Meshfree Lagrangian Advection Schemes for the Numerical Simulation of Transport Processes

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Abstract: *A novel concept for the numerical simulation of transport processes by meshfree methods is proposed. The resulting particle-based advection scheme is essentially a method of backward characteristics, which combines an adaptive semi-Lagrangian method with local interpolation by polyharmonic splines. This "extended abstract" gives a short introduction to the features of the basic algorithm, and it briefly addresses some of its theoretical and computational aspects. One numerical example concerning Burgers equation is provided for the purpose of illustration. Further details are discussed during the workshop.*

Keywords: Transport equations, method of characteristics, radial basis functions.

1 Introduction

Many physical phenomena in transport processes are modelled by time-dependent advection-diffusion equations of the form

$$\frac{\partial u}{\partial t} + \nabla f(u) = \epsilon \cdot \Delta u, \tag{1}$$

where for some domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$, and a compact time interval $I = [0, T]$, $T > 0$, the function $u : I \times \Omega \to \mathbb{R}$ is unknown. Moreover, $f(u) = (f_1(u), \ldots, f_d(u))^T$ denotes the *flux tensor*, and $\epsilon > 0$ is the *diffusion coefficient*.

One relevant example for a (nonlinear) flux function in (1) is $f(u) = \frac{1}{2}u^2 \cdot r$, with some steady flow direction r, which leads us to the viscous *Burgers equation*

$$\frac{\partial u}{\partial t} + u \nabla u \cdot r = \epsilon \cdot \Delta u. \tag{2}$$

The equation (2) was introduced in 1940 by Burgers for modelling free turbulences in fluid flow. Burgers equation (2) is a popular standard test case for the simulation of physical phenomena concerning shock wave propagation, see Section 4.

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In previous work [1, 2, 3], a particle-based concept for the *meshfree* simulation of multiscale phenomena in both linear and nonlinear transport processes is proposed. The resulting advection scheme relies on a *method of characteristics*, which combines an adaptive semi-Lagrangian method with local interpolation by polyharmonic splines. This particular advection scheme solves (1) numerically, on given initial conditions

$$u(0,x) = u_0(x), \qquad \text{for } x \in \Omega. \tag{3}$$

To this end, the method works with a finite set $\Xi \subset \Omega$ of nodes, each of which corresponds at a time $t \in I$ to one fluid particle. According to the basic concept of semi-Lagrangian advection, the equation (1) is integrated along the trajectories of the particles' streamlines. Moreover, the node set Ξ is adaptively modified during the simulation, where the required adaption rules rely on a customized a posteriori error estimator.

Details on the employed meshfree method of characteristics are explained in the following Section 2. Then, in Section 3, a very short discussion on polyharmonic splines is provided, where relevant results concerning the stability and approximation order of local polyharmonic spline interpolation are reviewed, and where also the abovementioned error estimator is introduced. For the purpose of illustration, a numerical example concerning Burgers equation is finally shown in Section 4. Further theoretical and computational aspects of the method, in combination with selected examples from relevant applications, are discussed during the workshop.

2 Meshfree Method of Characteristics

Starting point of our advection scheme is the Lagrangian form

$$\frac{du}{dt} = \epsilon \cdot \Delta u,$$

of (1), where $\frac{du}{dt} = \frac{\partial u}{\partial t} + \nabla f(u)$ is the *material derivative*. This leads us to the discretization

$$\frac{u(t+\tau,\xi) - u(t,\mathbf{x})}{\tau} = \epsilon \cdot \Delta u(t,\mathbf{x}), \tag{4}$$

where $\mathbf{x} \equiv \mathbf{x}(\xi)$ is the *upstream point*, corresponding to the node $\xi \in \Xi$. The upstream point $\mathbf{x}$ of ξ can be viewed as the position of a particle at time t, which by traversing along its trajectory, arrives at ξ at time $t + \tau$, where $\tau > 0$ denotes the time step size. By using some standard notation from dynamic systems, we can express the upstream point $\mathbf{x}$ of ξ as

$$\mathbf{x} = \Phi^{t,t+\tau}\xi, \tag{5}$$

where $\Phi^{t,t+\tau} : \Omega \to \Omega$ denotes the *continuous evolution* of the (backward) flow of the *ordinary differential equation* (ODE)

$$\dot{x} = \frac{dx}{dt} = v(t,x), \tag{6}$$

with $v = \frac{\partial f(u)}{\partial u}$ being the advection velocity.

Note that the exact location of $\mathbf{x}$ is usually unknown. Therefore, in order to compute an approximation $\tilde{\mathbf{x}} \approx \mathbf{x}$ numerically, we work with a specific *discrete evolution* $\Psi^{t,t+\tau}$ of the flow, corresponding to the continuous evolution $\Phi^{t,t+\tau}$ in (5). The operator $\Psi^{t,t+\tau}$ is given by any suitable numerical method for solving the above ODE (6), which allows us to express the resulting approximation $\tilde{\mathbf{x}}$ of $\mathbf{x}$ as

$$\tilde{\mathbf{x}} = \Psi^{t,t+\tau}\xi.$$

For the sake of brevity, we refrain from expanding details concerning the employed ODE solver of our preference, but rather refer to the previous papers [1, 2, 3]. Having computed $\tilde{\mathbf{x}} = \Psi^{t,t+\tau}\xi$, the desired approximation of $u(t+\tau,\xi)$ in (4) would thus be given by

$$u(t+\tau,\xi) = u(t,\tilde{\mathbf{x}}) + \tau \cdot \epsilon \Delta u(t,\tilde{\mathbf{x}}), \qquad \text{for } \xi \in \Xi. \tag{7}$$

In order to determine the *unknown* function values $u(t,\tilde{\mathbf{x}})$, $\Delta u(t,\tilde{\mathbf{x}})$ in the right hand side of (7), we work with local interpolation by using polyharmonic splines. Some selected details concerning the relevant background of this particular interpolation scheme are briefly discussed in the following Section 3. For the moment be it sufficient to say that, on any given upstream point approximation $\tilde{\mathbf{x}}$, we determine a neighbouring set $\mathcal{N} \subset \Xi$ of current nodes around $\tilde{\mathbf{x}}$, all of whose values $u(t,\nu)$, $\nu \in \mathcal{N}$, are known. Then, we compute a polyharmonic spline interpolant s satisfying

$$s(\nu) = u(t,\nu), \qquad \text{for all } \nu \in \mathcal{N}, \tag{8}$$

before we replace (7) by

$$u(t+\tau,\xi) = s(\tilde{\mathbf{x}}) + \tau \cdot \epsilon \Delta s(\tilde{\mathbf{x}}), \qquad \text{for } \xi \in \Xi.$$

Altogether, the advection step $t \to t+\tau$ is accomplished as follows.

Algorithm 1 (Method of Characteristics).

INPUT: *Time step* τ, *nodes* Ξ, *values* $\{u(t,\xi)\}_{\xi\in\Xi}$.

FOR *each* $\xi \in \Xi$ **DO**

(a) *Compute the upstream point approximation* $\tilde{\mathbf{x}} = \Psi^{t,t+\tau}\xi$;

(b) *Determine the value* $s(\tilde{\mathbf{x}}) \approx u(t,\tilde{\mathbf{x}})$ *by local interpolation, i.e., solve (8);*

(c) *Advect by letting* $u(t+\tau,\xi) = s(\tilde{\mathbf{x}}) + \tau \cdot \epsilon \Delta s(\tilde{\mathbf{x}})$.

OUTPUT: *The values* $u(t+\tau,\xi)$, *for all* $\xi \in \Xi$, *at time* $t+\tau$.

3 Polyharmonic Spline Interpolation

In order to solve the *local* interpolation problem (8), we prefer to work with *polyharmonic splines*, which are popular tools for multivariate interpolation from scattered data. In this particular interpolation scheme, the interpolant s in (8) has the form

$$s = \sum_{\nu \in \mathcal{N}} c_\nu \cdot \phi_{d,k}(\| \cdot - \nu \|) + p, \qquad p \in \mathcal{P}_k^d,$$

where $\| \cdot \|$ denotes the Euclidean norm on $\mathbb{R}^d$, and the polyharmonic spline $\phi_{d,k}$ is given by

$$\phi_{d,k}(r) = \begin{cases} r^{2k-d} \log(r), & \text{for } d \text{ even}, \\ r^{2k-d}, & \text{for } d \text{ odd}, \end{cases}$$

with $2k > d$. Moreover, $\mathcal{P}_k^d$ denotes the linear space of all d-variate polynomials of order at most k. We remark that the interpolation problem (8) has under constraints

$$\sum_{\nu \in \mathcal{N}} c_\nu p(\nu) = 0, \qquad \text{for all } p \in \mathcal{P}_k^d,$$

a unique solution, provided that the points in $\mathcal{N}$ are $\mathcal{P}_k^d$-*unisolvent*, i.e., for $p \in \mathcal{P}_k^d$,

$$p(\nu) = 0 \quad \text{for all } \nu \in \mathcal{N} \qquad \Longrightarrow \qquad p \equiv 0.$$

The stability and the approximation order of *local* polyharmonic spline interpolation has recently been discussed in [4]. One of the key observation in [4] is that the Lagrange basis $(\lambda_\nu(x))_{\nu \in \mathcal{N}}$, and thus the *Lebesgue constant*

$$\Lambda(U, \mathcal{N}) = \max_{x \in U} \sum_{\nu \in \mathcal{N}} |\lambda_\nu(x)|, \qquad \text{for } \mathcal{N} \subset U \subset \Omega,$$

of the interpolation scheme is invariant under uniform scalings. This in turn leads to a *stable* algorithm for solving (8). Moreover, it shows that the *approximation order* of local polyharmonic spline interpolation around any $\tilde{\mathbf{x}}$ is k, i.e., for any point $\tilde{\mathbf{x}} + h(x - \tilde{\mathbf{x}}) \in U$, $h > 0$, and a fixed local neighbourhood U of $\tilde{\mathbf{x}}$ we have

$$|s^h(\tilde{\mathbf{x}} + h(x - \tilde{\mathbf{x}})) - u(t, \tilde{\mathbf{x}} + h(x - \tilde{\mathbf{x}}))| = \mathcal{O}(h^k), \quad h \to 0, \qquad \text{for } u(t, \cdot) \in C^k,$$

where s^h denotes the unique polyharmonic spline interpolant satisfying

$$s^h(\tilde{\mathbf{x}} + h(\nu - \tilde{\mathbf{x}})) = u(t, \tilde{\mathbf{x}} + h(\nu - \tilde{\mathbf{x}})), \qquad \text{for all } \nu \in \mathcal{N}.$$

For further details on local polyharmonic spline interpolation, we refer to [4].

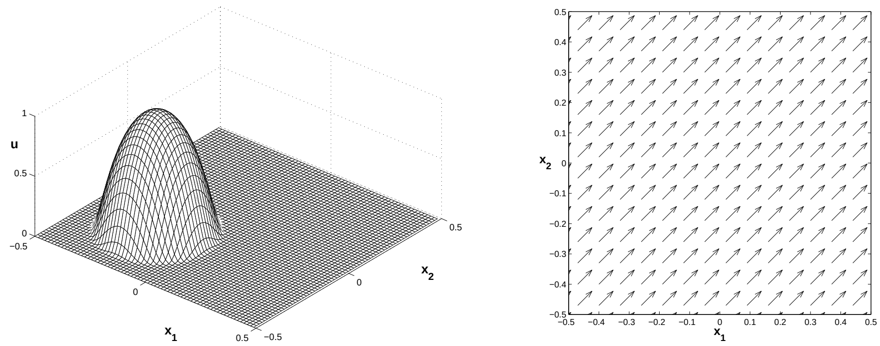
Polyharmonic spline interpolation is also used in order to adaptively modify the current node set $\Xi \equiv \Xi(t)$ after each advection step of Algorithm 1, yielding a modified node set $\Xi \equiv \Xi(t + \tau)$. To this end, we work with an *error indicator*, which assigns to each current node $\xi \in \Xi(t)$ a *significance value*

$$\eta(\xi) = |s_{\mathcal{N} \setminus \xi} - u(t, \xi)|, \qquad \text{for } \xi \in \Xi,$$

where $s_{\mathcal{N} \setminus \xi}$ denotes the polyharmonic spline interpolant which interpolates the values $u(t, \nu)$, $\nu \in \mathcal{N}$, at a set $\mathcal{N} \subset \Xi \setminus \xi$ of current nodes in the neighbourhood of ξ. The error indicator $\eta : \Xi \to \mathbb{R}$ thus evaluates the local approximation quality around the nodes in $\Xi(t)$. The modification of $\Xi(t)$ is then accomplished by the removal of nodes with small significances, *coarsening*, whereas in the neighbourhood of nodes with large significances new nodes are inserted, *refinement*. For further details concerning the implementation of these adaption rules, see [2].

4 Numerical Example: Burgers Equation

We use Burgers equation (2) in order to illustrate the efficacy of the meshfree method of characteristics, Algorithm 1, in combination with the abovementioned adaption rules. In this test case, we define for $R = 0.25$ and $c = (0.3, 0.3)$ the initial condition in (3) by $u_0(x) = \exp\left(\frac{\|x-c\|^2}{\|x-c\|^2-R^2}\right)$, for $\|x - c\| < R$, and $u_0(x) = 0$, otherwise. Moreover, we let $\Omega = [0, 1]^2$. Figure 1 shows the initial condition and the flow field $r = (1, 1)$, being aligned along the diagonal in the computational domain Ω.



(a) **(b)**

Figure 1: Burgers equation. **(a)** Initial condition u_0, and **(b)** flow field $r = (1, 1)$.

In this simulation, a constant time step size $\tau = 0.004$ is selected, and we let $I = [0, 330\tau]$. A plot of the numerical solution u at the three time steps $t_{110} = 110\tau$, $t_{220} = 220\tau$, and $t_{330} = 330\tau$ is shown in Figure 2, along with the corresponding distribution of the node set $\Xi \equiv \Xi(t)$. Observe that the propagation of the shock front is well-captured by the adaptive node distribution, which helps to reduce the required computational costs for the simulation at good approximation quality. This in turn confirms the utility of the adaption rules yet once more. Further properties of the method and its relevant applications are discussed during the workshop.

References

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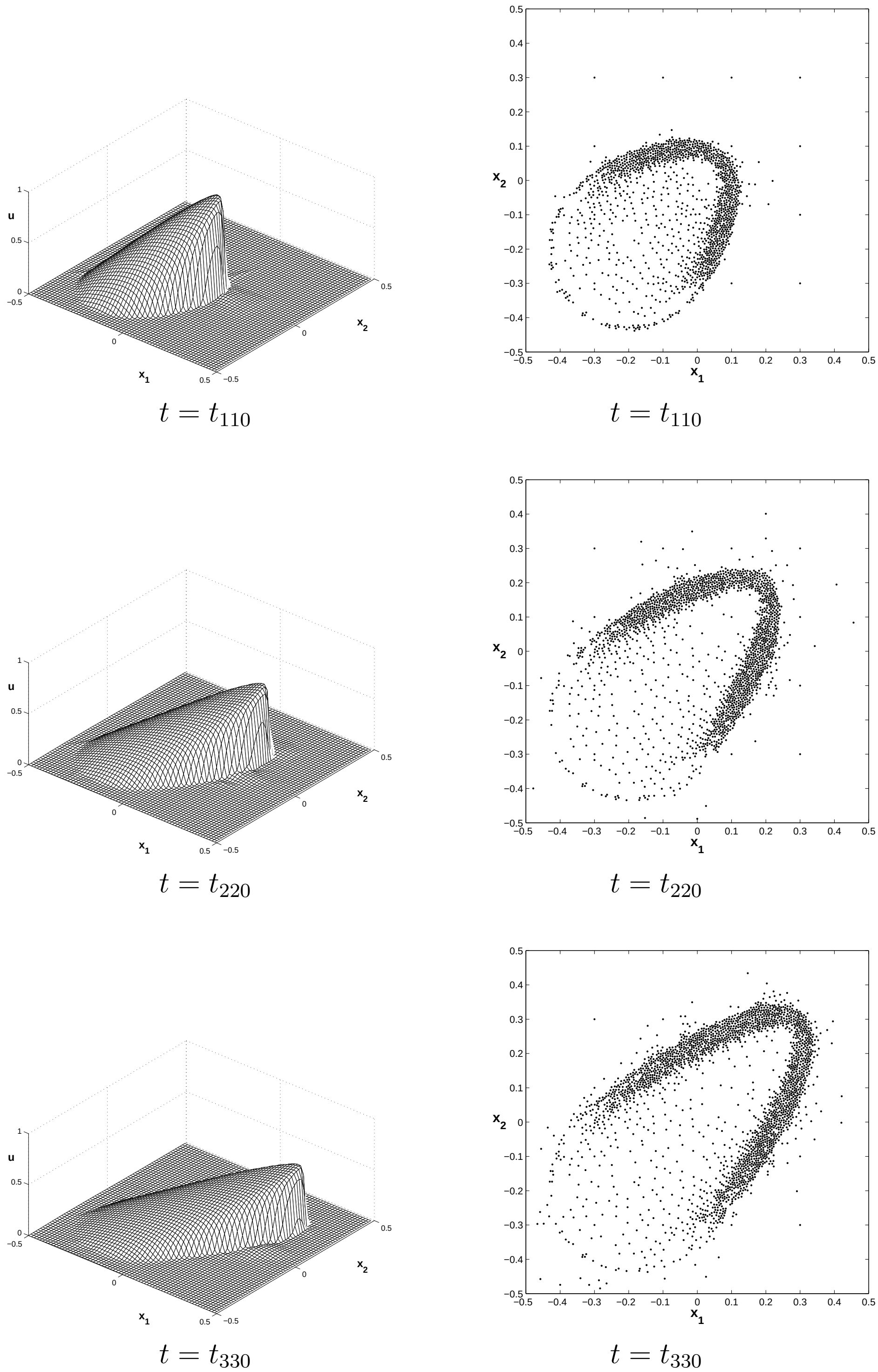

Figure 2: Burgers equation. Evolution of the solution u at three different time steps, $t_{110} = 110\tau$, $t_{220} = 220\tau$, and $t_{330} = 330\tau$ (left column), and the corresponding node distribution (right column).