Hybrid fluid/kinetic modeling for plasma

WENO method for plasma simulation

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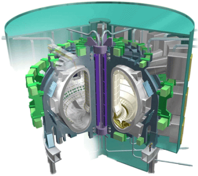
What is plasma or rarefied gas ?

- System of interacting particles
- Plasma : hot gas, electrons separated from atoms $\rightarrow$ electric field
- Examples of plasmas :
  - neons, ITER, nebula
- Examples of rarefied gas :
  - atmospheric entry (Soyouz, CST-100 Starliner, ...)



Outline

Models

Microscopic model: simulation of all particles

$(t, x_i(t), v_i(t)), i = 1, \dots, N$

✓ accuracy ✗ computational time and memory

Macroscopic model: plasma $\approx$ fluid

$(\rho, u, T)(t, x)$ thermodynamic variables

✗ accuracy ✓ computational time and memory

Kinetic model: simulation in phase space

$f(t, x, v)$ distribution of density in phase space

$\sim$ accuracy $\sim$ computational time and memory

Study only on macroscopic and kinetic models

Macroscopic model

Euler's equations:

$$\partial_t U + \nabla_x \cdot \mathcal{F}(U) = S_E(U)$$

- $U = U(t, x)$
- Vector $U = (\rho, \rho u, e)^T$ thermodynamic variables
- $S_E(U)$ source term that includes electric field E

Kinetic model

Vlasov-BGK's equation:

$$\partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = \frac{1}{\varepsilon} Q(f,f)$$

Transport (x, v) + stiff term $\frac{1}{\varepsilon}$

- $f = f(t, x, v)$ density distribution in phase space
- $Q(f, f)$ collision operator (BGK) $Q(f, f) = \mathcal{M}_{[U]} - f$
- $\mathcal{M}_{[U]}$: velocity distribution at equilibrium
- $\varepsilon \sim$ mean free path
  - If $\varepsilon \ll 1 \to$ Euler equations
  - If $\varepsilon \gg 1 \to$ no collision (what I do now)

Relation with macroscopic variables:

$$\int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} f(t,x,v)\,\mathrm{d}v = \int_{\mathbb{R}^d} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \mathcal{M}_{[U]}(t,x,v)\,\mathrm{d}v = U(t,x)$$

Electric field

Poisson's equation

$$\nabla_x \cdot E(x) = \rho(t,x) = \int_{\mathbb{R}^d} f(t,x,v)\,\mathrm{d}v$$

Periodic conditions in space: resolution by FFT
Maxwell's equation (magnetic field) soon! (one day)

Hybrid model

1. Micro-macro model (**mM**)

$$f = \underbrace{\mathcal{M}_{[U]}}_{\text{thermodynamic equilibrium state}} + \underbrace{g}_{\text{gap from equilibrium}}$$

2. Approximation of *micro* part (**mMh**) without interface between models (internship work)
   - Transition function $h(t, x)$ between fluid area Ω_F and kinetic area Ω_K

Building hybrid model

1. **mM** consisting of 2 equations:

macro: **mean** in v of kinetic model:

$$\partial_t U + \nabla_x \cdot \mathcal{F}(U) + \nabla_x \cdot \langle v m(v) g \rangle_v = S_E(U)$$

micro: **projection** of kinetic model on image of collision operator $Q(f,f) = \mathcal{M}_{[U]} - f$:

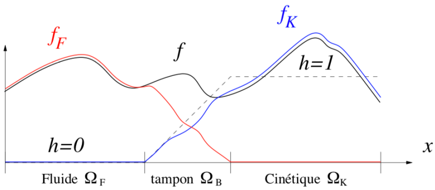
$$\partial_t g + (I - \Pi)[v \cdot \nabla_x (\mathcal{M}_{[U]} + g) + E \cdot \nabla_v (\mathcal{M}_{[U]} + g)] = -\frac{1}{\varepsilon} g$$

mM model is equivalent to kinetic model

Approximation of *micro* part

2. **Hypothesis:** $f = \mathcal{M}_{[U]}$ on $\Omega_F \Rightarrow g_F = 0$
New model: approximation of **micro**-macro by domain decomposition

$$\Omega = \Omega_F \cup \Omega_K \qquad g = (1-h)g + hg = g_F + g_K$$



Approximated *micro* part

We multiply by h micro part to get:

$$\partial_t g_K + (I - \Pi)\left[v \cdot \nabla_x(\mathcal{M}_{[U]} + g_K) + E \cdot \nabla_v(\mathcal{M}_{[U]} + g_K)\right] = -\frac{1}{\varepsilon} g_K + \frac{g_K}{h}\partial_t h$$

Outside the support of h: $g_K = 0$

Why this model? save computational time (kinetic evaluation **only** on Ω_K)

Outline

Goals

- Transport in phase space $(x, v) \rightsquigarrow$ scheme easy to use in multi-d (d at least 2)
- Heavy gradient $\rightsquigarrow$ need high order scheme
- Stiff term in $\frac{1}{\varepsilon}$, $\varepsilon \in]0, 1] \rightsquigarrow$ need adapted time integrators
- Long time simulation $\rightsquigarrow$ need stability of space+time scheme

Explicit Euler method

Unstable with 5^{th}-order WENO method:

- [Wang, R., & Spiteri, R. (2007) SINUM]

Amplification term is small enough to be *controlled* by very small Δt.
If stiff term $\rightsquigarrow$ IMEX:

$$f^{n+1} = f^n - dt(v\partial_x + E\partial_v)(f^n) + \frac{1}{\varepsilon}(\mathcal{M}_{[U^{n+1}]} - f^{n+1})$$

CFL upwind-IMEX: $\frac{\Delta x}{v_{\max}}$

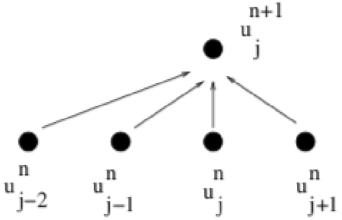
Runge-Kutta 3th order method

Stable with 5^{th}-order WENO method (see later)
If stiff term $\rightsquigarrow$ exponential formulation:

$$\partial_t(e^{\frac{t}{\varepsilon}} g) + (I - \Pi)\left((v\partial_x + E\partial_v)(e^{\frac{t}{\varepsilon}}(g + \mathcal{M}_{[U]}))\right) = 0$$

and Lawson scheme or IFRK method

Compact scheme



- High order 6 points scheme $(u^n_{j-3}, \ldots, u^n_{j-2})$
- Based on **1** polynomial of degree 5

It doesn't work very well (implementation bug ?) and it oscillates with discontinuity (not important for us) or heavy gradient (strong problem for filamentation).

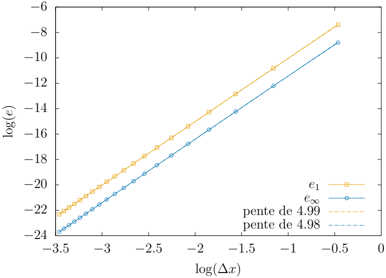
Numerical order

$$\partial_t u + \partial_x u = 0$$

initial: $u(t=0,x) = cos(x)$
solution: $u(t=t_i,x) = cos(x-t_i)$

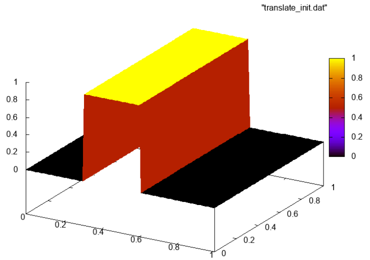
Δx	Δt	T_f
$\frac{2\pi}{N}$	$10^{-5}\Delta x$	1

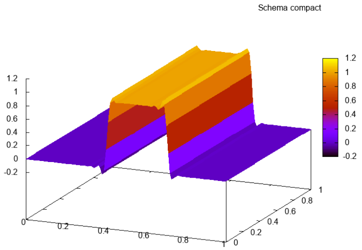
$N = 10, \ldots, 200$



Simplest test

Transport in 1 direction of a discontinuity





Initial condition

Result

WENO method

- High order 6 points scheme
- Based on **3** ENO approximations (of lower order) combined with non-linear weights (indicator of smoothness)

BUT: Unstable with explicit Euler method [Wang, R., & Spiteri, R. (2007) SINUM]

Numerical order

$$\partial_t u + \partial_x u = 0$$

initial: $u(t=0,x) = cos(x)$
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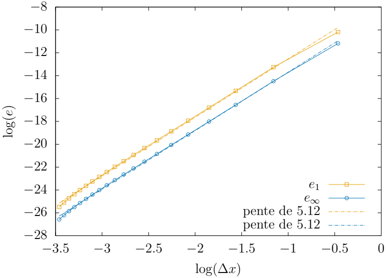

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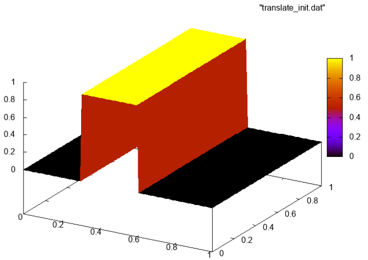
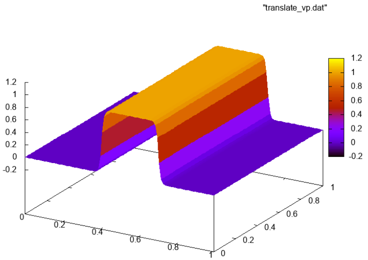


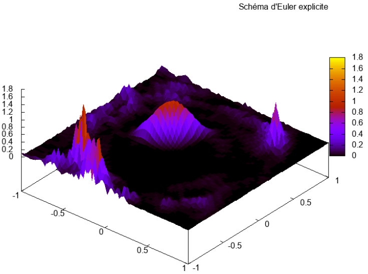


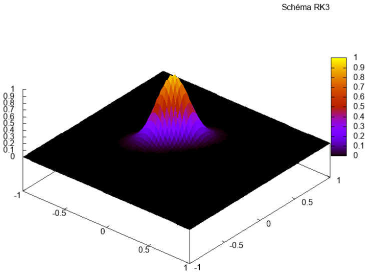
Initial condition

Result

Instability illustration

Gaussian rotation





Explicit Euler method RK3 method

grid: 100×100 $\Delta t = 0.3\Delta x$ $T_f = 15$

[Wang, R., & Spiteri, R. (2007) SINUM]

Steps of proof of instability

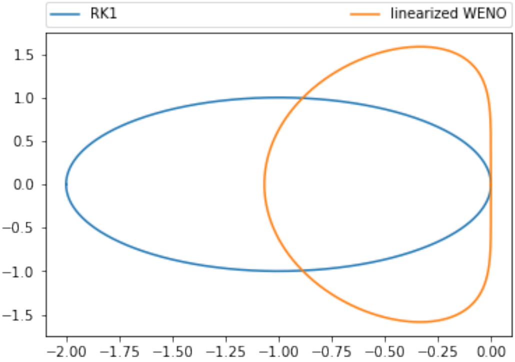
1. Von Neumann analysis : $f^n_{j+k} \to e^{ik\phi}$ ($\phi \equiv \kappa\pi\Delta x$)
2. Linearized WENO scheme (weight $\approx \mathcal{O}(\Delta x^2)$):

$$z(\phi) = \tilde{z}(\phi) + M(\epsilon_i, \phi)$$

   with $M(\epsilon_i, \phi) = \mathcal{O}(\Delta x^2)$
3. Draw $\tilde{z}(\phi)$ with some RK stability curve and conclude.

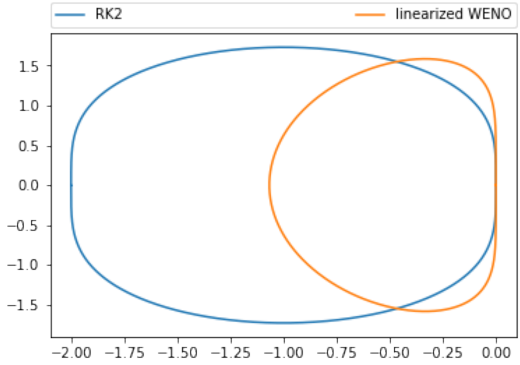
Stability of RKN-WENO

RK1-WENO



Stability of RKN-WENO

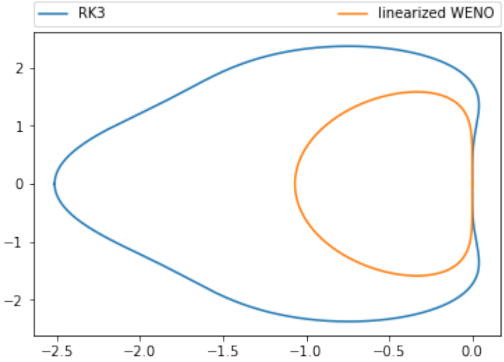
RK2-WENO



possible stability: $\Delta t = 1.73 \Delta x^{5/3}$ [Motamed, M., & Macdonald, C. & Ruuth S. (2010) J. Sci. Comput.]

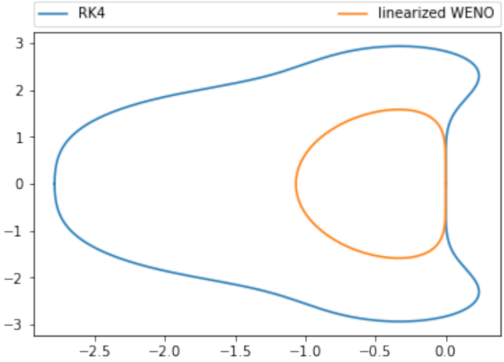
Stability of RKN-WENO

RK3-WENO (CFL: 1.433)



Stability of RKN-WENO

RK4-WENO (CFL: 1.731)



Outline

Sod shock tube

Fluid regime validation

boundary: Neumann in space x, periodic in velocity v

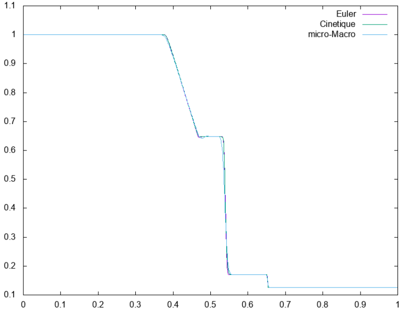
initial condition: discontinuity in ρ and T:

$$U(t=0,x) = \begin{cases} U_L = (\rho_L, u_L, T_L) = (1,0,1) & ,x \leq \frac{1}{2} \\ U_R = (\rho_R, u_R, T_R) = (0.125, 0, 0.8) & ,x > \frac{1}{2} \end{cases}$$

$$f(t=0,x,v) = \mathcal{M}_{[U(t=0,x)]}(x,v) \qquad g(t=0,x,v) = 0$$

Models and schemes validation

$\rho(t = 0.067, x)$

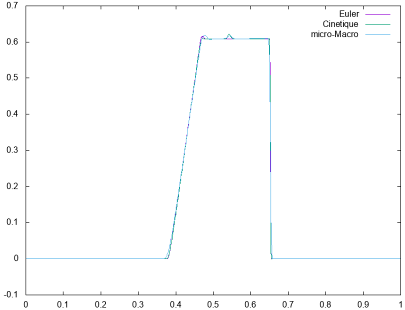


domain: $[0,1] \times [-18,18]$ grid: 1000×64 $\varepsilon = 10^{-4}$

$\Delta x = 10^{-3}$ $\Delta v = 0.5625$ $\Delta t = \frac{1}{2}\frac{\Delta x}{v_{\max}} = 2.77 \cdot 10^{-5}$

Models and schemes validation

$u(t = 0.067, x)$



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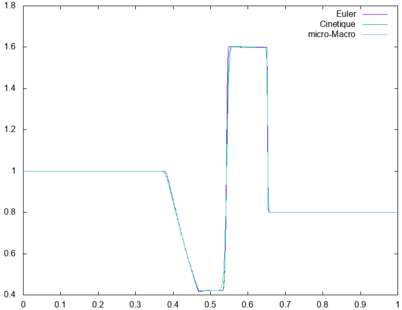
Models and schemes validation

$T(t = 0.067, x)$



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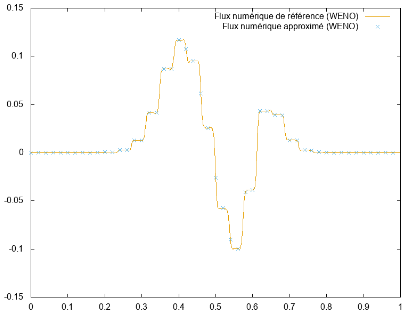
Simulation : Sod shock tube, kinetic mode: $\varepsilon = 1$

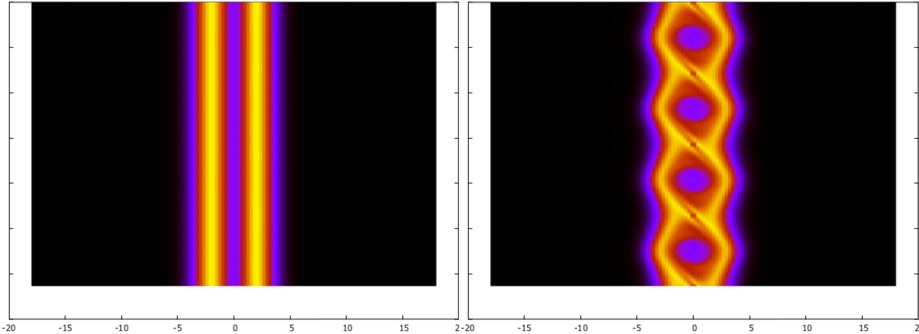


domain: $[0,1] \times [-18,18]$ grid: 1000×64 $\varepsilon = 1$

$\Delta x = 10^{-3}$ $\Delta v = 0.5625$ $\Delta t = \frac{1}{2}\frac{\Delta x}{v_{\max}} = 2.77 \cdot 10^{-5}$

Computing time: divided by 2

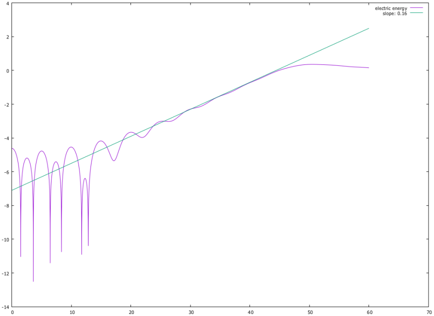
Numerical test: two streams



Initial condition Result

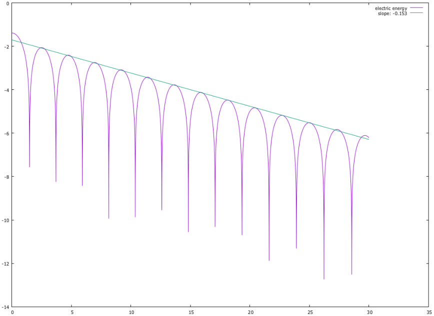
Numerical test: two streams

Electric energy



Numerical test: Landau damping

Electric energy

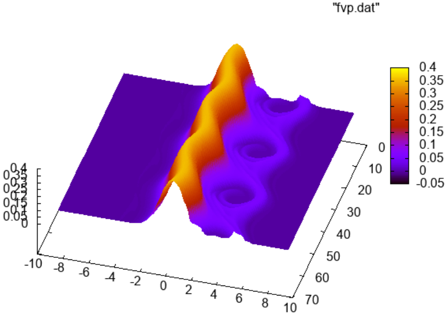


Bump on Tail (BoT)

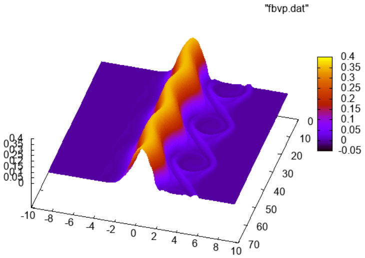
Cold and hot particles splitting (not same as micro-macro splitting)

$$f = f_c + f_h \qquad f = \mathcal{M}_{[U]} + g$$

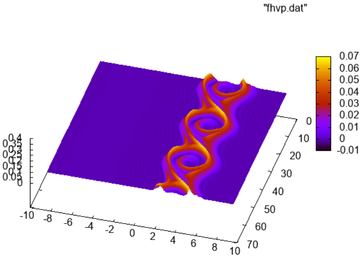
What we expect: $f_c = \mathcal{M}_{[U]}$, $f_h = g \dots$



BoT: f_c, f_h



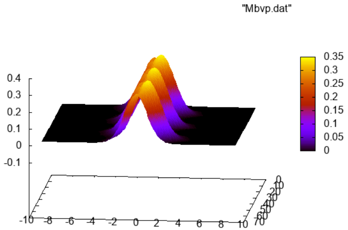
f_c

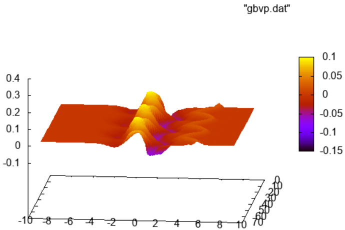


f_h

BoT: f_c mM, f_h kinetic

mM on $f_c = \mathcal{M}_{[U_c]} + g_c$, **kinetic** on f_h

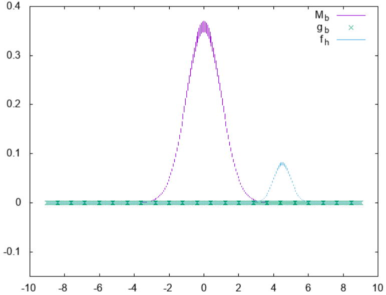




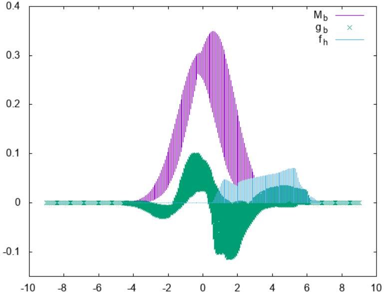
$\mathcal{M}_{[U_c]}$ g_c

BoT: f_c mM, f_h kinetic

mM on $f_c = \mathcal{M}_{U_c} + g_c$, **kinetic** on f_h



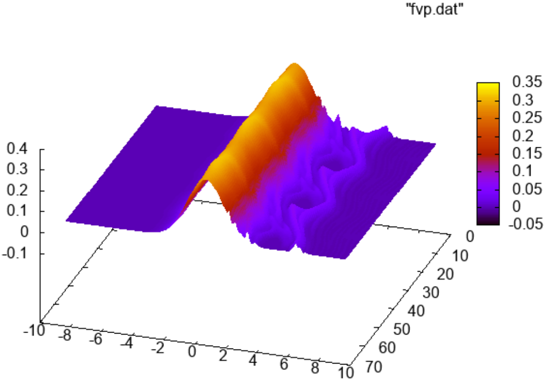
Initial condition



Result

BoT: f_c fluid approximation

approximation : $f_c = \mathcal{M}_{[U_c]}$, $g_c = 0$



BoT: f_c fluid approximation

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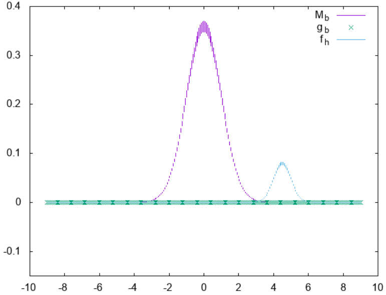
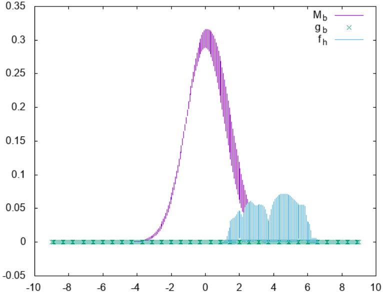


Initial condition



Result

Ideas

- Physicist idea (IPP Garching): $f_c = \delta_{v-u_c}$
- Computer scientist idea: reduce grid in v around effective data for f_h

Outline

Conclusion

✓ WENO approved!

- High order, no oscillation, no problem in multi-D (CFL ?)
- Works well with RK3 (even with stiff term)
- Could be use for Euler part

Future works

- Still a grid in phase space for 1Dx 3Dv or 3Dx 3Dv? (MC? PIC?)
- Code refactoring: some optimization and adaptive grid (no global variables) (Julia? C++?)
- Better understanding of SSPRK(3,3) diffusion, stability of couple of time-space schemes
- Automatic study of different schemes (*SymPy* & *NodePy*)
- Approve approximation of f_c with conservative variables, and integrate Dirac modeling

Tank you for your attention

Outline

Construction de la fonction $h(t, x)$

Euler's equations

WENO scheme

Discrétisation du modèle micro-macro approximé

Détermination *a priori* de la fonction h :
Zone *hors équilibre* au cours du temps :

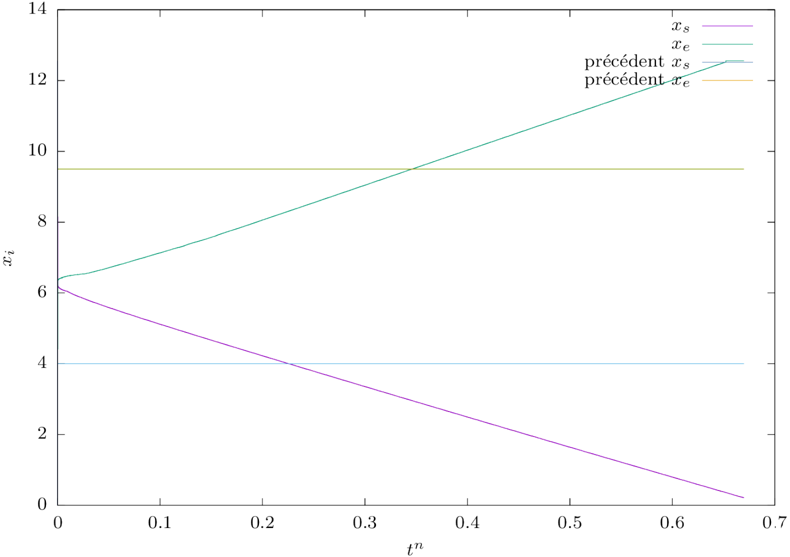
$$\operatorname{supp} h(t,x) = \Omega_K(t)$$

Étude du support numérique (seuil à 10^{-5}) de $(G_i^n)_3$:

$$\mathscr{I}^n = \left\{ i \in [\![0, N_x]\!], \left|\langle vm(v) g^n \rangle_{x=x_i}\right| > 10^{-5} \right\}$$

Étude de g_K limitée à $[\![i_s^n, i_e^n]\!] = \mathscr{I}^n$

Étude du support de h



Outline

Construction de la fonction $h(t, x)$

Euler's equations

WENO scheme

Euler's equations

$$\partial_t U + \nabla_x \cdot \mathcal{F}(U) = S_E(U)$$

$$\mathcal{F}(U) = \begin{pmatrix} \rho u \\ \rho u \otimes u + p\mathbb{I}_d \\ u(e+p) \end{pmatrix} \qquad S(U) = \begin{pmatrix} 0 \\ \rho E \\ 2\rho u E \end{pmatrix}$$

pressure: $p = 2(e - \frac{1}{2}\rho|u|^2)$

Outline

WENO scheme

Model:

$$\partial_t u + \partial_x(au) = 0$$

We would approximate $\partial_x(au)_{|x=x_i, v=v_k}$:

$$\partial(au)_{|x=x_i, v=v_k} \approx \frac{1}{\Delta x}(\hat{u}_{i+\frac{1}{2},k} - \hat{u}_{i-\frac{1}{2},k})$$

WENO flux

$$\begin{aligned}\hat{u}^{+}_{i+\frac{1}{2},k} &= w_0^{+}\left(\frac{2}{6}u^{+}_{i-2,k} - \frac{7}{6}u^{+}_{i-1,k} + \frac{11}{6}u^{+}_{i,k}\right)\\ &+ w_1^{+}\left(-\frac{1}{6}u^{+}_{i-1,k} + \frac{5}{6}u^{+}_{i,k} + \frac{2}{6}u^{+}_{i+1,k}\right)\\ &+ w_2^{+}\left(\frac{2}{6}u^{+}_{i,k} + \frac{5}{6}u^{+}_{i+1,k} - \frac{1}{6}u^{+}_{i+2,k}\right)\end{aligned}$$

and

$$\begin{aligned}\hat{u}^{-}_{i+\frac{1}{2},k} &= w_2^{-}\left(-\frac{1}{6}u^{-}_{i-1,k} + \frac{5}{6}u^{-}_{i,k} + \frac{2}{6}u^{-}_{i+1,k}\right)\\ &+ w_1^{-}\left(\frac{2}{6}u^{-}_{i,k} + \frac{5}{6}u^{-}_{i+1,k} - \frac{1}{6}u^{-}_{i+2,k}\right)\\ &+ w_0^{-}\left(\frac{11}{6}u^{-}_{i+1,k} - \frac{7}{6}u^{-}_{i+2,k} + \frac{2}{6}u^{-}_{i+3,k}\right)\end{aligned}$$

WENO weights

$$w_n^{\pm} = \frac{\tilde{w}_n^{\pm}}{\sum_{m=0}^{2} \tilde{w}_m^{\pm}}, \quad \tilde{w}_n^{\pm} = \frac{\gamma_n}{(\epsilon + \beta_n^{\pm})^2}$$

$$\gamma_0 = \frac{1}{10}, \quad \gamma_1 = \frac{3}{5}, \quad \gamma_2 = \frac{3}{10}$$

$\epsilon = 10^{-6}$ numerical value to prevent the denominator from being 0

WENO Indicator of Smoothness

$$\beta_0^+ = \frac{13}{12}(u^+_{i-2,k} - 2u^+_{i-1,k} + u^+_{i,k})^2 + \frac{1}{4}(u^+_{i-2,k} - 4u^+_{i-1,k} + 3u^+_{i,k})^2$$
$$\beta_1^+ = \frac{13}{12}(u^+_{i-1,k} - 2u^+_{i,k} + u^+_{i+1,k})^2 + \frac{1}{4}(u^+_{i-1,k} - u^+_{i+1,k})^2$$
$$\beta_2^+ = \frac{13}{12}(u^+_{i,k} - 2u^+_{i+1,k} + u^+_{i+2,k})^2 + \frac{1}{4}(3u^+_{i,k} - 4u^+_{i+1,k} + u^+_{i+2,k})^2$$

and

$$\beta_0^- = \frac{13}{12}(u^-_{i+1,k} - 2u^-_{i+2,k} + u^-_{i+3,k})^2 + \frac{1}{4}(3u^-_{i+1,k} - 4u^-_{i+2,k} + u^-_{i+3,k})^2$$
$$\beta_1^- = \frac{13}{12}(u^-_{i,k} - 2u^-_{i+1,k} + u^-_{i+2,k})^2 + \frac{1}{4}(u^-_{i,k} - u^-_{i+2,k})^2$$
$$\beta_2^- = \frac{13}{12}(u^-_{i-1,k} - 2u^-_{i,k} + u^-_{i+1,k})^2 + \frac{1}{4}(u^-_{i,k} - 4u^-_{i,k} + 3u^-_{i+1,k})^2$$