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Dynamic Optimal Transport with Optimal Star-Shaped Graphs

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ABSTRACT

We study an optimal transport problem in a compact convex set $\Omega \subset \mathbb{R}^d$ where bulk transport is coupled to dynamic optimal transport on a metric graph $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$ which is embedded in Ω. We prove the existence of solutions for fixed graphs. Next, we consider varying graphs, yet only for the case of star-shaped ones. Here, the action functional is augmented by an additional penalty that prevents the edges of the graph from overlapping. This allow us to preserve the graph topology and thus to rely on standard techniques in calculus of variations in order to show the existence of minimizers.

1 | Introduction

Metric graphs play an important role in the modeling of real-world phenomena such as gas or road networks [1, 2]. In particular, the theory of optimal transport has proven to be a useful tool to analyze transportation on such graphs. In recent years, several related formulations have been studied, see e.g., [3], where the authors provide a complete analysis of optimal transport on metric graphs with Kirchhoff–Neumann conditions at the vertices. Furthermore, Burger et al. [4] studied a transport metric that allows for mass storage on the vertices. These studies are strongly motivated by and related to a transport distance involving bulk and surface transport that was introduced in [5]. Related gradient flows with respect to these distances have also been studied, again in [3] and, for the case with vertex dynamics, in [6]. Independently, dynamic optimal transportation with non-linear mobilities was studied in [7], see also [8] for the case of a volume filling-mobility.

In the present article, we combine these approaches into a model, which consists of transport in a compact and convex domain $\Omega \subset \mathbb{R}^d$, coupled to optimal transport on a metric graph. The introduction of mobilities allows to impose lower and upper bounds on the mass densities, leading to a more versatile model. The coupled problem is motivated by the planning of traffic routes. A particular focus lies on networks where, due to pre-existing infrastructure or connections to other transportation networks, one city is highlighted as a central point. We assume that traveling along the graph is cheaper than traveling in the bulk domain. However, there is an additional cost to entering the graph, that can be thought of as the cost of train tickets or waiting times between different connections. An example of such a system can be found in French railroad planning, where Paris is associated with the accentuated center of the graph. This article extends the results of [9], where a coupled dynamic optimal transport problem between bulk and a second domain, which is the graph of a function (a single road), is analyzed. The resulting problem is understood as a dynamic optimal transportation problem together with an additional penalty functional allowing for an optimization over the metric graph as well.

To introduce our model, we first consider an arbitrary metric graph $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$ that is embedded in some convex and compact domain $\Omega \subset \mathbb{R}^d$ with initial and final data given as non-negative Radon measures μ_0 and μ_1 on Ω and ρ_0 and ρ_1 on G such that $\mu_0(\Omega) + \rho_0(\mathsf{G}) = 1 = \mu_1(\Omega) + \rho_1(\mathsf{G})$. This means that each vertex

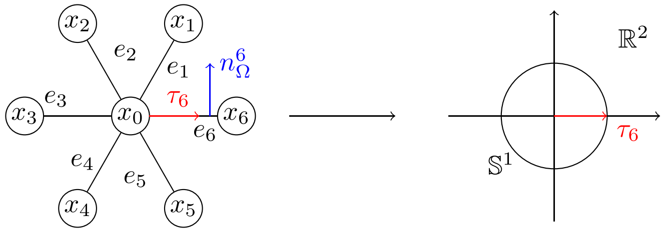

FIGURE 1 | A star-shaped metric graph embedded into $\mathbb{R}^2$ with $\mathsf{V}_{\text{out}} = \{v_1, \ldots, v_6\} = \mathsf{V} \setminus \{v_0\}$, normal $n_\Omega^6 = (0,1)^T$ and tangent $\tau_6 = (1,0)^T$.

$v \in \mathsf{V}$ can be identified with a point $x_v \in \Omega$, and we think of edges as straight lines connecting these points. For a rigorous definition, see Section 2. Any measure ρ_t on G can be determined by its values on the edges, thus we identify $\rho_t = (\rho_t^e)_{e\in\mathsf{E}}$. Now, the evolution of mass on the coupled system can be expressed, formally, by solutions of the following system of continuity equations:

$$\begin{cases} \partial_t \mu_t + \nabla \cdot J_t = 0 & \text{in } \Omega \\ J_t \cdot n_\Omega^e = f_t^e & \text{for } e \in \mathsf{E} \\ \partial_t \rho_t^e + \nabla \cdot V_t^e = f_t^e & \text{for } e \in \mathsf{E} \\ V_t^e n_e^v = G(v) = J_{t\,|\{x_v\}} \cdot \tau_e & \text{for } v \in \mathsf{V}_{\text{out}} \\ \sum_{e\in\mathsf{E}(v)} V_t^e n_e^v = 0 & \text{for } v \in \mathsf{V} \setminus \mathsf{V}_{\text{out}} \end{cases} \tag{1}$$

where $n_\Omega^e \in \mathbb{S}^{d-1}$ denotes the normal to the edges $e \in \mathsf{E}$, $\tau_e \in \mathbb{S}^{d-1}$ denotes the tangent to the embedded edge in Ω, and $n_e^v \in \{0, \pm 1\}$ is defined as in (2), prescribing an orientation to each edge. For an illustration, see Figure 1. In particular, we impose a non-homogeneous continuity equation on each edge, coupling them in the interior vertices $\mathsf{V} \setminus \mathsf{V}_{\text{out}}$ with homogeneous Neumann conditions, allowing for conservation of mass. For the outer vertices $\mathsf{V}_{\text{out}} \subset \mathsf{V}$, we allow an additional exchange of mass with the bulk region Ω. We denote by $\mathsf{CE}(\mathsf{G})$ the set of weak solutions to (1). Now, the evolution of this system is governed by quadratic costs and non-linear mobilities imposing bounds on the mass measures μ_t and ρ_t. The resulting (formal) action functional reads as

$$\begin{aligned} &\mathcal{A}_{\mathsf{G}}(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \\ &= \int_\Omega \frac{|J_t|^2}{m_\Omega(\mu_t)}\, d\lambda_\Omega + \sum_{e\in\mathsf{E}} \left(\int_e \alpha_1 \frac{|V_t^e|^2}{m_{\mathsf{G}}(\rho_t^e)} + \alpha_2 \frac{|f_t^e|^2}{m_{\mathsf{G}}(\rho_t^e)}\, d\lambda_e \right) \\ &\quad + \alpha_3 \sum_{v\in\mathsf{V}_{\text{out}}} \sum_{e\in\mathsf{E}(v)} \int_{\{x_v\}} \frac{|G_t^e(x_v)|^2}{m_{\mathsf{G}}(\rho^e_{t\,|x_v})}\, d\lambda_v, \end{aligned}$$

where m_Ω and m_{G} are mobility functions and λ_Ω, λ_e, and λ_v are fixed reference measures, necessary as the mobilities lead to a loss of 1-homogenity of the functional. We then consider the dynamic problem

$$\inf_{(\mu_t, J_t, \rho_t, V_t, f_t, G_t)\in\mathsf{CE}(\mathsf{G})} \mathcal{A}_{\mathsf{G}}(\mu_t, J_t, \rho_t, V_t, f_t, G_t).$$

We refer to Section 3 for a rigorous definition of weak solutions to the coupled system (1) and for the resulting dynamic problem.

In order to account for varying graphs in the second part of this work, we restrict our analysis to the case of star-shaped metric graphs. For such, there exists a unique central vertex $v_0 \in \mathsf{V}$, which is contained in all edges and we define $\mathsf{V}_{\text{out}} = \mathsf{V} \setminus \{v_0\}$. Thus, all edges can be written as $e = (v_0, v)$ for some $v \in \mathsf{V}_{\text{out}}$. Throughout minimization, we fix the connectivity information and only optimize over the placement of the vertices. For this to result in a well-defined metric graph, we need to prevent vertices from colliding and edges from crossing. To this end we introduce the additional penalty functional

$$R(x_{v_0}, \ldots, x_{N_{\mathsf{V}}-1}) := \sum_{i=1}^{N_{\mathsf{V}}-1} \left(\frac{1}{|x_{v_i} - x_{v_0}|} + \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{N_{\mathsf{V}}-1} \frac{1}{\alpha_{x_{v_i}, x_{v_j}}} \right),$$

where $N_V = |\mathsf{V}|$ and $\alpha_{x_{v_i}, x_{v_j}}$ is the unsigned angle between the edges (v_0, v_i) and (v_0, v_j) at the central vertex v_0. The augmented problem now reads

$$\inf_{\mathsf{G}} \inf_{\mathsf{CE}(\mathsf{G})} \int_0^1 \mathcal{A}_{\mathsf{G}}(\mu_t, J_t, \rho_t, V_t, f_t, G_t)\, dt + cR(x_{v_0}, x_{v_1}, \ldots, x_{v_{N_{\mathsf{V}}-1}})$$

and its rigorous definition is given in Section 4.

The article is structured as follows. In Section 2, we introduce some notation as well as measures on metric graphs. In Section 3, we define the notion of weak solutions to the coupled system as well as the dynamic formulation. Additionally, we prove existence of minimizers. In the last part, in Section 4, we analyze the dynamic problem for varying graphs where we restrict our considerations to star-shaped metric graphs and optimize over the placement of vertices. Again, we prove existence of minimizers.

2 | Notation

In order to rigorously define the coupled dynamic system, we start by introducing some notation.

Let $\Omega \subset \mathbb{R}^d$ be a compact and convex subset of $\mathbb{R}^d$ and $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ be a combinatorial graph, where V denotes the *set of nodes* and E is the *set of edges* $e = (v, w)$ for $v, w \in \mathsf{V}$. The number of nodes is denoted by $N_{\mathsf{V}} := |\mathsf{V}|$ and the number of edges by $N_{\mathsf{E}} := |\mathsf{E}|$. We define $\mathsf{E}(v) := \{e \in \mathsf{E} \mid v \in e\}$ as the set of edges containing $v \in \mathsf{V}$. Moreover, we introduce the set of *outer vertices* $\mathsf{V}_{\text{out}} := \{v \in \mathsf{V} \mid |\mathsf{E}(v)| = 1\}$ and the set of *outer edges* $\mathsf{E}_{\text{out}} := \{e \in \mathsf{E} \mid \exists\, v \in \mathsf{V}_{\text{out}} \text{ s.t. } v \in e\}$. With an additional map $l : \mathsf{E} \to (0, +\infty)$, associating a positive length l_e to each edge e of the graph, the combinatorial graph turns into a *metric graph* $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$. By defining the outer normal

$$n_e^v := \begin{cases} -1 & : e = (v, w) \\ 0 & : v \notin e \\ +1 & : e = (w, v) \end{cases} \tag{2}$$

and therefore fixing an orientation, we can identify edges with closed intervals $[0, l_e]$. In order to rigorously define the coupling between a domain and a metric graph, we need to embed the graph.

Definition 2.1. Let $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ be a combinatorial graph and $\Omega \subset \mathbb{R}^d$ be a compact and convex set. A collection of distinct points $x_v \in \Omega$ for $v \in \mathsf{V}$ is called an *embedding* of the graph, defining edges as straight lines, and we say that the graph G is *embedded into* Ω if the embedding has no intersecting edges. We say that a metric graph $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$ is *embedded into* Ω if it is embedded as a combinatorial graph and if $|x_w - x_v| = l_e$ for all $e \in \mathsf{E}$.

For an embedded metric graph, we denote the tangent vector of an edge $e = (v, w) \in \mathsf{E}$ by

$$\tau_e := \frac{x_w - x_v}{l_e} = \frac{x_w - x_v}{|x_w - x_v|} \tag{3}$$

and we write $[x_v, x_w] = \{x_v + t\tau_e \mid t \in [0, l_e]\} \subset \Omega$ for the interval defined by an edge $e = (v, w)$ of an embedded metric graph. Abusing notation, we identify $e = [x_v, x_w]$ throughout the article.

Functions on metric graphs are defined by their restriction to each edge. We introduce the sets

$$\Omega_\mathsf{E} := \bigsqcup_{e=(v,w)\in\mathsf{E}} [x_v, x_w], \quad \mathsf{L} := \bigsqcup_{e=(v,w)\in\mathsf{E}} [0,1]$$
$$\text{and} \quad \Omega_\mathsf{V} := \bigsqcup_{v\in\mathsf{V}_{\text{out}}} \{x_v\} \tag{4}$$

given as disjoint unions. In order to guarantee a metric structure on the metric graph and therefore identifying it with a metric space, we define the new sets

$$\Omega_\mathsf{G} := \Omega_\mathsf{E} / \sim_\mathsf{E} \quad \text{and} \quad \mathsf{L}_\mathsf{G} := \mathsf{L} / \sim_\mathsf{L},$$

where $\sim_\mathsf{E}$ denotes the equivalence relation that identifies the same vertex on different edges and $\sim_\mathsf{L}$ is the corresponding identification in L. Note that in Ω_G each vertex $v \in \mathsf{V}$ can be identified uniquely, whereas there are multiple copies in Ω_E, one for each edge $e \in \mathsf{E}(v)$. Any map on a metric graph is given as $\varphi = (\varphi^e)_{e\in\mathsf{E}} : \Omega_\mathsf{E} \to \mathbb{R}$ or $\tilde{\varphi} = (\tilde{\varphi}^e)_{e\in\mathsf{E}} : \mathsf{L} \to \mathbb{R}$. Both can be related using the transformation maps $\gamma_e(s) := x_v + s l_e \tau_e$ and $\tilde{\gamma}_e(x) = \frac{|x-x_v|}{l_e}$ for $e = (v, w)$ as

$$\tilde{\varphi}^e(s) = \varphi^e(\gamma_e(s)) \quad \text{and} \quad \varphi^e(x) = \tilde{\varphi}^e(\tilde{\gamma}_e(x)). \tag{5}$$

Similar definitions can be given for Ω_G and L_G. Finally, we define $C^1([0,1] \times L) := C^1([0,1]; C(\mathsf{L}_\mathsf{G})) \cap C([0,1]; C^1(\mathsf{L}))$, that is, functions that are continuous in each vertex having derivatives on each edge.

We call a (metric or combinatorial) graph *star-shaped* if there exists an accentuated node $v_0 \in \mathsf{V}$ such that $E = \{(v_0, v) \mid v \in \mathsf{V} \setminus \{v_0\}\}$. The node v_0 is called *center of the graph*. In particular it holds that $\mathsf{E} = \mathsf{E}(v_0) = \mathsf{E}_{\text{out}}$ and $\mathsf{V}_{\text{out}} = \mathsf{V} \setminus \{v_0\}$.

In order to rigorously formulate the coupling between different domains, we need to extend measures defined on the graph to measures on Ω. Let $\mathcal{M}(U, \mathbb{R}^N)$ be the set of Radon measures on $U \subset \mathbb{R}^d$ with values in $\mathbb{R}^N$ and $\mathcal{M}_+(U, \mathbb{R}^N)$ the set of measures in $\mathcal{M}(U, \mathbb{R}^N)$ that are non-negative. Moreover, we denote by $\mathcal{M}_{[0,1]}(U, \mathbb{R}^N)$ a Borel measurable family of measures in U indexed by $t \in [0,1]$ with values in $\mathbb{R}^N$. We also consider measures with values in the tangent space of some edge $e \in \mathsf{E}$. In particular, given $x \in e$ the measures $V^e \in \mathcal{M}(e, T_x e)$ and $G^e(x_v) \in \mathcal{M}(\{x_v\}, T_{x_v} e)$ will occur in our formulation, where $T_x e$ is the tangent space to e in x. Note that we can represent such measures as

$$V^e = \tau_e \mathcal{V}^e \quad \text{or} \quad G^e(x_v) = \tau_e \mathcal{G}^e(x_v) \tag{6}$$

with $\mathcal{V}^e \in \mathcal{M}(e, \mathbb{R})$, $\mathcal{G}^e(x_v) \in \mathcal{M}(\{x_v\}, \mathbb{R})$. For any measure $\rho^e \in \mathcal{M}(e, \mathbb{R})$, we define its zero extension into Ω by duality as the measure $\bar{\rho}^e \in \mathcal{M}(\Omega, \mathbb{R})$ such that

$$\int_\Omega \phi \, d\bar{\rho}^e = \int_e \phi \, d\rho^e \tag{7}$$

for all $\phi \in C(\Omega)$. For measures $\rho \in \mathcal{M}(\Omega_\mathsf{E}, \mathbb{R})$ we define their extension as $\bar{\rho} = (\bar{\rho}^e)_{e\in\mathsf{E}}$ and for $\tilde{\rho} \in \mathcal{M}(\mathsf{L}, \mathbb{R})$ as $\overline{\tilde{\rho}} = (\overline{\tilde{\rho}^e \circ \tilde{\gamma}_e})_{e\in\mathsf{E}}$. Measures $\rho \in \mathcal{M}(\Omega_\mathsf{E}, \mathbb{R})$ can be identified with measures $\tilde{\rho} \in \mathcal{M}(\mathsf{L}, \mathbb{R})$ through the push-forward by the maps γ_e for $e \in E$. In particular, when it will be necessary to underline the dependence on γ_e we will write $\tilde{\rho} = \rho \circ \gamma_e$. Similar notions of extension and push-forward operations can be defined for measures defined on Ω_G and L_G with values in $\mathbb{R}^N$ for $N \in \mathbb{N}$.

With these notions, we are able to introduce the space of admissible tuples $(\mu_t, J_t, \rho_t, V_t, f_t, G_t)$ as the space $\mathcal{D}_{\text{adm}}(\mathsf{G})$ defined by

$$\begin{aligned}\mathcal{D}_{\text{adm}}(\mathsf{G}) := \; & \mathcal{M}_{[0,1]}(\Omega, \mathbb{R}) \times \mathcal{M}_{[0,1]}(\Omega, \mathbb{R}^d) \times \mathcal{M}_{[0,1]}(\Omega_\mathsf{G}, \mathbb{R}) \\ & \times \mathcal{M}_{[0,1]}(\Omega_\mathsf{E}, T_x e) \times \mathcal{M}_{[0,1]}(\Omega_\mathsf{E}, \mathbb{R}) \\ & \times \mathcal{M}_{[0,1]}(\Omega_\mathsf{V}, T_{x_v} e).\end{aligned}$$

Admissible initial or final measures are given as elements of the set

$$\mathcal{P}_{\text{adm}}(\mathsf{G}) := \{(\mu, \rho) \in \mathcal{M}_+(\Omega) \times \mathcal{M}_+(\Omega_\mathsf{G}) \mid \mu(\Omega) + \rho(\Omega_\mathsf{G}) = 1\}. \tag{8}$$

3 | Fixed Graph

In this section, we consider a fixed metric graph $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$, embedded in $\Omega \subset \mathbb{R}^d$ compact and convex. We rigorously define the dynamic problem and show existence of solutions to the formal transport problem (1) with minimal dynamic costs.

3.1 | Continuity Equation

We rigorously define the coupled continuity equations and show mass conservation of the entire system.

Definition 3.1. We say that a tuple $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathcal{D}_{\text{adm}}(\mathsf{G})$ satisfies the coupled continuity equations for admissible initial and final data $(\mu_0, \rho_0), (\mu_1, \rho_1) \in \mathcal{P}_{\text{adm}}(\mathsf{G})$ if

$$\int_0^1 \int_\Omega \partial_t \phi_t(x)\, d\mu_t dt + \int_0^1 \int_\Omega \nabla\phi_t(x)\, dJ_t dt - \sum_{e\in\mathsf{E}} \int_0^1 \int_0^1 \phi_t(\gamma_e(s))\, d\tilde{f}_t^e dt + \sum_{v\in\mathsf{V}_{\text{out}}} \sum_{e\in\mathsf{E}(v)} \int_0^1 \int_{\{x_v\}} \phi_t(x_v) n_e^v\, d\tilde{\mathcal{G}}_t^e(x_v) dt = \int_\Omega \phi_1(x)\, d\mu_0 - \int_\Omega \phi_0(x)\, d\mu_1$$

for all $\phi_t \in C^1([0,1]\times\Omega)$ and

$$\sum_{e\in\mathsf{E}} \left(\int_0^1 \int_0^1 \partial_t \psi_t^e(s)\, d\tilde{\rho}_t^e dt + \int_0^1 \int_0^1 \nabla\psi_t^e(s) l_e\, d\tilde{\mathcal{V}}_t^e dt + \int_0^1 \int_0^1 \psi_t^e(s)\, d\tilde{f}_t^e dt \right) - \sum_{v\in\mathsf{V}_{\text{out}}} \sum_{e\in\mathsf{E}(v)} \int_0^1 \int_{\{x_v\}} \psi_t^e(x_v) n_e^v\, d\tilde{\mathcal{G}}_t^e(x_v) dt = \sum_{e\in\mathsf{E}} \left(\int_0^1 \psi_1^e(s)\, d\tilde{\rho}_0^e - \int_0^1 \psi_0^e(s)\, d\tilde{\rho}_1^e \right)$$

for all $\psi_t = (\psi_t^e)_{e\in\mathsf{E}} \in C^1([0,1]\times L)$ such that $\psi_t^e(\tilde{\gamma}_e(x_v)) =: \psi_t(v)$ for all $e \in \mathsf{E}(v)$, meaning that the map is continuous over vertices. We denote by $\mathsf{CE}(\mathsf{G})$ the set of such solutions on the graph G.

We can show that solutions to this system satisfy a global continuity equation and therefore are mass preserving.

Proposition 3.2. *Suppose that* $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$. *Given* $\eta_t := \mu_t + \sum_{e\in\mathsf{E}} \bar{\rho}_t^e$ *and* $W_t := J_t + \sum_{e\in\mathsf{E}} \bar{V}_t^e$ *it holds that*

$$\partial_t \eta_t + \nabla\cdot W_t = 0 \tag{9}$$

weakly with initial data $\mu_0 + \sum_{e\in\mathsf{E}} \bar{\rho}_0^e$ *and final data* $\mu_1 + \sum_{e\in\mathsf{E}} \bar{\rho}_1^e$.

Proof. Let $\phi \in C^1([0,1]\times\Omega)$ be an arbitrary test function. For each edge $e \in \mathsf{E}$, we define $\psi_t^e = \phi_t \circ \gamma_e \in C^1([0,1]\times[0,1])$, which, by construction, induces the admissible test function $\psi_t = (\psi_t^e)_{e\in\mathsf{E}} \in C^1([0,1]\times \mathsf{L}_\mathsf{G})$. Moreover, $\frac{d}{ds}\psi_t^e(s) = \nabla\phi_t(\gamma_e(s)) \cdot l_e \tau_e$. We obtain

$$\begin{aligned} &\int_0^1 \int_\Omega \partial_t \phi_t(x)\, d\eta_t dt + \int_0^1 \int_\Omega \nabla\phi_t(x)\, dW_t dt \\ &= \int_0^1 \int_\Omega \partial_t \phi_t(x)\, d\mu_t dt + \int_0^1 \int_\Omega \nabla\phi_t(x)\, dJ_t dt \\ &\quad + \sum_{e\in\mathsf{E}} \left[\int_0^1 \int_0^1 \partial_t \psi_t(s)\, d\tilde{\rho}_t^e dt + \int_0^1 \int_0^1 \nabla\psi_t(s) \cdot l_e \tau_e\, d\tilde{V}_t^e dt \right] \\ &= \int_\Omega \phi_1(x)\, d\mu_1 - \int_\Omega \phi_0(x)\, d\mu_0 \\ &\quad + \sum_{e\in\mathsf{E}} \left(\int_0^1 \psi_1^e(s)\, d\tilde{\rho}_1^e - \int_0^1 \psi_0^e(s)\, d\tilde{\rho}_0^e \right) \end{aligned}$$

where the last equality follows by substituting the weak formulation from of Definition 3.1, thus proving the statement. ☐

3.2 | Dynamic Formulation

We will define the variational formulation that governs the evolution of the measures $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$ over time. It is given as a generalized kinetic energy functional with an additional mobility function defining upper and lower bounds on the mass densities.

Definition 3.3 (Admissible mobilities). We call a function $m : [0, +\infty) \to [0, +\infty) \cup \{-\infty\}$ *admissible mobility* if it is an upper semi-continuous and concave function with $\text{int}(\text{dom}(m)) = (a, b)$ for $0 \le a < b$ and $m(z) > 0$ for all $z \in (a, b)$.

We are now able to rigorously introduce the dynamic problem.

Definition 3.4. We define the following variational problem

$$\inf_{\mathsf{CE}(\mathsf{G})} \int_0^1 \mathcal{A}_\mathsf{G}(\mu_t, J_t, \rho_t, V_t, f_t, G_t)\, dt, \tag{BB}$$

where

$$\begin{aligned} \mathcal{A}_\mathsf{G}(\mu_t, J_t, \rho_t, V_t, f_t, G_t) &= \int_\Omega \Psi_\Omega\left(\frac{d\mu_t}{d\lambda_\Omega}, \frac{dJ_t}{d\lambda_\Omega}\right) d\lambda_\Omega \\ &\quad + \sum_{e\in\mathsf{E}} \left(\int_e \alpha_1 \Psi_\mathsf{G}\left(\frac{d\rho_t^e}{d\lambda_e}, \frac{d\mathcal{V}_t^e}{d\lambda_e}\right) + \alpha_2 \Psi_\mathsf{G}\left(\frac{d\rho_t^e}{d\lambda_e}, \frac{df_t^e}{d\lambda_e}\right) d\lambda_e \right) \\ &\quad + \alpha_3 \sum_{v\in\mathsf{V}_{\text{out}}} \sum_{e\in\mathsf{E}(v)} \int_{\{x_v\}} \times \Psi_\mathsf{G}\left(\frac{d\rho^e_{t\,|x_v}}{d\lambda_v}, \frac{d\mathcal{G}_t^e(x_v)}{d\lambda_v}\right) d\lambda_v \end{aligned}$$

for $\alpha_1, \alpha_2, \alpha_3 > 0$ describing the cost of transport along the graph (α_1) and entering or leaving the graph (α_2, α_3), respectively. Here, $\lambda_\Omega \in \mathcal{M}_+(\Omega)$, $\lambda_e \in \mathcal{M}_+(e)$, and $\lambda_v \in \mathcal{M}_+(\{x_v\})$ are non-negative Radon-measures such that $\mu_t, J_t \ll \lambda_\Omega$, $\rho_t^e, \mathcal{V}_t^e, f_t^e \ll \lambda_e$, and $\rho^e_{t\,|x_v}, \mathcal{G}_t^e(x_v) \ll \lambda_v$ for almost all $t \in [0,1]$. The action functionals are defined as

$$\Psi_\Omega(u, v) := \begin{cases} \frac{|v|^2}{m_\Omega(u)} & : m_\Omega(u) \neq 0 \\ 0 & : m_\Omega(u) = 0 = v \\ +\infty & : \text{else} \end{cases} \quad \text{and}$$

$$\Psi_\mathsf{G}(u, v) := \begin{cases} \frac{|v|^2}{m_\mathsf{G}(u)} & : m_\mathsf{G}(u) \neq 0 \\ 0 & : m_\mathsf{G}(u) = 0 = v \\ +\infty & : \text{else} \end{cases} \tag{10}$$

for admissible mobility functions m_Ω and m_G.

Remark 3.5. As shown in [7, Theorem 2.1], functionals of the form (BB) are convex and lower semi-continuous with respect to the weak convergence of measures.

Boundedness of the action $\mathcal{A}_\mathsf{G}$ allows proving further regularity results for the mass densities μ_t and ρ_t^e, $e \in \mathsf{E}$, following the same arguments as in [5, Theorem 3.5].

Proposition 3.6. *For $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$ with $\int_0^1 \mathcal{A}_\mathsf{G}(\mu_t, J_t, \rho_t, V_t, f_t, G_t)\,dt < +\infty$ the measures μ_t and ρ_t admit a weakly continuous representative. Suppose further that* $\mathrm{int}(\mathrm{dom}(m_\Omega)) = (a_\Omega, b_\Omega)$ *and* $\mathrm{int}(\mathrm{dom}(m_\mathsf{G})) = (a_\mathsf{G}, b_\mathsf{G})$ *and denote by μ_t, ρ_t^e the densities of the measures with respect to λ_Ω and λ_G. It holds that*

$$a_\Omega \le \mu_t \le b_\Omega,\ \lambda_\Omega - \text{a.e.} \quad \textit{and} \quad a_\mathsf{G} \le \rho_t^e \le b_\mathsf{G},\ \lambda_\mathsf{G} - \text{a.e.} \tag{11}$$

for every $t \in [0,1]$ and every $e \in \mathsf{E}$.

3.3 | Existence of Minimizers for a Fixed Graph

In this section, we will show well-posedness of (BB) using the direct method of the calculus of variations. From Remark 3.5, we infer lower semi-continuity. Compactness will follow from a Hölder estimate.

Proposition 3.7 (Hölder estimate). *Suppose that $\int_0^1 \mathcal{A}_\mathsf{G}(\mu_t, J_t, \rho_t, V_t, f_t, G_t)\,dt \le M$ for $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$, and a constant $M \ge 0$. Then, it holds that*

$$\|\mu_t - \mu_s\|_{C^1(\Omega)^*} \le C(b_\Omega, b_\mathsf{G}, M)|t-s|^{\frac{1}{2}} \tag{12}$$

$$\sum_{e \in \mathsf{E}} \|\rho_t^e - \rho_s^e\|_{C^1(e)^*} \le C(b_\Omega, b_\mathsf{G}, M)|t-s|^{\frac{1}{2}} \tag{13}$$

for a constant $C(b_\Omega, b_\mathsf{G}, M) > 0$ and for all $t, s \in [0,1]$.

Proof. The statement can be proven analogously to [9, Proposition 2.10] following arguments from [5, Proposition 3.5]. □

From the previously stated Hölder estimates we can infer compactness.

Proposition 3.8 (Compactness). *Given $(\mu_t^n, J_t^n, \rho_t^n, V_t^n, f_t^n, G_t^n) \in \mathsf{CE}(\mathsf{G})$, $n \in \mathbb{N}$ and $M \ge 0$ such that*

$$\sup_{n \in \mathbb{N}} \int_0^1 \mathcal{A}_\mathsf{G}(\mu_t^n, J_t^n, \rho_t^n, V_t^n, f_t^n, G_t^n)\,dt \le M, \tag{14}$$

there exists $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$ such that, up to a subsequence, the following convergences hold:

(i) $\mu_t^n \rightharpoonup \mu_t$ weakly in $\mathcal{M}(\Omega)$ for all $t \in [0,1]$
(ii) $\rho_t^n \rightharpoonup \rho_t$ weakly in $\mathcal{M}(\Omega_\mathsf{G})$ for all $t \in [0,1]$
(iii) $J_t^n \rightharpoonup J_t$ weakly in $\mathcal{M}([0,1] \times \Omega, \mathbb{R}^d)$
(iv) $\mathcal{V}_t^n \rightharpoonup \mathcal{V}_t$ in $\mathcal{M}([0,1] \times \Omega_\mathsf{E})$
(v) $f_t^n \rightharpoonup f_t$ in $\mathcal{M}([0,1] \times \Omega_\mathsf{E})$
(vi) $\mathcal{G}_t^n \rightharpoonup \mathcal{G}_t$ in $\mathcal{M}([0,1] \times \Omega_\mathsf{V})$.

Proof. The proof of (i) and (ii) follows from Proposition 3.7, Proposition 3.6 and an application of a generalized Arzela–Ascoli theorem, see [10, Proposition 3.3.1]. The remaining convergence results follow by standard estimates on the total variation of the measures and Prokhorov's theorem carried out in [9, Theorem 2.11]. Admissibility of the limit is a direct consequence of the weak convergence and disintegration properties. □

We are now in a position to show well-posedness of (BB).

Theorem 3.9. *Suppose that (BB) is finite. Then, there exists a minimizer $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$.*

Proof. This is a direct consequence of Remark 3.5, Proposition 3.8, and the direct method of calculus of variations. □

4 | Varying Graphs

In this section, we analyze the case of varying graphs restricting our considerations to star-shaped metric graphs. From now on, we suppose that $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$ is star-shaped with central vertex $v_0 \in \mathsf{V}$. We keep the connectivity of the graph fixed and we optimize the graph by varying the placement of the vertices inside of Ω. For given initial and final data, we are therefore looking for an optimal embedding of the combinatorial graph. Note that we allow the edge length to vary as well. In order for the continuity equation to be well-defined throughout the minimization, we need to prevent overlapping edges. For this reason, we impose an additional constraint on the unsigned angle $\alpha_{x_v, x_w} \in [0, 2\pi)$ between any pair of edges (v_0, v) and (v_0, w) at the common central node v_0. The angle can be calculated as

$$\alpha_{x_v, x_w} = \left| \arccos \frac{\langle x_v - x_{v_0}, x_w - x_{v_0} \rangle}{|x_v - x_{v_0}||x_w - x_{v_0}|} \right| \tag{15}$$

and we approach an overlap of two edges if this angle is small. However, this does not prevent the nodes from collapsing in the center x_{v_0}. Therefore, we add an additional Coulomb-type potential in order to obtain lower bounds on the distances $|x_v - x_{v_0}|$ for $v \in \mathsf{V}$. The resulting penalty functional reads

$$R(x_{v_0}, x_{v_1}, \dots, x_{v_{N_\mathsf{V}-1}}) := \sum_{i=1}^{N_\mathsf{V}-1} \left(\frac{1}{|x_{v_i} - x_{v_0}|} + \frac{1}{2} \sum_{\substack{j=1 \\ j \ne i}}^{N_\mathsf{V}-1} \frac{1}{\alpha_{x_{v_i}, x_{v_j}}} \right) \tag{16}$$

inducing the variational problem BB_G> as $c > 0$ allows for different scalings. The following properties are direct consequences of the definition of the penalty functional.

Proposition 4.1. *Any representation $x_{v_0}, x_{v_1}, \dots, x_{v_{N_\mathsf{V}-1}} \in \Omega$ of a star-shaped metric graph with $R(x_{v_0}, x_{v_1}, \dots, x_{v_{N_\mathsf{V}-1}}) < +\infty$ is embedded in the sense of Definition 2.1. In particular, there is no overlap between different edges and there exists a lower bound $d > 0$ such that $|x_{v_i} - x_{v_j}| \ge d$ for all $i, j \in \{0, \dots, N_\mathsf{V} - 1\}$, $i \ne j$.*

Remark 4.2. If the penalty functional is finite, it is continuous with respect to the strong norm convergence of the vertices. In particular, it is lower semi-continuous.

When varying the graph, we need to account for changes in the initial and final data. To do so, let $\eta_0, \eta_1 \in \mathcal{P}(\Omega)$ be given. We define $\rho_k := \eta_{k|\Omega_\mathsf{G}}$ and $\mu_k = \eta_k - \bar{\rho}_k$ for $k = 0, 1$. Since

$$\mu_k(\Omega) + \sum_{e\in\mathsf{E}} \rho_k^e(e) = \eta_k(\Omega \setminus \Omega_\mathsf{G}) + \eta_k(\Omega_\mathsf{G}) = 1 \tag{17}$$

we constructed a pair of admissible initial and final data $(\mu_k, \rho_k) \in \mathcal{P}_{\text{adm}}(\mathsf{G})$, $k = 0, 1$. In this way, initial and final data can be defined independently of the graph.

For the minimization we need to assume compatibility conditions for the mobilities and reference measures along varying graphs as well.

Assumption 4.3. We make the following additional assumptions:

1. The mobilities m_Ω and m_G do not depend on the graph.
2. It holds that $\sup_{\mathsf{G}\text{ embedded}} \sum_{e\in\mathsf{E}} \|\lambda_e\|_{\mathcal{M}(e)} < +\infty$ and $\sup_{\mathsf{G}\text{ embedded}} \sum_{v\in\mathsf{V}} \|\lambda_v\|_{\mathcal{M}(\{x_v\})} < +\infty$.
3. For $x_{v_i}^n \to x_{v_i}$ as $n \to \infty$, $i \in \{0, \ldots, N_\mathsf{V} - 1\}$ it holds that $\lambda_{e^n} \rightharpoonup \lambda_e$ and $\lambda_{v^n} \rightharpoonup \lambda_v$.

An admissible family can be obtained from fixed reference measures $(\lambda_e)_{e\in\mathsf{E}} \in \mathcal{M}(\mathsf{L})$ by defining $\lambda_{e^n} \in \mathcal{M}(e^n)$ for $e^n \in E^n$, $n \in \mathbb{N}$, using the push-forward under $\gamma_{e^n} : [0,1] \to e^n$. In the same way, we can construct measures on V^n for $n \in \mathbb{N}$.

Under these assumptions, we are able to show a similar compactness result to Theorem 3.8.

Proposition 4.4 (Compactness for varying graphs). *Given a family of embedded, star-shaped metric graphs $\mathsf{G}^n = (\mathsf{V}^n, \mathsf{E}^n)$ with nodes $x_{v_i}^n \to x_{v_i}$ as $n \to \infty$, $i \in \{0, \ldots, N_\mathsf{V} - 1\}$ and measures $(\mu_t^n, J_t^n, \rho_t^n, V_t^n, f_t^n, G_t^n) \in \mathsf{CE}(\mathsf{G}^n)$ such that*

$$\sup_{n\in\mathbb{N}} \int_0^1 \mathcal{A}_\mathsf{G}(\mu_t^n, J_t^n, \rho_t^n, V_t^n, f_t^n, G_t^n)\, dt + cR(x_{v_0}^n, x_{v_1}^n, \ldots, x_{v_{N_\mathsf{V}-1}}^n) < +\infty \tag{18}$$

there exist measures $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$ such that, up to subsequences

- *(i)* $\mu_t^n \rightharpoonup \mu_t$ *weakly in* $\mathcal{M}(\Omega)$ *for all* $t \in [0,1]$
- *(ii)* $\rho_t^n \circ \gamma^n \rightharpoonup \rho_t \circ \gamma$ *weakly in* $\mathcal{M}(\mathsf{L}_\mathsf{G})$ *for all* $t \in [0,1]$
- *(iii)* $J_t^n \rightharpoonup J_t$ *weakly in* $\mathcal{M}([0,1] \times \Omega, \mathbb{R}^d)$
- *(iv)* $\mathcal{V}_t^n \circ \gamma^n \rightharpoonup \mathcal{V} \circ \gamma$ *in* $\mathcal{M}([0,1] \times \mathsf{L})$
- *(v)* $f_t^n \circ \gamma^n \rightharpoonup f_t \circ \gamma$ *in* $\mathcal{M}([0,1] \times \mathsf{L})$
- *(vi)* $\mathcal{G}_t^n \circ \gamma^n \rightharpoonup \mathcal{G}_t \circ \gamma$ *in* $\mathcal{M}([0,1] \times \Omega_\mathsf{V})$.

Proof. By composition of the measures $\rho_t^n, \mathcal{V}_t^n, f_t^n$, and $\mathcal{G}_t^n$ with the change of variables maps γ^n through the push-forward operation, the whole sequence of measures is defined on a common domain instead of varying graphs. The remainder of the proof follows as in Theorem 3.8 applied to the resulting push-forward measures. The norm-convergence of the vertices implies $C^1([0,1])$-convergence of the maps γ_e^n for all $e \in \mathsf{E}$, thus the change of variables can be reversed in the limit, concluding the proof. □

With compactness and lower semi-continuity at hand, we can prove well-posedness.

Theorem 4.5. *Suppose that* (BB_G) *is finite. Then, there exists an embedded star-shaped metric graph $\mathsf{G} = (\mathsf{V}, \mathsf{E}, l)$ and a family of measures $(\mu_t, J_t, \rho_t, V_t, f_t, G_t) \in \mathsf{CE}(\mathsf{G})$ minimizing* (BB_G).

Proof. Let G^n be a minimizing sequence of graphs with corresponding measures $(\mu^n, J^n, \rho^n, V^n, f^n, G^n) \in \mathsf{CE}(\mathsf{G}^n)$. Each graph is embedded with the embedding given by a family of vertices $\{x_{v_0}^n, x_{v_1}^n, \ldots, x_{v_{N_\mathsf{V}-1}}^n\} \subset \Omega$, defining the sequences $(x_{v_i}^n)_{n\in\mathbb{N}}$ for $i \in \{0, \ldots, N_\mathsf{V} - 1\}$. Compactness of $\Omega \subset \mathbb{R}^d$ allows to apply the Bolzano–Weierstrass theorem to each of these sequences. Therefore, there exists a family of limiting points $x_{v_i} \in \Omega$ for $i \in \{0, \ldots, N_\mathsf{V} - 1\}$ such that, up to a subsequence, $x_{v_i}^n \to x_{v_i}$ for $i \in \{0, 1, \ldots, N_\mathsf{V} - 1\}$. Now, Proposition 4.4 and Proposition 4.2 allow the application of the direct method, proving the theorem. □

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Conflicts of Interest

None of the authors have a conflict of interest to disclose.

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