Optimal Control of Macroscopic Models for Phase Transitions

Sven-Joachim Kimmerle

Institute of Mathematics and Computer Applications
Department of Aerospace Engineering
University of the Federal Armed Forces Munich
sven-joachim.kimmerle@unibw.de

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Motivation

Phase transitions

(-) Destroy material properties
(+ ) Possibility to design materials

Example: Final heat treatment in the production of GaAs \((Dreyer, Duderstadt ’08)\)

► Unwanted droplets precipitate
► Large droplets grow, small droplets shrink
► Goal: Control resulting droplet distribution by temperature

Example: Ageing of polymers \((Lion, Johlitz 2012)\)

► Thermooxidative processes enhance decomposition of polymer chains
► Cross-linking processes in the polymer network
► Goal: Control resulting fraction of intact polymer by injection of ageing inhibition chemicals
Models for phase transitions - Hierarchy

**Models for phase transitions**

**Continuum models**
- Phase field (/Diffuse-interface) models
  - Allen-Cahn
  - Cahn-Hilliard
- Sharp-interface models
  - Mullins-Sekerka, vol.-diffusion/interf.-reaction regime, conserv. total mass/volume

**Atomic models**
- Becker-Döring

**Macroscopic models**
- (in)homogeneous Lifshitz-Slyozov(-Wagner), volume-diffusion regime
  interface-reaction regime

Homogenization limit
Models for phase transitions - with control

Models for phase transitions

Continuum models
- Phase field (Diffuse-interface) models
  - Allen-Cahn (Farshbaf-Shaker)
  - Cahn-Hilliard (Hintermüller & Wegner)
- Sharp-interface models
  - Mullins-Sekerka, vol.-diffusion/interf.-reaction regime, conserv. total mass/volume

Atomic models
- Becker-Döring

Macroscopic models
- (in)homogeneous Lifshitz-Slyozov(-Wagner), interf.-reaction regime, ...
LSW model with mechanics

(Dis-)Advantages of models:

- Phase-field models: **numerically suitable, arbitrary topologies**, but artificially smeared out interface

- Sharp-interface models: caption spatial structure, but topological restrictions, high computational costs

- Macroscopic models: comprise **efficient & important effects, low computational costs**, but no spatial structure

LSW model, generalized with mechanics (K. 2009)

- Surface tension AND bulk stresses

- Microstructure of the solid crystal

- Minimal droplet volume $V_{\min} > 0$

- Realistic model, not restricted to GaAs

- Derived from **thermodynamical** principles, $\rightarrow$ clear how to control physically
Optimal control problem - LSW - Cost function

Find states (droplet volume distribution & “mean field volume”)

\[ \nu_t(V) \in C^0_{\text{weak}}([t_0, t_f]; (C^0_0(0, \infty))^*), \quad \overline{V}(t) \in C^0([t_0, t_f]; \mathbb{R}), \]

an initial control parameter (total mass) \[ u_0 \in \mathbb{R}^+, \]

and a control (temperature difference) \[ u_1(t) \in L^\infty([t_0, t_f]; \mathbb{R}^+), \]

s.t. the

Cost function

\[
J(\nu_{tf}, u_1) = \frac{\alpha_0}{2} \left\| u_1 \right\|_{L^2(t_0, t_f)}^2 + \alpha_1 \int_{V_{\text{min}}}^\infty d\nu_{tf}(V) + \alpha_2 \int_{V_{\text{min}}}^\infty V \, d\nu_{tf}(V) \\
+ \frac{\alpha_3}{2} \int_{V_{\text{min}}}^\infty \left| V \int_{V_{\text{min}}}^\infty d\nu_{tf}(S) - \int_{V_{\text{min}}}^\infty S \, d\nu_{tf}(S) \right|^2 \, d\nu_{tf}(V)
\]

where \( \alpha_k \geq 0, 0 \leq k \leq 3 \) and \( \sum_k \alpha_k > 0, \)

is minimized under the following constraints:
Optimal Control of Macroscopic Models for Phase Transitions
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Opt. control pb. - LSW - PDAE system (Vol.-diff.-controlled regime)

LSW equation (Balance of mass/substance at interfaces)

\[ \partial_t \nu_t(V) + a(V, V, u_1) \partial_V \nu_t(V) = 0 \text{ in } (V_{\text{min}}, \infty), \text{ a.e. in } [t_0, t_f], \]

with

\[ a(V, V, u_1) = V^{1/3} \frac{\mu_l(V, u_1) - \mu_l(V, u_1)}{X(V, u_1)} \]

Small droplets dissolve

\[ \nu_t(V) = 0 \text{ in } [0, V_{\text{min}}], \text{ in } [t_0, t_f], \]

Initial condition

\[ \nu(t_0, V) = \nu_0(V) \text{ in } [0, \infty). \]

Algebraic equation (AE) (Global conservation of mass/substance)

\[ \bar{V}(t) = \zeta \left( \frac{u_0 - \int_{V_{\text{min}}}^{\infty} \rho_L(V, u_1) V \, d\nu_t(V)}{X_0 u_0 - \int_{V_{\text{min}}}^{\infty} \eta_L(V, u_1) V \, d\nu_t(V) }, u_1 \right) \text{ in } [t_0, t_f], \]
Optimal control problem - LSW - Constraints

Pure state constraints

\[ a) \quad \nu_t(V) \geq 0 \quad \forall V \in [0, \infty) \quad \forall t \in [t_0, t_f], \]
\[ b) \quad V(t) \geq 0 \quad \forall t \in [t_0, t_f], \]

Box constraints for the controls

\[ u_{\text{min},0} \leq u_0 \leq u_{\text{max},0}, \]
\[ u_{\text{min},1} \leq u_1(t) \leq u_{\text{max},1} \quad \forall t \in [t_0, t_f], \]

where \( 0 < u_{\text{min},j} < u_{\text{max},j} < \infty, j = 0, 1. \)
Optimal control problem - LSW - Constraints

Pure state constraints

\[ a) \quad \nu_t(V) \geq 0 \quad \forall V \in [0, \infty) \quad \forall t \in [t_0, t_f], \]
\[ b) \quad \overline{V}(t) \geq 0 \quad \forall t \in [t_0, t_f], \]

Box constraints for the controls

\[
\begin{align*}
u_{\text{min},0} \leq & \quad u_0 \leq u_{\text{max},0}, \\
u_{\text{min},1} \leq & \quad u_1(t) \leq u_{\text{max},1} \quad \forall t \in [t_0, t_f],
\end{align*}
\]

where \( 0 < u_{\text{min},j} < u_{\text{max},j} < \infty, \quad j = 0, 1. \)

Optimal control problem with measure-valued partial differential algebraic equation with switch from PDE to algebraic equation (K. 2012)
Assumptions / Other regime

Assumptions:

- $X(V, u_1)$ strictly positive function, smooth, monotone decreasing in $V$
- Chemical potential of a precipitate $\mu_I(V, u_1)$, smooth, strictly monotone decreasing in $V$
- $\zeta$ nonlinear, smooth, strictly monotone function
  
  AE for $\overline{V}$ has index 1
- Total mass density in the liquid $\rho_L(V, u_1)$, smooth, strictly monotone decreasing in $V$
- Arsenic mass density $\eta_L(V, u_1)$, smooth, strictly monotone decreasing in $V$

Interface-reaction-controlled regime:

- Different type of Stefan condition enters LSW eq., $\propto V^{4/3}$
Ageing of polymers

Let $\Omega \subset \mathbb{R}^3$ open, bounded. Find states (polymer fractions & oxygen concentration & mechanical displacement)

$$\{p_k\}, \ c \in C^1([t_0, t_f]; \mathbb{R}^+), \ U \in C^1([t_0, t_f]; W^1,\infty(\Omega; \mathbb{R}^3))$$

and a control (concentration of injected chemicals)

$$u(t) \in L^\infty([t_0, t_f]; \mathbb{R}^+),$$

s.t. a suitable cost functional $J$ is minimized under the following constraints:

$$\dot{p} = f(p, c, U, u) \quad \text{a.e. in } [t_0, t_f],$$

$$\dot{c} - \nabla \cdot (\mu(c) \nabla c) = g(p, c, \nabla c, U, u) \quad \text{in } \Omega, \text{ a.e. in } [t_0, t_f],$$

$$\nabla \cdot S(U) = h(p, c, U, \nabla U, u) \quad \text{in } \Omega, \text{ a.e. in } [t_0, t_f],$$

+ algebraic equations for $p$ (conservation of mass, $0 \leq p_k \leq 1$)
+ initial conditions on $p, c$ + boundary conditions on $U, c$
+ constraints on the states & the control.
Optimal control problem - How to solve it?

Optimal control problem

Direct methods – First discretize then optimize (FDTO)
- Finite volume methods
- Characteristics: Mean field model
  - Adjoint approach
  - Sensitivity approach
  - Analysis

Indirect methods – First optimize then discretize (FOTD)
- Optimality system (KKT conditions)
  - Adjoint approach
  - Sensitivity approach
  - Numerics
  - Analysis

Same result?
First discretize then optimize (FOTD)

Special initial condition: start with $N_0$ distinct volumes $V_i^0$

$$
\nu_0(V) = \frac{1}{N_0} \sum_{i=1}^{N_0} \delta_{V_i^0}(V),
$$

$\hookrightarrow$ Solve PDAE for $N_0$ characteristics:

Mean field model, (without control Dreyer & K. 2009)
First discretize then optimize (FOTD)

Special initial condition: start with $\mathcal{N}_0$ distinct volumes $V_i^0$

$$\nu_0(V) = \frac{1}{\mathcal{N}_0} \sum_{i=1}^{\mathcal{N}_0} \delta_{V_i^0}(V),$$

→ Solve PDAE for $\mathcal{N}_0$ characteristics:

Mean field model, (without control Dreyer & K. 2009)

$\mathcal{N}(t)$ number of droplets at time $t$ with $V > V_{\text{min}}$

$t_j$ first time when $V_j \leq V_{\text{min}}$, otherwise $t_j = \infty$

Keep record of dissolved droplets s.t. number of states doesn’t change with time
Optimal control problem for mean field model

Find states \( V_i(t), 1 \leq i \leq \mathcal{N}_0, \) \( \bar{V}(t) \in C^0([t_0, t_f]; \mathbb{R}), \)

an initial control parameter \( u_0 \in \mathbb{R}^+, \)

and a control \( u_1(t) \in L^\infty([t_0, t_f]; \mathbb{R}^+), \)

s.t. the cost functional \( J \) is minimized under the following constraints:
Optimal control problem for mean field model

Find states \( V_i(t), 1 \leq i \leq N_0, \ \bar{V}(t) \in C^0([t_0, t_f]; \mathbb{R}), \)

an initial control parameter \( u_0 \in \mathbb{R}^+ \),

and a control \( u_1(t) \in L^\infty([t_0, t_f]; \mathbb{R}^+) \),

s.t. the cost functional \( J \) is minimized under the following constraints:

**Mean field model - Droplet evolution**

\[
\frac{\partial t}{V_i(t)} = a(\bar{V}, V_i, u_1) \quad \text{in} \quad [t_0, t_f] \setminus \bigcup_{1 \leq j \leq N_0} \{ t_j \}, \\
V_i(t^+) = V_i(t^-) \quad \text{in} \quad \left( \bigcup_{1 \leq j \leq N_0} \{ t_j \} \right) \cap [t_0, t_f], \\
V_i(t) = 0 \quad \text{in} \quad [t_0, t_f],
\]

for \( V_i > V_{\text{min}} \), otherwise

**Initial condition**

\[
V_i(t_0) = V_i^0 \quad \forall 1 \leq i \leq N_0,
\]
Optimal control problem for mean field model (continued)

Mean field model - Conservation of mass/substance

\[
\overline{V}(t) = \zeta \left( u_0 - \frac{1}{N_0} \sum_{i=1}^{N} \rho_L(V_i, u_1) V_i \right) \left( \frac{X_0 u_0 - \frac{1}{N_0} \sum_{i=1}^{N} \eta_L(V_i, u_1) V_i}{X_0 u_0} \right) u_1 \quad \forall t \in [t_0, t_f]
\]

Pure state constraints

\[
\{V_i(t)\}_{1 \leq i \leq N_0}, \overline{V}(t) \geq 0 \quad \forall t \in [t_0, t_f]
\]

Box constraints for the controls

as above

Solvable under reasonable assumptions (on \(X, \mu_I, \zeta, \rho_L, \eta_L, u_{min,0/1}, u_{max,0/1}\))
Numerical methods

1) **Sensitivity-based approach**, suitable for few variables & many constraints
2) **Adjoint-based approach**, suitable for many variables & few constraints

Implementation in OCODE 1.5 (OCPID-DAE) *(Gerds 2010)*

The algebr. equation (AE) for $V$ or the AE $V_i = 0$ for $V_i < V_{min}$ have index 1:

- replace it by ODE & suitable initial condition
- At times $t_j$ use AE to determine $V(t_j +)$ or $V_i(t_j +) = 0$.

Methods:

- (i) Replace AE for $V$ and $V_i < V_{min}$, use Runge-Kutta with fixed, suff. small time step
- (ii) Using DSRTSE (DASSL)
  - a) Keeping both AE
  - b) Replace only AE for $V_i < V_{min}$
  - c) Replace only AE for $V$

Feasibility:

- (i) & (ii)b): Reliable at switching points
- (i): For high accuracy time steps might be very small
- (ii): Problems with large time steps $\rightarrow$ Slow
Theoretical results with sensitivity approach - Algorithm (ii) b)

Sensitivities $S_{im} = (V_i)_{um}$, $l = 0, \ldots, N_0$, $m = 0, 1$, where $V_0 := \overline{V}$
W.l.o.g. $V_1 < V_2 < \ldots < V_i < \ldots < V_{N_0}$.

Sensitivity ODEs - $\overline{V}$ as algebraic variable

$$
S_0.(t_0) = (\overline{V}_0)'_{u}, \quad S_i.(t_0) = 0, \quad 1 \leq i \leq N_0
$$

$$
S_0.(t) = \sum_{k=1}^{N(t)} \zeta'_{V_k}(\{V_i\}, u)S_k.(t) + \zeta'_u(\{V_i\}, u)
$$

$$
\dot{S}_i.(t) = a'_{\overline{V}}(\overline{V}, V_i, u_1)S_0.(t) + a'_{V_i}(\overline{V}, V_i, u_1)S_i.(t) + (0, a'_{u_1}(\overline{V}, V_i, u_1)), \quad 1 \leq i \leq N(t)
$$

Update of Sensitivities:

$$
S_i.(t_j+) = \frac{a(\overline{V}, V_i, u_1)[t_j+] - a(\overline{V}, V_i, u_1)[t_j-]}{a(\overline{V}, V_j, u_1)[t_j-]}S_j.(t_j-) + S_i.(t_j-), \quad 1 \leq i < N(t_j-) = j
$$

$$
S_i.(t) = 0, \quad \forall t \geq t_i+
$$
Theoretical results with sensitivity approach - Algorithm (ii) b)

Sensitivities $S_{lm} = (V_l)'_{um}, l = 0, \ldots, \mathcal{N}_0, m = 0, 1$, where $V_0 := \overline{V}$

W.l.o.g. $V_1 < V_2 < \ldots < V_i < \ldots < V_{\mathcal{N}_0}$.

**Sensitivity ODEs - $\overline{V}$ as algebraic variable**

\[
S_0.(t_0) = (\overline{V}_0)'_u, \quad S_i.(t_0) = 0, \quad 1 \leq i \leq \mathcal{N}_0
\]

\[
S_0.(t) = \sum_{k=1}^{\mathcal{N}(t)} \zeta_{V_k}'(\{V_i\}, u)S_k.(t) + \zeta_0'(\{V_i\}, u)
\]

\[
\dot{S}_i.(t) = a_{\overline{V}}'(\overline{V}, V_i, u_1)S_0.(t) + a_{V_i}'(\overline{V}, V_i, u_1)S_i.(t) + (0, a_{u_1}'(\overline{V}, V_i, u_1)), \quad 1 \leq i \leq \mathcal{N}(t)
\]

**Update of Sensitivities:**

\[
S_i.(t_j+) = \frac{a(\overline{V}, V_i, u_1)[t_j+] - a(\overline{V}, V_i, u_1)[t_j-]}{a(\overline{V}, V_j, u_1)[t_j-]}S_j.(t_{j-}) + S_i.(t_{j-}), \quad 1 \leq i < \mathcal{N}(t_{j-}) = j
\]

\[
S_i.(t) = 0, \quad \forall t \geq t_j+
\]

Now discretize also time

Standard result for discretized DAE system applicable for typical data
Numerical results with sensitivity approach - Algorithm (i)

Radii \( r_i = \left(\frac{3}{4\pi}\right)^{1/3} V_i \), initially 50 (yellow), 220 (cyan), 320 (magenta), 520 (blue), 590 (green), “Mean field radius” (red), in \([10^{-9} \text{ m}]\) vs. time [1 s]. Top left: long-time behaviour (up to 1500 s). Top right: short-time behaviour (up to 150 s). Bottom left: Control by temperature \([10^2 \text{ K}]\) vs. time [1 s]. Bottom right: Volume fraction \(1/\mathcal{N}_0 \sum_{i=1}^{\mathcal{N}_0} V_i(t) [10^{-18} \text{ m}^3]\). \(\alpha_2 = 1, \alpha_j = 0, j \neq 2\). (K. 2012).
Theoretical results with adjoint approach - Case (i)

**Theorem:** Existence of adjoints / multiplicators; Necessary opt. cond.

W.l.o.g. $\alpha_0 = \alpha_2 = 1$, $\alpha_1 = \alpha_3 = 0$. Let $(\mathbf{V}, \{\mathbf{V}_i\}, \mathbf{u}) \in W^{1,\infty}([t_0, t_f], \mathbb{R}^{N_0+1}) \times \mathbb{R} \times L^\infty([t_0, t_f], \mathbb{R})$ a (weak) local minimum of the mean field control problem. Let $t_f$ s.t. $N_{t_f} =\text{const}$. Further $u \in \mathcal{U}$, closed, convex, with $\text{int}(\mathcal{U}) \neq \emptyset$ and $\xi = \frac{d}{dt} \zeta$.

Then there exist $l_0 \in \mathbb{R}^+$, $\lambda \in BV([t_0, t_f], \mathbb{R}^{N_0+1})$, $\mu \in NBV([t_0, t_f], \mathbb{R}^{N_0})$, s.t.

1. $(l_0, \lambda, \mu) \neq 0$
2. $\dot{\lambda}_2 = -\lambda_2 \xi'_V(\mathbf{V}, \{\mathbf{V}_i\}, \mathbf{u}) - \sum_{i=3}^{N_0+2} \lambda_i a'_V(\mathbf{V}, \mathbf{V}_i, \mathbf{u}_1)$, $\lambda_i$ diff. a.e. in $[t_0, t_f]$ with $\dot{\lambda}_i = -\lambda_2 \xi'_{V_i}(\mathbf{V}, \{\mathbf{V}_i\}, \mathbf{u}) - \lambda_i a'_{V_i}(\mathbf{V}, \mathbf{V}_i, \mathbf{u}_1) + \mu_i$ ($3 \leq i \leq N_0 + 2$)
3. $\lambda_2$ cont. in $t_j$, $1 \leq j \leq N_0$, $\lambda_i(t_j+) - \lambda_i(t_j-) = \mu_i(t_j+) - \mu_i(t_j-)$
4. $\lambda_2(t_f) = 0$, $\lambda_i(t_f) = \frac{l_0}{N_0}$
5. $(\lambda_2 \xi'_{V_0}(\mathbf{V}, \{\mathbf{V}_i\}, \mathbf{u}), l_0 \mathbf{u}_1 + \lambda_2 \xi'_{u_1}(\mathbf{V}, \{\mathbf{V}_i\}, \mathbf{u}) + \sum_i \lambda_i a'_{u_1}(\mathbf{V}, \mathbf{V}_i, \mathbf{u}_1)) \cdot (u - \mathbf{u}) \geq 0 \forall u \in \mathcal{U}$
6. $\mu_i$ strictly monotone increasing s.t. $\mu = \text{const}$ on $(t_i, t_f)$

Remarks to the proof: Consider $H = \frac{l_0}{2} u_1^2 + \lambda_2 \xi(\mathbf{V}, \{V_i\}, u) + \sum_{i=3}^{N_0+2} \lambda_i a(\mathbf{V}, V_i, u_1)$; apply Fritz-John conditions (KKT conditions - Regularity criterion fulfilled?)
Numerical results with adjoint approach - Algorithm (i)

Top left: State (as radius) $r_4 = (3/(4\pi)V_4)^{1/3}$, initially 520, in $[10^{-9} \text{ m}]$ vs. time [1 s], with corresponding adjoint $\lambda_4$ (bottom left), in $[\text{m}^{-1}]$, and multiplier $\mu_4$ (top right), in [1]. Bottom right: Adjoint corresponding to “mean field radius”, in $[\text{m}^{-1}]$. Plots calculated \textit{a posteriori}.
Initial control parameter: $u_0 = u_{\text{min},0}$

Control $u_1$ of bang-bang type

Control $u_1$ enters mainly in $X$

Different terms in $J$:

- $\alpha_1$-term: Depends on $\alpha_2$-term
- $\alpha_2$-term: Makes most sense to control
- $\alpha_3$-term: No impact for large $t_f$

(since $V_i = \overline{V}$ unstable stationary point)

**Adjoint-based approach:** Non-trivial switching conditions for adjoints
First optimize then discretize (FOTD)

Well-posedness for classical LSW equation without control (Niethammer, Pego 2000):
Existence, Uniqueness & Continuous dependence on initial data $\nu_0$; No shocks
First optimize then discretize (FOTD)

Well-posedness for classical LSW equation without control (Niethammer, Pego 2000):
Existence, Uniqueness & Continuous dependence on initial data $\nu_0$; No shocks

Assumption: Control-to-state operator

$$\mathbb{R}^+ \times L^\infty([t_0, t_f]; \mathbb{R}^+) \ni u \mapsto y := (\nu_t, \overline{V}) \in \mathcal{C}^0_{weak}([t_0, t_f]; C_0^0(0, \infty)^*) \times \mathcal{C}^0([t_0, t_f]; \mathbb{R})$$

is well-defined and Fréchet differentiable

Consider reduced problem for $u$
First optimize then discretize (FOTD)

Well-posedness for classical LSW equation without control (Niethammer, Pego 2000):
Existence, Uniqueness & Continuous dependence on initial data $\nu_0$; No shocks

Assumption: Control-to-state operator

$$R^+ \times L^\infty([t_0, t_f]; R^+) \ni u \mapsto y := (\nu_t, \bar{V}) \in C^0_{\text{weak}}([t_0, t_f]; C^0_0(0, \infty)^*) \times C^0([t_0, t_f]; R)$$

is well-defined and Fréchet differentiable

Consider reduced problem for $u$

**Adjoint-based approach**, suitable for many variables & few constraints
Adjoint-based approach

Let $\alpha_0 = \alpha_2 = 0, \alpha_1 = \alpha_3 = 1$. Replace here AE for $\overline{V}$ by ODE:

Expect $\lambda \in (C^0_{weak}([t_0, t_f]; C^0_0(0, \infty)^*))^* \times rca([t_0, t_f]; \mathbb{R}^+)$. 

But

$$\partial_t \lambda_1(t, V) + \partial_V \left( a(\overline{V}(u), V, u_1)\lambda_1(t, V) \right) = 0 \text{ in } (V_{min}, \infty), \text{ a.e. in } [t_0, t_f],$$

$$\lambda_1(t_f, \cdot) \equiv 0$$

yields $\lambda_1 \in C^0([0, t_f]; L^1(\mathbb{R})) \cap L^\infty([0, t_f] \times \mathbb{R})$.

Besides

$$\partial_t \lambda_2(t, V) + \xi'_V(\overline{V}(u), \nu_t(\cdot; u), u)\lambda_2(t, V)$$

$$= -\partial_V \left( a'_V(\overline{V}(u), V, u_1)\lambda_1(t, V) \right) \nu_t(V; u) \text{ in } (V_{min}, \infty), \text{ a.e. in } [t_0, t_f],$$

$$\lambda_2(t_f, \cdot) \equiv 0.$$
Adjoint-based approach

Let $\alpha_0 = \alpha_2 = 0, \alpha_1 = \alpha_3 = 1$. Replace here AE for $V$ by ODE:

Expect $\lambda \in (C^0_{weak}([t_0, t_f]; C^0_0(0, \infty)^*))^* \times rca([t_0, t_f]; \mathbb{R}^+)$.  

But

$$\partial_t \lambda_1(t, V) + \partial_V \left( a(V(u), V, u_1)\lambda_1(t, V) \right) = 0 \text{ in } (V_{min}, \infty), \text{ a.e. in } [t_0, t_f],$$

$$\lambda_1(t_f, \cdot) \equiv 0$$

yields $\lambda_1 \in C^0([0, t_f]; L^1(\mathbb{R})) \cap L^\infty([0, t_f] \times \mathbb{R})$.

Besides

$$\partial_t \lambda_2(t, V) + \xi'_V(V(u), \nu_t(\cdot; u), u)\lambda_2(t, V)$$

$$= -\partial_V \left( a'_V(V(u), V, u_1)\lambda_1(t, V) \right) \nu_t(V; u) \text{ in } (V_{min}, \infty), \text{ a.e. in } [t_0, t_f],$$

$$\lambda_2(t_f, \cdot) \equiv 0.$$  

Work in progress ...
Optimal control problem for (generalized) LSW as PDAE

- FDTO - Mean field model: Well-posed optimization problem; Numerical solution; Considered different contributions to cost function
- FOTD - Adjoint LSW problem
Outlook

Open questions:

▶ FDTO
  ▶ Mean field model: Optimal solution depends on $N_{tf}$
  ▶ More efficient algorithms for long-time behaviour, finite volume discretization

▶ FOTD
  ▶ Continue analysis ...
  ▶ Sensitivity-based approach feasible ?

▶ First optimize then discretize (FOTD) vs. first discretize then optimize (FDTO)

Similar situations in:

▶ Traffic flow (Colombo, Herty, Mercier 2011),
▶ Highly re-entrant manufacturing systems (Coron, Kawski, Wang 2010),
▶ Aerospace dynamics / Gas dynamics
▶ ...
Acknowledgements / References

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Thank you for your attention