Mathematical Analysis of Marine Ecosystem Models

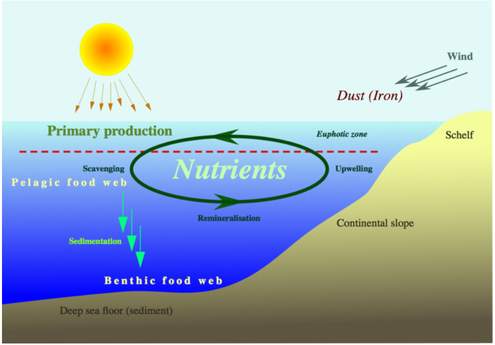
Christina Roschat

Christian-Albrechts-Universität zu Kiel, Cluster of Excellence "The Future Ocean"

June 15, 2015

Why ecosystem models?

- Oceans are a carbon sink
- Marine ecosystems influence concentrations of carbon, phosphorus...
- Models express processes in marine ecosystems



Model equations

Marine ecosystem model equation

$$\left.\begin{aligned} \partial_t y_j + \operatorname{div}(\mathbf{v} y_j) - \operatorname{div}(\kappa \nabla y_j) + d_j(y,u) &= 0 \quad \text{in } Q_T \\ \nabla y_j \cdot (\kappa \eta) + b_j(y,u) &= 0 \quad \text{on } \Sigma \end{aligned}\right\} j = 1, \ldots, s$$

with

- $\Omega \subset \mathbb{R}^n$, $n \leq 3$, open, bounded, $\Gamma := \partial\Omega$
- $Q_T := \Omega \times [0,T]$ and $\Sigma := \Gamma \times [0,T]$
- $\mathbf{v} \in L^\infty(0,T; H^1(\Omega)^n)$ with $\operatorname{div}(\mathbf{v}(t)) = 0$ in Ω and $\mathbf{v}(t) \cdot \eta = 0$ on Γ
- $\kappa \in L^\infty(Q_T)$ with $\kappa_{\min} := \operatorname{ess\,inf}_{(x,t)} \kappa(x,t) > 0$
- Reaction terms d and b with $d(0,u) = 0 = b(0,u)$
- $u \in \mathbb{R}^p$ parameter vector

Example: The PO_4-DOP model by Parekh et al. (2006)

Two model variables $y = (y_1, y_2)$ $(s = 2)$

Domain Ω is 3-dimensional

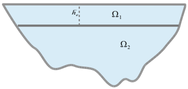


Figure : Domain Ω

Reaction terms differ in the upper and the lower part of Ω:

$$d_1(y,u) := \begin{cases} -\lambda y_2 + G(y_1) & \text{in } \Omega_1 \times [0,T], \\ -\lambda y_2 - (1-\nu)E(y_1) & \text{in } \Omega_2 \times [0,T]. \end{cases}$$

$$d_2(y,u) := \begin{cases} \lambda y_2 - \nu G(y_1) & \text{in } \Omega_1 \times [0,T], \\ \lambda y_2 & \text{in } \Omega_2 \times [0,T]. \end{cases}$$

with

$$G(y_1) := \alpha \frac{y_1}{|y_1| + K_P} \frac{I\mathrm{e}^{-x_3 K_W}}{|I\mathrm{e}^{-x_3 K_W}| + K_I} \quad \text{Consumption}$$

$$E(y_1) := \frac{\beta}{\bar{h}_e} \left(\frac{x_3}{\bar{h}_e} \right)^{-\beta - 1} \int_0^{\bar{h}_e} G(y_1) d\tilde{x}_3 \quad \text{Export (non-local)}$$

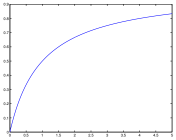


Figure : Half saturation function

Parameter identification

Aim: Model output reproduces observed data y_d

Corresponding optimal control problem

$$\min_{(y,u)} J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2}|u - u_{ref}|^2_{\mathbb{R}^p}, \quad \gamma \geq 0$$

subject to

$$\int_0^T \{\langle y_j', w_j\rangle + (\kappa \nabla y_j, \nabla w_j) + (\mathbf{v} \cdot \nabla y_j + d_j(y,u), w_j) + (b_j(y,u), w_j)\} dt = 0$$

$$(w_j \in L^2(0,T; H^1(\Omega)),\ j = 1, \ldots, s)$$

appropriate initial condition

$$u_{i\,\min} \leq u_i \leq u_{i\,\max}, \quad i = 1, \ldots, p.$$

Definitions

- A weak solution of each model equation belongs to the space

$$W(0,T) := \{v \in L^2(0,T;H^1(\Omega)) : v' \in L^2(0,T;H^1(\Omega)^*)\}$$

- Let $y_0 \in L^2(\Omega)^s$. A weak solution $y \in W(0,T)^s$ is called transient if

$$y_j(0) = y_0^j \quad \text{for all } j = 1, \ldots, s.$$

- A weak solution $y \in W(0,T)^s$ is called periodic if

$$y_j(0) = y_j(T) \quad \text{for all } j = 1, \ldots, s.$$

Outline

1 Transient solutions of general model equations

2 Periodic solution for the N-DOP model

3 Quadratic reaction terms

4 Parameter identification: Existence of optimal parameters and optimality conditions

Outline

1 Transient solutions of general model equations

2 Periodic solution for the N-DOP model

3 Quadratic reaction terms

4 Parameter identification: Existence of optimal parameters and optimality conditions

Generalized model equations

General transient problem

$$\left.\begin{array}{rcll} \partial_t y_j + \mathrm{div}(\mathbf{v} y_j) - \mathrm{div}(\kappa \nabla y_j) + d_j^1(y,u) + d_j^2(y,u) & = & q_Q & \text{in } Q_T \\ \nabla y_j \cdot (\kappa \eta) + b_j^1(y,u) + b_j^2(y,u) & = & q_\Sigma & \text{on } \Sigma \\ y_j(0) & = & y_{0j} & \text{in } \Omega \end{array}\right\} j = 1, \ldots, s$$

with

- $d^i : L^2(Q_T)^s \times \mathbb{R}^p \to L^2(Q_T)^s$ and $b^i : L^2(Q_T)^s \times \mathbb{R}^p \to L^2(\Sigma)^s$ continuous reaction terms ($i = 1, 2$)
- General inhomogeneities $q_Q, q_\Sigma \in L^2(0, T; H^1(\Omega)^*)^s$
- Initial value $y_0 \in L^2(\Omega)^s$

Result about existence and uniqueness

Theorem

Assuming that

- $d^1(\,.\,,u), b^1(\,.\,,u)$ *Lipschitz continuous*
- $d^2(\,.\,,u), b^2(\,.\,,u)$ *monotone and bounded*
- $d^i(0,u) = b^i(0,u) = 0$

there is a unique weak solution $y \in W(0,T)^s$ *of the general transient problem. Furthermore, the estimate*

$$\|y\|_{W(0,T)^s} \leq C(\|q_Q\|_{L^2(Q_T)^s} + \|q_\Sigma\|_{L^2(\Sigma)^s} + \|y_0\|_{L^2(\Omega)^s})$$

holds with a constant $C > 0$ *independent of* y, y_0.

Proof (idea):

- Fix Lipschitz continuous terms $d^1(z,u), b^1(z,u)$ with $z \in C([0,T], L^2(\Omega))^s$
- Solve monotone equation with standard methods
- Find solution of whole problem with Banach's Fixed Point Theorem

Result about existence and uniqueness

Theorem

Assuming that

- $d^1(\,.\,,u), b^1(\,.\,,u)$ *Lipschitz continuous*
- $d^2(\,.\,,u), b^2(\,.\,,u)$ *monotone and bounded*
- $d^i(0,u) = b^i(0,u) = 0$

there is a unique weak solution $y \in W(0,T)^s$ *of the general transient problem. Furthermore, the estimate*

$$\|y\|_{W(0,T)^s} \leq C(\|q_Q\|_{L^2(Q_T)^s} + \|q_\Sigma\|_{L^2(\Sigma)^s} + \|y_0\|_{L^2(\Omega)^s})$$

holds with a constant $C > 0$ *independent of* y, y_0.

Proof (idea):

- Fix Lipschitz continuous terms $d^1(z,u), b^1(z,u)$ with $z \in C([0,T], L^2(\Omega))^s$
- Solve monotone equation with standard methods
- Find solution of whole problem with Banach's Fixed Point Theorem

Outline

1 Transient solutions of general model equations

2 Periodic solution for the N-DOP model

3 Quadratic reaction terms

4 Parameter identification: Existence of optimal parameters and optimality conditions

Typical result for periodic solvability

Existence theorem of Gajewski et al., 1974

Let $V \subset H \subset V^*$ be an evolution triple , $X := L^2(0,T;V)$. If $A : X \to X^*$ is a continuous, monotone and coercive operator, the problem

$$y' + Ay = f, \quad y(0) = y(T),$$

has a solution $y \in L^2(0,T;V)$ with $y' \in L^2(0,T;V^*)$ for every $f \in X^*$.

Definitions:

- A monotone $:\Leftrightarrow \langle Ay - Az, y - z\rangle \geq 0$ for all $y, z \in X$
- A coercive $:\Leftrightarrow \frac{\langle Ay, y\rangle}{\|y\|_X} \to \infty$ if $\|y\|_X \to \infty$

Conservation of mass

Problems with standard existence theorem:

1. Coercivity usually not fulfilled by ecosystem model equations
2. Proof of existence not sufficient (trivial function is a periodic solution)

Idea: take into account the model's conservation of mass:

- An s-dimensional vector of concentrations y has a constant mass $C \in \mathbb{R}$ if

$$\mathrm{mass}(y(t)) := \sum_{j=1}^{s} \int_{\Omega} y_j(t) dx = C \quad \text{for all } t \in [0, T].$$

- The solution of an ecosystem model has a constant mass if

$$\sum_{j=1}^{s} [\int_{\Omega} d_j(y, u, t) dx + \int_{\Gamma} b_j(y, u, t) ds] = 0 \quad \text{for almost all } t \text{ and all } (y, u)$$

Conservation of mass

Problems with standard existence theorem:

1. Coercivity usually not fulfilled by ecosystem model equations
2. Proof of existence not sufficient (trivial function is a periodic solution)

Idea: take into account the model's conservation of mass:

- An s-dimensional vector of concentrations y has a constant mass $C \in \mathbb{R}$ if

$$\mathrm{mass}(y(t)) := \sum_{j=1}^{s} \int_\Omega y_j(t)dx = C \quad \text{for all } t \in [0, T].$$

- The solution of an ecosystem model has a constant mass if

$$\sum_{j=1}^{s} [\int_\Omega d_j(y,u,t)dx + \int_\Gamma b_j(y,u,t)ds] = 0 \quad \text{for almost all } t \text{ and all } (y,u)$$

Model of N-DOP type

Formulation as operator equation

$$y_1' + B(y_1) - \lambda y_2 + F_1(y) = 0$$
$$y_2' + B(y_2) + \lambda y_2 + F_2(y) = 0$$

with

- Operators $B, F_1, F_2 : L^2(0,T;H^1(\Omega)) \to L^2(0,T;H^1(\Omega)^*)$, defined by

$$\langle B(y), v\rangle := \int_0^T (\kappa \nabla y, \nabla v)_{L^2(\Omega)^3} dx + (\mathrm{div}(\mathbf{v}y), v)_{L^2(\Omega)} dt,$$
$$\langle F_j(y), v\rangle := \int_0^T \{(\tilde{d}_j(y,u), v)_{L^2(\Omega)} + (\tilde{b}_j(y,u), v)_{L^2(\Gamma)}\} dt$$

  for $j = 1, 2$ and $y, v \in L^2(0,T;H^1(\Omega))$ (parameter vector u fixed)

- $\lambda > 0$

Existence of nontrivial periodic solutions

Theorem

Let $C \in \mathbb{R}$. Assuming that

- $\tilde{d}, \tilde{b}$ *are continuous*
- $\sum_{j=1}^{2} [\int_{\Omega} \tilde{d}_j(y,u,t)dx + \int_{\Gamma} \tilde{b}_j(y,u,t)ds] = 0$ *for almost all* t *and all* (y,u)
- $\max\{\|\tilde{d}_j(y,u)\|_{L^2(Q_T)}, \|\tilde{b}_j(y,u)\|_{L^2(\Sigma)}\} \leq M$ *for all* (y,u), $j = 1,2$

there is at least one periodic weak solution $y \in W(0,T)^2$ *of the model equation of* N-DOP *type with*

$$\text{mass}(y(t)) = C \quad \textit{for all } t \in [0,T].$$

In particular, there is a nontrivial periodic solution.

Outline of the proof 1

Step 1:

Fix $z \in L^2(Q_T)^2$ and solve the linearized equations

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 &= -F_1(z) \\ y_2' + B(y_2) + \lambda y_2 &= -F_2(z) \\ y(0) &= y(T) \\ \mathrm{mass}(y(t)) &= C \text{ for all } t \in [0,T] \end{aligned}$$

1. Find unique periodic solution $y_2(z) \in W(0,T)$ of the second equation
   - $y_2 \mapsto B(y_2) + \lambda y_2$ is monotone and coercive in $L^2(0,T;H^1(\Omega))$
2. Find unique periodic solution $S(z)$ with $\mathrm{mass}(S(z)) = 0$ of the sum equation

$$S' + B(S) = -F_1(z) - F_2(z)$$

   - B, restricted to functions with mass 0, is monotone and coercive
   - $S(z) \in W(0,T)$ because of conservation of mass
3. Define periodic solution of first equation by $y_1(z) := S(z) - y_2(z) + |\Omega|^{-1}C$

Outline of the proof 1

Step 1:

Fix $z \in L^2(Q_T)^2$ and solve the linearized equations

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 &= -F_1(z) \\ y_2' + B(y_2) + \lambda y_2 &= -F_2(z) \\ y(0) &= y(T) \\ \mathrm{mass}(y(t)) &= C \text{ for all } t \in [0,T] \end{aligned}$$

1. Find unique periodic solution $y_2(z) \in W(0,T)$ of the second equation
   - $y_2 \mapsto B(y_2) + \lambda y_2$ is monotone and coercive in $L^2(0,T;H^1(\Omega))$
2. Find unique periodic solution $S(z)$ with $\mathrm{mass}(S(z)) = 0$ of the sum equation

   $$S' + B(S) = -F_1(z) - F_2(z)$$

   - B, restricted to functions with mass 0, is monotone and coercive
   - $S(z) \in W(0,T)$ because of conservation of mass
3. Define periodic solution of first equation by $y_1(z) := S(z) - y_2(z) + |\Omega|^{-1}C$

Outline of the proof 2

Step 2:

Solution of nonlinear equation = fixed point of operator

$$A : L^2(Q_T)^2 \to L^2(Q_T)^2; z \mapsto y(z) = (y_1(z), y_2(z))$$

Schauder Fixed Point Theorem

Let M be a nonempty, closed, bounded, convex subset of a Banach space X, and suppose $A : M \to M$ is a compact operator. Then A has a fixed point.

The theorem is applicable because

- $y(z)$ is bounded independently of z in $W(0,T)^2$ (boundedness assumptions)
- In particular, A maps a closed ball $M \subset L^2(Q_T)^2$ into itself
- A is continuous
- $A(\tilde{M})$ is bounded in $W(0,T)^2$ and therefore compact in $L^2(Q_T)^2$

□

Outline of the proof 2

Step 2:

Solution of nonlinear equation = fixed point of operator

$$A : L^2(Q_T)^2 \to L^2(Q_T)^2; z \mapsto y(z) = (y_1(z), y_2(z))$$

Schauder Fixed Point Theorem

Let M be a nonempty, closed, bounded, convex subset of a Banach space X, and suppose $A : M \to M$ is a compact operator. Then A has a fixed point.

The theorem is applicable because

- $y(z)$ is bounded independently of z in $W(0,T)^2$ (boundedness assumptions)
- In particular, A maps a closed ball $M \subset L^2(Q_T)^2$ into itself
- A is continuous
- $A(\tilde{M})$ is bounded in $W(0,T)^2$ and therefore compact in $L^2(Q_T)^2$

□

Simplified numerical model

- PO_4-DOP model on a 2-D domain (unit square)
- Implementation of Navier-Stokes equations (Griebel et al., 1995) extended by ecosystem model equations and periodical forcing (wind)

Computation of a periodic solution via "fixed point iteration":

Data: Initial concentration c_0 with mass C
Result: Initial value of a periodic solution
Initialize residual res;
while *res* $> \epsilon$ **do**
  Compute transient solution $y = (y_0, \ldots, y_N)$ with initial value $y_0 = c_i$;
  $c_{i+1} = y_N$;
  res $= \|c_i - c_{i+1}\|$;
end

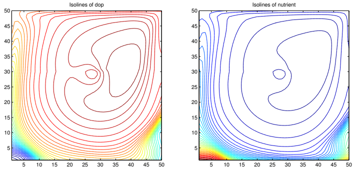


Figure : Typical concentrations

Test: Run this iteration starting with random c_0 (with mass C)
Result: Every test run yields the same solution

Simplified numerical model

- PO_4-DOP model on a 2-D domain (unit square)
- Implementation of Navier-Stokes equations (Griebel et al., 1995) extended by ecosystem model equations and periodical forcing (wind)

Computation of a periodic solution via "fixed point iteration":

Data: Initial concentration c_0 with mass C
Result: Initial value of a periodic solution
Initialize residual res;
while *res* $> \epsilon$ **do**
  Compute transient solution $y = (y_0, \ldots, y_N)$ with initial value $y_0 = c_i$;
  $c_{i+1} = y_N$;
  res $= \|c_i - c_{i+1}\|$;
end

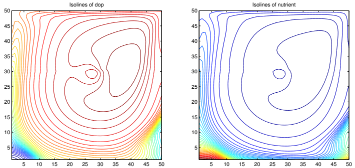


Figure : Typical concentrations

Test: Run this iteration starting with random c_0 (with mass C)
Result: Every test run yields the same solution

Outline

1 Transient solutions of general model equations

2 Periodic solution for the N-DOP model

3 Quadratic reaction terms

4 Parameter identification: Existence of optimal parameters and optimality conditions

$NPZD$ model (Version of Rückelt et al., 2010)

- Model variables $y = (y_1, y_2, y_3, y_4)$ ($s = 4$)

- Reaction terms

$$
\begin{aligned}
d_1(y) &= J(y_1, y_2)y_2 - \gamma_m y_4 - \Phi_m^z y_3 \\
d_2(y) &= (\Phi_m^p - J(y_1, y_2))y_2 + G(y_2)y_3 \\
d_3(y) &= \Phi_m^* |y_3| y_3 + (\Phi_m^z - \beta G(y_2))y_3 \\
d_4(y) &= \gamma_m y_4 - (1-\beta)G(y_2)y_3 - \Phi_m^* |y_3| y_3 - \Phi_m^p y_2
\end{aligned}
$$

with the abbreviations

$$
\begin{aligned}
G(y_2) &= \frac{g\epsilon y_2^2}{g + \epsilon y_2^2} \\
J(y_1, y_2) &= \min\{\bar{\mu}(y_2), \frac{y_1}{|y_1| + K_N}\}
\end{aligned}
$$

($\bar{\mu}(y_2)$ incidence of light)

- Homogeneous Neumann boundary conditions: $b(y, u) = 0$ (conservation of mass condition is satisfied)

Transient solutions

Theorem

Given initial values $y_0 \in L^\infty(\Omega)^4$, the $NPZD$ model equations have a unique transient solution $y \in (W(0,T) \cap L^\infty(Q_T))^4$.

Proof (ideas):

- Adapt technique of Raymond and Zidani (1999)
- Truncate the quadratic term $|y_3|y_3$ and fix the factors $J(z_1, z_2), G(z_2)$ $(z \in C([0,T]; L^2(\Omega))^4)$
- The truncated solutions $y(k,z) \in W(0,T)^4$ are L^∞ according to a proposition by Raymond and Zidani
- For $\hat{k}$ larger than upper bound, $y(z) = y(\hat{k}, z)$ solves the non-truncated equation
- A fixed point of $z \mapsto y(z)$ is a solution of the original problem (Banach's Fixed Point Theorem)

Transient solutions

Theorem

Given initial values $y_0 \in L^\infty(\Omega)^4$, the $NPZD$ model equations have a unique transient solution $y \in (W(0,T) \cap L^\infty(Q_T))^4$.

Proof (ideas):

- Adapt technique of Raymond and Zidani (1999)
- Truncate the quadratic term $|y_3|y_3$ and fix the factors $J(z_1, z_2), G(z_2)$ $(z \in C([0,T]; L^2(\Omega))^4)$
- The truncated solutions $y(k,z) \in W(0,T)^4$ are L^∞ according to a proposition by Raymond and Zidani
- For $\hat{k}$ larger than upper bound, $y(z) = y(\hat{k}, z)$ solves the non-truncated equation
- A fixed point of $z \mapsto y(z)$ is a solution of the original problem (Banach's Fixed Point Theorem)

Problems with periodic solutions

1. Weak formulation with quadratic reaction terms is not well-defined in the usual spaces

2. Existence of truncated solutions? Boundedness in L^∞?
   (Initial value of periodic solution: $y(0) \in L^2(\Omega)^4$)

3. An existence theorem is not sufficient (as before)

Are there other techniques to prove periodic solvability?

Problems with periodic solutions

1. Weak formulation with quadratic reaction terms is not well-defined in the usual spaces
2. Existence of truncated solutions? Boundedness in L^∞?
   (Initial value of periodic solution: $y(0) \in L^2(\Omega)^4$)
3. An existence theorem is not sufficient (as before)

Are there other techniques to prove periodic solvability?

Outline

1 Transient solutions of general model equations

2 Periodic solution for the N-DOP model

3 Quadratic reaction terms

4 Parameter identification: Existence of optimal parameters and optimality conditions

The parameter identification problem

Given: y_d = data, u_{ref} = reference parameters, $\gamma \geq 0$

Problem:

$$\min_{(y,u)} J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q)^s} + \frac{\gamma}{2}|u - u_{ref}|^2_{\mathbb{R}^p}$$

$$\text{s. t.} \qquad e(y,u) = 0$$

$$u \in U_{ad}$$

with

$$e : W(0,T)^s \times \mathbb{R}^p \to L^2(0,T;H^1(\Omega)^*)^s \times L^2(\Omega)^s :$$

$$e_1(y,u) = y' + B(y) + d(u,y) + b(u,y)$$

$$e_2(y,u) = y(0) - y_0$$

or $y(0) - y(T)$ (depending on problem)

$$U_{ad} = \{u \in \mathbb{R}^p : u_{i\,\min} \leq u_i \leq u_{i\,\max} \text{ for all } i = 1, \ldots, p\}$$

Existence of an optimal parameter vector

- Existence follows from a standard theorem (Hinze et al., 2009)
- Theorem holds in both the periodic and the transient case if reaction terms are continuous on $L^2(Q_T)^s \times \mathbb{R}^p$
- Uniqueness only in case that (y_d, u_{ref}) is an optimal control (relevant for tests) under one of the conditions
  - $\gamma > 0$
  - $y = z \Rightarrow u = v$ for all admissible pairs $(y, u), (z, v)$

First order optimality condition - Transient case 1

Given: optimal parameter $\bar{u} \in U_{ad}$

Further assumptions

- d and b are continuously Fréchet-differentiable
- Fréchet-derivatives are Lipschitz continuous on $L^2(Q_T)^s$
- Lipschitz constants are independent of time

Transient state equation is uniquely solvable $\Rightarrow$ well-defined and continuously Fréchet-differentiable control-to-state map

$$\mathcal{S} : \mathbb{R}^p \to L^2(Q_T)^s, u \mapsto y$$

Reduced cost function $\quad f : \mathbb{R}^p \to \mathbb{R}$ with $f(u) := J(\mathcal{S}(u), u)$

First order optimality condition - Transient case 1

Given: optimal parameter $\bar{u} \in U_{ad}$

Further assumptions

- d and b are continuously Fréchet-differentiable
- Fréchet-derivatives are Lipschitz continuous on $L^2(Q_T)^s$
- Lipschitz constants are independent of time

Transient state equation is uniquely solvable $\Rightarrow$ well-defined and continuously Fréchet-differentiable control-to-state map

$$\mathcal{S} : \mathbb{R}^p \to L^2(Q_T)^s, u \mapsto y$$

Reduced cost function $\quad f : \mathbb{R}^p \to \mathbb{R}$ with $f(u) := J(\mathcal{S}(u), u)$

First order optimality condition - Transient case 2

First order optimality condition = variational inequality

$$f'(\bar{u})(u-\bar{u}) \geq 0 \quad \text{for all } u \in U_{ad}$$

(U_{ad} convex and f Fréchet-differentiable)

Define adjoint state $p \in W(0,T)^s$ by $p(T) = 0$ and

$$\int_0^T \{-\langle p_j', w_j \rangle + (\nabla p_j, \kappa \nabla w_j) + (p_j, \mathbf{v} \cdot \nabla w_j + d_y'(\bar{u}, \mathcal{S}(\bar{u}))w_j) + (p_j, b_y'(\bar{u}, \mathcal{S}(\bar{u}))w_j)\}dt = \int_0^T (\mathcal{S}(\bar{u})_j - y_{dj}, w_j)dt$$

for all $w_j \in L^2(0,T;H^1(\Omega))$, $j = 1, \ldots, s$

The left hand side is equal to

$$f'(\bar{u})(u-\bar{u}) = (p, [d_u'(\bar{u}, \mathcal{S}(\bar{u})) + b_u'(\bar{u}, \mathcal{S}(\bar{u}))](u-\bar{u}))_{L^2(Q_T)^s} + \gamma(\bar{u} - u_{ref}, u - \bar{u})_{\mathbb{R}^p}$$

First order optimality condition - Transient case 2

First order optimality condition = variational inequality

$$f'(\bar{u})(u - \bar{u}) \geq 0 \quad \text{for all } u \in U_{ad}$$

(U_{ad} convex and f Fréchet-differentiable)

Define adjoint state $p \in W(0,T)^s$ by $p(T) = 0$ and

$$\int_0^T \{-\langle p_j', w_j\rangle + (\nabla p_j, \kappa \nabla w_j) + (p_j, \mathbf{v} \cdot \nabla w_j + d_y'(\bar{u}, \mathcal{S}(\bar{u}))w_j) + (p_j, b_y'(\bar{u}, \mathcal{S}(\bar{u}))w_j)\}dt = \int_0^T (\mathcal{S}(\bar{u})_j - y_{dj}, w_j)dt$$

for all $w_j \in L^2(0,T;H^1(\Omega))$, $j = 1, \ldots, s$

The left hand side is equal to

$$f'(\bar{u})(u - \bar{u}) = (p, [d_u'(\bar{u}, \mathcal{S}(\bar{u})) + b_u'(\bar{u}, \mathcal{S}(\bar{u}))](u - \bar{u}))_{L^2(Q_T)^s} + \gamma(\bar{u} - u_{ref}, u - \bar{u})_{\mathbb{R}^p}$$

First order optimality condition - Periodic case (N-DOP model) 1

Problem: Control-to-state map not well-defined (solution of state equation not unique)

Thus: Adjoint state as a Lagrange multiplier

Problem adapted to model of N-DOP type:

$$\min_{(y,u)} J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q)^2} + \frac{\gamma}{2}|u - u_{est}|^2_{\mathbb{R}^p}$$

s. t. $\quad e(y,u) = 0$ in $Z := (W(0,T)^*)^2 \times L^2(\Omega)^2$

$\quad u \in U_{ad}$

with

$$\begin{aligned} e_1(y,u) &= y_1' + B(y_1) - \lambda y_2 - F_1(y,u) \\ e_2(y,u) &= y_2' + B(y_2) + \lambda y_2 - F_2(y,u) \\ e_3(y,u) &= y(0) - y(T) \end{aligned}$$

Optimal control $(\bar{y}, \bar{u}) \in W(0,T)^2 \times U_{ad}$ with $e(\bar{y}, \bar{u}) = 0$

First order optimality condition - Periodic case (N-DOP model) 2

Regularity condition (Zowe-Kurcyusz, 1979)

For all $z \in Z$ there exists $(y, u) \in W(0,T)^2 \times U_{ad}$ with

$$e'(\bar{y}, \bar{u})((y - \bar{y}, u - \bar{u})) = z$$

- Let $z = (z_1, z_2, z_0) \in Z = (W(0,T)^*)^2 \times L^2(\Omega)^2$
- Define $u := \bar{u} \in U_{ad}$
- Remaining task: Find $y \in W(0,T)^2$ with $e'(\bar{y}, \bar{u})((y - \bar{y}, 0)) = z$, i.e.

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 - F_{1y}'(\bar{u}, \bar{y}) y_1 &= z_1 + \bar{y}_1' + B(\bar{y}_1) - \lambda \bar{y}_2 - F_{1y}'(\bar{u}, \bar{y}) \bar{y}_1 \\ y_2' + B(y_2) + \lambda y_2 - F_{2y}'(\bar{u}, \bar{y}) y_2 &= z_2 + \bar{y}_2' + B(\bar{y}_2) + \lambda \bar{y}_2 - F_{2y}'(\bar{u}, \bar{y}) \bar{y}_2 \\ y(0) &= y(T) + z_0 \end{aligned}$$

Problem: “Inhomogeneous” periodicity condition

First order optimality condition - Periodic case (N-DOP model) 2

Regularity condition (Zowe-Kurcyusz, 1979)

For all $z \in Z$ there exists $(y, u) \in W(0,T)^2 \times U_{ad}$ with

$$e'(\bar{y}, \bar{u})((y - \bar{y}, u - \bar{u})) = z$$

- Let $z = (z_1, z_2, z_0) \in Z = (W(0,T)^*)^2 \times L^2(\Omega)^2$
- Define $u := \bar{u} \in U_{ad}$
- Remaining task: Find $y \in W(0,T)^2$ with $e'(\bar{y}, \bar{u})((y - \bar{y}, 0)) = z$, i.e.

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 - F_{1y}'(\bar{u}, \bar{y}) y_1 &= z_1 + \bar{y}_1' + B(\bar{y}_1) - \lambda \bar{y}_2 - F_{1y}'(\bar{u}, \bar{y}) \bar{y}_1 \\ y_2' + B(y_2) + \lambda y_2 - F_{2y}'(\bar{u}, \bar{y}) y_2 &= z_2 + \bar{y}_2' + B(\bar{y}_2) + \lambda \bar{y}_2 - F_{2y}'(\bar{u}, \bar{y}) \bar{y}_2 \\ y(0) &= y(T) + z_0 \end{aligned}$$

Problem: “Inhomogeneous” periodicity condition

Summary

- Mostly standard proofs in the transient case – large class of ecosystem models covered
- Periodic case
  - Existence for one important model class (N-DOP type)
  - Open questions concern uniqueness and quadratic reaction terms
  - Proof highly adapted to the model class in question
- Missing uniqueness of periodic models equations leads to problems with optimality conditions