A Newton – Like Finite Element Scheme for Stationary Compressible Gas and Particle – Laden Gas Flows

Marcel Gurris

Dortmund University of Technology

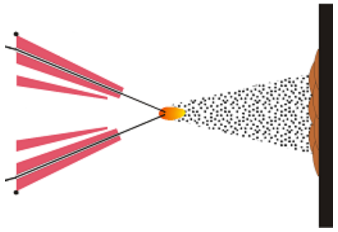
marcel.gurris@math.uni-dortmund.de

Contents & Goals

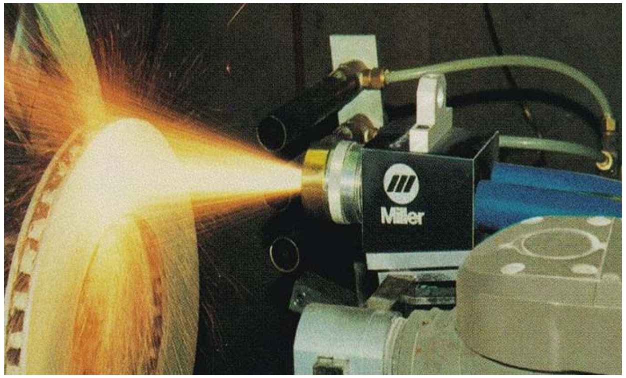
Aims

- Simulation of the gas-particle in arc spraying equipment
- High-resolution (semi-) implicit FEM-TVD schemes
- Stationary solutions

Experimental setup



Brake disk coating



Contents

- FEM discretization
- Semi-implicit pseudo time stepping and Newton-like schemes
- Boundary conditions
- Preconditioner
- Numerical results

The Euler Equations

Euler equations:

$$\partial_t \begin{bmatrix} \rho \\ \rho\mathbf{u} \\ \rho E \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho\mathbf{u} \\ \rho\mathbf{u} \otimes \mathbf{u} + \mathbf{I}P \\ \mathbf{u}(\rho E + P) \end{bmatrix} = 0$$

The 2 – Fluid Model

Gas phase:

$$\partial_t \begin{bmatrix} \alpha_g \rho_g \\ \alpha_g \rho_g \mathbf{u}_g \\ \alpha_g \rho_g E_g \end{bmatrix} + \nabla \cdot \begin{bmatrix} \alpha_g \rho_g \mathbf{u}_g \\ \alpha_g \rho_g \mathbf{u}_g \otimes \mathbf{u}_g + \alpha_g \mathbf{I} P \\ \alpha_g \mathbf{u}_g \left(\rho_g E_g + P \right) \end{bmatrix} = \begin{bmatrix} 0 \\ -\mathbf{F}_D \\ -\mathbf{u}_p \cdot \mathbf{F}_D - Q_T \end{bmatrix}$$

Particulate phase:

$$\partial_t \begin{bmatrix} \alpha_p \rho_p \\ \alpha_p \rho_p \mathbf{u}_p \\ \alpha_p \rho_p E_p \end{bmatrix} + \nabla \cdot \begin{bmatrix} \alpha_p \rho_p \mathbf{u}_p \\ \alpha_p \rho_p \mathbf{u}_p \otimes \mathbf{u}_p \\ \alpha_p \rho_p \mathbf{u}_p E_p \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{F}_D \\ \mathbf{u}_p \cdot \mathbf{F}_D + Q_T \end{bmatrix}$$

Saturation condition:

$$\alpha_g + \alpha_p = 1$$

- Two-way coupling via volume fractions and interfacial forces

High – Resolution Schemes

High – order scheme:

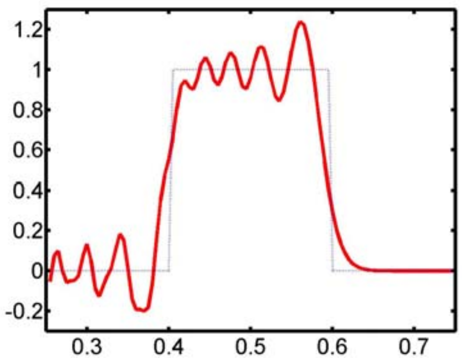
$$M_C \frac{dU}{dt} = KU$$

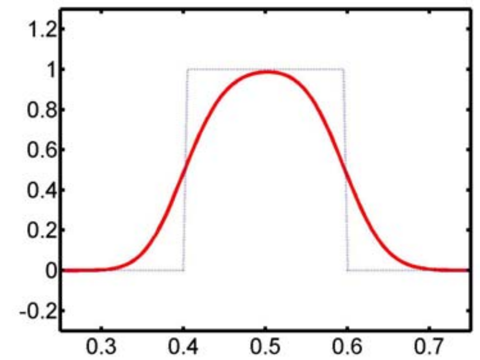
Low – order scheme:

$$M_L \frac{dU}{dt} = KU + DU = LU$$

- Oscillatory
- Second order

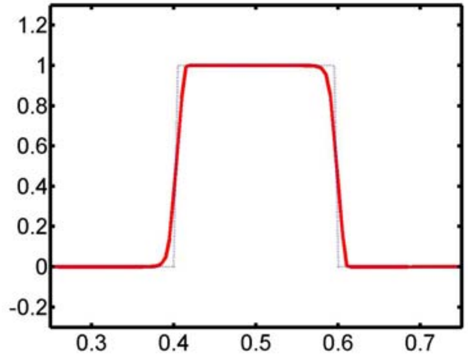
- Non – oscillatory
- First order





High – resolution scheme:

$$M_L \frac{dU}{dt} = KU + DU + F^{*}U = K^{*}U$$



- Non - oscillatory
- Less diffusive
- Variable order

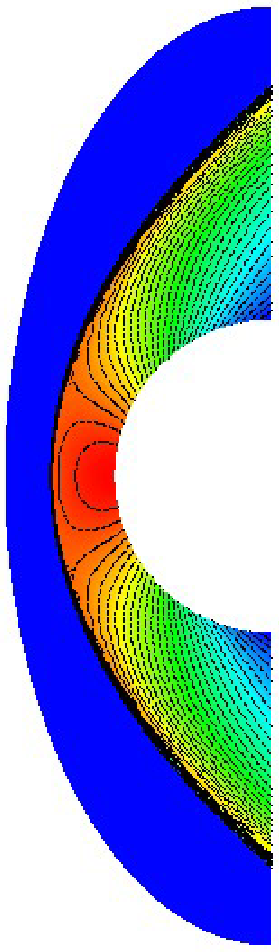
High – Resolution Scheme: Validation

Circular Cylinder at M=10:

- Riemann solvers fail
- Carbuncle phenomenon
- Oscillations at the bow shock

→ **No troubles with our scheme**

Gas density



Treatment of Source Terms

Mass lumping: $M_C S \Rightarrow M_L S$

Douglas – Rachford splitting

$$M_L \frac{\tilde{U} - U^n}{\Delta t} = \tilde{F} + M_L S^n$$

$$\frac{U^{n+1} - \tilde{U}}{\Delta t} = S^{n+1} - S^n$$

- Time step independent steady–state solutions
- Restrictive time step constraints
- Slow convergence

Strongly coupled strategy

$$M_L \frac{U^{n+1} - U^n}{\Delta t} = F^{n+1} + M_L S^{n+1}$$

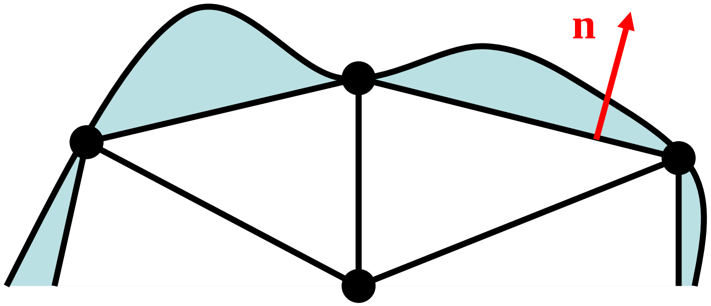
- Time step independent steady–state solutions
- No time step constraints
- Fast convergence

Weak Neumann – Type Boundary Conditions

Integration by parts:

$$\sum_j m_{ij} \frac{dU_j}{dt} = \sum_j \mathbf{c}_{ji} \cdot \mathbf{F}_j - \int_{\partial\Omega} \varphi_i \mathbf{n} \cdot \mathbf{F}_h ds, \quad \forall i$$

- Implicit treatment possible
- Unconditionally stable
- Uniquely defined outward normal
- Boundary conditions locally satisfied

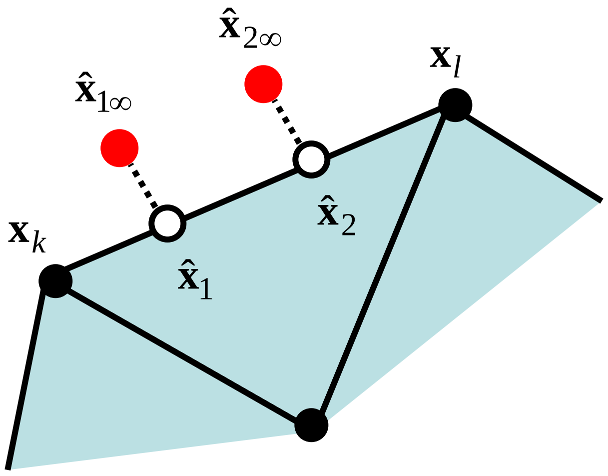


$$\int_{\partial\Omega} \varphi_i \mathbf{n} \cdot \mathbf{F}_h ds$$ → Evaluation of the boundary flux by solution of a boundary Riemann problem → $$\int_{\partial\Omega} \varphi_i \mathbf{n} \cdot \tilde{\mathbf{F}}_h ds$$

Boundary Flux & Boundary Integral

Evaluation of the boundary integral:

- Ghost nodes
- Edgewise integration



Roe flux:

$$F_{i\infty} = \frac{F_i + F_\infty}{2} - \frac{1}{2}\left|A_{i\infty}\right|\left(U_\infty - U_i\right)$$

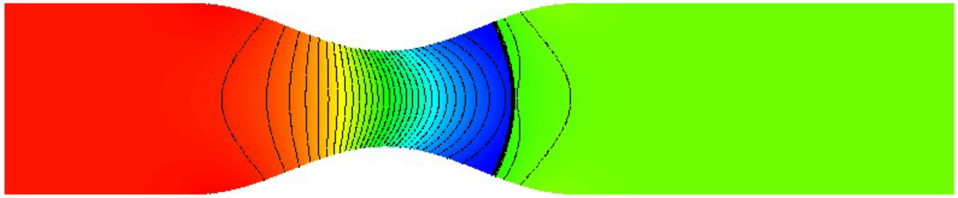
- Consistent with interior discretization
- U_∞ defined by the Riemann invariants
- Boundary conditions for incoming Riemann invariants

Verification

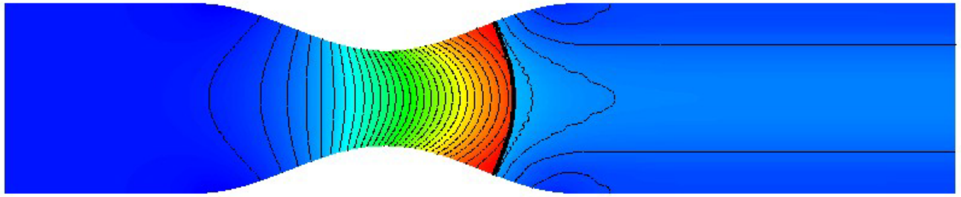
Nozzle with „pressure - outlet“:

- Subsonic inlet and outlet
- Outlet pressure: $P_{out} = 2/3$
- Convergence

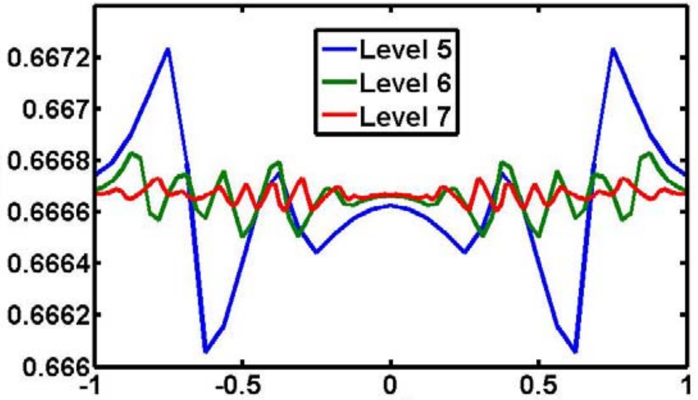
Pressure (red: P=1, blue: P=0.13)



Mach number (red: M=2.03, blue: M=0.27)



Computed outlet pressure



Convergence Analysis: „Pressure – Outlet“

Outlet pressure:

Level	NVT	NEL	NVT^{out}	E_2^{out}	p^{out}
5	5313	5120	33	$2.50 \cdot 10^{-3}$	1.32
6	20865	20480	65	$1.00 \cdot 10^{-3}$	1.12
7	82689	81920	129	$4.62 \cdot 10^{-4}$	

$$E_2^{out} = \frac{\left\| P_h - P_{out} \right\|_{2,\Gamma_{out}}}{\left\| P_{out} \right\|_{2,\Gamma_{out}}}$$

$$p^{out} = \frac{\log\left(\frac{\left\| P_h - P_{out} \right\|_{2,\Gamma_{out}}}{\left\| P_{h/2} - P_{out} \right\|_{2,\Gamma_{out}}} \right)}{\log(2)}$$

Strong vs. Weak Boundary Conditions

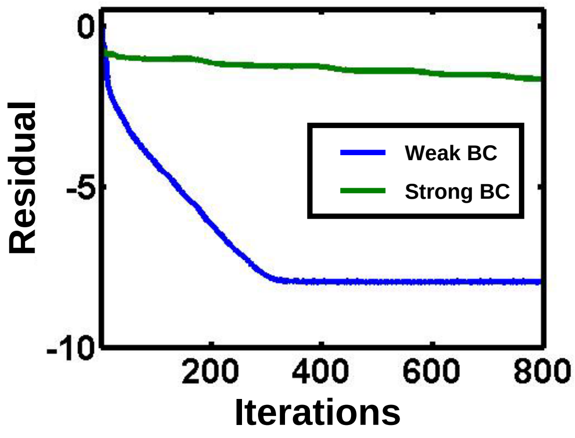
Strong Dirichlet – type BC:

- Semi – explicit
- Deterioration of matrix properties
- Very restrictive time step constraints
- Slow convergence

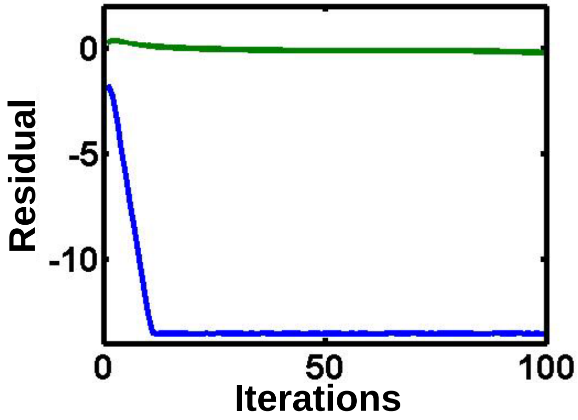
Weak Neumann – type BC:

- Imlicit
- Preservation of matrix properties
- Unconditionally stable
- Fast convergence

High – resolution scheme



Low – order scheme



Implicit Solver & Newton´s Method

Backward Euler scheme:

$$M_L \frac{U^{n+1} - U^n}{\Delta t} = (F+S)^{n+1}$$

Taylor series:

$$(F+S)^{n+1} = (F+S)^n + \left(\frac{\partial(F+S)}{\partial U}\right)^n \left(U^{n+1} - U^n\right) + O\left(\left\|U^{n+1} - U^n\right\|^2\right)$$

Semi – implicit scheme:

$$\left[\frac{M_L}{\Delta t} - \left(\frac{\partial(F+S)}{\partial U}\right)^n\right]\left(U^{n+1} - U^n\right) = (F+S)^n$$

Newton´s method:

$$-\left(\frac{\partial(F+S)}{\partial U}\right)^n \left(U^{n+1} - U^n\right) = F^n + S^n$$

- Omitting the lumped mass matrix yields Newton´s method
- Second order convergence if F sufficiently smooth

Approximate Jacobian

$$F_i^{\text{low}} = \sum_j \mathbf{c}_{ji} \cdot \mathbf{F}_j - B_i + D_{ij}\left(U_j - U_i\right)$$

Fluxes:

- Low – order approximation
- Parameter – free
- Increased robustness due to improved matrix properties

$$\frac{\partial F_i^{low}}{\partial U_j} \approx \mathbf{c}_{ji} \cdot \frac{\partial \mathbf{F}_j}{\partial U_j} - \frac{\partial B_i}{\partial U_j} + D_{ij}$$

$$B_i = \int_{\partial\Omega} \varphi_i \mathbf{n} \cdot \mathbf{F}_h \, ds$$

Source terms:

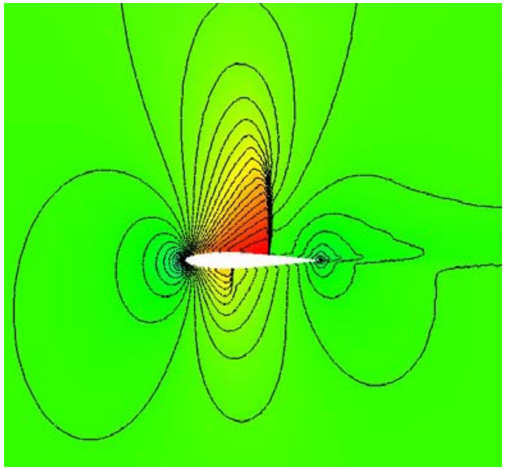
- Linearization
- Non – smooth terms are assumed constant
- Jacobian known analytically

Nonlinear Convergence Analysis: NACA 0012

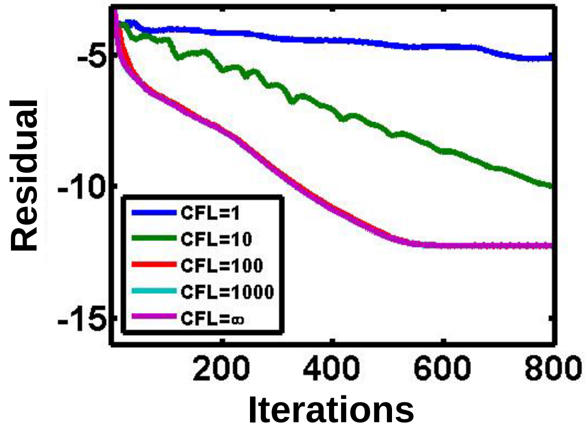
Configuration:

- Angle of attack: $\alpha = 1.25^{\circ}$
- Free stream Mach number: $M_{\infty} = 0.8$
- Convergence despite oscillatory correction factors
- No evidence of divergence

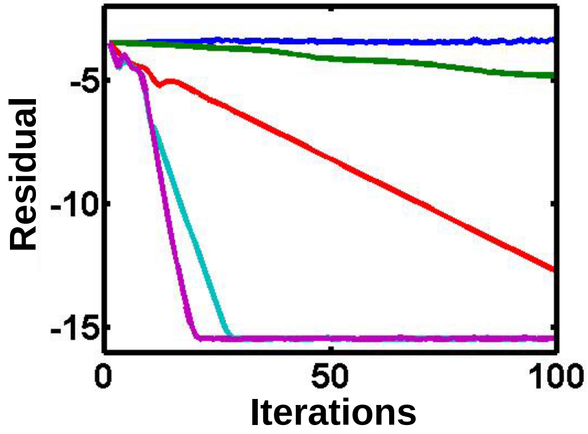
Mach number (blue, M=0.02, red: M=1.36)



High – resolution scheme



Low – order scheme

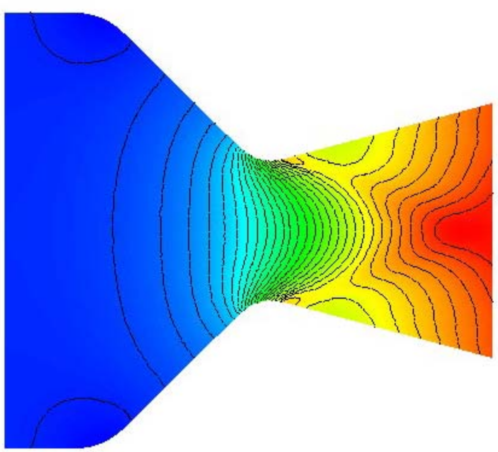


2-Fluid Model

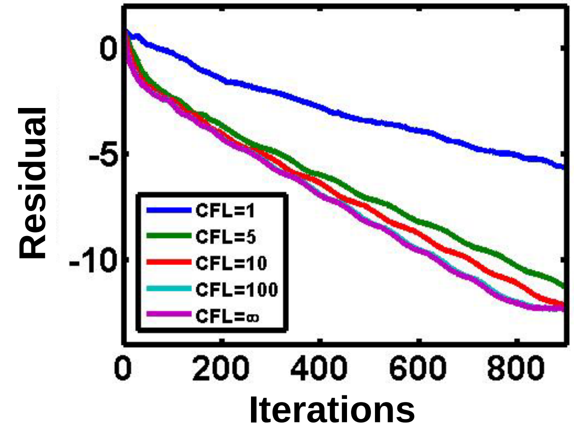
Nozzle flow:

- Subsonic inlet, supersonic outlet
- Wide range of Mach numbers
- Convergence to steady – state

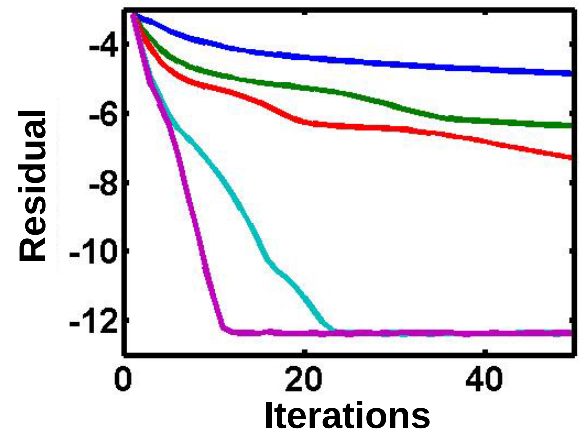
Mach number (blue, M=0.1, red: M=2.22)



High – resolution scheme



Low – order scheme



Conclusions & Outlook

Conclusions

- High - resolution FEM – TVD scheme
- Stationary solutions
- Wide range of Mach numbers
- Newton – like iterative solver
- Unconditional stability
- Improved boundary conditions
- Gain of efficiency due to strongly coupled strategy

Outlook

- Adaptivity
- Nonlinear multigrid
- 3D extension