Universität der Bundeswehr München

A hybrid semi implicit solver using real-gas thermodynamics applicable to a wide range of Mach numbers

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OUTLINE

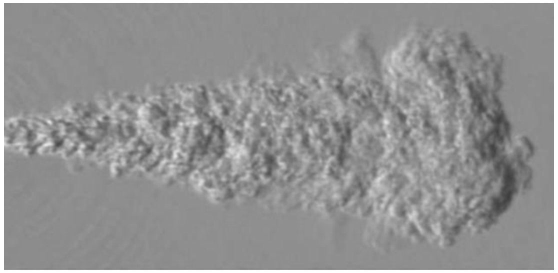
I. Motivation - High Pressure Injection Modeling

Advantages of Natural Gas:
- Better mixture formation
- Higher compression ratio
- Lean burning capabilities
- Lower fuel costs
- Higher durability of engine lubricant

} →

- Better performance
- Higher efficiency
- Less pollutant emission

Operating points:
- Injection pressures up to p = 500 bar
- Back pressures from p = 50 to 200 bar
- Injection temperatures at around T = 300 K



Numerical Challenges:
- Assumption of Ideal Gas <u>invalid</u>, supercritical fluid
  → Real-gas thermodynamics
- High pressure ratios
  → Subsonic, transonic and supersonic flow field
  → Wide range of Mach numbers
  → Rapidly changing fluid properties

II. Numerical Models - Hybrid Kurganov-Tadmor Scheme[1]

Conservation of:

Mass: $$\frac{\partial \rho}{\partial t} + \underline{\boldsymbol{\nabla} * [\boldsymbol{u}\rho]} = 0$$

Momentum: $$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \underline{\boldsymbol{\nabla} * [\boldsymbol{u}(\rho \boldsymbol{u})]} + \nabla p + \boldsymbol{\nabla} * \boldsymbol{T} = \boldsymbol{0}$$

Energy: $$\frac{\partial (\rho E)}{\partial t} + \underline{\boldsymbol{\nabla} * [\boldsymbol{u}(\rho E)]} + \underline{\boldsymbol{\nabla} * [\boldsymbol{u}p]} + \boldsymbol{\nabla} * (\boldsymbol{T} * \boldsymbol{u}) + \boldsymbol{\nabla} * \boldsymbol{j} = 0$$

Equation of State (EoS): $p = f(v, T)$

Integration over control volume, standard PISO form:

$$\int_V \boldsymbol{\nabla} * [\boldsymbol{u}\boldsymbol{\Psi}]\, dV = \int_S d\boldsymbol{S} * [\boldsymbol{u}\boldsymbol{\Psi}] \approx \sum_f \boldsymbol{S_f} * \boldsymbol{u_f}\boldsymbol{\Psi_f} = \sum_f \phi_f \boldsymbol{\Psi_f}$$

ρ ... density

$\boldsymbol{u}$ ... velocity

p ... pressure

$\boldsymbol{T}$ ... viscous stress tensor

E ... total energy density

$\boldsymbol{j}$ ... diffusive flux of heat

v ... specific volume

T ... Temperature

— Convective terms

$\boldsymbol{\Psi}$ ... transferable value

ϕ ... volumetric flux

f ... index of a face of a cell

$\boldsymbol{S_f}$ ... face area vector

II. Numerical Models - Hybrid Kurganov-Tadmor Scheme[1]

$$\int_V \boldsymbol{\nabla} * [\boldsymbol{u}\boldsymbol{\Psi}]\, dV = \int_S d\boldsymbol{S} * [\boldsymbol{u}\boldsymbol{\Psi}] \approx \sum_f \boldsymbol{S_f} * \boldsymbol{u_f}\boldsymbol{\Psi_f} = \sum_f \phi_f \boldsymbol{\Psi_f}$$

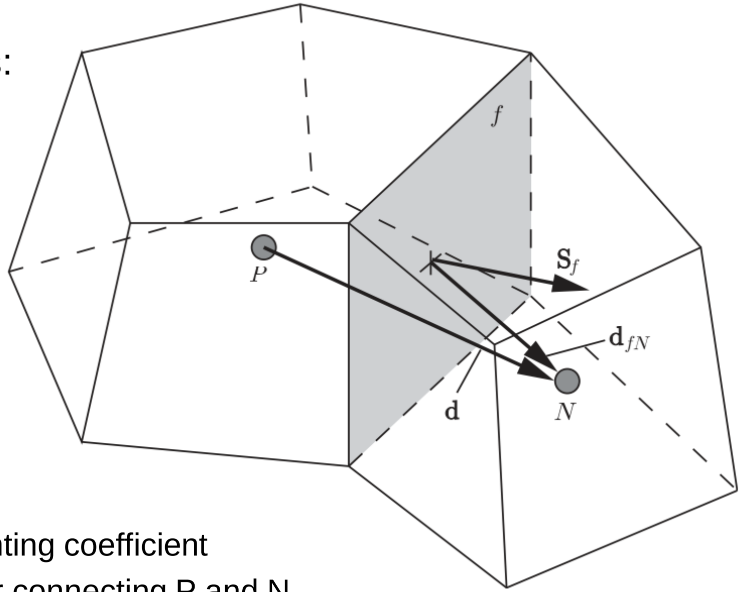
<u>Incompressible:</u>

$\boldsymbol{u_f}$ ⟶ linear interpolation from neighbouring cells

$\boldsymbol{\Psi_f}$ ⟶ interpolation according to one of many schemes:

$$\boldsymbol{\Psi_f} = w_f * \boldsymbol{\Psi_P} + (1 - w_f)\boldsymbol{\Psi_N}$$

$$w_f = |\boldsymbol{S_f} * \boldsymbol{d_{fN}}| / |\boldsymbol{S_f} * \boldsymbol{d}|$$



<u>Compressible:</u>

fluid properties are not only transported by the flow
→ propagation of waves
→ stabilization of flux interpolation

w ... weighting coefficient
$\boldsymbol{d}$ ... vector connecting P and N
$\boldsymbol{d_{fN}}$ ... vector connecting center of face to centroid of the cell N

II. Numerical Models - Hybrid Kurganov-Tadmor Scheme[1]

$$\int_V \boldsymbol{\nabla} * [\boldsymbol{u\Psi}]\, dV = \int_S d\boldsymbol{S} * [\boldsymbol{u\Psi}] \approx \sum_f \boldsymbol{S_f} * \boldsymbol{u_f}\boldsymbol{\Psi_f} = \sum_f \phi_f \boldsymbol{\Psi_f}$$

Split of interpolation in two directions ***f+*** & ***f-***

$$\sum_f \phi_f \boldsymbol{\Psi_f} = \sum_f [\underbrace{\alpha_{f+}\phi_{f+}\boldsymbol{\Psi_{f+}}}_{f+} + \underbrace{\alpha_{f-}\phi_{f-}\boldsymbol{\Psi_{f-}}}_{f-} + \underbrace{\omega_f(\boldsymbol{\Psi_{f-}} - \boldsymbol{\Psi_{f+}})}_{\text{additional diffusion term}}]$$

$$\alpha_{f+} = \frac{\varphi_{f+}}{\varphi_{f+} + \varphi_{f-}} \qquad \alpha_{f-} = \frac{\varphi_{f-}}{\varphi_{f+} + \varphi_{f-}}$$

$$\omega_f = \alpha_{f+}\varphi_{f-}$$

$$\varphi_{f+} = \max(c_{f+}|S_f| + \phi_{f+}, c_{f-}|S_f| + \phi_{f-}, 0)$$

$$\varphi_{f-} = \max(c_{f+}|S_f| - \phi_{f+}, c_{f-}|S_f| - \phi_{f-}, 0)$$

$$c = \sqrt{\frac{M_w}{\rho}\frac{c_p}{c_v}\left(\frac{\partial p}{\partial v}\right)_T}$$

α ... weighting factor

φ ... volumetric flux associated with local speeds of propagation

c ... local speeds of propagation

M_w ... molecular weight

$\boldsymbol{c_p}, \boldsymbol{c_v}$ ... specific heats

ρ ... density

ω_f ... diffusive volumetric flux

II. Numerical Models - Hybrid Kurganov-Tadmor Scheme[1]

$$\sum_f \phi_f \boldsymbol{\Psi}_f = \sum_f [\boldsymbol{\Psi}_{f+}(\alpha_{f+}\phi_{f+} + \alpha_{f+}\varphi_{f-}) + \boldsymbol{\Psi}_{f-}(\alpha_{f-}\phi_{f-} + \alpha_{f+}\varphi_{f-})]$$

volume fluxes

q ... mass flux
ρ ... density
κ_f ... mixing function
M_f ... Mach number
CFL ... Courant-Friedrich-Levy criterion

$$\kappa_f = \min(\frac{M_f}{CFL}, 1)$$

general

$$q_f^P = \kappa_f * \rho_f^P * (\alpha_{f+}\phi_{f+} + \alpha_{f+}\varphi_{f-})$$

$$q_f^N = (1 - \kappa_f) * \rho_f^P * (\alpha_{f+}\phi_{f+} + \alpha_{f+}\varphi_{f-}) + \rho_f^N * (\alpha_{f-}\phi_{f-} + \alpha_{f+}\varphi_{f-})$$

incompressible
$\kappa_f = 0$

compressible
$\kappa_f = 1$

$$q_f^P = 0$$

$$q_f^N = \rho_f^P * (\alpha_{f+}\phi_{f+} + \alpha_{f+}\varphi_{f-}) + \rho_f^N * (\alpha_{f-}\phi_{f-} + \alpha_{f+}\varphi_{f-})$$

$$q_f^P = \rho_f^P * (\alpha_{f+}\phi_{f+} + \alpha_{f+}\varphi_{f-})$$

$$q_f^N = \rho_f^N * (\alpha_{f-}\phi_{f-} + \alpha_{f+}\varphi_{f-})$$

II. Numerical Models - Hybrid Kurganov-Tadmor Scheme[1]

convert non−uniform averages back to original grid: u_j^{n+1}

↑

exact evaluation of new cell averages for t^{n+1}: $w_{j+1/2}^{n+1}$

↑

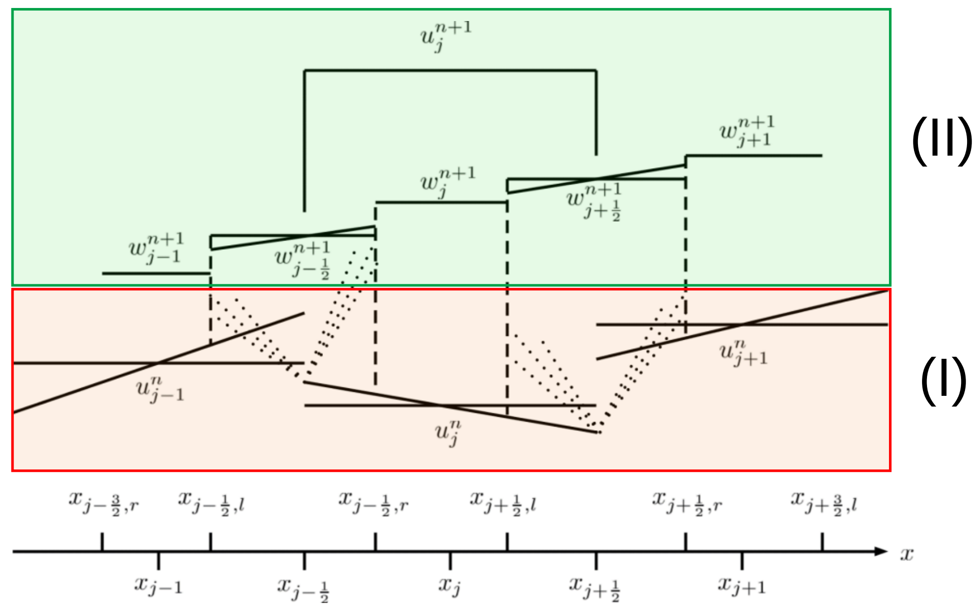
average over staggered control volumes $[x_{j+1/2,l}, x_{j+1/2,r}]$

↑

local speeds of propagation at cell boundaries $a_{j+1/2}^{n}$

↑

piecewise linear solution u_j^n,
reconstruct derivatives $(u_x)_j^n$



u ... conserved quantity
x ... coordinate
j ... cell index
n ... time step

II. Numerical Models - Real-Gas Thermodynamics

EoS: Peng-Robinson[2]

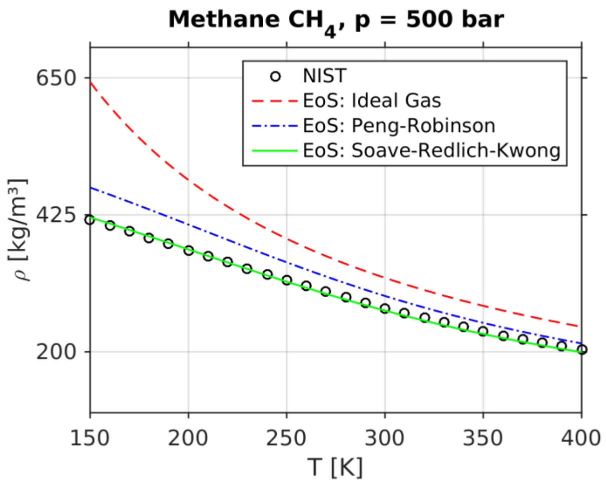
$$p = \frac{RT}{v - b_{PR}} - \frac{a_{PR}(T)}{v^2 + 2vb_{PR} - b_{PR}^2}$$

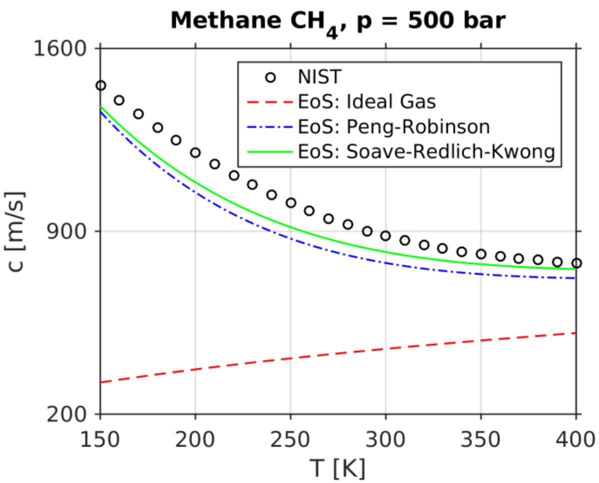
EoS: Soave-Redlich-Kwong[3]

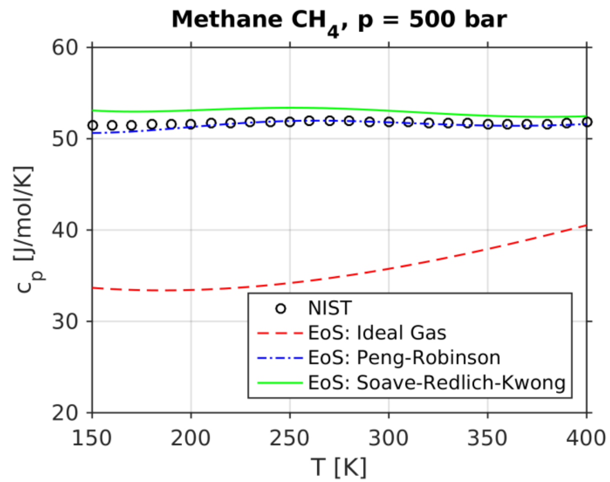
$$p = \frac{RT}{v - b_{SRK}} - \frac{a_{SRK}(T)}{v * (v + b_{SRK})}$$

Pressure correction for caloric properties:

$$h(T,p) = h_0(T) + \int_{p_0}^{p} \left(v - T \left(\frac{\partial v}{\partial T} \right)_p \right) dp \qquad c_p(T,p) = \left(\frac{\partial h}{\partial T} \right)_p$$







II. Numerical Models - Local Artificial Diffusivity (LAD)[4]

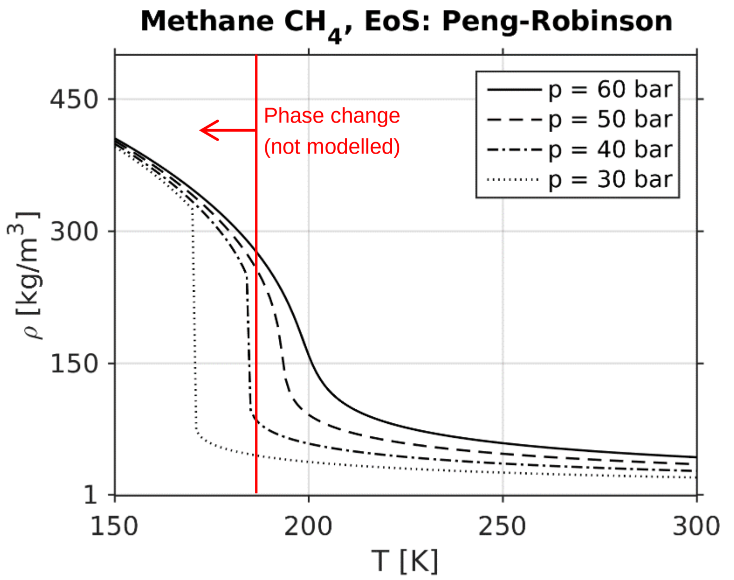
High pressure ratios and gradients:

- → Strong expansion in injector and/or chamber
- → Fluid close to or drop below critical point

$$\alpha_{eff} = \alpha_t + \alpha^*$$

$$\alpha^* = C_{AD} * \Delta x * \frac{T}{\rho * a_s} * \frac{\partial Z}{\partial x}$$

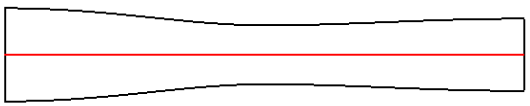
α_{eff} ... effective thermal diffusivity
α_t ... turbulent thermal diffusivity
α^* ... artificial thermal diffusivity
C_{AD} ... constant (0.01…0.1)
Δx ... grid spacing
T ... temperature
ρ ... density
a_s ... speed of sound
Z ... compressibility factor



Critical Properties of Methane CH_4:
p_{crit} = 45.992 bar
T_{crit} = 190.564 K
Z_{crit} = 0.286

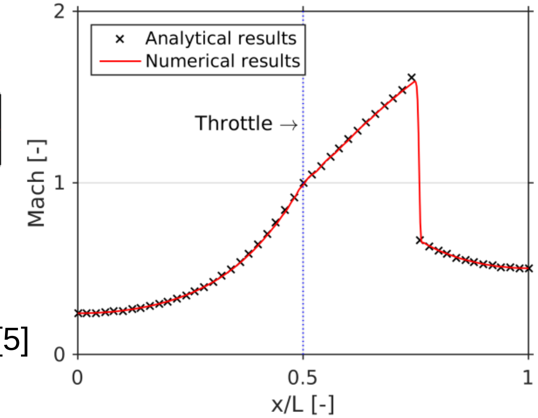
II. Numerical Models - Validation

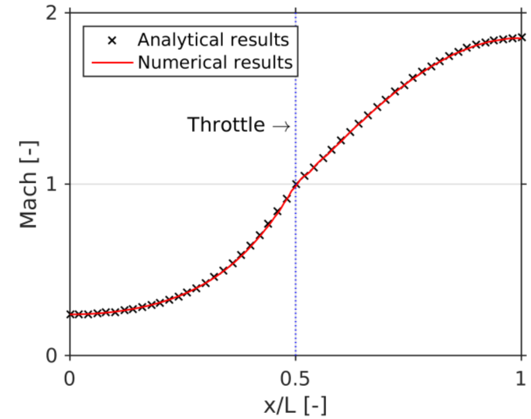
Flow field



- Converging-diverging nozzle
- Inviscid, non-heat conducting air

→ 1D, steady, compr. flow problem [5]





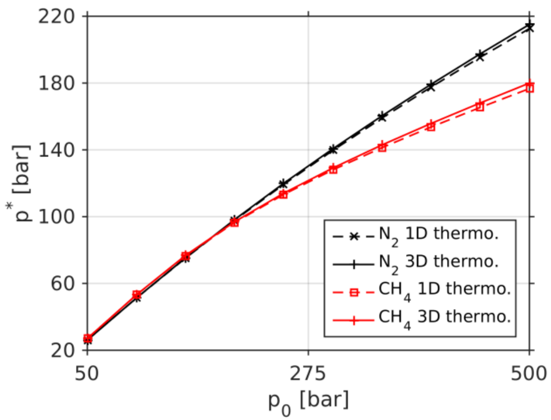
Two-steps validation

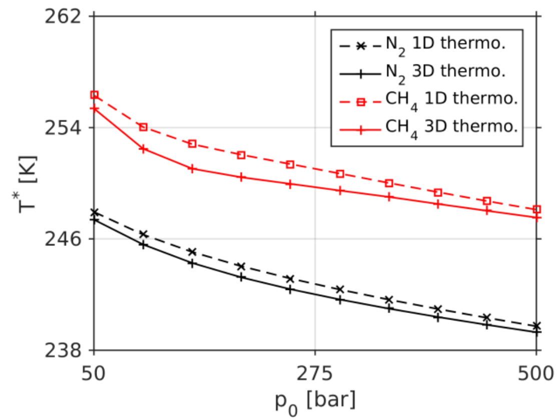
1D-Thermodynamics

- Converging nozzle
- assumption of isentropic flow

$$s_0 = s_{nozzle} = s^*$$

$$\rightarrow Ma = 1, p^*, T^*$$

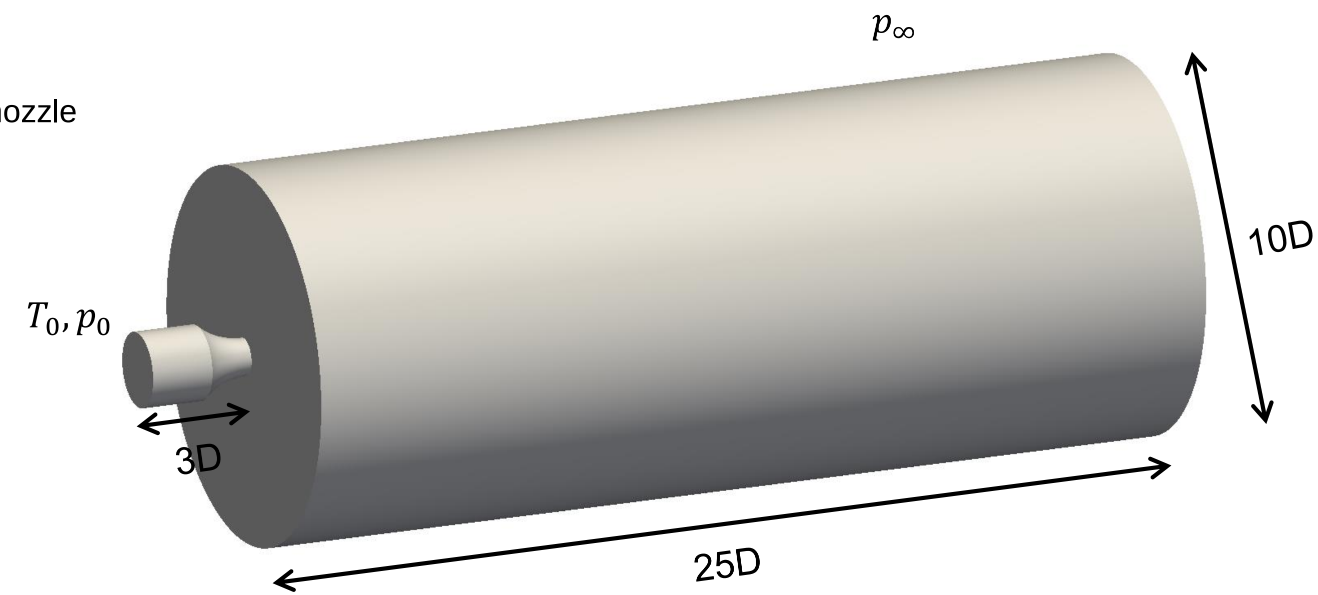




III. Test Case and Setup

Geometry:

- Simple axis-symmetric nozzle
- d_{nozzle} = 1 mm



Boundary Conditions:

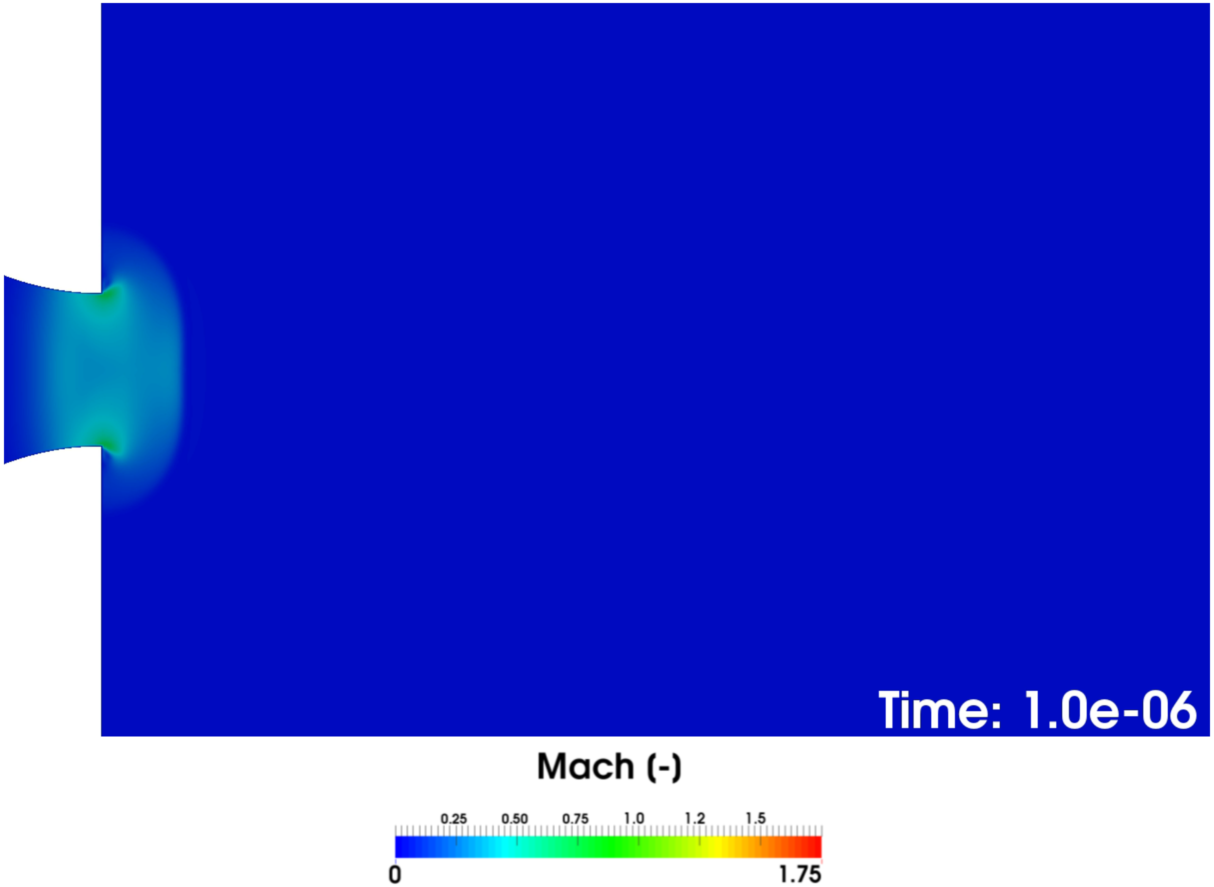
- Total inlet pressure
- Total inlet temperature
- Static outlet pressure

Numerical Setup:

- Pressure based URANS
- Equation of State: Peng-Robinson
- Viscosity Model: Chung
- Specific Heat Model: Janaf
- Turbulence Model: k-omega-SST
- Fluid: Methane CH_4
- Discretization: 1^{st} order in time
  2^{nd} order in space

IV. Results - Movie

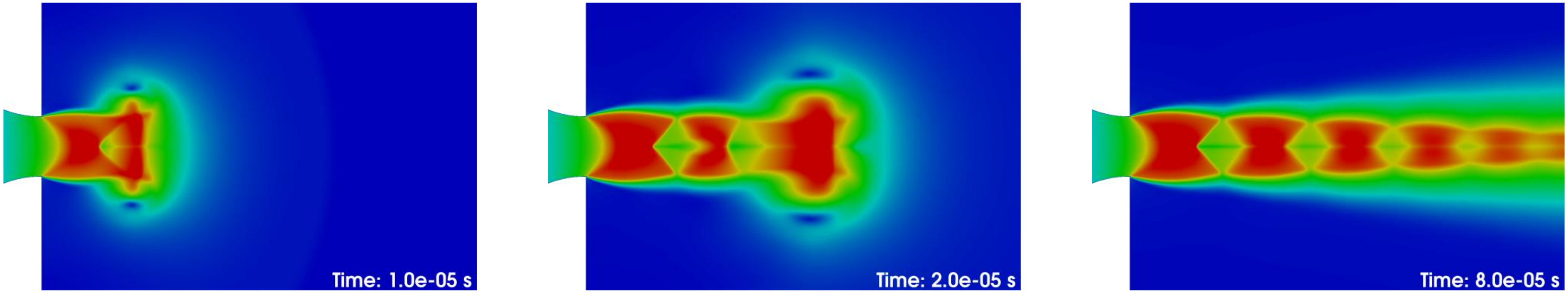
EoS: Peng-Robinson



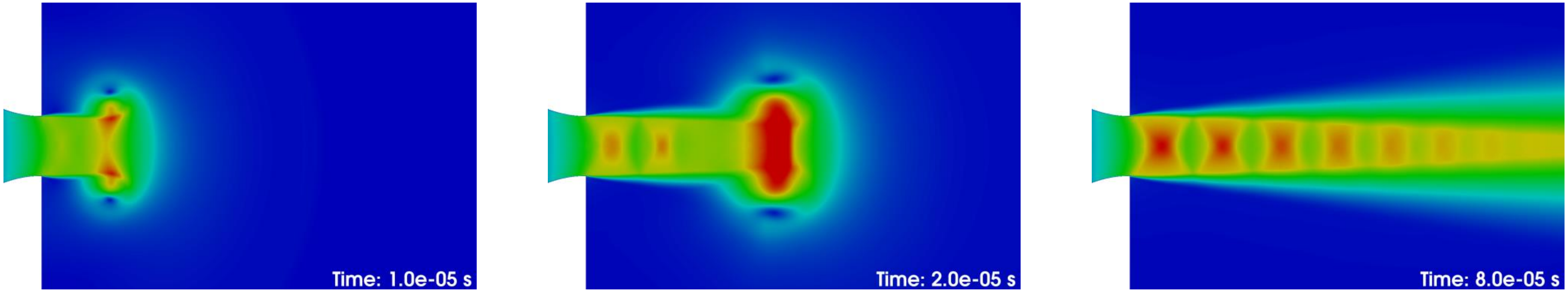
$p_{in,tot}$ = 400 bar
$T_{in,tot}$ = 300 K
$p_{out,stat}$ = 100 bar

IV. Results - Snapshots

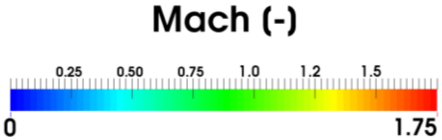
EoS: Ideal Gas



EoS: Peng-Robinson

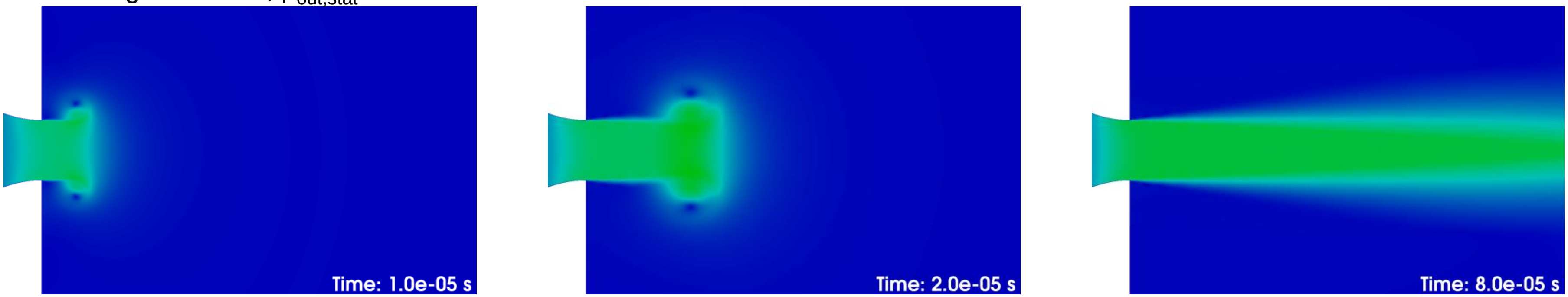


$p_{in,tot}$ = 400 bar
$T_{in,tot}$ = 300 K
$p_{out,stat}$ = 100 bar

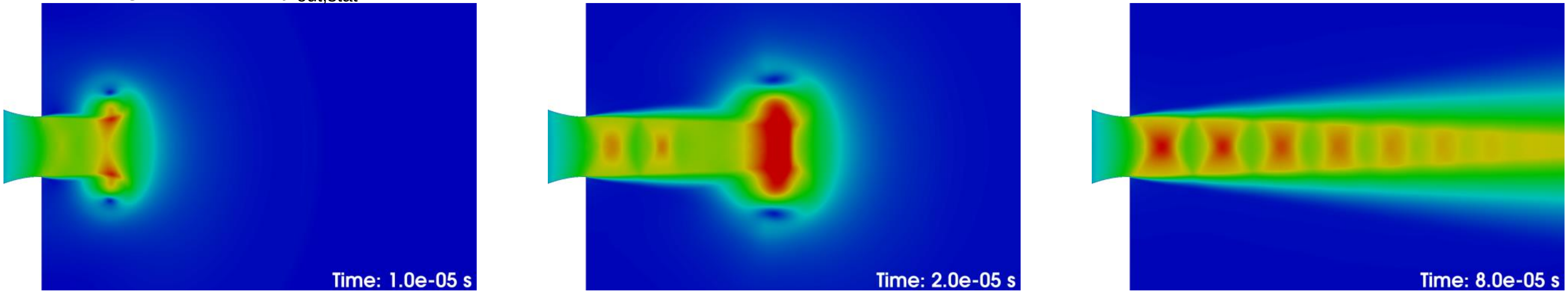


IV. Results - Snapshots

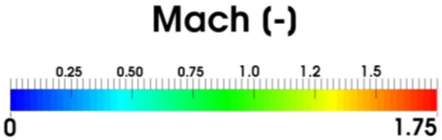
EoS: Peng-Robinson, $p_{out,stat}$ = 200 bar



EoS: Peng-Robinson, $p_{out,stat}$ = 100 bar



$p_{in,tot}$ = 400 bar
$T_{in,tot}$ = 300 K



V. Conclusion

Summary:

- Extension of Kurganov-Tadmor Numerical Scheme for use with real-gas thermodynamics
- Two cubic EoS: Peng-Robinson, Soave-Redlich-Kwong
- Fully validated
- Local artificial diffusivity used to stabilize simulations near critical point of fluid

→ Solver which is capable of simulating high pressure gas injections using real-gas thermodynamics

Future Work:

- Improvement of Local Artificial Diffusivity
- Phase-change models
- Equations for multi-species

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[1] M. Kraposhin, A. Bovtrikova, and S. Strijhak: *„Adaptation of Kurganov-Tadmor Numerical Scheme for Applying in Combination with the PISO Method in Numerical Simulation of Flows in a Wide Range of Mach Numbers“*

[2] D.-Y. Peng, D. B. Robinson: *„A New Two-Constant Equation of State“*

[3] G. Soave: *„Equilibrium constants from a modified Redlich-Kwong equation of state“*

[4] H. Terashima, S. Kawai, and N. Yamanishi: *„High-resolution numerical method for supercritical flows with large density variations”*

[5] J. D. Anderson: *„Modern Compressible Flow“*

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