LOCAL DISCRETE VELOCITY GRIDS FOR MULTI-SPECIES RAREFIED FLOW SIMULATIONS

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Introduction

Context: Deterministic simulations

Discrete velocity approximation for multi-species rarefied flows

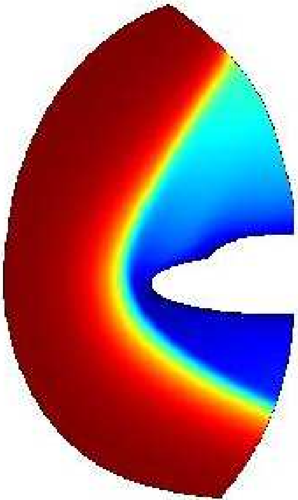
Global discrete velocity grid (Cartesian) commonly used for the whole computational domain (Kyoto group, Aristov et al., etc.)

Pb: For practical applications in aerodynamics, grid unadapted
$\Rightarrow$ computational ressources (memory storage and CPU time) huge

One solution: adaptative methods in the velocity variable.
Rarefied gases: [F.Filbet, T.Rey], [K.Xu], [V.Kolobov],
$\Rightarrow$ [S. Brull, L. Mieussens]

Motivations

To reduce numerical cost $\Rightarrow$ adaptative method in the velocity variable



Velocity grids

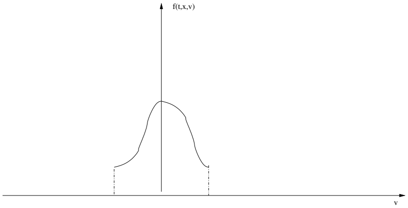


Figure: Small temperature or big mass

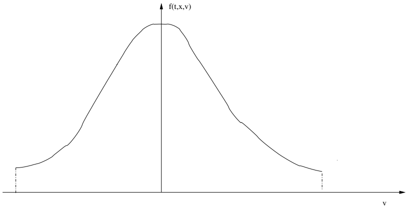
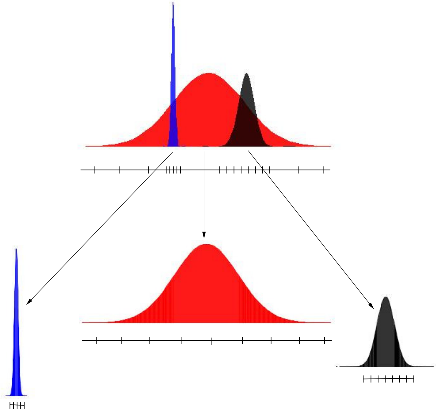


Figure: Big temperature or small mass

Local velocity grid

Idea: define a velocity grid different forall t and x and for each species



Numerical approximation of velocity domains

- Objective: Derive a deterministic numerical method using dynamic local velocity grids for gas mixtures in 1d case
  Generalisation of [S.Brull, L.Mieussens, 2014] (single species)

- $v \in \mathbb{R} \Rightarrow$ Choice of a suitable subset $\subset \mathbb{R} \Rightarrow$ depend on velocities, temperatures and molecular masses

- $(\alpha,\ t^n,\ x_i) \Rightarrow$ Local discrete velocity grids (LDV):
  $\mathcal{V}_i^{\alpha,n}$: velocity grid for species α, at time t_n, and space point x_i
  $\mathcal{V}_i^{\alpha,n} = \{(v_{i,k}^{\alpha,n})_k, k \in \{1, ..., N_v\}\} \Rightarrow$ possibility of $N_v(i)$

  f^α: distribution of species $\alpha \Rightarrow f_{i,k}^{\alpha,n} \simeq f^\alpha(t^n, x_i, v_{i,k}^{\alpha,n})$
  $\Rightarrow f_i^{\alpha,n}$ is known only on $\mathcal{V}_i^{\alpha,n}$

Multi-species kinetic model

- Gas mixture of N species of molecular masses $m^1, ..., m^N$

$$\text{Reduced mass:} \quad \mu^{\alpha\beta} = \frac{m^\alpha m^\beta}{m^\alpha + m^\beta}$$

- $f^\alpha(t, x, v) : \mathbb{R}_+ \times \Omega \times \mathbb{R} \mapsto \mathbb{R}_+$: distribution function of species α
- Multi-species kinetic equation, for $\alpha \in \{1, ..., N\}$:

$$\partial_t f^\alpha + \partial_x(v f^\alpha) = \mathcal{C}^\alpha(f^1, ..., f^N), \quad t \in \mathbb{R}_+, \ x \in \Omega \subset \mathbb{R}, \ v \in \mathbb{R},$$

- Macroscopic quantities:

$$\int_{\mathbb{R}} f^\alpha \mathrm{d}v = n^\alpha, \qquad \int_{\mathbb{R}} m^\alpha v f^\alpha \mathrm{d}v = m^\alpha n^\alpha u^\alpha = \rho^\alpha u^\alpha,$$

$$\int_{\mathbb{R}} m^\alpha \frac{v^2}{2} f^\alpha \mathrm{d}v = E^\alpha = \frac{1}{2} m^\alpha n^\alpha (u^\alpha)^2 + \frac{1}{2} n^\alpha k_B T^\alpha$$

BGK operator for multi-species flows

- BGK operator [Andries, Aoki, Perthame, 2001]:

$$\mathcal{C}^\alpha := \nu^\alpha \left(\overline{M}^\alpha(f^1, ..., f^N) - f^\alpha \right), \quad \alpha \in \{1, \dots, N\}$$

- $\overline{M}^\alpha(f) = \frac{n^\alpha}{\sqrt{2\pi k_B \frac{\overline{T}^\alpha}{m^\alpha}}} \exp\left(-\frac{(v-\overline{u}^\alpha)^2}{2k_B \frac{\overline{T}^\alpha}{m^\alpha}}\right)$

- Fictitious mixture velocities $\overline{u}^\alpha$ and temperatures $\overline{T}^\alpha$:

$$\overline{u}^\alpha = u^\alpha + \frac{2}{\nu^\alpha m^\alpha} \sum_{\beta=1}^{N} \mu^{\alpha\beta} \chi^{\alpha\beta} n^\beta \left(u^\beta - u^\alpha \right)$$

$$\overline{T}^\alpha = T^\alpha - \frac{m^\alpha}{2 n^\alpha k_B} (\overline{u}^\alpha - u^\alpha)^2 + \frac{2}{\nu^\alpha n^\alpha k_B} \sum_{\beta=1}^{N} \frac{2\mu^{\alpha\beta}\chi^{\alpha\beta} n^\beta}{m^\alpha + m^\beta} \left(\varepsilon^\beta - \varepsilon^\alpha + m^\beta \frac{(u^\beta - u^\alpha)^2}{2} \right)$$

Properties of BGK operator

Model constructed to reproduce some exchanges of the Boltzmann operator for Maxwell molecules

$\Rightarrow$ BGK operator has the same moments w.r.t. $\{1; v; v^2\}$ per species as the Boltzmann operator for Maxwell molecules

Collision kernel

$$B^{\alpha\beta}(n \cdot (v - v_*), |v - v_*|) = \overline{B}^{\alpha\beta}(\omega), \ \omega = \frac{n \cdot (v - v_*)}{|v - v_*|}$$

Definition of $\chi^{\alpha\beta}$

$$\chi^{\alpha\beta} = \int_{S_2} \cos^2(\omega)\overline{B}^{\alpha\beta}(\omega)d\omega, \ \nu^{\alpha\beta} = \int_{S_2} \overline{B}^{\alpha\beta}(\omega)d\omega$$

Condition: $\nu^{\alpha} \geq \sum_{\beta=1}^{N} \chi^{\alpha\beta} n^{\beta} \Rightarrow \nu^{\alpha} = \sum_{\beta=1}^{N} \nu^{\alpha\beta} n^{\beta}$

The model satisfies H theorem

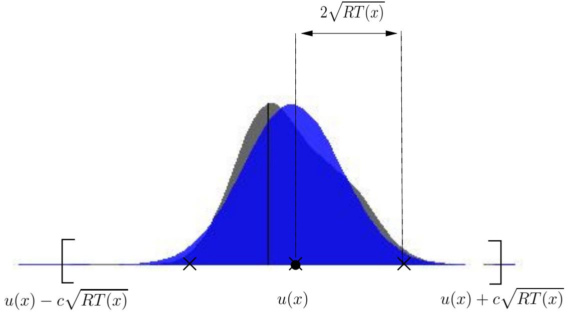
Computation of the discrete velocity grids

1^{st} **step:** Define $\mathcal{V}_i^{\alpha,n+1} = \{v_{i,1}^{\alpha,n+1}, \ldots, v_{i,N_v}^{\alpha,n+1}\}$

Bounds $(V_-)_i^{\alpha,n+1}$, $(V_+)_i^{\alpha,n+1}$ given by:

$$(V_\pm)_i^{\alpha,n+1} = u_i^{\alpha,n+1} \pm l_i^\alpha \sqrt{\frac{k_B T_i^{\alpha,n+1}}{m^\alpha}}, \quad l_i^\alpha \in \{4; 5\}$$

Remark: Correct bounds if f^α close to a Maxwellian distribution



Computation of the discrete velocity grids

Set of discrete velocities $\mathcal{V}_i^{\alpha,n+1} = \{v_{i,1}^{\alpha,n+1}, \dots, v_{i,N_v}^{\alpha,n+1}\}$, once the bounds $(V_-)_i^{\alpha,n+1}$, $(V_+)_i^{\alpha,n+1}$ have been computed:

$$v_{i,k}^{\alpha,n+1} = (V_-)_i^{\alpha,n+1} + (k-1)\frac{(V_+)_i^{\alpha,n+1} - (V_-)_i^{\alpha,n+1}}{N_v - 1}$$

$\Rightarrow$ Regular mesh in each local grid

$\Rightarrow$ Need to compute macroscopic quantities at time t^{n+1}

Computation of macroscopic quantities

- Semi-discretization of equation on f^α:

$$f_i^{\alpha,n+1}(v) = f_i^{\alpha,n}(v) - \frac{\Delta t}{\Delta x}(\phi_{i+\frac{1}{2}}^{\alpha,n}(v) - \phi_{i-\frac{1}{2}}^{\alpha,n}(v)) \\ + \Delta t \nu_i^{\alpha,n+1}(\overline{M}_i^{\alpha,n+1}(v) - f_i^{\alpha,n+1}(v))$$

- Upwind flux: $\phi_{i+\frac{1}{2}}^{\alpha,n}(v)$
- Computing moments of f^α $\Rightarrow$ Conservation laws

$\Rightarrow$ Computation of $n_i^{\alpha,n+1}$, $u_i^{\alpha,n+1}$, $T_i^{\alpha,n+1}$.

$\Rightarrow$ Computation of $\mathcal{V}_i^{\alpha,n+1}$

Conservation laws

$$\int_{\mathbb{R}} \begin{pmatrix} 1 \\ m_i v \\ \frac{1}{2} m_i v^2 \end{pmatrix} f_i^{\alpha,n+1}(v)dv = \int_{\mathbb{R}} \begin{pmatrix} 1 \\ m_i v \\ \frac{1}{2} m_i v^2 \end{pmatrix} f_i^{\alpha,n}(v)dv$$

$$- \int_{\mathbb{R}} \begin{pmatrix} 1 \\ m_i v \\ \frac{1}{2} m_i v^2 \end{pmatrix} \frac{\Delta t}{\Delta x}(\phi_{i+\frac{1}{2}}^{\alpha,n}(v) - \phi_{i-\frac{1}{2}}^{\alpha,n}(v))dv$$

$$+ \int_{\mathbb{R}} \begin{pmatrix} 1 \\ m_i v \\ \frac{1}{2} m_i v^2 \end{pmatrix} \Delta t \, \nu_i^{\alpha,n+1} (\overline{M}_i^{\alpha,n+1}(v) - f_i^{\alpha,n+1}(v))dv$$

Remark

$$\int_{\mathbb{R}} m_i v(\overline{M}_i^{\alpha,n+1}(v) - f_i^{\alpha,n+1}(v))dv \neq 0$$

$$\int_{\mathbb{R}} \frac{1}{2} m_i v^2(\overline{M}_i^{\alpha,n+1}(v) - f_i^{\alpha,n+1}(v))dv \neq 0$$

Conservation laws

- Equations on concentrations:

$$n_i^{\alpha,n+1} = n_i^{\alpha,n} - \frac{\Delta t}{\Delta x} \int_{\mathbb{R}} (\phi_{i+\frac{1}{2}}^{\alpha,n} - \phi_{i-\frac{1}{2}}^{\alpha,n}) \mathrm{d}v.$$

- Equations on momenta: $\forall \alpha \in \{1, ..., N\}$,

$$\rho_i^{\alpha,n+1} u_i^{\alpha,n+1} = \rho_i^{\alpha,n} u_i^{\alpha,n} - \frac{\Delta t}{\Delta x} \int_{\mathbb{R}} m^\alpha v (\phi_{i+\frac{1}{2}}^{\alpha,n} - \phi_{i-\frac{1}{2}}^{\alpha,n}) \mathrm{d}v$$
$$+ 2\Delta t n_i^{\alpha,n+1} \sum_{\beta=1}^{N} \mu^{\alpha\beta} \chi^{\alpha\beta} n_i^{\beta,n+1} (u_i^{\beta,n+1} - u_i^{\alpha,n+1})$$

- $(u_i^{\alpha,n+1})_\alpha$ coupled $\Rightarrow$ $N \times N$ linear system to solve for each x_i
- Equations on internal energies: $N \times N$ linear system coupling $(\varepsilon_i^{\alpha,n+1})_\alpha$ for each x_i

Computation of $f_i^{\alpha,n+1}$

Semi-discretization (variable v kept continuous):

$$
\begin{aligned}
f_i^{\alpha,n+1}(v) &= f_i^{\alpha,n}(v) - \frac{\Delta t}{\Delta x}(\phi_{i+\frac{1}{2}}^{\alpha,n}(v) - \phi_{i-\frac{1}{2}}^{\alpha,n}(v)) \\
&+ \Delta t \nu_i^{\alpha,n+1}(\overline{M}_i^{\alpha,n+1}(v) - f_i^{\alpha,n+1}(v))
\end{aligned}
$$

Computation of the Maxwellian
$(n_i^{\alpha,n+1}, u_i^{\alpha,n+1}, T_i^{\alpha,n+1}) \Rightarrow (\overline{u}_i^{\alpha,n+1}, \overline{T}_i^{\alpha,n+1}) \Rightarrow (\overline{M}_{i,k}^{\alpha,n+1})_k$

Implicitation of the BGK model $\Rightarrow$ AP scheme toward Euler
$\nu_i^{\alpha,n+1} = +\infty \Rightarrow$ kinetic scheme for Euler

Problem of grids

Computation of the flux $\phi^{\alpha,n}_{i+\frac{1}{2}}(v)$ on $\mathcal{V}^{\alpha,n+1}_i$

$$\phi^{\alpha,n}_{i+\frac{1}{2}}(v) = \frac{1}{2}\left(v\left(f^{\alpha,n}_{i+1}(v) + f^{\alpha,n}_i(v)\right) - |v|\left(f^{\alpha,n}_{i+1}(v) - f^{\alpha,n}_i(v)\right)\right)$$

$f^{\alpha,n}_i$, $f^{\alpha,n}_{i-1}$, $f^{\alpha,n}_{i+1}$ are not known on the same velocity grid

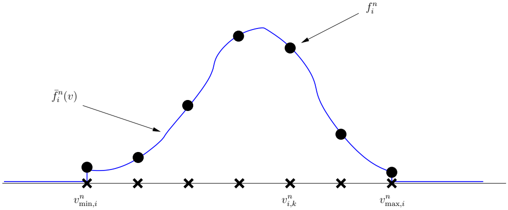
$$f^{\alpha,n}_i \leftrightarrow \mathcal{V}^{\alpha,n}_i, \quad f^{\alpha,n}_{i-1} \leftrightarrow \mathcal{V}^{\alpha,n}_{i-1}, \quad f^{\alpha,n}_{i+1} \leftrightarrow \mathcal{V}^{\alpha,n}_{i+1}, \qquad f^{\alpha,n+1}_i \leftrightarrow \mathcal{V}^{\alpha,n+1}_i$$

$\Rightarrow$ Pb to compute on $\mathcal{V}^{\alpha,n+1}_i$

How to communicate between the different grids $\mathcal{V}^{\alpha,n}_i$, $\mathcal{V}^{\alpha,n}_{i-1}$, $\mathcal{V}^{\alpha,n}_{i+1}$, $\mathcal{V}^{\alpha,n+1}_i$

Computation of $f_i^{\alpha,n+1}$

Reconstruction procedure



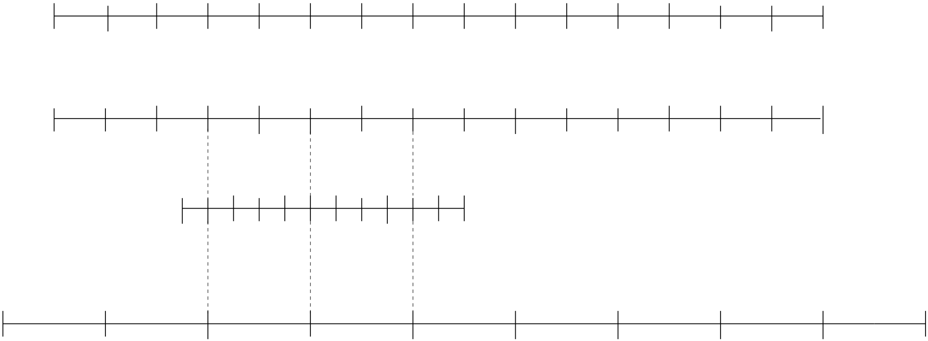
The scheme writes: $\forall\ v_{i,k}^{\alpha,n+1} \in \mathcal{V}_i^{\alpha,n+1}$

$$
\begin{aligned}
f_{i,k}^{\alpha,n+1} &= \overline{f}_i^{\alpha,n}(v_{i,k}^{\alpha,n+1}) - \frac{\Delta t}{\Delta x}\left(\overline{\phi}_{i+\frac{1}{2}}^{\alpha,n}(v_{i,k}^{\alpha,n+1}) - \overline{\phi}_{i-\frac{1}{2}}^{\alpha,n}(v_{i,k}^{\alpha,n+1})\right) \\
&+ \Delta t \nu_i^{\alpha,n+1}(\overline{M}_{i,k}^{\alpha,n+1} - f_{i,k}^{\alpha,n+1})
\end{aligned}
$$

$\overline{f}_i^{\alpha,n}$, $\overline{\phi}_{i+\frac{1}{2}}^{\alpha,n}$ interpolation on $\mathcal{V}_i^{\alpha,n+1}$ using ENO 4 scheme.

Shifted velocity grids (Motivations)

Aim: Obtain velocity grids with common points⇒ diminish interpolations



Choice: 0 belongs to all velocity grids

Shifted velocity grids (Constructions)

$$\Delta v_{\min}^{\alpha,0} = \min_i (\Delta v_i^{\alpha,0}).$$

Modifications of the steps

$$\overline{\Delta v}_i^{\alpha} = \lfloor \frac{\Delta v_i^{\alpha}}{\Delta v_{\min}^{\alpha,0}} \rceil \Delta v_{\min}^{\alpha,0}, \qquad \lfloor x \rceil : \text{ nearest integer to } x.$$

Modify bounds: $(\overline{V_{\min}})_i^{\alpha,0}$, $(\overline{V_{\max}})_i^{\alpha,0}$

$$(\overline{V_{\min}})_i^{\alpha,0} = \lfloor \frac{(V_{\min})_i^{\alpha,0}}{\overline{\Delta v}_i^{\alpha,0}} \rfloor \overline{\Delta v}_i^{\alpha,0}, \qquad (\overline{V_{\max}})_i^{\alpha,0} = \lceil \frac{(V_{\max})_i^{\alpha,0}}{\overline{\Delta v}_i^{\alpha,0}} \rceil \overline{\Delta v}_i^{\alpha,0}$$

$\lfloor x \rfloor$: integer part of x, $\lceil x \rceil$: integer part of $x + 1$

$(\overline{V_{\min}})_i^{\alpha,0}$, $(\overline{V_{\max}})_i^{\alpha,0}$, $\overline{\Delta v}_i^{\alpha,0}$ multiples of $\Delta v_{\min}^{\alpha,0}$

Shifted velocity grids (Constructions)

Aim: Obtain bounds and steps at t^{n+1} multiples of the same quantity

$$\Delta v_{\min}^{\alpha,n+1} = \min_i (\Delta v_i^{\alpha,n+1}).$$

1^{st} situation: $\Delta v_{\min}^{\alpha,n+1} \geq \Delta v_{\min}^{\alpha,n}$.

$$(\overline{\Delta v_{\min}})^{\alpha,n+1} = \lfloor \frac{(\Delta v_{\min})^{\alpha,n+1}}{\Delta v_{\min}^{\alpha,n}} \rceil \Delta v_{\min}^{\alpha,n}.$$

2^{nd} situation: $\Delta v_{\min}^{\alpha,n+1} \leq \Delta v_{\min}^{\alpha,n}$.

$$(\overline{\Delta v_{\min}})^{\alpha,n+1} = \frac{1}{\lfloor \frac{(\Delta v_{\min})^{\alpha,n+1}}{\Delta v_{\min}^{\alpha,n}} \rceil} \Delta v_{\min}^{\alpha,n}.$$

Test case: Blast waves

- Initial data:

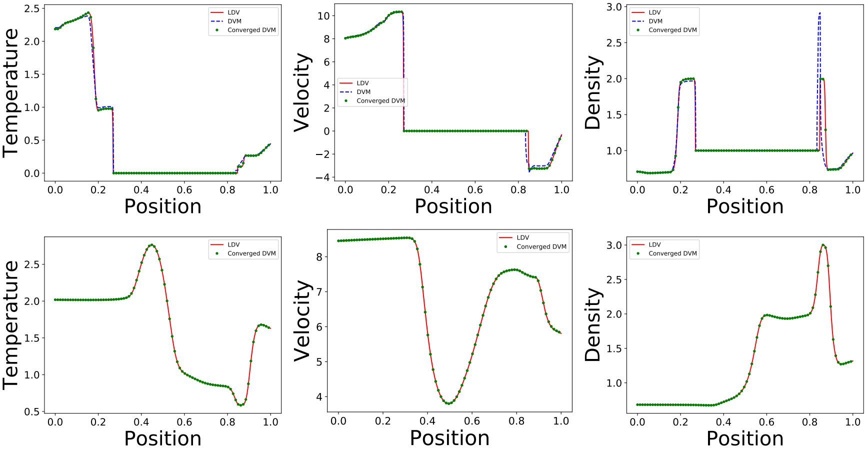
	ρ^α	u^α	T
$x \in [0, 0.1]$	1	0	4,8
$x \in [0.1, 0.9]$	1	0	$4, 8.10^{-5}$
$x \in [0.9, 1]$	1	0	$4, 8.10^{-1}$

- Simulation parameters:
  - Final time: $t_f = 0.05$
  - Velocity grids:

	l	N_v	CPU time
LDV	5	30	279s
DVM	5	200	516s

Two interacting blast waves

Before (up), after (down)



LDV: 30 points. DVM: 30 points. Converged DVM: 200 points

Test case: Shock waves

- Initial data:

	ρ^α	u^α	T
$x \in [0, 0.5]$	1	10^4	300
$x \in [0.5, 1]$	1	-10^4	300

- Simulation parameters:
  - Final time: $t_f = 10^{-5}$ s
  - Velocity grids:

	l	N_v	CPU time
LDV	5	30	147s
DVM	180	2000	1824s

Shock wave (Velocity)

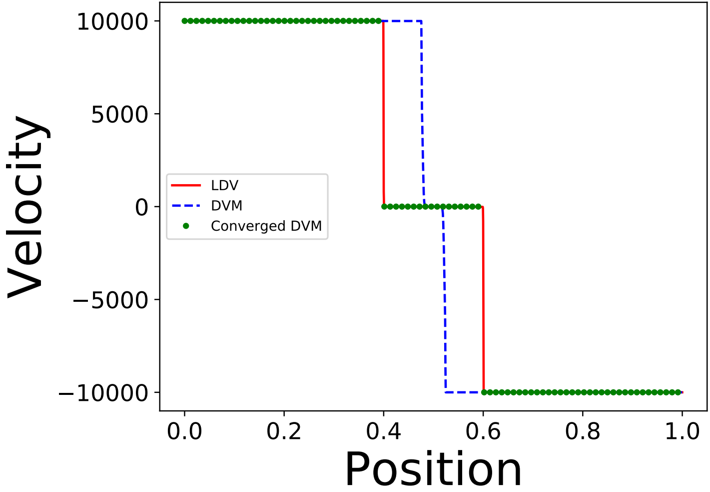


Figure: Velocity for a shock waves test case

Shock wave (Temperature)

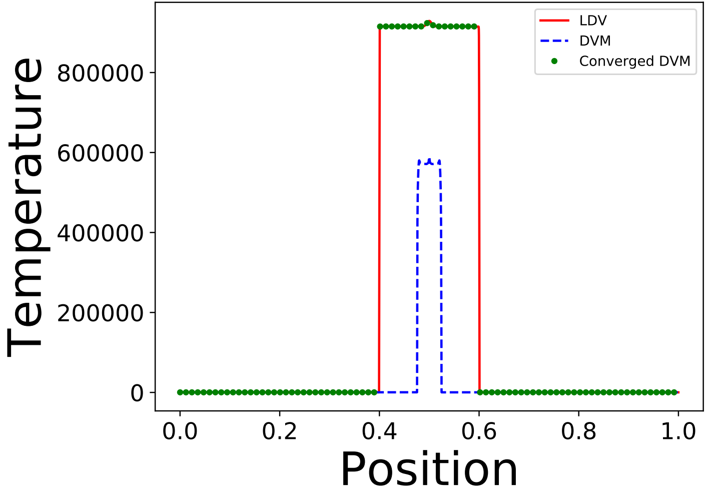
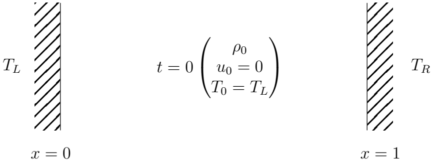


Figure: Temperature for a shock waves test case

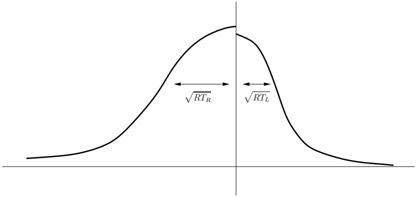
Heat transfert



$T = T_L = 300$ sur $[0, 1[$, $T(1) = T_R = 1000$, $\rho^\alpha = \rho_0$, $u^\alpha = 0$.

Diffuse boundary conditions $f(t, x = 0, v > 0) = -\frac{\langle v^- f \rangle}{\langle v^+ M_w \rangle} M_w$

For small t, the support of $f^\alpha(t, x \approx 1, v)$ is non symetric



Test case: Heat transfert

$Kn = 10$

- Initial data:

	ρ^α	u^α	T
$x \in [0, 1[$	1	0	300
$x = 1$	1	0	1000

- Simulation parameters:
  - Final time: $t_f = 1,3\,10^{-3}$
  - Velocity grids:

	l	N_v	CPU time
LDV	5	150	223s
SLDV	5	150	138s
DVM	20	600	274s

Extension of the grid: algorithm

Problem: If f^α is far from a Maxwellian ($K_n > 10^{-2}$)

Splitting between transport and collision

Transport step

- Computation of $f_{i,k}^{n+\frac{1}{2}}$ for each $v_{i,k}^{n+1}$ of $\mathcal{V}_i^{n+1}$
- $w = v_{i,1}^{n+1}$
- loop left
  - $w = w - \Delta v_i^{n+1}$
  - Compute $f_i^{n+\frac{1}{2}}(w)$ by the scheme

$$\frac{f_i^{n+\frac{1}{2}}(w) - \bar{f}_i^n(w)}{\Delta t} + w^+ \frac{\bar{f}_i^n(w) - \bar{f}_{i-1}^n(w)}{\Delta x} + w^- \frac{\bar{f}_{i+1}^n(w) - \bar{f}_i^n(w)}{\Delta x} = 0$$

  - If $f_i^{n+\frac{1}{2}}(w)$ too big add w to the grid and go on
- $w = v_{i,N_v(i)}^{n+1}$ + loop right

Collision step

Velocity-Converged case

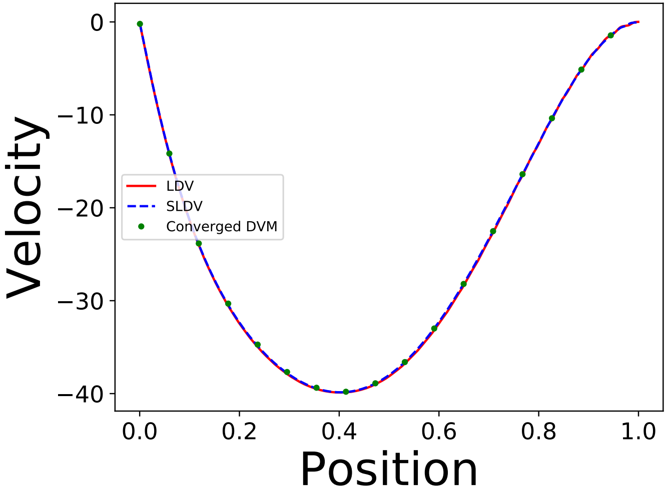


Figure: $l = 5$, $N_v = 150$ for LDV, SLDV. $l = 20$, $N_v = 600$ for reference DVM

Temperature-Converged case

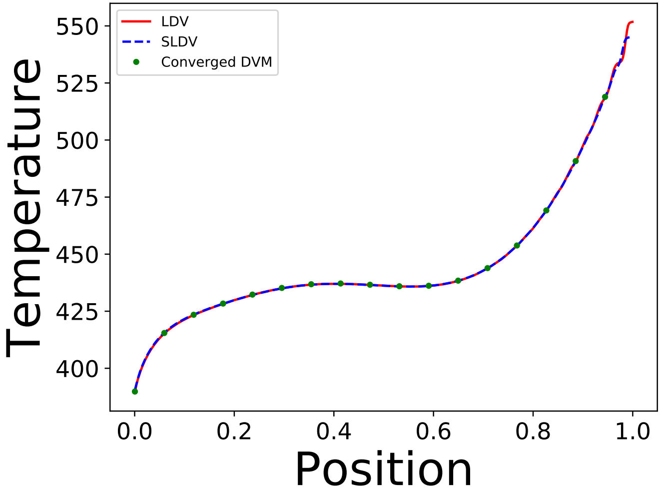


Figure: $l = 5$, $N_v = 150$ for LDV, SLDV. $l = 20$, $N_v = 600$ for reference DVM

Temperature-Non converged case

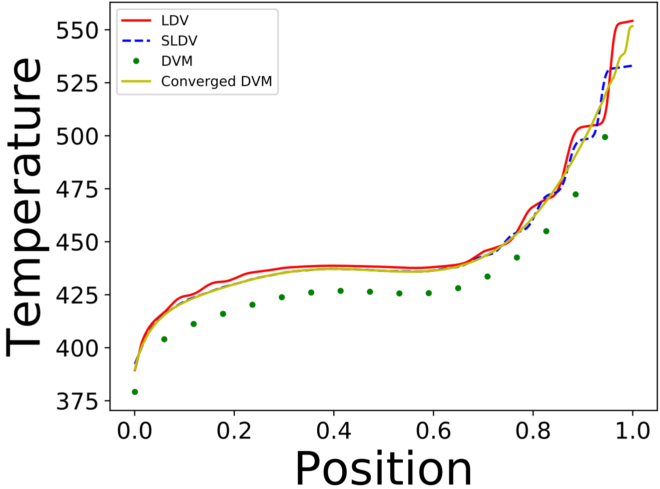


Figure: $l = 4$, $N_v = 50$ LDV, SLDV, DVM. $l = 20$, $N_v = 600$ for reference DVM

Conclusion

- Deterministic adaptative method for multi-species kinetic equations
- Very good results when compared to classical methods
- Related result: Reduce interpolation cost $\Rightarrow$ Shifted grids
- Perspectives

  $\hookrightarrow$ Higher dimensions

  $\hookrightarrow$ Implement other BGK models for Gas Mixtures:
  [S. Brull, V. Pavan, J. Schneider, 2012], [S. Brull, 2015]

  $\hookrightarrow$ Chemical reactions
  Implementation of the model [Groppi, Spiga, 2004]:
  Generalisation of [Andries, Aoki, Perthame] for slow chemical reactions
  [Bisi, Brull, Groppi, Prigent], in progress

Thank you for your attention.