Un schéma aux différences finies d'ordre élevé de l'équation de transport pour le HPC

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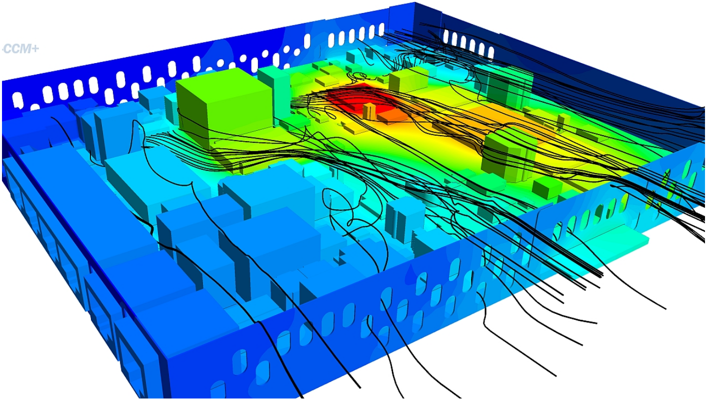
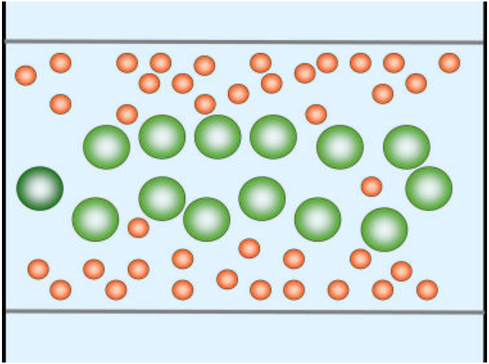
Transport de chaleur

$$D_t\theta = \kappa \Delta\theta \,. \tag{1}$$



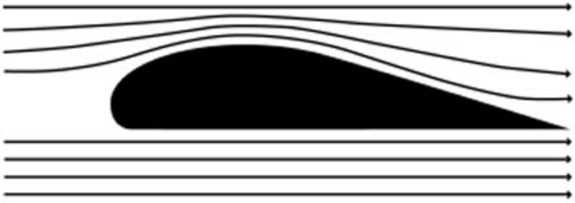
Advection diffusion de particules

$$D_t n = D \Delta n. \tag{2}$$



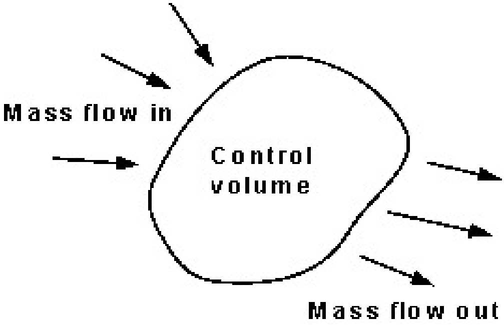
Mécanique des fluides

$$D_t\mathbf{u} = -\frac{1}{\rho}\nabla P + \nu\Delta\mathbf{u}. \tag{3}$$

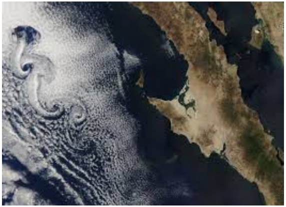


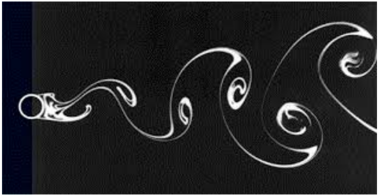
Phénomène de conservation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = D_t \rho + \rho \nabla \cdot \mathbf{u} = 0 \,. \tag{4}$$



Applications





Turbulence (théorie, aviation, voiture)

Convection thermique (géosciences, ventilation BTP)

Advection/diffusion (traçage de polluant)

Prévision météorologique

Trafic routier, divertissement etc.

L'équation

Équation d'advection :

$$D_t\Phi = \partial_t \Phi + u\partial_x \Phi\,. \tag{5}$$

Deux modélisations possibles :

Eulérienne $\Phi(x, t)$

Lagrangienne $\Phi(x(t), t)$

Deux écritures de dérivée :

$$\lim_{(\Delta t, \Delta x)\to 0} \frac{1}{\Delta t}\left[\Phi(x, t+\Delta t) - \Phi(x, t)\right] + \frac{u}{\Delta x}\left[\Phi(x, t) - \Phi(x-\Delta x, t)\right] \tag{6}$$

$$\lim_{\Delta t\to 0} \frac{1}{\Delta t}\left[\Phi(x(t+\Delta t), t+\Delta t) - \Phi(x(t) - u(x)\Delta t, t)\right] \tag{7}$$

Intérêt pour le calcul HPC des algorithmes Semi-Lagrangiens

Avantages :

Les équations sont locales

⇒ implémentations par domaine facilement parallélisable

Les équations ne nécessitent qu'une série de point fantômes

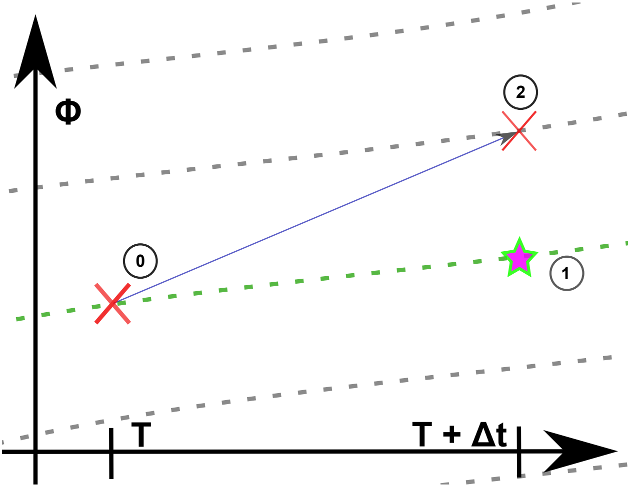
⇒ bonne gestion des conditions aux limites

⇒ coût de calcul et de mémoire faible

Inconvénients :

Ces algorithmes n'ont pas la convergence exponentielle des méthodes spectrales

Schéma $\mathscr{N}$ (n°2)



Erreur de $\mathcal{N}$

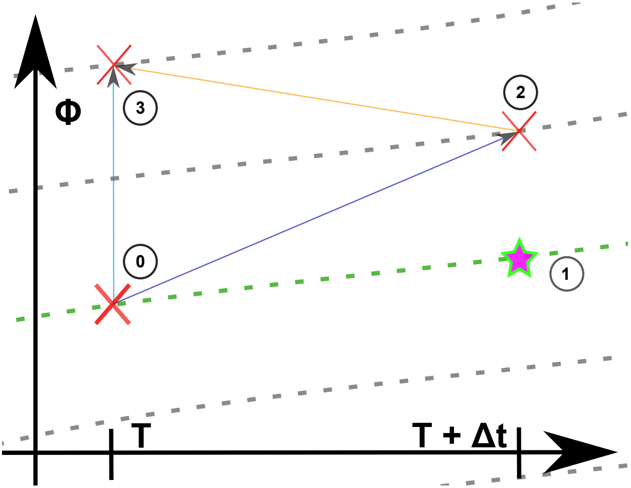


Schéma $\mathscr{A}$ (n°4)

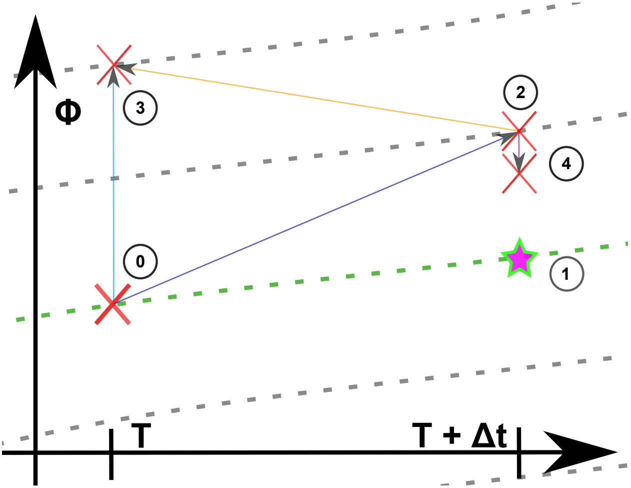


Schéma $\mathscr{B}$ (n°6)

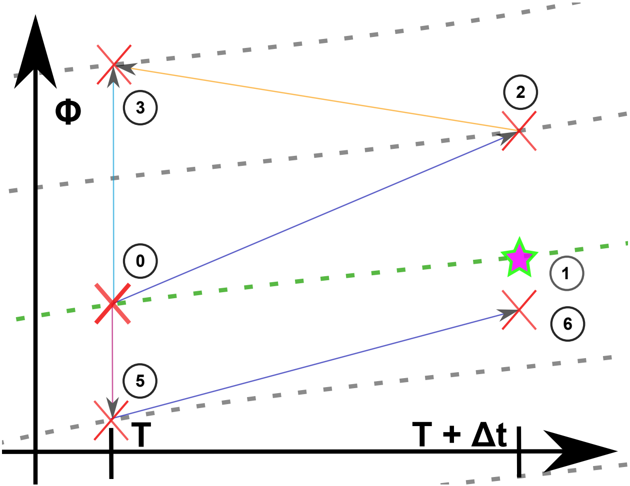
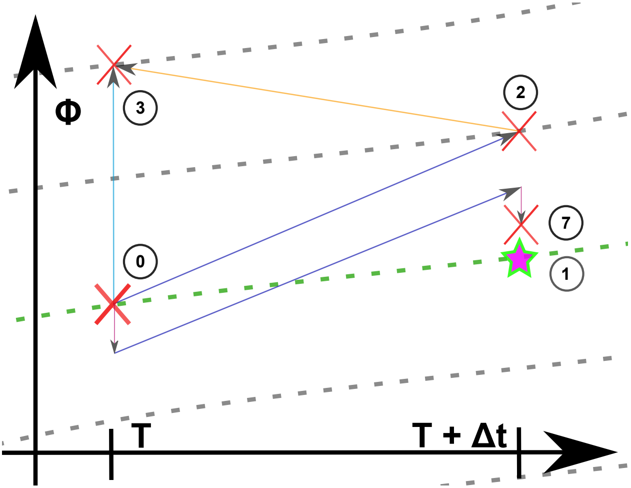


Schéma $\mathscr{C}$ (n°7)



Rappel : $\mathscr{N}$ (n°2), $\mathscr{A}$ (n°4), $\mathscr{B}$ (n°6), $\mathscr{C}$ (n°7)

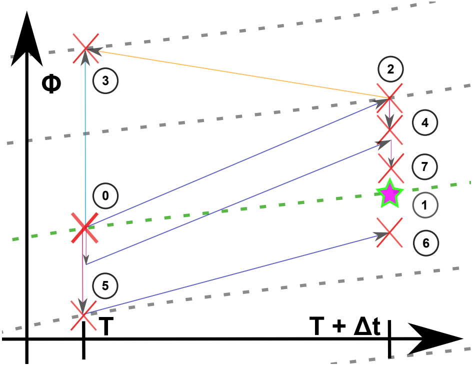


Schéma diffusif $\mathcal{N}$ (Upwind, CIR)

Algorithme 1d a vitesse constante :

$$\Phi_i^{n+1} = \mathcal{N}[\Phi^n] = L_+[\Phi^n]_i = \Phi_i^n - \Delta t\,(\mathbf{u}\cdot\nabla)\,\Phi_i^n \tag{8}$$

$$= (1-U)\Phi_i^n + U\Phi^n[i-1]\,. \tag{9}$$

Erreur :

$$D_t\Phi_{\mathcal{N}} = U(1-U)\frac{\Delta x^2}{2\Delta t}\partial_x^2\Phi\,. \tag{10}$$

Vitesse renormalisée voir la condition de CFL :

$$U = \frac{u\Delta t}{\Delta x}\,. \tag{11}$$

Stable : $CFL \leq 1$.

Schéma dispersif $\mathscr{A}$ (MacCormack)

Algorithme 1d a vitesse constante :

$$\Phi_{\mathscr{A}}^{n+1} = \mathscr{A}[\Phi^n] = L_+\left[\Phi^n\right] + \frac{1}{2}\left(\Phi^n - \bar{\Phi}^n\right) \text{ where } \bar{\Phi}^n = L_-\Big(L_+[\Phi^n]\Big). \quad (12)$$

Erreur :

$$D_t\Phi_{\mathscr{A}} = -U(1-U^2)\frac{(\Delta x)^3}{3!\Delta t}\partial_x^3\Phi - 3U^2(1-U^2)\frac{(\Delta x)^4}{4!\Delta t}\partial_x^4\Phi. \quad (13)$$

Stable : $CFL \leq 1$.
Temps de calcul : 2 itérations de $\mathscr{N}$

Schéma dispersif $\mathscr{B}$ (Dupont-Liu)

Algorithme 1d a vitesse constante :

$$\Phi_{\mathscr{B}}^{n+1} = \mathscr{B}[\Phi^n] = L_+\left[\Phi^n + \frac{1}{2}\left(\Phi^n - \bar{\Phi}^n\right)\right] = \frac{1}{2}L_+\left[3\Phi^n - \bar{\Phi}^n\right]. \tag{14}$$

Erreur :

$$D_t\Phi_{\mathscr{B}} = U(1-U)(2U-1)\frac{(\Delta x)^3}{3!\Delta t}\partial_x^3\Phi - 9U^2(1-U)^2\frac{(\Delta x)^4}{4!\Delta t}\partial_x^4\Phi. \tag{15}$$

Stable : $CFL \leq 1$.
Temps de calcul : 3 itérations de $\mathscr{N}$

Back and forth error compensation and correction methods for semi-Lagrangian schemes with application to level set interface computations Dupont, Liu - JSTOR, 2007

Schéma $\mathscr{C}$ (combinaison)

Algorithme 1d a vitesse constante :

$$\Phi_C = \mathscr{C}[\Phi^n] = (c_A\Phi_A + c_B\Phi_B) \,, \tag{16}$$

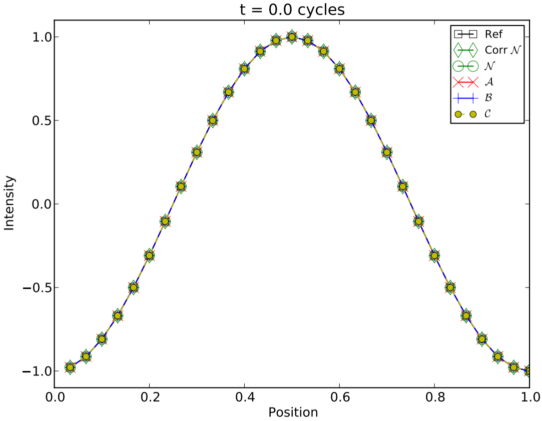
$$\text{with} \quad c_A = \frac{2U-1}{3U} = \frac{2}{3} - \frac{1}{3U} \quad \text{and} \quad c_B = \frac{1+U}{3U} = \frac{1}{3} + \frac{1}{3U} \,. \tag{17}$$

Erreur :

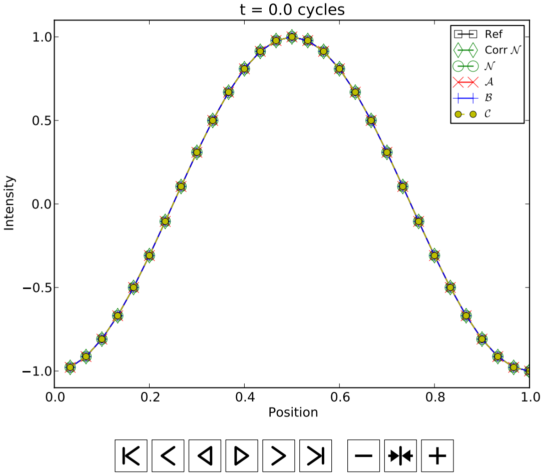
$$D_t\Phi_C = -(1+U)\,U(1-U)(2-U)\,\frac{(\Delta x)^4}{4!\Delta t}\,\partial_x^4\Phi \,. \tag{18}$$

Stable : $CFL \leq 1$.
Temps de calcul : 3 itérations de $\mathscr{N}$

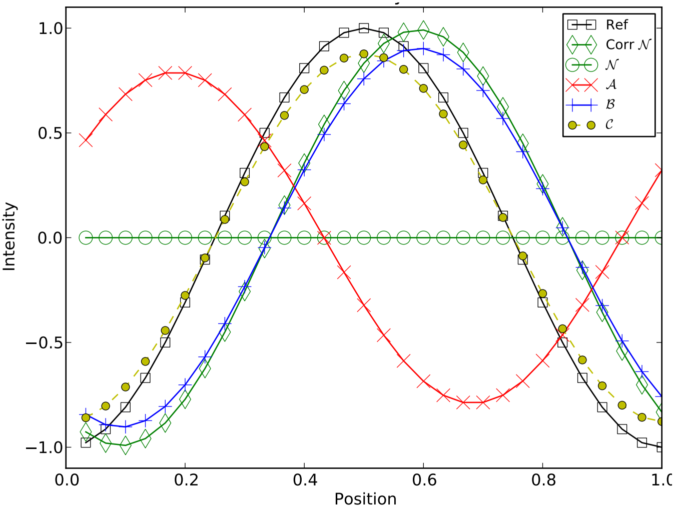
Transport 1d d'un profil harmonique (temps courts)



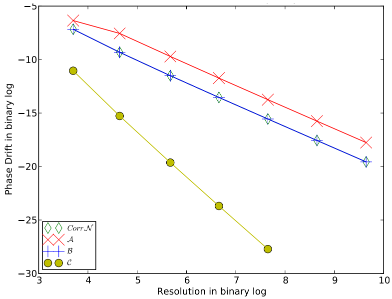
Transport 1d d’un profil harmonique (temps longs)



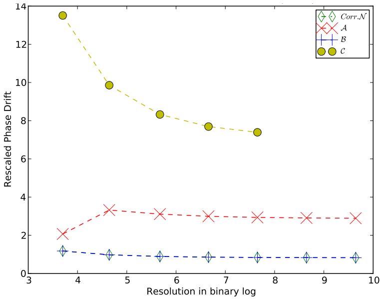
Transport 1d d'un profil harmonique



Dérive de phase

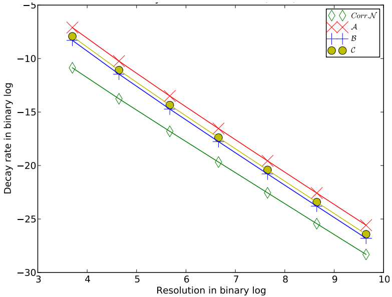


(a) Dérive de phase

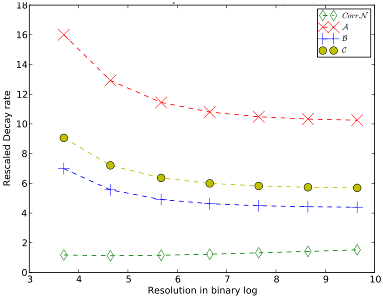


(b) Dérive de phase normalisée

Taux de décroissance



(c) Taux de décroissance



(d) Dérive de phase normalisée

Qu'est ce que la convection de R.-B.

Convection dite : “heated from below”

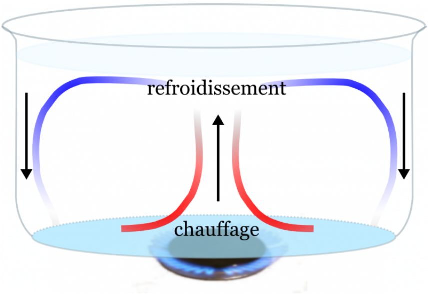


Schéma diffusif $\mathcal{N}$

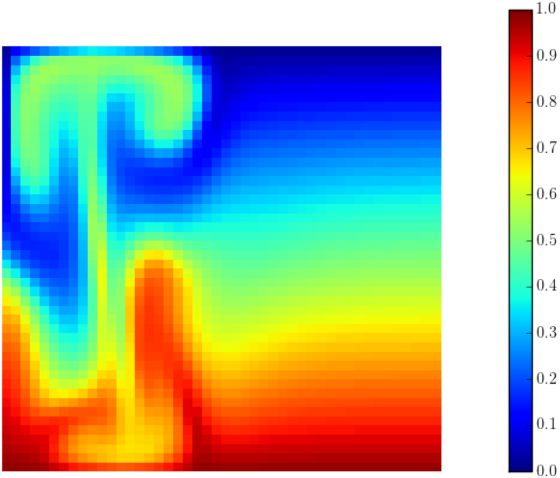


Schéma dispersif $\mathscr{A}$

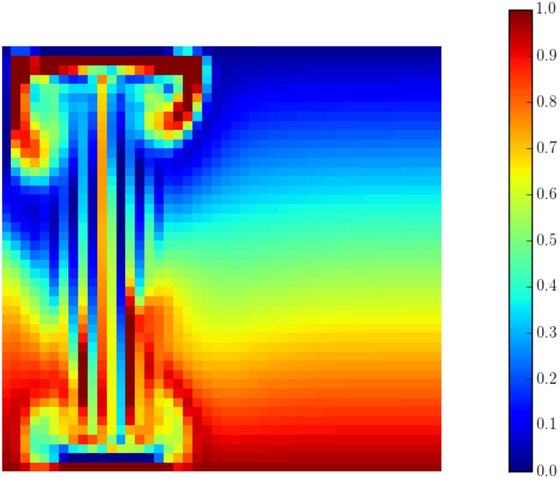


Schéma dispersif $\mathscr{B}$

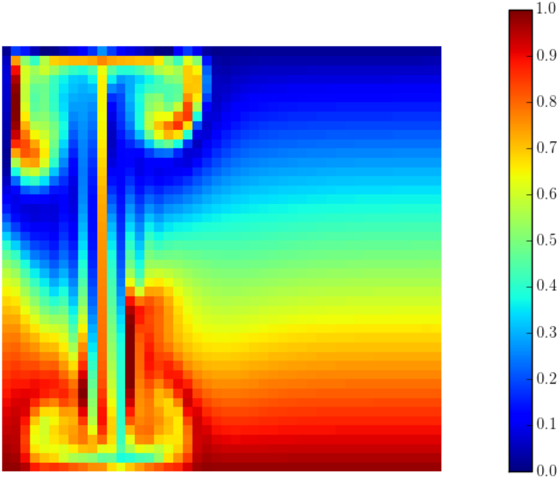
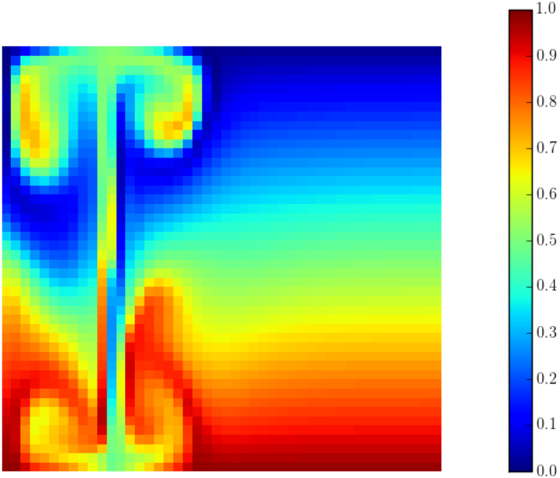
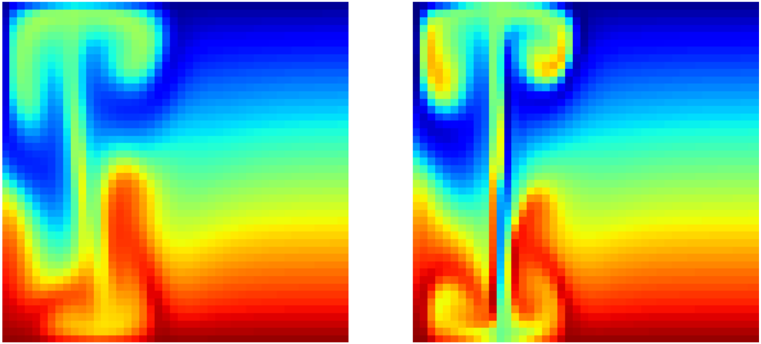


Schéma $\mathscr{C}$ (combinaison)



Comparaison des schémas $\mathscr{N}$ et $\mathscr{C}$



En bref

Schéma	Formule	Ordre de ∂_x	Erreur
$\mathscr{N}$	$L_+[\Phi]$	2	$U(1-U)\,\frac{(\Delta x)^2}{2!\Delta t}\,\partial_x^2\Phi$
$\mathscr{A}$	$L_+[\Phi]+\frac{1}{2}(\Phi-\bar{\Phi})$	3	$-U(1-(U)^2)\,\frac{(\Delta x)^3}{3!\Delta t}\,\partial_x^3\Phi$ $-3\,(U)^2\,(1-(U)^2)\,\frac{(\Delta x)^4}{4!\Delta t}\,\partial_x^4\Phi$
$\mathscr{B}$	$L_+\left[\Phi+\frac{1}{2}(\Phi-\bar{\Phi})\right]$	3	$U(1-U)(1-2U)\,\frac{(\Delta x)^3}{3!\Delta t}\,\partial_x^3\Phi$ $-9\,(U)^2\,(1-(U)^2)\,\frac{(\Delta x)^4}{4!\Delta t}\,\partial_x^4\Phi$
$\mathscr{C}$	$L_+\left[\Phi+\frac{1+U}{6U}(\Phi-\bar{\Phi})\right]+\frac{1-2U}{6U}(\Phi-\bar{\Phi})$	4	$-(1+U)\,U(1-U)(2-U)\,\frac{(\Delta x)^4}{4!\Delta t}\,\partial_x^4\Phi$

Table: 1D scheme comparative table

Variante pour l'équation de conservation

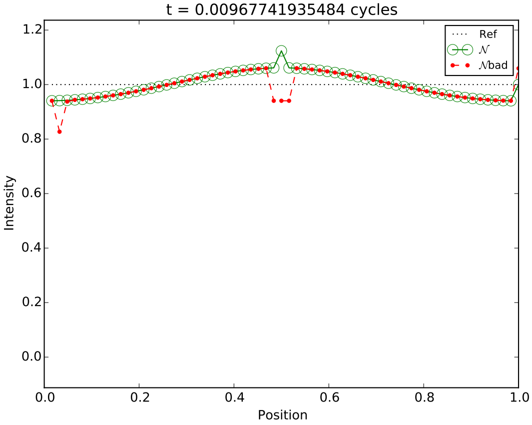
Modification simple (une transposition de matrice) utilisant le fait que l'équation de transport et de conservation sont adjointes
$\Rightarrow$ schéma conservatif ... mais non monotone

Cette méthode est bien adaptée aux équations de conservation-diffusion du type

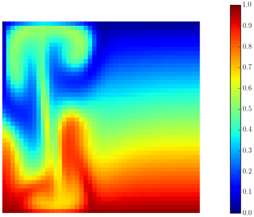
$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = D \Delta \rho \ . \tag{19}$$

Conservative Finite-Difference Methods on General Grids, M. Shashkov

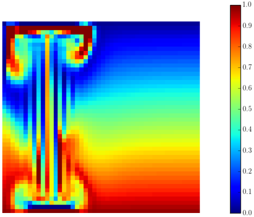
Test avec un profil de vitesse harmonique



Comparatif des algorithmes

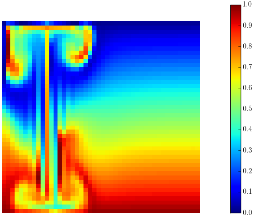


(e) N

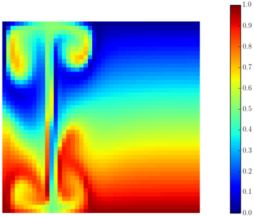


(f) A

Merci de votre attention

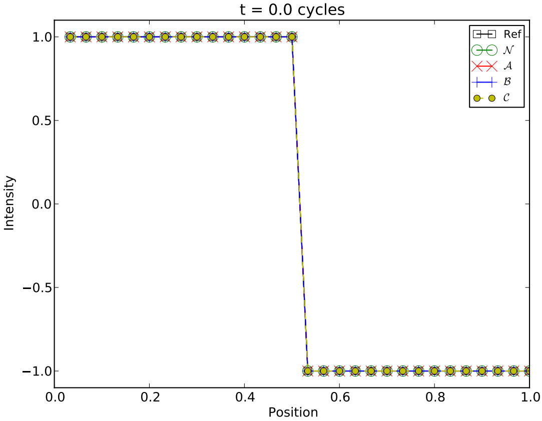


(g) B

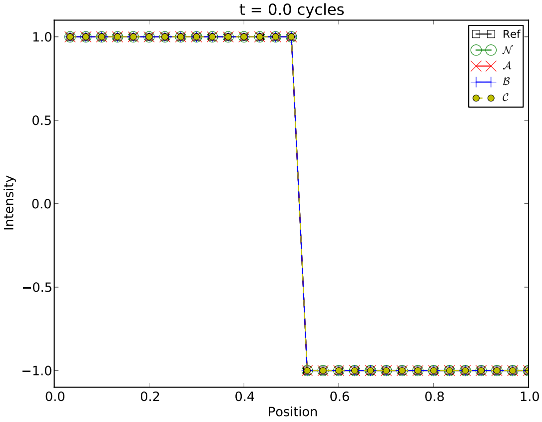


(h) C

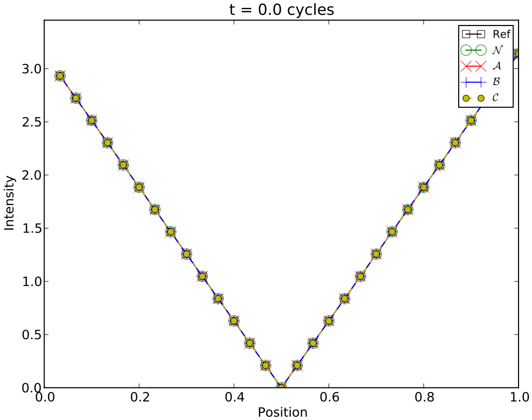
Heaviside 1d



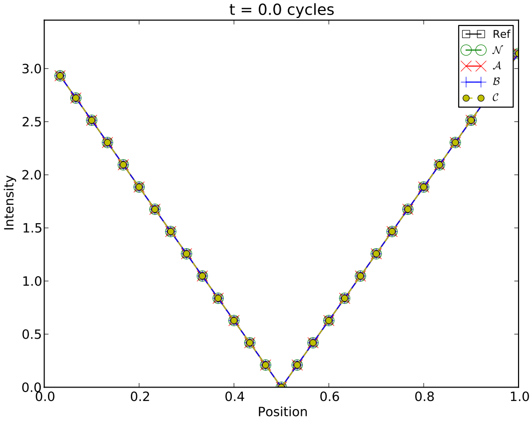
Heaviside 1d



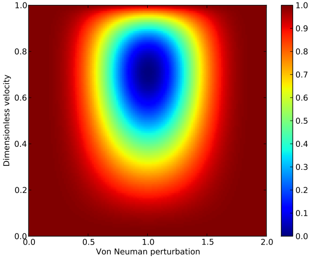
Triangles 1d



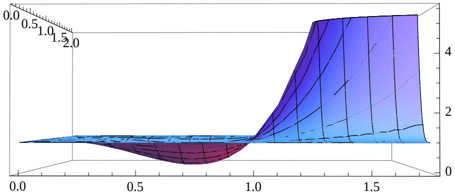
Triangles 1d



Stabilité $\mathscr{A}$ schéma



(i) Color-plot

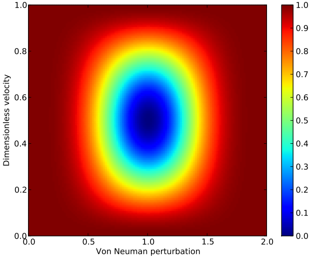


(j) 3D-plot

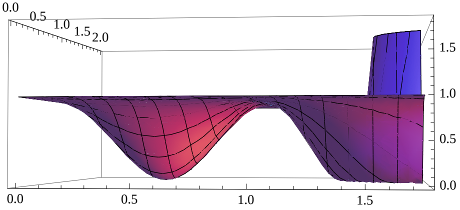
Facteur d'amplification de Von Neumann :

$$\xi_{\mathscr{A}}(\theta, U) = 1 - U^2 + U^2 \cos(\theta) - iU \sin(\theta)\,. \tag{20}$$

Stabilité $\mathscr{B}$ schéma



(k) Color-plot

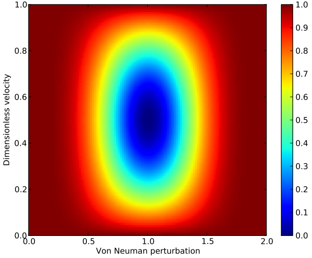


(l) 3D-plot

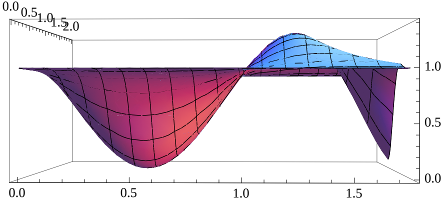
Facteur d'amplification de Von Neumann :

$$\xi_{\mathscr{B}}(\theta, U) = 1 - 2U\sin(\tfrac{1}{2}\theta)\Big[ie^{-i\frac{\theta}{2}}\Big(1 + U2[1-U]\sin^2(\tfrac{1}{2}\theta)\Big) + \sin(\tfrac{1}{2}\theta)\Big(U-1\Big)\Big]. \tag{21}$$

Stabilité $\mathscr{C}$ schéma



(m) Color-plot



(n) 3D-plot

Facteur d'amplification de Von Neumann :

$$\xi_{\mathscr{C}}(\theta, U) = 1 - \frac{2}{3}\sin\frac{\theta}{2}\left[U\left(3+2[1-U^2]\sin^2\frac{\theta}{2}\right)\sin\frac{\theta}{2} + \left(3+2U[1-U^2]\sin^2\frac{\theta}{2}\right)i\cos\frac{\theta}{2}\right]. \qquad (22)$$