Computational Modeling for Non-equilibrium Shock Tube Flows

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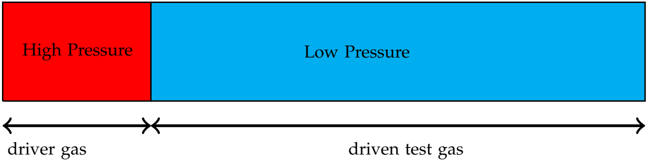
- Shock Waves in Internal Flows -

Shock tube problem



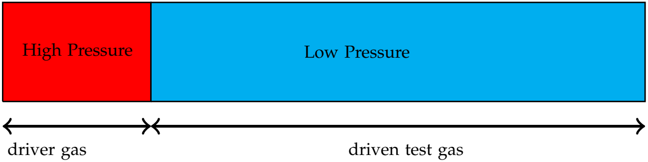
Schematic of shock tube problem

$$\partial_t \boldsymbol{u} + \partial_x [\boldsymbol{\mathcal{F}}(\boldsymbol{u})] = 0$$

$$\boldsymbol{u}(x,t) = \begin{cases} \boldsymbol{u}_l & x \leq x_0 \\ \boldsymbol{u}_l & x > x_0 \end{cases}$$

Gary Sod"*A Survey of Several Finite Difference Methods for Systems of Non-linear Hyperbolic Conservation Laws*"

Shock tube computational challenges :



Schematic of shock tube problem

- The heating process of the driver gas
- The diaphragm rupture
- Diaphragm fragments, residual soot from previous experiments and wall ablation due to high wall temperatures
- Turbulent multi-scale mixing between the hot jet of the driver gas and the cold driven tube
- Radiation cooling

Shock tube computational challenges :

- Conservation equations :

$$\partial_t \rho_s + \boldsymbol{\partial_x} \cdot (\rho_s \boldsymbol{u}) + \boldsymbol{\partial_x} \cdot \boldsymbol{\mathcal{F}_s} = \dot{\omega}_s \qquad s \in \mathcal{S},$$

$$\partial_t (\rho \boldsymbol{u}) + \boldsymbol{\partial_x} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\boldsymbol{I}) + \boldsymbol{\partial_x} \cdot \boldsymbol{\Pi} = \boldsymbol{0}$$

$$\partial_t (\mathcal{E}_{tr} + \mathcal{E}_{in} + \tfrac{1}{2}\rho \boldsymbol{u} \cdot \boldsymbol{u}) + \boldsymbol{\partial_x} \cdot (\mathcal{E}_{tr} + \mathcal{E}_{in} + \tfrac{1}{2}\rho \boldsymbol{u} \cdot \boldsymbol{u} + p)\boldsymbol{u}) + \boldsymbol{\partial_x} \cdot (\boldsymbol{\Pi} \cdot \boldsymbol{u} + \boldsymbol{\mathfrak{Q}}_{tr} + \boldsymbol{\mathfrak{Q}}_{in}) = \boldsymbol{0}$$

$$\partial_t (\mathcal{E}_{in}) + \boldsymbol{\partial_x} \cdot (\boldsymbol{u}\mathcal{E}_{in}) + \boldsymbol{\partial_x} \cdot (\boldsymbol{\mathfrak{Q}}_{in}) = \omega_{in}$$

- Large disparity between the space scale $\mathcal{O}$(meters), and time scale $\mathcal{O}$(nanoseconds) seconds.
- Stiffness is increased by the chemical and kinetics source terms governing the non-equilibrium processes

Physical models and Numerical methods

Physical models

- Thermal and chemical non equilibrium - Park's two-temperatures model
- Chapman-Enskog method for the transport properties.
- Stefan-Maxwell for the mass diffusion flux.

$\rightarrow$ The thermodynamics and transport properties are computed using *PLATO* library.

Numerical methods

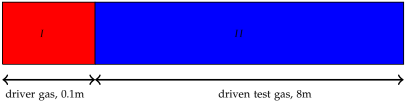
$$\partial_t(\mathbf{Q}) + \sum_{i\in\mathcal{D}}(\partial_i \mathbf{F}_i^c) + \sum_{i\in\mathcal{D}}(\partial_i \mathbf{F}_i^d) = \mathbf{S}$$

- Second order Finite Volume solver (Linear reconstruction using a least-squares method)
- The convective fluxes are computed using the $AUSM^{+UP}$ scheme.
- Crank-Nicolson scheme for time integration
- Generalized Minimum RESidual (GMRES) algorithm and Additive Schwartz pre-conditioner - PETSc library-

$\rightarrow$ Flow solver is *COOLFLuiD*

Unsteady simulation of EAST facility

- A two-dimensional uniform grid was used for this simulation - $\Delta x = 10^{-3} m$, $d_{wall} = 10^{-6}$.
- The wall is considered as isothermal at $T_w = 300K$ and no slip wall boundary conditions is applied.
- Wall condition is used at the end of the driver tube.
- Air -11 species - is used as a test gas, with the driver gas is composed of 99% of Helium and 1% Nitrogen.

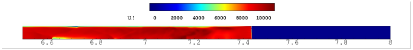


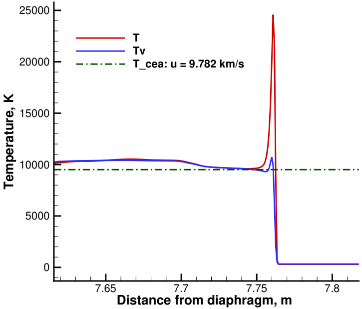
Schematic of NASA Ames' Electrical Arc shock Tube (EAST)

	driver	driven
	Y_{N_2} : 0.01	Y_{N_2} : 0.79
	Y_{He} : 0.99	Y_{O_2} : 0.21
ρ, kg/m^3	1.10546	3.0964 x 10^{-4}
T, K	6000	300
p, Pa	12.7116 x 10^6	26.771

Initial conditions at diaphragm rupture

Unsteady simulation of EAST facility



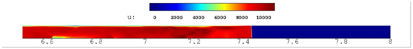


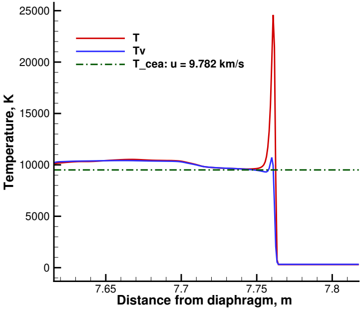
Bensassi et al. AIAA 2019-0798

Computational cost

- 100 Ivy-Bridge nodes -2000 cores-, on Pleiades, NASA Advanced Supercomputing (NAS)
- 12 TB data
- 120 days of continuous run and 7 months of monitoring the simulation

Unsteady simulation





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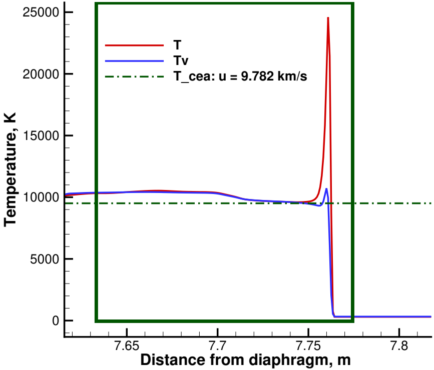
→ impractical to support a real-time experimental test campaign

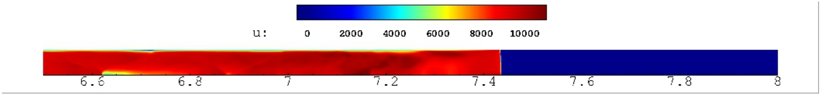
How to reduce the computational cost ?

How to reduce the computational cost ?

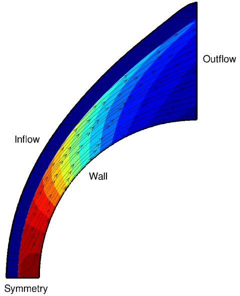
- Define a region of interest
- Reduce the computational space
- Reduce the time scale



Stagnation line approach

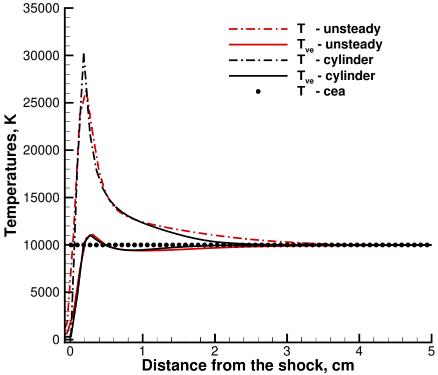


- Steady flow simulation over a 3m radius cylinder.
- Free steam conditions are the same as for the test gas
- Free stream velocity

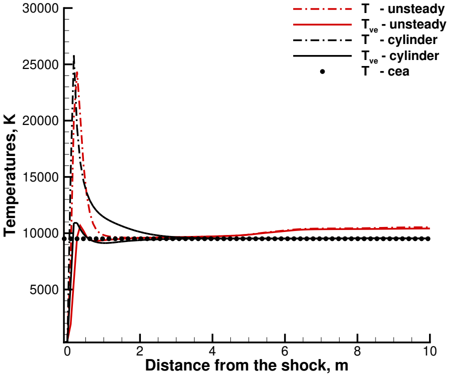


Case	I : inviscid	II : viscous
u_∞, km/s	10.065	9.782

Stagnation line approach vs Unsteady simulation



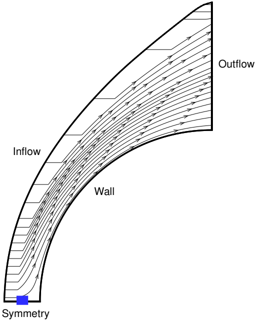
inviscid conditions



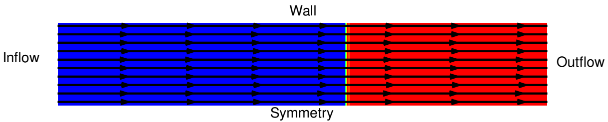
viscous conditions

Stagnation line approach : drawbacks

- Wall curvature effect
- no boundary layer in the post-shock region
- decreasing velocity near the wall
- The shock layer radiation requires a high grid resolution
  $\rightarrow$ increases drastically the number of degree of freedom



Local steady state shock tube

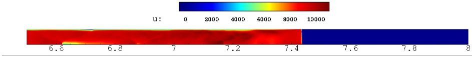


Computational domain and the stream lines, length of the domain is 0.3m

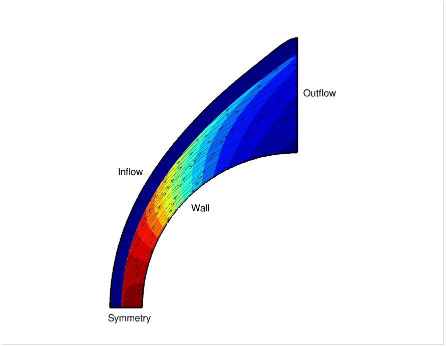
- Inflow condition is supersonic
- Outflow is subsonic
  $\rightarrow$The equilibrium post-shock pressure (*CEA*) is imposed at the outflow.

Different approaches

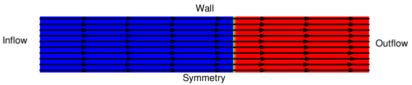
- Unsteady simulation of the complete shock tube



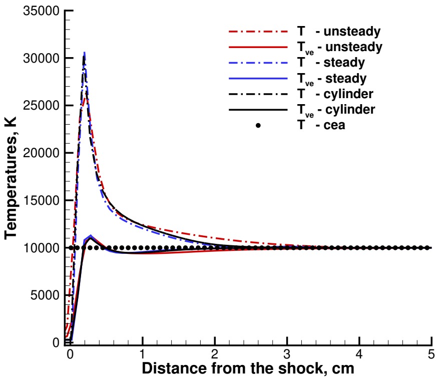
- steady simulation around a cylinder



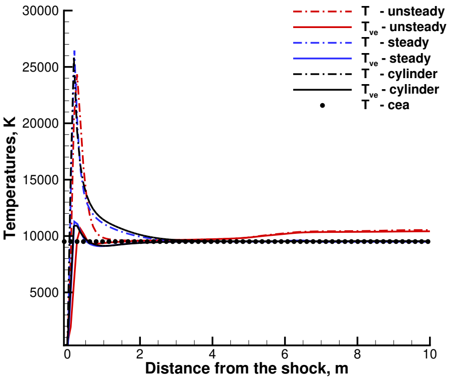
- Local steady state shock tube



Comparison of different approaches



inviscid conditions



viscous conditions

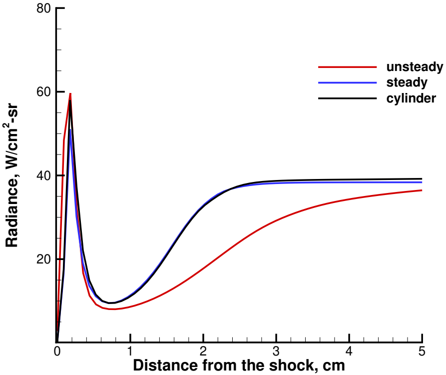
Radiation calculation

- The flow solution, i.e temperatures and number densities along the symmetry boundary condition (line of sight), is passed to *NEQAIR*.

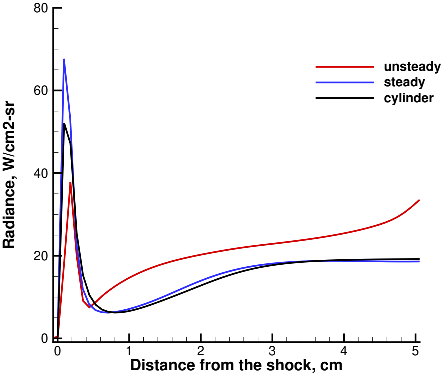
- *NEQAIR*, in shock tube mode, then produces the radiance perpendicular to the axis of the tube.

- The non-Boltzmann population of the radiating state is solved using *NEQAIR*'s non-Boltzmann option.

Radiance comparison



inviscid conditions



viscous conditions

Conclusion

- Explored different computational approaches for simulating non-equilibrium flows in shock tubes. Both steady and unsteady cases were considered.
- The cylinder case presents several disadvantages : wall curvature effect, no boundary layer in the post-shock region and decreasing velocity near the wall.
- The local steady-state shock tube approach alleviates several of the drawbacks of the cylinder approach. Good agreement was obtained between this approach and the cylinder
- Both steady cases showed some disagreement with the unsteady simulation.

Acknowledgments

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