Optimal Control of Macroscopic Models for Phase Transitions

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Contents

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 limit

Sharp-interface models
- Mullins-Sekerka, vol.-diffusion/interf.-reaction regime, conserv. total mass/volume

Atomic models

- Becker-Döring

Homogenization limit

Homogenization limit

Macroscopic models

- (in)homogeneous Lifshitz-Slyozov(-Wagner), volume-diffusion regime

interface-reaction regime

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

- **generalized** homog. Lifshitz-Slyozov-Wagner, vol.-diffusion regime (K.)
- (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")

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

an initial control parameter (total mass) $u_0 \in \mathbf{R}^+$,

and a control (temperature difference)

$$u_1(t) \in L^\infty([t_0, t_f]; \mathbf{R}^+),$$

s.t. the

Cost function

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

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

is minimized under the following constraints:

Opt. control pb. - LSW - PDAE system (Vol.-diff.-controlled regime)

LSW equation (Balance of mass/substance at interfaces)

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

$$\text{with } a(\overline{V}, V, u_1) = V^{1/3} \frac{\mu_I(\overline{V}, u_1) - \mu_I(V, u_1)}{\mathbb{X}(V, u_1)}$$

Small droplets dissolve $\quad \nu_t(V) = 0$ in $[0, V_{min}]$, 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)

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

Optimal control problem - LSW - Constraints

Pure state constraints

$$\begin{aligned} a)\ & \nu_t(V) \geq 0 && \forall V \in [0, \infty)\ \forall t \in [t_0, t_f], \\ b)\ & \overline{V}(t) \geq 0 && \forall t \in [t_0, t_f], \end{aligned}$$

Box constraints for the controls

$$\begin{aligned} u_{min,0} &\leq u_0 \leq u_{max,0}, \\ u_{min,1} &\leq u_1(t) \leq u_{max,1} \qquad \forall t \in [t_0, t_f], \end{aligned}$$

where $0 < u_{min,j} < u_{max,j} < \infty$, $j = 0, 1$.

Optimal control problem - LSW - Constraints

Pure state constraints

$$
\begin{aligned}
&a)\ \nu_t(V) \geq 0 \qquad \forall V \in [0, \infty)\ \forall t \in [t_0, t_f], \\
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\end{aligned}
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Box constraints for the controls

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\begin{aligned}
u_{min,0} &\leq u_0 \leq u_{max,0}, \\
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\end{aligned}
$$

where $0 < u_{min,j} < u_{max,j} < \infty$, $j = 0, 1$.

$\hookrightarrow$ Optimal control problem with measure-valued partial differential algebraic equation with switch from PDE to algebraic equation (K. 2012)

Assumptions / Other regime

Assumptions:

- $\mathbb{X}(V, u_1)$ strictly positive function, smooth, monotone decreasing in V
- Chemical potential of a precipitate $\mu_l(V, u_1)$, smooth, strictly monotone decr. in V
- ζ 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 decr. 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 $\Omega \subset \mathbf{R}^3$ open, bounded. Find states (polymer fractions & oxygen concentration & mechanical displacement)

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

and a control (concentration of injected chemicals)

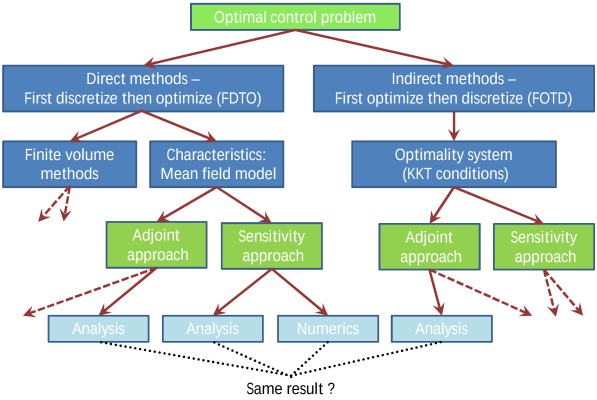
$$u(t) \in L^\infty([t_0, t_f]; \mathbf{R}^+),$$

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

$$\begin{aligned} \dot{p} &= f(p, c, U, u) && \text{a.e. in } [t_0, t_f], \\ \dot{c} - \nabla \cdot (\mu(c) \nabla c) &= g(p, c, \nabla c, U, u) && \text{in } \Omega, \text{ a.e. in } [t_0, t_f], \\ \nabla \cdot \mathbb{S}(U) &= h(p, c, U, \nabla U, u) && \text{in } \Omega, \text{ a.e. in } [t_0, t_f], \end{aligned}$$

+ 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?



First discretize then optimize (FOTD)

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

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

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

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

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

t_j first time when $V_j \leq V_{min}$, 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 $V_i(t), 1 \leq i \leq \mathcal{N}_0,\ \overline{V}(t)\ \in C^0([t_0, t_f]; \mathbf{R}),$

an initial control parameter $u_0 \in \mathbf{R}^+,$

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

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

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and a control $u_1(t) \in L^\infty([t_0, t_f]; \mathbf{R}^+)$,
s.t. the cost functional J is minimized under the following constraints:

Mean field model - Droplet evolution

$$\left.\begin{array}{lll} \partial_t V_i(t) = a(\overline{V}, V_i, u_1) & \text{in } [t_0, t_f] \setminus \cup_{1 \leq j \leq \mathcal{N}_0} \{t_j\}, & \\ V_i(t+) = V_i(t-) & \text{in } \left(\cup_{1 \leq j \leq \mathcal{N}_0} \{t_j\}\right) \cap [t_0, t_f], & \text{for } V_i > V_{min}, \\ V_i(t) = 0 & \text{in } [t_0, t_f], & \text{otherwise} \end{array}\right.$$

Initial conditon

$$V_i(t_0) = V_i^0 \quad \forall 1 \leq i \leq \mathcal{N}_0,$$

Optimal control problem for mean field model (continued)

Mean field model - Conservation of mass/substance

$$\overline{V}(t) = \zeta\left(\frac{u_0 - \frac{1}{\mathcal{N}_0}\sum_{i=1}^{\mathcal{N}} \rho_L(V_i, u_1)\, V_i}{X_0 u_0 - \frac{1}{\mathcal{N}_0}\sum_{i=1}^{\mathcal{N}} \eta_L(V_i, u_1)\, V_i}, u_1\right) \quad \forall t \in [t_0, t_f]$$

Pure state constraints

$$\{V_i(t)\}_{1\leq i\leq \mathcal{N}_0},\ \overline{V}(t) \geq 0 \quad \forall t \in [t_0, t_f]$$

Box constraints for the controls

as above

Solvable under reasonable assumptions (on $\mathbb{X}, \boldsymbol{\mu}_l, \zeta, \rho_L, \eta_L, u_{min,0/1}, u_{max,0/1}$)

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) (Gerdts 2010)

The algebr. equation (AE) for $\overline{V}$ 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 $\overline{V}(t_j+)$ or $V_i(t_j+) = 0$.

Methods:

(i) Replace AE for $\overline{V}$ 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 $\overline{V}$

Feasibility:

- (i) & (ii)b): Reliable at switching points
- (i): For high accuracy time steps might be very small
- (ii): Problems with large time steps $\longrightarrow$ Slow

Theoretical results with sensitivity approach - Algorithm (ii) b)

Sensitivities $S_{lm} = (V_l)'_{u_m}$, $l = 0, \ldots, \mathcal{N}_0$, $m = 0, 1$, 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

$$S_{0\cdot}(t_0) = (\overline{V}_0)'_u, \quad S_{i\cdot}(t_0) = 0,\ 1 \leq i \leq \mathcal{N}_0$$

$$S_{0\cdot}(t) = \sum_{k=1}^{\mathcal{N}(t)} \zeta'_{V_k}(\{V_i\}, u) S_{k\cdot}(t) + \zeta'_u(\{V_i\}, u)$$

$$\dot{S}_{i\cdot}(t) = a'_{\overline{V}}(\overline{V}, V_i, u_1) S_{0\cdot}(t) + a'_{V_i}(\overline{V}, V_i, u_1) S_{i\cdot}(t) + (0, a'_{u_1}(\overline{V}, V_i, u_1)),\ 1 \leq i \leq \mathcal{N}(t)$$

Update of Sensitivities:

$$S_{i\cdot}(t_j+) = \frac{a(\overline{V}, V_i, u_1)[t_j+] - a(\overline{V}, V_i, u_1)[t_j-]}{a(\overline{V}, V_j, u_1)[t_j-]} S_{j\cdot}(t_j-) + S_{i\cdot}(t_j-),\ 1 \leq i < \mathcal{N}(t_j-) = j$$

$$S_{i\cdot}(t) = 0, \quad \forall t \geq t_i+$$

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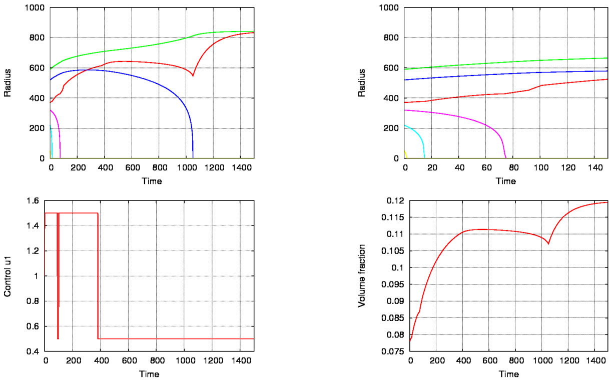
$$S_{i\cdot}(t) = 0, \quad \forall t \geq t_i+$$

Now discretize also time

Standard result for discretized DAE system applicable for typical data

Numerical results with sensitivity approach - Algorithm (i)



Radii $r_i = (3/(4\pi)V_i)^{1/3}$, initially 50 (yellow), 220 (cyan), 320 (magenta), 520 (blue), 590 (green), "Mean field radius" (red), in $[10^{-9}$ 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 $[10^2$ K] vs. time [1 s]. Bottom right: Volume fraction $1/\mathcal{N}_0 \sum_{i=1}^{\mathcal{N}_0} V_i(t)$ $[10^{-18}$ 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 $(\overline{V}, \{\hat{V}_i\}, \hat{u}) \in W^{1,\infty}([t_0, t_f], \mathbf{R}^{\mathcal{N}_0+1}) \times \mathbf{R} \times L^\infty([t_0, t_f], \mathbf{R})$ a (weak) local minimum of the mean field control problem. Let t_f s.t. $\mathcal{N}_{t_f} = const$. Further $u \in \mathcal{U}$, closed, convex, with $int(\mathcal{U}) \neq \emptyset$ and $\xi = \frac{d}{dt}\zeta$.

Then there exist $l_0 \in \mathbf{R}^+$, $\lambda \in BV([t_0, t_f], \mathbf{R}^{\mathcal{N}_0+1})$, $\mu \in NBV([t_0, t_f], \mathbf{R}^{\mathcal{N}_0})$, s.t.

(1) $(l_0, \lambda, \mu) \neq 0$

(2) $\dot{\lambda}_2 = -\lambda_2 \xi'_{\overline{V}}(\hat{\overline{V}}, \{\hat{V}_i\}, \hat{u}) - \sum_{i=3}^{\mathcal{N}_0+2} \lambda_i a'_{\overline{V}}(\hat{\overline{V}}, \hat{V}_i, \hat{u}_1)$, $\quad \lambda_i$ diff. a.e. in $[t_0, t_f]$ with
$\dot{\lambda}_i = -\lambda_2 \xi'_{V_i}(\hat{\overline{V}}, \{\hat{V}_i\}, \hat{u}) - \lambda_i a'_{V_i}(\hat{\overline{V}}, \hat{V}_i, \hat{u}_1) + \dot{\mu}_i \quad (3 \leq i \leq \mathcal{N}_0 + 2)$

(3) λ_2 cont. in t_j, $1 \leq j \leq \mathcal{N}_0$, $\quad \lambda_i(t_j+) - \lambda_i(t_j-) = \mu_i(t_j+) - \mu_i(t_j-)$

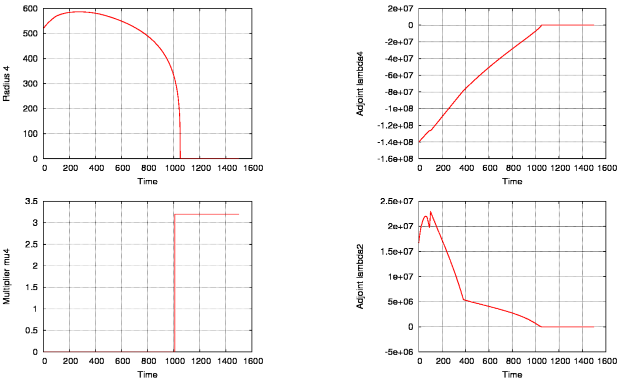
(4) $\lambda_2(t_f) = 0, \quad \lambda_i(t_f) = \frac{l_0}{\mathcal{N}_0}$

(5) $(\lambda_2 \xi'_{u_0}(\hat{\overline{V}}, \{\hat{V}_i\}, \hat{u}), l_0 \hat{u}_1 + \lambda_2 \xi'_{u_1}(\hat{\overline{V}}, \{\hat{V}_i\}, \hat{u}) + \sum_i \lambda_i a'_{u_1}(\hat{\overline{V}}, \hat{V}_i, \hat{u}_1)) \cdot (u - \hat{u}) \geq 0 \quad \forall u \in \mathcal{U}$

(6) μ_i strictly monotone increasing s.t. $\mu = const$ on (t_i, t_f)

Remarks to the proof: Consider $H = \frac{l_0}{2} u_1^2 + \lambda_2 \xi(\overline{V}, \{V_i\}, u) + \sum_{i=3}^{\mathcal{N}_0+2} \lambda_i a(\overline{V}, V_i, u_1)$;
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 $[10^{-9}$ m] vs. time [1 s], with corresponding adjoint λ_4 (bottom left), in $[\text{m}^{-1}]$, and multiplier μ_4 (top right), in [1]. Bottom right: Adjoint corresponding to "mean field radius", in $[\text{m}^{-1}]$. Plots calculated *a posteriori*.

Numerical results - Conclusions

Initial control parameter: $u_0 = u_{min,0}$

Control u_1 of bang-bang type

Control u_1 enters mainly in $\mathbb{X}$

Different terms in J:

- α_1-term: Depends on α_2-term
- α_2-term: Makes most sense to control
- α_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 ν_0; No shocks

First optimize then discretize (FOTD)

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Existence, Uniqueness & Continuous dependence on initial data ν_0; No shocks

Assumption: Control-to-state operator

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

is well-defined and Fréchet differentiable

Consider reduced problem for u

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

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

Besides

$$\begin{aligned} \partial_t \lambda_2(t, V) &+ \xi'_{\overline{V}}(\overline{V}(u), \nu_t(\cdot; u), u)\lambda_2(t, V)) \\ &= -\partial_V \left(a'_{\overline{V}}(\overline{V}(u), V, u_1)\lambda_1(t, V) \right) \nu_t(V; u) \text{ in } (V_{min}, \infty), \text{ a.e. in } [t_0, t_f], \end{aligned}$$

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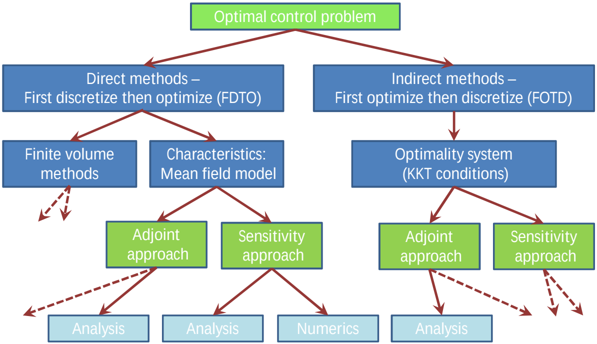
Besides

$$\begin{aligned} &\partial_t \lambda_2(t,V) + \xi'_{\overline{V}}(\overline{V}(u), \nu_t(\cdot; u), u)\lambda_2(t,V)) \\ &\qquad = -\partial_V \left(a'_{\overline{V}}(\overline{V}(u), V, u_1)\lambda_1(t,V) \right) \nu_t(V;u) \text{ in } (V_{min}, \infty), \text{ a.e. in } [t_0, t_f], \end{aligned}$$

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

Work in progress ...

Summary



- 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 $\mathcal{N}_{t_f}$
  - 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