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Vorwort

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In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe sollen sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen werden.

Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

ADJOINT BASED OPTIMAL CONTROL USING MESH-LESS DISCRETIZATIONS

JAN MARBURGER, NICOLE MARHEINEKE, AND RENÉ PINNAU

ABSTRACT. The paper at hand presents a combination of optimal control approaches for PDEs with mesh-less discretizations. Applying a classical Lagrangian type particle method on optimization problems with hyperbolic constraints, several adjoint-based strategies differing in the sequential order of optimization and discretization of the Lagrangian or, respectively, Eulerian problem formulation are proposed and compared. The numerical results confirm the theoretically predicted independence principle of the optimization approaches and and show the expected convergence behavior. Moreover, they exemplify the superiority of mesh-less methods to the conventional mesh-based approaches for the numerical handling and optimization of problems with time-dependent geometries and free moving boundaries.

Keywords. Mesh-less methods, particle methods, Eulerian-Lagrangian formulation, optimization strategies, adjoint method, hyperbolic equations

Subject (MSC). 49-99, 65K10, 76M28

1. Introduction

An easy numerical handling of time-dependent problems with complicated geometries, free moving boundaries and interfaces, or oscillating solutions is of great importance for many applications, e.g., in fluid dynamics (free surface and multiphase flows, fluid-structure interactions [22, 18, 24]), failure mechanics (crack growth and propagation [4]), magneto-hydrodynamics (accretion disks, jets and cloud simulation [6]), biophysics and -chemistry. Appropriate discretizations, so-called mesh-less methods, have been developed during the last decades to meet these challenging demands and to relieve the burden of remeshing and successive mesh generation being faced by the conventional mesh-based methods, [16, 10, 3]. The prearranged mesh is an artificial constraint to ensure compatibility of the mesh-based interpolant schemes, that often conflicts with the real physical conditions of the continuum model. Then, remeshing becomes inevitable, which is not only extremely time- and storage consuming but also the source for numerical errors and hence the gradual loss of computational accuracy. Apart from this advantage, mesh-less methods also lead to fundamentally better approximations regarding aspects, such as smoothness, nonlocal interpolation character, flexible connectivity, refinement and enrichment procedures, [16]. The common idea of mesh-less methods is the discretization of the domain of interest by a finite set of independent, randomly distributed particles moving with a characteristic velocity of the problem. Location and distribution of the particles then account for the time-dependent description of the geometry, data and solution. Thereby, the global solution is linearly superposed from the local information carried by the particles. In classical particle methods [20, 21], the respective weight functions are Dirac distributions which yield solutions in a distributional sense.

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In mesh-less Galerkin or partition of unity methods [3, 8], in contrast, compact patches or volumes are attached to every particle, whose union forms an open covering of the domain. On the patches, local weight functions are constructed via data fitting. Representing the influence of the particles in their respective neighborhoods, these functions provide a basis for a Galerkin or collocation discretization process. Depending on the fitting ansatz, the methods generalize finite element, volume and difference approaches, respectively,

Since there is a tremendous and even increasing need of optimization and optimal control in the mentioned applications [5, 13], the goal of this paper is a first combination of conventional optimization strategies for PDEs with mesh-less discretizations. We focus on the application of classical Lagrangian type particle methods on balance laws, in particular hyperbolic equations, and study the optimization results formally obtained from different strategies using an adjoint approach [12]. The investigated strategies tackle hereby the question of the numerical effect and computational effort when varying the sequential order of optimization and discretization on Lagrangian as well as Eulerian problem formulations.

This paper is organized in the following manner. After a brief introduction to particle methods in section 2, we present several adjoint-based optimization strategies differing in the sequential order of optimization and discretization (first optimization, then discretization versus first optimization, then discretization) for tracking-type problems with hyperbolic partial differential constraints in section 3. In particular, we formally derive the corresponding adjoint systems for a Lagrangian problem formulation, discuss their differences and compare them with the optimization results for the associated Eulerian formulation in section 4. In section 5 we apply the strategies exemplarily on one-dimensional problems, i.e., linear convection and nonlinear Burger equations. The numerical results confirm the theoretically predicted independence principle of the optimization approaches and show the expected convergence behavior. Moreover, they clearly emphasize the superiority of mesh-less methods to mesh-based ones in case of time-dependent geometry changes and huge deformations.

2. Lagrangian Type Particle Method

Particle methods are a special type of mesh-less methods. They originate from the numerical treatment of physics applications like Boltzmann equations [20, 21] (molecular dynamics, direct simulation Monte Carlo, see [16] and the references within) where the quantities of the conservation problem are approximated on a set of randomly distributed particles. Classically, they have been truly Lagrangian methods, i.e. the particles move with the convective velocity of the problem. This ansatz has been extended to mixed Lagrangian-Eulerian considerations such that the dynamics of the particles might also be prescribed by another characteristic velocity, e.g., the deformation velocity given by a free surface motion. Thus, the approach provides an easy numerical treatment of free moving boundaries and interfaces, complicated geometries and time dependencies, but is also restricted to (instationary) conservation problems. Stationary or elliptic problems might be handled by other mesh-less variants based on data fitting, e.g., Galerkin and partition of unity methods, such as smoothed particle hydrodynamics (SPH) [9, 19], moving least square (MLS) [14, 15] and moving least square particle hydrodynamics (MLSPH) [7], reproducing kernel particle method (RKPM) [17], partition of unity finite element method (PUFEM) [1, 2] and particle-partition of unity method [11] or finite point-set method (FPM) [24] (for more details about mesh-less (particle) methods see [16, 10, 3]).

The approximation idea common to mesh-less methods can be summarized as follows: Let the quantity of interest $y : \Omega \times [0,T] \to \mathbb{R}^m$, $\Omega \subset \mathbb{R}^n$, be approximated by N particles carrying the information of their position and the specific local quantity $(x_i, y_i) : [0,T] \to \Omega \times \mathbb{R}^m$, $i = 1, ..., N$, then

$$y(x,t) \simeq y_h(x,t) := \sum_{i=1}^{N} y_i(t)\, S_i(x,t;x_1^N(t)), \qquad x_1^N(t) := \{x_i(t)\}_{i=1,\dots,N}. \tag{1}$$

The spatial interpolation functions S_i represent the influence of the respective particles in their local neighborhood. In particle methods they are given by Dirac distributions $S_i(x,t;x_1^N(t)) = \delta(x - x_i(t))$, whereas in mesh-less Galerkin or partition of unity methods they are constructed via data fitting, satisfying $\sum_{i=1}^N S_i = 1$. Investigating particle methods on conservation laws, Raviart [23] derived convergence results $y_h \to y$ under the assumption of sufficiently uniform particle distributions for $N \to \infty$.

Following Raviart's approach, we focus on the discretization via a classical Lagrangian type particle method in this paper. This discretization can be interpreted as a method of characteristics for hyperbolic equations which requires a specific coordinate transformation between Lagrangian (material) and Eulerian (spatial) coordinates. A coordinate transformation or motion Φ is given by an invertible, regular mapping

$$\Phi : \hat{\Omega}^T = \hat{\Omega} \times (0,T] \to \mathbb{R}^n, \quad \hat{\Omega} \subset \mathbb{R}^n,$$

initialized with $\Phi(X,0) = X$ at time $t = 0$. We denote its derivative with respect to X by $\delta\Phi := \partial_X \Phi$ and assume $\det(\delta\Phi) > 0$. Consider the transformation-dependent domain

$$\Omega^T = \{(x,t) \,|\, x \in \Phi(\hat{\Omega},t),\, t \in (0,T]\}$$

with boundary $\partial\Omega^T = \{(x,t) \,|\, x \in \Phi(\partial\hat{\Omega},t),\, t \in (0,T)\}$. For every function $\omega : \Omega^T \to \mathbb{R}^m$, we define the associated mapping $\hat{\omega} : \hat{\Omega}^T \to \mathbb{R}^m$ with respect to the reference domain $\hat{\Omega}$ by

$$\hat{\omega}(X,t) := \omega(\Phi(X,t),t).$$

Then, the following relations hold

$$\begin{aligned} \partial_X \hat{\omega}(X,t) &= \partial_x \omega(\Phi(X,t),t)\, \delta\Phi(X,t), \\ \partial_t \hat{\omega}(X,t) &= \partial_X \hat{\omega}(X,t)(\delta\Phi(X,t))^{-1} \partial_t \Phi(X,t) + \partial_t \omega(\Phi(X,t),t). \end{aligned}$$

3. Optimization Strategies

In this section we study the two main adjoint-based approaches for the optimization of conservation problems using particle methods. In the first approach, we apply the adjoint based optimization formalism directly to the continuous (Eulerian or, respectively Lagrangian) formulation of the optimization problem and derive the optimality system to be discretized via a particle method. In the second approach, we proceed from the discrete Lagrange functional to deduce the respective adjoint system. For convenience, we restrict the following investigations to scalar-valued one-dimensional hyperbolic PDEs in order to embed the particle method into the method of characteristics using the convective velocity as particle motion. Certainly, they can be directly extended to vector-valued, higher dimensional as well as parabolic equations.

The minimization problem of interest reads for state y and control u variable:
Minimize

$$J(y,u) = \frac{1}{2}\int_{\mathbb{R}} |y(x,T) - y_d(x)|^2\,dx + \frac{\alpha}{2}\int_0^T\int_{\mathbb{R}} |u(x,t)|^2\,dx\,dt$$

subject to

$$\left.\begin{aligned} \partial_t y + \frac{d}{dx} f(y,x,t) &= u && \text{in } \mathbb{R}\times(0,T], \\ y(x,0) &= y_0(x) && \text{in } \mathbb{R}, \end{aligned}\right\} (\mathrm{CF_E})$$

where y_d denotes the desired state at time T and $\alpha > 0$ a regularization parameter in the tracking-type problem. The flux function f in the hyperbolic constraint is supposed to be sufficiently regular. Assuming a compact support for the initial condition $y(x,0) = y_0(x)$ on $\hat{\Omega} \subset \mathbb{R}$ and non-crossing characteristics, the full space optimization can be reduced onto the domain of problem-relevant characteristics Ω^T prescribed by the initial domain $\hat{\Omega}$ and the convective velocity $\partial_y f$ via the coordinate transformation Φ:

$$\partial_t \Phi(X,t) = \partial_y f(y(\Phi(X,t),t),\Phi(X,t),t) \quad \text{in } \hat{\Omega}^T, \qquad \Phi(X,0) = X \quad \text{in } \hat{\Omega}. \tag{2}$$

Then, we minimize

$$J(y,\Phi,u) = \frac{1}{2}\int_{\Phi(\hat{\Omega},T)} |y(x,T) - y_d(x)|^2\,dx + \frac{\alpha}{2}\int_{\Omega^T} |u(x,t)|^2\,dx\,dt$$

subject to

$$\begin{aligned} \partial_t y + \frac{d}{dx} f(y,x,t) &= u && \text{in } \Omega^T, \\ y(x,0) &= y_0(x) && \text{in } \Omega^0 = \hat{\Omega}. \end{aligned}$$

3.1. **Continuous Lagrangian Approach.** The coordinate transformation Φ in (2) implies a Lagrangian (material) formulation of the problem. In this formulation, the PDE-constraint reduces to a system of ODEs in $\hat{\Omega}^T$

$$\left.\begin{aligned} \partial_t \hat{y}(X,t) &= u(\Phi(X,t),t) - \partial_x f(\hat{y}(X,t),\Phi(X,t),t), \\ \hat{y}(X,0) &= y_0(X), \\ \partial_t \Phi(X,t) &= \partial_y f(\hat{y}(X,t),\Phi(X,t),t), \\ \Phi(X,0) &= X, \end{aligned}\right\} (\mathrm{CF_L})$$

where the control u exclusively affects the state $\hat{y}$ along the characteristics but not their run Φ themselves. Hence, we minimize the respective cost functional

$$\hat{J}(\hat{y},\Phi,u) = \frac{1}{2}\int_{\hat{\Omega}} |\hat{y}(X,T) - y_d(\Phi(X,T))|^2\,\delta\Phi\,dX + \frac{\alpha}{2}\int_{\hat{\Omega}^T} |u(\Phi(X,t),t)|^2\,\delta\Phi\,dX\,dt$$

subject to $(\mathrm{CF_L})$. For the control u and the desired state function y_d we avoid the substitution with the transformed (hatted) quantities, since we do not intend to change the setting. The quantities are defined in the spatial domain in an Eulerian sense and not on a reference set (material points) in a Lagrangian consideration. Therefore, we also evaluate them in Ω^T.

Dealing with a constrained optimization problem [12], we formulate the Karush-Kuhn-Tucker system by help of the Lagrangian functional associated to the minimization problem

$$\begin{aligned}\hat{L}(\hat{y},\Phi,u,\hat{p},z) &= \hat{J}(\hat{y},u,\Phi) + \langle \hat{y}(\cdot,0)-y_0(\cdot),\hat{p}(\cdot,0)\rangle + \langle \Phi(\cdot,0)-\cdot, z(\cdot,0)\rangle \\ &\quad + \langle \partial_t\hat{y} - u(\Phi,\cdot) + \partial_x f(\hat{y},\Phi,t),\hat{p}\rangle + \langle \partial_t\Phi - \partial_y f(\hat{y},\Phi,t), z\rangle,\end{aligned} \tag{3}$$

where $\hat{p}$, z denote the adjoint variables and $\langle .,. \rangle$ suitably chosen duality pairings. According to the Lagrange Multiplier theorem, the variations of the Lagrangian with respect to the state, control and adjoint variables vanish in the critical point which yields the first-order optimality system

$$\begin{aligned}&\partial_{\hat{y}}\hat{L}(\hat{y},\Phi,u,\hat{p},z)\varphi^{\hat{y}} = 0, \qquad \partial_{\hat{p}}\hat{L}(\hat{y},\Phi,u,\hat{p},z)\varphi^{\hat{p}} = 0, \qquad \partial_u\hat{L}(\hat{y},\Phi,u,\hat{p},z)\varphi^{u} = 0,\\ &\partial_{\Phi}\hat{L}(\hat{y},\Phi,u,\hat{p},z)\varphi^{\Phi} = 0, \qquad \partial_z\hat{L}(\hat{y},\Phi,u,\hat{p},z)\varphi^{z} = 0\end{aligned}$$

for all suitable test functions $\varphi^{\hat{y}},\varphi^{\Phi},\varphi^{\hat{p}},\varphi^{z} : \hat{\Omega}^T \to \mathbb{R}$ and $\varphi^u : \Omega^T \to \mathbb{R}$. This yields formally the continuous backward (adjoint) equations

$$\left.\begin{aligned}\partial_t\hat{p}(X,t) &= \partial_{xy}f(\hat{y},\Phi,t)\hat{p} - \partial_{yy}f(\hat{y},\Phi,t)z,\\ \hat{p}(X,T) &= -(\hat{y}(X,T) - y_d(\Phi(X,T)))\,\delta\Phi,\\ \partial_t z(X,t) &= -\partial_x u(\Phi,t)\hat{p} + \partial_{xx}f(\hat{y},\Phi,t)\hat{p} - \partial_{xy}f(\hat{y},\Phi,t)z,\\ z(X,T) &= (\hat{y}(X,T) - y_d(\Phi(X,T)))\partial_X y(X,T)\end{aligned}\right\} \quad (\mathrm{CB_L})$$

and the gradient of the reduced cost functional by help of the variational lemma

$$\nabla\tilde{J}(u) := \nabla\hat{J}(\hat{y}(u),\Phi(u),u) = \alpha u(x,t) - \hat{p}(\Phi^{-1}(x,t),t)(\,\delta\Phi(\Phi^{-1}(x,t),t))^{-1}.$$

Finally, both systems, $(\mathrm{CF_L})$ and $(\mathrm{CB_L})$, are discretized with a particle method. For this, we randomly distribute N particles at positions $\{X_i\}_{i=1,\dots,N}$ in Ω. Then, we obtain the corresponding discrete forward equations for the particle trajectories Φ_i and the carried local quantities y_i

$$\left.\begin{aligned}\partial_t y_i(t) &= u(\Phi_i(t),t) - \partial_x f(y_i(t),\Phi_i(t),t),\\ y_i(0) &= y_0(X_i),\\ \partial_t\Phi_i(t) &= \partial_y f(y_i(t),\Phi_i(t),t),\\ \Phi_i(0) &= X_i,\end{aligned}\right\} \quad (\mathrm{DF})$$

as well as the discrete backward (adjoint) equations

$$\left.\begin{aligned}\partial_t p_i(t) &= \partial_{xy}f(y_i(t),\Phi_i(t),t)p_i(t) - \partial_{yy}f(y_i(t),\Phi_i(t),t)z_i(t),\\ p_i(T) &= (y_i(T) - y_d(\Phi_i(T)))\,\delta\Phi_i(T),\\ \partial_t z_i(t) &= -\partial_x u(\Phi_i(t),t)p_i(t)\\ &\qquad + \partial_{xx}f(y_i(t),\Phi_i(t),t)p_i(t) - \partial_{xy}f(y_i(t),\Phi_i(t),t)z_i(t),\\ z_i(T) &= (y_i(T) - y_d(\Phi_i(T)))\partial_X y_i(T).\end{aligned}\right\} \quad (\mathrm{DB_{L1}})$$

Consequently, the Lagrangian type particle method yields two systems of $2N$ ODEs. Since the adjoint problem $(\mathrm{DB_{L1}})$ uses the same trajectories as the forward problem (DF), only the function values of the control u need to be interpolated. The discrete gradient reads

$$\nabla\tilde{J}_h(u) = \alpha u(x,t) - \sum_{i=1}^{N} p_i(t)\,\delta\Phi_i(t)^{-1}S_i(x,t;\Phi_1^N(t)) \tag{4}$$

using the solution of ($\mathrm{DB_{L1}}$).

3.2. **Discrete Lagrangian Approach.** Performing the optimization on the discretized system (DF), we state the discrete version of the cost functional

$$J_h(y_1^N, \Phi_1^N, u) = \frac{1}{2}\sum_{i=1}^N |y_i(T) - y_d(\Phi_i(T))|^2 h_i(\Phi_1^N) + \frac{\alpha}{2}\int_0^T \sum_{i=1}^N u(\Phi_i(t), t)^2 h_i(\Phi_1^N)\, dt$$

where the spatial integrals are approximated by a quadrature formula whose convergence order depends on the chosen weight functions $h_i(\Phi_1^N)$. In the particular one-dimensional case at hand, we use a finite difference scheme

$$h_i(\Phi_1^N(t)) := \frac{1}{2}(\Phi_{i+1}(t) - \Phi_{i-1}(t)).$$

Minimizing $J_h(y_1^N, \Phi_1^N, u)$ subject to (DF), the associated discrete Lagrange functional reads

$$\begin{aligned} L_h(y_1^N, \Phi_1^N, u, p_1^N, z_1^N) &= J_h(y_1^N, \Phi_1^N, u) \\ &\quad + \sum_{j=1}^N \big[(y_j(0) - y_0(X_j))p_j(0) + (\Phi_j(0) - X_j)z_j(0)\big] h_j(X_1^N) \\ + \int_0^T \sum_{j=1}^N \big[(\partial_t y_j &- u(\Phi_j(t), t) + \partial_x f(y_j, \Phi_j, t))p_j + (\partial_t \Phi_j - \partial_y f(y_j, \Phi_j, t))z_j\big] h_j(X_1^N)\, dt \end{aligned}$$

This is equivalent to a discretization of the continuous Lagrange functional in (3). Taking variations of L_h with respect to the states y_i, Φ_i and the control u we obtain the discrete adjoint equations

$$\left.\begin{aligned} \partial_t p_i &= \partial_{xy} f(y_i, \Phi_i, t)p_i - \partial_{yy} f(y_i, \Phi_i, t)z_i, \\ p_i(T) &= -(y_i(T) - y_d(\Phi_i(T)))\, \delta\Phi_i(t), \\ \partial_t z_i &= \alpha u(\Phi_i, t)\partial_x u(\Phi_i, t)\, \delta\Phi_i - \frac{\alpha}{4}(u(\Phi_{i+1}, t)^2 - u(\Phi_{i-1}, t)^2)h_i(X_1^N)^{-1} \\ &\quad - \partial_x u(\Phi_i, t)p_i + \partial_{xx} f(y_i, \Phi_i, t)p_i - \partial_{xy} f(y_i, \Phi_i, t)z_i, \\ z_i(T) &= (y_i(T) - y_d(\Phi_i(T)))\partial_x y_d(\Phi_i(T))\, \delta\Phi_i(T) \\ &\quad + \frac{1}{4}\big((y_{i+1}(T) - y_d(\Phi_{i+1}(T)))^2 - (y_{i-1}(T) - y_d(\Phi_{i-1}(T)))^2\big)h_i(X_1^N)^{-1} \end{aligned}\right\} (\mathrm{DB_{L2}})$$

and identify the gradient of the reduced cost functional as

$$\nabla \tilde{J}_h(u) = \alpha u(x,t) - \sum_{i=1}^N p_i(t)\, \delta\Phi_i(t)^{-1} S_i(x, t; \Phi_1^N)$$

in the discrete L^2-inner product.

3.3. **Continuous Eulerian Approach.** The application of a particle method induces a Lagrangian (material) formulation of the problem with ODEs for particle trajectories (characteristics) Φ and information $\hat{y}$, but the optimization is not necessarily restricted to this formulation. The adjoint equations can analogously be directly derived from the original Eulerian (spatial) formulation with the hyperbolic PDE constraint for y ($\mathrm{CF_E}$), then we get

$$\left.\begin{aligned} \partial_t p + \partial_y f(y,x,t)\partial_x p &= 0 && \text{in } \mathbb{R}\times(0,T], \\ p(x,T) &= -(y(x,T)-y_d(x)) && \text{in } \mathbb{R}. \end{aligned}\right\} (\mathrm{CB_E})$$

Since the forward and adjoint system are independent of each other, we have the freedom to apply two different particle discretizations $\{X_i\}_{i=1,\ldots,N}$ and $\{\bar{X}_j\}_{j=1,\ldots,M}$. This yields the already known forward system (DF) and the discrete adjoint system

$$\begin{aligned} \partial_t p_j(t) &= 0, \\ p_j(T) &= -(y(\bar{\Phi}_j(T),T) - y_d(\bar{\Phi}_j(T))), \\ \partial_t \bar{\Phi}_j(t) &= \partial_y f(y(\bar{\Phi}_j(t),t),\bar{\Phi}_j(t),t), \\ \bar{\Phi}_j(T) &= \bar{X}_j. \end{aligned}$$

As consequence, y has to be interpolated at the points $\bar{\Phi}_j(t)$ using for example (1). To avoid unnecessary computational errors on account of these interpolations one can restrict the computation to a single common discretization, setting $\bar{X}_i = \Phi_i(T)$, $m = n$. Then, the adjoint system reduces to

$$p_i(t) = -(y_i(T) - y_d(\Phi_i(T))). \quad \Big\} (\mathrm{DB_E})$$

The gradient of the reduced cost functional is identified as

$$\nabla \tilde{J}(u) = \alpha u(x,t) - p(x,t)$$

or, respectively, using the discrete values given by ($\mathrm{DB_E}$), as

$$\nabla \tilde{J}_h(u) = \alpha u(x,t) - \sum_{i=1}^{N} p_i(t) S_i(x,t;\Phi_1^N(t)). \tag{5}$$

4. Comparison of the Three Approaches

In the following we discuss the relation of the three optimization approaches and show that they are either equivalent or differ at most by an error of order of the discretization error.

4.1. **Comparison of Lagrangian Optimization Approaches.** The varying sequential order of optimization and discretization does not affect the forward system. It is the same in both approaches, in particular (DF). Hence, starting with the same particle distribution $\{X_i\}_{i=1,\ldots,N}$, the particle trajectories Φ_i and carried quantities y_i are identical. Also the form of the gradients and the evolution equations for the adjoints p_i in ($\mathrm{DB_{L1}}$) and ($\mathrm{DB_{L2}}$) coincide. The only apparent difference is the ODE for the adjoint trajectories z_i. To estimate its effect, we reintroduce the X-dependency of the particle quantities, i.e., we reinterpret $\Phi_i(t) = \Phi(X_i,t)$ and $y_i(t) = \hat{y}(X_i,t)$. Then, the evolution equation for z_i of ($\mathrm{DB_{L2}}$) can be rewritten as

$$\begin{aligned} \partial_t z_i &= \alpha u(\Phi_i,t)\partial_x u(\Phi_i,t)\,\delta\Phi_i - \frac{\alpha}{2}\frac{d}{dX}(u(\Phi(X_i,t),t)^2) + \mathcal{O}(h^2) \\ &\quad - \partial_x u(\Phi_i,t)p_i + \partial_{xx} f(y_i,\Phi_i,t)p_i - \partial_{xy} f(y_i,\Phi_i,t) z_i \\ &= -\partial_x u(\Phi_i,t)p_i + \partial_{xx} f(y_i,\Phi_i,t)p_i - \partial_{xy} f(y_i,\Phi_i,t) z_i + \mathcal{O}(h^2), \end{aligned}$$

$$
\begin{aligned}
z_i(T) &= (y_i(T) - y_d(\Phi_i(T)))\partial_x y_d(\Phi_i(T))\,\delta\Phi_i(T) + \frac{1}{2}\frac{d}{dX}\big((\hat{y}(X_i,T) - y_d(\Phi(X_i,T)))^2\big) + \mathcal{O}(h^2)\\
&= (y_i(T) - y_d(\Phi_i(T)))\partial_X y_i(T) + \mathcal{O}(h^2).
\end{aligned}
$$

Hence, ($\mathrm{DB_{L2}}$) just differs from ($\mathrm{DB_{L1}}$) in an discretization error of order $\mathcal{O}(h^2)$, $h = \max_i h_i(X_1^N)$, that enters the system by the approximation of the derivatives. Note that h refers to the initial particle distribution and is thus independent of time. Consequently, both strategies yield consistent discretizations of the continuous problem as expected.

4.2. **Comparison of Lagrangian and Eulerian Ansatz.** The Eulerian and Lagrangian formulations are transferable into each other using the coordinate transformation Φ. Hence, applying the same Lagrangian particle method the respective discrete forward systems are identical. The backward systems ($\mathrm{DB_{L1}}$) and ($\mathrm{DB_E}$) as well as the corresponding gradients (4) and (5), in contrast, seem to differ at the first glance, but there exists also a transformation between the adjoints as we will show in the following.

Therefore, we introduce $\bar{p}_i = p_i\,\delta\Phi_i^{-1}$ in the Lagrangian approach. Then, the gradient in (4) becomes

$$
\nabla\tilde{J}_h(u) = \alpha u(x,t) - \sum_{i=1}^{N} \bar{p}_i(t) S_i(x,t;\Phi_1^N(t)),
$$

which obviously coincides with (5). Rewriting the evolution equation for p_i of ($\mathrm{DB_{L1}}$) in terms of $\bar{p}_i$, we obtain

$$
\begin{aligned}
\partial_t\bar{p}_i &= \big[\partial_{xy} f(y_i,\Phi_i,t) - \partial_t(\,\delta\Phi_i)\,\delta\Phi_i^{-1}\big]\bar{p}_i - \partial_{yy} f(y_i,\Phi_i,t) z_i\,\delta\Phi_i^{-1},\\
\bar{p}_i(T) &= -(y_i(T) - y_d(\Phi_i(T))),
\end{aligned}
$$

since $\delta\Phi_i = \partial_X\Phi(X_i,t) \neq 0$. With the regularity of the coordinate transformation, $\partial_t(\,\delta\Phi_i) = \partial_X(\partial_t\Phi(X_i,t))$ is valid where the last expression can be deduced from the evolution equation for Φ in (DF)

$$
\partial_X(\partial_t\Phi(X_i,t)) = \partial_{yy} f(y_i,\Phi_i,t)\partial_X y_i + \partial_{xy} f(y_i,\Phi_i,t)\,\delta\Phi_i
$$

Inserting this relation yields

$$
\begin{aligned}
\partial_t\bar{p}_i &= -\partial_{yy} f(y_i,\Phi_i,t)\,\delta\Phi_i^{-1}\,(\bar{p}_i\partial_X y_i + z_i)\\
\bar{p}_i(T) &= -(y_i(T) - y_d(\Phi_i(T)))
\end{aligned}
$$

with arbitrary flux function f. Obviously, it holds that $(\bar{p}_i\partial_X y_i + z_i)(T) = 0$ in ($\mathrm{DB_{L1}}$). The evaluation of the derivative

$$
\begin{aligned}
\partial_t(\bar{p}_i\partial_X y_i + z_i) &\overset{\text{(DF)}}{=} [\partial_x u(\Phi_i(t),t)\,\delta\Phi_i - \partial_{xy} f(y_i,\Phi_i,t)\partial_X y_i - \partial_{xx} f(y_i,\Phi_i,t)\,\delta\Phi_i]\bar{p}_i\\
&\quad + \partial_X y_i\partial_t\bar{p}_i + \partial_t z_i\\
&\overset{(\mathrm{DB_{L1}})}{=} -\partial_{xy} f(y_i,\Phi_i,t)(\bar{p}_i\partial_X y_i + z_i) + \partial_X y_i\partial_t\bar{p}_i\\
&= -\frac{d}{dX}(\partial_y f(y_i,\Phi_i,t))\,\delta\Phi_i^{-1}\,(\bar{p}_i\partial_X y_i + z_i)
\end{aligned}
$$

results in an ordinary differential equation on the compact interval $[0,T]$, whose right-hand side is continuous in t and Lipschitz-continuous in $(\bar{p}_i\partial_X y_i + z_i)$. Hence, it has an unique solution which turns out to be the trivial solution due to the initial value. Consequently, $\partial_t\bar{p}_i = 0$, and the Lagrangian and Eulerian ansatz coincide as expected. The results of this

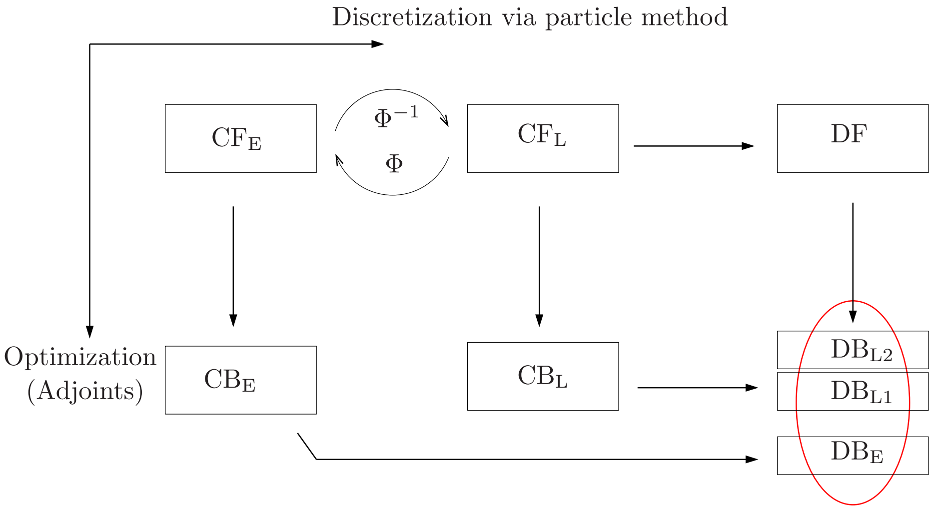


FIGURE 1. Independence principle: Conformity of optimization strategies

section are summarized in figure 1 that illustrates the investigated independence principle of the optimization approaches.

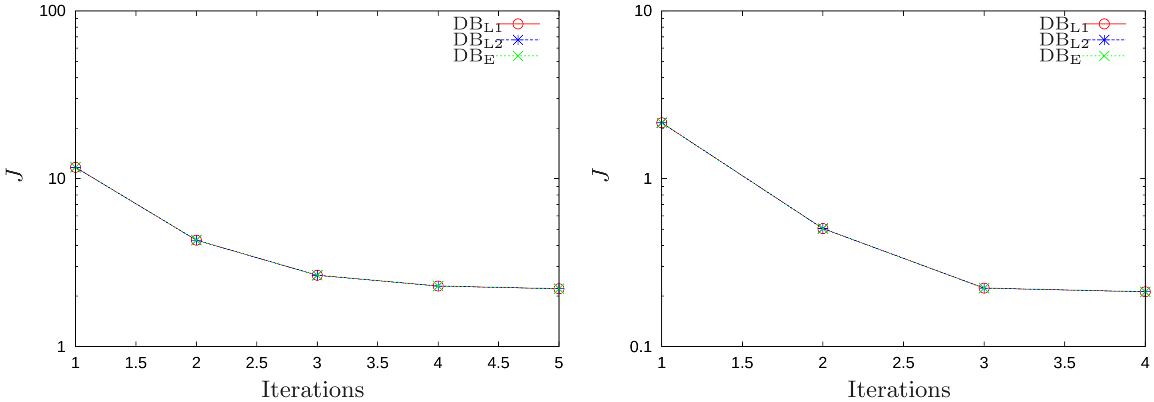
5. Numerical Results

After a short outline of the gradient algorithm used for the numerical implementation, we study the computational performance and correlations of the described optimization approaches in this section. Therefore, we apply the strategies on different test cases, i.e., linear convection and nonlinear Burger equations. We exclude the question of shock handling due to technical reasons that unnecessarily complicate the numerical implementation without bringing any insight into the optimization aspects.

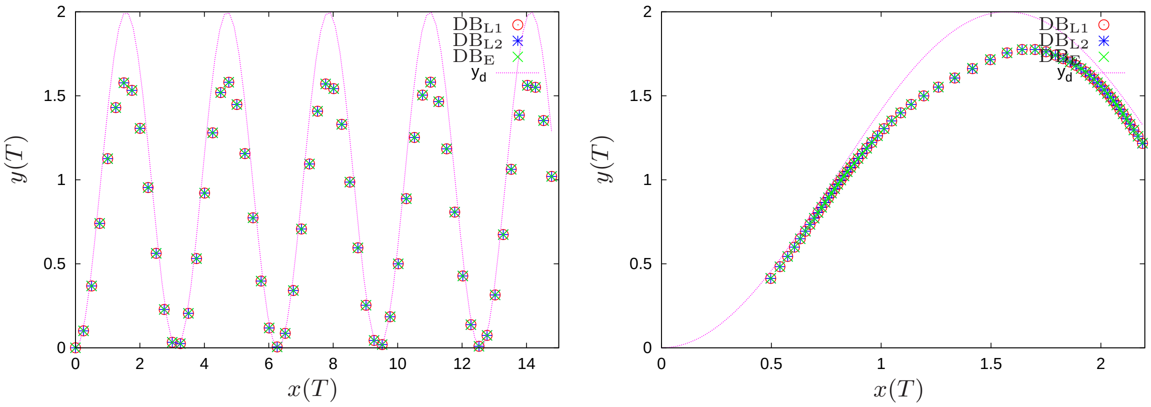
Gradient Algorithm.

(1) Initialize control function $u^{(0)}$, iteration counter $k = 0$, tolerance ϵ and set desired state y_d
(2) Generate particle set $\{X_i\}_{i=1,\dots,N}$ in $\hat{\Omega}$, e.g., equidistantly distributed
(3) Do
  (a) Given $u^{(k)}$ solve (DF) for $y_i^{(k)}$, $\Phi_i^{(k)}$
  (b) Solve (DB_{L1}), (DB_{L2}) or, respectively, (DB_E) for $p_i^{(k)}$, $z_i^{(k)}$
  (c) Determine a step size parameter $\tau > 0$, e.g., by Armijo's rule
  (d) Optional: Restrict u to be in a given range and forbid crossing characteristics
  (e) Set $u^{(k+1)} = u^{(k)} - \tau \nabla \tilde{J}_h(u^{(k)})$
while $J_h(y^{(k+1)}, \Phi^{(k+1)}, u^{(k+1)}) / J_h(y^{(k)}, \Phi^{(k)}, u^{(k)}) < 1 - \epsilon$

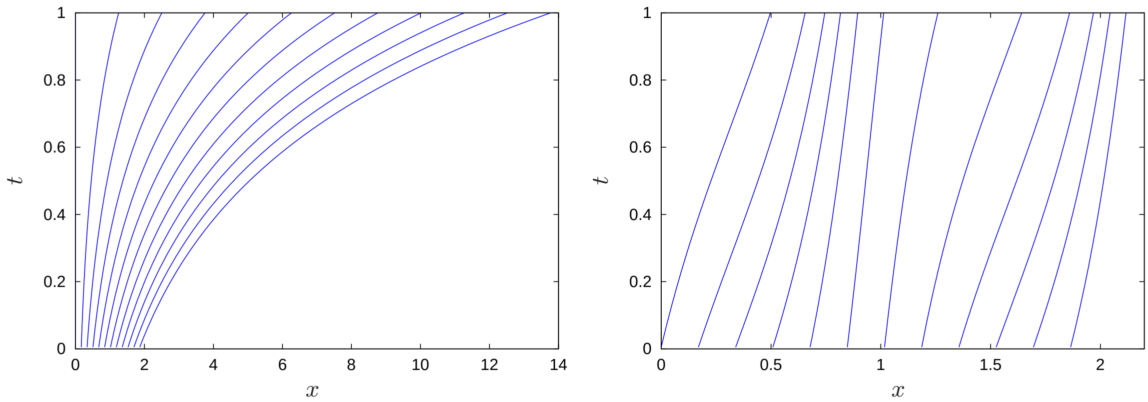
The following tests are evaluated on $\hat{\Omega}^T = [0, 2] \times [0, 1]$ with regularization $\alpha = 0.1$. The time integrations are performed with an implicit ODE solver using 200 time steps. The spatial discretization consists of 60 particles initially equidistantly distributed. Moreover, state and control function are initialized by $y_0 \equiv 0$, $u^{(0)} \equiv 0$ and the step size in the gradient algorithm



(a) Performance of cost functional



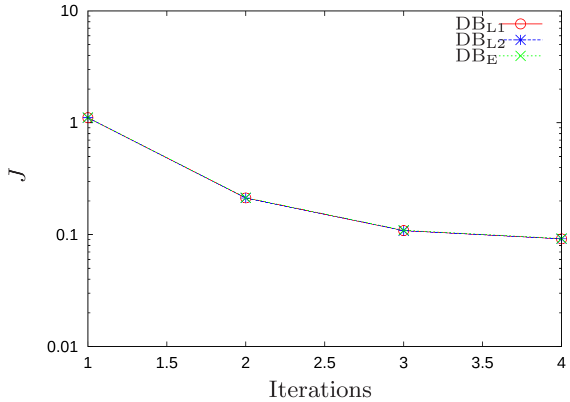
(b) Desired state y_d versus final results $y_i(T)$ of optimization strategies



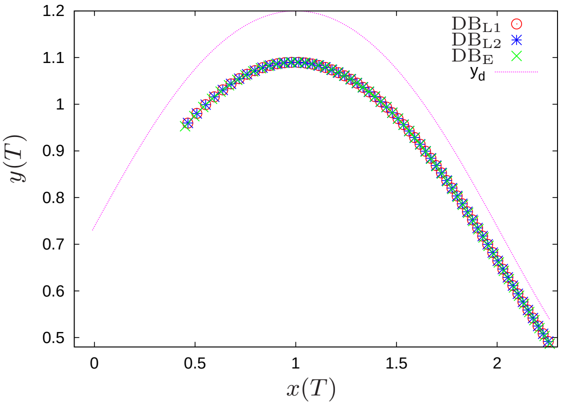
(c) Trajectories $\Phi_i(t)$ of $(\mathrm{DB_{L1}})$

FIGURE 2. Linear convection. Left: $f(y,x,t) = 2xy$. Right: $f(y,x,t) = 0.2(\sin(5x)+1.5)y$

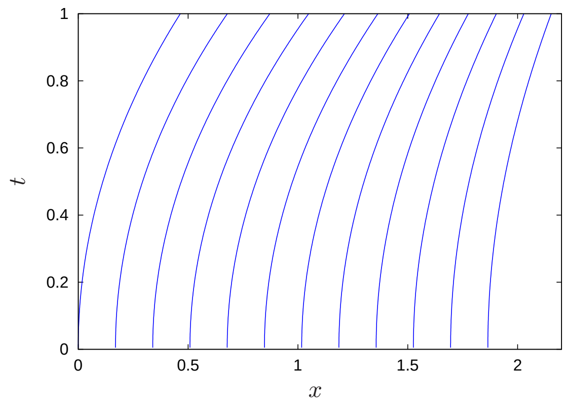
by $\tau_0 = 1$. For convenience the control is provided on a fine background grid during the simulation.



(a) Performance of cost functional



(b) Desired state y_d versus final results $y_i(T)$ of optimization strategies



(c) Trajectories $\Phi_i(t)$ of (DB$_{\mathrm{L1}}$)

FIGURE 3. Optimization results for Burger equation, $f(y, x, t) = y^2/2$

As exemplified for linear convection and nonlinear Burger equations in figures 2 and 3, respectively, all optimization strategies yield similar particle trajectories Φ_i and solutions y_i

while having comparable computational effort in the performance of gradient iterations and step-size reductions. Only, the evaluation of the adjoints in (DB_E) is obviously faster, since no ODEs for p_i and z_i need to be solved as in (DB_{Li}). Furthermore, the optimizations are in general independent of the number of particles. Just very big particle sets implying small distances to neighbor particles could cause an exceptional behavior since additional step-size reductions might be performed in the gradient algorithm to exclude the artificial crossing of characteristics, cf. step (3d).

The numerical deviations between the Lagrangian approaches varying in the sequential order of optimization and discretization, (DB_{L1}) and (DB_{L2}), lie in the order of the discretization $\mathcal{O}(h^2)$ as theoretically predated. This is illustrated for $f(y, x, t) = y^4/4$ in figure 4 where the resulting controls are compared in the L^2-sense (see 'o'-markers). Since h denotes the initial distance of two neighboring particles in $\hat{\Omega}$, the increase of particles goes proportionally to the decrease of h. As for the Eulerian ansatz, we find an agreement in the range of $\mathcal{O}(h)$. The small discrepancy that is finally kept between (DB_{L1})/(DB_{L2}) and (DB_E) for an increasing point number is carried into the simulations by the stopping criterion in the gradient algorithm (step (3)) since we use a constant tolerance ϵ. The good agreement of the approaches is not surprisingly, but in fact physically desirable since the optimization results should be independent of the problem formulation and the chosen strategy (figure 1). This independence principle is the basis for all black-box optimization tools applied on mesh-based methods in practice so far.

Apart from the approximation quality, the test cases show clearly the superiority of particle (mesh-less) methods to the conventional mesh-based methods. The particles are spread according to the coordinate transformation / convective motion and yield so an appropriate discretization adapted to Ω^T that varies over time, moreover particles at the boundary stay at the boundary. Hence, in case of big support changes as for $f(y, x, t) = 2xy$ in figure 2, the prearrangement of a sufficiently huge mesh covering the whole domain Ω^T or, respectively, the adaptive remeshing over time are avoided. Both variants are highly time- and storage-demanding and form therefore the major drawback in the numerical handling of time-dependent geometries with huge deformations or moving boundaries / interfaces using mesh-based methods. Similarly, in case of equation-driven oscillations of the solution, the resolution of particle methods is automatically adapted to the problem. However, adaptive strategies on the market that generate new particles and delete redundant ones might certainly even improve performance and approximation quality. The fact that the used Lagrangian type particle method yields ordinary differential equations in time has moreover the advantage that no accuracy is lost by the approximation of spatial derivatives of the system variables. But this advantage is annulled when parabolic equations or hyperbolic systems are considered.

6. Conclusion

In this paper we have combined optimal control approaches with mesh-less discretizations. Applying a classical Lagrangian type particle method on hyperbolic constrained optimization problems, we have presented several adjoint-based strategies differing in the sequential order of optimization and discretization of the Lagrangian or, respectively, Eulerian problem formulation. Their theoretical investigation and numerical application on linear and nonlinear test cases show their suitability for the handling of practically relevant and evidently more

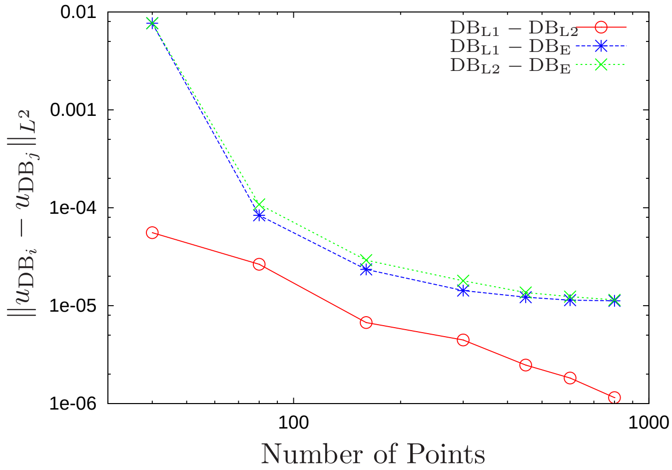


FIGURE 4. Convergence of the approaches to each other

demanding optimization problems as they might arise in the context of fluid dynamics, failure mechanics, biophysics and -chemistry where time dependencies, complex geometries, free moving boundaries and interfaces tremendously matter.

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