Smooth particle methods without smoothing

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Abstract

We present a novel class of particle methods with deformable shapes that achieve high-order convergence rates in the uniform norm without requiring remappings, extended overlapping or vanishing moments for the particles. Unlike classical convergence analysis, our estimates do not rely on the use of a smoothing kernel but rather on the uniformly bounded overlapping of the particles supports and on the smoothness of the characteristic flow. In particular, they also apply to heterogeneous particle decompositions such as piecewise polynomial bases on unstructured meshes. In the first-order case which simply consists of pushing forward linearly transformed particles (LTP) along the flow, we provide an explicit scheme and establish rigorous estimates that demonstrate the convergence in the uniform norm and the uniform boundedness of the resulting particle overlapping. To illustrate the flexibility of the method we develop an adaptive multilevel version where particles are dynamically refined based on a local error indicator. Numerical studies allow to assess the convergence properties of this new particle scheme in both its uniform and adaptive versions, by comparing it with traditional fixed-shape particle methods with or without remappings.

1 Introduction

Efficient and simple particle methods are extremely popular for the numerical simulation of transport equations involved in many physical problems ranging from fluid dynamics [7, 12] to kinetic (e.g., Vlasov) equations [13, 16]. However, particle methods also suffer from weak convergence properties that lead to important disadvantages in many practical cases. Specifically, it is known that they only converge in a strong sense when the particles present an extended overlapping, that is, when the number of overlapping particles tends to infinity as the mesh size $h$ of their initialization grid tends to 0, see e.g., Refs. [3, 24]. Moreover, convergence rates are known to be suboptimal and to require additional constraints (namely, vanishing moments) for the particle shape functions that prevent high orders to be achieved with positive shapes. In practice, extended particle overlapping can be expensive and it involves an additional parameter to be optimized, such as the overlapping exponent $q < 1$ for which the particles radius behaves like $h^q > h$. In Particle-In-Cell (PIC) codes for instance, taking $q < 1$ typically leads to increasing the number of particles per cell faster than the number of cells, since the latter determine the radius of the particles [19]. In Smoothed Particle Hydrodynamics (SPH) schemes it amounts to increasing the number of neighbors, i.e., interacting particles [23]. Because of these issues, many particle simulation methods do not meet the conditions of convergence which can result in numerically intensive simulations for acceptable results. Also, limited numerical resources often produce strong oscillations seen as a statistical noise that hamper interpretation of results and can further cause large scale errors.

To suppress noise, many methods (like the Denavit redeposition scheme [15], recently revisited as a Forward Semi-Lagrangian scheme (FSL), see e.g., Refs. [22, 10, 13]) use periodic remappings, i.e., particle re-initializations that smooth out the evolution. However, frequent remappings can introduce unwanted numerical diffusion which in many cases contradicts the benefit of using low-diffusion particle schemes, and to reduce this adverse effect some authors have introduced high-order adaptive remappings, see, e.g. Refs. [5, 26].

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In this article, we present a new class of particle methods with deformable shapes that converge in the uniform norm without requiring remappings, extended overlapping or vanishing moments for the particles. Unlike classical error estimates based on a smoothing kernel argument, our analysis applies to general particle collections with Lipschitz smoothness and bounded overlapping properties. In particular our estimates easily extend to the transport of heterogeneous “particle” approximations such as standard finite elements bases.

Our results are threefold. On a formal level first, we establish high-order convergence rates in $L^\infty$ for a class of transport operators where the particle shapes are deformed with polynomial mappings, the coefficients of which involve spatial derivatives of the backward flow. In particular, the first-order case is a linearly-transformed particle method (LTP) where the particles are deformed with the Jacobian matrices of the backward flow. It corresponds to a method already studied by Cohen and Perthame [9] who established its first-order convergence in $L^1$ but did not provide a numerical scheme for the deformation matrices. It can also be viewed as a modified version of Hou’s method [18] where instead of using a global deformation mapping, each particle is transported by the linearized flow around its trajectory. On a numerical level, we provide an explicit scheme for the LTP method that is based solely on pointwise evaluations of the forward flow, and we establish rigorous a priori estimates for both the transport error and the particle overlapping. To illustrate the flexibility of our approach we also present an adaptive multilevel LTP scheme where local estimates for the single-particle transport errors are used to decide which particles are dynamically refined, and a local correction filter for high-order positivity-preserving hierarchical approximations is presented. On a practical level we eventually present numerical results obtained with academic test cases. They show that a B-spline based LTP scheme converges with better rates compared to the traditional smoothed particle method (TSP) with extended overlapping. Here the convergence is sometimes improved by introducing periodic remappings, but compared with the FSL scheme we also show that optimal remapping frequencies are much lower with LTP, leading to lower numerical diffusion and computational cost. Finally we verify that our adaptive LTP scheme enhances the convergence of solutions with sharp edges by equi-distributing the transport error.

As we have pointed out, deforming the particles is not a new idea. Dynamic adaptation, i.e., refinement and coarsening of particles, also has a substantial history. In vortex methods for instance, Cottet, Koumoutsakos and others have introduced a variety of algorithms to handle particles with spatially varying sizes based on global or local mappings, see e.g. [11, 4]. In kinetic (PIC) schemes, Lapenta, Assous and others developed “re zoning” algorithms to increase or lower the number of particles per grid cell, while preserving the corresponding grid moments such as charge, current or energy density, see e.g. [20, 1]. And for pure transport problems, Bergdorf and Koumoutsakos [5] have studied a wavelet-based FSL scheme with adaptive, high-order remappings. However, although the list is not exhaustive we observe that these methods adapt the size of particles with fixed shape, and hence require high frequency remappings. A noteworthy exception is the Complex Particle Kinetic method developed by Bateson and Hewett for the simulation of plasmas [2, 17] where in addition to having their Gaussian shape transformed by the local shearing of the flow, particles can be fragmented to probe for emerging features, and merged where fine particles are no longer needed. When mature, our adaptive scheme should be compared with the above methods.

The outline of the article is as follows. In Section 2 we begin with a rapid overview of the main particle methods, introduce some notations and state our main results. In Section 3 we present a class of high-order particle methods with polynomial deformations, as well as a fully discrete LTP scheme, and we establish a priori estimates. Section 4 is then devoted to the description of an adaptive multilevel LTP scheme based on refinable B-splines, and numerical results are presented in Section 5.

Readers mostly interested in the practical aspects of the LTP scheme may prefer to first read Sections 2.3, 3.3 and 5.3. Its main properties are stated in Theorem 3.10 and its adaptive multilevel version is summarized in Algorithms 4.4 and 4.6.
2 A brief review of particle methods

To introduce some notations and state our main results we begin with a rapid overview of particle methods. Following [24] we consider the linear $d$-dimensional transport equation

$$\partial_t f(t,x) + u(t,x) \cdot \nabla f(t,x) = 0, \quad t \in [0,\tau], \quad x \in \mathbb{R}^d$$

(2.1)

associated with an initial data $f^0 : \mathbb{R}^d \to \mathbb{R}$, a final time $\tau$ and a velocity field $u : [0,\tau] \times \mathbb{R}^d \to \mathbb{R}^d$. In fluid problems for instance, we have $d = 2, 3$, while in kinetic formulations $\mathbb{R}^d$ is a phase space with $d \leq 6$, and $u$ is a generalized velocity field with components of velocity and acceleration. We assume that $u$ is smooth enough for the characteristic trajectories $X(t) = X(t,t_0,x_0)$, solutions to

$$X'(t) = u(t,X(t)), \quad X(t_0) = x_0,$$

(2.2)

to be defined on $[0,\tau]$ for all $x_0 \in \mathbb{R}^d$ and $t_0 \in [0,\tau]$, see, e.g., [24]. In particular, the corresponding characteristic flow $F_{t_0,t} : x_0 \mapsto X(t)$ is invertible and satisfies $F_{t,t_0} = (F_{t_0,t})^{-1}$. Solutions to (2.1) read then

$$f(t,x) = f(t_0, (F_{t_0,t})^{-1}(x)) \quad \text{for all } t_0, t \in [0,\tau] \text{ and } x \in \mathbb{R}^d.$$

For simplicity, we restrict ourselves to the incompressible case where $\text{div} \, u = 0$. In this case, the flow is measure preserving in the sense that its Jacobian matrix $J_{F_{t_0,t}}(x) = (\partial_j (F_{t_0,t}))_{1 \leq i,j \leq d}$ has a constant determinant equal to 1,

$$\det (J_{F_{t_0,t}}(x)) = 1 \quad \text{for all } t_0, t \in [0,\tau] \text{ and } x \in \mathbb{R}^d.$$

2.1 The traditional smoothed particle method (TSP)

In the standard “academic” particle method [24], numerical solutions are typically computed as follows: considering deterministic initializations for simplicity, the initial data $f^0$ is first approximated by a collection of particles on a regular (say, cartesian) grid of step $h > 0$,

$$f_{h,x}^0(x) := \sum_{k \in \mathbb{Z}^d} w_k(f^0) \varphi_\epsilon(x - x_k) \quad \text{with } x_k := hk$$

and with weights

$$w_k(f^0) := \int_{x_k + [ -\frac{h}{2}, \frac{h}{2}]^d} f^0(x) \, dx \quad \text{or } \quad w_k(f^0) := h^d f^0(x_k^0).$$

(2.3)

Here $\varphi_\epsilon = \epsilon^{-d} \varphi(\cdot/\epsilon)$ is a particle shape function with radius proportional to $\epsilon$, usually seen as a smooth approximation of the Dirac measure obtained by scaling a compactly supported “cut-off” function $\varphi$ for which a common choice is a B-spline. Particle centers are then updated at each time step $t^n = n\Delta t$ by following the flow $F^n = F_{t^n,t^{n+1}}$ or its numerical approximation, and the weights are kept constant, leading to

$$f_{h,x}^{n+1}(x) := \sum_{k \in \mathbb{Z}^d} w_k(f^n) \varphi_\epsilon(x - x_k^{n+1}) \approx f(t^{n+1},x) \quad \text{with } x_k^{n+1} := F^n(x_k^n).$$

In the classical error analysis [3, 24], the above process is seen as (i) an approximation (in the distribution sense) of the initial data by a collection of weighted Dirac measures, (ii) the exact transport of the Dirac particles along the flow, and (iii) the smoothing of the resulting distribution $\sum_k w_k(f^n) \delta_{x_k^n}$ with the convolution kernel $\varphi_\epsilon$. The classical error estimate reads then as follows: if for some prescribed integers $m > 0$ and $r > 0$, the cut-off $\varphi$ has $m$-th order smoothness and satisfies a moment condition of order $r$, namely if $\int \varphi = 1$, $\int |y|^r |\varphi(y)| \, dy < \infty$ and

$$\int y_1^{s_1} \ldots y_d^{s_d} \varphi(y_1, \ldots, y_d) \, dy = 0 \quad \text{for } s \in \mathbb{N}^d \text{ with } 1 \leq s_1 + \cdots + s_d \leq r - 1,$$

then there exists a constant $C$ independent of $f^0, h$ or $\epsilon$, such that for all $n \leq \tau/\Delta t$ we have

$$\|f(t^n) - f_{h,x}^n\|_{L^p} \leq C(\epsilon^r \|f^0\|_{W^{r,p}} + (h/\epsilon)^m \|f^0\|_{W^{m,p}})$$

(2.4)
with $1 \leq \mu \leq \infty$. More recently, Cohen and Perthame [9] observed that defining the weights as

$$w_k(f^0) := \int_{\mathbb{R}^d} f^0(x) \tilde{\varphi}_h(x - x_k^0) \, dx$$

with a weighting function \( \tilde{\varphi}_h = \tilde{\varphi}(\cdot/h) \) derived from a continuous and compactly supported \( \tilde{\varphi} \) such that

$$\sum_{k \in \mathbb{Z}^d} k_1^{s_1} \cdots k_d^{s_d} \tilde{\varphi}(y - k) = y_1^{s_1} \cdots y_d^{s_d} \quad \text{for } s \in \mathbb{N}^d \text{ with } 0 \leq s_1 + \cdots + s_d \leq m - 1,$$

one has the improved estimate

$$\|f(t^n) - f^0_h\|_{L^\mu} \leq C\left( \varepsilon \|f^0\|_{W^{s,\mu}} + (h/\varepsilon)^m \|f^0\|_{L^\mu}\right)$$

(2.6)

with a new constant that is again independent of \( f^0, h \) or \( \varepsilon \). Note that (2.6) is better than (2.4) in that \( m \) is not constrained by the smoothness of \( f^0 \), which allows to reach higher convergence rates. Indeed balancing the error terms in the above estimates suggests to take \( \varepsilon \sim h^q \) with

$$q = \frac{s}{m+\tau},$$

yielding a convergence in \( h^q \). In particular, if \( f^0 \in W^{s,\mu} \) for some integer \( s \) then the best possible rate with standard weights is only \( h^{s/2} \|f^0\|_{W^{s,\mu}} \), obtained with \( m = r = s \). With the improved weights instead, one can take a higher value for \( m \) and obtain estimates close to \( h^s \|f^0\|_{W^{s,\mu}} \). Moreover, the latter approach also allows to improve (i.e., reduce) the particle overlapping, since the corresponding exponents are \( q = \frac{1}{2} \) and \( \frac{m}{m+\tau} \approx 1 \), respectively. In either case, we see from the term \( h^n \|f^0\|_{W^{s,\mu}} \) in the estimates that extended particle overlapping does not only make the simulations more expensive, it also deteriorates their convergence order.

### 2.2 The forward semi-lagrangian scheme (FSL)

In Forward Semi-Lagragian schemes (the new name for the periodically remapped particle method introduced by Denavit [15]), extended overlapping is usually not required and particles have the same scale than their initialization grid, i.e., \( \varepsilon = h \). Instead, their weights and centers are re-initialized using a regular grid once every \( N_t \) time steps. Thus, denoting by

$$A_h : g \mapsto \sum_{k \in \mathbb{Z}^d} w_k(g) \varphi_h(x - x_k^0)$$

the particle approximation operator with again \( x_k^0 = hk \) and weights computed, e.g., as in (2.3), and by

$$T^n : \varphi_h(\cdot - x_k^n) \mapsto \varphi_h(\cdot - F^n(x_k^n))$$

the fixed-shape particle transport operator, the FSL scheme takes the form

$$f_{h}^{n+1} = \sum_{k \in \mathbb{Z}^d} w_k^{n+1} \varphi_h(\cdot - x_k^{n+1}) := T^n \tilde{f}_{h}^{n} \quad \text{with} \quad \tilde{f}_{h}^{n} := \begin{cases} A_h f_{h}^{n} \quad &\text{if } n \in N_t \mathbb{N} \\ f_{h}^{n} \quad &\text{otherwise}, \end{cases}$$

(2.7)

and where \( T^n \) has been extended to collections of particles by linearity.

### 2.3 The linearly-transformed particle method (LTP)

In this article we shall develop a lesser-known approach already studied by Cohen and Perthame [9] who observed that by transporting the particles with the linearized flow around their trajectories, one obtains a convergent method (in \( L^1 \)) with particles scaled with their initialization grid, and no remappings. On a formal level this amounts to defining linearly-transformed particles as

$$\varphi_{h,k}(t,x) := \varphi_h(J_k(t)(x - x_k(t)))$$

with

$$\begin{cases} x_k(t) := F_{0,t}(x_k) \\
J_k(t) := J_{F_{t,0}}(x_k(t)). \end{cases}$$

(2.8)

In practice, we observe that occasional remappings are needed for accurate solutions. We may then rewrite the numerical LTP scheme in a form similar to (2.7), but particles are now associated with
invertible $d \times d$ deformation matrices $D^n_k$ representing backward Jacobian matrices at $x^n_k$. Thus, numerical solutions read

$$f^n_h(x) = \sum_{k \in \mathbb{Z}^d} w^n_k \varphi^n_{h,k}(x) := \sum_{k \in \mathbb{Z}^d} w^n_k \varphi_h(D^n_k(x - x^n_k))$$ (2.9)

and transporting the particles consists in updating the deformation matrices $D^n_k$ together with the particle centers $x^n_k$, initialized as $D^0_k := I_d$ and $x^0_k := h_k$, respectively. In Section 3.3 we will describe a numerical method for doing so, that is solely based on pointwise evaluations of the (approximated) forward flow $F^n$. We may summarize our findings as follows.

**Main results.** The formal LTP method (2.8) converges with order 1 in $L^\infty$, and arbitrary orders can be reached with proper polynomial deformations which coefficients involve the derivatives of the backward flow (see Theorem 3.2). On the numerical side, an explicit implementation of the LTP transport operator based on finite-difference approximations of the forward Jacobian is also shown to converge with order 1 in $L^\infty$ with no remappings required (see Theorem 3.10). In practice this leads to improved convergence compared to both TSP and FSL schemes, with lower remapping frequencies than the latter (see Section 5.1). Moreover, local error estimates for the single-particle transport errors are established (in Theorem 3.10) that can be used for dynamic refinements in a multilevel particle framework (see Section 5.2).

In the sequel it will be convenient to use the maximum norm $\|x\|_\infty := \max_i |x_i|$ for vectors and the associated $\|A\|_\infty := \max_{ij} |A_{ij}|$ for matrices. For functions in Sobolev spaces $W^{m,\infty}(\omega)$ with $\omega \subset \mathbb{R}^d$ and integer index $m > 0$, we will use the semi-norm

$$|v|_{m,\omega} := \max_i \left\{ \sum_{l_1=1}^d \cdots \sum_{l_m=1}^d \|\partial_{l_1} \cdots \partial_{l_m} v_i\|_{L^\infty(\omega)} \right\},$$ (2.10)

and for conciseness we drop the domain when it is the whole space.

## 3 Particle methods without smoothing

In this section we present a class of particle methods that deviate from the “smoothed” approaches described in Sections 2.1 and 2.2 in the following sense.

- **Convergence** (including high-order) is proved without resorting to a smoothing kernel argument as with TSP schemes. Instead particles have their radius proportional to the meshsize $h$ of their initialization grid, which
  - (i) permits using not only one single particle shape but also heterogeneous collections such as standard finite element bases, as no vanishing moments or high-order smoothness is required;
  - (ii) allows to compute their weights with standard approximation schemes;
  - (iii) yields uniformly bounded numbers of overlapping particles.

- **Remappings** are not required for convergence as in FSL schemes, although they may improve the results in practice.

To simplify the presentation we focus on homogeneous spline particles, although heterogeneous bases could be used, see Remark 3.3 below. Thus, in Section 3.1 we first review one local approximation scheme with B-splines. In Section 3.2 we introduce particle transport operators $T^{(r)}$ with polynomial shape transformations that converge without smoothing arguments, and in Section 3.3 we describe one explicit implementation of the first-order operator $T^{(1)}$. In Section 3.4 we give a practical tool for localizing particles with linearly transformed supports, and in Section 3.5 we establish rigorous error estimates that prove both the uniform convergence and the uniformly bounded overlapping of the deformed particles.
3.1 High-order quasi-interpolations with B-spline particles

For simplicity, we consider homogeneous particles based on tensorized B-splines. Specifically, the univariate cardinal B-splines can be defined recursively as

\[ B_0 := \chi_{\left[ -\frac{1}{2}, \frac{1}{2} \right]} \quad \text{and} \quad B_p(x) := (B_{p-1} * B_0)(x) = \int_{-\frac{1}{2}}^{x+\frac{1}{2}} B_{p-1} \quad \text{for} \quad p \geq 1, \]

where \( \chi \) denotes the set characteristic function. Clearly, \( B_p \) is a piecewise polynomial of degree \( p \), it is globally \( C^{p-1} \) and supported on \( [-\frac{p+1}{2}, \frac{p+1}{2}] \). Moreover its integer translations span the space of cardinal splines of degree \( p \), see, e.g., \cite{13}. Thus \( B_1(x) = \max(1 - |x|, 0) \) is the traditional “hat-function”, \( B_3 \) is the centered cubic B-spline, and so on. Our reference particle shape function will be the tensorized, centered B-spline of odd degree \( p \),

\[ \varphi(x) := \prod_{i=1}^{d} B_p(x_i) \quad \text{supported on} \quad \text{supp}(\varphi) = [-c_p, c_p]^d \quad \text{with} \quad c_p := \frac{p+1}{2}. \quad (3.1) \]

Note that B-splines of odd degree are refinable on dyadic grids, which will be used in Section 4 to reformulate our particle method in a multilevel framework.

Since our particles are scaled with their initialization (or remapping) grid, we can use standard approximation schemes that rely on the fact that the span of their integer translates

\[ \varphi_{h,k}^p(x) = \varphi_h(x - x_0^p) = h^{-d} \varphi(h^{-1} x - k), \quad k \in \mathbb{Z}^d, \quad (3.2) \]

contains the space \( P_p \) of polynomials with coordinate degree less or equal to \( p \). Specifically, we shall consider quasi-interpolation schemes described by \cite{8} and \cite{25}, where high-order B-spline approximations are locally obtained by pointwise evaluations of the target function. In the univariate case they take the form

\[ A_h^{(1d)} : g \mapsto \sum_{k \in \mathbb{Z}} w_k(g) \varphi_{h,k}^0 \quad \text{with normalized weights} \quad w_k(g) := h^d \sum_{|l| \leq m_p} a_l g(x_{k+l}^0) \]

and symmetric coefficients \( a_l = a_{-l} \) defined in such a way that \( A_h^{(1d)} \) reproduces the space \( P_p^{(1d)} \). They can be computed with the iterative algorithm in \cite{8} Section 6: for the first orders we obtain

- \( m_p = 0 \) and \( a_0 = 1 \) for \( p = 1 \),
- \( m_p = 1 \) and \( (a_0, a_1) = (\frac{5}{6}, -\frac{1}{6}) \) for \( p = 3 \),
- \( m_p = 4 \) and \( (a_0, a_1, a_2, a_3, a_4) = (\frac{204}{225}, -\frac{1469}{225}, \frac{7}{225}, \frac{13}{3600}, \frac{1}{3600}) \) for \( p = 5 \).

In the multivariate case we can tensorize the above, as it is easily checked that the operator

\[ A_h : g \mapsto \sum_{k \in \mathbb{Z}^d} w_k(g) \varphi_{h,k}^0 \quad \text{with} \quad w_k(g) := h^d \sum_{|l| \leq m_p} a_l g(x_{k+l}^0), \quad a_l := \prod_{1 \leq i \leq d} a_{l_i} \quad (3.3) \]

reproduces any polynomial \( \pi \in P_p \). Moreover, we have

\[ \|A_h g\|_{L^\infty} \leq (2c_p)^d \|\varphi_h\|_{L^\infty} \sup_{k \in \mathbb{Z}^d} |w_k(g)| \leq (2c_p)^d \|\varphi\|_{L^\infty} \|a\|_{\ell^1} \|g\|_{L^\infty} \quad (3.4) \]

with \( \|a\|_{\ell^1} = \sum_{\|l\|_{\ell^\infty} \leq m_p} |a_l| \), by using the fact that no more than \( (2c_p)^d \) B-splines overlap. It follows that \( A_h \) is uniformly bounded in \( L^\infty \), with

\[ \|A_h\|_{L^\infty} := \sup_{g \neq 0} \frac{\|A_h g\|_{L^\infty}}{\|g\|_{L^\infty}} \leq (2c_p)^d \|\varphi\|_{L^\infty} \|a\|_{\ell^1}. \]

Using a localized version of (3.4), we write that for an arbitrary \( \pi \in P_q, q \leq p \),

\[ \|A_h g - g\|_{L^\infty(B_\infty(x_0^p, h))} \leq \|A_h(g - \pi)\|_{L^\infty(B_\infty(x_0^p, h))} + \|g - \pi\|_{L^\infty(B_\infty(x_0^p, h))} \leq \left( \|A_h\|_{L^\infty} + 1 \right) \|g - \pi\|_{L^\infty(B_\infty(x_0^p, h+c_p))} \]

where \( B_\infty(x, \rho) \) denotes the open cube of center \( x \) and radius \( \rho \). Taking for \( \pi \) the \( q \)-th Taylor expansion of \( g \) around \( x_k \), we thus find for all \( q \leq p \),

\[ \|A_h g - g\|_{L^\infty} \leq h^{q+1} c_A |g|_{q+1} \quad \text{with} \quad c_A = \left( \|A_h\|_{L^\infty} + 1 \right) (m_p + c_p)^{q+1} / (q + 1)! . \quad (3.5) \]
3.2 High-order particle transport with polynomial shape transformations

We now address the problem of transporting a collection of particles

\[ f_h^0 = \sum_{k \in \mathbb{Z}^d} w_k \phi_{h,k}^0 \approx f^0 \]

along the flow \( F = F_{0,\tau} \) associated with the whole time domain, with no remappings. Here we consider particles initially centered on the cartesian grid \([3.2]\), with weights satisfying

\[ |w_k| \leq c_w h^d \| f^0 \|_{L^\infty}, \quad k \in \mathbb{Z}^d \]  

(3.6)

with a fixed \( c_w > 0 \), as it should be with any standard approximation scheme (if \( f_h^0 = A_h f^0 \) we can take \( c_w = \| a \|_{L^1} \)). Moreover, to simplify the analysis we begin by forgetting the time discretization and consider that \( F \) is known and can applied exactly. (In Section 3.3 we will take into account the time approximation errors to study a discrete particle scheme.) Thus, in the traditional method which does not move. Since the other particles do not contribute to \( x \) with \( \theta \)

Since the exact transport operator reads

\[ T = T_{(0)} : \phi_{h,k}^0 \mapsto \phi_{h}(-\bar{x}_k) \quad \text{where} \quad \bar{x}_k := F(x_k^0). \]  

(3.7)

Since the exact transport operator reads

\[ T_{ex} : g \mapsto g(F^{-1}(-)), \]  

(3.8)

the approximation \([3.7]\) is exact for point (Dirac) particles. For finite-size particles however, the method does not converge. Take indeed \( p = 1 \) (i.e., \( \phi \) is the standard hat function), and consider the infinitely smooth problem where \( f^0 = 1 \) and \( u(t,x) = (-x_2,x_1) \) in two dimensions, over the time interval \([0, \frac{\pi}{2}]\). Then any reasonable initialization will give \( w_k = h^2 \), hence, \( f_h^0(x) = 1 \), and clearly the exact final solution is \( f(\frac{\pi}{2}, x) = 1 \). Now, at the final time the particle centers will have rotated of \( \tau = \frac{\pi}{4} \), therefore every particle with \( |k_1| + |k_2| = 1 \) will be centered on \((\cos(\theta + \frac{\pi}{4}), \sin(\theta + \frac{\pi}{4}))\) with \( \theta \in \frac{\pi}{2} \mathbb{N} \), and hence contributes to \( x = 0 \) with \( T_{(0)} \phi_{h,k}^0(0) = h^{-2}(1 - \frac{1}{\sqrt{2}})^2 \), in addition to \( \phi_{h,0} \) which does not move. Since the other particles do not contribute to \( x = 0 \), the final error satisfies

\[ \| (T_{(0)} - T_{ex}) f_h^0 \|_{L^\infty} \geq |T_{(0)} f_h^0(0) - 1| = 2(\sqrt{2} - 1)^2, \]  

regardless of \( h \).

To improve the accuracy of the transport operator we shall estimate its error, using as basic property that the transported particles are localized by a relation

\[ \text{supp}(T \phi_{h,k}^0) \subset B_{\infty}(\bar{x}_k, h\hat{\rho}_{h,k}), \]  

(3.9)

with radius factors uniformly bounded by \( \hat{\rho} := \sup_{h>0,k \in \mathbb{Z}^d} \hat{\rho}_{h,k} < \infty \). This clearly holds for \( T_{(0)} \), taking \( \hat{\rho}_{h,k} = c_p = \hat{\rho} \). If \( T \) is such that \([3.9]\) holds, then the particles overlap in a bounded way. Indeed for all \( x,k \) such that \( T \phi_{h,k}^0(x) \neq 0 \) we have \( \| k - h^{-1}F^{-1}(x) \|_{\infty} \leq h^{-1}|F^{-1}|_1 \| \bar{x}_k - x \|_{\infty} < \hat{\rho}_{h,k}|F^{-1}|_1 \), hence we may define an overlapping constant that satisfies

\[ \Theta := \sup_{h>0} \sup_{x \in \mathbb{R}^d} \# \{ k \in \mathbb{Z}^d : T \phi_{h,k}^0(x) \neq 0 \} \leq (2\hat{\rho}|F^{-1}|_1)^d. \]  

(3.10)

Moreover, it is easily seen that the particles transported with the exact operator \([3.8]\) also have a bounded overlapping constant: if \( k \) is such that \( T_{ex} \phi_{h,k}^0(x) \neq 0 \) then obviously \( \| k - h^{-1}F^{-1}(x) \|_{\infty} < c_p \), hence

\[ \Theta_{ex} := \sup_{h>0} \sup_{x \in \mathbb{R}^d} \# \{ k \in \mathbb{Z}^d : T_{ex} \phi_{h,k}^0(x) \neq 0 \} \leq (2c_p)^d. \]

In particular, we can decompose the global error \((T - T_{ex}) f_h^0\) in terms of local (single-particle) transport errors \( e_{h,k} = (T - T_{ex}) \phi_{h,k}^0 \), as

\[ \| (T - T_{ex}) f_h^0 \|_{L^\infty} \leq \hat{\Theta} \sup_{k \in \mathbb{Z}^d} \| w_k e_{h,k} \|_{L^\infty} \leq h^d c_w \| f^0 \|_{L^\infty} \hat{\Theta} \sup_{k \in \mathbb{Z}^d} \| e_{h,k} \|_{L^\infty} \]  

(3.11)
holds with $\hat{\Theta} := \Theta + \Theta_{ex}$, where we have used (3.6). We next localize the particles transported with the exact operator by writing

$$T_{ex}\varphi^0_{h,k}(x) \neq 0 \implies F^{-1}(x) \in \Sigma^0_{h,k} := \text{supp}(\varphi^0_{h,k}) = B_\infty(x^0_k, hc_p)$$

$$\implies \|x - \bar{x}_k\|_\infty \leq \|F|_{1,\Sigma^0_{h,k}}\|F^{-1}(x) - x^0_k\|_\infty < hc_p|F|_{1,\Sigma^0_{h,k}},$$

so that

$$\text{supp}(T_{ex}\varphi^0_{h,k}) = F(\Sigma^0_{h,k}) = F(B_\infty(x^0_k, hc_p)) \subset B_\infty(\bar{x}_k, hc_p|F|_{1,\Sigma^0_{h,k}}).$$  \hspace{1cm} (3.12)

Hence the localization $\text{supp}(\epsilon_{h,k}) \subset B_\infty(\bar{x}_k, h\tilde{\rho}_{h,k})$ for the error terms, with a new factor $\tilde{\rho}_{h,k} := \max\{\tilde{\rho}_{h,k}, cp|F|_1\} \leq \tilde{\rho} := \max\{\tilde{\rho}, cp|F|_1\}$. In the case of particle translations, i.e., for $T = T(0)$, it follows that

$$\|\epsilon_{h,k}\|_\infty = \sup_{x \in B_\infty(\bar{x}_k, h\tilde{\rho}_{h,k})} |\varphi_h(x - \bar{x}_k) - \varphi_h(F^{-1}(x) - x^0_k)|$$

$$\leq |\varphi_h|_1 \sup_{x \in B_\infty(\bar{x}_k, h\tilde{\rho}_{h,k})} \|F^{-1}(x) - (F^{-1}(\bar{x}_k) - \bar{x}_k)\|_\infty$$

$$\leq h^{-d} \tilde{\rho}_{h,k} |\varphi|_1 |F^{-1} - I|_{1,B_\infty(\bar{x}_k, h\tilde{\rho}_{h,k})}$$

where we have used the scaling $|\varphi_h|_1 \approx h^{-d-1} |\varphi|_1$, see (3.2). Thus, we find

$$\|(T(0) - T_{ex})f^0_h\|_\infty \leq c_w |\varphi|_1 |\hat{\Theta}|_1 |F^{-1} - I|_1\|f^0\|_\infty$$

for the fixed-shape particle method. Note that we can take $\hat{\Theta} = (2c_p)^d (1 + |F^{-1}|^d_1)$ and $\tilde{\rho} = cp|F|_1$ in the above estimate, indeed $\det(J_F(x)) = 1$ valid for all $x$ gives $1 \leq \|J_F(x)\|_\infty \leq |F|_1$. Not surprisingly, the above analysis fails short of proving the convergence of the method. But it suggests one way to improve its accuracy: letting indeed

$$\phi_k(s) = \phi_k(s; x) := (F^{-1} - I)(\bar{x}_k + s(x - \bar{x}_k))$$  \hspace{1cm} (3.14)

we may see the approximation $(F^{-1}(x) - x) \approx (F^{-1}(\bar{x}_k) - \bar{x}_k)$ involved in (3.13) as a zero-order Taylor expansion $\phi_k(1) \approx \phi_k(0)$, and consider replacing $\varphi_h(x - \bar{x}_k)$ by $\varphi_h(\Phi_{k,(r)}(x))$, $r \geq 1$, where

$$\Phi_{k,(r)}(x) := x - \bar{x}_k + \phi^{(r)}_k(0) + \cdots + \frac{1}{r!} \phi^{(r)}_k(0) \approx \Phi_{k,ex}(x) := F^{-1}(x) - x^0_k$$  \hspace{1cm} (3.15)

is formally an $r$-th order approximation. One could also consider expansions of the alternate $\hat{\phi}_k(s) := (I - F)(x^0_k + s(F^{-1}(x) - x^0_k))$ since $\phi_k(1) - \phi_k(0) = \phi_k(1) - \phi_k(0)$, but the particular form of (3.14) gives

$$\phi^{(r)}_k(s) = \sum_{l_1=1}^{d} \cdots \sum_{l_r=1}^{d} \left[ \partial_{l_1} \cdots \partial_{l_r}(F^{-1} - I)\bar{x}_k + s(x - \bar{x}_k) \right]^{r} \sum_{i=1}^{r}(x - \bar{x}_k)_{l_i},$$  \hspace{1cm} (3.16)

so that $\Phi_{k,(r)}$ is a polynomial mapping which coefficients involve evaluations of space derivatives of $F^{-1}$ at $\bar{x}_k$, which can be written in terms of the derivatives of $F$, at $F^{-1}(\bar{x}_k) = x^0_k$. Also, (3.16) allows to specify the accuracy of the Taylor expansions (3.15) as follows: for all $r \geq 1$ and every $x$ in a localized domain $\omega \subset B_\infty(\bar{x}_k, h\rho)$ with $\rho > 0$, we have

$$\|\Phi_{k,(r)}(x) - \Phi_{k,ex}(x)\|_\infty = \left\| \int_0^1 \left(\frac{1}{r!} \phi^{(r+1)}_k(s) ds \right) \right\|_\infty \leq h^{r+1} \frac{(\rho)^{r+1}}{(r+1)!} |F^{-1}|_{r+1,\omega}$$

(3.17)

where $\langle \omega \rangle$ denotes the convex hull of $\omega$.

For $r = 1$ we observe that $J_{F^{-1}}(\bar{x}_k) = (J_F(x^0_k))^{-1}$ is the Jacobian matrix of the backward flow, or equivalently, the matrix inverse of the forward Jacobian. The linearly-transformed particles are then defined as

$$T_{(1)}\varphi^0_{h,k}(x) := \varphi_h(\Phi_{k,(1)}(x)) = \varphi_h(J_k(x - \bar{x}_k)) \quad \text{with} \quad \begin{cases} \bar{x}_k := F(x^0_k) \\ J_k := (J_F(x^0_k))^{-1}. \end{cases}$$  \hspace{1cm} (3.18)
Since $\Phi_{k,(r)}$ is invertible the particles have a parallelogram support localized with
\[
\text{supp}(T(1)\varphi_{h,k}^0) = \bar{x}_k + J^{-1}_k(B_\infty(0,hc_p)) \subset B_\infty(\hat{\rho}_h,k, hc_p||J^{-1}_k||_\infty),
\]
i.e., (3.9) now holds with $\hat{\rho}_h,k = c_p||J^{-1}_k||_\infty \leq c_p F_1 = \hat{\rho}$. As a consequence the above analysis applies readily to $T(1)$, the only noticeable change being that instead of (3.13) we now write
\[
\|e_{h,k}\|_{L^\infty} = \sup_{x \in B_\infty(\bar{x}_h,k,\hat{\rho}_h,k)} |\varphi_h(\Phi_{k,(1)}(x)) - \varphi_h(\Phi_{k,ex}(x))|
\leq |\varphi_h|_1 \sup_{x \in B_\infty(\bar{x}_h,k,\hat{\rho}_h,k)} \|\Phi_{k,(1)}(x) - \Phi_{k,ex}(x)\|_\infty \leq h^{-(d-1)}(\bar{\rho}_h,k)^2 |\varphi_h|_1 |F^{-1}|_{2,B_\infty(\bar{x}_h,k,\hat{\rho}_h,k)}
\]
with $\bar{\rho}_h,k = c_p \max\{||J^{-1}_k||_\infty, |F|_{1,\Sigma^0_{h,k}}\} = c_p |F|_{1,\Sigma^0_{h,k}}$. Using (3.11) and (3.10) we thus find
\[
\| (T(1) - T_{ex}) f^0_h \|_{L^\infty} \leq h^{\frac{d}{2}} \hat{\Theta} c_{w,1} |\varphi_h|_1 |F^{-1}|_{2} \| f^0 \|_{L^\infty}
\]
for the formal LTP scheme, with $\hat{\rho} = c_p |F|_1$ and $\hat{\Theta} = (2 c_p)^d (1 + |F^{-1}|_1^2 |F|_1^2)$. 

**Remark 3.1.** When applied to a particle with general shape and support containing $x_k^0$, the LTP transport operator is defined as the exact transport for the linearized flow
\[
F_{x_k^0} : x \mapsto F(x_k^0) + J_F(x_k^0)(x - x_k^0),
\]
i.e., we set $T(1)\varphi_{h,k}^0 := T_{ex}[F_{x_k^0}]\varphi_{h,k}^0 = \varphi_{h,k}^0 \circ (F_{x_k^0})^{-1}$.

For larger values of $r$, care must be taken when defining $T(r)$. Indeed, $\Phi_{k,(r)}$ may not be invertible hence there is no guarantee that $\| x - \bar{x}_k \|_\infty \lesssim h$ in the support of $\varphi_h(\Phi_{k,(r)})$. To overcome this we define the transported particle as being restricted to some domain $\bar{\Sigma}_{h,k}$ that is a priori bounded, i.e., we set
\[
T(r)\varphi_{h,k}^0(x) = \varphi_h(\Phi_{k,(r)}(x))\chi_{\bar{\Sigma}_{h,k}}(x),
\]
where again $\Phi_{k,(r)}$ is the polynomial mapping defined by (3.15) and (3.16) and $\chi$ denotes the set characteristic function. To determine $\bar{\Sigma}_{h,k}$ we next observe that in order to carry out the error analysis, a convenient property is that
\[
F(\Sigma^0_{h,k}) \subset \bar{\Sigma}_{h,k} \subset B_\infty(\bar{x}_k,h\bar{\rho}_{h,k})
\]
for some $\bar{\rho}_{h,k}$. Indeed, from (3.12) this would give supp$(e_{h,k}) \subset \bar{\Sigma}_{h,k}$ and
\[
\|e_{h,k}\|_{L^\infty} = \sup_{x \in \bar{\Sigma}_{h,k}} |\varphi_h(\Phi_{k,(r)}(x)) - \varphi_h(\Phi_{k,ex}(x))| 
\leq |\varphi_h|_1 \sup_{x \in B_\infty(\bar{x}_h,k,\hat{\rho}_h,k)} \|\Phi_{k,(r)}(x) - \Phi_{k,ex}(x)\|_\infty \leq h^{-d} |\varphi_h|_1 (\hat{\rho}_h,k)^{r+1} |F^{-1}|_{r+1,B_\infty(\bar{x}_h,k,\hat{\rho}_h,k)}.
\]
Using (3.12) we see that an obvious solution to (3.21) is obtained with
\[
\bar{\Sigma}_{h,k} := B_\infty(\bar{x}_k,h\bar{\rho}_{h,k}) \quad \text{with} \quad \bar{\rho}_{h,k} := c_p |F|_{1,\Sigma^0_{h,k}}.
\]
However, one may want to restrict the particles to parallelogram supports that are closer to $F(\Sigma^0_{h,k})$ than the upper bound $B_\infty(\bar{x}_k,\hat{\rho}_{h,k})$. To this end we observe that for any $x \in F(\Sigma^0_{h,k})$, applying (3.17) gives
\[
\|\Phi_{k,(1)}(x)\|_\infty \leq \|F^{-1}(x) - x_k^0\|_\infty + \|\Phi_{k,(1)}(x) - \Phi_{k,ex}(x)\|_\infty \leq hc_p (1 + \lambda)
\]
as long as
\[
\lambda \geq \frac{1}{2} hc_p |F|_{1,\Sigma^0_{h,k}} |F^{-1}|_{2,F(\Sigma^0_{h,k})}.
\]
It follows that a finer solution to (3.21) is given by
\[
\left\{ \begin{array}{l}
\bar{\Sigma}_{h,k} := (\Phi_{k,(1)})^{-1}(B_\infty(0, hc_p (1 + \lambda))) = \bar{x}_k + (J_k)^{-1}(B_\infty(0, hc_p (1 + \lambda))) \\
\bar{\rho}_{h,k} := c_p |F|_{1,\Sigma^0_{h,k}} (1 + \lambda).
\end{array} \right.
\]
In either case, global estimates are easily derived from the above discussion.
Theorem 3.2. As above we consider B-spline particles (3.1)-(3.2) initially centered on regular nodes, and denote by \( F = F_{0,T} \) the exact characteristic flow associated with the transport equation (2.1). We let \( T_{(r)} \) be the \( r \)-th order particle transport operator defined as (3.18) for \( r = 1 \), or as (3.20) for \( r \geq 2 \), with restriction domain given by (3.23) or (3.24). In the latter case we take \( \lambda \geq \frac{1}{2}h_{cp}|F|_{2}^{-1}|F^{-1}|_{2} \), otherwise we set \( \lambda := 0 \). Then the transported particles are localized by

\[
\text{supp}(T_{(r)}\phi_{h,k}^{0}) \subset B_{\infty}(F(x_{k}^{0}), \hat{\rho}) \quad \text{with} \quad \hat{\rho} = c_{p}|F|_{1}(1 + \lambda)
\]

and their overlapping constant satisfies

\[
\Theta := \sup_{x \in \mathbb{R}^{d}} \# \{ \{ k \in \mathbb{Z}^{d} : T_{(r)}\phi_{h,k}^{0}(x) \neq 0 \} \} \leq (2\hat{\rho}|F^{-1}|_{1})^{d}.
\]

Moreover, the global transport error satisfies

\[
\| (T_{(r)} - T_{\text{ex}})f_{h}^{0} \|_{L_{\infty}} \leq h^{r}c_{w}|\phi|_{1} \hat{\Theta} \frac{(\hat{\rho})^{r+1}}{(r+1)!}|F^{-1}|_{r+1}\|f^{0}\|_{L_{\infty}}
\]

where \( \hat{\Theta} = (2c_{p})^{d} + \Theta \), and where \( c_{w} \) is the constant from (3.6).

Remark 3.3 (heterogeneous “particle” approximations). As previously pointed out, our arguments do not rely on a smoothing kernel unlike classical analysis of particle methods [3, 24], and the above estimates readily extend to the heterogeneous case where the “particles” \( \phi_{h,k} \) are not derived from a reference \( \phi \) but instead are defined as piecewise polynomials with global continuity constraints (e.g., standard finite element bases) on unstructured meshes of \( \mathbb{R}^{d} \), under the usual shape regularity and quasi-uniformity assumptions.

### 3.3 A finite difference implementation of the LTP method

We now describe and analyze an implementation of the particle transport operator \( T_{(1)} \) that only requires pointwise evaluations of some forward numerical flow

\[
F^{n} \approx F_{\text{ex}}^{n} = F_{\text{ex},n+1},
\]

given by an explicit solver for the ODE (2.2) over the time step \([t^{n}, t^{n+1}]\). Specifically, we consider the following approximations. First, the exact transport operator

\[
T_{\text{ex}}^{n} = T_{\text{ex}}[F_{\text{ex}}^{n}] : \phi_{h,k}^{n} \mapsto \phi_{h,k}^{n} \circ (F_{\text{ex}}^{n})^{-1},
\]

when applied to a linearly transformed particle \( \phi_{h,k}^{n} = \phi_{h}(D_{k}^{n}(\cdot - x_{k}^{n})) \) as in (2.9), is approached by the LTP transport operator according to Remark 3.1, i.e.,

\[
T_{(1)}[F_{\text{ex}}^{n}] : \phi_{h,k}^{n} \mapsto \phi_{h}(D_{k}^{n}J_{k,\text{ex}}^{n}(\cdot - F_{\text{ex}}^{n}(x_{k}^{n}))) \quad \text{with} \quad J_{k,\text{ex}}^{n} = (J_{F_{\text{ex}}^{n}}(x_{k}^{n}))^{-1}.
\]

The Jacobian matrices involved in the latter are then approached by a finite difference scheme, and finally the values of \( F_{\text{ex}}^{n} \) are replaced by those of the numerical flow \( F^{n} \). Thus, we set

\[
T_{h} : \phi_{h,k}^{n+1} \mapsto \phi_{h,k}^{n+1} = \phi_{h}(D_{h,k}^{n+1}(\cdot - x_{k}^{n+1}))
\]

with \( x_{k}^{n+1} := F^{n}(x_{k}^{n}) \) and \( D_{k}^{n+1} := D_{k}^{n}J_{k}^{n} \). Here \( J_{k}^{n} \approx (J_{F_{\text{ex}}^{n}}(x_{k}^{n}))^{-1} \) is a numerical approximation of the backward Jacobian matrix obtained by first approximating the forward Jacobian by a centered finite difference scheme,

\[
(\hat{J}_{k}^{n})_{i,j} := (2h)^{-1} \left( (F^{n})_{i}(x_{k}^{n} + he_{j}) - (F^{n})_{i}(x_{k}^{n} - he_{j}) \right) \approx \partial_{j}(F^{n})_{i}(x_{k}^{n})
\]

for \( i, j = 1, \ldots, d \), and then letting

\[
J_{k}^{n} := \det(\hat{J}_{k}^{n})^{\frac{1}{2}}(\hat{J}_{k}^{n})^{-1} \quad \text{or simply} \quad J_{k}^{n} := (\hat{J}_{k}^{n})^{-1},
\]

whether we want a conservative transport (i.e., where \( \int T_{h} \phi_{h,k}^{n} = \int \phi_{h,k}^{n} \)), or not.

Note that \( \det(J_{F_{\text{ex}}^{n}}) = 1 \) on \( \mathbb{R}^{d} \), therefore it is reasonable to assume that the \( d \times d \) matrix \( \hat{J}_{k}^{n} \) is invertible. In the following Lemma we establish a sufficient condition for this, together with some a priori estimates for the resulting approximations.
Lemma 3.4. Let \( e_{\Delta t}^n := \| F^n - F^n_{\text{ex}} \|_{L^\infty} \) be the error of the ODE solver, and write
\[
\mu_{1,k}^n := \| F^n_{\text{ex}} \|_{1,B_{h,k}^n} + h^{-1} d e_{\Delta t}^n, \quad \mu_{2,k}^n := \frac{1}{2} \| F^n_{\text{ex}} \|_{2,B_{h,k}^n} + d h^{-2} e_{\Delta t}^n,
\]
where \( B_{h,k}^n := B_{\infty}(x_k^n, h) \). Then the approximated Jacobian \( \tilde{J}_k^n \) is defined in (3.29) satisfies
\[
\| J_k^n - J(F^n_{\text{ex}}) \|_{\infty} \leq 2 d^2 h \mu_{2,k}^n (\theta_k^n)^{-2} (\mu_{1,k}^n)^{2(d-1)}
\]
and
\[
\| (J_k^n)^{-1} - J(F^n_{\text{ex}}) \|_{\infty} \leq h \mu_{2,k}^n \left( 1 + (\theta_k^n)^{-\frac{d+1}{d}} (\mu_{1,k}^n)^d \right)
\]
provided \( \theta_k^n > 0 \). In particular, for all \( \rho \geq 0 \) we have
\[
\sup_{x \in B_{\infty}(x_k^n, \rho h)} \| J_k^n (x - x_k^n) - (F^n_{\text{ex}})^{-1} (x - x_k^n) \|_{\infty} \leq h^2 C_{h,k}(\rho)
\]
with
\[
C_{h,k}(\rho) = 2 d^2 \rho \mu_{2,k}^n (\theta_k^n)^{-2} (\mu_{1,k}^n)^{2(d-1)} + \mu_{2,k}^n (\mu_{1,k}^n)^{d-1} + \frac{1}{2} \rho^2 \| (F^n_{\text{ex}})^{-1} \|_{1,2,B_{\infty}(x_k^n, \rho h)}
\]

Proof. For conciseness, we denote
\[
J^{n,\text{ex}}_k = J(F^n_{\text{ex}})^{-1}(F^n_{\text{ex}}(x_k^n)), \quad \tilde{J}^{n,\text{ex}}_k = J(F^n_{\text{ex}})^{-1}(x_k^n), \quad \tilde{J}^{n,*}_k = \left( \frac{(F^n_{\text{ex}}(x_k^n + h \epsilon_j))^2 - (F^n_{\text{ex}}(x_k^n))^2}{2h} \right)_{1 \leq i,j \leq d}
\]
The latter is the finite difference approximation of \( \tilde{J}^{n,*}_k \) obtained by substituting \( F^n \) by \( F^n_{\text{ex}} \) in (3.28), so that \( \| \tilde{J}^{n,*}_k - J^n_k \|_{\infty} \leq h^{-1} d e_{\Delta t}^n \). We observe that with the semi-norms (2.10) we have
\[
\| J^{n,\text{ex}}_k \|_{\infty}, \| \tilde{J}^{n,*}_k \|_{\infty} \leq \| F^n_{\text{ex}} \|_{1,1,B_{h,k}^n}
\]
hence
\[
\| J_k^n \|_{\infty} \leq \| \tilde{J}^{n,*}_k \|_{\infty} + \| J_k^n - J^{n,\text{ex}}_k \|_{\infty} \leq \| F^n_{\text{ex}} \|_{1,1,B_{h,k}^n} + h^{-1} d e_{\Delta t}^n = \mu_{1,k}^n.
\]
Next we write two Taylor formulas for \( s \mapsto F^n_{\text{ex}}(x_k^n + s \epsilon_j) \) with \( j = 1, \ldots, d \), namely
\[
F^n_{\text{ex}}(x_k^n + \sigma h \epsilon_j) = F^n_{\text{ex}}(x_k^n) + \sigma h \partial \sigma F^n_{\text{ex}}(x_k^n) + \int_0^{\sigma h} (\sigma h - s) \partial^2 \sigma F^n_{\text{ex}}(x_k^n + s \epsilon_j) ds, \quad \sigma = \pm 1.
\]
By taking their difference we obtain
\[
\| \tilde{J}^{n,*}_k - \tilde{J}^{n,\text{ex}}_k \|_{\infty} \leq \frac{1}{2} h \| F^n_{\text{ex}} \|_{2,2,B_{h,k}^n},
\]
Using det(\( \tilde{J}^{n,\text{ex}}_k \)) = 1 and the multilinearity of the determinant, we then find
\[
| \det(\tilde{J}^{n,\text{ex}}_k) - 1 | \leq d \| \tilde{J}^{n,\text{ex}}_k \|_{\infty} \max \{ \| \tilde{J}^{n,*}_k \|_{\infty}, \| \tilde{J}^{n,\text{ex}}_k \|_{\infty} \}^{d-1} \leq d \mu_{2,k}^n (\mu_{1,k}^n)^{d-1}
\]
which shows (3.30). From the cofactor's formula \( A^{-1} = \det(A)^{-1} C^t \) involving the transposed cofactor matrix we next write for \( \theta_k^n > 0 \)
\[
\| J_k^n \|_{\infty} \leq d \|\tilde{J}^{n,\text{ex}}_k \|_{\infty} \| \tilde{J}^{n,\text{ex}}_k \|_{\infty} \leq d \| F^n_{\text{ex}} \|_{1,1,B_{h,k}^n} \leq d (\mu_{1,k}^n)^{d-1}
\]
where we have used \( J^{n,\text{ex}}_k = (\tilde{J}^{n,\text{ex}}_k)^{-1} \). Similarly, we have
\[
\| (\tilde{J}^{n,\text{ex}}_k)^{-1} \|_{\infty} \leq d \|\tilde{J}^{n,\text{ex}}_k \|_{\infty} \| \tilde{J}^{n,\text{ex}}_k \|_{\infty} \leq d (\theta_k^n)^{-1} (\mu_{1,k}^n)^{d-1}
\]
hence in the non-conservative case, the approximated Jacobian satisfies
\[ \|J^n_k - J^n_{\text{ex},k}\|_\infty \leq \|J^{n,\text{ex}}_k\|_\infty \|\tilde{J}^n_k - \tilde{J}^{n,\text{ex}}_k\|_\infty \|J^n_k\|_\infty \leq d^2 h \mu^n_{2,k}(\theta^n_k)^{-1}(\mu^n_{1,k})^{2(d-1)}. \]

For the conservative case, we infer from \( \theta^n_k \leq \min\{1, \det(\tilde{J}^n_k)\} \) that for \( \alpha \leq 1 \),
\[ |1 - \det(\tilde{J}^n_k)^\alpha| = \left| \int_1^{\det(\tilde{J}^n_k)^\alpha} \alpha z^{\alpha-1} \, dz \right| \leq |\alpha|(|\theta^n_k|^{\alpha-1}|1 - \det(\tilde{J}^n_k)|. \] (3.38)

Taking \( \alpha = \frac{1}{d} \), we then obtain
\[ \|J^n_k - J^n_{\text{ex},k}\|_\infty = \|\det(\tilde{J}^n_k)^{-\frac{1}{d}}(\tilde{J}^n_k)^{-1} - (\tilde{J}^{n,\text{ex}}_k)^{-1}\|_\infty \]
\[ \leq |\det(\tilde{J}^n_k)^{-\frac{1}{d}} - 1||\tilde{J}^n_k\|_\infty + ||(\tilde{J}^{n,\text{ex}}_k)^{-1}\|_\infty ||J^n_k - \tilde{J}^{n,\text{ex}}_k||_\infty \]
\[ \leq dh \mu^n_{2,k}(\mu^n_{1,k})^{2(d-1)}((\theta^n_k)^{-\frac{1}{d} - 2} + d(\theta^n_k)^{-1}). \]

Estimate (3.31) is then easily derived from the above inequalities, using \( d \geq 1 \) and \( \theta^n_k \leq 1 \). Next, we note that (3.35) gives \( \|J^n_k\|^{-1} - (J_{\text{ex},k})^{-1}\|_\infty \leq h \mu^n_{2,k} \) in the non-conservative case, while in the conservative case it gives
\[ \|((J^n_k)^{-1} - (J^n_{\text{ex},k})^{-1})\|_\infty \]
\[ \leq |\det(\tilde{J}^n_k)^{-\frac{1}{d}} - 1||\tilde{J}^n_k\|_\infty + ||(\tilde{J}^{n,\text{ex}}_k)^{-1}\|_\infty \]
\[ \leq h \mu^n_{2,k}(\theta^n_k)^{-\frac{1}{d} - 1}(\mu^n_{1,k})^{d}) \]
where we have used (3.38) with \( \alpha = -\frac{1}{d} \), together with (3.36), (3.34). This shows that (3.32) is valid in both cases. To complete the proof we finally write
\[ \|J^n_k(x - x^{n+1}_k) - (F^n(x^{n+1}_k) - F^n(x^n_k))\|_\infty \leq \|J^n_k - J^n_{\text{ex},k}\|(x - x^{n+1}_k)\|_\infty \]
\[ + \|J^n_{\text{ex},k}(F^n(x^{n+1}_k) - F^n(x^n_k))\|_\infty + \|J^n_{\text{ex},k}(x - F^n(x^n_k))\|_\infty \]
\[ \leq 2h^2 d^2 \rho h^n \mu^n_{2,k}(\theta^n_k)^{-2}(\mu^n_{1,k})^{2(\nu-1)} + d(\mu^n_{1,k})^{d-1}e^n_{\Delta t} + \frac{(h \rho)^2}{2}(F^n)^{-1}_{2,B_\infty(x^{n+1}_k,\rho h)} \]
where we have used \( x^{n+1}_k = F^n(x^n_k) \) in the first inequality and (3.17) with \( r = 1 \) in the second one.

3.4 Intermission: localization of particles with deformed shape

In order to compute pointwise values of the density \( f^n_h(x) = \sum_k w^n_k \varphi^n_{h,k}(x) \), it is important to access every particle which support contain any given \( x \in \mathbb{R}^d \) in a reasonable amount of time. This can be done with a pre-processing algorithm that subdivides the phase space into simple domains such as dyadic cells \( \Omega_m = 2^{-j}(m + [0,1]^d), m \in \mathbb{Z}^d \), with \( 2^{-j} \approx h \), and then writes in the scope of every such cell the indices of the overlapping particles, namely
\[ K^n_m = \{ k \in \mathbb{Z}^d : \varphi^n_{h,k}(\Omega_m) \neq 0 \}, \quad m \in \mathbb{Z}^d. \] (3.39)

In practice, one can run a cell marking algorithm for each unstructured particle \( \varphi^n_{h,k} \), starting with the cell \( \Omega_m \) containing \( x^n_k \), i.e. \( m = \lfloor 2^{-j}x^n_k \rfloor \), and recursively testing whether the adjacent cells overlap the parallelogram support of \( \varphi^n_{h,k} \). To perform this test we can use the following result with \( A = (D^n_k)^{-1}, B = B_{\infty}(0, h \rho_p) \) and \( B^t = B_{\infty}(2^{-j}(m + \frac{1}{2}) - x^n_k, 2^{-j-1}) \).

Lemma 3.5. Let \( B = \prod_{i=1}^d [x_i - r_i, x_i + r_i] \) and \( B^t = \prod_{i=1}^d [x'_i - r'_i, x'_i + r'_i] \) be two orthotopes aligned with the coordinate axes, and \( A \) an invertible \( d \times d \) matrix. We have
\[ AB \cap B^t \neq \emptyset \iff |(Ax - x')_i| \leq r_i + r'_i \text{ and } |(x - A^{-1}x')_i| \leq r_i + r'_i \quad \text{for } i = 1 \ldots d \]
with \( \tilde{r}_i := \sum_{j=1}^d |A_{i,j}|r_j \) and \( \tilde{r}'_i := \sum_{j=1}^d |A^{-1}_{i,j}|r'_j \).
Proof. Observe that \( \tilde{B} := \prod_{i=1}^{d} [(A x)_i - \tilde{r}_i, (A x)_i + \tilde{r}_i] \) and \( \tilde{B}' := \prod_{i=1}^{d} [(A^{-1} x)_i - \tilde{r}_i, (A^{-1} x)_i + \tilde{r}_i] \) are the smallest orthotopes aligned with the coordinate axes that contain \( AB \) and \( A^{-1}B' \), respectively. Since the above two sets of inequalities hold if and only if \( \tilde{B} \) and \( B \) intersect \( \tilde{B}' \) and \( B' \) respectively, the \( \Rightarrow \) direction is easily checked. In order to prove the \( \Leftarrow \) direction we make use of the fact that two disjoint convex polytopes can always be separated by the hyperplane supported by one \( d-1 \) dimensional face of one polytope. Thus, if \( AB \) and \( B' \) are disjoint, we can choose a face of \( B' \) or a face of \( AB \). This respectively implies that \( \tilde{B} \cap B' = \emptyset \) or \( B \cap \tilde{B}' = \emptyset \), and hence ends the proof. \( \square \)

### 3.5 A priori estimates for a fully discrete LTP scheme

In this section we establish a priori estimates for the fully discrete particle scheme consisting of an initialization step using the B-spline quasi-interpolation (3.3), and of a series of transport steps using the LTP transport operator (3.27)-(3.29), with no remappings. Thus, we consider

\[
f_h^0 := A_h f^0 \quad \text{and} \quad f_h^{n+1} := T_h^n f_h^n \quad \text{for} \quad n = 0, \ldots, N - 1,
\]

with \( \Delta t = \tau / N \). \( L^\infty \) convergence of this scheme will be established in Theorem 3.10 together with uniform bounds for the particle overlapping. A local (single-particle) error estimate will be shown as well, that will be of practical use in the adaptive multilevel LTP scheme described in Section 4.

To express our estimates in terms of the smoothness of the velocity field \( u \), we begin with local bounds for the characteristic flow.

**Lemma 3.6.** Given a domain \( \omega \subset \mathbb{R}^d \), an integer \( m \) and two instants \( s, t \in [0, \tau] \), we denote

\[
|u|_{m, (s, t, \omega)} := \sup_{t' \in [s, t]} |u(t', \cdot)|_{m, F_{s, t'}}(\omega)
\]

where \( F_{s, t'} \) is the flow of \( u \) between \( s \) and \( t' \), as above. Then we have

\[
|F_{s, t} - I|_{1, \omega} \leq c_{1, u} \exp(c_{1, u}) \quad \text{and} \quad |F_{s, t}|_{2, \omega} \leq c_{2, u} \exp(c_{1, u})(1 + c_{1, u} \exp(c_{1, u}))
\]

where \( c_{m, u} = |t - s| |u|_{m, (s, t, \omega)} \) for \( m = 1, 2 \).

**Proof.** Rewriting (2.2) as \( \partial_t F_{s, t}(x) = u(t, F_{s, t}(x)) \), we obtain that for \( i, l = 1, \ldots, d \),

\[
\partial_i \partial_l (F_{s, t} - I)_i(x) = \partial_i \partial_l (F_{s, t})_i(x)
\]

\[
= \sum_{l' = 1}^{d} \partial_{l'} u_i(t, F_{s, t}(x)) \partial_l (F_{s, t})_{l'}(x)
\]

\[
= \sum_{l' = 1}^{d} \partial_{l'} u_i(t, F_{s, t}(x)) \partial_l (F_{s, t} - I)_{l'}(x) + \partial_{l'} u_i(t, F_{s, t}(x))
\]

In particular, using \( F_{s, s} = I \) we find

\[
\partial_i (F_{s, t} - I)_i(x) = \int_s^t \left[ \sum_{l' = 1}^{d} \partial_{l'} u_i(t', F_{s, t'}(x)) \partial_l (F_{s, t'} - I)_{l'}(x) + \partial_{l'} u_i(t', F_{s, t'}(x)) \right] dt',
\]

so that taking the supremum over \( x \in \omega \), summing over \( l = 1, \ldots, d \) and taking the maximum over \( i = 1, \ldots, d \) yields

\[
|F_{s, t} - I|_{1, \omega} \leq |u|_{1, (s, t, \omega)} \left( |t - s| + \int_s^t |F_{s, t'} - I|_{1, \omega} \, dt' \right)
\]

\[
\leq |t - s| |u|_{1, (s, t, \omega)} \exp \left( |t - s| |u|_{1, (s, t, \omega)} \right)
\]

where the second inequality follows from the Gronwall Lemma in integral form. This shows the inequality. In particular, using \( |I|_{1, \omega} = 1 \) this shows that

\[
|F_{s, t}|_{1, \omega} \leq 1 + |t - s| |u|_{1, (s, t, \omega)} \exp \left( |t - s| |u|_{1, (s, t, \omega)} \right).
\]

Turning to the second derivatives, using again \( F_{s, s} = I \) we write

\[
\partial_i \partial_j (F_{s, t})_i(x) = \int_s^t \left[ \sum_{l' = 1}^{d} \partial_{l'} u_i(t', F_{s, t'}(x)) \partial_j (F_{s, t'})_{l'}(x) \partial_i (F_{s, t'})_{l'}(x)
\]

\[
+ \sum_{l' = 1}^{d} \partial_{l'} u_i(t', F_{s, t'}(x)) \partial_j (F_{s, t'})_{l'}(x) \partial_i (F_{s, t'})_{l'}(x) \right] dt'
\]
so that taking the supremum over \( x \in \omega \), summing over \( l_1, l_2 = 1, \ldots, d \) and taking the maximum over \( i = 1, \ldots, d \) now gives

\[
|F_{s,t}|_{2,\omega} \leq |u|_{2,(s,t,\omega)} \int_{s}^{t} |F_{s,t'}|_{2,\omega} \, dt' + |u|_{1,(s,t,\omega)} \int_{s}^{t} |F_{s,t'}|_{2,\omega} \, dt'
\]

\[
\leq |u|_{2,(s,t,\omega)} \left( \int_{s}^{t} |F_{s,t'}|_{2,\omega} \, dt' \right) \exp \left( \|t-s\|u|_{1,(s,t,\omega)} \right)
\]

\[
\leq c_{2,u}(1 + c_{1,u} \exp(c_{1,u}))\exp(c_{1,u})
\]

where we have used again the Gronwall Lemma, and \((3.41)\).

**Corollary 3.7.** For a given domain \( \omega \subset \mathbb{R}^d \), we denote

\[
\nu_{1,\omega} := |u|_{1,\xi} \exp(\Delta t|u|_{1,\xi}) \quad \text{and} \quad \nu_{2,\omega} := |u|_{2,\xi} \exp(\Delta t|u|_{1,\xi})(1 + \Delta t \nu_{1,\omega}),
\]

where \( \xi = (t^n, t^{n+1}, \omega) \). Then we have

\[
|(F^n_{\text{ex}})^{-1}|_{1,F^n_{\text{ex}}(\omega)} = |F^n_{\text{ex}}|_{1,\omega} \leq 1 + \Delta t \nu_{1,\omega}, \quad |(F^n_{\text{ex}})^{-1}|_{2,F^n_{\text{ex}}(\omega)} = |F^n_{\text{ex}}|_{2,\omega} \leq \Delta t \nu_{2,\omega}.
\]

\[(3.42)\]

In particular, denoting \( \nu_i^n := \nu_{i,2,\omega} \) yields

\[
|(F^n_{\text{ex}})^{\pm 1}|_{1} \leq 1 + \Delta t \nu_1^n, \quad |(F^n_{\text{ex}})^{\pm 1}|_{2} \leq \Delta t \nu_2^n.
\]

\[(3.43)\]

**Proof.** The first estimate follows from \( F_{v^{n+1}}(F^n_{\text{ex}}(x)) = F_{v^n}(x) \) and Lemma 3.6. The second one follows from the fact that \( F^n_{\text{ex}} \) is a diffeomorphism.

**Assumption 3.8.** In view of Lemma 3.6 and Corollary 3.7, one can expect that the error resulting from the linearization of the flow around \( x^n_{k+1} \) behaves like

\[
\|J^n_k(x - x^n_{k+1}) - (F^n_{\text{ex}})^{-1}(x - x^n_{k})\| \lesssim \Delta t(h^2(1 + \Delta t \nu_1^n + h^{-1}c_{\Delta t}^n)^{(d-1)}(\nu_2^n + h^{-2}c_{\Delta t}^n)}
\]

so that it seems natural to ask that \( h^{-2}c_{\Delta t}^n \sim \Delta t \). In the sequel we will assume that \( h \) and \( \Delta t \) are such that

\[
h^{-2}c_{\Delta t}^n \leq \alpha \Delta t,
\]

\[(3.44)\]

where \( \alpha > 0 \) is a fixed constant. Note that if an \( r \)-th order ODE solver is used to compute the numerical flow, the above condition reads \( \Delta t \leq C \alpha h^\frac{2}{r} \) with a constant \( C \) depending on the smoothness of \( u \), typically through \( |u|_{r+1,\xi}(c_{\Delta t}^n, \mathbb{R}^d) \).

For the subsequent analysis it will be convenient to introduce the following measures of the velocity smoothness,

\[
\begin{align*}
\kappa_{1,1,h} := & \nu_{1,2,h,k} + h\alpha_k, \\
\kappa_{2,1,h} := & \frac{1}{2}\nu_{2,2,h,k} + \alpha_k, \\
\kappa_{3,1,h} := & 2d(1 + \Delta t k_{3,1,h})^{d-1}\kappa_{2,2,h,k}, \\
\kappa_{4,1,h} := & 2d^2(1 + \Delta t k_{3,1,h})^{d-2}(1 + \Delta t k_{3,1,h})^{2(d-1)}k_{2,2,h,k},
\end{align*}
\]

\[(3.45)\]

as well as space-global versions \( \kappa_{1,h} := \nu_{1,2} + h\alpha \), \ldots, and finally the time-global counterparts \( \kappa_{i,h} \), \( i = 1, \ldots, 4 \), obtained by replacing \( \Delta t \) with \( \tau \), and using

\[
\nu_1 = |u|_{1,\xi} \exp(\Delta t|u|_{1,\xi}) \quad \text{and} \quad \nu_2 := |u|_{2,\xi} \exp(\Delta t|u|_{1,\xi})(1 + \Delta t \nu_1)
\]

\[(3.46)\]

where \( \xi = (0, \tau, \mathbb{R}^d) \). Equipped with the local measures \((3.45)\) we derive the following estimates from Lemma 3.6.

**Corollary 3.9.** Provided \( h \) and \( \Delta t \) satisfy \((3.44)\) and the additional mild condition

\[
h\Delta t \kappa_{3,1,h} \leq 1,
\]

\[(3.47)\]

the finite difference scheme \((3.28)\) computes an invertible matrix \( J^n_k \) satisfying

\[
|\det(J^n_k)|^{-1} \leq (\theta_k^n)^{-1} \leq 1 + h\Delta t \kappa_{3,1,h}.
\]

\[(3.48)\]
therefore the operator $T^n_k$ is well defined by\[3.27]-\[3.29]. Moreover, the linearized flow based on the approximated backward Jacobian $J^n_k$ satisfies the local estimate

\[
\sup_{x \in B_{\infty}(x^{n+1,\rho}),\rho} \| J^n_k(x - x^{n+1}_k) - ((F^n_{\text{ex}})^{-1})(x - x^n_k) \|_\infty \leq h^2 \Delta t C^n_{h,k}(\rho) \tag{3.49}
\]

for all $\rho \geq 0$, with $C^n_{h,k}(\rho) = \rho c^{\alpha}_{1,h,k} + \kappa^n_{1,h,k} + \frac{1}{2} \rho^2 \nu^n_{2,(F^n_{\text{ex}})^{-1}}(B_{\infty}(x^{n+1,k},\rho))$.

**Proof.** According to $(3.42)$, we have

$$C^n_{h,k}(\rho)=\rho c^{\alpha}_{1,h,k} + \kappa^n_{1,h,k} + \frac{1}{2} \rho^2 \nu^n_{2,(F^n_{\text{ex}})^{-1}}(B_{\infty}(x^{n+1,k},\rho)),$$

with constants $c^{\alpha}_{f,t}$ towards the solution $L$ that conditions $(3.47)$.

Let $\Theta_{\text{ex}}$ be such that \[3.47\] holds then from Lemma 3.4 and the definitions $(3.45)$. which shows the invertibility of $\tilde{J}^n_k$ and also gives $(3.48)$, hence the first claim. The local estimate $(3.49)$ follows then from Lemma 3.4 and the definitions $(3.45)\).\]

We are now in position to state a priori estimates for the fully discrete LTP scheme. Again, we emphasize that although the following result is established for B-spline particles, the same arguments apply to more general approximation settings such as continuous finite element basis functions, see Remark 3.3.

**Theorem 3.10.** Let $h > 0$ be lower than a fixed but arbitrary $\tilde{h}$, and $\Delta t := \tau/N$ be such that conditions $(3.47)$ and $(3.44)$ hold for some fixed $\alpha > 0$. Then if the velocity field $u$ is in $L^\infty([0,\tau];W^{2,\infty}(\mathbb{R}^d))$, the numerical densities computed by the particle scheme $(3.40)$ converge towards the solution $f$ of equation $(2.1)$, with

\[
\| f^n_h - f(t^n) \|_{L^\infty} \leq h(c_T \| f^0 \|_{L^\infty} + c_A \| f^0 \|_{1}) \quad \text{for} \quad n = 0, \ldots, N, \tag{3.51}
\]

with constants $c_T, c_A$ independent of $h$ and $\Delta t$, that are specified in the proof. The particles $\varphi^n_{h,k} = \varphi(D^n_k(: - x^n_k))$ composing $f^n_h$ have uniformly bounded supports,

$$\text{supp}(\varphi^n_{h,k}) \subset B_{\infty}(x^n_{h,k}; h\rho_h) \quad \text{with} \quad \rho_h = c_p \exp(\tau(n_\rho/\Delta t)),$$

in particular, $\rho_h \to c_p \exp(\tau(n_\rho/\Delta t))$ as $h \to 0$. Moreover, the overlapping constant of the particles $\Theta_{h,k} := \sup_{n \leq \infty, x \in \mathbb{R}^d} \#\{(k \in \mathbb{Z}^d : \varphi^n_{h,k}(x) \neq 0)\}$ satisfies

\[
\Theta_{h,k} \leq (2 \exp(\tau(n_\rho/\Delta t)) (\rho_h + h\tau(n_\rho/\Delta t)))^d \to (2c_p \exp(2d\tau(n_\rho/\Delta t)) \quad \text{as} \quad h \to 0. \tag{3.53}
\]

Finally, the single-particle transport errors can be estimated by local indicators,

\[
(T^n_h - T^n_{\text{ex}})\varphi^n_{h,k} \leq h^{-d} \Delta t \| \varphi \|_{1} \| D^n_k \|_{\infty} C^n_{h,k}(\rho^n_{h,k}) \tag{3.54}
\]

where $C^n_{h,k}$ is as in Corollary 3.7, and where

$$\rho^n_{h,k} = \alpha h \Delta t + \rho_h \| (D^n_k)^{-1} \|_{\infty} \max \{ (1 + h \Delta t \kappa^n_{3,h,k}(\rho_h))^{\frac{1}{4}} (1 + \Delta t \kappa^n_{1,h,k}(\rho_h)), 1 + \Delta t \nu^n_{1,\Sigma_{h,k}} \}. \tag{3.55}
$$

**Proof.** Following the main lines of the error analysis in Section 3.2 for all $n$ and $k$ we let

$$e_{h,k}^n := (T^n_h - T^n_{\text{ex}})\varphi^n_{h,k} = \varphi^n_{h,k} - T^n_{\text{ex}}\varphi^n_{h,k},$$

denote the particle transport error, and we define the corresponding overlapping constant as

$$\tilde{\Theta}_{h,k} := \sup_{n \leq \infty, x \in \mathbb{R}^d} \#\{(k \in \mathbb{Z}^d : e_{h,k}^n(x) \neq 0)\}.$$\]

Thus, using the bound $|w_k(f^0)| \leq h^d \| a \|_{1} \| f^0 \|_{L^\infty}$ satisfied by the weights in $(3.3)$ we have

\[
\| (T^n_h - T^n_{\text{ex}})f^n_h \|_{L^\infty} \leq \| \sum_{k \in \mathbb{Z}^d} w_k(f^0)e_{h,k}^{n+1} \|_{L^\infty} \leq h^d \| a \|_{1} \| f^0 \|_{L^\infty} \tilde{\Theta}_{h,k} \sup_{k \in \mathbb{Z}^d} \| e_{h,k}^{n+1} \|_{L^\infty}. \tag{3.57}
\]

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Next we claim that the local transport errors have their supports bounded with
\[ \text{supp}(\rho^{n+1}_{h, k}) \subset B_\infty(x^n_k, h\rho^{n+1}_{h, k}), \]  
(3.58)
where \( \rho^{n+1}_{h, k} \) is defined as in (3.55). Using Corollary 3.9 this gives
\[
\| \rho^{n+1}_{h, k} \|_{L^\infty} = \sup_{x \in B_\infty(x^n_k, h\rho^{n+1}_{h, k})} \left| \varphi_h(D^n_{k}\jmath^n_k(x, x^n_k)) - \varphi_h(D^n_{k}\jmath^n_k(F^n_{\text{ex}})^{-1}(x)) \right|
\]
\[
\leq \| \varphi_h \|_{L^\infty} \sup_{x \in B_\infty(x^n_k, h\rho^{n+1}_{h, k})} \| J^n_{k}(x, x^n_k) - ((F^n_{\text{ex}})^{-1}(x)) \|_{\infty}
\]
\[
\leq h^{-\delta} \Delta t \| \varphi_h \|_{L^\infty} \| D^n_{k}\|_{L^\infty} C^n_{h, k}(\rho^{n+1}_{h, k})
\]
where we have used \( \| \varphi_h \|_{L^\infty} = h^{-\delta} \| \varphi_h \|_{L^\infty} \). This is our local estimate (3.54). To derive a global estimate we observe that
\[ \| (T^n_{h} - T^n_{\text{ex}}) f^n_h \|_{L^\infty} \leq \Delta t h \beta(h, \Delta t) \| f^0 \|_{L^\infty} \]
holds with
\[ \beta(h, \Delta t) := \| a \|_{\ell^1} \Theta(h, \varphi) \sup_{n \leq \Delta t} \left\{ \| D^n_{k}\|_{L^\infty} C^n_{h, k}(\rho^{n+1}_{h, k}) \right\}. \]
(3.59)
It follows that the global error \( f^{n+1}_h - f(t^{n+1}) = T^n_{h} f^n_h - T^n_{\text{ex}} f(t^n) \) is bounded by
\[
\| f^{n+1}_h - f(t^{n+1}) \|_{L^\infty} \leq \| (T^n_{h} - T^n_{\text{ex}}) f^n_h \|_{L^\infty} + \| T^n_{\text{ex}}(f^n_h - f(t^n)) \|_{L^\infty}
\]
\[
\leq \| T^n_{h} - T^n_{\text{ex}} \|_{L^\infty} \sup_{n \leq \Delta t} \left\{ \| D^n_{k}\|_{L^\infty} \right\}
\]
(3.60)
\[ \leq \sum_{m=0}^n \| (T^m_{h} - T^m_{\text{ex}}) f^m_h \|_{L^\infty} + \| f^m_h - f^0 \|_{L^\infty}
\]
where we have used the fact that \( T^m_{\text{ex}} \) is an exact transport operator in the second inequality, and estimate (3.5) with \( q = 1 \) in the last one. In particular we can take
\[ c_A = \frac{1}{2}(m_p + c_p)^2((2c_p)^d \| \varphi \|_{L^\infty} \| a \|_{\ell^1} + 1). \]
It order to bound \( \beta(h, \Delta t) \) independently of \( h \) and \( \Delta t \) we next observe that the deformation matrices involved in the scheme (3.27) verify
\[ D^n_{k} = j^n_k \cdots j^1_k^{-1} \quad \text{with} \quad j^n_k = \begin{cases} \det(j^n_k)^{-\frac{1}{d}}(j^n_k)^{-1} & \text{in the conservative case, or} \\ (j^m_k)^{-1} & \text{in the non-conservative case.} \end{cases} \]
Using estimates (3.48), (3.34) and (3.50) we then observe that
\[ |\det(j^m_k)|^{-\frac{1}{d}} \leq (\theta^m_k)^{-\frac{1}{d}} \leq (1 + h\Delta t \kappa^m_{3, h})^{-\frac{1}{d}}, \quad \| j^m_k \|_{L^\infty} \leq \mu^m_{1, k} \leq (1 + h\Delta t \kappa^m_{1, h}). \]
(3.61)
It follows that
\[ \| (D^n_k)^{-1} \|_{L^\infty} \leq (1 + h\Delta t \kappa^m_{3, h})^{\frac{n}{d}} (1 + \Delta t \kappa^m_{1, h})^{\frac{n}{d}} \leq \exp(\tau(h\kappa^m_{3, h} + \kappa^m_{1, h})) \]
(3.62)
holds for \( n \leq N \), in both the conservative and the non-conservative cases. To obtain a bound for \( \| (D^n_k)^{-1} \|_{L^\infty} \) we cannot repeat the above steps because our estimate (3.37) for \( \| (j^m_k)^{-1} \|_{L^\infty} \) is too weak. However we can use the cofactor formula for \( D^n_k \) directly. Indeed, by construction we have \( \det(D^n_k) = 1 \) in the conservative case, and in the non-conservative case we infer from (3.48) that
\[ \| \det(D^n_k) \| \leq \prod_{m=0}^{n-1} |\det(j^m_k)|^{-1} \leq (1 + h\Delta t \kappa^m_{3, h}) \leq \exp(\tau(h\kappa^m_{3, h} + \kappa^m_{1, h})) \]
and we observe that (3.62) becomes \( \| (D^n_k)^{-1} \|_{L^\infty} \leq \exp(\tau \kappa^m_{1, h}) \). Using the cofactor formula we then find in both cases that
\[ \| D^n_k \|_{L^\infty} \leq d \| \det(D^n_k) \| (D^n_k)^{-1} \|_{L^\infty} \leq d \exp \left( \tau(h\kappa^m_{3, h} + \kappa^m_{1, h}(d - 1)) \right). \]
(3.63)
This allows to bound the particles support. We indeed observe that
\[
\Sigma_{h,k}^n := \text{supp}(\varphi_{h,k}^n) = x_k^n + (D_k^n)^{-1}(B_{\infty}(0, hc_p)) \subset B_{\infty}(x_k^n, hc_p\|D_k^n\|_\infty),
\]
which shows the uniform estimate (3.52). From (3.54) we also derive that
\[
\text{supp}(T_{ex}^n, \varphi_{h,k}^n) = F_0^n(\Sigma_{h,k}^n) \subset B_{\infty}(x_k^{n+1}, \epsilon_{\Delta t} + hc_p\|D_k^n\|_\infty\||F_{ex}^n|1, \Sigma_{h,k}^n|),
\]
which allows to localize the particle transport error \(\epsilon_{h,k}^{n+1}\) with
\[
\text{supp}(\epsilon_{h,k}^{n+1}) \subset B_{\infty}(x_k^n, \epsilon_{\Delta t} + hc_p\|D_k^n\|_\infty\max\{|J_h^n|_\infty, |F_{ex}^n|1, \Sigma_{h,k}^n\}).
\]
Using (3.41), (3.61) and (3.42) this proves our claim (3.58). Turning next to the particle overlapping we consider an arbitrary \(x \in \mathbb{R}^d\), and for a given \(n \leq N\) we denote \(x^n = x\) and recursively set \(x^m := (F_{ex}^n)^{-1}(x^{n+1})\) for \(m = n-1, \ldots, 0\). Using (3.43) and (3.44) we see that
\[
\|x^n - x_k^n\|_\infty \leq \|(F_{ex}^n)^{-1}|_{x_k^n}\|_\infty \|x^n - F_{ex}^n(x_k^n)\|_\infty \\
\leq (1 + \Delta t\nu_1)(\|x^n - x_k^n\|_\infty + \epsilon_{\Delta t}^n) \\
\leq \cdots \\
\leq (1 + \Delta t\nu_1)^n (\|x^n - x_k^n\|_\infty + nh^2\Delta t\alpha).
\]
In particular, for \(k\) such that \(\varphi_{h,k}^n(x) \neq 0\) we have \(\|x - x_k^n\|_\infty \leq h\rho_h\) according to (3.52), hence
\[
\|h^{-1}x^n - k\|_\infty = h^{-1}\|x^n - x_k^n\|_\infty < \exp(\tau\nu_1)(\rho_h + h\tau\alpha).
\]
This proves the estimate (3.53) on the particles overlapping. As for the particle transport errors (3.56) we have
\[
\tilde{\Theta}_h \leq 2\Theta_h,
\]
given that the particle overlapping is not increased by the exact transport operator. From (3.62) and \(\nu_1 \leq \kappa_{1,h}\) we then observe that
\[
\tilde{\rho}_h^n \leq \alpha h\Delta t + \rho_h \leq \alpha \bar{h}\tau + \rho_h =: \bar{\rho}_h
\]
holds for all \(\Delta t \leq \tau, n \leq \tau/\Delta t, k \in \mathbb{Z}^2\) and \(h \leq \bar{h}\). In particular, the above discussion gives
\[
\beta(h, \Delta t) \leq \|a\|_{\ell^1} |\varphi| 2(2\exp(\tau\nu_1)(\bar{\rho}_h))^{d}d\exp(\tau(h\kappa_{3,h} + \kappa_{1,h}(d - 1)))C_{\tilde{\rho}}(\bar{\rho}_h),
\]
where we have set \(C_{\tilde{\rho}}(\rho) = \rho\kappa_{4,h} + \kappa_{5,h} + \frac{1}{2}\rho^2\nu_2^{\alpha}\). This latter bound provides us with a constant \(c_T\) for the global estimate (3.51), which completes the proof. \(\square\)

4 Adaptive transport with multilevel particles

To illustrate the flexibility of our approach we now describe one adaptive multilevel version of our LTP scheme, where the goal is to save computational effort without deteriorating the order of accuracy of the simulations. To implement that principle we use a hierarchy of particles with dyadic scales \(h = 2^{-j}\), corresponding to integer levels \(j = j_0, \ldots, j_{\max}\). For notational simplicity we will label with \(j\) the objects that were previously labelled with their resolution \(h\), or that depended implicitly on it. For instance, particles with resolution \(h = 2^{-j}\) will now be denoted
\[
\varphi_{j,k}^n = \varphi_j(D_j^n(x_{j,k}^n)),
\]
instead of \(\varphi_{h,k}^n\) as in equation (2.9).

In Section 4.1 we first present one B-spline version of the common hierarchical approach for building adaptive approximations with prescribed error tolerance \(\varepsilon\), and in Section 4.2 we suggest a local filter that makes the resulting adaptive approximations positivity-preserving, without noticeable loss of accuracy. In Section 4.3 we then describe a dynamic strategy for refining the particles in the course of their transport, so that the associated transport error is on the order of the prescribed tolerance.
4.1 Adaptive approximations with multilevel B-splines

To build adaptive B-spline approximations of a given function \( g \), we reformulate the quasi-interpolation operator \([3.3]\) in a hierarchical setting. Specifically, writing

\[
A_j : g \mapsto \sum_{k \in \mathbb{Z}^d} w_{j,k}(g) \phi_{j,k} \quad \text{with} \quad w_{j,k}(g) := 2^{-jd} \sum_{||l||_\infty \leq m_p} a_l g(2^{-j}(k + l)), \tag{4.1}
\]

we replace the approximation \( g \approx A_{j_{\max}} g \) by a recursive process where we start from \( g_{j_0} := A_{j_0} g \) and define \( g_j \) by correcting \( g_{j-1} \) for \( j = j_0 + 1, \ldots, j_{\max} \), i.e.,

\[
g_j := g_{j-1} + A_j(g - g_{j-1}).
\]

In such a framework, adaptivity is classically obtained by restricting the corrections in the regions where the residual is larger than the prescribed tolerance. This idea can be realized by discarding small particles: indeed, using

\[
A_j^\varepsilon : g \mapsto \sum_{k : w_{j,k}(g) > \varepsilon} w_{j,k}(g) \phi_{j,k}^0 \quad \text{with} \quad \varepsilon_j(\varepsilon) := 2^{-dj}(2c_p)^d ||\varphi||_{L^\infty}^{-1}
\]
gives an acceptable error, as

\[
\| (A_j^\varepsilon - A_j) g \|_{L^\infty} \leq \| \sum_{k : w_{j,k}(g) \leq \varepsilon_j(\varepsilon)} w_{j,k}(g) \phi_{j,k}^0 \|_{L^\infty} \leq 2^d (2c_p)^d ||\varphi||_{L^\infty} \varepsilon_j(\varepsilon) = \varepsilon.
\]

Moreover, the adaptive correction process only needs to be applied in the regions where the residual is significant. Specifically, let

\[
\Omega_j^+ := \{ x : |(g - g_{j-1})_j(x) | > c^+ \varepsilon \} \quad \text{and} \quad K_j^+ := \{ k : 2^{-j}(k + m_p[-1,1]^d) \cap \Omega_j^+ \neq \emptyset \}
\]

where \( c^+ := (2c_p)^d ||\varphi||_{L^\infty} ||a||_{\ell^1}^{-1} \). It is then easily seen that

\[
|w_{j,k}(g - g_{j-1})| \leq \varepsilon_j(\varepsilon) \quad \text{for} \quad k \notin K_j^+.
\]

In practice the set \( K_j^+ \) may not be readily computable, but it is possible to find some reasonable approximations \( K_j^* \) that contains it. The resulting scheme for adaptive quasi-interpolation with multilevel B-splines reads then as follows.

**Algorithm 4.1** (Adaptive B-spline quasi-interpolation, \( A_\varepsilon : g \mapsto g_{j_{\max}} \)).

1. Initialize the algorithm with \( g_{j_0} := 0 \) and pre-activate every coarse particle (i.e., make it a candidate for a possible selection) by letting \( K_j^* := \mathbb{Z}^d \).

2. For \( j = j_0, \ldots, j_{\max} \), do:

   (a) for \( k \in K_j^* \), compute \( w_{j,k}^* = w_{j,k}(g - g_{j-1}) \) as in \([4.1]\), then set

   \[
g_j := g_{j-1} + \sum_{k \in K_j} w_{j,k}^* \phi_{j,k} \quad \text{where} \quad K_j := \{ k \in K_j^* : |w_{j,k}^*| > \varepsilon_j(\varepsilon) \};
\]

   (b) if \( j < j_{\max} \), pre-activate particles at the finer level for possible selection by determining \( K_{j+1}^* \)

   (c) if the option is set, apply the positive correction filter (see Algorithm 4.2 below).

To determine the set \( K_{j+1}^* \) of candidate particles, a naive approach would evaluate local values of the residual \( g - g_j \). However this is somehow redundant with the computation of the weights \( w_{j+1,k}^* \) at the next level, therefore it should be avoided. Instead, we observe that \( K_{j+1}^* \) can be built as follows.

**Algorithm 4.2** (Pre-activation of particles in \( K_{j+1}^* \), for \( j = j_0, \ldots, j_{\max} - 1 \)).
1. Initialize the set with $K_{j+1}^* = \emptyset$.

2. For $k \in K_j^*$, do:
   
   (a) if $k \in K_j$ has been selected, add $\{2k + l : \|l\|_\infty \leq m_p + 2c_p\}$ to $K_{j+1}^*$
   
   (b) otherwise, evaluate the residual $r_{j,k} := \|g - g_{j-1}\|_{L^\infty(B_{\infty2}(2^{-i}k,2^{-i-1}))}$ and add $\{2k + l : \|l\|_\infty \leq m_p\}$ to $K_{j+1}^*$ if $r_{j,k} > c^+\varepsilon$.

Proposition 4.3. The sets built in Algorithm 4.2 do satisfy

$$K_{j+1}^+ \subset K_j^*,$$

$j = j_0, \ldots, j_{\text{max}} - 1$.

Proof. Take $k \in K_{j+1}^+$. By definition there is an $x$ such that $\|(g-g_j)(x)\| > c^+\varepsilon$ and $\|2^{i+1}x - k\|_\infty \leq m_p$. Then if $k$ has not been added to $K_{j+1}^*$ on step 2a, it is easily seen that $\|2^ix - k\|_\infty > c_p$ holds for all $k' \in K_j$. In particular we have $\|(g-g_{j-1})(x)\| = \|(g-g_j)(x)\| > c^+\varepsilon$, hence $x \in \Omega_j^+$. Take now $k''$ such that $\|k'' - 2^ix\|_\infty < 1 \varepsilon$ (this is possible up to choosing another $x$ close to the first one, as $g - g_{j-1}$ is continuous). This gives $r_{j,k''} > c^+\varepsilon$ and $k'' \in K_{j+1}^+$, by definition of the latter. Now, it also gives $\|2^ik'' - k\|_\infty \leq 2\|k'' - 2^ix\|_\infty + \|2^{i+1}x - k\|_\infty < m_p + 1$. Since we can assume as an induction hypothesis that $K_j^+ \subset K_j^*$ (it is valid for $K_{j_0}^* = Z^d$), $k$ must have been added to $K_{j+1}^*$ on step 2a.

Finally we note that the main loop in Algorithm 4.2 can be merged with step 2a from Algorithm 4.1. In particular, the local residuals $r_{j,k}$ can be evaluated while computing the weights $w_{j,k}$.

### 4.2 Positivity preserving hierarchical approximations

If the target function $g$ is nonnegative, one may want its particle approximation to be nonnegative as well. However, it is easily seen that the above scheme is likely to yield some negative weights. A first reason for this is that the single-level scheme (4.1) is not positive for $p > 1$. A second reason is due to the hierarchical framework: wherever $g_{j-1}$ is below the target, the residual takes negative values which are likely to be approximated by negative level-$j$ particles.

The latter issue can be addressed by locally decreasing $g_{j-1}$ in the neighborhood of a negative weight $w_{j,k}$. So as to increase the residual and hopefully correct the negativity of $w_{j,k}$. Since B-spline particles satisfy a refinement equation

$$\varphi_{j',k'} = \sum_{\|l\|_\infty \leq c_p} \sigma_l \varphi_{j'+1,2k'+l}, \quad (4.2)$$

it is possible to do so by refining coarse particles which contributions to $\varphi_{j,k}$ will increase its weight. An attractive feature of such corrections is that they do not require new evaluations of the target function, or iterative approximations of updated residuals. Let us specify one such algorithm. Because it may be necessary to refine particles over several levels, it is useful to derive multilevel scaling relations from (4.2),

$$\varphi_{j',k'} = \sum_{\|l\|_\infty \leq s_s} \sigma_l^{(s)} \varphi_{j'+\delta,2^\delta k'+1}, \quad (4.3)$$

with multilevel refinement coefficients satisfying

$$\sigma_l^{(s)} := \sum_{\|m\|_\infty \leq s_{s-1}} \sigma_m^{(s-1)} \sigma_{l-2m}, \quad s_1 := 2s_{s-1} + 1,$$

and initialized with $\sigma^{(1)} = \sigma$, $s_1 = c_p$. Indeed, we can observe that if all the particles at the level $j - \delta$, $\delta \geq 1$, were to be refined up to level $j$, the resulting increase to $w_{j,k}$ would be

$$C_{j-\delta}(j,k) = \sum_{k' \in Z^d} \sigma_{k'-2^\delta k'}^{(s)} w_{j-\delta,k'}.$$
Therefore, letting \( S'_j(j, k) := w_{j,k} + \sum_{j' = j}^{j-1} C'_{j'}(j, k) \) we define the correction level associated to some given negative weight \( w_{j,k} \) as

\[
\mathcal{J}_{\text{cor}}(j, k) := \begin{cases} 
\max \left\{ j' < j : S'_j(j, k) \geq 0 \right\} & \text{if } S'_{j_0}(j, k) \geq 0, \\
\infty & \text{otherwise.}
\end{cases}
\] (4.4)

It corresponds to the coarser level from which neighboring particles should be refined in order to correct the weight \( w_{j,k} \). Obviously, it is not necessary to refine every such coarse particle, since only those satisfying \( \|k - 2^j k'\|_\infty \leq s_0 \) do contribute to \((j, k)\). Moreover, we do not need to fully refine them up to level \( j \). Instead, the same increase to \( w_{j,k} \) can be obtained by refining them one level at a time, and only considering those contributing to \((j, k)\) in the process, namely those \((j', k')\) with \( \|2^{-j'} k' - k\|_\infty \leq s_{j-j'} \). Thus we see that these corrections are indeed local.

We also observe that for \( p > 1 \), it may happen that some weights remain negative despite the corrections. In this case we suggest to simply discard those weights after correcting them. Clearly this may deteriorate the approximation accuracy, but in a hierarchical framework one can hope that finer layers of details will essentially correct the resulting errors. In practice indeed we have observed such a behavior, see Section 5.2. Let us now summarize the above correction filter, to be applied to the weights \( w_{j', k'} \), \( j' = j_0, \ldots, j \), computed on step 2a of Algorithm 4.1. Note that here we compute the correction levels before refining the contributing particles so as not to break the possible symmetries in the particle grid.

**Algorithm 4.4** (Positive correction filter). Let \( K_{j}^{<0} := \{ k \in K_{j} : w_{j,k} < 0 \} \) denote the indices of the active particles to correct at level \( j \). Then,

1. if \( j > j_0 \),
   
   (a) set \( \mathcal{J}_{\text{cor}}(j, k) < j \) as in (4.4), for all \( k \in K_{j}^{<0} \);
   
   (b) then, refine the contributing particles. Namely, for \( k \in K_{j}^{<0} \) and \( j' = \mathcal{J}_{\text{cor}}(j, k), \ldots, j-1 \), refine every particle \((j', k')\) such that \( \|2^{-j'} k' - k\|_\infty \leq s_{j-j'} \) by setting
   
   \[ w_{j'+1,2k'+1} := w_{j'+1,2k'+1} + \sigma w_{j', k'}, \quad \text{for all } \|l\|_\infty \leq s_1, \quad \text{and} \quad w_{j', k'} := 0 ; \]

2. for all \( k \in K_{j}^{<0} \), set \( w_{j,k} := \max\{0, w_{j,k}\} \).

**Remark 4.5.** We observe that there is no need to pre-activate new finer particles after running the above correction algorithm, i.e., the set \( K_{j+1}^* \) built in Algorithm 4.2 still verifies Proposition 4.3. Indeed, the refinements on step 1b do not change the approximation \( g_j \), nor the residual. The only change to \( g_j \) occurs when discarding a negative weight \( w_{j,k} \). There, a significant error may be introduced but since \( k \) is in \( K_j \), a finer patch has already been pre-activated on step 2a of Algorithm 4.2.

### 4.3 Dynamic particle refinement without remapping

In order to achieve some prescribed accuracy when transporting the multilevel particles

\[
f^n_{\text{max}} = \sum_{j=j_0}^{j_{\text{max}}} \sum_{k \in \mathbb{Z}^d} w^n_{j,k} \varphi_j(D^n_{j,k}(\cdot - x^n_{j,k})),
\]

it is in general necessary to refine some of them over time. Indeed, the errors induced by the discrete transport operator depend on the local smoothness of the flow, and on the level of the particles. However, at the initialization step their resolution is essentially driven by the local smoothness of \( f^0 \). Rather than follow a conservative approach and automatically refine patches of particles to resolve the emerging features that may appear in the solutions, we propose to use the local error estimate (3.54) to determine which particles are admissible for discrete transport, and which need to be refined. Given that both the number of levels and the number of overlapping particles per level are uniformly bounded, we have \( \| (T^n_{\text{ex}} - T^n_{\text{ex}}) f^n_{\text{max}} \|_{L^\infty} \lesssim \sup_{j,k} \| w^n_{j,k} \|_{L^\infty} \| e^n_{j,k} \|_{L^\infty} \) hence a particle \( w^n_{j,k} \) will be said admissible for transport if it satisfies

\[
|w^n_{j,k}| \eta^n_{j,k} \leq C_T \varepsilon,
\] (4.5)
where \( \eta_{j,k}^n \) is a computable estimate for the transport error, see (4.7) below, and \( C_T \) is an ad-hoc constant.

We next observe that, although it is possible from (4.2) to represent exactly a deformed particle by a few finer ones, using

\[
\varphi_j(D^n_{j,k}(x - x^1_{j,k})) = \sum_{\|\| \leq c_p} \sigma_l \varphi_{j+1}(D^n_{j,k}(x - x^l_{j,k,l}))
\]

where \( x^l_{j,k,l} := x^1_{j,k} + 2^{-j-1}(D^n_{j,k})^{-1} l \), refining inadmissible particles in such a way can result in a significant increase of their total number. Assume indeed that every level-\( j \) particle needs to be refined in \( f^n \). Since there is no reason why we should have \( D^n_{j,k} = D^n_{j,k'} \) and \( x^l_{j,k,l} = x^l_{j,k',l'} \) for \( k' \) and \( l' \) such that \( 2k + l = 2k' + l' \), replacing every \( \varphi_{j,k}^n \) by its exact finer representation is likely to add \( \sim 2^{d_j} (2c_p + 1)^d \) new level-\( (j + 1) \) particles, which is much more than the particles involved by a uniform discretization at level \( j + 1 \), and similar phenomena may happen on further time steps as well.

For that reason we propose to refine inadmissible particles \( \varphi_{j,k}^n \) in a “retroactive” fashion. Namely, we represent them by the level-\( (j + 1) \) particles that would have been present in \( f^n \) if the original (structured) \( \varphi_{j,k}^n \) had been refined from the start, that is, at the last remapping step. Note that some of those fine particles may already be present in \( f^n \), and in such a case it suffices to update their weight. In particular, this approach allows to refer to any particle by its multilevel space-time index without ambiguity: for all \( j, k, n \) we indeed have \( \varphi_{j,k}^n = \varphi_j(D^n_{j,k}(\cdot - x^1_{j,k})) \) with particle center and deformation matrix given by

\[
x^1_{j,k} = F^{n-1}(x^n_{1,k}) = (F^{n-1} \ldots F^{n_0})(2^{-j} k) \quad \text{and} \quad D^n_{j,k} = D^{n-1}_{j,k} \cdot D^{n-1}_{j,k} = \prod_{m=n_0}^{n-1} J^n_{j,k}
\]

where \( n_0 \) is the last remapping step and \( J^n_{j,k} \) is defined by (3.28)–(3.29).

It remains to give one error indicator \( \eta_{j,k}^n \) for the local admissibility condition (4.5). In the numerical tests shown in Section 5 we have used local estimates

\[
|u^n_{1,x^n_{j,k}}| := \max_{1 \leq l \leq d} \sum_{l=1}^d |\Delta^j_t u_i(t^n)(x^n_{j,k})|, \quad |u^n_{2,x^n_{j,k}}| := \max_{1 \leq l \leq d} \sum_{l_1,l_2=1}^d |\Delta^j_{t_1} u_i(t^n)(x^n_{j,k})|
\]

based on the finite differences

\[
\Delta^j_t u(t^n)(x) = 2^j (u(t^n, x + 2^{-i-1}e_l) - u(t^n, x - 2^{-i-1}e_l)) \quad \text{and} \quad \Delta^j_{t_1} u = \Delta^j_{t_1} \Delta^j_{t_2}.
\]

We mimic the local smoothness measures from Lemma 3.6 and Corollary 3.7 with

\[
\begin{cases}
\hat{\nu}_{1,(j,k)}^n := |u^n_{1,x^n_{j,k}}| \exp(\Delta t |u^n_{1,x^n_{j,k}}|) \\
\hat{\nu}_{2,(j,k)}^n := |u^n_{2,x^n_{j,k}}| \exp(\Delta t |u^n_{2,x^n_{j,k}}|(1 + \Delta t \hat{\nu}_{1,(j,k)}^n))
\end{cases}
\]

and define coefficients \( \kappa_{i,(j,k)}^n \), \( i = 1, \ldots, 4 \), consistent with (3.45). Following (3.54) we finally take

\[
\eta_{j,k}^n = 2^{d-1} \Delta t |\varphi|_1 \|D^n_{j,k}||\| C^m_{j,k}(\hat{\rho}^{n+1})
\]

where we have set \( C^m_{j,k}(\tilde{\rho}) := \tilde{\rho} \kappa_{1,(j,k)}^n + \kappa_{3,(j,k)}^n + \frac{1}{2} \tilde{\rho}^2 \hat{\nu}_{2,(j,k)}^n \) and

\[
\hat{\rho}^{n+1} := \alpha 2^{-\frac{j}{2}} \Delta t + c_p \|D^n_{j,k}|||^{1} (1 + h \Delta t \kappa_{3,(j,k)}^n) \frac{1}{2} (1 + \Delta t \kappa_{1,(j,k)}^n)
\]

Note that neglecting the small terms in (4.7) gives

\[
\eta_{j,k}^n \approx 2^{d-1} \Delta t |\varphi|_1 \|D^n_{j,k}||\| \left[|u^n_{2,x^n_{j,k}}| \right]^{1} (\frac{1}{2} \tilde{\rho}^2 + d^2 \tilde{\rho} + d + \alpha(d\tilde{\rho} + 1))
\]

where \( \tilde{\rho} = c_p \|D^n_{j,k}|||^{1} \approx \hat{\rho}^{n+1} \) and \( \alpha \) is the constant from assumption (3.44). We summarize our adaptive transport algorithm for multilevel particles as follows.
Algorithm 4.6 \((T^n_f : f_{j_{\text{max}}}^n \mapsto f_{j_{\text{max}}}^{n+1})\). For \(j = j_0, \ldots, j_{\text{max}}\), and then for \(k \in \mathbb{Z}^d\) such that \(w_{j,k}^n \neq 0\), do:

1. if \(j = j_{\text{max}}\) or if the admissibility condition (4.5) is met, then the particle is transported by setting \(w_{j,k}^{n+1} := w_{j,k}^n\), \(x_{j,k}^{n+1} := F^n(x_{j,k}^n)\) and \(D_{j,k}^n := D_{j,k}^n J_{j,k}^n\) according to (3.27)-(3.29);
2. otherwise, it is dynamically refined by adding \(\sigma_l w_{j,k}^n\) to \(w_{j,k}^{n+1,2k+l}\) for every \(l\) such that \(\parallel l \parallel \leq c_p\) (which may involve the activation of new particles according to (4.6)) and by finally setting \(w_{j,k}^n := 0\).

Remark 4.7. One disadvantage of the above strategy is the need to apply the numerical flows from past time steps, namely \(F^n_0, \ldots, F^n_{n-1}\), when refining a particle at time step \(n\). However it is useful from a theoretical point of view. Practical procedures involving local approximations of the time-integrated flow are currently being tested and will be presented in a forthcoming article.

5 Numerical experiments

In this section we compare the numerical performances of the different particle methods, using Leveque’s swirling velocity field [21] in two dimensions,

\[
\begin{align*}
    u_0(t, x) &= -\sin^2(\pi x_0) \sin(2\pi x_1) g(t), \\
    u_1(t, x) &= \sin^2(\pi x_1) \sin(2\pi x_0) g(t)
\end{align*}
\]

where \(g(t) = \cos(\pi t / T), t \in [0, T]\). The corresponding flow is easily pictured from the space pattern shown in Figure 1, and from the symmetry of \(g\) with respect to \(T/2\) which reverts the solutions to their initial state at \(t = T\). We will take \(T = 2.5\) which corresponds to a moderate stretching at \(t = T/2\) (see Figures 2, 3 and 6 below) and a fixed time step \(\Delta t = T/100\).

Although the time symmetry may simplify the measure of the numerical errors, we note that by considering only the final accuracy one misses the intermediate errors resulting from the inaccurate transport of the particle shapes, which yields biased estimates for particle methods with no remappings. Therefore, we shall only use the time symmetry in Section 5.2 when assessing the performances of the uniform and adaptive versions of the linearly transformed particle (LTP) scheme, with at least one remapping. In Section 5.1 where the traditional smoothed particle method (TSP) is compared to the forward semi-lagrangian (FSL) and the LTP schemes, we will only solve the equation on the half interval \([0, T/2]\), and hence measure the numerical errors at the instant of maximal stretching, using a reference numerical solution obtained with significantly higher space and time resolution.

![Figure 1: Leveque’s swirling velocity field (5.1) shown in the computational domain \([0, 1]^2\) at time \(t = 0\).](image-url)
5.1 Numerical comparison of the TSP, FSL and LTP schemes

To compare the LTP scheme with the classical TSP and FSL methods reviewed in Section 2, we consider the two following cases.

- A smooth hump centered on \( c = (0.5, 0.75) \) given by
  \[
  f^0(x) = \frac{1}{2} (1 + \text{erf}(a + b||x - c||_2)) \quad \text{with} \quad a = 3.43, \ b = 21.43. \tag{5.2}
  \]
  Here \( ||\cdot||_2 \) is the Euclidean norm and \( \text{erf}(s) = \frac{2}{\sqrt{\pi}} \int_0^s e^{-y^2} \, dy \) is the standard “error function” that smoothly spans \([-1, 1]\), see Figure 2.

- A discontinuous Zalesak’s slotted disk centered on \( c' = (0.5, 0.7) \),
  \[
  f^0(x) = H(0.15 - ||x - c'||_2)(1 - (1 - H(|x_0 - 0.5| - 0.02))(1 - H(x_1 - 0.8))) \tag{5.3}
  \]
  where \( H(s) = \chi_{s \geq 0} \) denotes the Heaviside step function, see Figure 4.

In Figures 3 and 4 the relative errors are plotted versus the average number of active particles at \( t = T/2 \), in order to avoid a biased measure for the TSP method as explained above. For the smooth hump case we measure the errors in \( L^\infty \), and for the discontinuous Zalesak disk we use the \( L^1 \) norm. Here all three methods have been run with B-spline particles of degree \( p = 1 \) or 3, initialized (and remapped, in the FSL and LTP cases) with the quasi-interpolation scheme of corresponding order. For the TSP method we show the effect of varying the overlapping exponent \( q \) such that \( \epsilon = h^q \), see Section 2.1 and for the FSL and LTP schemes we plot the runs corresponding to decreasing remapping frequencies, i.e., increasing values of the number \( N_r \) of time steps between two remappings. Observe that the higher \( q \) or \( N_r \), the cheaper the simulations. In every set of curves we have used a thick line to emphasize the cheapest run: for the TSP scheme that corresponds to the case \( q = 1 \) (particles radii are proportional to the initial meshsize) and for the FSL and LTP schemes that corresponds to the case with no remappings. Note that the FSL and TSP method coincide with such parameters.

From these plots we make the following observations. First, we see that a necessary condition for the TSP method to converge is indeed that particles present an extended overlapping. That is, the ratio \( \epsilon/h \) must go to \( +\infty \) as \( h \) goes to 0. Moreover, the convergence is relatively slow and is not much improved with third-order B-splines, although they help for moderate particle overlapping \( (q \approx 0.8) \). This is not surprising since the theoretical convergence analysis requires vanishing moments for high-order accuracy, which the B-splines do not have.

Second, our numerical tests confirm the announced practical condition for the FSL scheme to converge: remapping frequency must be high. On the plus side, we note that on the smooth test case, the FSL scheme exhibits significantly higher convergence rates than the TSP method when \( B_3 \) particles are used. However, to our view the method is severely hampered by the following dilemma: for values of \( N_r \) close to 1, problems with sharp edges such as the discontinuous Zalesak disk give rise to a strong numerical diffusion that can be seen (especially with \( B_3 \) particles) from the increase of the number of active particles and from the deterioration of the accuracy: decreasing the remapping frequencies helps reducing that effect, but doing so always leads to a loss of convergence (the lower the frequency, the sooner the stagnation).

Finally, we see that the LTP scheme always converges as expected from our analysis, including in the cheap, non-remapped runs, although remappings do improve the accuracy in the smooth test case (Figure 5). Moreover, the convergence rates are significantly higher than with the TSP method, and in the smooth case the benefit of using \( B_3 \) splines is obvious, just as in the FSL method. In the discontinuous case (Figure 5) we observe that lowering the remapping frequency strongly reduces the numerical diffusion (especially with \( B_3 \) particles), and in fact also improves the numerical accuracy. The striking result is that the loss of convergence observed in every FSL run using a low remapping frequency is completely suppressed in the LTP runs.

5.2 Numerical study of an adaptive LTP scheme

To assess the ability of our adaptive particle strategy to improve the computational efficiency, we compare its convergence curves to those of the uniform LTP scheme, using the two following cases.
Figure 2: Profile of the exact solution at $t = 0$ or $T$ (left) and $T/2$ (right) for the smooth hump

Figure 3: Convergence curves (relative $L^\infty$ errors at $t = T/2$ vs. average number of active particles) for the smooth hump test case shown in Figure 2, using the TSP, FSL and LTP schemes with B-spline particles of degree 1 and 3. Triangles represent slopes of 0.5 and 1.
Figure 4: Profile of the exact solution at $t = 0$ or $T$ (left) and $T/2$ (right) for the Zalesak’s slotted disk [5,3].

Figure 5: Convergence curves (relative $L^1$ errors at $t = T/2$ vs. average number of active particles) for the Zalesak’s test case shown in Figure 4 using the TSP, FSL and LTP schemes with B-spline particles of degree 1 and 3. Triangles represent slopes of 0.5 and 1.
• The smooth hump shown in Figure 2.

• A smoothed version of the discontinuous Zalesak’s slotted disk, designed so as to get solutions of highly non uniform smoothness that still can be approximated in the uniform norm. Indeed our adaptive refinement strategies are aimed at balancing the local errors in this norm and they have no reason to exhibit better convergence properties when the error is measured using another norm. The initial data $f^0$ is then obtained by substituting the discontinuous Heaviside step function $H(s) = \chi_{\{s \geq 0\}}$ in (5.3) with a smooth approximation $H_\epsilon(s) = \frac{1}{2}(1 + \text{erf}(s/\epsilon))$, where the transition zone has approximate diameter of $4\epsilon$. In the numerical tests we take $\epsilon = 0.01$, see Figure 6.

In Figure 7 we plot for both cases the $L^\infty$ convergence curves obtained with the uniform LTP scheme using various values of $N_r$ as above, and those obtained with our adaptive particle method using the optimal value $N_r = 25$ as found from the uniform runs, and levels $j = j_0, \ldots, j_{\text{max}}$ with $j_0 = 5$ and $j_{\text{max}} = 9$. Since we now consider particle methods with at least one remapping step, numerical accuracy is measured on the final time $t = T$ where the exact solutions revert to their initial state. The prescribed tolerance $\varepsilon$ varies in order to get different points in the “adaptive” convergence curves and we have fixed the constant $C_T$ in Condition (4.5) to 2, to optimize the numerical performances. However we note that a proper study of how the parameters $C_T$ and $N_r$ should be set in the general case remains to be done.

Figure 6: Profile of the exact solution at $t = 0$ or $T$ (left) and $T/2$ (right) for the smoothed Zalesak’s slotted disk.

Figure 7: $L^\infty$ convergence curves for the smooth hump (left) and the smoothed Zalesak’s slotted disk (right) in Leveque’s swirling flow. The relative $L^\infty$ errors are plotted vs. the average number of particles. Here the adapt curves correspond to adaptive runs and are obtained by varying the tolerance $\varepsilon$. The other curves are obtained by varying the uniform resolution $h$, as in Section 5.1. In the right panel the runs labelled adapt + use the positive correction filter (Algorithm 4.4) in each adaptive remapping. Triangles represent slopes of 0.5 and 1.
Figure 8: Particle centers (left) and level maps (right) at $t = T/2$ for the smooth hump test case shown in Figure 2 before (top) and after (bottom) being remapped on a hierarchy of cartesian grids with resolution levels $j = 5, \ldots, 9$ at $t = T/2$. Here the prescribed tolerance $\varepsilon$ is set so as to get an average number of particles corresponding to a uniform run of level $j = 7$, see Figure 9 below.

Figure 9: Final error distributions obtained for the smooth hump test case with a uniform run of level $j = 7$ using about $10^{164}$ particles in average (left), and the adaptive run shown on Figure 8 using about $10^{498}$ particles in average (right).
Figure 10: Particle centers (left) and level maps (right) for the smoothed Zalesak’s slotted disk shown in Figure 6 before (top) and after (bottom) being remapped on a hierarchy of cartesian grids with resolution levels $j = 5, \ldots, 9$ at $t = T/2$. Again the prescribed tolerance $\varepsilon$ is set so as to get an average number of particles corresponding to a uniform run of level $j = 7$, see Figure 11 below.

Figure 11: Final error distributions obtained for the smooth Zalesak’s slotted disk with a uniform run of level $j = 7$ using about 11864 particles in average (left), and the adaptive run shown on Figure 10, using about 11964 particles in average (right).
From Figure 7 we see that using adaptive particles with dynamic refinements yields a clear gain in terms of active particles number. Moreover, in the Zalesak case where the numerical solutions are likely to strongly oscillate in the vicinity of the sharp edges, we also plot a series of runs obtained with our multilevel correction Algorithm 4.4 that enforces positive weights, hence positive particles. The resulting observation is that the numerical efficiency does not seem to suffer much from this local (and somewhat crude) positivity-preserving filter.

To illustrate the behavior of the adaptive particle method, we also show on Figures 8 and 10 the distribution of active particle centers and associated level maps \(x \rightarrow \max \{j : \sum_{k \in \mathbb{Z}^d} |w_{j,k}^n \varphi_{j,k}^n| \neq 0\}\) at \(t = T/2\) (before and after remapping the particles).

Finally, one relevant feature of our adaptive particle scheme is shown on Figures 9 and 11, for the smooth hump and the smoothed Zalesak disk, respectively. There we have plotted the final error distributions obtained with uniform and adaptive runs using similar numbers of active particles (the adaptive runs correspond to those shown in Figures 8 and 10). In both cases we verify that resorting to adaptive particles does not only reduce the maximum error, but also balances the error distribution over the computational domain, as it should be.

6 Conclusion and further work

We have introduced a formal class of particle methods for transport problems with polynomial deformations of arbitrary degree \(r\), and established their \(L^\infty\) convergence with order \(r\), based on the smoothness of the underlying velocity field. In the first order case we have presented a fully discrete scheme for the resulting LTP scheme, along with local and global error estimates. Our preliminary numerical results demonstrate the improved convergence rate of the LTP scheme compared to the traditional “smoothed” particle method (TSP) with extended overlapping, and the need of lower remapping frequencies compared to the FSL scheme, leading to lower numerical diffusion and computational cost. On a practical level, implementing the FSL scheme is made simple by the fact that it only involves pointwise evaluations of the forward flow, a building block in any particle scheme. We also note that pointwise evaluations of the deformed particle collections can be made computationally efficient by following the procedure described in Section 3.4.

In a near future we shall present extensions of the LTP scheme that deal with non-linear transport problems arising in, e.g., plasma physics [6], and we will further investigate the properties of our adaptive multilevel scheme.

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