Ghostcells eingestellt. Eine mögliche Alternative für Verfahren hoher Ordnung ist die Reduzierung der Ordnung zum Rand hin. Dann kann man dann den Rand direkt determinieren ( $u=0\dots$ ).

Bei der Verwendung von GhostCells spielt die Tatsache eine große Rolle, dass die verwendeten Gitter in den meisten Fällen krummlinig sind. Die Forderung  $\frac{\partial p}{\partial n}$  ist somit nicht trivial krummlinigen Koordinaten-System (KoS). Man stelle sich z.B. vor, dass eine Gitterlinie unter einem scharfen Winkel auf den Rand trifft. Verfolgt man jetzt die Ideologie, dass die Druckwerte gespiegelt werden, so erzeugt man dadurch ungewollt einen Rand der orthogonal zu dieser Gitterlinie ist. Als besonders klares Beispiel kann die Simulation eines Riemann Problems betrachtet werden. Ein Gebiet mit Riemann-Startbedingungen und freien Rändern erzeugt bei schrägen Gitterlinien am Rand eine Krümmung des Stoßes, weil die unsteten Druckverläufe am Rand falsch gespiegelt werden. Als Folge erfüllen die Ghostcells im kartesischen Koordinatensystem nicht die Forderung  $\frac{\partial p}{\partial n}$  und ein Druckgradient stellt sich ein.

Ein Gedanke, dieses Problem zu umgehen, ist die Spiegelung der Metrik. Eine gespiegelte Metrik und gespiegelte Strömungsgrößen  $p, \rho, u, v, w$  führen zu einer direkten Kontrolle der

Flüsse. Allerdings gibt es Probleme bei den Impulsflüssen, da hier das Produkt aus  $u,v,w$  und  $\theta$  steht. Ein Vorzeichenverlust ist die Folge. Dies kann korrigiert werden, indem eine Hilfsvariable (BC\_Corrector in SHOCK) verwendet wird, aber dennoch sind diese Randbedingungen von zwei Fehlern geprägt. Auf diese Weise sind die Flüsse symmetrisch. Im Weiteren kann gezeigt werden, dass bei der verwendeten Approximation  $\frac{\partial F}{\partial x} = \frac{F_{i+1/2}-F_{i-1/2}}{\Delta x}$  die Ableitung gleich 0 wird sofern die optimalen Koeffizienten für das WENO Verfahren eingesetzt werden. (Klioutchnikov hat eine entsprechende Umformung). Die Wand befindet sich zwischen dem ersten realen Gitterpunkt und der ersten GhostCell. Für die anderen Randbedinungen werden die GhostCells extrapoliert und die Metrik berechnet wird. Hier ist auf zwei Dinge zu achten:

- 1. Das Gitter muss zum Rand orthogonal sein.
- 2. Die Gitterabstände am Rand müssen symmetrisch zum Rand sein (keine Extrapolation mit konstantem Abstand).

Nur wenn sowohl Abstand als auch Winkel zum Rand (Wand) in einer GhostCell so sind, dass sie am Rand gespiegelt einer realen Gitterzelle entsprechen, ist eine Spiegelung der Strömungsgrößen  $p,\rho,u,v,w$  aus eben dieser realen Gitterzelle in die GhostCell zulässig.

Bei Einhaltung dieser Anforderungen an das Gitter spielt es keine Rolle ob  $\theta_{1,2,3}$  oder  $u,v,w$  gespiegelt werden, da die Metrik der GhostCells entsprechend der Metrik des realen Gebietes ist und eine Umrechnung von  $\theta_{1,2,3}$  nach  $u,v,w$  und umgekehrt möglich ist.

**Metrikspiegelung:** Die Spiegelung der Metrik für Slip und Non-Slip Walls geschieht unter Berücksichtigung der Flüsse. Damit ist gemeint, dass die Flussgrößen nur dann antimetrisch sein können wenn die Metrik antimetrisch ist. Die Geschwindigkeiten in Form von  $\theta_{1,2,3}$  und  $u,v,w$  haben allerdings das bekannte Problem, dass das Minuszeichen verschwinden kann. Dies kann vermieden werden, indem die Hilfsvariable BC\_Corrector verwendet wird.

**Anmerkung:** Der Geschwindigkeitsvektor besitzt im kartesischen KoS die achsenparallelen Komponenten  $u,v,w$  und im krummlinigen die achsenparallelen Komponenten  $\theta_{1,2,3}$ .

$$\begin{pmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{pmatrix} \cdot \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u\xi_x + v\xi_y + w\xi_z \\ u\eta_x + v\eta_y + w\eta_z \\ u\zeta_x + v\zeta_y + w\zeta_z \end{pmatrix} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix}$$

## D. Ähnlichkeitsgrößen

Mach-Zahl	Ma	$\frac{\text{Stroemungsgeschwindigkeit}}{\text{Schallgeschwindigkeit}}$	$\frac{v}{c}$	$\frac{m/s}{m/s}$
Reynolds-Zahl	Re	$\frac{\text{Tragheitskraft}}{\text{Zachigkeitskraft}}$	$\frac{\rho \cdot v \cdot l}{\mu}$	$\frac{kg/m^3 \cdot m/s \cdot m}{kg/s \cdot m}$
Prandtl-Zahl	Pr	$\frac{\text{Impulstransport}}{\text{Waermetransport}} = \frac{\text{kinematischer Viskositaet}}{\text{Temperaturleitfahigkeit}}$	$\frac{\nu}{a}$	$\frac{m^2/s}{m^2/s}$
Schmidt-Zahl	Sc	$\frac{\text{Impulstransport}}{\text{Stofftransport}} = \frac{\text{kinematischer Viskositaet}}{\text{Diffusionskoeffizient}}$	$\frac{\nu}{D}$	$\frac{m^2/s}{m^2/s}$
Strouhal-Zahl	Sr	$\frac{\text{Wirbelabloesefrequenz und Groesse des umstroemten Hindernisses}}{\text{Stroemungsgeschwindigkeit}}$	$\frac{f \cdot l}{v}$	$\frac{1/s \cdot m}{m/s}$