# The Transport PDE and Mixed-Integer Linear Programming

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**Abstract.** Discrete, nonlinear and PDE constrained optimization are mostly considered as different fields of mathematical research. Nevertheless many real-life problems are most naturally modeled as PDE constrained mixed integer nonlinear programs. For example, nonlinear network flow problems where the flow dynamics are governed by a transport equation are of this type. We present four different applications together with the derivation of the associated transport equations and we show how to model these problems in terms of mixed integer linear constraints.

**Keywords.** Transport Equation, Partial Differential Equation, Mixed-Integer Linear Programming, Modeling, Nonlinear Constraints.

## 1 Introduction

Continuous and discrete optimization are currently two distinct fields of mathematics. From time to time, discrete optimizers try to cope with a problem which has some intrinsic nonlinear continuous structure, sometimes modeled using partial differential equations. Then they most likely would try to get rid of these continuous parts, such that a pure combinatorial problem remains. Similarly, if a person with a background in continuous optimization gets involved with a problem that involves discrete and combinatorial aspects, he would most likely try to relax the discontinuities to some continuous constraints, in order to apply some well-understood methods of the field. For both of them it is true that *if one only has a hammer, the world is full of nails.*

In this article we try to bridge the gap between these two fields. Since the authors are both working in discrete optimization, our view is naturally biased. We assume that our readers have a similar background, which in particular means that we will explain the derivation of the partial differential equations involved, but we do not explain linear programming based branch-and-cut methods.

In the sequel we will present four different applications. All involve the transport of quantities of certain good in given network structures. Hence when it

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comes to modeling these processes it is no surprise that the corresponding models all have a structural similarity. In our case this is the so called *transport equation*, which is a partial differential equation that describes the flow of particles on an edge of the network. Although the transport equation is ubiquitous, the models differ however in the complexity of the dynamics that are involved. We proceed from the simplest dynamics to more complex ones. At the one end we have a simple linear transport of the particles that goes only in the direction of the flow, whereas at the other end a nonlinear behavior and new phenomena such as backward shock waves might occur.

## 2 The Transport Equation

We are interested in the flow of particles on a given network. The flow evolves over time. Time is denoted by $t$. We think of the edges as one dimensional objects. Therefore every location in the network can be described by a single coordinate, denoted by $x$. We assume that the number of particles is so large that we cannot consider them individually. Furthermore we think of the particles as being small with respect to the network size - think of cars in a street network or gas molecules in a pipeline network. Hence to count them we consider their *density* $\rho(x,t)$, which is defined as the number of particles per unit length in $x$ at a certain time $t$. Depending only on the density we want to describe the *flow* of the particles $f(\rho)$ on the arcs of the network. Per definition, flow is measured in number of particles per unit time. A positive flow, $f(\rho) > 0$, means that the particles are moving in direction of the arc.

Since $\rho(x,t)$ describes the "concentration" of particles at position $x$ at time $t$, the number of particles in a section of an edge between positions $x_1$ and $x_2$ is given by

$$\int_{x_1}^{x_2} \rho(x,t)dx. \tag{1}$$

Similarly we can express how many particles flow through position $x$ during a time interval from $t_1$ to $t_2$, namely by computing

$$\int_{t_1}^{t_2} f(\rho(x,t))dt. \tag{2}$$

The perhaps most fundamental laws in physics are the conservation laws (energy conservation, for example), stating that a considered system is always close in the sense that nothing is lost or gained. Everything happens only by transformation. This is also valid for our applications, where we assume a mass balance, that is, the number of particles between $x_1$ and $x_2$ at time $t_2$ equals the number of particles in this section that were already there at some time $t_1$ before $t_2$, plus or minus the inflow or outflow at $x_1$ and $x_2$, respectively. Expressed as an equation, material balance can be stated as

$$\int_{x_1}^{x_2} \rho(x,t_2)dx = \int_{t_1}^{t_2} f(\rho(x_1,t))dt + \int_{x_1}^{x_2} \rho(x,t_1)dx - \int_{t_1}^{t_2} f(\rho(x_2,t))dt, \tag{3}$$

for all $t_1 < t_2$ and $x_1 < x_2$. Here "$x_1 < x_2$" means that $x_1$ is closer to the tail and $x_2$ is closer to the head of the arc under consideration.

From the fundamental theorem of calculus we obtain

$$\rho(x, t_2) - \rho(x, t_1) = \int_{t_1}^{t_2} \frac{\partial}{\partial t} \rho(x, t) dt, \tag{4}$$

and also

$$f(\rho(x_2, t)) - f(\rho(x_1, t)) = \int_{x_1}^{x_2} \frac{\partial}{\partial x} f(\rho(x, t)) dx, \tag{5}$$

assuming that the functions involved are sufficiently smooth. In view of equation (3) we integrate (4) and (5) with respect to the "missing" variables, and get

$$\int_{x_1}^{x_2} \rho(x, t_2) - \rho(x, t_1) dx = \int_{x_1}^{x_2} \int_{t_1}^{t_2} \frac{\partial}{\partial t} \rho(x, t) dt dx, \tag{6}$$

and

$$\int_{t_1}^{t_2} f(\rho(x_2, t)) - f(\rho(x_1, t)) dt = \int_{t_1}^{t_2} \int_{x_1}^{x_2} \frac{\partial}{\partial x} f(\rho(x, t)) dx dt, \tag{7}$$

respectively. Replacing the left-hand sides of (6) and (7) in (3) by their right-hand sides gives

$$\int_{x_1}^{x_2} \int_{t_1}^{t_2} \frac{\partial}{\partial t} \rho(x, t) + \frac{\partial}{\partial x} f(\rho(x, t)) dt dx = 0. \tag{8}$$

Since (8) is valid for every segment $x_1, x_2$ and for each time interval $t_1, t_2$, and also assuming that the partial derivatives of order one are continuous functions, we obtain from an elementary integration property of continuous functions the equation

$$\frac{\partial}{\partial t} \rho(x, t) + \frac{\partial}{\partial x} f(\rho(x, t)) = 0. \tag{9}$$

This partial differential equation of order one is called the *transport equation*. It is the basis for all applications and models presented in the sequel.

## 3 Applications

In this section we give four examples and models where the transport equation shows up in practice. We concentrate here on describing the modeling of transport equations and leave out all further side constraints that show up in the practical applications. For details of the whole models we refer to the corresponding papers.

### 3.1 Production Network Planning

Our study of production networks was initially motivated by a practical problem, the manufacturing of tooth brushes in a multi-step assembly line with queues [1,2,3,4]. Unfinished products are transported on small pallets on conveyer belts between different manufacturing units. Each unit is equipped with a buffer (a waiting queue). The queues are in front of each processor. In the model they do not have a physical length. The layout of the production line is modeled by a graph $G = (V, A)$, where the processors correspond to the arcs. Each processor $j \in A$ is operating at a certain constant speed $v^j$. Note that for each arc $j$ we have individual flow and density functions $f^j$ and $\rho^j$, respectively. Then, the transport of pallets within a processor is modeled by the transport equation

$$\frac{\partial}{\partial t}\rho^j(x,t) + \frac{\partial}{\partial x} f^j(\rho^j(x,t)) = 0,\ \forall\, j \in A, x \in [a^j, b^j], t \geq 0. \tag{10}$$

Note that one can show that $f^j(\rho^j(x,t)) = v^j \rho^j(x,t)$, see [1], hence the transport equation simplifies to the linear PDE constraint

$$\frac{\partial}{\partial t}\rho^j(x,t) + v^j \cdot \frac{\partial}{\partial x}\rho^j(x,t) = 0,\ \forall\, j \in A, x \in [a^j, b^j], t \geq 0. \tag{11}$$

Besides the transport equation (11), the production network planning problem contains several other side constraints.

Among them are that each processor has an upper capacity limit. In addition to the modeling of the flow-density-behavior inside a processor, the combination of arcs at junctions (vertices) of merging or dispersing type must be considered. At each junction the incoming flow is directly send to the queues of the subsequent processors. The actual change of the queue size of each processor at each time equals its inflow minus its outflow, and hence can be described by an ordinary differential equation. The objective is to maximize the pallets in the network. New pallets are only introduced via one a-priori known arc in the network. Details of the model maybe found in [5].

### 3.2 Traffic

The main modeling difference in the evolution of traffic flow compared to the flow of pallets on a production line is the structure of the transport equation. For traffic flow it is common to use the Lighthill-Whitham equations [6]:

$$\forall j \in A, x \in [a_j, b_j], t \geq 0 : \frac{\partial}{\partial t}\rho^j(x,t) + \frac{\partial}{\partial x} f^j(\rho^j(x,t)) = 0, \tag{12}$$

with

$$f^j(\rho) = \rho \cdot u(\rho), \tag{13}$$

where $u(\rho)$ is the *fundamental diagram of traffic flow.* This diagram defines an idealistic relation between the traffic flow (in cars per hour) and the traffic density (in cars per km). It has the property that for zero density the flow is also zero, since there are no vehicles on the road, and with an increasing number of vehicles, the density and the flow also increase. At some point, when the number of vehicles gets too large, a situation of maximum density is reached when the vehicles can't move. This is the jam density, and the corresponding flow is zero. Somewhere between zero density and jam density the flow reaches a maximum. The fundamental diagram is for example

$$u(\rho) = \hat{\rho} - \rho, \tag{14}$$

which leads to a parabolic flow-density relationship. Here $\hat{\rho}$ is the density of maximum flow.

Similar to the production network additionally constraints are the flow conservation in the traffic network. A typical objective is to minimize the average time that the cars spent in the network. Note that by solving this problem we obtain a solution that shows the full dynamic behavior of traffic flows. Unfortunately this problem is at the same time too difficult to be solved numerically. Thus we derived simplified models that do not show the all dynamic aspects of the flow, but at the same time are more easier to solve, see [5] for details.

### 3.3 Gas Networks

The task in gas network optimization is to route the gas through the network to satisfy the consumers' demands such that the costs for the control elements, that is fuel gas consumption of the compressors, is minimized.

We model a dynamic gas transport network by means of a directed finite graph $G = (V, A)$. The set of arcs is partitioned into different sets for the various components in the network, e.g., compressors, valves, and pipes.

The gas flow in a pipe is governed by the system of Euler equations supplemented by a suitable equation of state. In several situations, we can assume a nearly constant temperature $T = \bar{T}$ of the gas - e.g., pipes in Germany are typically at least one meter beneath the ground. In such a situation, an isothermal flow is an appropriate model. Assuming ideal gas behavior, the Euler equations reduce to the continuity and the momentum equation. On each pipe of the network we have

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho v) = 0\,, \tag{15}$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2) + \frac{\partial}{\partial x}p = -g\rho\frac{\partial}{\partial x}h - \frac{\lambda}{2D}\rho|v|v\,. \tag{16}$$

The two terms on the right-hand side of (16) describe the influence of gravity and friction. Here, $g$ is the acceleration constant, $\partial_x h$ is the slope of the pipe, $\lambda$ is the pipe friction value, and $D$ is the diameter of the pipe.

The friction factor $\lambda$ is implicitly given by the Prandtl-Colebrook law,

$$\frac{1}{\sqrt{\lambda}} = -2\,\log_{10}\left(\frac{2.51}{Re\,\sqrt{\lambda}} + \frac{k}{3.71\,D}\right), \tag{17}$$

with the Reynolds number $Re = D\rho|v|/\eta$, where $\eta$ is the dynamic viscosity of the gas, and with the roughness $k$ of the pipe.

This system of partial differential equations has to be completed by initial, boundary and coupling conditions across the whole network. The objective function is to minimize the fuel gas consumption of the compressors, which is turn are described by further highly nonlinear functions. For details of the model we refer to [7].

### 3.4 Water Networks

In water supply networks, we are dealing with pressurized water networks. Due to the incompressibility of water, pressure $p$ can equivalently be expressed as an elevation difference

$$\Delta h = \frac{p}{g\rho}, \tag{18}$$

where $g$ is the gravity constant and $\rho$ is the constant water density. In water management, pressure is therefore often measured by the elevation above sea level, called the head $h$, which is the sum of the actual geodetic height and the elevation difference corresponding to the hydraulic pressure. For this kind of network, the governing equations in all pipes are the so-called water hammer equations [8]:

$$\frac{\partial h}{\partial t} + \frac{a^2}{gA}\frac{\partial q}{\partial x} = 0\,, \tag{19}$$

$$\frac{\partial q}{\partial t} + gA\frac{\partial h}{\partial x} = -\lambda\frac{q|q|}{2DA}\,, \tag{20}$$

where $(h, q)$ is the state vector consisting of the piezometric head and the flow. Again, $g$ is the gravitational constant, $a$ is the speed of sound in the pipe, $A$ and $D$ are the cross-sectional area and the diameter of the pipe. The term on the right-hand side of (20) models the influence of friction. As for the gas networks, the friction coefficient $\lambda$ is implicitly given by (17).

Analogously to the other models from above, we enforce conservation of mass and consistency of the pressure head as coupling conditions. The objective functions is to minimize the energy consumption of the pumps, which gives rise to further nonlinearities. Details of the model can be found in [7].

## 4 Transforming into MIP Model

We have seen in the four applications above how the transport equation shows up and as a consequence how the applications can be modeled as an optimization problem over partial differential equations. Note that in the first two applications no discrete variables are involved and we are left with a pure PDE optimization problem, whereas in other two applications on gas and water network optimization discrete variables are necessary modeling the switching of valves, pumps, and compressors.

Motivated by the latter two applications where discrete variables cannot be avoided, we want to show how to transform the PDE models into mixed integer programming models. The way to this is done two steps. In the first step the PDE systems are transformed into a system of differential algebraic equations (DAEs) by applying some finite difference scheme. These equations are of linear or nonlinear behavior. In the first case we are already done and obtained a mixed integer linear programming formulation. In the second case, the nonlinear equations still must be approximated by piecewise linear functions.

Each of the two steps is well studied in the literature. We show the first step on our first application, the production line problem, and give hints and references for the other three.

We introduce a discretization for the time steps $T := \{t_0, \ldots, t_N\}$ with $t_n := n\Delta t$ for $n \in \{0, 1, \ldots, N\}$, where $\Delta t$ is a constant step size (see below), and $N = T/\Delta t$. From now on, the time is not running continuously, but in discrete time steps. For each processor $j$ and each time $t_n$ we introduce two variables $\alpha_n^j, \beta_n^j \in \mathbb{R}_+$, that describe the density of pallets at the two ends of a processor at time step $t_n$, i.e., $\alpha_n^j := \rho^j(a^j, t_n), \beta_n^j := \rho^j(b^j, t_n)$. With $\Delta x := L^j := b^j - a^j$ the upwind scheme

$$\frac{\rho^j(x, t + \Delta t) - \rho^j(x, t)}{\Delta t} + v^j \cdot \frac{\rho^j(x, t) - \rho^j(x - \Delta x, t)}{\Delta x} = 0, \tag{21}$$

can be rewritten as

$$\beta_{n+1}^j = \beta_n^j - \frac{v^j \Delta t}{L^j} \cdot (\beta_n^j - \alpha_n^j), \ \forall\, j \in A, n \in \{0, \ldots, T\}. \tag{22}$$

Note that (22) is already a linear equation and thus step two above is no longer necessary. The same principle can be used for the traffic flow problem as well as the gas and water network optimization problems except that the discretization step must be performed with more care, since the transportation equation is a nonlinear PDE in all cases and complemented in addition by the momentum equations in the latter two applications. We refer for details to [5,7].

For the inclusion of nonlinear constraints into the mixed-integer linear framework by piecewise linear functions, which is necessary in the second step from above, we apply well-known techniques from the literature, such as the convex combination method [9], the incremental method [10], the SOS method [11], the logarithmic approach [12], and their respective generalizations to higher dimensions [13,14].

## 5 Conclusions

We presented four different models and applications of the transport PDE. We indicated how to model these applications as PDE optimization as well as mixed-integer linear optimization problems. For all models we applied appropriate methods, such as adjoint calculus for PDE optimization or branch-and-cut for MILP optimization. Tests on medium to large scale instances indicate that for the production network planning problem both the continuous and the discrete model yield exactly the same solution. In the case of the traffic network flow problem, the continuous models became too difficult to solve even for medium size instances. Thus it is appropriate to solve linear approximations for large scale instances. In the case of water and gas network problems, the linearized models hardly cope with the dynamics of the flow, yielding either high running times, or inaccurate solutions.

A promising future direction is to combine the advantages of both worlds by using the mixed-integer approach to decide on the correct combinatorics and the PDE approach to get the physics straight.

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