

# Topological derivative method for control of wave equation on networks

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**Abstract**—The dynamical, boundary optimal control problems on networks are considered. The domain of definition for the distributed parameter system is given by a graph  $G$ . The optimal cost function for control problem is further optimized with respect to the shape and topology of the graph  $\Omega$ . The small cycle is introduced and the topological derivative of the cost with respect to the size of the cycle is determined. In this way, the singular perturbations of the graph can be analyzed in order to change the topology  $\Omega$ . The topological derivative method in shape and topology optimization is a new tool which can be used to minimize the shape functionals under the Partial Differential Equations (PDEs) constraints. The topological derivative is used as well for solution of optimum design problems for graphs. In optimal control problems the topological derivative is used for optimum design of the domain of integration of the state equation. As an example, optimal control problems are considered on a cross with a small cycle. The state equation is the wave equation on the graph. The boundary control problem by Neumann conditions at a boundary vertex is solved for a tracking cost function. The shape functional is given by the optimal value of the control cost. The topological derivative of the shape functional is determined for the steady state model with the size of a cycle  $\varepsilon \rightarrow 0$ . Numerical results for a model problem are presented.

**Index Terms**—Distributed parameter system, optimal control, shape optimization, topological derivative, network modeling, optimality system.

## I. INTRODUCTION

The shape and topology optimization techniques are an important tool for the modeling and optimum design of distributed parameter systems, see e.g., [1], [2], [3], [4], [5], [6], for representative monographs and papers. However, such techniques are used only a little in control and design of networks modeled on graphs [7], [8], [9], (in general, on the so-called stratified spaces). The technique of self-adjoint extensions for the wave equation [10] is not really used for the graphs. We refer to [11] for some results in this direction.

The networks of distributed parameter systems are of common use e.g., in gas or water transportations modeling and control. The distributed parameter systems on graphs are usually governed by systems of nonlinear Partial Differential Equations on edges with the continuity and Kirchhoff conditions at the vertices of the associated graphs.

We consider the wave equation on a planar graph  $G := \{E, V\}$ . The geometrical domain of the tree  $G$  is denoted by  $\Omega$ . The perturbations of the tree by a small cycle of the size  $\varepsilon \rightarrow 0$  at the interior vertex  $P_0 \in V$  are considered for purposes of optimum design of the graph. When the nucleation of a small cycle is considered, the graph  $G$  is decomposed into two subgraphs  $G^0$  and  $G_\varepsilon$ . The geometrical domain  $\Omega_\varepsilon$  is associated with the domain decomposition of  $G$  of the form  $G^0 \cup G_\varepsilon$ . The topology variations of the network are governed by a small cycle  $G_\varepsilon$  for  $\varepsilon \rightarrow 0$ , in another words, a small cycle is introduced at some interior node  $P_0 \in V$  of  $G$  in order to evaluate the topological derivative of a given shape function. The subgraph of domain decomposition with the cycle is denoted by  $G_\varepsilon := \{E_\varepsilon, V_\varepsilon\}$ , the geometrical domain for the perturbed graph  $G^0 \cup G_\varepsilon$  is denoted by  $\Omega_\varepsilon$ . The graph  $G$  with vertices  $V$  is partitioned into boundary vertices  $V_B$  and vertices of junction  $V_J$ . Let  $I_E := \{1, \dots, n_E\}$  and  $I_V := \{1, \dots, n_V\}$  denote the set of edge indices and the set of vertex indices, respectively. In short, we have

$$V = V_B \cup V_J = \{P_1, P_2, P_3, \dots, P_{n_V}\}, \\ E = \{E_1, E_2, E_3, \dots, E_{n_E}\}.$$

As for the direction, we denote  $n_{E_i}(P_j)$  where  $n_{E_i}$  is the outward-pointing normal of the vertex  $P_j$ , thus

$$n_{E_i}(P_j) = \begin{cases} -1 & \text{if node } P_j \text{ is the start node of } E_i, \\ +1 & \text{if node } P_j \text{ is the end node of } E_i, \\ 0 & \text{otherwise.} \end{cases}$$

On a boundary vertex,  $P_1 \in V$  the Neumann control is applied. Given the shape functional  $\Omega \rightarrow J(\Omega)$ , the topological derivative at the interior vertex  $P_0 \in V$  is defined by the following limit, if the limit exists,

$$\mathcal{J}(P_0) := \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (J(\Omega_\varepsilon) - J(\Omega)). \quad (1)$$

The existence of limit in (1) implies the expansion of the shape functional

$$J(\Omega_\varepsilon) = J(\Omega) + \varepsilon \mathcal{J}(P_0) + o(\varepsilon). \quad (2)$$

## II. BOUNDARY CONTROL PROBLEM FOR WAVE EQUATION

The main ideas are presented in a simple case of a tree with singular perturbation given by a cycle. We need to explain the dynamical control problem on such a graph from one side, and the technique of shape and topology optimization from the other. The technique requires the notions of shape derivative, shape gradient, and topological derivative for a model of control problem. In optimal control, we use the optimality system [12] which is used to evaluate an optimal control and the optimal value of the cost function.

Let us start with the control problem for the wave equation on the interval  $I_\varepsilon := [0, 1 + \varepsilon]$ , where  $\varepsilon \rightarrow 0$  is the shape parameter. We assume that  $\varepsilon \in [-0.1, 0.1]$ . The state equation

$$y_{tt} - y_{xx} = 0, \text{ on } (0, T) \times (0, 1 + \varepsilon), \quad (3)$$

is supplemented with the initial conditions

$$y(0, x) = y^0(x), \quad y_t(0, x) = y^1(x) \quad (4)$$

and the boundary conditions

$$y_x(t, 0) = u(t), \quad y(t, 1 + \varepsilon) = 0. \quad (5)$$

The solution  $y := y_\varepsilon$  of the state equation depends on the small parameter because its domain of integration depends on  $\varepsilon$ . The derivative of  $\varepsilon \rightarrow y_\varepsilon$  is denoted by  $\dot{y}$ .

**Remark** For given control  $u$  the derivative  $\dot{y}$  is given by the following system for, say  $\varepsilon = 0$ ,

$$\dot{y}_{tt} - \dot{y}_{xx} = 0, \text{ in } I = (0, 1) \quad (6)$$

supplemented with the initial conditions

$$\dot{y}(0, x) = 0, \quad \dot{y}_t(0, x) = 0 \quad (7)$$

and the boundary conditions

$$\dot{y}_x(t, 0) = 0, \quad \dot{y}(t, 1) = -y_x(t, 1). \quad (8)$$

If the optimal control  $u := u_\varepsilon$  admits the derivative  $\dot{u}$ , then we should replace the homogeneous Neumann condition in (8) by the nonhomogeneous condition  $\dot{y}_x(t, 0) = \dot{u}(t)$ .

We assume that the functions  $y^0, y^1$  are defined on  $\mathbb{R}$ . The tracking type cost functional takes the form

$$J(u) = \int_0^T \int_0^{1+\varepsilon} \chi(x)(y_\varepsilon(x) - z(x))^2 dx dt + |u - \zeta|_{H^m(0, T)}^2, \quad (9)$$

where  $\chi(x)$  is the characteristic function of  $[0, 0.9]$ , i.e.,  $\chi(x) = 1$  on  $[0, 0.9]$  and  $\chi(1-x) = 0$ ,  $m = 2, 3$  and  $\{z, \zeta\}$  is a steady state  $z$  ( $\varepsilon = \varepsilon_0$ ) and the control  $\zeta$  for the wave equation. Thus,  $z = z(x)$ ,  $x \in I = [0, 1]$  and  $\zeta \in \mathbb{R}$  are given by the solution of ODE

$$z''(x) = 0 \quad \text{in } (0, 1), \quad z'(0) = \zeta, \quad z(1) = 0, \quad (10)$$

and we extend  $z(x) = 0$ ,  $x > 1$ , the extended function is also denoted by  $z(x)$ .

The unique optimal control is given by an optimality system [12]. We are interested in the derivative of the optimal value

of the cost with respect to the shape parameter  $\varepsilon$  at  $\varepsilon = 0^+$ . The sensitivity analysis of the control problems for the wave equation is considered, e.g., in [11].

## III. BOUNDARY CONTROL ON THE CROSS WITH VARIABLE LENGTHS OF EDGES.

First, we consider the regular perturbations  $\Omega_\varepsilon$  of the shape  $\Omega$  of a graph  $G$ . Let us consider for example the cross  $G_\varepsilon$ ,  $|\varepsilon| \leq 0.1$ , with three edges of the length  $|E_1| = 1 - 2\varepsilon$ ,  $|E_2| = |E_3| = 1 + \varepsilon$ , so the total length of the graph is constant  $|E_1| + |E_2| + |E_3| = 3$ . The geometrical domain of the associated graph is denoted by  $\Omega_\varepsilon$ .

We are interested in the derivatives of the optimal cost and of the optimality system with respect to the shape parameter  $\varepsilon \rightarrow \Omega_\varepsilon$ .

Assume for simplicity that the initial conditions are homogeneous. The state equations read

$$y := y_\varepsilon \in V_\varepsilon := V(\Omega_\varepsilon)$$

$$(y_{tt}(t), \varphi)_{\Omega_\varepsilon} + a_\varepsilon(y(t), \varphi) = ((Lu)(t), \varphi)_{\Omega_\varepsilon}, \quad \forall \varphi \in V_\varepsilon$$

The cost functional is defined on the subset  $\Omega_0 := \Omega \setminus \overline{\mathcal{O}(P_0)}$  which independent of  $\varepsilon$ . It means that the small cycle is included in  $\mathcal{O}(P_0)$  for all admissible  $-c \leq \varepsilon \leq c$ , for some small  $c \in \mathbb{R}$ . Thus, we introduce the characteristic function  $\chi$  of  $\Omega_0$ ,

$$J(u) = \frac{1}{2} \int_0^T \int_{\Omega} \chi(y - z)^2 + \frac{1}{2} |u|_m^2.$$

The control is in  $H^m(0, T)$  for  $m = 2, 3$ . The space  $H^2(0, T)$  is used in order to obtain the unique optimal control. For the existence of the topological derivative with respect to the size of a small cycle we need more regularity, hence the control space is  $H^3(0, T)$ .

The solution of control problem for fixed shape parameter is given by the associated optimality system. The optimality system is derived e.g., in the framework of the Lagrangian formalism. This is the coupled system of the state equation, adjoint state equation, and the optimality condition. In our case, the optimality system is reduced to two coupled wave equations and admits a unique solution. In addition, the optimality system is differentiable with respect to the shape parameter.

## IV. SINGULAR PERTURBATION OF THE GRAPH AT THE CENTRAL VERTEX BY A SMALL CYCLE

We consider the cross with six edges of the length  $|E_1| = |E_2| = |E_3| = 1 - \varepsilon$ , and  $|E_4| = |E_5| = |E_6| = \varepsilon$  for  $\varepsilon \rightarrow 0^+$ , so the total length of the graph is constant  $|E_1| + |E_2| + |E_3| + |E_4| + |E_5| + |E_6| = 3$ .

We are interested in the derivatives of the optimal cost and of the optimality system with respect to the shape parameter to the shape parameter at  $\varepsilon = 0^+$ . In this way, we evaluate the *Topological Derivative of the Optimal Cost* for the singular perturbation of the graph by a small cycle.

The topological derivative for nucleation of a cycle in the graph is obtained for the model problem. This result is stronger compared to the known results [7], [8]. For example, the cost in [9] is the energy for the network of Timoshento beams. In our case, the shape function is governed by the optimal value of the cost for control problem, so it is a cost different from the elastic energy.

The PDEs models on graphs are usually systems of nonlinear Partial Differential Equations on edges with the continuity and Kirchhoff conditions at the vertices of the associated graphs. In the wave equation, we obtain the following transmission conditions (Abbreviate  $y_{E_i}$  as  $y_i$ )

$$y_i(P_j) = y_k(P_j), \forall i, k \in I_E, j \in n_V \quad (\text{Continuity})$$

$$\sum_{E_i} (y_i)_x(P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V \quad (\text{Kirchhoff})$$

## V. NUMERICAL RESULT

Now we present the numerical results of the example on  $\Omega_\varepsilon$  (See Fig. 1). There is a boundary control  $u(t)$  at vertical  $P_1$ , i.e.,  $\frac{\partial y_1}{\partial x}(t, 0) = u(t)$ .

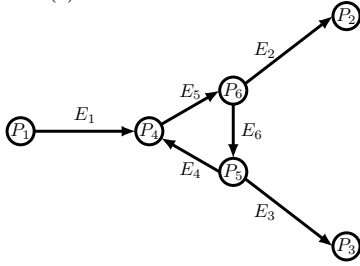


Fig. 1. Tripod directed network with a cycle.

We want to solve the optimality system. It means that we solve two coupled wave equations. The control is replaced by the adjoint state from the optimality condition.

1. Compute the solution of the steady-state equation. We use the solution of the steady-state equation in the cost function. In this graph, we assume the perturbation be  $\varepsilon_0$ .

$$\begin{cases} -z_i'' = 0, x \in [0, L_i] \\ z_1'(0) = \zeta, z_2(L_2) = z_3(L_3) = 0 \\ z_i(P_j) = z_k(P_j), \forall i, k \in I_E, j \in n_V \\ \sum_{E_i} z_i'(P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V \end{cases} \quad (11)$$

2. Discretize the scalar elliptic problem governed by optimality condition to obtain the optimal control  $u(t) := \mathcal{L}[p](t)$  in function of adjoint state  $p$ :

$$u \in H^2(0, T) : \int_0^T u_{tt} w_{tt} = - \int_0^T p(t, 0) w(t), \quad (12)$$

$$\forall w(t) \in H^2(0, T)$$

$$u(0) = u(T) = \zeta, \quad u_t(0) = u_t(T) = 0.$$

3. Solve state equation coupled with the adjoint equation by the Neumann boundary condition:

$$\begin{cases} (y_i)_{tt} - (y_i)_{xx} = 0, t \in [0, T], x \in [0, L_i], \forall i \in I_E \\ y_i(0, x) = y_{i,0}(x), (y_i)_t(0, x) = y_1(x), \\ (y_1)'(t, 0) = \mathcal{L}(t), (y_2)(t, L_2) = 0, (y_3)(t, L_3) = 0, \\ y_i(t, P_j) = y_k(t, P_j), \forall i, k \in I_E, j \in n_V \\ \sum_{E_i} y_i'(t, P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V \end{cases} \quad (13)$$

where  $\mathcal{L}(t) = \mathcal{L}[p](t)$  is defined at 2.

4. Adjoint equation is coupled with the state equation by the right-hand side; the direction of time  $t$  is reversed if compared with the state equation because the final conditions are given instead of the initial conditions;

$$\begin{cases} (p_i)_{tt} = (p_i)_{xx} + z_i - y_i \text{ in } t \in [0, T], x \in [0, 1], i \in I_E \\ p_i(T, x) = 0, (p_i)_t(T, x) = 0, \\ (p_1)'(t, 0) = 0, (p_2)(t, L_2) = 0, (p_3)(t, L_3) = 0, \\ p_i(t, P_j) = p_k(t, P_j), \forall i, k \in I_E, j \in n_V \\ \sum_{E_i} p_i'(t, P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V. \end{cases} \quad (14)$$

We use a finite-difference approximation for the time derivative. A first and second-order approximation is given by the central difference formula.

$$\begin{aligned} \dot{y}(t, x) &\approx \frac{y(t + \Delta t, x) - y(t - \Delta t, x)}{2\Delta t}, \\ \ddot{y}(t, x) &\approx \frac{y(t + \Delta t, x) - 2y(t, x) + y(t - \Delta t, x)}{(\Delta t)^2}, \end{aligned} \quad (15)$$

where  $\Delta t$  is the time step.

Denote  $y^n \approx y(n\Delta t, x)$ , and  $u^n \approx u(n\Delta t)$ . Then, the implicity scheme of the weak form will be

$$\begin{cases} \left( \frac{y^{n+1} - 2y^n + y^{n-1}}{(\Delta t)^2}, \varphi \right)_{L^2(0,1)} \\ + a \left( \frac{y^{n+1} + y^{n-1}}{2}, \varphi \right) = u^{n+1} \varphi(0), \forall \varphi, \varphi(1) = 0, \\ \frac{y^1 - y^{-1}}{2\Delta t} \approx y_t(0, x) = y^1(x), \quad y^0 = y^0(x). \end{cases} \quad (16)$$

Then we use the Hermite finite element space discretization. On the unit interval  $[0, 1]$ , there exist four Hermite Shape Functions with cubic order, denoted by  $h_{00}$ ,  $h_{01}$ ,  $h_{10}$ , and  $h_{11}$  (Eq. 17). These functions are referred to as hat functions on the reference unit, and they are graphically displayed in Fig 2.

$$\begin{aligned} h_{00} &= 2x^3 - 3x^2 + 1, h_{01} = -2x^3 + 3x^2, \\ h_{10} &= x^3 - 2x^2 + x, h_{11} = x^3 - x^2. \end{aligned} \quad (17)$$

Let  $0 = x_0 < x_1 < \dots < x_{N_i} = L_i$  be a local mesh on one edge interval  $[0, L_i]$  which consisting of  $N_i$  subintervals of length  $h_i$ . After mapping from the reference unit to the

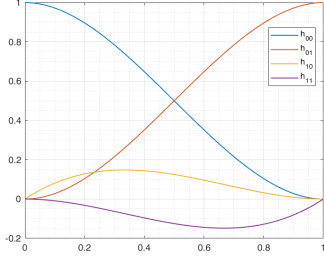


Fig. 2. The four Hermite basis functions on the unit interval  $[0, 1]$ .

local interval, the hat function can be given by  $H_{1,i}$  and  $H_{2,i}$  as follows:

$$H_{1,i} = \begin{cases} -2\left(\frac{x-x_{i-1}}{h_i}\right)^3 + 3\left(\frac{x-x_{i-1}}{h_i}\right)^2 & \text{in } [x_{i-1}, x_i]; \\ 2\left(\frac{x-x_i}{h_i}\right)^3 - 3\left(\frac{x-x_i}{h_i}\right)^2 + 1 & \text{in } [x_i, x_{i+1}]; \\ 0 & \text{otherwise.} \end{cases}$$

$$H_{2,i} = \begin{cases} \left(\frac{x-x_{i-1}}{h_i}\right)^3 - \left(\frac{x-x_{i-1}}{h_i}\right)^2 & \text{in } [x_{i-1}, x_i]; \\ \left(\frac{x-x_i}{h_i}\right)^3 - 2\left(\frac{x-x_i}{h_i}\right)^2 + \frac{x-x_i}{h_i} & \text{in } [x_i, x_{i+1}]; \\ 0 & \text{otherwise.} \end{cases}$$

Each base function is continuous, piecewise cubic. For  $H_{1,i}$ , it takes a unit value at its own node  $x_i$ , while being zero at all other nodes. For  $H_{2,i}$ , its derivative takes a unit value at its own node  $x_i$ , while being zero at all other nodes (See Fig. 3). The ansatz function  $y_h(x)$  is constructed as a

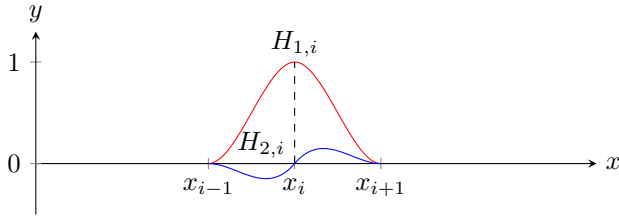


Fig. 3. Illustration of shape functions (red:  $H_{1,i}$ , blue:  $H_{2,i}$ )

linear combination of two sets of basis functions,  $H_{1,j}(x)$  and  $H_{2,j}(x)$ , that are defined over the set of nodes  $x_j$ .

$$y(t, x) \approx y_h(t, x) = \sum_{j=0}^{N_i} Y_j H_{1,j}(x) + \sum_{j=0}^{N_i} \tilde{Y}_j H_{2,j}(x).$$

At the  $j$ -th node  $x_j$ , there are two degrees of freedom  $Y_j$  and  $\tilde{Y}_j$ , where  $Y_j$  is the value of  $y_h(x)$  at  $x_j$  and  $\tilde{Y}_j$  is the corresponding derivative value.

For convenience, denote

$$Y^n = (Y_1(n\Delta t), \dots, Y_{N+1}(n\Delta t), \tilde{Y}_1(n\Delta t), \dots, \tilde{Y}_{N+1}(n\Delta t))^T$$

be a column vector. Then, the equation (16) can be written as

$$\begin{cases} \left(M_{N_h} + \frac{1}{2}\Delta t^2 K_{N_h}\right) Y^{n+1} = \\ 2M_{N_h} Y^n - \left(M_{N_h} + \frac{1}{2}\Delta t^2 K_{N_h}\right) Y^{n-1} - \Delta t^2 u^n \\ n = 0, 1, \dots, T \\ Y^{-1} = Y^1 - 2\Delta t(y_1(0), \dots, y_1(1), y_1'(0), \dots, y_1'(1))^T, \\ Y^0 = (y_0(0), \dots, y_0(1), y_0'(0), \dots, y_0'(1))^T, \end{cases}$$

where  $M_{N_h}$  is the mass matrix and  $K_{N_h}$  is the stiffness matrix. Similarly, we have the numerical scheme for adjoint state  $p$  and optimal condition.

One way to handle this problem is to use an iterative procedure. To this end, we introduce the fixed point algorithm:

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**Algorithm 1** Fixed point algorithm

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1. Choose  $u^0$
  2. **For**  $i = 1$  until satisfied
    - a. solve state equation for  $y_i$
    - b. solve adjoint equation for  $p_i$
    - c. solve optimal condition for  $u_i$
  3. Terminate with the (approximate) fixed point  $\hat{u}, \hat{y}, \hat{p}$ .
- 

Set  $\zeta = 1, T = 1, \varepsilon = 0.01, \varepsilon_0 = 0.001$ . The final state  $y$  of the network can be shown in Fig. 4 generated by MATLAB with the initial value:

$$\begin{aligned} y_1^0(x) &= x^2 + \zeta x - \zeta L_1 - L_1^2; \\ y_2^0(x) &= -\frac{1}{L_2}(L_1 + \frac{1}{2}\zeta)x^2 + (L_1 + \frac{1}{2}\zeta)x; \\ y_3^0(x) &= -\frac{1}{L_3}(L_1 + \frac{1}{2}\zeta)x^2 + (L_1 + \frac{1}{2}\zeta)x; \\ y_4^0(x) &= x^4 - 2\varepsilon x^3 + \varepsilon^2 x^2; \\ y_5^0(x) &= -\frac{1}{\varepsilon^2}(2L_1 + \zeta)x^3 - \frac{2}{\varepsilon}(2L_1 + \zeta)x^2 + (2L_1 + \zeta)x; \\ y_6^0(x) &= -\frac{1}{\varepsilon^2}(2L_1 + \zeta)x^3 - \frac{3}{2\varepsilon}(2L_1 + \zeta)x^2 + (L_1 + \frac{1}{2}\zeta)x; \\ y_i^1(x) &= 0, i = 1, 2, \dots, 6 \end{aligned}$$

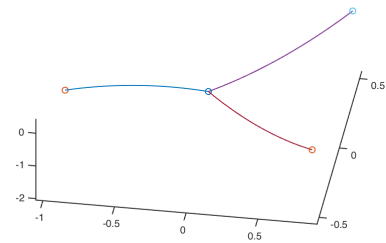


Fig. 4. Final state for wave equation.

## VI. STEADY STATE BOUNDARY CONTROL PROBLEM.

We evaluate the topological derivative of shape functional for the steady state distributed parameter system.

Let us consider the control problem for  $G$  with control at  $P_1$ , i.e.,  $\frac{dy_1}{dx}(0) = u$ . We assume that at  $P_2, P_3$  there are homogeneous Dirichlet conditions. The state equation on  $G = \{V, E\}$  is defined in weak form by

$$\begin{aligned} y \in H : a(y, \phi) &= \langle L(u), \phi \rangle \quad \forall \phi \in H, \\ H &= \{ \phi, \phi'_i \in L^2(0, L_i), \phi_2(0) = \phi_3(0) = 0, \\ &\text{continuity at interior vertices.} \} \end{aligned} \quad (18)$$

We apply the domain decomposition method associated with the decomposition of graph  $G = G^0 \cup G_\varepsilon$  (See Fig. 5). Here,  $G_\varepsilon = \{E_\varepsilon, V_\varepsilon\}$  contains a small cycle.  $E_\varepsilon = \{E_{\varepsilon,1}, E_{\varepsilon,2}, \dots, E_{\varepsilon,6}\}$ ,  $V_\varepsilon = \{Q_1, Q_2, Q_3, P_4, P_5, P_6\}$ ,  $|E_{\varepsilon,1}| = |E_{\varepsilon,2}| = |E_{\varepsilon,3}| = \varepsilon_{\max} - \varepsilon = 1 - \varepsilon$ ,  $|E_{\varepsilon,4}| = |E_{\varepsilon,5}| = |E_{\varepsilon,6}| = \varepsilon$ . In this way the dependence of the solutions to the state equation with respect to the small parameter  $\varepsilon \rightarrow 0$  is explicitly given in the weak form of the state equation.

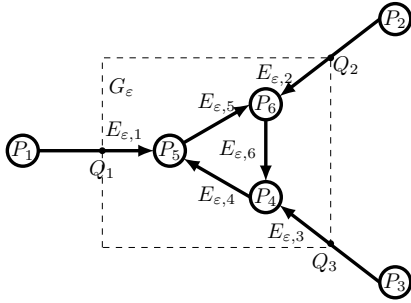


Fig. 5. Tripod directed network with a cycle with domain decomposition.

The model defined on  $G_\varepsilon$  is  $-w''_i = 0$  on  $E_{\varepsilon,i}$ . We determine on  $G_\varepsilon$  the Dirichlet-to-Neumann nonlocal operator given by a matrix  $(\Lambda_\varepsilon)_{3 \times 3}$  by the solution for the boundary conditions

$$w_i(0) = w_i(Q_i) = a_i$$

and

$$b = -\Lambda a,$$

where  $a = \text{col}\{a_1, a_2, a_3\}$ ,  $b = \text{col}\{b_1, b_2, b_3\}$ ,  $b_i = \frac{dw_i}{dx}(0) = \frac{dw_i}{dx}(Q_i)$ .

We need the Green's formula for a single beam  $E_i = Q_i - P_i$  in order to identify the Steklov-Poincaré operator. We assume that the vertex  $Q_i$  is a boundary vertex and the vertex  $P_i$  is the interior vertex for the subgraph  $G_\varepsilon$ .

Let us return to Green's formula for the bilinear form  $a_i(w_i, \phi_i)$  associated with the system. We have

$$\int_0^{L_i} w'_i \phi'_i = - \int_0^{L_i} w''_i \phi_i + (N_i w_i \phi_i)_{x=0}^{x=L_i}, \quad (19)$$

where  $w_i \mapsto N_i w_i$  is the Neumann operator  $N_i$  on  $E_i$ . Here,  $N_i w_i = w'_i$ .

**Proposition 1.** *If we know the exact solution  $y_a$  for the Dirichlet problem on the graph  $G_\varepsilon$  with the polynomials on the edges, it follows that the associated energy for such a*

*solution takes the form  $a(y_a, y_a) = -a^\top \Lambda_\varepsilon \cdot a$ , thus the energy functional for the graph  $G$  reads*

$$\phi \mapsto a(\Omega; \phi, \phi) = a(\Omega^0; \phi, \phi) - \phi(L-1)^\top \Lambda_\varepsilon \cdot \phi(L-1).$$

*The restriction of the state equation to  $\Omega^0$  can be considered under assumption that the control  $u$  is supported in  $\Omega^0$  and the state is observed in  $\Omega^0$ . Thus, the state equation becomes:*

*Find  $y \in H(\Omega^0)$  such that*

$$a(\Omega^0; y, \phi) - y(L-1)^\top \Lambda_\varepsilon \cdot \phi(L-1) = (L(u), \phi)_{\Omega^0}, \quad (20)$$

*for all test functions  $\phi \in H(\Omega^0)$ .*

**Remark 1.** *It is surprising that the vector  $\tilde{a} = \text{col}(1, 1, 1)^\top$  i.e., such that  $\tilde{a}_1 = \tilde{a}_2 = \tilde{a}_3 = 1$ , is in the kernel of  $\Lambda_\varepsilon$ . Indeed, the associated energy on  $G_\varepsilon$  for the constant solutions on edges equals zero,*

$$-\tilde{a}^\top \Lambda_\varepsilon \cdot \tilde{a} = 0.$$

*On the other hand, the bilinear form on the left hand side of elliptic state equation (20) is coercive provided that there is at least one Dirichlet boundary vertex of the graph  $G^0$ .*

Now we combine the coupling conditions at inner vertices to compute  $\Lambda_\varepsilon$ . It's easy to know that the solutions on  $E_{\varepsilon,i} = [0, L_{\varepsilon,i}]$  are given by

$$w_i(x) = \alpha_i x + \beta_i, \quad x \in [0, L_{\varepsilon,i}].$$

So  $a_i = w_i(0) = \beta_i$ ,  $b_i = \frac{dw_i(0)}{dx} = \alpha_i$ ,  $b = \Lambda_\varepsilon a \iff \alpha = \Lambda_\varepsilon \beta$ .

Considering the Kirchhoff and continuity at  $P_4, P_5, P_6$  respectively, we have

$$\begin{aligned} (1-\varepsilon)\alpha_1 + \beta_1 &= \varepsilon\alpha_4 + (1-\varepsilon)\alpha_3 + \beta_3, \\ (1-\varepsilon)\alpha_2 + \beta_2 &= \varepsilon\alpha_5 + (1-\varepsilon)\alpha_1 + \beta_1, \\ (1-\varepsilon)\alpha_3 + \beta_3 &= \varepsilon\alpha_6 + (1-\varepsilon)\alpha_2 + \beta_2, \\ \alpha_1 + \alpha_4 - \alpha_5 &= 0, \\ \alpha_2 + \alpha_5 - \alpha_6 &= 0, \\ \alpha_3 + \alpha_6 - \alpha_4 &= 0. \end{aligned} \quad (21)$$

Then we get

$$\alpha_1 = -\frac{-2\beta_1 + \beta_2 + \beta_3}{2\varepsilon - 3}, \alpha_2 = -\frac{\beta_1 - 2\beta_2 + \beta_3}{2\varepsilon - 3}, \alpha_3 = -\frac{\beta_1 + \beta_2 - 2\beta_3}{2\varepsilon - 3}. \quad (22)$$

Hence

$$\Lambda_\varepsilon = \frac{1}{2\varepsilon - 3} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \quad (23)$$

**Remark 2.**  $\Lambda_\varepsilon$  is negative semidefinite because with the identical Dirichlet conditions, the solution is constant so the energy is zero.

The cost functional is

$$J(u) = \frac{1}{2} \sum_{i=1}^3 \int_0^{L_i-1} (y_i - z_i)^2 + \frac{1}{2} |u - \zeta|^2.$$

Finally, the optimality system becomes

$$\begin{cases} \sum_{i=1}^3 \int_0^{L_i-1} y_i \phi_i + a(\Omega^0; p, \phi) \\ -\phi(L-1)^\top \Lambda_\varepsilon p(L-1) = \sum_{i=1}^3 \int_0^{L_i-1} z_i \phi_i, \\ a(\Omega^0; y, \phi) - p_1(0) \phi_1(0) \\ -y(L-1)^\top \Lambda_\varepsilon \phi(L-1) = -\zeta \phi_1(0). \end{cases}$$

We use the finite element method to solve the optimality system for control problem. Set  $\zeta = 1, \varepsilon_0 = 0.5$ . The optimal value of the cost is depicted in Figure 6. It can be seen that cost functional is zero when  $\varepsilon = \varepsilon_0$ . And the derivative of  $J$  with respect to  $\varepsilon$  is less than 0 as  $\varepsilon$  approaches 0. This is the information which allows for the topology variations by nucleation of a small cycle at an interior vertex of the graph.

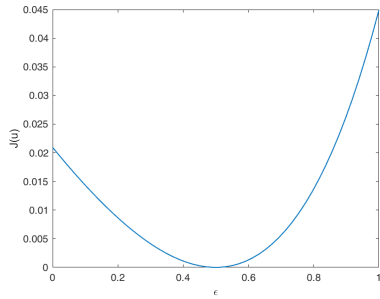


Fig. 6. The shape functional for  $\varepsilon \in [0, 1]$

## VII. CONCLUSIONS

The bilevel optimization problems are considered on metric graphs. The state equation is the second order wave equation. The steady state problems are ordinary differential equations. The optimal control problems are solved by solution of optimality systems. For the steady state problems, the topological derivatives are obtained for the topology variations by nucleation of a small cycle. Numerical results of optimization are presented for the wave equation and for the steady state problem.

The domain decomposition technique is used in mathematical modeling of distributed parameter systems defined on graphs. Such a system is called a network and its model includes a graph  $G = \{V, E\}$  along with the state equations on edges  $E$ . Such a model is used e.g., in the analysis of real life large scale gas networks with quasilinear hyperbolic equations on the edges. At the interior nodes of the graph there are prescribed two conditions, the continuity of solutions as well as the continuity of fluxes, the latter condition is called the Kirchhoff condition. The geometrical domain associated with the system is denoted by  $\Omega$  and the shape and topology optimization problems are considered on the network. The shape functional is given by an optimal cost of control problem defined on the network. Thus, the optimization problem is bilevel, at a lower level an optimal control problem, and at a higher level a shape and topology optimization problem.

The topology optimization means the variations of the network form e.g., by nucleations of cycles. Therefore, the state equation at the higher level, for the shape and topology optimization takes the form of the optimality system for optimal control problem. Domain decomposition technique allows us to replace the singular domain perturbation of  $\Omega$  by a regular perturbation of the bilinear form for the elliptic problem considered on  $\Omega^0$ . The perturbation of bilinear form is given by the Dirichlet-to-Neumann operator which is also called the Steklov-Poincaré operator. In the case considered the nonlocal operator is represented by a *semidefinite positive matrix*  $-\Lambda_\varepsilon$  which is determined explicitly (23). In this way the evaluation of topological derivatives for the shape functional becomes simple and it does not require e.g., the compound asymptotic method used for the purposes of asymptotic analysis in singularly perturbed domains. The domain decomposition technique for networks on graphs is employed to obtain the topological derivative of shape function. The topological derivative is defined as the limit for  $\varepsilon \rightarrow 0^+$  of the shape cost derivative with respect to  $\varepsilon$ , see Figure 6.

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