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Frédérique Charles. Particle methods for transport equations: foundations and improved reconstruction methods. École thématique. Italy. 2022. <hal-04204747v2>

HAL Id: hal-04204747

<https://hal.science/hal-04204747v2>

Submitted on 2 May 2025

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Particle methods for transport equations : foundations and improved reconstruction methods

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Abstract. We present here two methods for improving the accuracy of the solution reconstruction in particle methods. First, we recall the mathematical theory of the transport equation, which is used in the following, and the principle of the smooth particle method. We then present the LTP method, where the shape functions of the particles are transformed according to a local expansion in order to follow the local variation of the flow. This method allows to obtain a strong convergence for the reconstructed solution without extensive overlapping of the particles. We then present a second method, the FBL method, which uses the backward Lagrangian representation of the solution and also the local expansions of the flow around the particles. The convergence analysis shows a theoretical gain of at least one order of convergence compared to the LTP method.

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Introduction

Transport equations are widely used to describe the motion and evolution of various physical quantities, such as mass, momentum and energy, in a wide range of scientific and engineering disciplines. For example, these equations are commonly found in fluid dynamics, plasma physics, and atmospheric sciences.

Particle methods are popular for solving these transport equations, especially for kinetic equations where the dimension of the phase space can be large. Indeed, they are quite easy to implement, even for high dimensions, and the computational cost is lower than that of Eulerian methods (such as finite differences, finite volumes...) and forward semi-Lagrangian schemes. The principle of particle methods is to advance numerical "particles", which are considered as markers of the flow, along approximated characteristic lines. An approximation to the solution of the transport equation is then constructed using these particles and a smooth shape function around the particles. Although conceptually simple, the standard smooth particle method suffers from a lack of strong convergence, which in practice leads to noisy numerical solutions. More precisely, the strong convergence of the method is obtained when the size h of the particle grid tends to zero under the condition that the size of the particle support tends to zero as h^q , with $q < 1$ [34]. In practice, this means that under this condition the number of particles whose supports overlap tends to infinity as h tends to zero, which makes the reconstruction of the approximate solution very costly.

Several strategies have been developed to reduce the oscillations caused by the lack of strong convergence without creating a large overlap of particle supports. One of them is to perform out regular projections on a grid in order to reinitialise the particles (known as remapping) [26]; with remapping at each time step, we obtain the forward semi-Lagrangian method [24, 18, 33]. These remappings have a regularising effect but also introduce numerical diffusion, although this is mitigated by the use of high-order interpolation kernels [22, 20] or adaptive remapping methods [2, 37] or other methods: weight averaging [1, 16], artificial viscosity [19] and the use of wavelets [3, 14].

We present here two quite different methods for reducing the numerical noise of the numerical solutions reconstructed using particles, based on local

asymptotic expansions of the flow.

The first section introduces the mathematical foundations of the theory of characteristics for linear transport equations. In particular, the notion of measure solution to these equations is crucial to the understanding of particle methods.

The second section presents the principle of the smooth particle method and convergence estimates. In particular, we see that strong convergence can be obtained under a restrictive condition between the size of the initial particle lattice and the width of the shape function support.

In the third section, we present the Linearly Transformed Particle (LTP) method, introduced by Campos-Pinto in [6]. The principle of this method is to deform the shape functions of the particles locally according to the linearisation of the flow around each particle. An LTP approximation is then introduced, where the shape functions of the smooth particle approximation are replaced by the deformed shape functions. We prove the strong convergence of this method for a passive advection equation, and briefly present some extensions of the method to nonlinear problems [8, 7].

The last section is dedicated to the presentation of the Forward-Backward Lagrangian method introduced in [9], which can be seen as hybrid between a particle method and a semi-Lagrangian method. Since the deformation of the shape functions in the LTP method could lead to a loss of locality in the reconstruction, we introduce a global approximation of the backward flow, using the local linearisations around the particles and a partition of unity. We study this method on an advective equation for a passive flow, and we prove a gain of one order of convergence in space compared to the LTP method.

Notations

The integrations are here with respect to the Lebesgue measure dx on the Lebesgue subsets of \mathbb{R}^d . We introduce the Sobolev space defined for any connected open set $\Omega \subset \mathbb{R}^d$ with a Lipschitz continuous boundary

$$W^{r,p}(\Omega) := \left\{ g : \Omega \rightarrow \mathbb{R}^m, g \in L^p(\Omega), D^\alpha g := \frac{\partial^{|\alpha|} g}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}} \in L^p(\Omega), |\alpha| \leq r \right\}$$

provided with the norm

$$\|g\|_{W^{r,p}(\Omega)} := \left(\sum_{|\alpha| \leq r} \int_{\Omega} \|D^\alpha g(x)\|_{\infty}^p \right)^{1/p}, \quad 1 \leq p < +\infty$$

$$\|g\|_{W^{r,\infty}(\Omega)} := \max_{|\alpha| \leq r} \sup_{x \in \Omega} \|D^\alpha g(x)\|_{\infty}, \quad p = +\infty.$$

We shall also employ the seminorms

$$|g|_{W^{r,p}(\Omega)} := \left(\sum_{|\alpha|=r} \int_{\Omega} \|D^{\alpha}g(x)\|_{\infty}^p \right)^{1/p}, \quad 1 \leq p < +\infty$$

$$|g|_{W^{r,\infty}(\Omega)} := \max_{|\alpha|=r} \sup_{x \in \Omega} \|D^{\alpha}g(x)\|_{\infty}, \quad p = +\infty.$$

Throughout these notes the symbol C refers to a generic constant $C > 0$.

1 Theory of characteristics

1.1 Transport equation

We consider a transport equation

$$\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) + a_0 \rho = 0 \quad (1.1)$$

where $\mathbf{a} = (a_1, \dots, a_d)$ is called the advection field. We assume throughout these notes that we have (at least)

$$a_i \in \mathcal{C}([0, T], W^{1,\infty}(\mathbb{R}^d) \cap \mathcal{C}^1(\mathbb{R}^d)) \text{ for } 1 \leq i \leq d, \quad \text{and } a_0 \in L_{\text{loc}}^{\infty}([0, T] \times \mathbb{R}^d). \quad (1.2)$$

If $a_0 = 0$, we get an equation known as the conservation equation

$$\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) = 0. \quad (1.3)$$

We will also consider the transport equation in a different form

$$\partial_t u + \mathbf{a} \cdot \nabla_x u = 0, \quad (1.4)$$

which we will call the advection equation by convenience. Note that equation (1.4) is a particular case of (1.1), when we take $a_0 = -\operatorname{div}_x(\mathbf{a})$.

Definition 1.1. A characteristic associated with the differential operator $\partial_t + \mathbf{a} \cdot \nabla_x = \frac{\partial}{\partial t} + \sum_{i=1}^d a_i \frac{\partial}{\partial x_i}$ is a function $X \in \mathcal{C}^1(I, \mathbb{R}^d)$ (where I is an interval of \mathbb{R}) satisfying

$$X'(s) = \mathbf{a}(s, X(s)) \quad \forall s \in I. \quad (1.5)$$

The Cauchy-Lipschitz theorem gives a sufficient condition on the advection field \mathbf{a} to obtain existence and uniqueness of equation (1.5) with an initial condition (see [38] for example).

Theorem 1.2. Assume (1.2). Then for all $t \in [0, T]$ and $x \in \mathbb{R}^d$, there exists an unique characteristic associated with $\partial_t + \mathbf{a} \cdot \nabla_x$ defined on $[0, T]$ and satisfying $X(t) = x$. We denote it by $X(s; t, x)$, and we have

$$X \in \mathcal{C}^1([0, T]_s \times [0, T]_t \times \mathbb{R}_x^d).$$

Moreover, $\partial_s \nabla_x X$ and $\nabla_x \partial_s X$ exist and are equal in $\mathcal{C}([0, T]_s \times [0, T]_t \times \mathbb{R}_x^d)$, where $\nabla_x X = (\partial_{x_i} X_j)_{1 \leq i \leq d, 1 \leq j \leq d}$.

Note that the existence and uniqueness of the characteristic can be obtained under weaker conditions on \mathbf{a} (see [38],[28]). However, here we are interested here in a situation where there is sufficient regularity.

We will use the following notations :

- ▷ $F^{t,s}(x) := X(s; t, x)$ is the flow map between t and s , starting from x ,
- ▷ $J^{t,s}(x) = \left(\partial_{x_j} F_i^{t,s}(x) \right)_{i,j} = (\nabla_x X(s; t, x))^\top$ is the jacobian matrix of the flow,
- ▷ $j^{t,s}(x) = \det(J^{t,s}(x))$ is the jacobian of the flow.

We now have the following properties on the flow.

Theorem 1.3. Under assumption (1.2), we have

- (i) For all t_1, t_2, t_3 in $[0, T]$, $F^{t_2, t_3} \circ F^{t_1, t_2} = F^{t_1, t_3}$.
- (ii) The flow map is a \mathcal{C}^1 diffeomorphism of \mathbb{R}^d , with inverse $(F^{t,s})^{-1} = F^{s,t}$.
- (iii) The jacobian matrix verifies

$$\partial_s J^{t,s}(x) = D\mathbf{a}(s, F^{t,s}(x)) J^{t,s}(x) \quad (1.6)$$

and its determinant verifies

$$\partial_s j^{t,s}(x) = \operatorname{div}_x(\mathbf{a})(s, F^{t,s}(x)) j^{t,s}(x). \quad (1.7)$$

- (iv) The flow verifies

$$\partial_t F^{t,s}(x) + (\mathbf{a}(t, x) \cdot \nabla_x) F^{t,s}(x) = 0. \quad (1.8)$$

Proof. Property (i) is a direct consequence of the definition of $F^{t,s}$ and the uniqueness in Theorem 1.2. We deduce (ii) by taking $t_1 = t_3 = t$ and $t_2 = s$ in (i). To prove property (iii), we denote \bar{M} the comatrice of a matrix M , and we recall that the differential of the determinant is given by $D_M \det(H) = \text{Tr}(\bar{M}^\top H)$. Then

$$\partial_s j^{t,s}(x) = \text{Tr} \left(\overline{J^{t,s}(x)}^\top \partial_s J^{t,s}(x) \right).$$

Moreover, since the flow verifies $\partial_s F^{t,s}(x) = \mathbf{a}(s, F^{t,s}(x))$, we have

$$\begin{aligned} \partial_s J^{t,s}(x) &= \partial_s \left(\partial_{x_j} F_i^{t,s}(x) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} = \left(\partial_{x_j} \partial_s F_i^{t,s}(x) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} \\ &= \left(\partial_{x_j} (a_i(s, F^{t,s}(x))) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} \\ &= \left(\sum_{k=1}^d \partial_{x_k} a_i(s, F^{t,s}(x)) \partial_{x_j} F_k^{t,s}(x) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} \\ &= \left(\partial_{x_j} a_i(s, F^{t,s}(x)) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} J^{t,s}(x). \end{aligned}$$

Then

$$\begin{aligned} \partial_s j^{t,s}(x) &= \text{Tr} \left(\overline{J^{t,s}(x)}^\top \left(\partial_{x_j} a_i(s, F^{t,s}(x)) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} J^{t,s}(x) \right) \\ &= \text{Tr} \left(\left(\partial_{x_j} a_i(s, F^{t,s}(x)) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} \overline{J^{t,s}(x)}^\top J^{t,s}(x) \right) \\ &= j^{t,s}(x) \text{Tr} \left(\left(\partial_{x_j} a_i(s, F^{t,s}(x)) \right)_{\substack{1 \leq i \leq d \\ 1 \leq j \leq d}} \right) \\ &= j^{t,s}(x) \text{div}_x(\mathbf{a})(s, F^{t,s}(x)). \end{aligned}$$

To prove (iv), we start from the relation

$$X(t_3; t_1, x) = X(t_3; t_2, X(t_2; t_1, x))$$

that we differentiate with respect to t_2 . Then for all i we get (here we denote ∂_1 and ∂_2 the derivative according to the first and second variable of X respectively)

$$0 = \partial_2 X_i(t_3; t_2, X(t_2; t_1, x)) + \sum_{k=1}^d \partial_{x_k} X_i(t_3; t_2, X(t_2; t_1, x)) \underbrace{\partial_1 X_k(t_2; t_1, x)}_{=a_k(t_2, X(t_2; t_1, x))}.$$

With the change of variable $y = X(t_2; t_1, x)$ we then get

$$0 = \partial_2 X_i(t_3; t_2, y) + \sum_{k=1}^d \partial_{x_k} X_i(t_3; t_2, y) a_k(t_2, y), \quad \text{for } 1 \leq i \leq d$$

that is

$$0 = \partial_2 X(t_3; t_2, y) + (\mathbf{a}(t_2, y) \cdot \nabla_x) X(t_3; t_2, y) \quad \text{for all } t_2, t_3 \in \mathbb{R}, y \in \mathbb{R}^d.$$

By taking $t_3 = s$ and $t_2 = t$ we obtain

$$0 = \partial_t X(s; t, y) + (\mathbf{a}(t, y) \cdot \nabla_x) X(s; t, y)$$

which correspond to (1.8). \square

Corollary 1.4. *The jacobian verifies*

$$j^{t,s}(x) > 0 \quad \text{for all } x \in \mathbb{R}^d, t \in \mathbb{R}, s \in \mathbb{R} \quad (1.9)$$

$$j^{t_2, t_3}(F^{t_1, t_2}(x)) j^{t_1, t_2}(x) = j^{t_1, t_3}(x) \quad \text{for all } t_1, t_2, t_3 \in [0, T]. \quad (1.10)$$

Proof. For a given $x \in \mathbb{R}^d$ and $s \in \mathbb{R}$, function $t \mapsto j^{t,s}(x)$ is a continuous functions such that $j^{t,s}(x) \neq 0$ (since the flow map is a \mathcal{C}^1 diffeomorphism of \mathbb{R}^d) and $j^{s,s}(x) = 1$. It leads to inequality (1.9). Relation (1.10) is obtained by differentiating relation (i) of Theorem 1.3 with respect to x . \square

Remark 1.5. Note that in particular (take $t_1 = t_3 = t$, $t_2 = s$) we have

$$[j^{t,s}(x)]^{-1} = j^{s,t}(F^{t,s}(x)).$$

1.2 Classical solutions

Theorem 1.6. *Assume (1.2).*

(i) *If $u^0 \in \mathcal{C}^1(\mathbb{R}^d)$, there exists an unique solution $u \in \mathcal{C}^1([0, T] \times \mathbb{R}^d)$ to*

$$\partial_t u + \mathbf{a} \cdot \nabla u = 0, \quad u(0, \cdot) = u^0 \quad (1.11)$$

given by

$$u(t, x) = u^0(F^{t,0}(x)). \quad (1.12)$$

(ii) *If $a_0, \operatorname{div}_x(\mathbf{a}) \in \mathcal{C}^0([0, T] \times \mathbb{R}^d)$, and $\rho^0 \in \mathcal{C}^1(\mathbb{R}^d)$, there exists an unique solution $\rho \in \mathcal{C}^1([0, T] \times \mathbb{R}^d)$ to*

$$\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) + a_0 \rho = 0, \quad \rho(0, \cdot) = \rho^0 \quad (1.13)$$

given by

$$\rho(t, x) = \rho^0(F^{t,0}(x)) j^{t,0}(x) \exp\left(-\int_0^t a_0(r, F^{t,r}(x)) dr\right). \quad (1.14)$$

Proof.

(i) If $u \in C^1([0, T] \times \mathbb{R}^d)$ verifies (1.11), we have for all $\tau \in \mathbb{R}$ and $y \in \mathbb{R}^d$

$$\begin{aligned} \frac{d}{ds} u(s, F^{\tau, s}(y)) &= \partial_t u(s, F^{\tau, s}(y)) + \partial_s F^{\tau, s}(y) \cdot \nabla_x u(s, F^{\tau, s}(y)) \\ &= 0 \end{aligned}$$

since $\partial_s F^{\tau, s}(y) = \mathbf{a}(s, F^{\tau, s}(y))$. Then u is constant along the characteristics : $u(s, F^{\tau, s}(y)) = u(0, F^{\tau, 0}(y))$. By setting $x = F^{\tau, s}(y)$, we obtain

$$u(s, x) = u(0, F^{\tau, 0}(F^{s, \tau}(x))) = u(0, F^{s, 0}(x)).$$

Conversely, let u defined by (1.12). Then

$$\begin{aligned} \partial_t u(t, x) + \mathbf{a}(t, x) \cdot \nabla_x u(t, x) &= (\partial_t + \mathbf{a}(t, x) \cdot \nabla_x) F^{t, 0}(x) \cdot \nabla_x u^0(F^{t, 0}(x)) \\ &= 0 \end{aligned}$$

thanks to (1.8).

(ii) Let $\rho \in C^1([0, T] \times \mathbb{R}^d)$ a solution of (1.13). Then for any $\tau \in \mathbb{R}$ and $y \in \mathbb{R}^d$

$$\begin{aligned} \frac{d}{ds} \rho(s, F^{\tau, s}(y)) &= \partial_t \rho(s, F^{\tau, s}(y)) + \nabla_x \rho(s, F^{\tau, s}(y)) \cdot \partial_s F^{\tau, s}(y) \\ &= -(\operatorname{div}_x(\mathbf{a}) + a_0)(s, F^{\tau, s}(y)) \rho(s, F^{\tau, s}(y)) \\ &= -\left(\frac{\partial_s j^{\tau, s}(y)}{j^{\tau, s}(y)} + a_0(s, F^{\tau, s}(y)) \right) \rho(s, F^{\tau, s}(y)), \end{aligned}$$

thanks to (1.7), and consequently

$$\frac{d}{ds} [\rho(s, F^{\tau, s}(y)) j^{\tau, s}(y)] = -a_0(s, F^{\tau, s}(y)) j^{\tau, s}(y) \rho(s, F^{\tau, s}(y)).$$

Then

$$\rho(s, F^{\tau, s}(y)) j^{\tau, s}(y) = \rho(0, F^{\tau, 0}(y)) j^{\tau, 0}(y) \exp\left(-\int_0^s a_0(r, F^{\tau, r}(y)) dr\right).$$

Moreover, relation (1.10) with $t_1 = \tau$, $t_3 = 0$, $t_2 = s$ gives

$$j^{s, 0}(F^{\tau, s}(y)) j^{\tau, s}(y) = j^{\tau, 0}(y). \quad (1.15)$$

Finally, by setting $x = F^{\tau, s}(y)$ we get

$$\begin{aligned} \rho(s, x) &= \rho(0, F^{\tau, 0}(F^{s, \tau}(x))) j^{s, 0}(F^{\tau, s}(F^{s, \tau}(x))) \exp\left(-\int_0^s a_0(r, F^{\tau, r}(F^{s, \tau}(x))) dr\right) \\ &= \rho(0, F^{s, 0}(x)) j^{s, 0}(x) \exp\left(-\int_0^s a_0(r, F^{s, r}(x)) dr\right). \end{aligned}$$

Conversely, let ρ defined by (1.14). Then if we introduce

$$g(t, x) := \rho(t, x)[j^{t,0}(x)]^{-1} \left(\int_0^t a_0(r, F^{t,r}(x)) dr \right) = \rho(0, F^{t,0}(x)),$$

then $g(0, x) = \rho(0, x)$, and g is constant along characteristics : for all $t, s \in \mathbb{R}$ and $x \in \mathbb{R}^d$,

$$g(s, F^{t,s}(x)) = \rho^0(F^{s,0}(F^{t,s}(x))) = \rho^0(F^{t,0}(x)) = g(t, x).$$

For $\tau \in \mathbb{R}$ we set $y = F^{0,\tau}(x)$ and $t = 0$, previous relation writes :

$$g(s, F^{\tau,s}(y)) = g(0, F^{\tau,0}(y)).$$

Then

$$\rho(s, F^{\tau,s}(y))[j^{s,0}(F^{\tau,s}(y))]^{-1} \left(\int_0^s a_0(r, F^{s,r}(F^{\tau,s}(y))) dr \right) = \rho(0, F^{\tau,0}(y))$$

that is, using (1.15)

$$\rho(s, F^{\tau,s}(y))j^{\tau,s}(y) = \rho(0, F^{\tau,0}(y))j^{\tau,0}(y) \left(- \int_0^s a_0(r, F^{\tau,r}(y)) dr \right).$$

Then

$$\frac{d}{ds} [\rho(s, F^{\tau,s}(y))j^{\tau,s}(y)] = -a_0(s, F^{\tau,s}(y))\rho(s, F^{\tau,s}(y))j^{\tau,s}(y)$$

and we can obtain that ρ is solution of equation (1.13). □

1.3 Weak solutions

We introduce L the differential operator defined, for $v \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}^d)$, by

$$Lv := \frac{\partial v}{\partial t} + \operatorname{div}_x(\mathbf{a}v) + a_0v,$$

and L^* its formal adjoint : $L^*v = -\frac{\partial v}{\partial t} - \mathbf{a} \cdot \nabla_x(v) + a_0v$. We denote

$$\langle v, \psi \rangle = \int_0^T \int_{\mathbb{R}^d} v(t, x)\psi(t, x) dx dt.$$

Note that for v and $\psi \in \mathcal{C}_c^1(]0, T[\times \mathbb{R}^d)$

$$\langle Lv, \psi \rangle = \langle v, L^*\psi \rangle \quad \text{for } v \text{ and } \psi \in \mathcal{C}_c^1(]0, T[\times \mathbb{R}^d).$$

Definition 1.7. We say that $\rho \in L^1((0, T) \times \mathbb{R}^d)$ is a weak solution of (C) with initial condition $\rho(0, \cdot) = \rho^0$ if

$$\langle \rho, L^* \psi \rangle = \int_{\mathbb{R}^d} \rho^0(x) \psi(0, x) dx \quad \forall \psi \in \mathcal{C}_c^1([0, T] \times \mathbb{R}^d).$$

Theorem 1.8 (Weak solutions). *Assume (1.2). If $\rho^0 \in L^1(\mathbb{R}^d)$, $a_0 \in \mathcal{C}((0, T); L^\infty(\mathbb{R}^d))$ then equation (1.1) with initial condition $\rho(0, \cdot) = \rho^0$ has a unique weak solution $\rho \in \mathcal{C}([0, T], L^1(\mathbb{R}^d))$ given by*

$$\rho(t, x) = \rho^0 \left(F^{t,0}(x) \right) j^{t,0}(x) \exp \left(- \int_0^t a_0(s, F^{t,s}(x)) ds \right). \quad (1.16)$$

Proof. Let ρ defined by (1.16). Then for all $\psi \in \mathcal{C}_c^1([0, T] \times \mathbb{R}^d)$

$$\begin{aligned} \langle \rho, L^* \psi \rangle &= \int_0^T \int_{\mathbb{R}^d} \rho^0 \left(F^{t,0}(x) \right) j^{t,0}(x) \exp \left(- \int_0^t a_0(s, F^{t,s}(x)) ds \right) (L^* \psi)(t, x) dx dt \\ &= \int_0^T \int_{\mathbb{R}^d} \rho^0(y) \exp \left(- \int_0^t a_0(s, F^{0,s}(y)) ds \right) (L^* \psi)(t, F^{0,t}(y)) dx dt \end{aligned}$$

with the change of variable $y = F^{t,0}(x)$. We note that

$$\begin{aligned} &\frac{d}{dt} \left[\exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) \psi(t, F^{0,t}(x)) \right] \\ &= [-a_0(t, F^{0,t}(x)) \psi(t, F^{0,t}(x)) + \frac{\partial \psi}{\partial t}(t, F^{0,t}(x)) + \underbrace{\nabla_x F^{0,t}(x)}_{\mathbf{a}(t, F^{0,t}(x))} \cdot \nabla_x \psi(t, F^{0,t}(x))] \\ &\quad \times \exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) \\ &= -(L^* \psi)(t, F^{0,t}(x)) \exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right). \end{aligned} \quad (1.17)$$

Then

$$\begin{aligned} \langle \rho, L^* \psi \rangle &= - \int_{\mathbb{R}^d} \int_0^T \frac{d}{dt} \left[\exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) \psi(t, F^{0,t}(x)) \right] dt dx \\ &= \int_{\mathbb{R}^d} \rho^0(x) \psi(0, x) dx. \end{aligned}$$

We conclude that ρ is a weak solution of equation (1.1). \square

Theorem 1.9 (Measures solutions). If $\rho^0 \in \mathcal{L}(\mathbb{R}^d)$, and under the same assumptions on \mathbf{a} and a_0 as in Theorem 1.8, then $\rho \in \mathcal{L}(\mathbb{R}^d)$ defined by

$$\langle \rho, \psi \rangle = \left\langle \rho^0, x \mapsto \int_0^T \psi(t, F^{0,t}(x)) \exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) dt \right\rangle$$

for all $\psi \in \mathcal{C}_c^1([0, T] \times \mathbb{R}^d)$, is a weak solution of equation (C) with initial condition $\rho(0, \cdot) = \rho^0$.

Proof. Let ρ defined by

$$\langle \rho, \psi \rangle = \left\langle \rho^0, x \mapsto \int_0^T \psi(t, F^{0,t}(x)) \exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) dt \right\rangle$$

for all $\psi \in \mathcal{C}_c([0, T] \times \mathbb{R}^d)$. Then

$$\langle \rho, L^* \psi \rangle = \left\langle \rho^0, x \mapsto \int_0^T (L^* \psi)(t, F^{0,t}(x)) \exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) dt \right\rangle$$

and using (1.17) we get

$$\begin{aligned} \langle \rho, L^* \psi \rangle &= - \left\langle \rho^0, x \mapsto \int_0^T \frac{d}{dt} \left[\exp \left(- \int_0^t a_0(s, F^{0,s}(x)) ds \right) \psi(t, F^{0,t}(x)) \right] dt \right\rangle \\ &= \left\langle \rho^0, \psi(0, \cdot) \right\rangle. \end{aligned}$$

□

Remark 1.10. If $\rho \in L^1((0, T) \times \mathbb{R}^d)$ is a weak solution of (C), then it is also a measure solution :

$$\begin{aligned} &\int_{\mathbb{R}^d} \int_0^T \rho(t, x) \psi(t, x) dt dx \\ &= \int_{\mathbb{R}^d} \int_0^T \rho^0(F^{t,0}(x)) j^{t,0}(x) \exp \left(- \int_0^t a_0(s, F^{t,s}(x)) ds \right) \psi(t, x) dt dx \\ &= \int_{\mathbb{R}^d} \int_0^T \rho^0(y) \exp \left(- \int_0^t a_0(s, \underbrace{F^{t,s}(F^{0,t}(y))}_{F^{0,s}(y)}}) ds \right) \psi(t, F^{0,t}(y)) dt dx \\ &= \left\langle \rho^0, y \mapsto \int_0^T \psi(t, F^{0,t}(x)) \exp \left(- \int_0^t a_0(s, F^{0,s}(y)) ds \right) dt \right\rangle \end{aligned}$$

with the change of variable $y = F^{t,0}(x)$ of jacobien $j^{t,0}(x)$.

Remark 1.11. For $a_0 = 0$, then the measure solution of (1.3) correspond to the push-forward of ρ^0 by the flow map: $\rho(t, x) = \left(F^{0,t} \# \rho^0\right)(t, x)$.

We deduce from Theorem 1.9 the following Corollary, on which is based the principle of particle methods.

Corollary 1.12. Let $\rho^0 = \sum_{k \in K} \omega_k^0 \delta(x - x_k^0)$, with $K \subset \mathbb{Z}^d$, and $(X_k(s))_{k \in K}$, be trajectories starting from $(x_k^0)_{k \in K}$:

$$\frac{dX_k}{ds} = \mathbf{a}(s, X_k(s)), \quad X_k(0) = x_k^0, \quad k \in K$$

Then $\rho(t, x) = \sum_{k \in K} \omega_k(t) \delta(x - X_k(t))$, with

$$\omega_k(t) = \omega_k^0 \exp\left(-\int_0^t a_0(s, X_k(s)) ds\right),$$

is a measure solution of $\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) + a_0 \rho = 0$. In particular, for $a_0 = 0$, $\rho(t, x) = \sum_{k \in K} \omega_k^0 \delta(x - X_k(t))$ is a measure solution of $\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) = 0$.

2 Smooth Particle method

2.1 Particle approximation of the solution

Here we describe here the method without any time discretisation. Starting from an approximation of the initial condition ρ^0 given by

$$\rho_{\text{part}}^0 = \sum_{k \in \mathbb{Z}^d} \omega_k^0 \delta(x - x_k^0), \quad (2.1)$$

we introduce the particle approximation of the solution of (1.1) at time t with initial condition ρ_{part}^0 given by Corollary 1.12 :

$$\rho_{\text{part}}(t, x) = \sum_{k \in \mathbb{Z}^d} \omega_k(t) \delta(x - X_k(t)) \quad (2.2)$$

where $X_k(t) = F^{0,t}(x_k^0)$, that is the solution of

$$X_k'(t) = \mathbf{a}(t, X_k(t)), \quad X_k(0) = x_k^0 \quad (2.3)$$

and ω_k the solution of

$$\omega_k'(t) = -a_0(t, X_k(t)) \omega_k(t), \quad \omega_k(0) = \omega_k^0. \quad (2.4)$$

From an heuristic point of view, it is equivalent to defining positions $(x_k^0)_{k \in \mathbb{Z}^d}$ and weights $(\omega_k^0)_{k \in \mathbb{Z}^d}$ of particles such that (2.1) is a "good" approximation of ρ^0 ; and then then pushing these particles forward along characteristic lines. If $a_0 \neq 0$, the weight of the particles are modified.

Approaching ρ^0 with the measure (2.1) corresponds to finding $(x_k^0)_{k \in \mathbb{Z}^d}$ and weights $(\omega_k^0)_{k \in \mathbb{Z}^d}$ such that

$$\int_{\mathbb{R}^d} \rho^0(x) \psi(x) dx \simeq \sum_{k \in \mathbb{Z}^d} \omega_k^0 \psi(x_k^0) \quad (2.5)$$

for all test functions $\psi \in \mathcal{C}_c^0(\mathbb{R}^d)$. This corresponds to the classical problem of numerical quadrature.

In the following, we will take the set positions $(x_k^0)_{k \in \mathbb{Z}^d}$ on a regular grid, i.e $x_k^0 = hk$ ($k \in \mathbb{Z}^d$) with $h > 0$, and take for ω_k^0 an approximation of $\int_{B_k} \rho^0(x) dx$, with $B_k := x_k + [-\frac{h}{2}, \frac{h}{2}]^d$. In practice, if ρ^0 is compactly supported, one can restrict the sum in (2.5) to a finite subset $K \in \mathbb{Z}^d$.

The following Theorem gives a weak convergence result of the measure approximation of the solution in the case that the chosen quadrature method to discretize $\int_{B_k} \rho^0(x) dx$ is a midpoint quadrature.

Theorem 2.1 (Raviard). *Let $\rho^0 \in \mathcal{C}(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$, $a_i \in \mathcal{C}(0, T; W^{1, \infty}(\mathbb{R}^d))$ for $1 \leq i \leq d$, $a_0 \in \mathcal{C}((0, T); L^\infty(\mathbb{R}^d))$ and $\rho \in L^1((0, T) \times \mathbb{R}^d)$ the weak solution of*

$$\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) + a_0 \rho = 0.$$

For $k \in \mathbb{Z}^d$, let $x_k^0 = hk$, $\omega_k^0 = h^d \rho^0(x_k)$,

$$\rho_{\text{part}, h}^0(x) = \sum_{k \in \mathbb{Z}^d} \omega_k^0 \delta(x - x_k^0),$$

and for any $k \in \mathbb{Z}^d$, let X_k and ω_k the solutions of

$$\begin{aligned} X_k'(t) &= \mathbf{a}(t, X_k(t)), & X_k(0) &= x_k^0 \\ \omega_k'(t) &= -a_0(t, X_k(t)) \omega_k(t), & \omega_k(0) &= \omega_k^0. \end{aligned}$$

Then $\rho_{\text{part}, h}$ defined by

$$\rho_{\text{part}, h}(t, x) = \sum_{k \in \mathbb{Z}^d} \omega_k(t) \delta(x - X_k(t))$$

verifies for any $t \in [0, T]$ and for all $\psi \in \mathcal{C}_c(\mathbb{R}^d)$

$$\lim_{h \rightarrow 0} \langle \rho(t, \cdot) - \rho_{\text{part}, h}(t, \cdot), \psi \rangle = 0.$$

Proof. Thanks to Theorem 1.8 and the change of variable $y = F^{t,0}(x)$, we can write

$$\int_{\mathbb{R}^d} \rho(t, x) \psi(x) dx = \int_{\mathbb{R}^d} \rho^0(y) \exp\left(-\int_0^t a_0(s, F^{0,s}(y)) ds\right) \psi(F^{0,t}(y)) dy$$

for all $\psi \in \mathcal{C}_c(\mathbb{R}^d)$. Moreover,

$$\langle \rho_{\text{part},h}(t, \cdot), \psi \rangle = \sum_k \omega_0^k \exp\left(-\int_0^t a_0(s, F^{0,s}(x_k^0)) ds\right) \psi(F^{0,t}(x_k^0)),$$

Then $\langle \rho(t, \cdot) - \rho_{\text{part},h}(t, \cdot), \psi \rangle$ can be written under the following form:

$$\langle \rho(t, \cdot) - \rho_{\text{part},h}(t, \cdot), \psi \rangle = \sum_k E_k(g(t, \cdot)),$$

with

$$E_k(g) = \int_{B_k} g dx - h^d g(x_k)$$

and

$$g(t, x) = \rho_0(x) \exp\left(-\int_0^t a_0(s, F^{0,s}(x)) ds\right) \psi(F^{0,t}(x)).$$

Let $f \in \mathcal{C}_c^\infty(\mathbb{R}^d)$, $k \in \mathbb{Z}^d$, and $\tilde{f}_k(\xi) = f(x_k + h\xi)$. We have

$$\int_{B_k} f(x) dx - h^d f(x_k) = h^d \int_{[-1/2, 1/2]^d} \tilde{f}_k(\xi) d\xi - h^d \tilde{f}_k(0)$$

and a Taylor expansion of \tilde{f}_k around 0 gives

$$\tilde{f}_k(\xi) = \tilde{f}_k(0) + D\tilde{f}_k(0)(\xi) + \frac{1}{2} \int_0^1 D^2 \tilde{f}_k(t\xi)(\xi)(\xi) dt.$$

Then

$$\left| \int_{[-1/2, 1/2]^d} \tilde{f}_k(\xi) - \tilde{f}_k(0) \right| \leq C |\tilde{f}_k|_{W^{2,p}(B(0,1/2))} \leq Ch^{2-d/p} |f|_{W^{2,p}(B_k)}$$

for any $p > 1$, and

$$E_k(f) \leq Ch^d h^{2-d/p} |f|_{W^{2,p}(B_k)} \leq Ch^{2+d/q} |f|_{W^{2,1}(B_k)}$$

with $q = \frac{p}{p-1}$. Finally we get

$$\sum_{k \in \mathbb{Z}^d} E_k(f) \leq Ch^{2+\frac{d}{q}} |f|_{W^{2,1}(\mathbb{R}^d)},$$

which proves that $\sum_{k \in \mathbb{Z}^d} E_k(f) \rightarrow_{h \rightarrow 0} 0$ for all $f \in \mathcal{C}_c^\infty(\mathbb{R}^d)$. Since $g(t, \cdot) \in \mathcal{C}_c(\mathbb{R}^d)$, a density argument allows to conclude. \square

2.2 Smooth particle approximation

The result 2.1 is unfortunately of little interest for the numerical approximation of functions. We would like to be able to obtain at least a continuous approximation of the solution of (1.1). To do this, we introduce, for $\varepsilon > 0$, an even cut-off function $\varphi_\varepsilon \in \mathcal{C}(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ such that $\varphi_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \delta$ and

$$\int_{\mathbb{R}^d} \varphi_\varepsilon(x) dx = 1.$$

In general, φ_ε is defined thanks to a function ϕ continuous and compactly supported, by setting $\varphi = \phi \otimes \cdots \otimes \phi$, and $\varphi_\varepsilon(x) = \frac{1}{\varepsilon^d} \varphi\left(\frac{x}{\varepsilon}\right)$. For example, one can take for ϕ a B-spline function (see [6]) : the B-splines can be defined recursively by

$$B^1(x) = \begin{cases} (1 - |x|) & \text{for } |x| \leq 1 \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad B^m(x) = \int_{x-1/2}^{x+1/2} B^{m-1}(y) dy.$$

Other functions such as truncated Gaussian [31] or Wendland functions [25, 29] are also used. We can now introduce a smooth particle approximation of ρ with

$$\rho_{h,\varepsilon}(t, x) = \rho_h \star \varphi_\varepsilon(t, x) = \sum_{k \in \mathbb{Z}^d} \omega_k(t) \varphi_\varepsilon(x - X_k(t)). \quad (2.6)$$

Since (2.6) could involve an infinite number of particles, one may wonder if it makes sense. The following lemma gives a sufficient condition.

Lemma 2.2. *We take $\varphi_\varepsilon(x) = \frac{1}{\varepsilon^d} \varphi\left(\frac{x}{\varepsilon}\right)$ with $\varphi \in \mathcal{C}_c(\mathbb{R}^d)$. Under assumptions of Theorem 1.2, then the smooth particle approximation $\rho_{h,\varepsilon}(t, \cdot)$ (2.6) is well defined for all $t \in [0, T]$ and is a continuous function.*

Proof. Let assume that $\text{Supp}(\varphi) \subset [-L, L]^d$, for $L > 0$. Let $x \in \mathbb{R}^d$ and $t \geq 0$ fixed, and $k \in \{j \in \mathbb{Z}^d, \|X_j(t) - x\|_\infty \leq L\varepsilon\}$. Then, since the flow map is a \mathcal{C}^1 diffeomorphism,

$$\|x_k^0 - F^{t,0}(x)\|_\infty = \|F^{t,0}(X_k(t)) - F^{t,0}(x)\|_\infty \leq |F^{t,0}|_{W^{1,\infty}(B(x,L\varepsilon))} L\varepsilon$$

which implies that $k \in B\left(\frac{F^{t,0}(x)}{h}, \frac{\varepsilon}{h} L |F^{t,0}|_{W^{1,\infty}(B(x,L\varepsilon))}\right)$. Then there exists only a finite number of indices $k \in \mathbb{Z}^d$ such that $X_k(t)$ belongs to the support of the function $y \mapsto \varphi_\varepsilon(x - y)$, and (2.6) makes sense. \square

Remark 2.3. In the general case, it is sufficient to have $\sum_{k \in \mathbb{Z}^d} |\omega_k(t)| < +\infty$ for (2.6) to be well defined.

In all that follows, we will assume that $\varphi_\varepsilon(x) = \frac{1}{\varepsilon^d} \varphi\left(\frac{x}{\varepsilon}\right)$ where φ is at least continuous and compactly supported. For a given $h > 0$, the value of $\varepsilon > 0$ must be chosen so that $\|\rho_{h,\varepsilon}(t, \cdot) - \rho(t, \cdot)\|$ (for a given norm) is optimised. Intuitively, we're faced with the following dilemma: on the one hand, if the radius of the shape functions is too small compared to the minimum distance between the particles, the reconstructed $\rho_{h,\varepsilon}$ cancels out between the particles and then exhibits oscillations. On the other hand, if the radius is too large, the reconstructed solution is too spread out and lacks precision. Even if the particles are initially equidistant, they then become inhomogeneously distributed.

We now want to estimate the error between the solution of (1.1) and the smooth particle approximation. The following classical Lemma (see [34] for example) gives an estimate of the convolution error:

Lemma 2.4. *Assume that there exists an integer $r \geq 1$ such that for all $\alpha \in \mathbb{N}^d$, $1 \leq |\alpha| := \alpha_1 + \dots + \alpha_d \leq r - 1$,*

$$\begin{aligned} (i) \quad & \int_{\mathbb{R}^d} \varphi(x) dx = 1 \\ (ii) \quad & \int_{\mathbb{R}^d} x_1^{\alpha_1} \dots x_d^{\alpha_d} \varphi(x_1, \dots, x_d) dx = 0, \\ (iii) \quad & \int_{\mathbb{R}^d} \|x\|^r |\varphi(x)| dx < +\infty \end{aligned} \tag{2.7}$$

Then there exists $C > 0$ such that for all $f \in W^{r,p}(\mathbb{R}^d)$, $1 \leq p \leq +\infty$,

$$\|f \star \varphi_\varepsilon - f\|_{L^p(\mathbb{R}^d)} \leq C \varepsilon^r |f|_{W^{r,p}(\mathbb{R}^d)}. \tag{2.8}$$

Now, by splitting the error between the convolution error and the quadrature error for $x \rightarrow \rho(t, x) \varphi_\varepsilon(x)$, we get (see [34] for the detailed proof):

Theorem 2.5. *Assume there exist $r, m \in \mathbb{N}$, $m > d$, such that $\varphi \in W^{m,1}(\mathbb{R}^d) \cap W^{m,\infty}(\mathbb{R}^d)$ and conditions (2.7) are satisfied. We denote $l = \max(r, m)$ and we further assume moreover that*

- ▷ $a_1, \dots, a_d, a_0 + \operatorname{div}_x(\mathbf{a}) \in L^\infty(0, T; W^{l,\infty}(\mathbb{R}^d))$
- ▷ $\rho^0 \in W^{l,p}(\mathbb{R}^d)$

then the following error estimate holds, for $1 \leq p \leq \infty$:

$$\sup_{t \in [0, T]} \|\rho_{h,\varepsilon}(t, \cdot) - \rho(t, \cdot)\|_{L^p(\mathbb{R}^d)} \leq C_T \left(\varepsilon^r |\rho^0|_{W^{r,p}(\mathbb{R}^d)} + \left(\frac{h}{\varepsilon}\right)^m |\rho^0|_{W^{m,p}(\mathbb{R}^d)} \right). \tag{2.9}$$

The estimate (2.9) has been improved in [17] for a certain choice of the weights ω_k (we then get $\|\rho^0\|_{L^p(\mathbb{R}^d)}$ instead of $|\rho^0|_{W^{m,p}(\mathbb{R}^d)}$ in (2.9), which allows to weaken the assumptions on ρ^0). However, these estimates lead to a strong convergence of the approximate solution only for $\varepsilon \sim h^s$, with $0 < s < 1$ when ε and h tend to 0 (the optimal choice is $s = \frac{m}{m+r}$). Numerically, this means an increasing overlap of particle supports and a number of particles (of the order of $\frac{1}{h^d}$) that increases non-linearly as we decrease ε . With $\varepsilon = h$, one has only a weak convergence of the approximate solution, which may show unwanted oscillations. Figure 1 shows the appearance of oscillations in the reconstructed solution when $\varepsilon = h$. Figure 2 shows the evolution of the L^∞ error between the SP approximation and the exact solution as a function of time, for different values of h and for $\varepsilon = h^s$, with $s \in \{0.5, 0.75, 1\}$. We can see that for a given h , the error is initially smaller when $s = 1$, but quickly becomes larger than for other values of $s < 1$. Furthermore, the error increases drastically after a certain time, regardless of the value of $s \leq 1$.

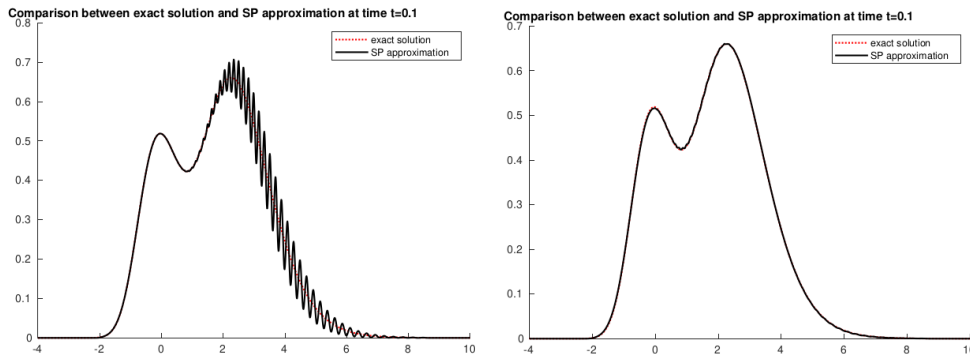


Figure 1: Comparison between the exact solution of the one-dimensional equation (1.1), with $a(t, x) = x^2$ and $\rho^0(x) = e^{-(x-2)^2} + 0.5e^{-x^2}$, and the Smooth Particle approximation, with $h = 0.1$ and φ a B3-spline. On the left picture $\varepsilon = h$, and on the right picture $\varepsilon = h^{0.75}$.

3 Lineary Transformed Particle method

In this section we present a density reconstruction method for noise reduction. This method, introduced by Campos-Pinto in [6], is based on a local deformation of the shape functions φ_ε . The idea of deforming the shapes of particles was introduced by Hou in [30], but without any explicitation. In [17],

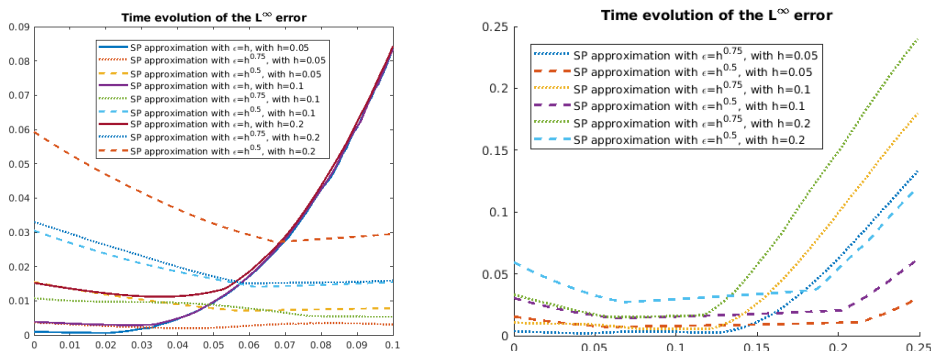


Figure 2: Time evolution of the L^∞ error between the exact solution of the one-dimensional equation (1.1) (with $a(t, x) = x^2$ and $\rho^0(x) = e^{-(x-2)^2} + 0.5e^{-x^2}$) and the Smooth Particle approximation, for $h \in \{0.01, 0.1, 0.2\}$ and $\varepsilon \in \{h, h^{0.75}, h^{0.5}\}$, between 0 and $T = 0.1$ (left), and between 0 and $T = 0.25$ (right). Here φ is a B3-spline.

Cohen and Perthame take up this idea by introducing "deformed cells" by the flow and obtain, for $\varepsilon = h$, a strong convergence in L^1 norm of their method for a passive flow to order 1 in h . Campos-Pinto then specified these deformations in [6] by introducing local developments to order r around each particle, and in particular developed the LTP (Linearly Transformed Particle) method that we present here. We assume here that the advection flow \mathbf{a} and the function a_0 are given and smooth enough (hypothesis (1.2)), so that the characteristics are well defined and smooth.

3.1 The LTP method

We first define an approximation of the initial condition, similar to the Smooth Particle approximation with $\varepsilon = h$. The Smooth Particle approximation of the initial conditions of the equations (1.1) and (1.4) respectively writes

$$\rho_h^0(x) = \sum_{k \in \mathbb{Z}^d} \omega_k^0 \varphi_{h,k}^0(x), \quad \text{and} \quad u_h^0(x) = \sum_{k \in \mathbb{Z}^d} \omega_k^0 \varphi_{h,k}^0(x), \quad (3.1)$$

with $x_k^0 = hk$, $k \in \mathbb{Z}^d$, and

$$\varphi_{h,k}^0(x) = \frac{1}{h^d} \varphi\left(\frac{x - x_k^0}{h}\right). \quad (3.2)$$

In the following we assume that

$$\varphi \in \mathcal{C}_c(\mathbb{R}^d) \cap W^{1,\infty}(\mathbb{R}^d) \quad \text{and} \quad \int_{\mathbb{R}^d} \varphi(x) dx = 1. \quad (3.3)$$

We then introduce a time discretisation $(t^n)_{0 \leq n \leq N}$ of $[0, T]$, and we assume that the time numerical schemes for discretising ODE (2.3) (the "particle pusher") and (2.4) are given for all $k \in \mathbb{Z}^d$. We denote $(x_k^n)_{k \in \mathbb{Z}^d, 0 \leq n \leq N}$ and $(\omega_k^n)_{k \in \mathbb{Z}^d, 0 \leq n \leq N}$ the approximations with the chosen time scheme, that is respectively the positions and weights of the particles at time t^n .

The idea of the method is to transform the shape $\varphi_{h,k}^0$ with a linearised flow around each particle. For each $k \in \mathbb{Z}^d$, we introduce \mathcal{J}_k^n an (invertible) approximation of the Jacobian $J^{0,t^n}(x_k^0)$, and we denote $D_k^n = (\mathcal{J}_k^n)^{-1}$ the deformation matrix around the k -th particle. We define an approximation of the local expansion at order 1 of the forward flow around x_k^0 by

$$\mathcal{F}_{h,k,1}^n : x \mapsto x_k^n + \mathcal{J}_k^n(x - x_k^0) \quad (3.4)$$

and an approximation of the local expansion of order 1 of the backward flow around x_k^n by :

$$\mathcal{B}_{h,k,1}^n = (\mathcal{F}_{h,k,1}^n)^{-1} : x \mapsto x_k^0 + D_k^n(x - x_k^n). \quad (3.5)$$

LTP approximation of the advection equation (1.4) Thanks to the theorem 1.6, the solution at time t^n of the equation (1.4) with initial condition $\varphi_{h,k}^0$ is $\varphi_{h,k}^0(F^{t^n,0}(x))$, which we approximate by $\varphi_{h,k}^0(\mathcal{B}_{h,k,1}^n)$.

By linearity, we then define the LTP approximation of the solution of the equation with initial condition u^0 (approached by (3.1)) by

$$u_{h,\text{LTP}}^n(x) = \sum_k \omega_k^0 \varphi_{h,k}^n(x), \quad (3.6)$$

with

$$\varphi_{h,k}^n(x) := \varphi_{h,k}^0(\mathcal{B}_{h,k,1}^n(x)) = \varphi_h(D_k^n(x - x_k^n)). \quad (3.7)$$

LTP approximation of the transport equation (1.1) In this case, the classical solution at time t of the transport equation (1.1) is given by

$$\rho_h(t, x) = \rho^0(F^{t,0}(x)) \det(J^{t,0}(x)) \exp\left(-\int_0^t a_0(r, F^{t,r}(x)) dr\right).$$

We then introduce the LTP approximation of the solution of the equation (1.1) with initial condition ρ^0 (approached by (3.1)) by

$$\rho_{h,\text{LTP}}^n(x) = \sum_k \omega_k^n \varphi_{h,k}^n(x), \quad (3.8)$$

with

$$\varphi_{h,k}^n(x) := \det((\mathcal{J}_k^n)^{-1}) \varphi_{h,k}^0(\mathcal{B}_{h,k,1}^n(x)) = \det(D_k^n) \varphi_h(D_k^n(x - x_k^n)). \quad (3.9)$$

We recall that the weight ω_k^n is computed thanks to the discretisation of the ODE (2.4), and is therefore an approximation of

$$\omega_k(t^n) = \exp\left(-\int_0^{t^n} a_0(r, F^{t^n,r}(x_k^0)) dr\right) \omega_k^0.$$

Remark 3.1. If $a_0 = 0$, then the LTP approximation of the conservative equation $\partial_t \rho + \operatorname{div}_x(\mathbf{a}\rho) = 0$ writes

$$\rho_{h,\text{LTP}}^n(x) = \sum_k \omega_k^0 \varphi_{h,k}^n(x) = \sum_k \omega_k^0 \det(D_k^n) \varphi_h(D_k^n(x - x_k^n)).$$

and the method is of course mass-preserving :

$$\int_{\mathbb{R}^d} \rho_{h,\text{LTP}}^n(x) dx = \int_{\mathbb{R}^d} \rho_h^0(x) dx.$$

Remark 3.2. The advection equation (1.4) can also be written as a transport equation (1.1), with $a_0 = -\operatorname{div}_x(\mathbf{a})$. From the point of view of the transport equation, the LTP approximation is given by

$$\rho_{h,\text{LTP}}^n(x) = \sum_k \omega_k^n \det(D_k^n) \varphi_h(D_k^n(x - x_k^n)).$$

Here ω_k^n is an approximation of $\omega_k(t^n)$, where $\omega_k(0) = \omega_k^0$ and

$$\omega_k'(t) = -a_0(t, F^{0,t}(x_k^0)) \omega_k(t) = \operatorname{div}_x(\mathbf{a})(t, F^{0,t}(x_k^0)) \omega_k(t),$$

and $\det(D_k^n)$ is an approximation of the determinant of the Jacobian of the backward flow $j^{t^n;0}(x_k^n)$, which, thanks to (1.10), is equal to $(j^{0,t^n}(x_k^0))^{-1}$. Furthermore, thanks to (1.7), $j^{0,t^n}(x_k^0)$ is the solution at time t^n and for $x = x_k^0$ of

$$\partial_t j^{0,t}(x) = \operatorname{div}_x(\mathbf{a})(t, F^{0,t}(x)) j^{0,t}(x).$$

with $j^{0,0}(x) = 1$. Then $\omega_k^n \det(D_k^n)$ is an approximation of $\omega_j(t) (j^{0,t}(x_k^0))^{-1} = \omega_k^0$, which shows that this point of view is consistent with the LTP approximation of the advection equation (3.6).

Remark 3.3. In practice, the approximated matrix \mathcal{J}_k^n can be computed by finite difference over the positions of the particles :

$$\mathcal{J}_k^n = \left(\frac{(x_{k+e_j}^n - x_{k-e_j}^n)_i}{2h} \right)_{1 \leq i, j \leq d}, \quad D_k^n = (\mathcal{J}_k^n)^{-1} \quad (3.10)$$

(see [6] for more details), or by computing a stepwise approximation of $J^{t^{n-1}, t^n}(x_k^{n-1})$, for example using (1.6) (see [7]).

Remark 3.4. One could think to introduce $\mathcal{B}_{h,k,2}^n$, the second order local expansion around x_k^0 , which takes the form

$$(\mathcal{B}_{h,k,2}^n(x))_i = (x_k^0)_i + (D_k^n(x - x_k^n))_i + (x - x_k^n)^t Q_{k,i}^n(x - x_k^n), \quad (3.11)$$

for $1 \leq i \leq d$, where $Q_{k,i}$ is an approximation of the Hessian matrix of the i th component of the backward flow starting from x_k^n . However, if we define $\varphi_{h,k,2}^n(x) = \varphi_h(\mathcal{B}_{h,k,2}^n(x) - x_k^0)$, we can have $\varphi_{h,k,2}^n(x) \neq 0$ while x is far away from x_k^n (since the quadratic mapping $x \mapsto D_k^n(x - x_k^n) + ((x - x_k^n)^t Q_{k,i}^n(x - x_k^n))_{1 \leq i \leq d}$ is not invertible), which in practice leads to strong oscillations, because the expansion only takes place in the vicinity of the particle. However, it is possible to restrict the particle supports to the regions where this flow is locally invertible (see [6]).

3.2 Error estimate for a passiv flow

We present here the error analysis of the method for a passive advection equation, i.e. the equation (1.4) with given advection field \mathbf{a} and a_0 . The extension for some nonlinear equations is presented in section 3.4. Moreover, we focus here on the error induced by the LTP approximation and we do not consider the error due to the time discretisation of the particles trajectories. We therefore assume that $x_k^n = F^{0, t^n}(x_k^0)$ for all $k \in \mathbb{Z}^d$ and $n \in \{0, \dots, N\}$.

Initialization error First we estimate the error between u^0 and u_h^0 . Let us introduce

$$A_{h,p} : g \mapsto \sum_{k \in \mathbb{Z}^d} \omega_k^0(g) \varphi_{h,k}(x), \quad \text{with } \omega_k^0(g) = h^d \sum_{\|l\|_\infty \leq m_p} a_l g(x_{k+l}^0). \quad (3.12)$$

where the coefficients a_l are chosen so as to be exact on polynomials of degree less than or equal to $p \in \mathbb{N}$, i.e.

$$A_{h,p}(\Pi) = \Pi \quad \forall \Pi \in \mathcal{P}_p(\mathbb{R}^d). \quad (3.13)$$

We refer to [8] for examples of such operators. For example, for $p = 1$ and a shape function such that $\varphi(0) = 1$ one can take $m_1 = 0$, $a_0 = 1$.

Proposition 3.5. *Suppose that $A_{h,p}$ satisfies (3.13), with $\varphi \in \mathcal{C}_c(\mathbb{R}^d)$. Then for any integer $q \leq p+1$, there exists $C = C(p, q)$ such that for all $g \in W^{q, \infty}(\mathbb{R}^d)$*

$$\|A_{h,p}g - g\|_{L^\infty(\mathbb{R}^d)} \leq Ch^q |g|_{W^{q, \infty}(\mathbb{R}^d)}. \quad (3.14)$$

Proof. First, we show that $A_{h,p}$ is uniformly bounded in L^∞ . Since $\varphi \in \mathcal{C}_c(\mathbb{R}^d)$, if we introduce L so that $\text{Supp}(\varphi) \in [-L, L]$, we have $\#\{j \in \mathbb{Z}^d, x_j \in \text{Supp}(\varphi_{h,k})\} \leq 2L$, and then

$$\begin{aligned} \|A_{h,p}g\|_{L^\infty} &\leq 2L \sup_{k \in \mathbb{Z}^d} |\omega_k(g)| \|\varphi\|_{L^\infty(\mathbb{R}^d)} \\ &\leq 2L \sup_{\|l\|_\infty \leq m_p} |a_l| \|\varphi\|_{L^\infty(\mathbb{R}^d)} \|g\|_{L^\infty(\mathbb{R}^d)} \end{aligned}$$

Then, for $k \in \mathbb{Z}^d$ and Π the $(q-1)$ -th Taylor expansion of g around x_k^0 , we have $A_{h,p}\Pi = \Pi$ and

$$\begin{aligned} \|A_{h,p}g - g\|_{L^\infty(B_\infty(x_k^0, h))} &\leq \|A_{h,p}(g - \Pi)\|_{L^\infty(B_\infty(x_k^0, h))} + \|\Pi - g\|_{L^\infty(B_\infty(x_k^0, h))} \\ &\leq (\|A_{h,p}\|_\infty + 1) \|\Pi - g\|_{L^\infty(B_\infty(x_k^0, h))} \\ &\leq Ch^q |g|_{W^{q, \infty}(B_\infty(x_k^0, h))} \end{aligned}$$

where C depends on $\|A_{h,p}\|_\infty$, q , d , but not k . We then get (3.14). \square

Estimate on the deformation matrix

Lemma 3.6. *Let $F^{s,t}$ be a flow map such that $t \mapsto F^{0,t} \in L^\infty([0, T], W^{2, \infty}(\mathbb{R}^d))$ and such that the Jacobian of the flow is bounded by below : there exists $\alpha > 0$ such that*

$$\alpha \leq \det(J^{s,t}(x)) \quad \forall (s, t) \in [0, T] \times [0, T], x \in \mathbb{R}^d. \quad (3.15)$$

Let \mathcal{J}_k^n be calculated by

$$\mathcal{J}_k^n = \left(\frac{(F^{0,tn}(x_{k+e_j}^0) - F^{0,tn}(x_{k-e_j}^0))_i}{2h} \right)_{1 \leq i, j \leq d}$$

and $D_k^n = (\mathcal{J}_k^n)^{-1}$. Then there exist $h^* > 0$ and C (depending on $\sup_{t \in [0, T]} \|F^{0,t}\|_{W^{2, \infty}(\mathbb{R}^d)}$) and α) such that for all $0 < h < h^*$:

$$\sup_{0 \leq n \leq N} \sup_{k \in \mathbb{Z}^d} \|D_k^n\| \leq C. \quad (3.16)$$

Proof. A Taylor expansion of F^{0,t^n} around x_k^0 gives

$$\left\| \mathcal{J}_k^n - J^{0,t^n}(x_k^0) \right\| \leq \frac{1}{2} \|F^{0,t^n}\|_{W^{2,\infty}(\mathbb{R}^d)} h \quad (3.17)$$

and also $\|\mathcal{J}_k^n\| \leq \|F^{0,t^n}\|_{W^{1,\infty}(\mathbb{R}^d)}$. We then use the following property of linear algebra (see Lemma A.2 in [9]): there exists $C > 0$ (depending on d and the chosen norm for $\|\cdot\|$ on $\mathcal{M}_d(\mathbb{C})$) such that for $A, B \in \mathcal{M}_d(\mathbb{C})$,

$$|\det(A) - \det(B)| \leq C(\|A\| + \|B\|)\|A - B\|. \quad (3.18)$$

Then

$$\begin{aligned} |\det(\mathcal{J}_k^n) - \det(J^{0,t^n}(x_k^0))| &\leq C(\|\mathcal{J}_k^n\| + \|J^{0,t^n}(x_k^0)\|)\|\mathcal{J}_k^n - J^{0,t^n}(x_k^0)\| \\ &\leq Ch. \end{aligned}$$

where C depends on $\sup_{t \in [0, T]} \|F^{0,t}\|_{W^{2,\infty}(\mathbb{R}^d)}$. Thanks to the hypothesis (3.15), we deduce that there exists $h^* > 0$ (also depending on $\sup_{t \in [0, T]} \|F^{0,t}\|_{W^{2,\infty}(\mathbb{R}^d)}$) such that for all $0 < h < h^*$, for all $k \in \mathbb{Z}^d$ and $0 \leq n \leq N$, $\det(\mathcal{J}_k^n) \geq \alpha/2$. Furthermore, the coefficients of $\bar{\mathcal{J}}_k^n$, the comatrix of \mathcal{J}_k^n , can be bounded by those of \mathcal{J}_k^n . Then

$$\|D_k^n\|_\infty = \frac{1}{|\det(\mathcal{J}_k^n)|} \left\| \bar{\mathcal{J}}_k^n \right\|_\infty \leq C,$$

where C depends on α and $\sup_{t \in [0, T]} \|F^{0,t}\|_{W^{2,\infty}(\mathbb{R}^d)}$, but not on k and n . \square

Estimates on the flows We analyse here two quantities :

▷ the error on the Forward flow

$$e_F^n = \sup_k \|F^{0,t^n} - \mathcal{F}_{h,k,1}^n\|_{L^\infty(S_{h,k}^0)}, \quad \text{with } S_{h,k}^0 = \text{Supp}(\varphi_{h,k}^0),$$

▷ and the error on the Backward flow

$$e_B^n = \sup_k \|F^{t^n,0} - \mathcal{B}_{h,k,1}^n\|_{L^\infty(\Sigma_{h,k}^n)}, \quad \text{where } \Sigma_{h,k}^n = F^{0,t^n}(S_{h,k}^0) \cap \mathcal{F}_{h,k,1}^n(S_{h,k}^0).$$

Lemma 3.7. *Let $\mathbf{a} = (a_i)_{1 \leq i \leq d}$ an advection field with $a_i \in \mathcal{C}([0, T]; \mathcal{C}^1(\mathbb{R}^d) \cap W^{1,\infty}(\mathbb{R}^d))$ and $\text{div}(\mathbf{a}) = 0$. We assume that $F^{s,t}$, the flow map associated with the characteristic equation (1.5), satisfies $t \mapsto F^{0,t} \in L^\infty([0, T], W^{2,\infty}(\mathbb{R}^d))$. Let $x_k^n = F^{0,t^n}(x_k^0)$, \mathcal{J}_k^n computed by (3.10), and $\mathcal{F}_{h,k,1}^n$ and $\mathcal{B}_{h,k,1}^n$ respectively*

the approximated Forward and Backward flows respectively, given by (3.4) and (3.5). Then there exists $C > 0$ (depending on $\sup_{t \in [0, T]} \|F^{0, t}\|_{W^{2, \infty}(\mathbb{R}^d)}$ and $\sup_{t \in [0, T]} |F^{t, 0}|_{W^{1, \infty}(\mathbb{R}^d)}$) such that

$$e_F^n \leq Ch^2$$

and $h^* > 0$ such that for $0 < h < h^*$

$$e_B^n \leq Ch^2.$$

Proof. First, the regularity assumed on \mathbf{a} and the theorem 1.2 allow to obtain that $(t, x) \mapsto F^{0, t}(x)$ and $(t, x) \mapsto F^{t, 0}(x) \in \mathcal{C}([0, T], W^{2, \infty}(\mathbb{R}^d))$. Furthermore, since $\operatorname{div}(\mathbf{a}) = 0$, we have $j^{0, t^n}(x_k^0) = \det(J^{0, t^n}(x_k^0)) = 1$, thanks to (1.7), and the hypothesis (3.15) is verified with $\alpha = 1$.

For $x \in S_{h, k}^0$, we have $\|x - x_k^0\| \leq Lh$, and we split $F^{0, t^n}(x) - \mathcal{F}_{h, k, 1}^n(x)$ into two terms : the error due to the linearisation of order 1 around x_k^0

$$e_1(x) := F^{0, t^n}(x) - F^{0, t^n}(x_k^0) - J^{0, t^n}(x_k^0)(x - x_k^0)$$

and the error resulting from the approximation of $J^{0, t^n}(x_k^0)$

$$e_2(x) := \left(J^{0, t^n}(x_k^0) - \mathcal{J}_k^n \right) (x - x_k^0).$$

We can estimate e_1 directly from

$$\|e_1\|_{L^\infty(S_{h, k}^0)} \leq |F^{0, t^n}|_{W^{2, \infty}} \|x - x_k^0\|_\infty^2 \leq C |F^{0, t^n}|_{W^{2, \infty}} h^2.$$

Then thanks to (3.17) we have

$$\|e_2\|_{L^\infty(S_{h, k}^0)} \leq \frac{1}{2} |F^{0, t^n}|_{W^{2, \infty}(\mathbb{R}^d)} h \|x - x_k^0\|_\infty \leq C |F^{0, t^n}|_{W^{2, \infty}(\mathbb{R}^d)} h^2.$$

We then get

$$\sup_{0 \leq n \leq N} e_F^n \leq C \sup_{t \in [0, T]} |F^{0, t}|_{W^{2, \infty}(\mathbb{R}^d)} h^2.$$

We now estimate e_B^n . For $y \in \mathcal{F}_{h, k, 1}^n(S_{h, k}^0)$, let $x = \mathcal{B}_{h, k, 1}^n(x) \in S_{h, k}^0$. We have

$$\begin{aligned} F^{t^n, 0}(y) - \mathcal{B}_{h, k, 1}^n(y) &= F^{t^n, 0}(\mathcal{F}_{h, k, 1}^n(x)) - x \\ &= F^{t^n, 0}(\mathcal{F}_{h, k, 1}^n(x)) - F^{t^n, 0}(F^{0, t^n}(x)) \end{aligned}$$

and then

$$\|F^{t^n, 0}(y) - \mathcal{B}_{h, k, 1}^n(y)\|_\infty \leq |F^{t^n, 0}|_{W^{1, \infty}(\mathbb{R}^d)} e_F^n.$$

For $y \in F^{0,t^n}(S_{h,k}^0)$, let $x = F^{t^n,0}(y)$. We have

$$\begin{aligned} F^{t^n,0}(y) - \mathcal{B}_{h,k,1}^n(y) &= x - \mathcal{B}_{h,k,1}^n(F^{0,t^n}(x)) \\ &= x - x_k^0 - D_k^n(F^{0,t^n}(x) - x_k^n) \\ &= D_k^n \left(\mathcal{J}_k^n(x - x_k^0) - F^{0,t^n}(x) - x_k^n \right) \end{aligned}$$

and then

$$\begin{aligned} \|F^{t^n,0}(y) - \mathcal{B}_{h,k,1}^n(y)\|_\infty &\leq \|D_k^n\| \|\mathcal{F}_{h,k,1}^n(x) - F^{0,t^n}(x)\|_\infty \\ &\leq \|D_k^n\| e_F^n. \end{aligned}$$

Finally, thanks to (3.16), we get for $0 < h < h^*$,

$$e_B^n \leq C e_F^n \leq C h^2.$$

□

Overlapping estimate For a given $x \in \mathbb{R}^d$, we denote $\mathcal{K}_n(x)$ the set of overlapping particles at location x

$$\mathcal{K}_n(x) := \{k \in \mathbb{Z}^d, x \in F^{0,t^n}(S_{h,k}^0) \cup \mathcal{F}_{h,k,1}^n(S_{h,k}^0)\},$$

and

$$\kappa_n := \sup_{x \in \mathbb{R}^d} \#\mathcal{K}_n(x).$$

We can estimate κ_n with e_F^n .

Lemma 3.8. Assume that $(t, x) \mapsto F^{t,0}(x) \in L^\infty([0, T]; W^{1,\infty}(\mathbb{R}^d))$. Then there exists $C > 0$ ($= \max(1, \sup_{t \in [0, T]} |F^{t,0}|_{W^{1,\infty}(\mathbb{R}^d)})$) such that

$$\kappa_n \leq C \left(1 + \frac{e_F^n}{h}\right)^d. \quad (3.19)$$

Proof. Let $x \in \mathbb{R}^d$ and $k \in \mathcal{K}_n(x)$. Let $z = F^{t^n,0}(x)$ and $y = \mathcal{B}_{h,k,1}^n(x)$. If $x \in F^{0,t^n}(S_{h,k}^0)$, then $z \in S_{h,k}^0$ and thus $|z - kh| = |z - x_k^0| \leq h$. Otherwise $x \in \mathcal{F}_{h,k,1}^n(S_{h,k}^0)$, and $y = \mathcal{B}_{h,k,1}^n(x) \in S_{h,k}^0$. Then

$$\begin{aligned} \|z - x_k^0\|_\infty &\leq \|F^{t^n,0}(x) - y\|_\infty + \|y - x_k^0\|_\infty \\ &\leq \|F^{t^n,0}(\mathcal{F}_{h,k,1}^n(y)) - F^{t^n,0}(F^{0,t^n}(y))\|_\infty + h \\ &\leq |F^{t^n,0}|_{W^{1,\infty}(\mathbb{R}^d)} \|\mathcal{F}_{h,k,1}^n(y) - F^{0,t^n}(y)\|_\infty + h \\ &\leq |F^{t^n,0}|_{W^{1,\infty}(\mathbb{R}^d)} e_F^n + h. \end{aligned}$$

It follows that for $x \in F^{0,t^n}(S_{h,k}^0) \cap \mathcal{F}_{h,k,1}^n(S_{h,k}^0)$,

$$\left\| k - \frac{F^{t^n,0}(x)}{h} \right\|_{\infty} \leq 1 + |F^{t^n,0}|_{W^{1,\infty}(\mathbb{R}^d)} \frac{e_F^n}{h},$$

and we obtain (3.19). \square

Convergence theorem We now prove a result for the convergence of the LTP method for the advection equation [6].

Theorem 3.9 (Campos-Pinto, 2014). *Let $u^n = u(t^n, \cdot)$ be the solution of (1.4) at time t^n with initial condition u^0 , and $u_{h,LTP}^n$ given by (3.6) with $x_k^n = F^{0,t^n}(x_k^0)$, $\omega_k^0 = A_{h,1}(u^0)$, and \mathcal{J}_k^n computed by (3.10). We assume that $u^0 \in W^{1,\infty}(\mathbb{R}^d)$, $\operatorname{div}(\mathbf{a}) = 0$, $(t, x) \mapsto F^{0,t}(x) \in L^\infty(0, T; W^{2,\infty}(\mathbb{R}^d))$, and $(t, x) \mapsto F^{t,0}(x) \in L^\infty(0, T; W^{1,\infty}(\mathbb{R}^d))$. Then there exists $h^* > 0$ and $C > 0$ (depending on $\sup_{t \in [0, T]} \|F^{0,t}\|_{W^{2,\infty}(\mathbb{R}^d)}$, $|\varphi|_{W^{1,\infty}}$ and $|F^{t^n,0}|_{W^{1,\infty}(\mathbb{R}^d)}$, $\|u^0\|_{W^{1,\infty}}$, $|\varphi|_{W^{1,\infty}}$) so that for $0 < h \leq h^*$,*

$$\sup_{0 \leq n \leq N} \|u_{h,LTP}^n - u^n\|_{L^\infty(\mathbb{R}^d)} \leq Ch.$$

Proof. For a given $x \in \mathbb{R}^d$ and $n \in \{0, \dots, N\}$, we can write

$$\begin{aligned} u(t^n, x) - u_{h,LTP}^n(x) &= \\ & \underbrace{u^0(F^{t^n,0}(x)) - \sum_k \omega_k^0 \varphi_{h,k}^0(F^{t^n,0}(x))}_{=: T_1(x)} + \underbrace{\sum_k \omega_k^0 \left(\varphi_h(F^{t^n,0}(x) - x_k^0) - \varphi_h(D_k^n(x - x_k^n)) \right)}_{=: T_2(x)}. \end{aligned} \quad (3.20)$$

The first term is estimated thanks to the error of discretisation of the initial condition (3.14):

$$|T_1(x)| \leq \|A_{h,1}u^0 - u^0\|_{L^\infty(\mathbb{R}^d)} \leq Ch|u^0|_{W^{1,\infty}(\mathbb{R}^d)}.$$

We can now estimate $|T_2(x)|$ in (3.20).

$$\begin{aligned} |T_2(x)| &\leq \left| \sum_k \omega_k^0 \left(\varphi_h(F^{t^n,0}(x) - x_k^0) - \varphi_h(D_k^n(x - x_k^n)) \right) \right| \\ &\leq |\varphi_h|_{W^{1,\infty}} \sum_{k \in \mathcal{K}_n(x)} |\omega_k^0| \|F^{t^n,0}(x) - \mathcal{B}_{h,k,1}^n(x)\|_{\infty} \\ &\leq \frac{1}{h^{d+1}} |\varphi|_{W^{1,\infty}} \kappa_n h^d \|u^0\|_{\infty} e_B^n. \end{aligned}$$

We can conclude using lemmas 3.7 and 3.8. \square

3.3 Numerical comparisons between the LTP method and the SP method

Let us first return to the numerical example shown in Figures 1 and 2. Figure 3 shows the suppression of spurious oscillations obtained by the LTP method compared with the SP method, as well as the error control over time. Figure 4 shows a comparison between the convergence curves (in L^∞ norm) with respect to h for the LTP method on the one hand, and the SP method on the other. The LTP method converges linearly, while the SP method does not converge for $h = \varepsilon$ (as expected), and has a lower order of convergence for $h = \varepsilon^s$, where $s < 1$.

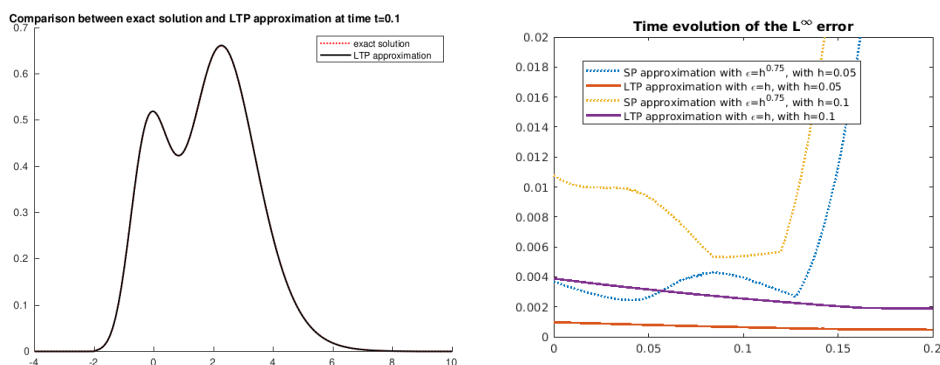


Figure 3: LTP method for the one-dimensional equation (1.1), with $a(t, x) = x^2$ and $\rho^0(x) = e^{-(x-2)^2} + 0.5e^{-x^2}$. Here φ is a B3-spline. Left : comparison at time $t = 0.1$ between the exact solution of the and the LTP approximation, with $h = 0.1$. Right : time evolution between 0 and $T = 0.2$ of the L^∞ error for the LTP approximation on one hand and the SP approximation with $\varepsilon = h^{0.75}$ on the other hand, for $h \in \{0.05, 0.1\}$.

Figure 5 shows a numerical comparison between the LTP approximation and the SP approximation (for $\varepsilon = h$ and $\varepsilon = h^{0.9}$) of a 2d transport equation. As in the 1d example of Figure 1, oscillations are observed for the SP approximation with $\varepsilon = h$, while the SP approximation with $\varepsilon = h^{0.9}$ solution exhibits numerical diffusion and a lack of precision compared to the LTP approximation.

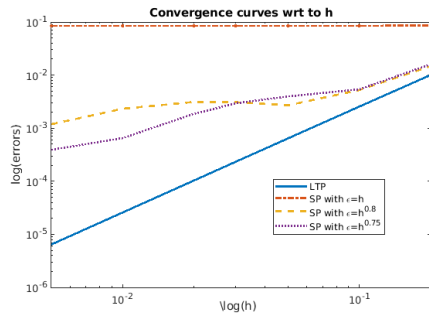


Figure 4: Convergence curves (in L^∞ norm) with respect to h for the LTP method (with $\varepsilon = h$) and the SP method with $\varepsilon = h^s$, with $s \in \{0.75, 0.8, 1\}$.

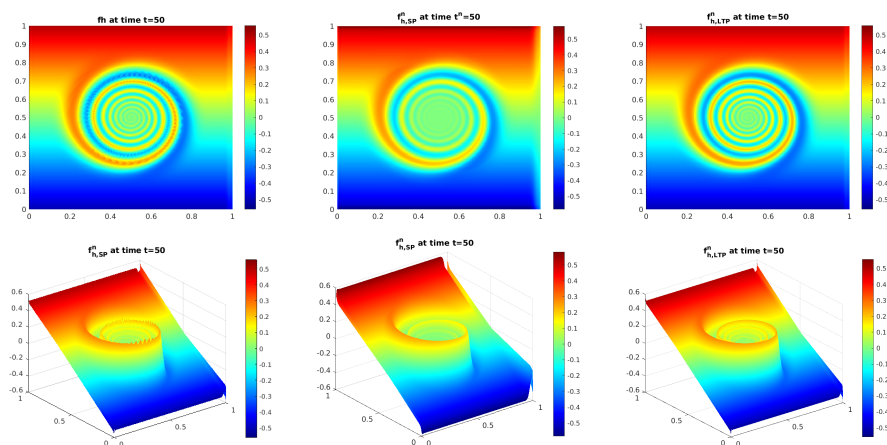


Figure 5: Numerical approximation at time $T = 50$ of the solution of the 2d transport equation (1.4) with $a(t, x) = \left(1 - \frac{1}{0.4} \|x - (0.5, 0.5)\|_2\right)_+^3 \begin{pmatrix} 0.5 - x_2 \\ x_1 - 0.5 \end{pmatrix}$ and $u^0(x, y) = x_2 - 0.5$. From left to right : SP approximation with $\varepsilon = h$, SP approximation with $\varepsilon = h^{0.9}$, LTP approximation with $\varepsilon = h$. The figures in the first line correspond to a top view, the figures in the second line to a 3d view. Here we take the following numerical parameters : 251×251 particles, a time step $\Delta t = 0.5$, and a period of remapping $\Delta t_r = 3$.

3.4 Application to nonlinear equations

We present here some applications of the LTP method to nonlinear transport equations where the advection field depends on the solution: $\mathbf{a} = \mathbf{a}(\rho)$. In

this situation, one has to reconstruct an approximation of the advection field $\mathbf{a}(\rho(t^n, \cdot))$ at each time step of the time scheme. This can be done for example with a Particle-In-Cell (PIC) method (see [35]).

Vlasov-Poisson system The LTP method has been used for the first time to approach a nonlinear problem in [10] for the 1d-1v Vlasov-Poisson system in a periodic spatial domain :

$$\begin{cases} \frac{\partial f}{\partial t} + v \partial_x f - E \partial_v f = 0, & (t, x, v) \in [0, T] \times \mathbb{R} \times \mathbb{R} \\ \partial_x E(t, x) = 1 - \int_{\mathbb{R}} f(t, x, v) dv & (t, x) \in [0, T] \times \mathbb{R} \end{cases} \quad (3.21)$$

supplemented with an initial condition $f(0, \cdot, \cdot) = f^0 \geq 0$, and a zero-mean field condition $\int_0^L E(t, x) dx = 0$ for all $T \geq 0$.

Note that since $\mathbf{a}(t, x, v) = (v, -E(t, x))^t$, we have $\operatorname{div}_{x,v}(\mathbf{a}) = 0$ and the first equation of (3.21) can be written either on conservative (1.3) either on advective form (1.4).

Using standard arguments from [36] (see, e.g., [21], Theorem 1) we easily verify that with the above conditions the system (3.21) has a unique solution (f, E) . This solution is L -periodic with respect to x and has the same order of smoothness as f^0 , namely, $(f, E) \in W^{2,\infty}([0, T] \times \mathbb{R}^2) \times W^{2,\infty}([0, T] \times \mathbb{R}^2)$.

The convergence of the method applied to this problem was then studied in [8]. A strong convergence of the approximated density $f_{h,LTP}^n$ is obtained, which improves the standard estimates of Cottet and Raviart [21] applied to the case of Smooth Particles with bounded overlapping (that is, by taking $\varepsilon \sim h$).

Theorem 3.10. *Assume that $f^0 \in W^{2,\infty}(\mathbb{R}^2)$ is L -periodic with respect to x , has a bounded support in v -dimension, and satisfies a global neutrality relation: $\int_0^L (\int_{\mathbb{R}} f^0(x, v) dv - 1) dx = 0$. Let $E_h^{n,1}$, $z_k^n = (x_k^n, v_k^n)$ and $f_{h,LTP}^n$ be the approximate electric field, trajectories (in phase space) and density, respectively, given by the scheme introduced in [8]. Provided that $\Delta t \lesssim \sqrt{h}$, the errors on the electric field and the trajectories of the particles verify*

$$\sup_{0 \leq n \leq T/\Delta t} \|E_h^{n,1} - E(t_{n+1/2})\|_{L^\infty} + \sup_k \|z_k^n - F^{0,t_n}(z_k^0)\| \leq C_T (h^2 + \Delta t^2)$$

and the LTP approximation of the space phase density $f_{h,LTP}^n$ satisfies

$$\|f_{h,LTP}^n - f(t^n, \cdot)\|_{L^\infty(\mathbb{R}^2)} \leq C_T \left(h + \frac{\Delta t^2}{h} \right)$$

where the constant C_T depends on $\|f\|_{W^{2,\infty}([0,T] \times [0,L] \times [-v_{max}, v_{max}])}$.

Figure 6 shows the comparison between the SP and the LTP approximations of the solution of the Vlasov-Poisson system (3.21) with the initial condition

$$f_0(x, v) = (1 - \alpha \cos(kx)) \frac{1}{2\pi} e^{-v^2/2}. \quad (3.22)$$

Here again we see that the oscillations are smoothed.

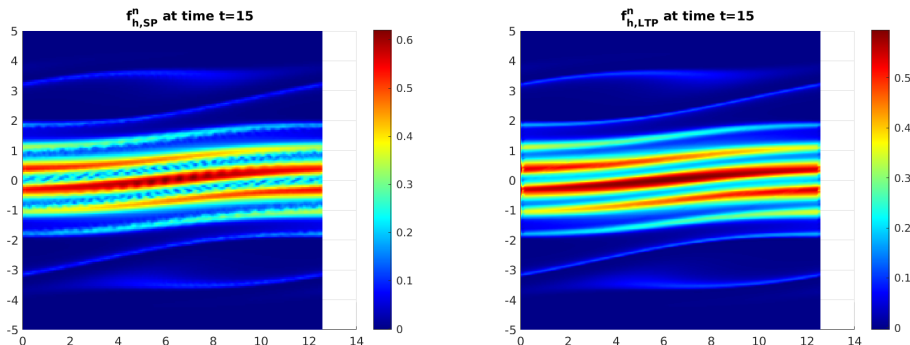


Figure 6: Strong Landau Damping test case (Vlasov-Poisson system (3.21) with initial conditions (3.22)), with $\alpha = k = 0.5$. Left picture : SP method with $\varepsilon = h$, right picture : LTP method. For both the number of particles is 150×150 , $\Delta t = 1/8$, and the period of remapping is $\Delta t_r = 3$.

Aggregation equation Here we consider an equation modelling particle aggregation, which is written in the form of a nonlinear transport equation

$$\partial_t \rho + \operatorname{div}(\mathbf{u}\rho) = 0, \quad \rho(0, \cdot) = \rho^0 \quad \mathbf{u}(t, x) = -(\nabla_x \mathcal{W} \star \rho(t))(x) \quad (3.23)$$

where $\mathcal{W} : \mathbb{R}^d \rightarrow \mathbb{R}$ is an interaction potential. Two types of potential are considered here.

- ▷ Regular potentials, when $\nabla \mathcal{W} \in W^{1,\infty}(\mathbb{R}^d)$. In this case it is easy to see that as soon as $\rho^0 \in L^1(\mathbb{R}^d)$ the velocity field is Lipschitzian, with

$$\sup_{0 \leq t \leq T} \|\mathbf{u}(t, \cdot)\|_{W^{1,\infty}(\mathbb{R}^d)} \leq C \|\rho^0\|_{L^1} \|\nabla \mathcal{W}\|_{W^{1,\infty}(\mathbb{R}^d)}.$$

The well-posedness of (3.23) in this context has been studied in [5]. If $\rho^0 \in W^{1,1}(\mathbb{R}^d)$, $\rho^0 \geq 0$ then there exists a unique solution of (3.23) which verifies $\rho \in L^\infty(0, T, W^{1,1}(\mathbb{R}^d))$, $\rho \geq 0$ for all $T > 0$. In addition, the approach introduced by Dobrushin [27] can be applied and leads to the existence of measure solutions [11, 12].

▷ Singular potentials. For these, we assume that $\nabla\mathcal{W} \in W_{\text{loc}}^{1,q}(\mathbb{R}^d)$, as well as the following properties

$$|D^2\mathcal{W}(x)| \leq \frac{C}{|x|^\alpha}, \quad |D^2\mathcal{W}(x)| \leq \frac{C}{|x|^{\alpha+1}}, \quad (3.24)$$

with $-1 < \alpha < d-1$, and $1 \leq q \leq \frac{d}{\alpha+1}$. This is the case, for example, of the attractive-repulsive potential

$$\mathcal{W}_{ab}(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b}, \quad \text{with} \quad 2-d < b < a < 2.$$

The assumptions $\nabla\mathcal{W} \in W_{\text{loc}}^{1,q}(\mathbb{R}^d)$ and (3.24) guarantee that the velocity field is Lipschitzian in x (locally in time) for densities in $L^1(\mathbb{R}^d) \cap L^p(\mathbb{R}^d)$, where p is the conjugate exponent of q . Under these assumptions, it has been shown [4] that if $\rho^0 \in W^{1,1} \cap W^{1,p}(\mathbb{R}^d)$, $1 \leq q \leq d/(\alpha+1)$, $\rho^0 \geq 0$, then there exists a time T^* such that for $0 \leq T < T^*$, $\rho \in L^\infty(0, T, W^{1,1} \cap W^{1,p}(\mathbb{R}^d))$. In this case, it is possible to have *blow-up* in finite time.

Discretisations of the equation (3.23) have been proposed in [23] by a particle method, in [32] by a finite volume method, or in [13] by methods using the gradient Float structure of the equation.

In [7], a numerical scheme with LTP reconstruction of the approximated density is introduced. In the case of regular potential, the strong convergence in L^1 and L^∞ norm for $\rho_{h,\text{LTP}}^n$ is proved (Theorem 3.11), as well as the convergence (without any condition on the time step) of measured solutions (Theorem 3.12) for the distance d_{BL} defined by

$$d_{BL}(\rho_1, \rho_2) := \sup \left\{ \left| \int_{\mathbb{R}^d} \psi d\rho_1 - \int_{\mathbb{R}^d} \psi d\rho_2 \right| : \psi \in W^{1,\infty}(\mathbb{R}^d) \text{ and } \|\psi\|_{W^{1,\infty}} \leq 1 \right\}.$$

Theorem 3.11. *Assume that $\Delta t \lesssim h$. If $\rho^0 \in W^{1,1}(\mathbb{R}^d)$, $\rho^0 \geq 0$ and $\nabla\mathcal{W} \in W^{1,\infty}(\mathbb{R}^d)$, then there exists C (depending on $d, T, \|\nabla\mathcal{W}\|_{W^{1,\infty}}$ and $\|\rho^0\|_{W^{1,1}}$ only) such that*

$$\max_{0 \leq n \leq N} \|\rho(t_n, \cdot) - \rho_{h,\text{LTP}}^n\|_{L^1} \leq C \left(\|\rho^0 - \rho_h^0\|_{L^1} + h + \frac{\Delta t}{h} \right)$$

Furthermore, if $\rho^0 \in L^\infty(\mathbb{R}^d)$ then we also have convergence in L^∞ norm.

$$\max_{0 \leq n \leq N} \|\rho(t_n, \cdot) - \rho_{h,\text{LTP}}^n\|_{L^\infty} \leq C \left(\|\rho^0 - \rho_h^0\|_{L^\infty} + \|\rho^0 - \rho_h^0\|_{L^1} + h + \frac{\Delta t}{h} \right).$$

Theorem 3.12. *If $\rho^0 \in \mathcal{M}(\mathbb{R}^d)$ and $\nabla\mathcal{W} \in W^{1,\infty}(\mathbb{R}^d)$ then there exists C depending only on $d, T, \|\nabla\mathcal{W}\|_{W^{1,\infty}}$ such that*

$$\max_{0 \leq n \leq \frac{T}{\Delta t}} d_{BL}(\rho(t^n, \cdot), \rho_{h,LTP}^n) \leq C(d_{BL}(\rho^0, \rho_h^0) + h + \Delta t).$$

In the case of a singular potential, the convergence is proved (up to the blow-up time) in L^1 and L^p norms (depending on the regularity of the potential).

Theorem 3.13. *Assume that the potential $\mathcal{W} \in W_{loc}^{1,q}(\mathbb{R}^d)$ verifies (3.24). Consider $\rho^0 \in W^{2,p}(\mathbb{R}^d)$, with $1/p + 1/q = 1$, and ρ a solution of (3.23) defined on a time interval $[0, T]$, such that $\rho \in L^\infty(0, T; (W^{1,1} \cap W^{1,p} \cap L^\infty)(\mathbb{R}^d))$. It is assumed that $\Delta t \lesssim h^2 \leq 1$. Then there exist $h_* > 0$ and C independent of h and Δt such that*

$$\sup_{0 < h \leq h_*} \sup_{0 \leq n \leq N} \|\rho(t^n, \cdot) - \rho_{h,LTP}^n\| \leq Ch,$$

with $\|\cdot\| := \|\cdot\|_{L^1} + \|\cdot\|_{L^p}$.

We note in the theorems 3.12 and 3.13 a constraint between h and Δt to obtain convergence. However, this is not as restrictive as a CFL condition. Moreover, the use of a higher-order time scheme to discretise of particle trajectories may be able to weaken this constraint.

3.5 Conclusion on the LTP method

The LTP method allows to obtain strong convergence of the approximate solution, and improves the quality of the reconstruction. However, in practice, it still requires some regular remappings, although less frequent than in a standard particle method. Indeed, the supports of the particle shape functions $\varphi_{h,k}^n$ can stretch too far in one direction (if the deformation matrix D_k^n has an eigenvalue that is significantly smaller than the others), leading to a loss of locality in the reconstruction. The accuracy of the approximate density is compromised, and the CPU cost of reconstruction also increases.

4 Forward-Backward Lagrangian method

4.1 The FBL method

The Forward Backward Lagrangian method proposed in [9] is based on the solution expression (1.1) or (1.4), where $F^{t^n,0}$, the backward flow between t^n and 0, is reconstructed from the displacement of particles. These particles,

pushed forward as in a particle method, can only be seen as weightless and "formless". Shape functions are no longer used here.

Here, as in section 3.1 we describe the method for a passive flow \mathbf{a} and without taking into consideration the time solver of (2.3) to calculate the positions of the particles $(x_k^n)_{k \in \mathbb{Z}^d, n \geq 0}$. The principle of the method is as follows:

- (i) To each particle of position x_k^n we associate the polynomial backflow $\mathcal{B}_{h,k}^n$ obtained by local Taylor expansion around x_k^n , to order 1 as in $\mathcal{B}_{h,k,1}^n$ given by (3.5), or to higher order as in

$$\mathcal{B}_{h,k,2}^n : x \mapsto x_k^0 + D_k^n(x - x_k^n) + \frac{1}{2} \left((x - x_k^n)^t (Q_k^n)_i (x - x_k^n) \right)_{1 \leq i \leq d}, \quad (4.1)$$

where $(Q_k^n)_i$ is an approximation of the Hessian matrix of the i th component of the backward flow from t^n to 0.

- (ii) From these local approximations, a global approximation of the backward flow is constructed. To do this, we can consider a partition of the unit using a compactly supported, positive function S that satisfies

$$\sum_{i \in \mathbb{Z}^d} S(x - i) = 1, \quad x \in \mathbb{R}^d. \quad (4.2)$$

This is the case, for example, with B-splines [6]. We then introduce a grid \mathcal{G}_F to reconstruct the flow (noting the nodes $\xi_i = ih_F$, $i \in \mathbb{Z}^d$ to avoid confusion with the particle initialisation grid) and the function

$$S_{h_F,i}(x) = S\left(\frac{x - \xi_i}{h_F}\right).$$

For each node of \mathcal{G}_F we define $k^*(n, i)$ the index of the particle closest to the node ξ_i :

$$k^*(n, i) := \operatorname{argmin}_{k \in \mathbb{Z}^d} \|x_k^n - \xi_i\|_\infty, \quad (4.3)$$

and we introduce the global approximation of the flow by

$$\mathcal{B}_h^n(x) := \sum_{i \in \mathbb{Z}^d} \mathcal{B}_{h,k^*(n,i)}^n(x) S_{h_F,i}(x), \quad (4.4)$$

and possibly (in the case of the equation (1.1)) a global approximation of the backward Jacobian $\det(J^{t_n,0}(x))$.

$$j_{B,h}^n(x) = \sum_{i \in \mathbb{Z}^d} \det(D_{k^*(n,i)}^n) S_{h_F,i}(x). \quad (4.5)$$

(iii) We use the initial density (or an interpolation of the density at the last remapping time) to define the approximate density

$$u_{h,\text{FBL}}^n(x) := u^0(\mathcal{B}_h^n(x)) \quad (4.6)$$

for equation (1.4) or

$$\rho_{h,\text{FBL}}^n(x) := \rho^0(\mathcal{B}_h^n(x)) j_{B,h}^n(x) \quad (4.7)$$

for equation (1.1).

In (3.5) and (4.1) the approximate Jacobian (and possibly Hessian) matrices of the forward flow (which give the approximations D_k^n and $Q_{k,i}^n$, see Appendices A and B of [9]) can be computed by finite differences of the particle positions x_k^n on the initialisation grid as in (3.10), or by an approximate expression (as in the schemes for the Vlasov-Poisson and aggregation equations we considered in 3.4).

Remark 4.1. The FBL method has some similarities with semi-Lagrangian methods. However, unlike a classical semi-Lagrangian method, it is the backward flow between t^n and 0, or a remapping instant, that is approximated (and not the one between t^{n+1} and t^n).

4.2 Errors estimates for a passiv flow

We present the following theorem from [9] for the equation (1.4) with a passive advection flow \mathbf{a} , assuming exact particle trajectories, i.e. $x_k^n = F^{0,t^n}(x_k^0)$ for $k \in \mathbb{Z}^d$. Here we take $h_F = h$ to simplify.

Theorem 4.2. *Assume that $u^0 \in W^{1,\infty}(\mathbb{R}^d)$, $\text{div}(\mathbf{a}) = 0$, and that the exact forward and reverse flows verify $t \mapsto F^{0,t} \in L^\infty([0, T], W^{2,\infty}(\mathbb{R}^d))$ and $t \mapsto F^{t,0} \in L^\infty([0, T], W^{2,\infty}(\mathbb{R}^d))$. Let $u^n = u(t^n, \cdot)$ be the solution of (1.4) with initial condition u^0 at time t^n . Then there exists h^* such that for $0 < h \leq h^*$ the FBL approximation for (1.4) of order 1 verifies*

$$\sup_{0 \leq n \leq N} \|u_{h,\text{FBL}}^n - u^n\|_{L^\infty(\mathbb{R}^d)} \leq C_1 h^2, \quad (4.8)$$

where the constant C_1 depends on $|\rho^0|_{W^{1,\infty}(\mathbb{R}^d)}$, $\sup_{t \in [0, T]} \|F^{0,t}\|_{W^{2,\infty}(\mathbb{R}^d)}$ and

$\sup_{t \in [0, T]} \|F^{t,0}\|_{W^{2,\infty}(\mathbb{R}^d)}$. Furthermore, if $t \mapsto F^{0,t} \in L^\infty([0, T], W^{3,\infty}(\mathbb{R}^d))$ and $t \mapsto F^{t,0} \in L^\infty([0, T], W^{3,\infty}(\mathbb{R}^d))$, the approximation to order 2 verifies

$$\|u_{h,\text{FBL}}^n - u^n\|_{L^\infty(\mathbb{R}^d)} \leq C_{2,n} h^3, \quad (4.9)$$

where the constant C_2 depends on $|\rho^0|_{W^{1,\infty}(\mathbb{R}^d)}$, $\sup_{t \in [0,T]} \|F^{0,t}\|_{W^{3,\infty}(\mathbb{R}^d)}$ and

$$\sup_{t \in [0,T]} \|F^{t,0}\|_{W^{3,\infty}(\mathbb{R}^d)}.$$

We prove here only the estimate (4.8) which corresponds to an asymptotic expansion of the backward flow at order 1. The proof of (4.9) for an asymptotic expansion of order 2 is similar, using estimates on the Hessian matrices of the forward and backward flows proved in [9].

Proof. Using the property (4.2) and the positivity of the function S , we have

$$\begin{aligned} |u_{h,FBL}^n(x) - u(t^n, x)| &= |u^0(\mathcal{B}^n(x) - u^0(F^{t^n,0}(x)))| \\ &\leq |u^0|_{W^{1,\infty}(\mathbb{R}^d)} \left\| \mathcal{B}^n(x) - F^{t^n,0}(x) \right\|_{\infty} \\ &\leq |u^0|_{W^{1,\infty}(\mathbb{R}^d)} \left\| \sum_{i \in \mathbb{Z}^d} \left(\mathcal{B}_{h,k^*(n,i)}^n(x) - F^{t^n,0}(x) \right) S_{h,i}(x) \right\|_{\infty} \\ &\leq |u^0|_{W^{1,\infty}(\mathbb{R}^d)} e_{B,FBL}^n \end{aligned}$$

where we denote

$$e_{B,FBL}^n = \sup_{i \in \mathbb{Z}^d} \|\mathcal{B}_{h,k^*(n,i)}^n - F^{t^n,0}\|_{L^\infty(\text{Supp}(S_{h,i}))}$$

with $S_{h,i}(x) = S\left(\frac{x - \xi_i}{h}\right)$. Let $n \in \{0, \dots, N\}$, $i \in \mathbb{Z}^d$, and $x \in \text{Supp}(S_{h,i})$. We have

$$\begin{aligned} \mathcal{B}_{h,k^*(n,i)}^n(x) - F^{t^n,0}(x) &= x_{k^*(n,i)}^0 + D_{k^*(n,i)}^n(x - x_{k^*(n,i)}^n) - F^{t^n,0}(x) \\ &= \underbrace{x_{k^*(n,i)}^0 + J^{t^n,0}(x_{k^*(n,i)}^n)(x - x_{k^*(n,i)}^n) - F^{t^n,0}(x)}_{=: A_{i,n}} \\ &\quad + \underbrace{D_{k^*(n,i)}^n \left(J^{0,t^n}(x_{k^*(n,i)}^0) - \mathcal{J}_{k^*(n,i)}^n \right) J^{t^n,0}(x_{k^*(n,i)}^n)(x - x_{k^*(n,i)}^n)}_{=: B_{i,n}} \end{aligned}$$

The first term can be estimated thanks to the error of the second order Taylor expansion of the Backward flow around $x_{k^*(n,i)}^n$:

$$\|A_{i,n}\|_{\infty} \leq \frac{1}{2} |F^{t^n,0}|_{W^{2,\infty}(\mathbb{R}^d)} \|x - x_{k^*(n,i)}^n\|_{\infty}^2$$

and the second thanks to the error on the Jacobian (3.17) and the lemma 3.6: for $0 < h < h^*$, we have

$$\|B_{i,n}\|_{\infty} \leq C |F^{0,t^n}|_{W^{2,\infty}(\mathbb{R}^d)} |F^{t^n,0}|_{W^{1,\infty}(\mathbb{R}^d)} \|x - x_{k^*(n,i)}^n\|_{\infty} h$$

(where C does not depend on $n \in \{0, \dots, N\}$ and $i \in \mathbb{Z}^d$). Let $y_i = F^{t^n, 0}(\xi_i)$, and k_i° the grid node index closest to y_i , which is such that $\|x_{k_i^\circ} - y_i\|_\infty \leq h$. Then, according to the definition (4.3) of $k^*(n, i)$

$$\begin{aligned} \|F^{0, t^n}(x_{k^*(n, i)}^0) - \xi_i\|_\infty &\leq \|F^{0, t^n}(x_{k_i^\circ}) - \xi_i\|_\infty \\ &\leq \|F^{0, t^n}(x_{k_i^\circ}^0) - F^{0, t^n}(y_i)\|_\infty \\ &\leq |F^{0, t^n}|_{W^{1, \infty}(\mathbb{R}^d)} h, \end{aligned}$$

and thus, since $x \in \text{Supp}(S_{i, h})$

$$\|x - x_{k^*(n, i)}^n\|_\infty \leq (L_S + |F^{0, t^n}|_{W^{1, \infty}(\mathbb{R}^d)}) h,$$

where L_S is the diameter of the support of S . Returning to the estimates of $\|A_{i, n}\|_\infty$ and $\|B_{i, n}\|_\infty$, we then get

$$\|\mathcal{B}_{h, k^*(n, i)}^n(x) - F^{t^n, 0}(x)\|_\infty \leq Ch,$$

where C depends on $\sup_{t \in [0, T]} |F^{0, t}|_{W^{1, \infty}(\mathbb{R}^d)}$, $\sup_{t \in [0, T]} |F^{0, t}|_{W^{2, \infty}(\mathbb{R}^d)}$ and $\sup_{t \in [0, T]} |F^{t, 0}|_{W^{1, \infty}(\mathbb{R}^d)}$.

This allows us to finally obtain (4.8). □

We thus gain one order in h compared to the LTP method [6]. This gain comes from the fact that the error estimate now includes $|\rho^0|_{W^{1, \infty}(\mathbb{R}^d)}$ (or the norm of the density reconstructed at a remapping time) and no longer the terms $|\varphi_{h, k}^n|_{W^{1, \infty}(\mathbb{R}^d)}$, which are of the order of $\frac{1}{h}$. Moreover, in the case of a linear transport equation such as the one shown here, we can see that the gain in order obtained by increasing the order of the asymptotic expansion relies on the regularity of the flow (and hence of $\mathbf{a}(t, x)$), and does not require greater regularity of the solution (and hence of the initial condition), as is the case for semi-Lagrangian methods [15].

Remark 4.3. It can also be shown (see [9]) that the regularity of the approximate solution is preserved. Under the same assumptions as in theorem 4.2, the FBL reconstruction of order $r \in \{1, 2\}$ verifies that

$$\|u_{h, \text{FBL}}^n\|_{W^{q, \infty}} \leq C_n \|u^0\|_{W^{q, \infty}}, \quad \text{for } 1 \leq q \leq r + 1$$

where the constant C_n depends on the forward and reverse flows F^{0, t_n} and $F^{t_n, 0}$ but not on h .

Remark 4.4. The error estimates (4.8) and (4.8) do not depend on Δt as we have not introduced time discretisation for the resolution of (2.3). We can consider the case of the method with fixed number R of remappings, with

the assumption that the interpolation or approximation operator $A_{h,p}$ satisfies (3.14). The error after r remappings $e_r := \max_{m_{r-1} \leq n \leq m_r} \|\rho_{h,\text{FBL}}^n\|_{W^{1,\infty}}$, where $(m_r)_{1 \leq r \leq R+1}$ are the remapping time indices, verifies [9]

$$\max_{1 \leq r \leq R+1} e_r \leq CT \| \|A_{h,p}\| \|_{\infty}^R \frac{h^2}{\Delta r},$$

where $\Delta r = T/(R+1)$. This estimate can then explode if $\| \|A_{h,p}\| \|_{\infty} > 1$ and the number of remappings is proportional to the time step when time discretisation is introduced. In practice, however, this is not necessary.

4.3 Numerical illustrations of the FBL method

In Figure 7, we illustrate the gain in the order of convergence for the FBL method, as well as its robustness when the initial condition is less regular. We first note that the order of convergence found numerically agrees well with that proved theoretically. Furthermore, while the order of convergence of the Backward Semi-Lagrangian (BSL) method is reduced when the initial condition is less regular, that of the FBL methods is not affected. This is consistent with the Theorem 4.2, which shows that the order of convergence depends on the regularity of the flow but not on the regularity of the initial condition. The accuracy of the BSL method for a non- \mathcal{C}^1 initial condition is also illustrated in Figure 8. Furthermore, as expected, this method preserves the positivity of the solution.

Acknowledgments. The author acknowledge support by the ANR MUFFIN ANR-19-CE46-0004.

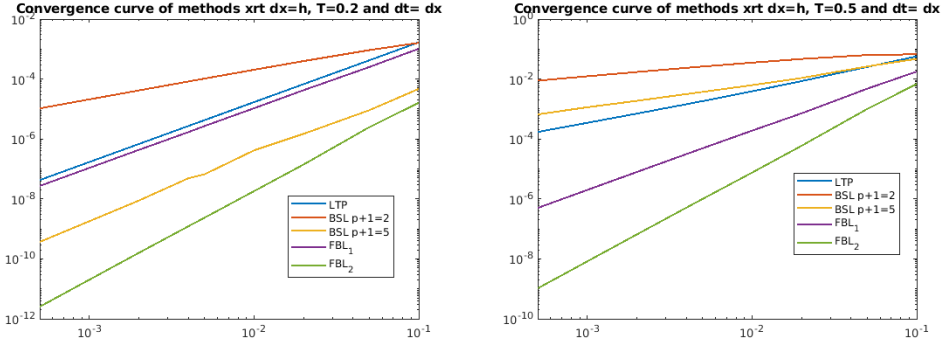


Figure 7: L^∞ convergence curves with respect to $\Delta x = h$, for the 1-d advection equation (1.4) with $a(t, x) = x^2$, for various numerical schemes : LTP, FBL_1 (with an asymptotic expansion of order 1), FBL_2 (with an asymptotic expansion of order 2), and Backward Semi-Lagrangian schemes (BSL) with 2 or 5 interpolation points and a grid of size Δx . Left picture : the initial condition u^0 is a B3 spline, and right picture : $u^0 = \max(0, -4x^2 + 8x - 3)$.

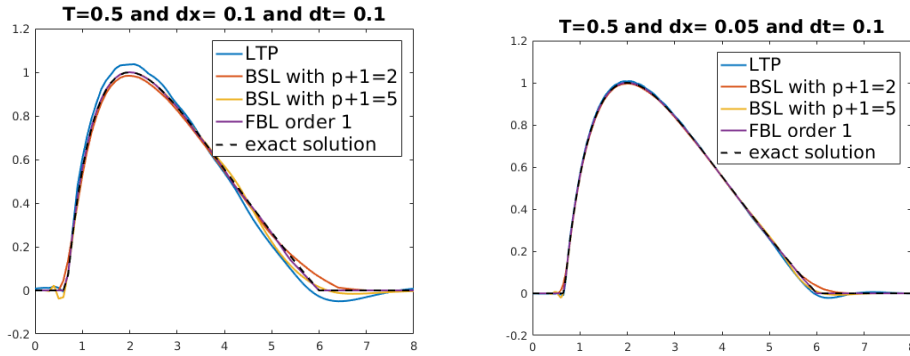


Figure 8: Comparison between the exact solution of the 1-d advection equation (1.4) with $a(t, x) = x^2$ and the approximate solutions with different numerical methods : LTP, FBL_1 (with an asymptotic expansion at order 1), FBL_2 (with an asymptotic expansion at order 2), and Backward Semi-Lagrangian schemes (BSL) with 2 or 5 interpolation points and a grid of size Δx . The initial condition is $u^0 = \max(0, -4x^2 + 8x - 3)$. Left picture : $h = \Delta x = 0.1$, right picture : $h = \Delta x = 0.05$.

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