

# NONLOCAL CONSERVATION LAWS (NLCL) – MODELING, SIMULATION AND OPTIMAL CONTROL

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## Motivation and applications

- ▶ Main applications:
  - ▶ traffic flow: adjusting velocity of flow at a current location based on the foregoing traffic situation.
  - ▶ chemical engineering: growing of particles depending on the surface area or concentration of synthesized products.
- ▶ Temporal development of the state in the given spatial variables (also in the broad sense) depending on the information on the whole considered domain.
- ▶ Further applications: crowd dynamics, pedestrian flow, sedimentation processes, opinion formation, supply chains, etc.

## Mathematical models: NLCL on $\mathbb{R}^n$ ...

For  $(t, \mathbf{x}) \in (0, T) \times \mathbb{R}^n$ ,  $n \in \mathbb{N}_{\geq 1}$  and  $T \in \mathbb{R}_{>0}$

$$q_t(t, \mathbf{x}) + \operatorname{div}_{\mathbf{x}} \left( \lambda \left[ W[q, \gamma, \mathcal{A}] \right] (t, \mathbf{x}) q(t, \mathbf{x}) \right) = h(t, \mathbf{x}) + g(t, \mathbf{x}) q(t, \mathbf{x})$$

$$q(0, \mathbf{x}) = q_0(\mathbf{x})$$

$$W[q, \gamma, \mathcal{A}](t, \mathbf{x}) := \iint_{\mathcal{A}(t)} \gamma(t, \mathbf{x}, \mathbf{y}) q(t, \mathbf{y}) d\mathbf{y}$$

$$\lambda[w](t, \mathbf{x}) := \lambda(w(t, \mathbf{x}), t, \mathbf{x}).$$

### Description of terms

- ▶  $q$ : traffic density, particle size distribution (PSD), etc.
- ▶  $q_0$ : initial datum.
- ▶  $\lambda$ : velocity function, growth function (in particle synthesis).
- ▶  $W$ : nonlocal impact (look ahead behavior, mass of particles, etc.).
- ▶  $\gamma$ : nonlocal weight.
- ▶  $g$ : damping term (rate of vehicles on highway exits, outflow rate of particles, etc.).
- ▶  $h$ : further source/sink term (vehicles on highway access, inflow of new nuclei, etc.).
- ▶  $\mathcal{A}$ : nonlocal integration area. For  $K \in \mathbb{R}_{>0}$  be  $\mathcal{A} \in C([0, T]; \mathcal{M}_K^n)$  with

$$\mathcal{M}_K^n := \{ \mathcal{B} \in \mathcal{M}^n : \mathcal{H}^{n-1}(\partial \mathcal{B}) \leq K \}$$

and  $\mathcal{M}^n$  the set of all Lebesgue measurable subsets in  $\mathbb{R}^n$  which are bounded or whose complement is bounded.

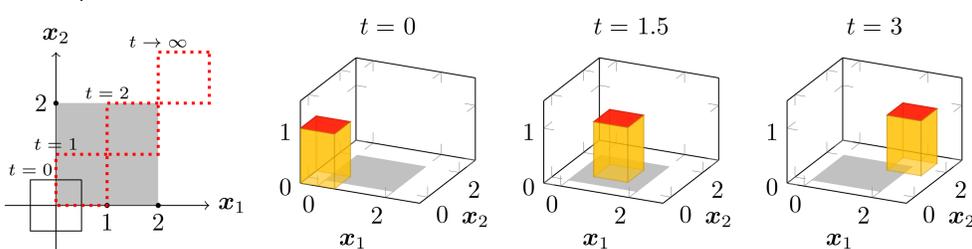


Figure 1: Graphical illustration of the nonlocal impact. Here, the speed of a generic cuboid moving in diagonal direction linearly depends on the partial volume of the cuboid located over the gray area. The motion can be described by an appropriate NLCL. **Left:** Development from the top. **Remaining:** Development from the side (cf. [3]).

## ... and on bounded domains in $\mathbb{R}$

For  $(t, x) \in (0, T) \times (0, 1)$ , and  $T \in \mathbb{R}_{>0}$

$$q_t(t, x) = -\partial_x \left( \lambda \left[ W[q, v, \gamma_\eta] \right] (t, x) q(t, x) \right)$$

$$q(0, x) = q_0(x)$$

$$\lambda \left[ W[q, v, \gamma_\eta] \right] (t, 0) q(t, 0) = \lambda \left[ W[q, v, \gamma_\eta] \right] (t, 0) u(t)$$

$$W[q, v, \gamma_\eta](t, x) := \int_x^{x+\eta} \gamma_\eta(t, x, y) \begin{pmatrix} q(t, y) & y \in (0, 1) \\ v(t, y) & \text{else} \end{pmatrix} dy$$

### Further explanations and comments

- ▶  $\eta$ : nonlocal reach (view horizon).
- ▶  $u$ : boundary datum (inflow of new vehicles at beginning of road).
- ▶ Integration area in nonlocal term depending on  $x$ .
- ▶ Nonnegative velocity function  $\lambda$ . Thus, upper boundary condition more general than assuming  $q(t, 0) = u(t)$  and no boundary condition in  $x = 1$  to be prescribed. However,  $v$  determining the velocity of the outflow represents a kind of "boundary condition".

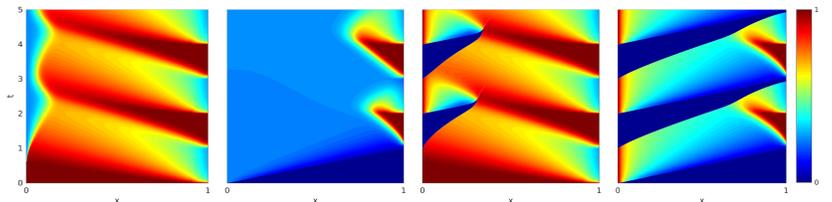


Figure 2: Simulation of different traffic scenarios with Greenshields' flux function  $\lambda[w] \equiv 1 - w$ ,  $v$  representing traffic lights on the right end, green only for  $t \in (1, 2) \cup (3, 4)$ , and a given  $\gamma_\eta$ . **From left to right:**  $(q_0, u) = (1, \frac{1}{4})$ ,  $(q_0, u) = (0, \frac{1}{4})$ ,  $(q_0, u) = (1, 1 - v)$  and  $(q_0, u) = (0, 1 - v)$  (cf. [4]).

## Analytical properties

- ▶ No fully local behavior anymore, i.e., solution has to be known on the nonlocal integration area to process in time.
- ▶ Still finite propagation of mass but infinite information flow.
- ▶ None of the usual existence results (Kruřkov, etc.) applicable.
- ▶ Existence of weak solutions provable by a fixed-point argument in the nonlocal term.
- ▶ No Entropy condition required for uniqueness.
- ▶ Additional conditions on data can guarantee existence of solution on any finite time horizon (maximum principle, etc.).
- ▶ No smoothing of solutions (as with Kruřkov, i.e., in contrast to the regularizing effect to solutions of local conservation laws for positive times), thus preservation of regularity.
- ▶ IBVP: very good approximation of the Lighthill–Whitham–Richards traffic flow model, significantly more reasonable due to the look ahead behavior.

## Optimal control in chemical engineering

- ▶ Optimization of cost functionals depending on the solution of NLCL.
- ▶ Controls as time-dependent process conditions: temperature profiles, inflow/outflow rates,...
- ▶ Cost functionals: minimizing the difference between the resulting particle size distribution (PSD) and a target PSD, minimizing the relative standard deviation, maximizing the yield,...
- ▶ Model- and gradient-based optimization possible due to a differentiable numerical scheme.

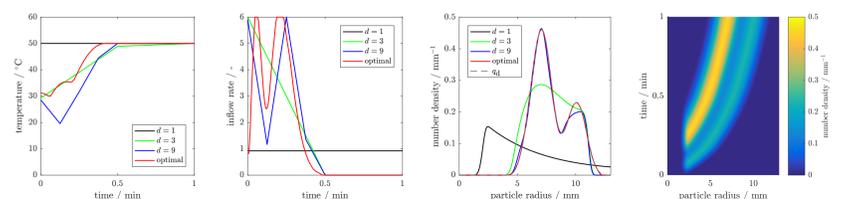


Figure 3: Final time  $L^2$ -tracking of fluidized bed spray granulation process with monomodal initial datum and bimodal target by adjusting process temperature and inflow rate. **From left to right:** optimization of controls for different degrees of freedom  $d$ , final PSD and top view of temporal development of the solution (cf. [6]).

## Ongoing and further research

- ▶ Convergence of solutions of NLCL to local conservation laws (see the poster *The singular limit of nonlocal conservation laws to local conservation laws* by Coclite et al. and [1]).
- ▶ NLCL incorporating time delays for encoding data, e.g., of routing apps.
- ▶ NLCL with feedback terms for synthesis processes with residence time distribution reactors.
- ▶ Nonlocal (non mass preserving) transport equations.

## Selected publications

- [1] Coclite, G. M., Coron, J. M., De Nitti, N., Keimer, A., & Pflug, L. (2020). A general result on the approximation of local conservation laws by nonlocal conservation laws: The singular limit problem for exponential kernels. ArXiv preprint: 2012.13203.
- [2] Keimer, A., & Pflug, L. (2017). Existence, uniqueness and regularity results on nonlocal balance laws. *Journal of Differential Equations*, 263(7), 4023-4069.
- [3] Keimer, A., Pflug, L., & Spinola, M. (2018). Existence, uniqueness and regularity of multi-dimensional nonlocal balance laws with damping. *Journal of Mathematical Analysis and Applications*, 466(1), 18-55.
- [4] Keimer, A., Pflug, L., & Spinola, M. (2018). Nonlocal scalar conservation laws on bounded domains and applications in traffic flow. *SIAM Journal on Mathematical Analysis*, 50(6), 6271-6306.
- [5] Spinola, M., Keimer, A., Segets, D., Leugering, G., & Pflug, L. (2020). Model-based optimization of ripening processes with feedback modules. *Chemical Engineering & Technology*, 43(5), 896-903.
- [6] Spinola, M., Keimer, A., Segets, D., Pflug, L., & Leugering, G. (2020). Modeling, Simulation and Optimization of Process Chains. In *Dynamic Flowsheet Simulation of Solids Processes* (pp. 549-578). Springer, Cham.

