A Newton-Picard Inexact SQP Method for Time-Periodic PDE Constrained Optimization

A. Potschka A. Küpper
H.G. Bock M. Diehl S. Engell
E. Kostina J.P. Schlöder

Interdisciplinary Center for Scientific Computing, University of Heidelberg

Department of Biochemical and Chemical Engineering, TU Dortmund

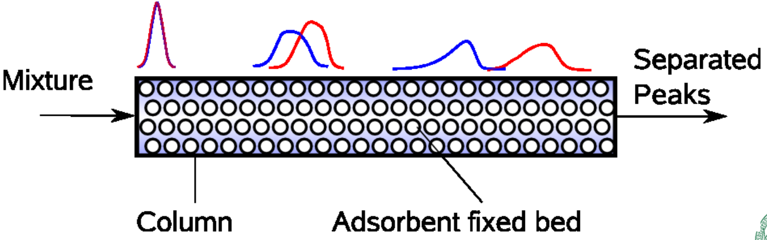
OPTEC, K.U. Leuven, Belgium Philipps-University Marburg

GAMM Workshop on PDE Constrained Optimization of Certain and Uncertain Processes
Trier, June 4, 2009

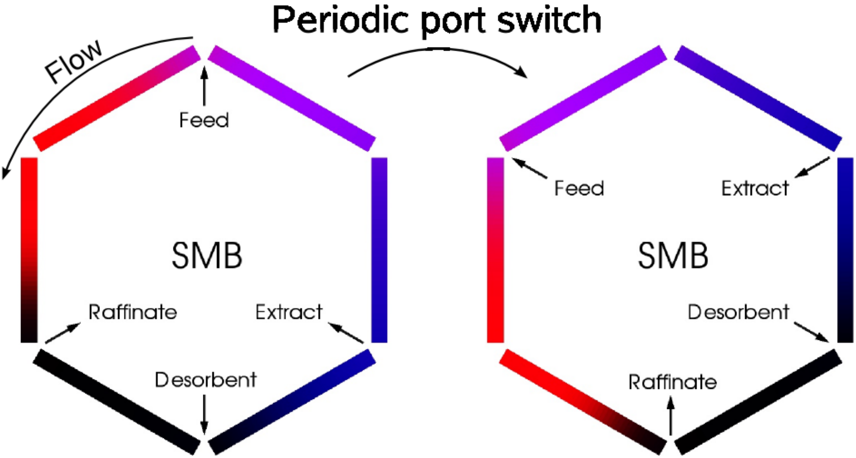
Outline

Simulated Moving Bed Processes (SMB)

- Goal: Separation of two chemical species in a solution
  - Distillation not possible
  - Eg. Glucose/fructose separation, enantiomere separation
- Used in: Soft drinks, pharmacy
- Preparative chromatography:
  Separation by different adsorption properties
- Simple batch form:



Simulated Moving Bed Principle I



- Control: Port flows, switching period
- Fixed controls: Process attains cyclic/periodic steady state

Simulated Moving Bed II

Advantages:

- Chemical: Better separation properties
- Economical: Continuous process
  $\Rightarrow$ Continuous production

Goal:

- Optimize cyclic steady state (CSS)

SMB Model

- General Rate Model (1D) [Gu, 1990, 1995]
- System of diffusion-advection-adsorption equations
- Main difficulty: Highly nonlinear coupling via algebraic isotherm equations
- E.g. Bi-Langmuir isotherm equation

$$q_i = \frac{H_i^1 c_{p,i}}{1 + \sum_{m=1}^2 k_m^1 c_{p,m}} + \frac{H_i^2 c_{p,i}}{1 + \sum_{m=1}^2 k_m^2 c_{p,m}}$$

Constrained Optimization Problem

- Optimize cyclic steady state (CSS)

$$
\begin{aligned}
\min_{y,u,T} \quad & f(y(T),u) \\
\text{s.t.} \quad & \partial_t y = L(y,u) \quad \text{in } [0,T]\times\Omega, \quad \text{plus BC on } \partial\Omega, \\
& y(0) - Py(T) = 0, \\
& h_1(y(T)) \geq 0, \quad (\text{range}(h_i) \subset \mathbb{R}^m), \\
& h_2(u(t),T) \geq 0, \quad t \in [0,T]
\end{aligned}
$$

- Main difficulty:
  Boundary value constraint on y

Discretize then Optimize

- Discretize states in space and controls in time
- Parametrize states in time by Shooting technique
  $\Rightarrow$ Large scale NLP
- Solved by Inexact SQP
- Generation of forward and adjoint directional derivatives via Internal Numerical Differentiation/Automatic Differentiation
- q: Discretized controls plus parameters and switch period
- s: Discretized initial state
- $\hat{s}(t; s, q)$: Parametrized state

Inexact SQP (a.k.a. adjoint-based SQP)

[Griewank & Walther 2002, Diehl et al. 2008, Wirsching 2006]

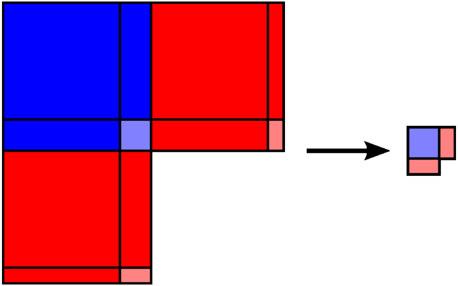
- SQP: Sequentially solve Quadratic Programs with approximated Hessians
- Inexact SQP: Also approximate constraint Jacobians
- Solve QP-KKT systems in each iteration:

$$\begin{pmatrix} H_{ss} & H_{sq} & A_s^{\mathrm{T}} & B_s^{\mathrm{T}} \\ H_{qs} & H_{qq} & A_q^{\mathrm{T}} & B_q^{\mathrm{T}} \\ A_s & A_q & 0 & 0 \\ B_s & B_q & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta s \\ \Delta q \\ -\Delta\lambda \\ -\Delta\mu_{\text{active}} \end{pmatrix} = - \begin{pmatrix} \nabla_s L \\ \nabla_q L \\ s - P\hat{s}(T; s, q) \\ h_{\text{active}}(s, q) \end{pmatrix}$$

- Calculation of ∇L by adjoint solve
- Quasi Newton Hessian approximation H (BFGS)
- Newton-Picard projective approximation for A_s (data-sparse)

Elimination of states from QP

- Use data-sparse A_s to directly eliminate Δs and periodicity constraint from QP: $\Delta s = C\Delta q + r$



- Solve small QP with standard active set QP solver
- Recover Δs
- Recover $\Delta\lambda$ by KKT transformation rules (requires one additional adjoint solve)

Newton-Picard Approximation

- Consider discretized periodicity constraint for s with fixed q:

$$s - P\hat{s}(T; s, q) = 0$$

- Use Newton-type method:

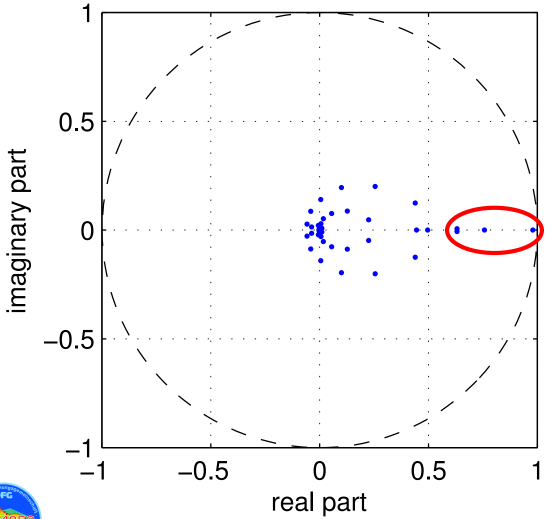
$$A_s^k \Delta s^k = -\left(s^k - P\hat{s}(T; s^k, q)\right), \quad s^{k+1} = s^k + \Delta s^k$$

- Full Newton: $A_s^k = \mathbb{I} - M^k$, where

$$M^k = P \frac{\mathrm{d}\hat{s}}{\mathrm{d}s}(T; s^k, q)$$

is the so called monodromy matrix

Typical Spectrum of the SMB M



- Cluster of EV around 0
- Few large EV
- Idea: Calculate M only for "slow" EV
- Picard for fast EV
- Philosophy: High-dimensional discretization but low-dimensional dynamics

Newton-Picard [Lust et al. 1998]

- Use expensive Newton method on "slow" modes
- Use inexpensive functional (Picard) iteration on "fast" modes
- Let orthonormal $V_p \in \mathbb{R}^{n_s \times p}$ span the "slow" invariant subspace, i.e. the p-dimensional dominant subspace of M
- Approximation of $\mathbb{I} - M$:

$$A_s = \mathbb{I} - M V_p V_p^{\mathrm{T}},$$

- For A_s and A_s^{-1}, only the action MV_p is needed
- Can be evaluated by p directional forward derivatives of DE
- Algorithmically, V_p is only approximated with a piggy-back Subspace Iteration simultaneously with the Newton-type method
- Picard contraction can be improved by introduction of a shift [Potschka et al. 2008]

Local Convergence I

- By increasing p, A_s can be ameliorated
- Algorithmically, an estimate for the inexactness is available from the Subspace Iteration for V_p

$$\sigma_{\mathrm{r}}(A_s - (\mathbb{I} - M)) < \lambda_p$$

Local Convergence II [Wirsching et al., 2006]

Assumptions:

- $w^* = (s^*, q^*, \lambda^*, \mu^*)$ KKT-point
- LICQ and strict complementarity holds in w^*
- H_k positive definite, bounded
- Exact KKT matrix $\hat{K}(w_k)$, approximate K_k
- K_k^{-1} uniformly bounded for all k
- There exists $\kappa < 1$ such that

$$\left\| K_{k+1}^{-1} \left(K_k - \hat{K}(w_k + \alpha \Delta w_k) \right) \Delta w_k \right\| \leq \kappa \left\| \Delta w_k \right\|, \quad \forall \alpha \in [0, 1]$$

- Full steps

Then:

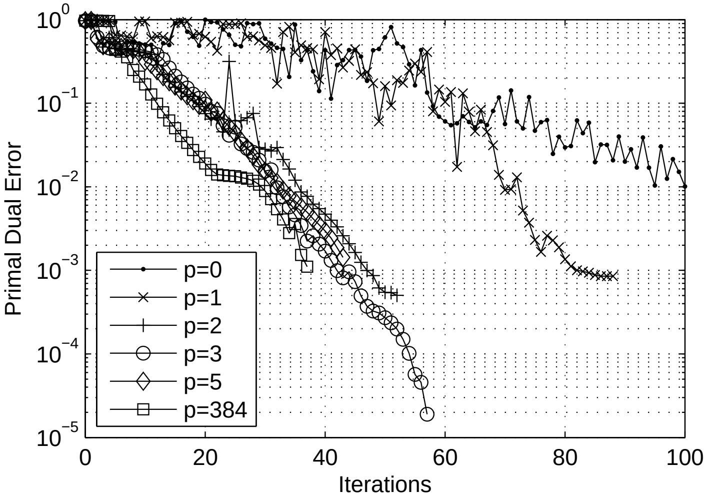
- Stationary active set and q-linear convergence in a neighborhood of w^* with convergence rate κ

Complexity Analysis

Per Iteration	Newton-Picard iSQP	SQP
Forward solves	1	1
Forward dir. der.	$n_u \frac{3M+1}{2} + S \cdot p + 1$	$n_u \frac{M+1}{2} + n_s$
Adjoint solves	$3\ (2)$	0

- M control intervals (typically $\leq$ 20)
- p dimension of subspace (typically 1–20)
- S subspace iterations (typically 1–5)
- Effort for linear algebra negligible
- Number of solves per Newton-Picard iSQP iteration independent of n_s

Numerical Convergence of Newton-Picard iSQP



Summary

- Newton-Picard Inexact SQP Method: Simultaneous approach for solution of time-periodic PDE optimization problems
- Exploitation of low-dimensional dynamics of a high-dimensional discretization
- Used to solve SMB application