
Model hierarchies and optimization for dynamic flows on networks

S. Göttlich and A. Klar

Department of mathematics, TU Kaiserslautern

Fraunhofer ITWM, Kaiserslautern



Collaborators:

P. Degond (Toulouse)

M. Herty (Aachen)

B. Piccoli (Rome)

C. Ringhofer (Tempe)

A. Fügenschuh, A. Martin (Darmstadt)

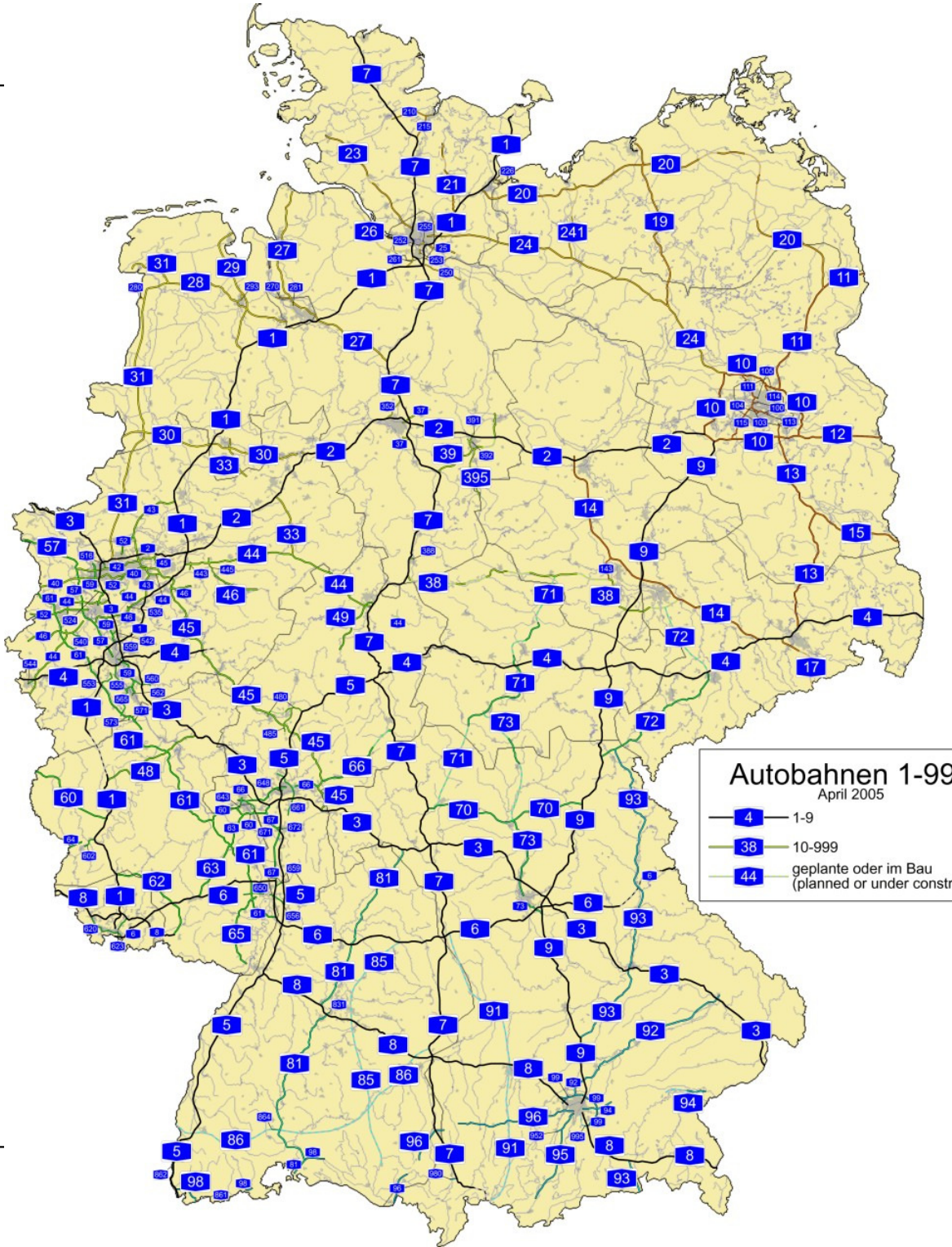
R. Borsche, A. Dittel, U. Ziegler (TU / ITWM Kaiserslautern)



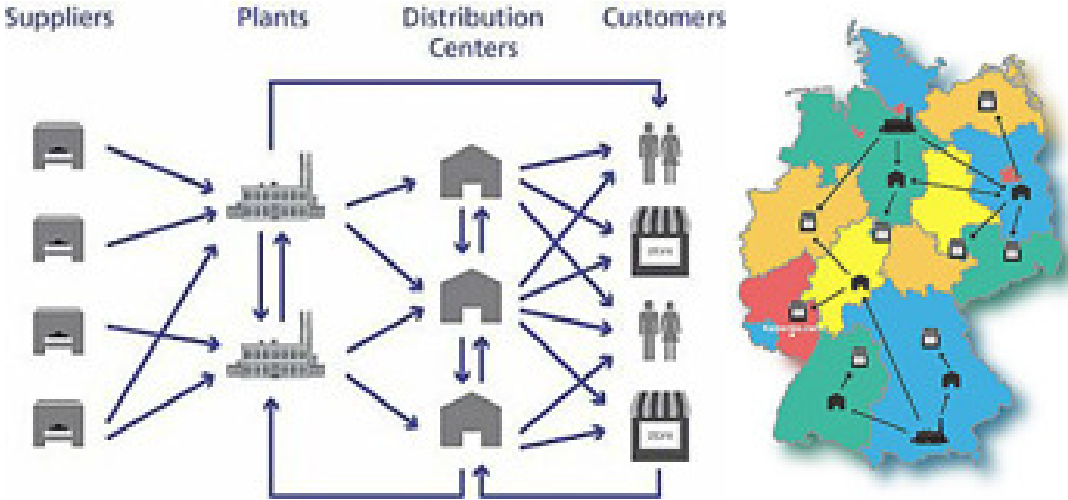
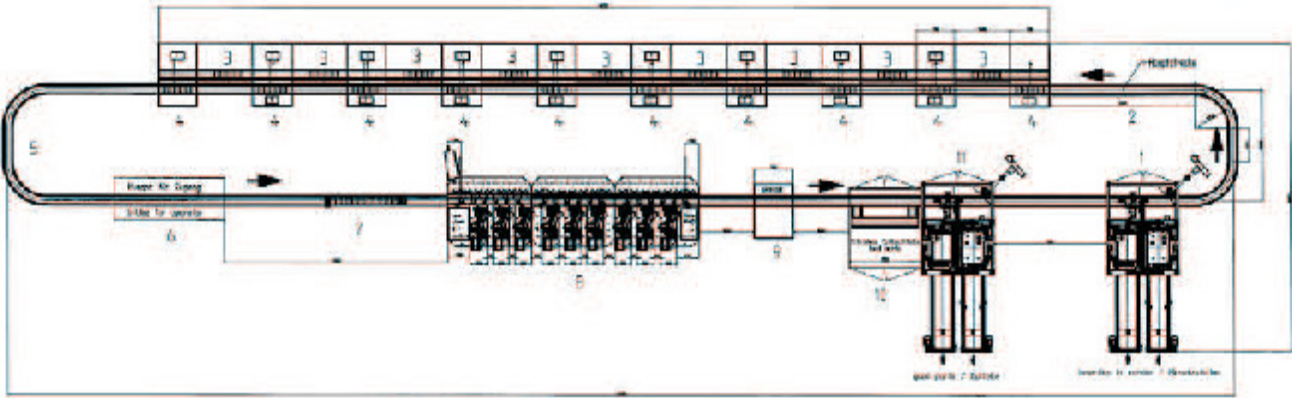
Introduction



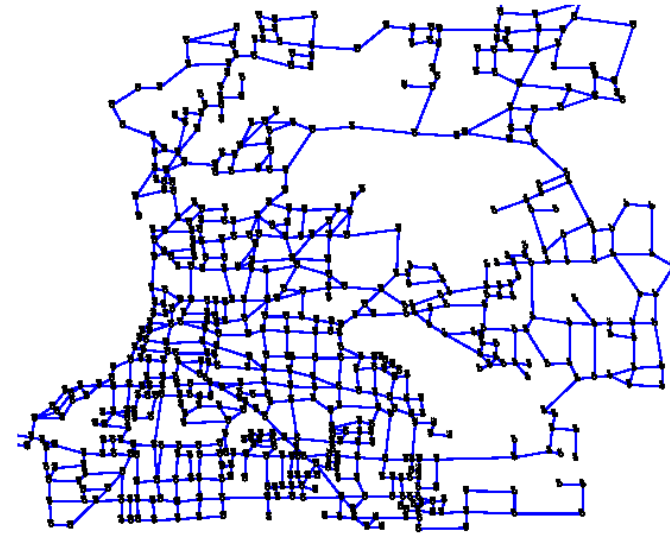
Example: Traffic Networks



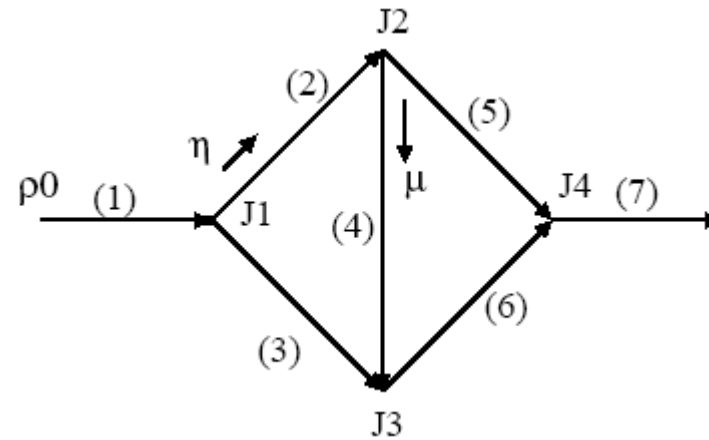
Example: Supply-Chains



Example: Gas/Water Networks



Networks



General Tasks:

- Modelling: Determine dynamics on the arcs, coupling conditions
- Model reduction, simplified models
- Optimization of throughput, etc.

Contents of the course

1. Dynamic models for traffic flow, supply chains and gas flow
2. PDE Network models (dynamics at junctions/coupling conditions)
 1. Scalar equations: LW-type traffic models and supply-chain models
 2. System of equations: Multipolicy sc, gas dynamics, higher order traffic models
3. Model reduction: Simplified network models
4. Optimization and control
 1. Continuous approaches / adjoints
 2. Discrete optimization, large scale networks
 3. Numerical comparison of the two approaches



1. Dynamic models for traffic flow, supply chains and gas/water flow



Traffic flow



Traffic flow: Microscopic models

Ordinary differential equations/Follow the leader $(x_i(t), v_i(t))$

$$\begin{aligned}\underline{x}_i &= v_i, \\ \underline{v}_i &= \frac{v_{i+1} - v_i}{(x_{i+1} - x_i)^{\gamma+1}} + \frac{1}{T} \left[V\left(\frac{1}{x_{i+1} - x_i}\right) - v_i \right]\end{aligned}$$

Kinetic/Vlasov/mean field models $f(x, v, t)$

$$\partial_t f + v \partial_x f = C(f)$$

$$\partial_t f + v \partial_x f + \partial_v (B[f]f - D[f] \partial_v f) = 0$$



Macroscopic/fluid dynamic equations

Lighthill-Whitham

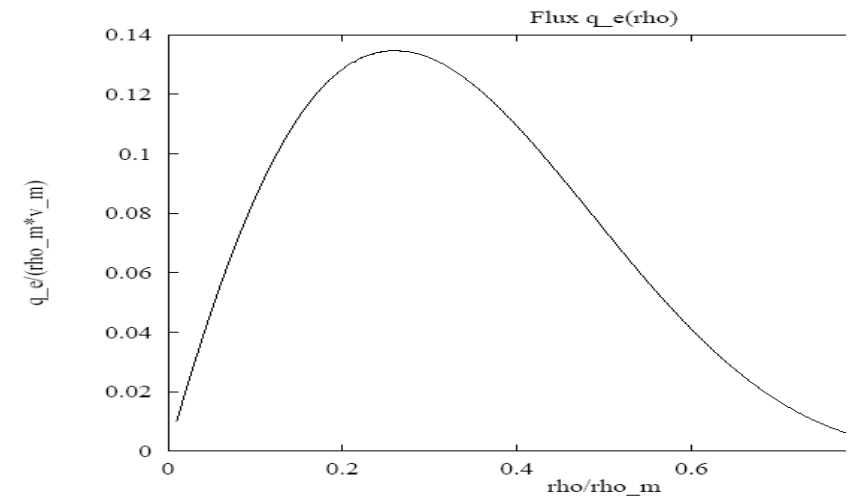
Basic equations:

$$\partial_t \rho(x, t) + \partial_x f(\rho(x, t)) = 0$$

$$f(\rho) = \rho V^e(\rho)$$

$\rho(x, t)$: density of vehicles

$V^e(\rho)$: **Equilibrium velocity**



Second order models (Aw-Rascle):

$$\begin{aligned}\partial_t \rho + \partial_x(\rho u) &= 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2) + c(\rho) \partial_x u &= S(\rho, u).\end{aligned}$$

$$S(\rho, u) \sim \frac{\rho}{T} [V^e(\rho) - u].$$

$u(x, t)$: mean velocity of vehicles

$c(\rho)$: anticipation factor $c(\rho) = -\rho^{\gamma+1}$

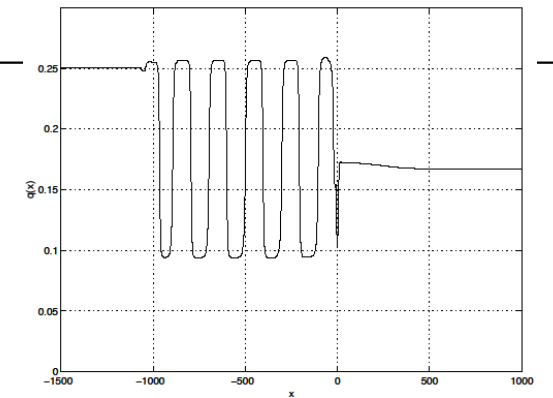
Derivation from FtL-mode

See also: Zhang, Greenberg, Colombo, ...



Stop and go waves, traffic instabilities

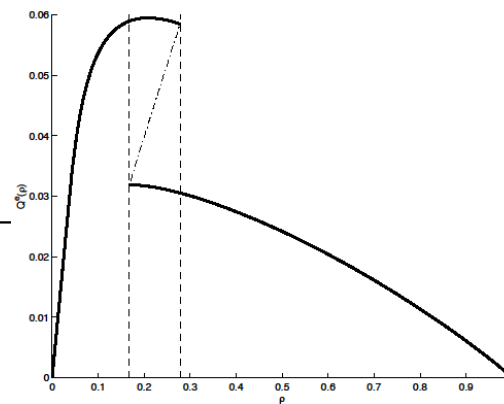
Many attempts, revised Aw-Rascle equations:



$$\partial_t \rho + \partial_x(\rho u) = 0$$

$$\partial_t(\rho u) + \partial_x(\rho u^2) + c(\rho) \partial_x u = S^{ex}(\rho, u).$$

$$S^{ex}(\rho, u) \sim \frac{\rho}{\tau} \begin{cases} u_1^e(\rho) - u & , \quad \rho < R(u) \\ u_2^e(\rho) - u & , \quad \rho \geq R(u). \end{cases}$$



Derivation from kinetic mode

Supply chains



Supply-Chain Models:

Microscopic models (~Follow the leader)

Discrete event simulations: track each item, equations for processing time of each part

Problem: Simulation and optimization is computationally expensive

Macroscopic/fluid dynamic models (~Lighthill-Whitham)

(Armbruster, Degond, Ringhofer):

Assume many parts in DES, dynamics for product density by PDE



Microscopic models: discrete event

M processors, each supplier m is linked to only one previous supplier $m - 1$.

$\tau(m, n)$: arrival time of part n at supplier m

$T(m)$: processing time.

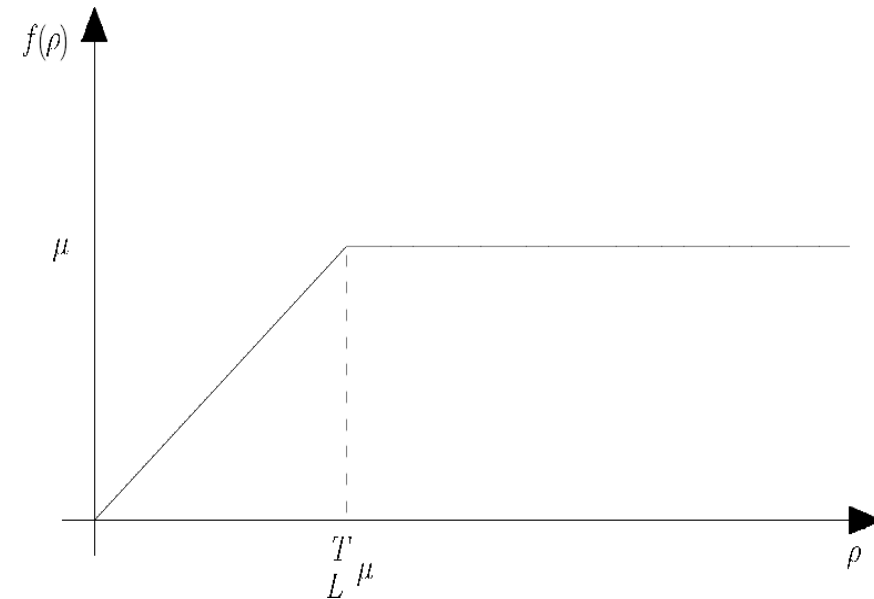
$\mu(m)$: maximal processing rate.

$$\tau(m + 1, n) = \max\left\{\tau(m, n) + T(m), \tau(m + 1, n - 1) + \frac{1}{\mu(m)}\right\}$$



Basic equations for Supply Chains

Basic equations:



$$\partial_t \rho(x, t) + \partial_x f(\rho(x, t)) = 0$$

$$f(\rho) = \min\{\mu, v\rho(x, t)\}$$

ρ : density of parts

μ : maximum processing capacity

V : processing velocity

Derivation from DES



Gas / Water



(Macroscopic) Equations for Gasflow

Isothermal Euler equations with friction

$$\partial_t \rho + \partial_x(\rho u) = 0$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + a^2 \rho) = -f_g \frac{q|q|}{2D\rho}$$

$$\partial_t U + \partial_x F(U) = R(U)$$

with

$$U = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}.$$

Similar for water flow (different pressure law): St. Venant/Shallow Water



2. Network models based on partial differential equations

2. 1. Scalar equations: Lighthill-Whitham type traffic models and supply chain models



Traffic models



Traffic: Network model and coupling conditions

Dynamic equations on each arc: Lighthill-Whitham

$$\partial_t \rho_i(x, t) + \partial_x f_i(\rho_i(x, t)) = 0 \quad \forall i \in I, x \in [a_i, b_i], t \geq 0$$

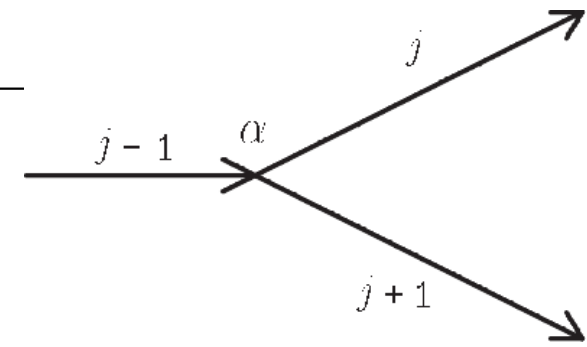
$$\rho_i(0, t) = \rho_{i,0}(x) \quad \forall x \in [a_i, b_i]$$

$$f_i(\rho) = \rho V_i^e(\rho) : \text{Fundamental diagram}$$

Additionally: conditions at the junctions



Conditions at the junctions (general approach)



1. Consider waves emerging out of the junctions
2. Equality of in- and outgoing fluxes

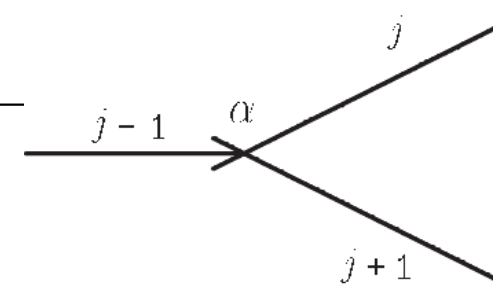
$$\sum_{i=1}^n f_i(\rho_i(b_i, t)) = \sum_{i=n+1}^{n+m} f_i(\rho_i(a_i, t)) \quad \forall t$$

3. Include wishes of drivers (α_{ki} : percentage of drivers from road i to road k)

$$0 < \alpha_{kn} < 1 \text{ and } \sum_{k=n+1}^{n+m} \alpha_{ki} = 1, \quad \forall i.$$

$$f_k(\rho_k(a_k, t)) = \sum_{i=1}^n \alpha_{ki} f_i(\rho_i(b_i, t)) \quad \forall k = n+1, \dots, n+m.$$

Further conditions at the junctions



FIFO (First in first out): Engineering literature, Piccoli et al.

4. Maximize ingoing flow

$$\sum_{i=1}^n f(\rho_i).$$



Other approaches:

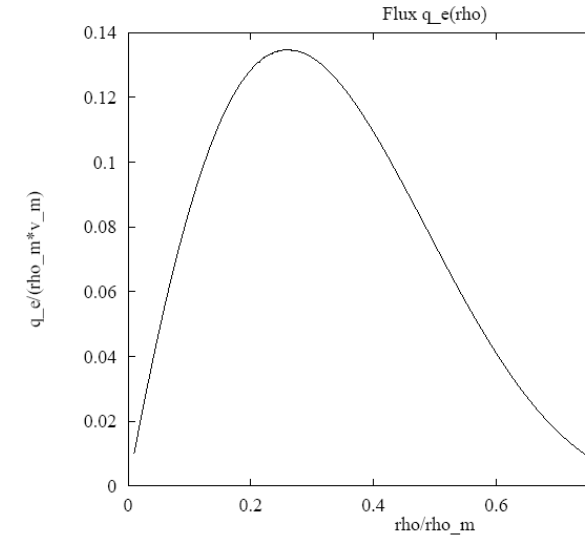
NON FIFO: J.P. Lebacque

or

Detailed multilane modelling of the junction,
determination of new states as asymptotic states
of the multilane problem



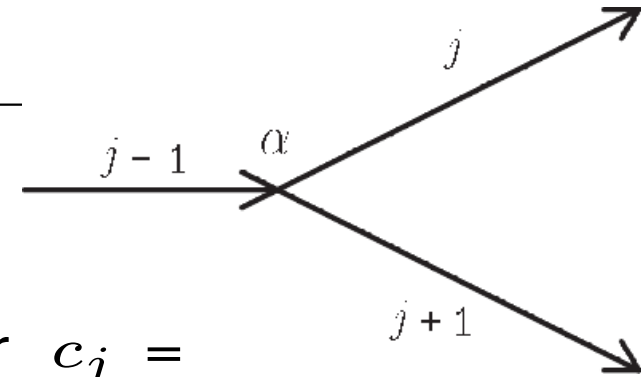
Waves out of the junction



$$\begin{array}{ll}
 \bar{\rho}_i \in [\sigma, 1] & \rho_{i,0} \geq \sigma \quad i = 1, \dots, n \\
 \bar{\rho}_i \in \{\rho_{i,0}\} \cup [\tau(\rho_{i,0}), 1] & \rho_{i,0} \square \sigma \quad i = 1, \dots, n \\
 \bar{\rho}_i \in [0, \sigma] & \rho_{i,0} \square \sigma \quad i = n+1, \dots, n+m \\
 \bar{\rho}_i \in [0, \tau(\rho_{i,0})] \cup \{\rho_{i,0}\} & \rho_{i,0} \geq \sigma \quad i = n+1, \dots, n+m
 \end{array}$$

$\tau(\rho)$ is the unique number $\tau(\rho) \neq \rho$, s.t. $f(\rho) = f(\tau(\rho))$. Thus $\rho < \sigma \Rightarrow \tau(\rho) > \sigma$ and vice versa.

Example (FIFO)



c_j : maximal flux on road j , i.e. either $c_j = f(\rho_{j,0})$ or $c_j = f(\sigma)$.

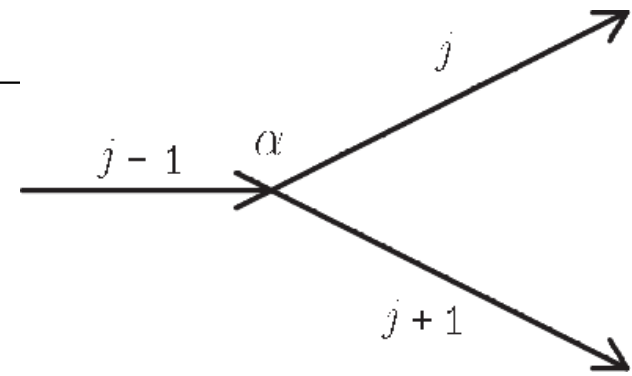
(1) $\gamma_1 \in \mathbb{R}_+ = [0, c_1]$, $\alpha_{j,1} \gamma_1 \in \mathbb{R}_+$ for $j = 2, 3$.

(2) Maximize γ_1 w.r.t. (1).

(3) $\gamma_j = \alpha_{j,1} \gamma_1$, $j = 2, 3$. $\gamma_1 = \min\{c_1, c_2/\alpha_{2,1}, c_3/\alpha_{3,1}\}$.

Typical situation: If road 2 is full, then $c_2 = 0$, i.e. $\gamma_1 = 0$

Example (NON FIFO)



(1) $\gamma_j \in -j$ and $\gamma_j/\alpha_{j,1} \in -1$ for $j = 2, 3$.

(2) Maximize γ_j w.r.t. (1) for $j = 2, 3$.

(3) $\gamma_1 = \sum_{j=2}^3 \gamma_j$. $\gamma_j = \min\{\alpha_{j,1}c_1, c_j\}$, $j = 2, 3$

Typical situation: If road 2 is full, then $c_2 = 0$ and γ_1 must not ! be equal to 0.

Traffic: Theory

Holden et al.

Piccoli et al.

etc.

Existence of weak network solutions



Supply chain models



Network Models

- Production network as directed graph
- Each processor is described by an arc e described by the interval $[a^e, b^e]$.
- Dynamics of the processor is described by

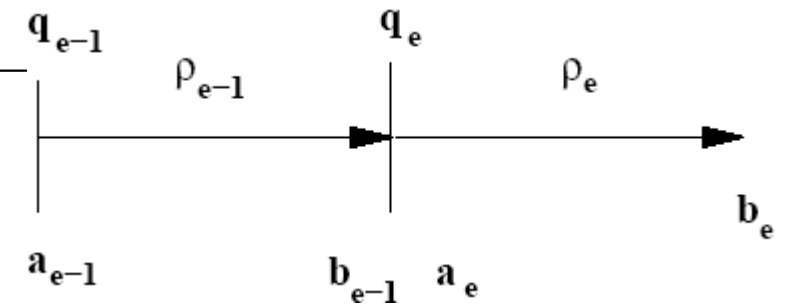
$$\partial_t \rho(x, t) + \partial_x f(\rho(x, t)) = 0$$

$$f(\rho) = \min\{\mu, v\rho(x, t)\}$$

- v, μ constant for each processor
- Add equation for queues in front of the processor



Consecutive Processors



$$\partial_t \rho_e(x, t) + \partial_x f_e(\rho_e(x, t)) = 0, \quad f_e(\rho) = v_e \rho$$

$$f_e(\rho_e(a_e, t)) = \begin{cases} \min\{f_{e-1}(\rho_{e-1}(b_{e-1}, t)), \mu_e\} & q_e(t) = 0 \\ \mu_e & q_e(t) > 0 \end{cases}$$

Inflow is whatever is in the queue, but at most the maximal capacity

$$\partial_t q_e(t) = f_{e-1}(\rho_{e-1}(b_{e-1}, t)) - f_e(\rho_e(a_e, t))$$

rate of change of queue e = Inflow from arc $e-1$ – inflow to processor e

Reformulation of the dynamics:

Regularization (Ringhofer et al.)

$$f_e(\rho_e(a_e, t)) = \min\left\{\mu_e; \frac{q_e(t)}{\epsilon}\right\}$$

$q \leq \epsilon\mu$:

$$f_e(\rho_e(a_e, t)) = \frac{q_e}{\epsilon}, \quad \partial_t q_e(t) = f_{e-1}(\rho_{e-1}(b_{e-1}, t)) - \frac{q_e}{\epsilon},$$
$$q_e \sim \epsilon f_{e-1}(\rho_{e-1}(b_{e-1}, t))$$

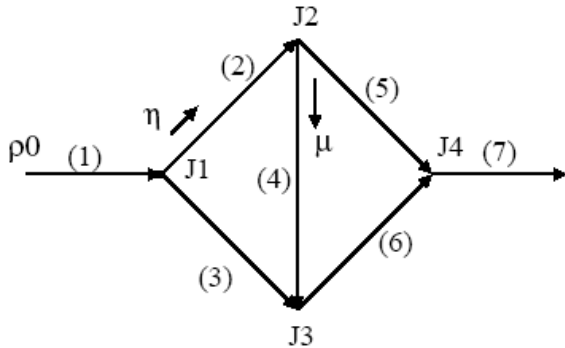
$q > \epsilon\mu$:

$$f_e(\rho_e(a_e, t)) = \mu_e$$



General networks

Directed graph, arc e is described by the interval $[a^e, b^e]$.



For a vertex the set of all ingoing arcs is δ^- , δ^+ is the set of all outgoing arcs.

Distribution of total mass flux:

$A(t) \in \mathbb{R}^{|\delta^+|}$ having entries $A_e(t) \in [0, 1]$ and satisfying $\sum_{e \in \delta^+} A_e(t) = 1$.

Equation for queues:

$$\partial_t q^e(t) = A_e(t) \left(\sum_{\tilde{e} \in \delta^-} f^{\tilde{e}}(\rho^{\tilde{e}}(b^{\tilde{e}}, t)) \right) - f^e(\rho^e(a^e, t))$$

General networks:

Dynamics in processor e: $\partial_t \rho^e + v^e \partial_x \rho^e = 0, \quad v^e \rho^e(a^e, t) = \min\left\{\mu^e; \frac{q^e(t)}{\epsilon}\right\}$

$$\partial_t q^e(t) = \sum_{\tilde{e} \in \delta^-} A_e(t) f^{\tilde{e}}(\rho^{\tilde{e}}(b^{\tilde{e}}, t)) - \min\left\{\mu^e; \frac{q^e(t)}{\epsilon}\right\}$$

The second equation is rephrased as

Dynamics in queue e: $\partial_t q^e(t) = h^e(\rho, A) - \min\left\{\mu^e; \frac{q^e(t)}{\epsilon}\right\}$

Release rule queue to processor :

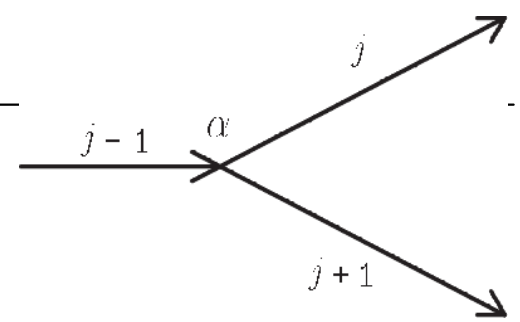
Inflow is whatever is in the queue but at most the maximal capacity

Geometry of network:

h^e (controllable) inflow to arc e with controls A



Example: Dispersing junction



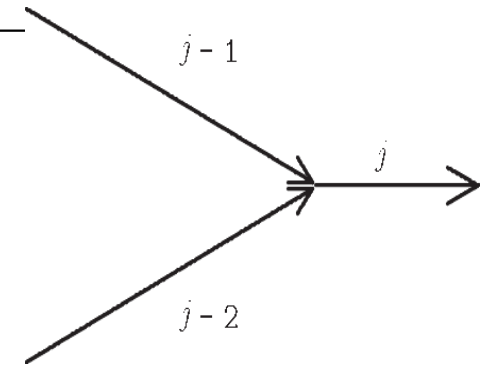
$$\partial_t q_j = \alpha f_{j-1}(\rho_{j-1}(b_{j-1}, t)) - f_j(\rho_j(a_j, t))$$

$$\partial_t q_{j+1} = (1 - \alpha) f_{j-1}(\rho_{j-1}(b_{j-1}, t)) - f_{j+1}(\rho_j(a_j, t))$$

$$f_j(\rho_j(a_j, t)) = \begin{cases} \min\{\alpha f_{j-1}(\rho_{j-1}(b_{j-1}, t)), \mu_j\} & q_j(t) = 0 \\ \mu_j & q_j(t) > 0 \end{cases}$$

$$f_{j+1}(\rho_j(a_j, t)) = \begin{cases} \min\{(1 - \alpha) f_{j-1}(\rho_{j-1}(b_{j-1}, t)), \mu_{j+1}\} & q_{j+1}(t) = 0 \\ \mu_{j+1} & q_{j+1}(t) > 0 \end{cases}$$

Example: Merging Junctions



$$\partial_t q_j(t) = f_{j-2}(\rho_{j-2}(b_{j-1}, t)) + f_{j-1}(\rho_{j-1}(b_{j-1}, t)) - f_j(\rho_j(a_j, t))$$

$$f_j(\rho_j(a_j, t))$$

$$= \begin{cases} \min\{f_{j-2}(\rho_{j-2}(b_{j-1}, t)) + f_{j-1}(\rho_{j-1}(b_{j-1}, t)), \mu_j\} & q_j(t) = 0 \\ \mu_j & q_j(t) > 0 \end{cases}$$

Theory

Theorem (Piccoli et al.):

There exists a unique solution $(\rho^e(x, t), q^e(t))$ on the network, such that $\rho^e \in C^{0,1}(0, T; L^1(a^e, b^e))$ is a weak solution to the pde and $q^e \in W^{1,1}([0, T])$.

Remark: proof by construction of approximate solutions via front-tracking,
estimate on number of interaction at vertices (between waves and waves with queues),
estimate on total variation of solutions

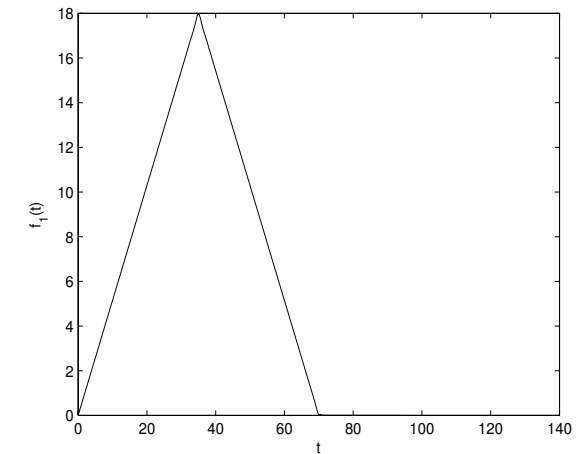
Remark: Uniqueness of solutions using arguments as in Bressan/Crasta/Piccoli.



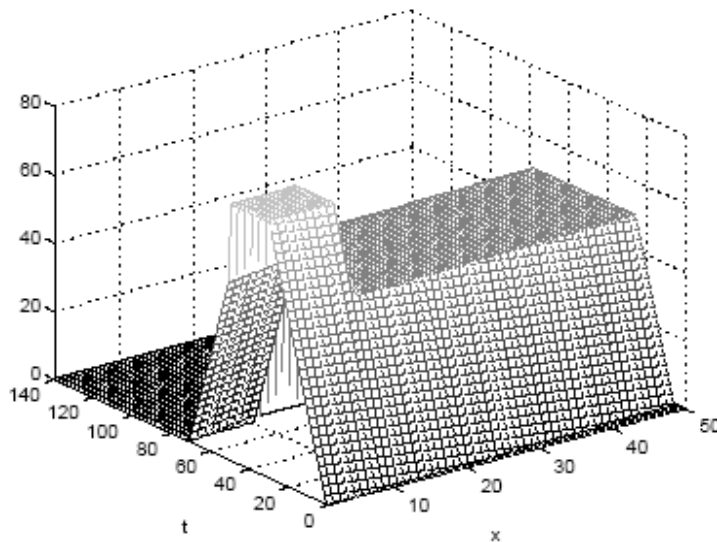
Numerical Example

Processor j	N_j	μ_j	T_j	L_j
1	10	25	1	1
2	10	15	1	0.2
3	30	10	3	0.6
4	10	15	1	0.2

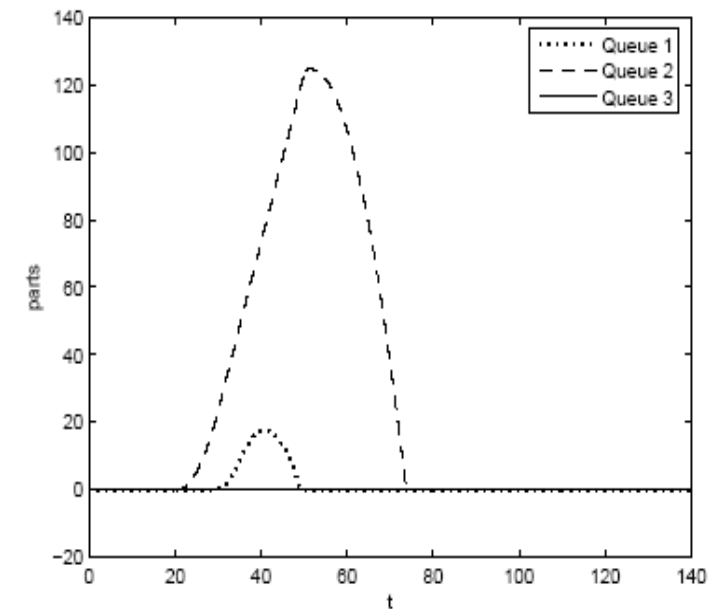
Inflow:



Density



Queues 1,2,3:



Comparison of CPU times:

Model	Parameters		CPU Time			
DES	$K = 3$ $T_{max} = 100$ $\Delta t = 0.5$	$n=10000$	2.0229	0.010014	0.91331	2.9442
DES		$n=50000$	9.6238	0.020029	4.6267	14.2705
DES		$n=100000$	19.0374	0.040058	9.4937	28.5711
PDE		$\Delta x = 0.1$				1.4220



2.2. System of equations: Multipolicy supply chains, gas dynamic equations, higher order traffic models



Multipolicy supply chains



Network Models with multiple policies

Equations: Armbruster, Degond, Ringhofer

Idea: Fluxes with higher priority (e.g. time to due-date) are preferred.

Example: $K = 2$ Y_1 (high priority)
 $Y_1 < Y_2$ Y_2 (low priority)

$$\partial_t \rho_k + \partial_x f_k = 0,$$

$$\partial_t(\rho_k Y_k) + \partial_x f_k Y_k = 0,$$

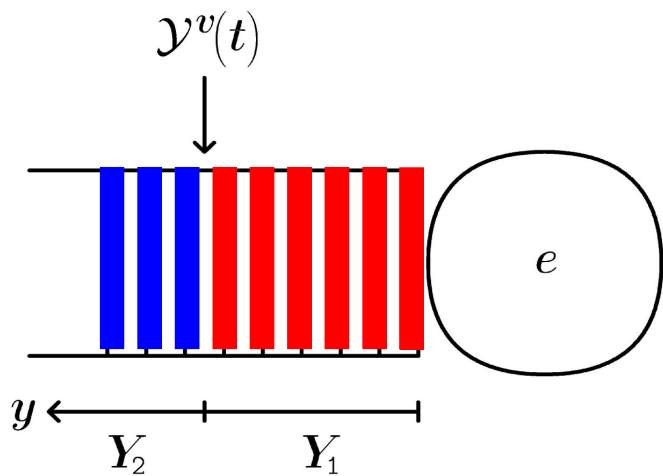
1. If $\mu < \rho_1 v_1$, then $f_1 = \mu$ and $f_2 = 0$.
2. If $\rho_1 v_1 < \mu < \rho_1 v_1 + \rho_2 v_2$, then $f_1 = \rho_1 v_1$ and $f_2 = \mu - \rho_1 v_1$.
3. If $\rho_1 v_1 + \rho_2 v_2 \leq \mu$, then $f_k = \rho_k v_k$, $k = 1, 2$.



Network Models with multiple policies

Idea: Use above equations to describe dynamics inside a processor and define coupling conditions using queues as before.

New: Introduce a pointer-function $\mathcal{Y}^\nu(t)$ which indicates the lowest priority which is still processed on the outgoing processor.



$$\mathcal{Y}^\nu(t) = \begin{cases} Y_1 & \text{if } q_1^e(t) \neq 0 \text{ or if } \mu^e < f_1^{e-1}(x_\nu^{e-1}, t) \\ Y_2 & \text{if } q_1^e(t) = 0, q_2^e(t) \neq 0 \text{ or if } \\ & f_1^{e-1}(x_\nu^{e-1}, t) < \mu^e \leq f_1^{e-1}(x_\nu^{e-1}, t) + f_2^{e-1}(x_\nu^{e-1}, t) \\ \infty & \text{if } q_1^e(t) = q_2^e(t) = 0 \text{ and if } f_1^{e-1}(x_\nu^{e-1}, t) + f_2^{e-1}(x_\nu^{e-1}, t) \leq \mu^e \end{cases}$$

Gas /Water



Gas Networks

Isothermal Euler equations with friction

$$\begin{aligned}\partial_t \rho_j + \partial_x(\rho_j u_j) &= 0, \\ \partial_t(\rho_j u_j) + \partial_x(\rho_j u_j^2 + a^2 \rho_j) &= -f_g \frac{q_j |q_j|}{2D \rho_j}.\end{aligned}$$

or without friction

$$\partial_t U_j + \partial_x F(U_j) = 0,$$

with

$$U_j = \begin{pmatrix} \rho_j \\ q_j \end{pmatrix}, \quad F(U_j) = \begin{pmatrix} q_j \\ q_j / \rho_j + a^2 \rho_j \end{pmatrix}.$$

Water: St. Venant

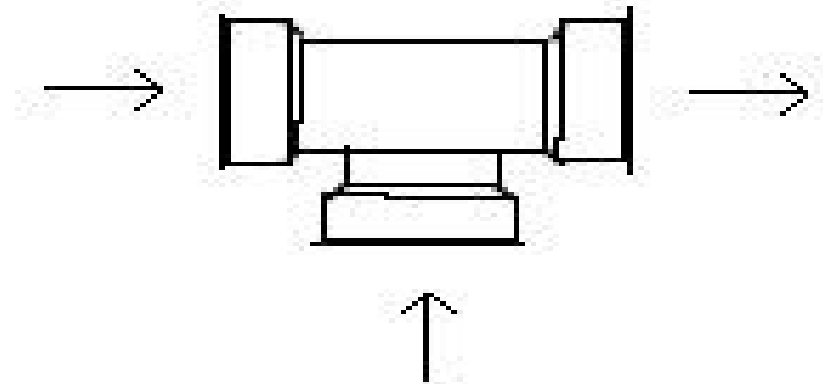


Gas network model: Coupling conditions I

Equality of fluxes:

$$\sum_{j=1 \dots n} q_j(b_j, t) = \sum_{j=n+1 \dots m} q_j(a_j, t).$$

Further conditions are necessary!



Gas network model: Coupling conditions II

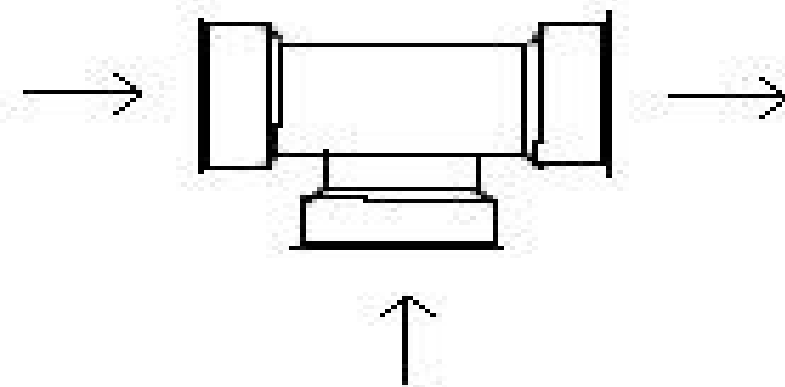
Equality of pressure at the vertex:

$$a^2 \rho_j = a^2 \rho_{j'}.$$

Equality of momentum (not physical)

Partial conservation of momentum

Engineering approach: Minor losses in pressure



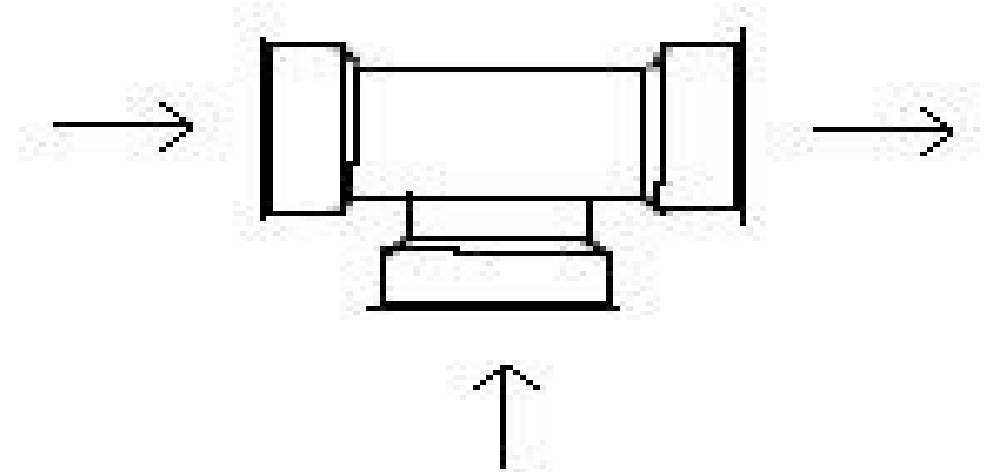
Theorem (special cases):

Consecutive pipes 1,2. Under suitable conditions (subsonic) there exists a unique weak entropic solution $U_j(x, t), j = 1, 2$ with the following properties

1. Equality of fluxes is satisfied for all times $t > 0$, at the vertex, $q_1(b_1, t) = q_2(a_2, t)$.
2. Pressure equality $a^2 \rho_1(b_1, t) = a^2 \rho_2(a_2, t)$.
3. The flux at the interface $q_1(b_1, t)$ is maximal subject to the other two conditions



General theorem



Colombo, Herty et al.

includes

equality of pressure (subsonic), equality of momentum,...



Discussion

Remark: In contrast to traffic networks the distribution of flow for a dispersing junction can not be chosen, but is implicitly given.

Remark: Engineers do not care too much about the above considerations!

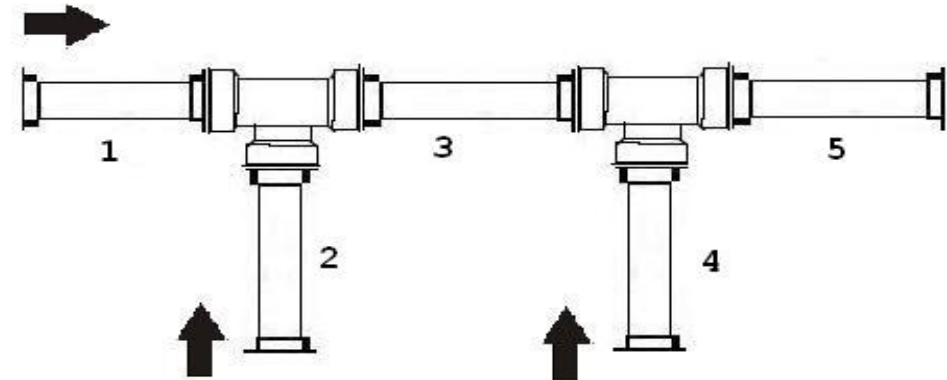
For real world applications the pressure at the vertex is reduced by so called minor losses. This is modelled by a pressure drop factor depending on geometry, flow and density at the intersection.

Realistic coupling conditions by 3-D simulations



Example: Numerical Results

Equality of pressure



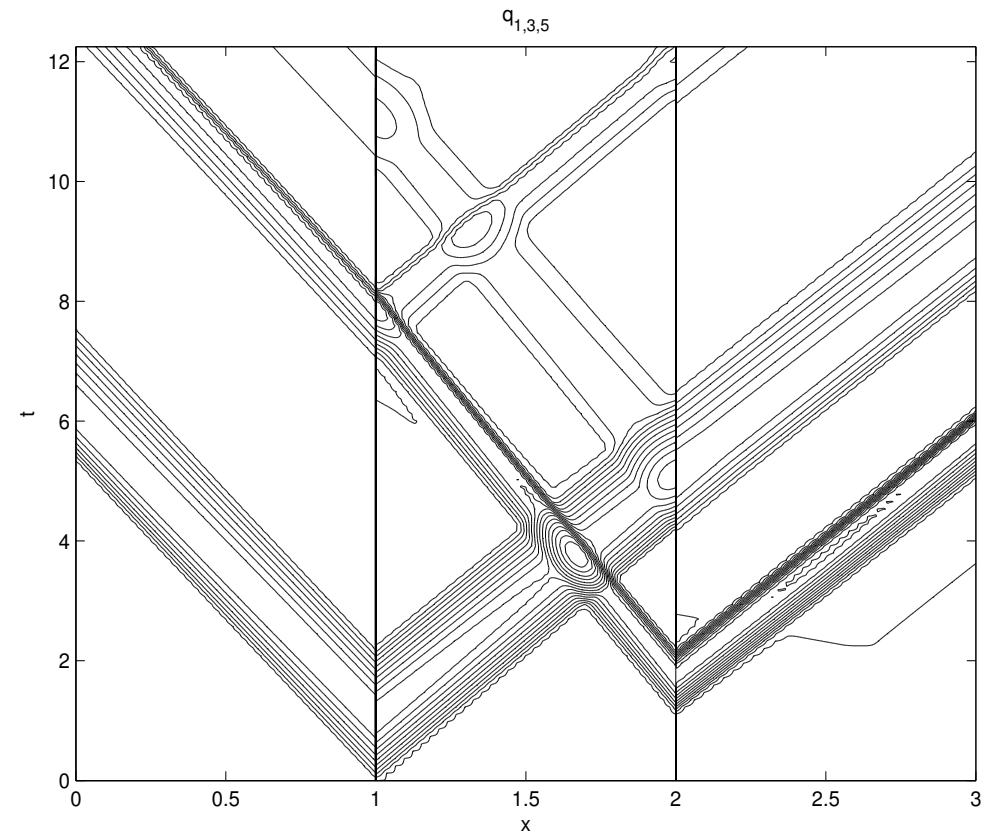
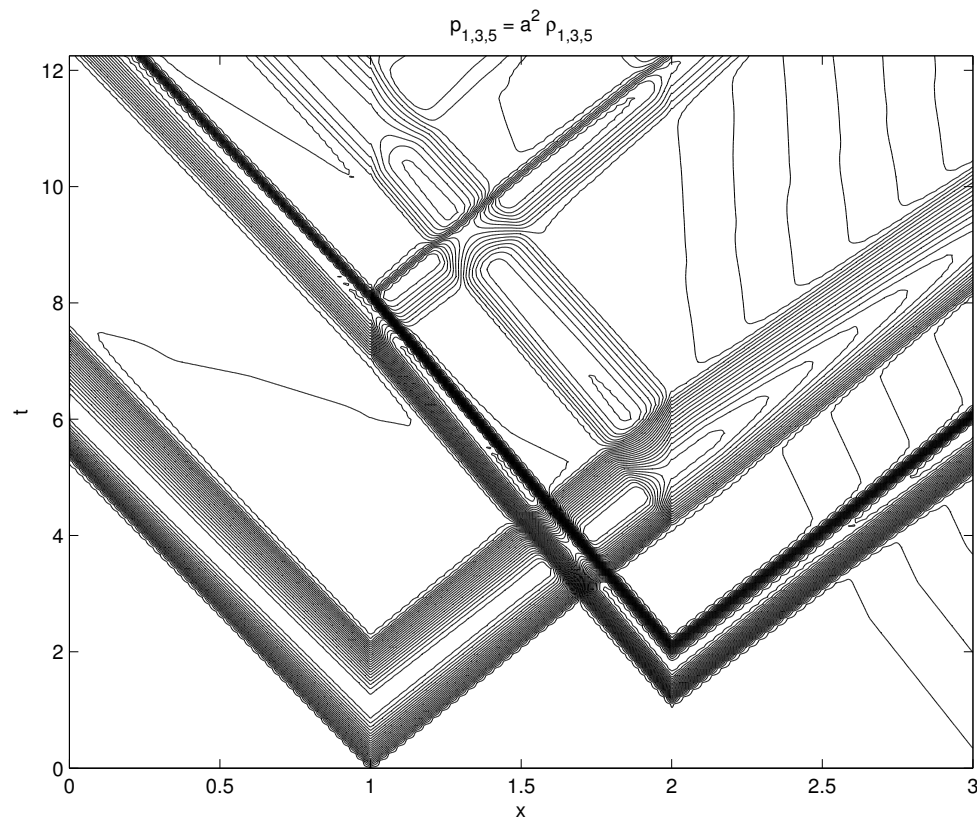
Pressure increase on the two vertical pipes 2 and 4

$$U_2^0(x) = \begin{cases} (4, 2) & x < \frac{1}{2} \\ (4 + \frac{1}{2} \sin(\pi(2x - 1)), 2) & x > \frac{1}{2} \end{cases}$$

$$U_4^0(x) = \begin{cases} 4 + \frac{1}{2} \sin(4\pi(x - \frac{1}{4})), 2 & \frac{1}{2} < x < \frac{3}{4} \\ (4, 2) & \text{else} \end{cases}$$

Initial conditions on pipes 1, 3, 5 are $(4, 2)$, $(4, 4)$, $(4, 6)$.

Numerical Results



Extension: Water network including surface flow

Network flow:

St. Venant equations

Surface flow:

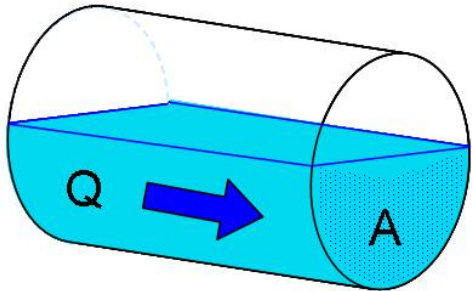
2-D Shallow Water equations



Example: Water network including surface flow

Network flow: St. Venant equations

$$\partial_t A + \partial_x Q = 0$$



$$\partial_t Q + \partial_x \left(\frac{Q^2}{A} + p(A, r) \right) = 0$$

Surface flow: 2-D Shallow Water equations

$$\partial_t h + \partial_x (hu) + \partial_y (hv) = S_c^1$$

$$\partial_t (hu) + \partial_x \left(hu^2 + \frac{g}{2} h^2 \right) + \partial_y (huv) = S_c^2$$

$$\partial_t (hv) + \partial_x (huv) + \partial_y \left(hv^2 + \frac{g}{2} h^2 \right) = S_c^3$$

Example: Water network including surface flow

Coupling in the network:

Equal heights

$$\begin{aligned} h(A_1) &= h(A_2) \\ &\vdots \\ h(A_{n-1}) &= h(A_n) \end{aligned}$$

Conservation of mass

$$\sum_{i=1}^n Q_i = -Q_D + S_C$$

Dropshaft equation

$$Q_D = |A_J| \partial_t h(A_1)$$

store mass

A_J : Dropshaft cross section



Example: Water network including surface flow

Coupling the network to the surface:

In the network

$$S_C = \gamma \int_{A_J} \left(h(\vec{x}, t) - |h(A_1(0, t)) - d|_+ \right) d\vec{x}$$

On the surface

mass

$$S_c^1 = -\gamma \chi_J \left(h(\vec{x}, t) - |h(A_1(0, t)) - d|_+ \right)$$

(conserved)

momentum

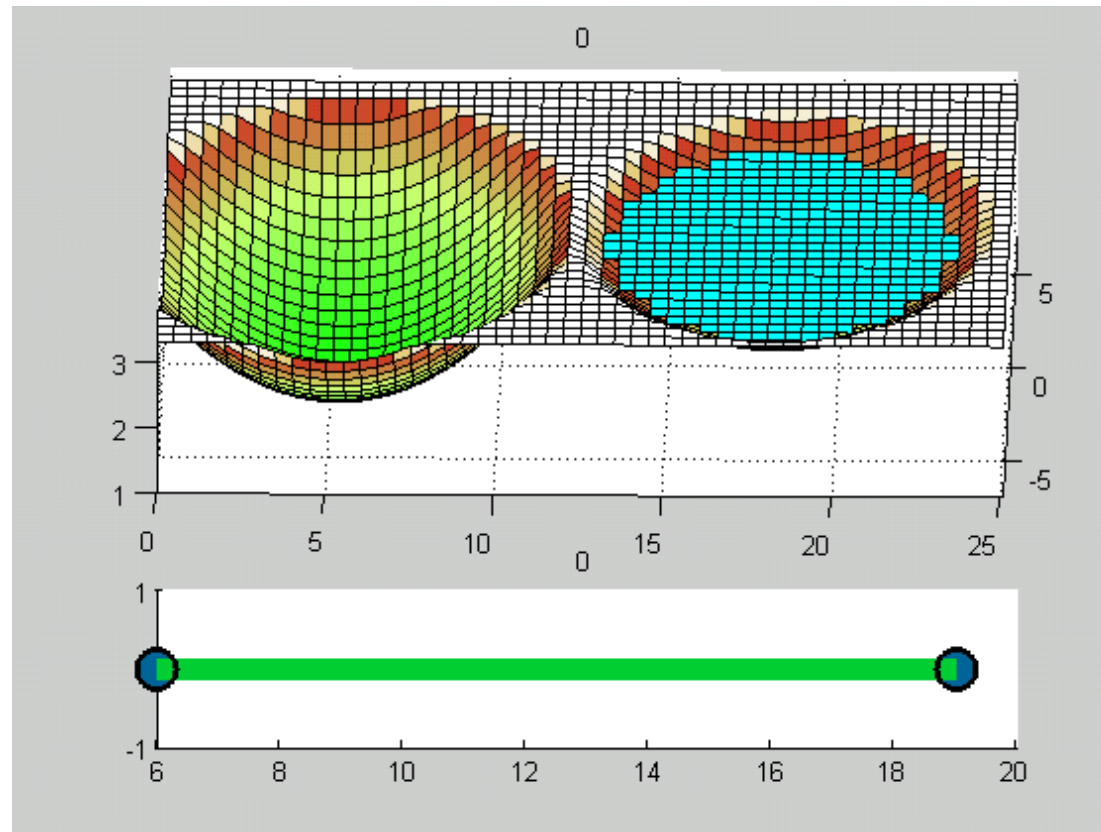
$$S_c^2 = -\gamma \chi_J \left| h(\vec{x}, t) - |h(A_1(0, t)) - d|_+ \right|_+ u(\vec{x}, t)$$

(not conserved)

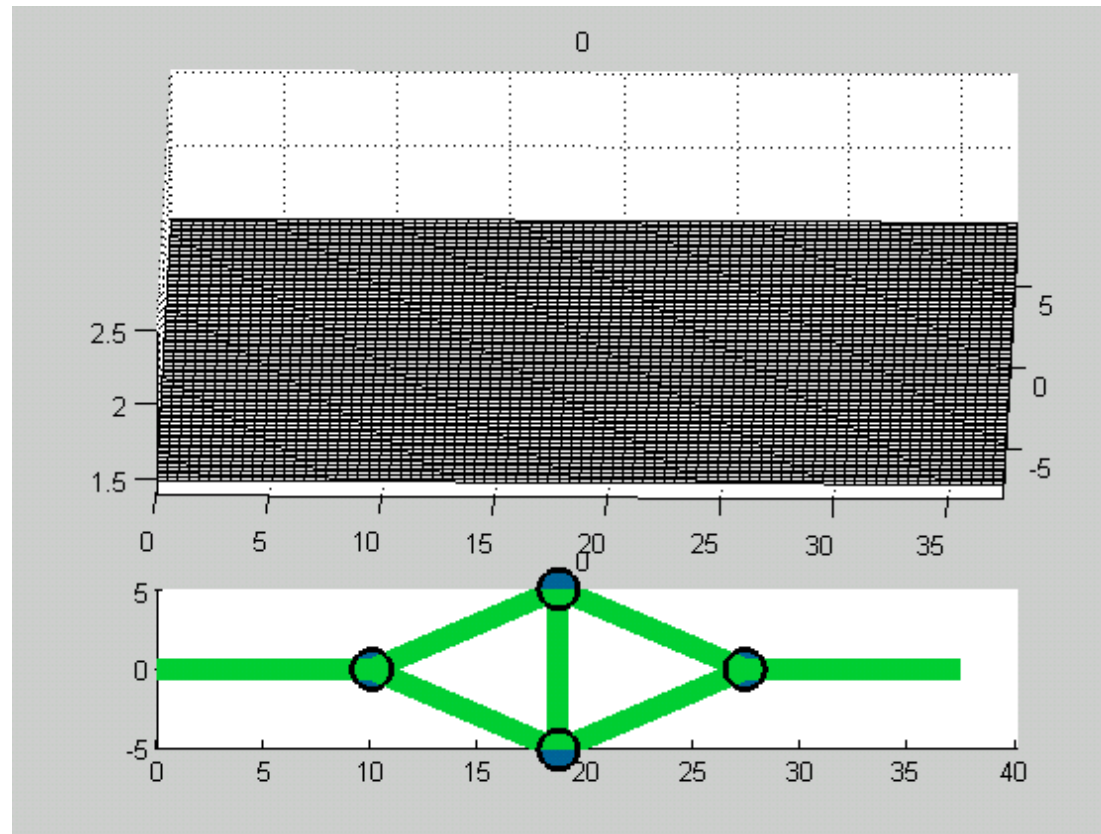
$$S_c^3 = -\gamma \chi_J \left| h(\vec{x}, t) - |h(A_1(0, t)) - d|_+ \right|_+ v(\vec{x}, t)$$



Numerical example 1: Two connected pools (R. Borsche)



Example 2: Diamond under street (R. Borsche)



Traffic flow



Higher order traffic models

Discussion of Riemann problems at the junction

Herty, Rascle

Garavello, Piccoli

Expensive for large networks compared to Lighthill-Whitham



3. Simplified network models

Traffic: Simplified model

Model 1: ODE

3-point discretization of hyperbolic problem \Rightarrow

$$\begin{aligned}\partial_t \rho_j^{(a)}(t) &= -\frac{2}{L} \left(f_j(\rho_j(m, t)) - f_j(p_j^a(t)) \right) \\ \partial_t \rho_j^{(b)}(t) &= \frac{2}{L} \left(f_j(\rho_j(m, t)) - f_j(p_j^b(t)) \right)\end{aligned}$$

with

$$\rho_j^{(a)}(t) \sim \frac{2}{b-a} \int_a^m \rho_j(x, t) dx: \text{ average density}$$

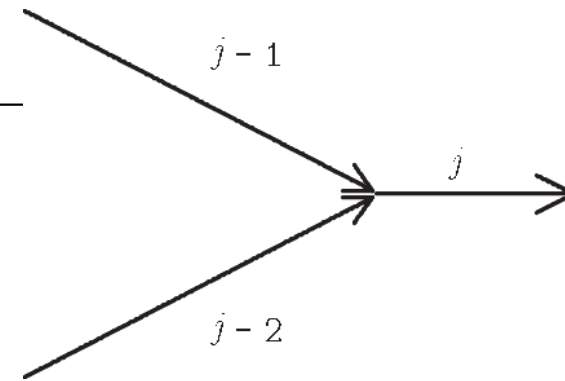
$$\rho_j(m, t) \sim \frac{1}{2} \left(\rho_j^{(a)}(t) + \rho_j^{(b)}(t) \right): \text{ density at mid-point}$$

$$p_j^{a/b}(t) \text{ density at endpoint given by coupling conditions)}$$



Traffic: Simplified models

Model 2: Algebraic model



Track waves to obtain nonlinear system of equations, compute/approximate arrival times of waves at junctions

$$t_j = \left(t_l + \frac{L_l}{s_l}\right) \frac{\rho_{l,0}}{\rho_{l,0} + \rho_{k,0}} + \left(t_k + \frac{L_k}{s_k}\right) \frac{\rho_{k,0}}{\rho_{k,0} + \rho_{k,0}},$$
$$s_j = \frac{f(\rho_j)}{\rho_j}.$$

Approximation of arrival times for a junction with two ingoing and one outgoing road (single ingoing wave)



Supply chains

See section on optimization



Gas/water networks

Hierarchy of simplified equations

Shallow water equations

Neglecting nonlinear terms (inertia) and gravity

Stationary models / pressure drop (algebraic models)

Improved algebraic models



Water networks

Shallow water equations

$$\begin{aligned}0 &= \frac{\partial \varrho}{\partial t} + \frac{\partial q}{\partial x} \\0 &= \frac{\partial q}{\partial t} + \frac{\partial}{\partial x} \left(\frac{q^2}{\varrho} + p \right) + g\varrho \frac{dh(x)}{dx} + \frac{\lambda(q)}{2D} \frac{|q|q}{\varrho} \\ \varrho &= \frac{M}{RT} \frac{p}{z(p, T)}\end{aligned}$$



Gas/water networks

Neglecting nonlinear terms (inertia) and gravity and time derivative for q

$$0 = \frac{\partial}{\partial t} \frac{p}{z(p, T)} + \frac{RT}{M} \frac{\partial}{\partial x} q$$
$$0 = \frac{p}{z(p, T)} \frac{\partial}{\partial x} p + \frac{RT}{2DM} \lambda(q) |q| q .$$

Integrating the second equation over the whole length L of the pipe finally yields:



Gas/water networks

Stationary models /pressure drop equations (algebraic models)

$$F(p_0) - F(p_L) = \frac{RTL}{2DM} \lambda(q) |q| q .$$

with

$$F(p) = \int^p \frac{\varphi}{z(\varphi, T)} d\varphi .$$

Further approximations yield the pressure drop equation:

$$\text{sign}(q) |q|^{b_q} = ap_0^{b_0} - bp_L^{b_L} .$$



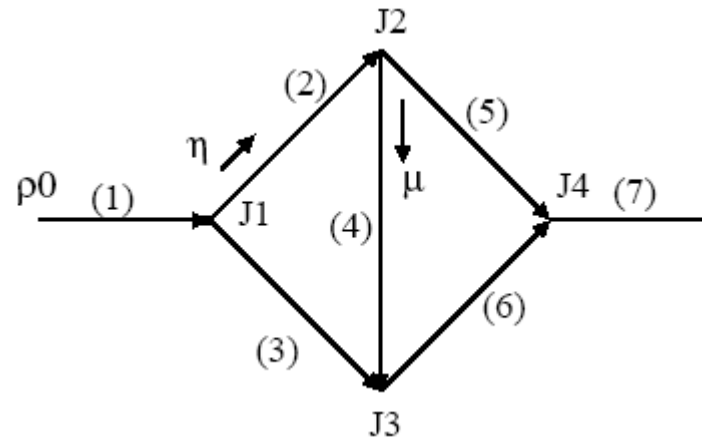
4. Optimization and control

4.1 Continuous approaches

Traffic Flow



Traffic flow networks



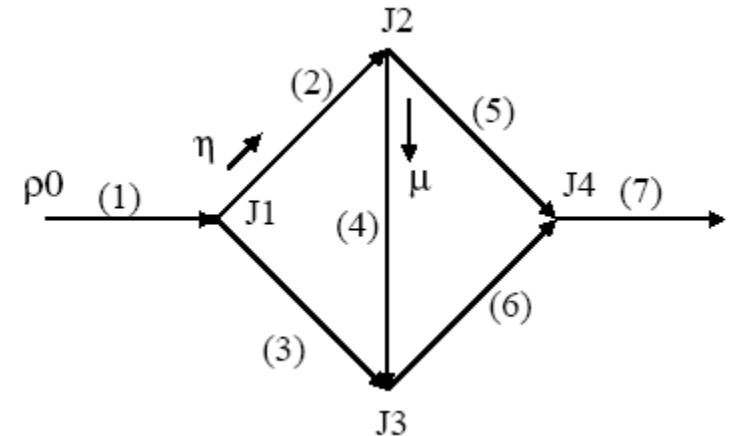
Goal: Optimization of outgoing flow (i.e. flux on road (7))

Method:

Distribute traffic at the junctions (J_1, J_2) in a suitable way

Traffic: Optimization of PDE model

$$J_1 : \eta = \eta(t), \quad J_2 : \mu = \mu(t)$$



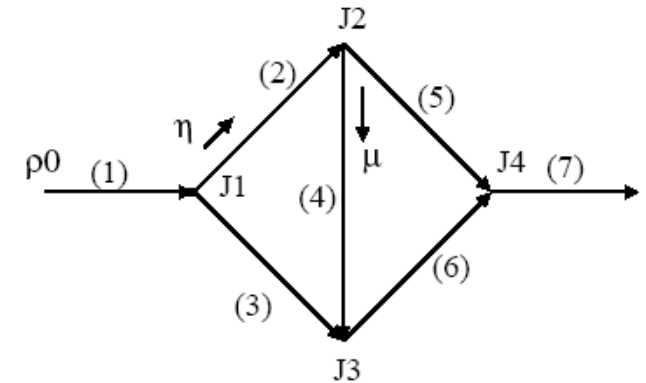
$$G(\mu, \eta) = \sum_{j=1}^J \int_0^T \int_{a_j}^{b_j} \rho_j(t, x) dt dx \rightarrow \min$$

subject to $(\mu, \eta) \in (0, 1) \times (0, 1)$



Traffic: Optimization of PDE model

Numerical solution: Front tracking algorithm, Godunov
upwind discretization



Optimization: General Functional

$$\min_{A(t)} \sum \int_0^T \int_{a^e}^{b^e} \mathcal{F}(\rho^e(x, t), q^e(t)) dx dt, \quad \mathcal{F}(\rho^e, q^e) = \rho^e(x, t) + q^e(t),$$

Methods

Methods for Optimization:

1. Quasi-Newton, Finite difference approximation of functional-derivative
2. adjoint calculus, solve first order optimality system numerically, Computation of adjoint equations

Computational costs:

Adjoint calculus: similar to costs of the network simulation

Finite differences: proportional to number of control parameters times costs of the network simulation



Computation times for global optimization with adjoint approach

Model and Scheme	Parameters	CPU time
Godunov scheme for pde model	N=100	135.65 s
Godunov scheme for pde model	N=50	45.17 s
ODE-Model (2-point discretization)	N=3	3.39 s

Improved optimization procedures:

Instantaneous control: use only solution at the next time step
to optimize the system



Comparison for example network

Differences of the simplified (algebraic) model to PDE model:

See later

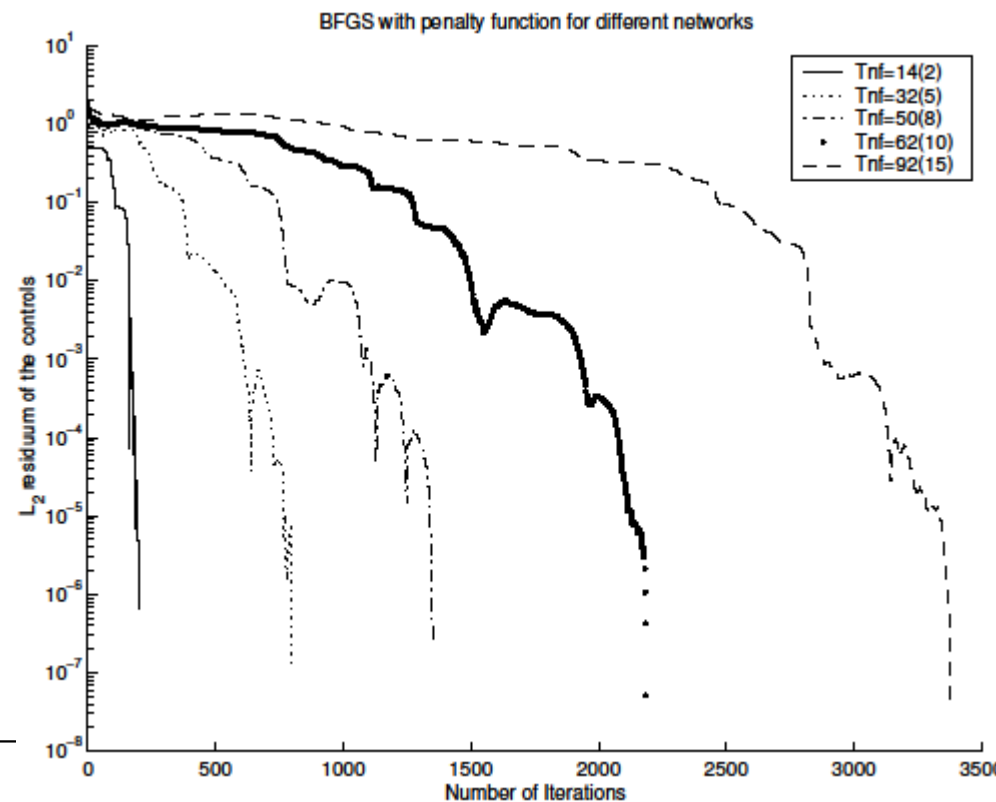
Computation times:

PDE, Discrete Differences with Godunov Scheme	N=100	135.655s
PDE, Discrete Differences for Front-Tracking	mk=25	45.172s
PDE, Discrete Differences with Godunov Scheme	N=50	45.172s
ODE Model	N=100	7.753s
PDE, Discrete Differences for Front-Tracking	mk=5	6.183s
ODE Model	N=50	3.391s
Algebraic model		0.149s



Large Networks

Convergence history for algebraic model with \$2\$ to \$15\$ junctions

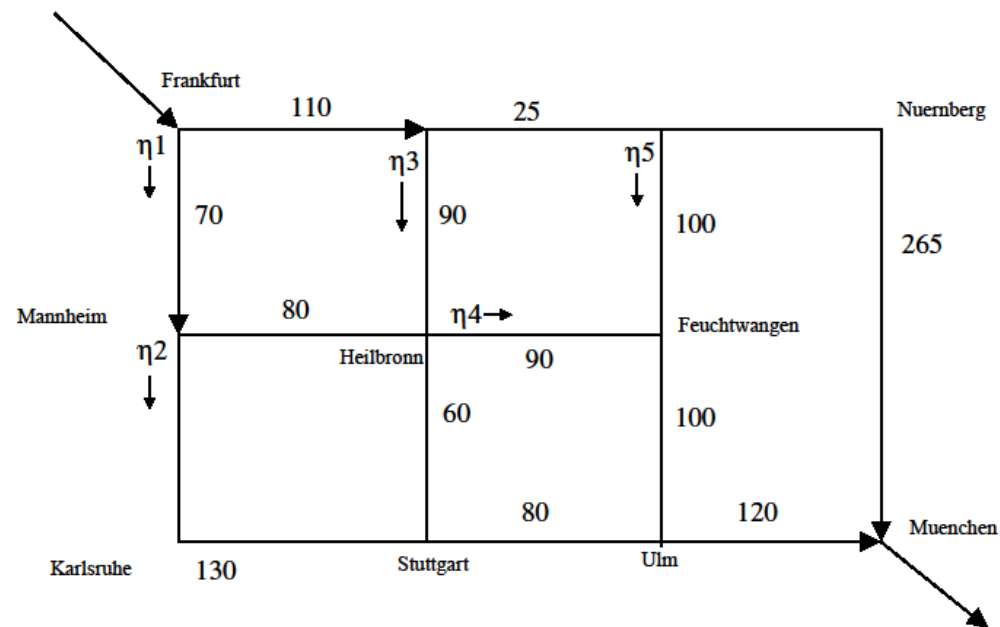


Further Example

"Realistic" network (Frankfurt - München)

Congestion between Mannheim and Stuttgart

Optimal parameters (free/ congested)



$$\eta_1 = 0.57 / 0.27$$

$$\eta_2 = 1.0 / 0.37$$

$$\eta_3 = 0.0 / 0.0$$

$$\eta_4 = 1.0 / 0.04$$

$$\eta_5 = 0.0 / 0.42$$

Outgoing flow (free/ congested)

$$0.74 / 0.73$$



Supply Chains



Supply chains: Optimal control problem

$$\min_{A(t)} \sum \int_0^T \int_{a^e}^{b^e} \mathcal{F}(\rho^e(x, t), q^e(t)) dx dt, \quad \mathcal{F}(\rho^e, q^e) = \rho^e(x, t) + q^e(t),$$

$$\partial_t \rho^e + v^e \partial_x \rho^e = 0, \quad v^e \rho^e(a^e, t) = \psi^e(q^e)$$

$$\partial_t q^e(t) = h^e(\rho, A) - \psi^e(q^e)$$

$$\psi^e(q^e) = \min\left\{\mu^e; \frac{q^e}{\epsilon}\right\}$$

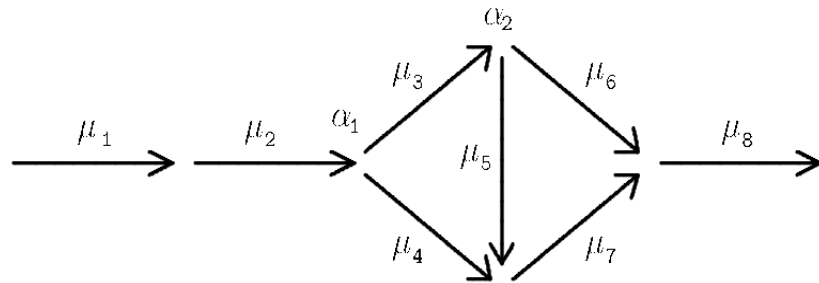
Approach: Adjoint calculus for the network system

- Derive first order optimality system
- Discretize optimality system
- Solve numerically with descent algorithm, etc.

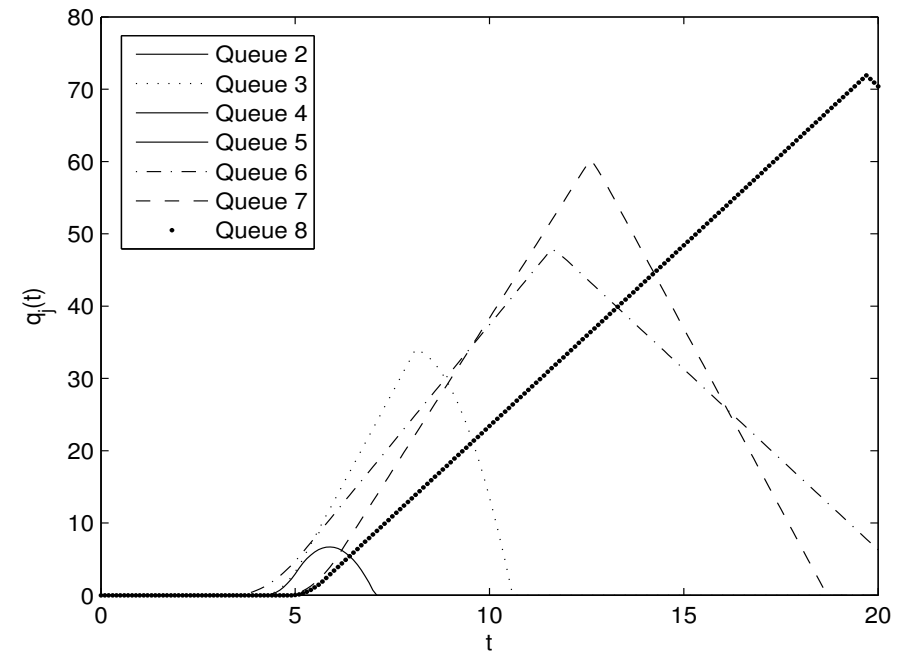
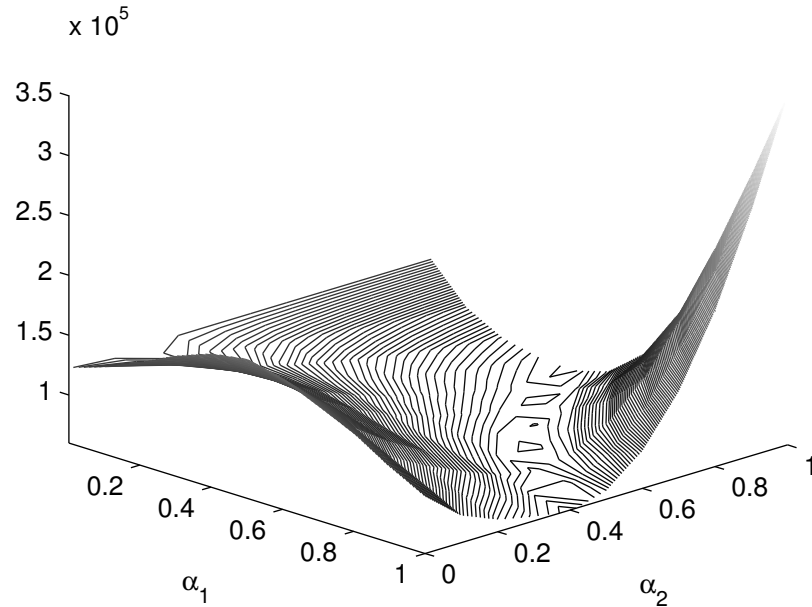


Supply chains: Optimization of PDE models

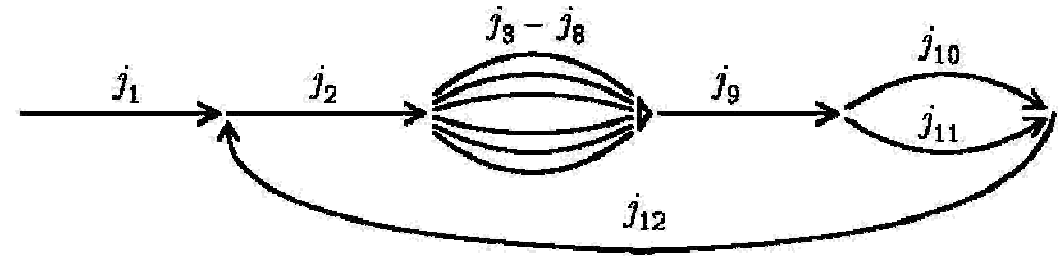
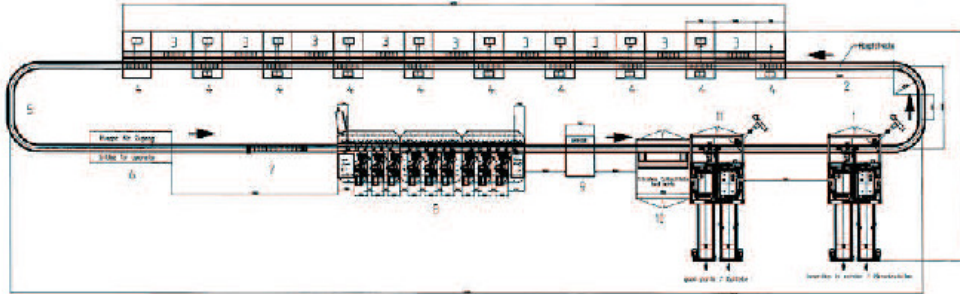
Example 1 (Optimization of distribution rates):



$$J(\vec{\alpha}, \vec{\rho}, \vec{q}) := \sum_{j=2}^8 \int_0^{T_{max}} q_j^2(t) dt,$$



Example 2 (Braun, Frankfurt)



$$\sum_t -\frac{1}{t+1} g_t^{12}$$

Processor	μ^e	v^e	L^e	\bar{q}^e
1	100	0.01333	1	100
2	0.71	0.35714	1.5	18
3 - 8	0.06666	0.01333	1	8
9	0.71	0.04762	3	1
10 - 11	0.24	0.1119	1.5	1
12	0.71	0.35714	1.5	1

Gas / Water



Optimal control of gas/water flows

Colombo, Herty,

Control for example by compressor stations

Two pipes connected with a compressor

Customers require certain pressure and flow

Control P through a modified coupling condition:

$$P = q_1 \left(\left(\frac{p(\rho_1)}{p(\rho_2)} \right)^k - 1 \right), \quad q_1 = q_2$$



4.2 Mixed-Integer, Linear Programming

Traffic



Traffic: Simplified models

Track waves to obtain nonlinear system of equations

Arrival times:

$$t_j = \left(t_l + \frac{L_l}{s_l}\right) \frac{\rho_{l,0}}{\rho_{l,0} + \rho_{k,0}} + \left(t_k + \frac{L_k}{s_k}\right) \frac{\rho_{k,0}}{\rho_{k,0} + \rho_{k,0}}, \quad s_j = \frac{f(\rho_j)}{\rho_j}.$$

Functional:

$$\sum_{j=1}^J \int_0^T \int_{a_j}^{b_j} \rho_j(t, x) dt dx = \sum_{j=1}^J (T - t_j) L_j \rho_{j,0} - \frac{\rho_{j,0}}{2s_j} L_j^2$$



Rewriting model in terms of fluxes on the arcs and Linearization gives

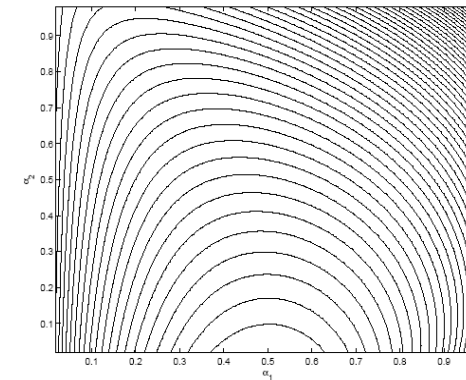
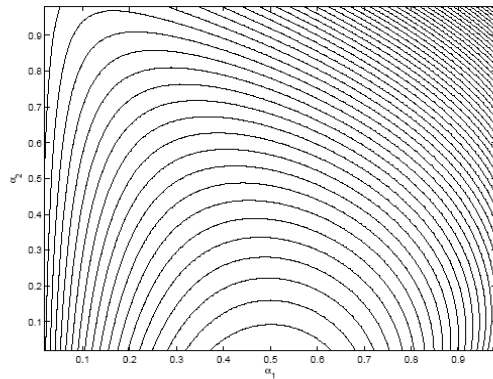
Mixed integer program (MIP)

Fast numerical treatment by combinatorial methods or CPLEX etc.

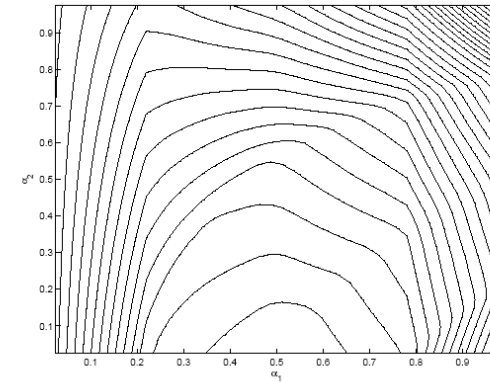
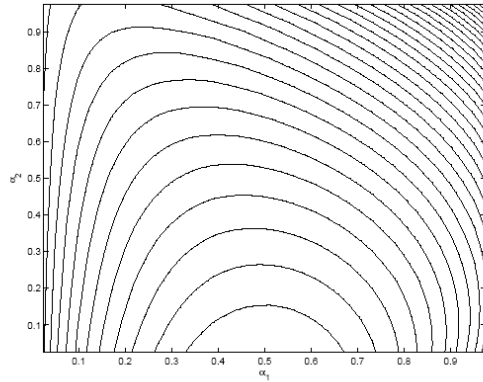


Comparison of models: **PDE** versus **MIP** for **Free Flow**

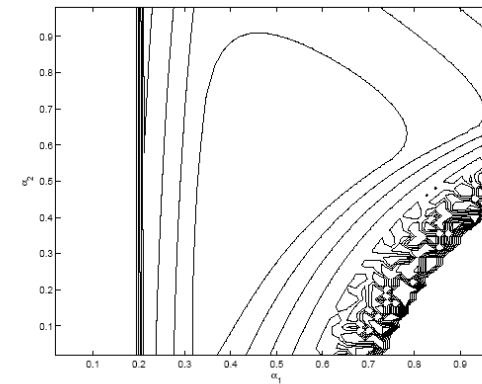
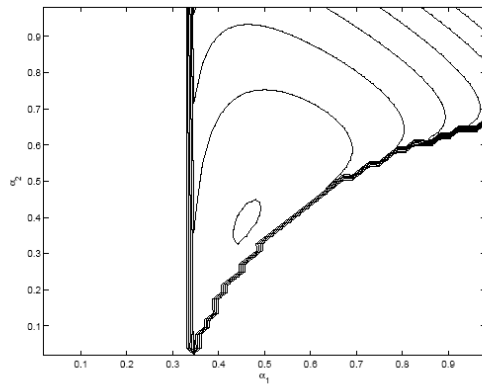
$$G(\mu, \eta) = \sum_{j=1}^J \int_0^T \int_{a_j}^{b_j} \rho_j(t, x) dt dx$$



Coarse versus fine linear discretization



PDE versus simplified model (Jam situation)

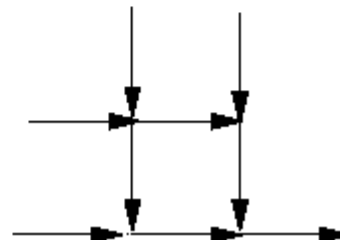
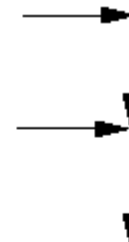
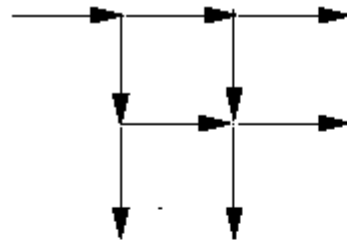


Comparison of computation times for simple network

Model and Scheme	Parameters	CPU time
Godunov scheme for pde model	$N=100$	135.65 s
Godunov scheme for pde model	$N=50$	45.17 s
ODE-Model	$N=3$	3.39 s
Simplified nonlinear model		0.05 s
Linear Model with dynamics	$D_q = D_t = 100, N_i \cdot N_j = 25$	0.02 s
Linear Model without dynamics	$D_q = 100$	0.01 s



Large networks



Computation times for large network optimization

Model	# Roads	D_q	D_t	$N_i N_j$	Gap	CPU time
Simplified nonlinear model	240	n.a.	n.a.	n.a.	n.a.	6 s
Linear with dynamics		10	10	25	1%	11 m
		10	10	25	10%	3.8 m
		10	10	9	0.1%	2.6 m
		10	10	9	10%	57 s
Linear without dynamics		100	n.a.	n.a.	0.1%	<0.01 s
Simplified nonlinear model	1'500	n.a.	n.a.	n.a.	n.a.	57 m
Linear with dynamics		10	10	25	10%	4.7 h
		10	10	9	10%	26 m
		5	5	9	10%	5 m
Linear without dynamics		1000	n.a.	n.a.	0.1%	24.98 s
		100	n.a.	n.a.	0.1%	12.75 s
		5	n.a.	n.a.	0.1%	1.8 s
Simplified nonlinear model	15'000	n.a.	n.a.	n.a.	n.a.	>4d
Linear with dynamics		5	5	9	10%	6.2 h
Linear without dynamics		100	n.a.	n.a.	n.a.	22.79 m
		10	n.a.	n.a.	n.a.	7.33 m
Linear without dynamics	150'000	10	n.a.	n.a.	n.a.	16.77 h



Supply chains

Supply chains: Simplified models

Much simpler: piecewise linear flux functions

Two point discretization yields MIP or even LP depending on the model:

Very fast algorithms for very large problems



Approach: Mixed-Integer, Linear Programming

- Simplification of the dynamics (2-point discretization on each arc)
- Linear dynamics in processor and queue yield discretized linear equations except for

$$\psi^e(q^e) = \min\left\{\mu^e; \frac{q^e}{\epsilon}\right\}$$

- Rewrite ψ using binary variables
- Discretized optimization problem is a large scale mixed-integer problem



Remarks:

- The functional needs to be linear (otherwise more binary variables are needed)
- The problem is solved using CPLEX
- Suitable preprocessing routines for CPLEX can be derived from PDE Ansatz
- Further reduction to linear programmes in special cases



Model extensions are easy in MIP formulation:

Finite size buffers

$$q_t^e \leq \text{const} , \forall e, t.$$

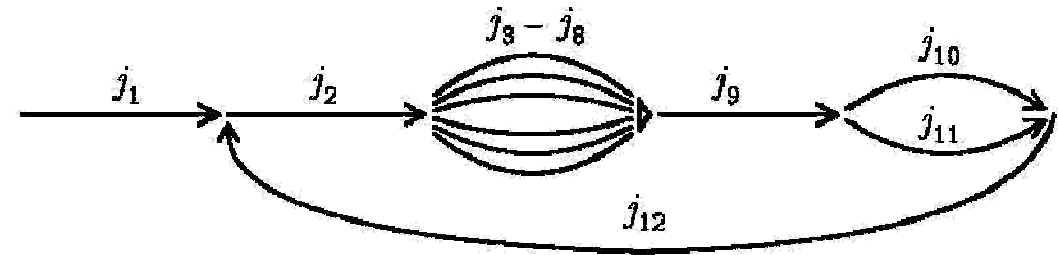
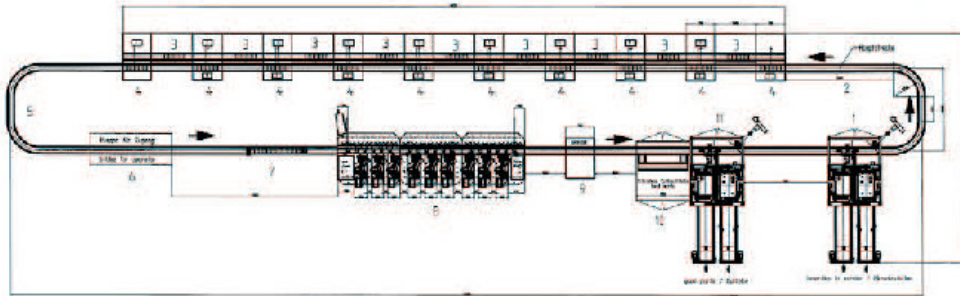
Optimal inflow profile

$$\max \sum_{e=1,t} f_t^e,$$

Maintenance shut-down



Example I (Braun, Frankfurt)



$$\sum_t -\frac{1}{t+1} g_t^{12}$$

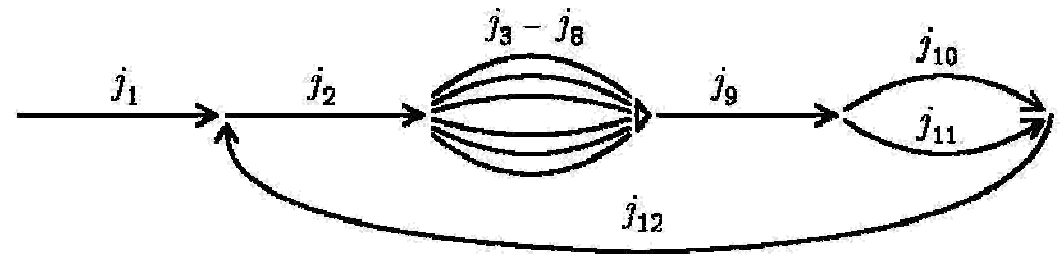
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2	0.71	0.35714	1.5	18
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9	0.71	0.04762	3	1
10 - 11	0.24	0.1119	1.5	1
12	0.71	0.35714	1.5	1



Numerical results II (Comparison of CPU times, small networks)

Comparison of MIP/CPLEX and adjoint/gradient approach

Same optimal functional value

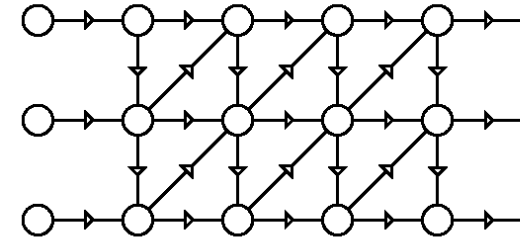


NT	Adjoint	MIP
200	7.31	5.52
400	26.10	17.06
800	45.10	68.09
2000	124.58	592.61

See following talks

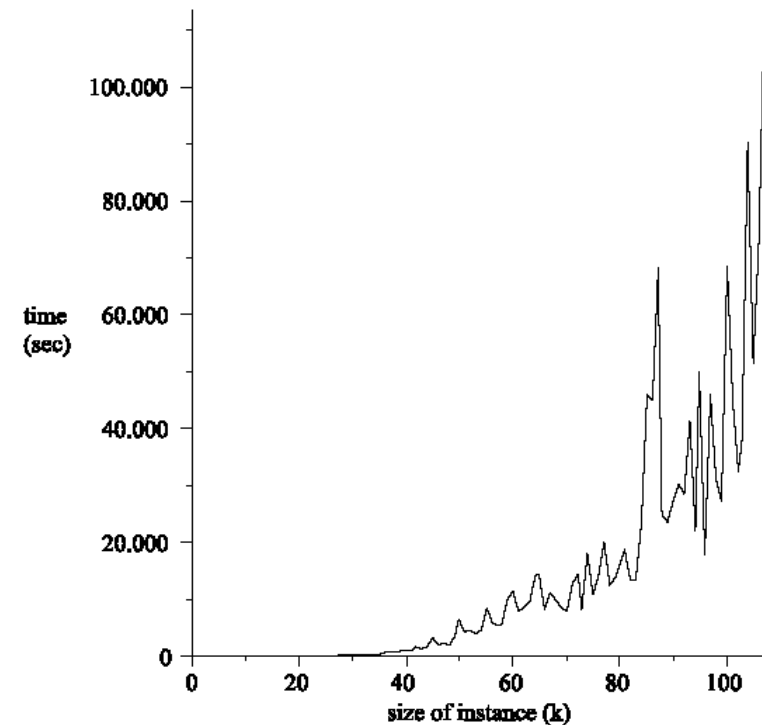
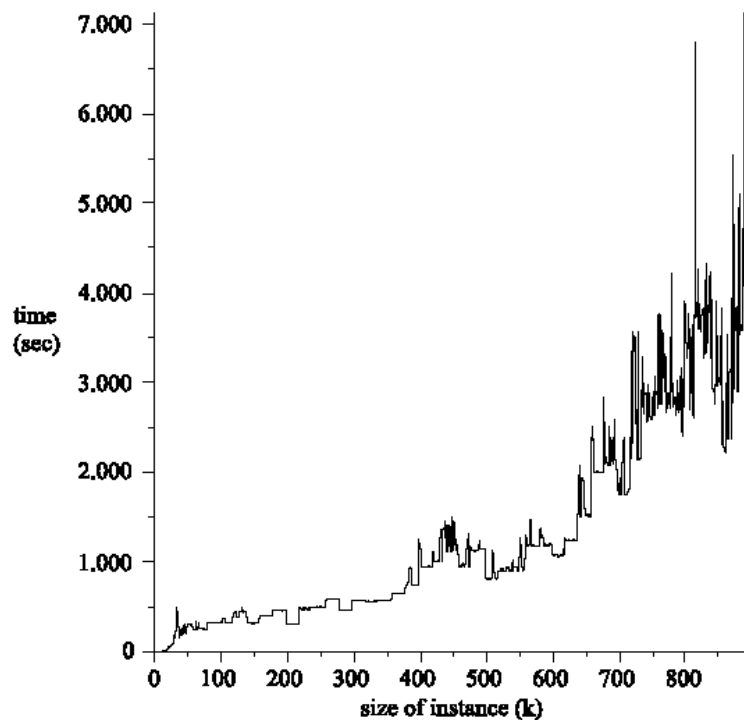


Numerical results III (Large scale, MIP, CPLEX)



„PDE solution“ not feasible

Computing times for $k \times 2$ networks with $100+k$, $100+k/20$ time steps:



Remark: LP allows for larger networks.



Gas / water



Mixed Integer Models for Gas/Water

simplified models for gas / water lead after piecewise linearization again to

Mixed integer problems



discrete optimization community

Further topics / current work:

Numerical improvements:

- Multilevel approaches, hybrid methods
- Preprocessing techniques for MIP (U. Ziegler, A. Dittel)

Extensions:

- Stochastic effects (S. Martin)
- supply chains: Nonlinear dynamics at nodes, Multi-policy networks
- gas/water: numerical realization / optimization for full problem /coupling to surface flow(R. Borsche)

