Interior-Point Methods for Dynamic Optimization

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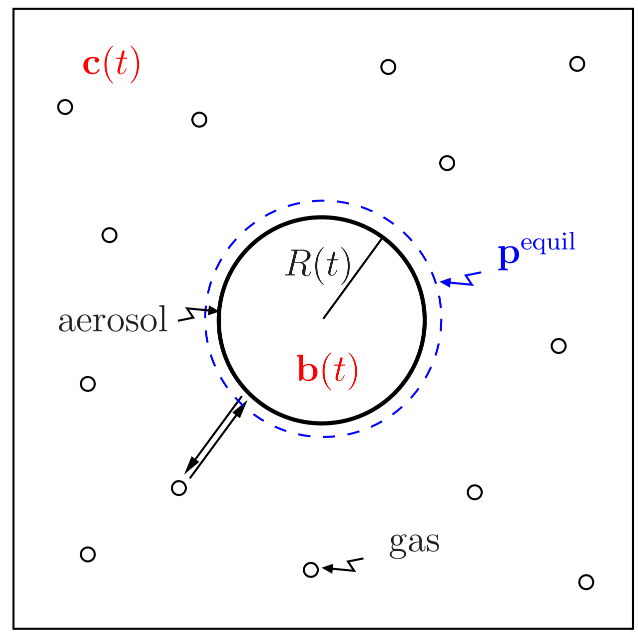
Motivations

- Modeling and computation of the physical state and chemical composition of atmospheric aerosol particles.
- *"The chemical and physical properties of aerosols are needed to estimate and predict direct and indirect climate forcing"*, (IPCC, 2001).

- Constrained optimization problem models the thermodynamic equilibrium.
- Differential equations model the mass transfer between the particle and the gas.



Model Problem

$$
\begin{aligned}
\frac{d}{dt}\mathbf{b}(t) \quad &= \quad f(t, \mathbf{b}(t), \mathbf{z}(t)), \quad \mathbf{b}(0) = \mathbf{b}_0, \\
\mathbf{z}(t) = \arg\min_{\mathbf{z}^\star} \quad & \quad g(\mathbf{z}^\star) \\
\text{s. t.} \quad & \quad A\mathbf{z}^\star = \mathbf{b}(t), \\
& \quad \mathbf{z}^\star \geq 0.
\end{aligned}
$$

i.e. $\mathbf{z}(t)$ is the **global minimum** of the optimization problem at time $t \in (0, T)$.

- Coupling between an optimization problem and a differential equation.
- Minimization of the internal energy of the particle, under mass conservation constraints and positiveness of the concentrations.
- The inequality constraints imply that the variables $\mathbf{z}(t)$ are truncated and not smooth.

Time Discretization

- Consider a time step h, a time discretization $t^0 = 0 < t^1 < t^2 < \ldots < t^n = nh < \ldots$ and $\mathbf{b}^n \simeq \mathbf{b}(t^n)$, $\mathbf{z}^n \simeq \mathbf{z}(t^n)$.
- An implicit first order discretization of the differential equation reads, for all $n \geq 0$:

$$
\begin{aligned}
\frac{\mathbf{b}^{n+1} - \mathbf{b}^n}{h} \quad &= \quad f(t^{n+1}, \mathbf{b}^{n+1}, \mathbf{z}^{n+1}), \qquad \mathbf{b}^0 = \mathbf{b}_0, \\
\mathbf{z}^{n+1} = \arg\min_{\mathbf{z}^\star} \quad & \quad g(\mathbf{z}^\star), \\
\text{s. t.} \quad & \quad A\mathbf{z}^\star = \mathbf{b}^{n+1}, \\
& \quad \mathbf{z}^\star \geq 0.
\end{aligned}
$$

- Coupling of the optimization problem with one additional algebraic relation.
- The optimization problem is replaced with the relaxed first order (Karush-Kuhn-Tucker) conditions.

Interior-Point Method and KKT conditions

$$
\begin{aligned}
&\frac{\mathbf{b}^{n+1}-\mathbf{b}^{n}}{h} = f(t^{n+1},\mathbf{b}^{n+1},\mathbf{z}^{n+1}),\\
&\nabla g(\mathbf{z}^{n+1}) + A^T\boldsymbol{\lambda}^{n+1} - \boldsymbol{\theta}^{n+1} = 0,\\
&A\mathbf{z}^{n+1} = \mathbf{b}^{n+1},\\
&\boldsymbol{\theta}^{n+1}\mathbf{z}^{n+1} = 0,\\
&\boldsymbol{\theta}^{n+1} \geq 0, \quad \mathbf{z}^{n+1} \geq 0.
\end{aligned}
$$

- $\boldsymbol{\lambda}^{n+1}$ is the Lagrange multiplier related to the equality constraint.
- $\boldsymbol{\theta}^{n+1}$ is the Kuhn-Tucker multiplier related to the inequality constraint.
- Equivalence for convex optimization, but not necessarily for the non-convex case.

Interior-Point Method and KKT conditions

$$\frac{\mathbf{b}^{n+1} - \mathbf{b}^n}{h} = f(t^{n+1}, \mathbf{b}^{n+1}, \mathbf{z}^{n+1}),$$
$$\nabla g(\mathbf{z}^{n+1}) + A^T \boldsymbol{\lambda}^{n+1} - \boldsymbol{\theta}^{n+1} = 0,$$
$$A\mathbf{z}^{n+1} = \mathbf{b}^{n+1},$$
$$\boldsymbol{\theta}^{n+1}\mathbf{z}^{n+1} = \nu,$$
$$\boldsymbol{\theta}^{n+1} > 0, \quad \mathbf{z}^{n+1} > 0.$$

- ν is a penalty parameter, which tends to zero **at each time step.**
- Algorithm provides a sequence $\mathbf{z}^{n+1} > \mathbf{0}$ for all $n \geq 0$ and converges ultimately to a point $\mathbf{z}^{n+1}$ possibly on the boundary.

Newton System

- At each time step and for a given value of ν, a Newton method is used to solve the system of nonlinear equations.

$$\begin{bmatrix} \frac{1}{h}\mathbf{I} - \nabla_{\mathbf{b}^{n+1}} f & -\nabla_{\mathbf{z}^{n+1}} f & -\nabla_{\boldsymbol{\lambda}^{n+1}} f \\ 0 & \nabla^2 g(\mathbf{z}^{n+1}) + \frac{\nu}{(\mathbf{z}^{n+1})^2} & A^T \\ -\mathbf{I} & A & 0 \end{bmatrix} \begin{bmatrix} \mathbf{p_b} \\ \mathbf{p_z} \\ \mathbf{p}_{\boldsymbol{\lambda}} \end{bmatrix} = \begin{bmatrix} \mathbf{r_b} \\ \mathbf{r_z} \\ \mathbf{r}_{\boldsymbol{\lambda}} \end{bmatrix}$$

- Newton method incorporated in the interior-point iterations (decreasing values of the parameter ν).
- Resolution of the linear system with direct decomposition techniques, with control of the inertia (Sequential quadratic programming or Schur complement techniques).

Cold-Start vs. Warm-Start

When the objective function is non-convex:

- With **cold-start techniques**, the optimization algorithm converges to the global minimum.
  - Accurate detection of active/inactive constraints.
- However, with **warm-start techniques**, the optimization algorithm may converge to a local minimum.
  - Bifurcation to branches of local minima.
  - Activation/deactivation of inequality constraints can be missed!
- Tracking techniques for the time of activation/deactivation of the constraints $\mathbf{z} \geq 0$.
  - Automatic detection of discontinuities to allow large time steps.

Tracking of Activations

- Activation/deactivation of an inequality constraint $\mathbf{z}_i \geq 0$ require event location techniques.
  - Deactivation: $\mathbf{z}_i > 0 \rightarrow \mathbf{z}_i = 0$.
  - Activation: $\mathbf{z}_i = 0 \rightarrow \mathbf{z}_i > 0$.

- Two steps procedure:
  - Find the fraction of time step to reach activation/deactivation.
  - Compute the variables at the time of impact with high order methods (in order to conserve the accuracy of the algorithm).

- First order approximation:

$$0 = \mathbf{z}_i(t^n + h^\star) = \mathbf{z}_i(t^n) + h^\star \frac{d\mathbf{z}_i}{dt}(t^n) + \mathcal{O}((h^\star)^2),$$

Tracking of Activations

- Activation/deactivation of an inequality constraint $\mathbf{z}_i \geq 0$ require event location techniques.
  - Deactivation: $\mathbf{z}_i > 0 \rightarrow \mathbf{z}_i = 0$.
  - Activation: $\mathbf{z}_i = 0 \rightarrow \mathbf{z}_i > 0$.
- Two steps procedure:
  - Find the fraction of time step to reach activation/deactivation.
  - Compute the variables at the time of impact with high order methods (in order to conserve the accuracy of the algorithm).
- First order approximation:

$$h^\star \simeq -\frac{\mathbf{z}_i(t^n)}{\dfrac{d\mathbf{z}_i}{dt}(t^n)}.$$

Sensitivity Analysis

- Approximation of $\dfrac{d\mathbf{z}_i}{dt}(t^n)$ by differentiation of the KKT system:

$$\begin{bmatrix} \nabla^2 g(\mathbf{z}_\alpha) + \dfrac{\nu}{(\mathbf{z}^{n+1})^2} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \dfrac{d\mathbf{z}}{dt}(t^n) \\ \dfrac{d\boldsymbol{\lambda}}{dt}(t^n) \end{bmatrix} = \begin{bmatrix} 0 \\ \dfrac{d\mathbf{b}}{dt}(t^n) \end{bmatrix}$$

- The right-hand side is approximated by the numerical fluxes

$$\frac{d\mathbf{b}}{dt}(t^n) \simeq f(t^n, \mathbf{b}^n, \mathbf{z}^n) \qquad \text{or}$$

$$\frac{d\mathbf{b}}{dt}(t^n) \simeq f(t^n, \mathbf{b}^n, \mathbf{z}^n) + \frac{h^\star}{2h}\left(f(t^n, \mathbf{b}^n, \mathbf{z}^n) - f(t^{n-1}, \mathbf{b}^{n-1}, \mathbf{z}^{n-1})\right).$$

- Second order sensitivity analysis to approximate the second term in the Taylor expansion (future work).

Multistep Techniques

- Once the time step $h^\star$ is obtained, multisteps methods are used for the approximation of the differential variables $\mathbf{b}$ satisfying $\dfrac{d\mathbf{b}}{dt}(t) = f(t, \mathbf{b}(t), \mathbf{z}(t))$ at time $t^n + h^\star$ (Adams 2-steps).
- Predictor:

$$\tilde{\mathbf{b}}^{n+1}(h^\star) = \mathbf{b}^n + h^\star \left[\left(1 + \frac{h^\star}{2h}\right) f(t^n, \mathbf{b}^n, \mathbf{z}^n) - \frac{h^\star}{2h} f(t^{n-1}, \mathbf{b}^{n-1}, \mathbf{z}^{n-1}) \right]$$

- Corrector:

$$\mathbf{b}^{n+1} = \mathbf{b}^n + \frac{1}{2} h^\star \left(f(t^n + h^\star, \tilde{\mathbf{b}}^{n+1}(h^\star), \tilde{\mathbf{z}}^{n+1}(h^\star)) + f(t^n, \mathbf{b}^n, \mathbf{z}^n) \right)$$

Application : Phase Equilibrium Problem

- Global optimization problem for the modeling of phase separation into different liquid phases.

$$
\begin{aligned}
\min_{\mathbf{n}_\alpha} \quad & \sum_{\alpha=1}^{N+1} g(\mathbf{n}_\alpha) \\
\text{s. t.} \quad & \sum_{\alpha=1}^{N+1} \mathbf{n}_\alpha = \mathbf{b}, \\
& \mathbf{n}_\alpha \geq 0, \quad \alpha = 1, \ldots, N+1.
\end{aligned}
$$

- $\mathbf{n}_\alpha$ is the chemical concentration in the phase α.
- g is homogeneous of degree one.
- Split $\mathbf{n}_\alpha = y_\alpha \mathbf{x}_\alpha$, where y_α is the total number of moles in phase α and $\mathbf{x}_\alpha$ is the mole-fraction.

Application : Phase Equilibrium Problem

- Global optimization problem for the modeling of phase separation into different liquid phases.

$$\begin{array}{ll} \displaystyle\min_{y_\alpha \mathbf{x}_\alpha} & \displaystyle\sum_{\alpha=1}^{N+1} y_\alpha g(\mathbf{x}_\alpha) \\ \text{s. t.} & \displaystyle\sum_{\alpha=1}^{N+1} y_\alpha \mathbf{x}_\alpha = \mathbf{b}, \\ & y_\alpha \geq 0, \quad \alpha = 1, \ldots, N+1. \\ & \mathbf{e}^T \mathbf{x}_\alpha = 1, \quad \mathbf{x}_\alpha > 0, \quad \alpha = 1, \ldots, N+1. \end{array}$$

- y_α is the total number of moles in phase α and $\mathbf{x}_\alpha$ is the (normalized) mole-fraction.
- Global optimization corresponds to the determination of the convex envelope of the function g, or to the determination of the supporting tangent plane.

Application : Phase Equilibrium Problem

- Global optimization problem for the modeling of phase separation into different liquid phases.

$$
\begin{aligned}
\min_{y_\alpha \mathbf{x}_\alpha} \quad & \sum_{\alpha=1}^{N+1} y_\alpha g(\mathbf{x}_\alpha) \\
\text{s. t.} \quad & \sum_{\alpha=1}^{N+1} y_\alpha \mathbf{x}_\alpha = \mathbf{b}, \\
& y_\alpha \geq 0, \quad \alpha = 1, \ldots, N+1. \\
& \mathbf{e}^T \mathbf{x}_\alpha = 1, \quad \mathbf{x}_\alpha > 0, \quad \alpha = 1, \ldots, N+1.
\end{aligned}
$$

- The inequality constraints $y_\alpha \geq 0$ are treated with an interior-point approach.
- Introduction of a log/barrier penalization term

Application : Phase Equilibrium Problem

- Global optimization problem for the modeling of phase separation into different liquid phases.

$$\min_{y_\alpha \mathbf{x}_\alpha} \quad \sum_{\alpha=1}^{N+1} y_\alpha g(\mathbf{x}_\alpha) - \nu \sum_{\alpha=1}^{N+1} \ln(y_\alpha)$$

$$\text{s. t.} \quad \sum_{\alpha=1}^{N+1} y_\alpha \mathbf{x}_\alpha = \mathbf{b},$$

$$\mathbf{e}^T \mathbf{x}_\alpha = 1, \quad \mathbf{x}_\alpha > 0, \quad \alpha = 1, \ldots, N+1.$$

- **Result:** A KKT point is a global minimum if and only if $\nabla^2 g(\mathbf{x}_\alpha) > 0$ when $y_\alpha > 0$.
- **Result:** For a "good" initial guess of the primal and dual variables and the relaxation parameter, the interior-point method converges to the global optimum.

Dynamic Optimization

- Coupling of the evolution of the gas concentrations with the optimization problem for the modeling of mass transfer.

$$
\begin{aligned}
\frac{d}{dt}\mathbf{b}(t) &= \mathbf{h}\left(\mathbf{b}^{\mathrm{tot}} - \mathbf{b}(t) - \mathbf{C}\exp\left(\nabla g(\mathbf{x}_\alpha(t))\right)\right) \\
\min_{y_\alpha(t),\mathbf{x}_\alpha(t)} &\quad \sum_{\alpha=1}^{N+1} y_\alpha(t) g(\mathbf{x}_\alpha(t)) - \nu \sum_{\alpha=1}^{N+1} \ln(y_\alpha(t)) \\
\text{s. t.} &\quad \sum_{\alpha=1}^{N+1} y_\alpha(t)\mathbf{x}_\alpha(t) = \mathbf{b}(t), \\
&\quad \mathbf{e}^T\mathbf{x}_\alpha(t) - 1 = 0, \quad \mathbf{x}_\alpha(t) > 0, \quad \alpha = 1, \ldots, N+1,
\end{aligned}
$$

Dynamic Optimization

- Discretization in time to obtain an extended optimization problem at each time step.

$$
\begin{aligned}
\frac{\mathbf{b}^{n+1}-\mathbf{b}^{n}}{h} \quad &= \quad \mathbf{h}\left(\mathbf{b}^{tot}-\mathbf{b}^{n+1}-\mathbf{C}\exp\left(\nabla g(\mathbf{x}_\alpha^{n+1})\right)\right) \\
\min_{y_\alpha^{n+1},\mathbf{x}_\alpha^{n+1}} \quad & \quad \sum_{\alpha=1}^{N+1} y_\alpha^{n+1} g(\mathbf{x}_\alpha^{n+1}) - \nu \sum_{\alpha=1}^{N+1} \ln(y_\alpha^{n+1}) \\
\text{s. t.} \quad & \quad \sum_{\alpha=1}^{N+1} y_\alpha^{n+1}\mathbf{x}_\alpha^{n+1} = \mathbf{b}^{n+1}, \\
& \quad \mathbf{e}^T\mathbf{x}_\alpha^{n+1} - 1 = 0, \quad \mathbf{x}_\alpha^{n+1} > 0, \quad \alpha = 1,\ldots,N+1,
\end{aligned}
$$

Dynamic Optimization

- Replacement of the optimization problem by its first order optimality conditions.

$$\frac{\mathbf{b}^{n+1} - \mathbf{b}^n}{h} = \mathbf{h}\left(\mathbf{b}^{tot} - \mathbf{b}^{n+1} - \mathbf{C}\exp\left(-\boldsymbol{\lambda}^{n+1}\right)\right)$$

$$y_\alpha^{n+1}\left(\nabla g(\mathbf{x}_\alpha^{n+1}) + \boldsymbol{\lambda}^{n+1}\right) + \zeta_\alpha^{n+1}\mathbf{e} = 0, \quad \alpha = 1, \ldots, N+1,$$

$$g(\mathbf{x}_\alpha^{n+1}) + (\boldsymbol{\lambda}^{n+1})^T\mathbf{x}_\alpha^{n+1} - \frac{\nu}{y_\alpha^{n+1}} = 0, \quad \alpha = 1, \ldots, N+1,$$

$$\sum_{\alpha=1}^{N+1} y_\alpha^{n+1}\mathbf{x}_\alpha^{n+1} - \mathbf{b}^{n+1} = 0, \quad \mathbf{e}^T\mathbf{x}_\alpha^{n+1} - 1 = 0$$

- The introduction of the interior-point parameter $\nu \to 0$ induces discontinuities in the trajectories.

Newton System

$$\begin{bmatrix} \mathbf{H_b} & 0 & 0 & \mathbf{B} & 0 \\ 0 & y_\alpha \nabla^2 g(\mathbf{x}_\alpha) & \nabla g(\mathbf{x}_\alpha) + \boldsymbol{\lambda} & y_\alpha & \mathbf{e} \\ 0 & (\nabla g(\mathbf{x}_\alpha) + \boldsymbol{\lambda})^T & \dfrac{\nu}{(y_\alpha)^2} & (\mathbf{x}_\alpha)^T & 0 \\ -\mathbf{I} & (y_\alpha)^T & \mathbf{x}_\alpha & 0 & 0 \\ 0 & \mathbf{e}^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{p_b} \\ \mathbf{p_x} \\ \mathbf{p}_y \\ \mathbf{p}_{\boldsymbol{\lambda}} \\ \mathbf{p}_{\zeta_\alpha} \end{bmatrix} = \begin{bmatrix} \mathbf{r_b} \\ \mathbf{r_x} \\ \mathbf{r}_y \\ \mathbf{r}_{\boldsymbol{\lambda}} \\ \mathbf{r}_{\zeta_\alpha} \end{bmatrix}$$

- Karush-Kuhn-Tucker Newton system is block-structured and ill-conditioned.
- $\mathbf{H_b}$ is positive definite.
- Design of numerical algebra techniques, via sequential quadratic programming or Schur complement techniques.
- System can be symmetrized with a change of variables.

SQP Algorithm

- The KKT system can be expressed as the convex problem:

$$\min_{\mathbf{p_b}} \left\{ \frac{1}{2}\mathbf{p_b}^T \mathbf{H_b} \mathbf{p_b} + \tilde{\mathbf{r}}_\mathbf{b}^T \mathbf{p_b} + \mathcal{G}(\mathbf{p_b}) \right\},$$

where $\mathcal{G}(\mathbf{p_b})$ is the optimum value of a quadratic problem:

$$\min_{\mathbf{p}_{\mathbf{x}_\alpha}, \mathbf{p}_{y_\alpha}} \quad \frac{1}{2}\sum_{\alpha=1}^{P} (\mathbf{p}_{\mathbf{x}_\alpha} \ \ \mathbf{p}_{y_\alpha})^T \begin{pmatrix} y_\alpha \nabla^2 g(\mathbf{x}_\alpha) & \nabla g(\mathbf{x}_\alpha) + \boldsymbol{\lambda} \\ (\nabla g(\mathbf{x}_\alpha) + \boldsymbol{\lambda})^T & \dfrac{\nu}{y_\alpha^2} \end{pmatrix} \begin{pmatrix} \mathbf{p}_{\mathbf{x}_\alpha} \\ \mathbf{p}_{y_\alpha} \end{pmatrix}$$

$$+ \sum_{\alpha=1}^{N+1} (\tilde{\mathbf{r}}_{\mathbf{x}_\alpha} \ \ \tilde{\mathbf{r}}_{y_\alpha})^T \begin{pmatrix} \mathbf{p}_{\mathbf{x}_\alpha} \\ \mathbf{p}_{y_\alpha} \end{pmatrix}$$

$$\text{s. t.} \quad \sum_{\alpha=1}^{N+1} y_\alpha \mathbf{p}_{\mathbf{x}_\alpha} + \sum_{\alpha=1}^{P} \mathbf{x}_\alpha \mathbf{p}_{y_\alpha} = \mathbf{r}_{\boldsymbol{\lambda}} + \mathbf{p_b}, \quad \sum_{\alpha=1}^{N+1} \mathbf{e}^T \mathbf{p}_{\mathbf{x}_\alpha} = \mathbf{r}_\zeta.$$

SQP Algorithm

- The KKT system can be expressed as the convex problem:

$$\min_{\mathbf{p_b}} \left\{ \frac{1}{2}\mathbf{p_b}^T \mathbf{H_b} \mathbf{p_b} + \tilde{\mathbf{r}}_\mathbf{b}^T \mathbf{p_b} + \mathcal{G}(\mathbf{p_b}) \right\},$$

- **Result:** In a neighborhood of a KKT point, the displacements $\mathbf{p}_{\mathbf{x}_\alpha}$, $\alpha = 1, \ldots, P$ and $\mathbf{p_y} = (\mathbf{p}_{y_\alpha})_{\alpha=1}^P$ are linear functions of $\mathbf{p}_g$:

$$\begin{aligned} \mathbf{p_y} &= \tilde{\mathbf{A}}_\mathbf{y} \mathbf{p}_g + \tilde{\mathbf{B}}_\mathbf{y} \\ \mathbf{p}_{\mathbf{x}_\alpha} &= \tilde{\mathbf{A}}_{\mathbf{x}_\alpha} \mathbf{p}_g + \tilde{\mathbf{B}}_{\mathbf{x}_\alpha}, \quad \alpha = 1, \ldots, P. \end{aligned}$$

SQP Algorithm

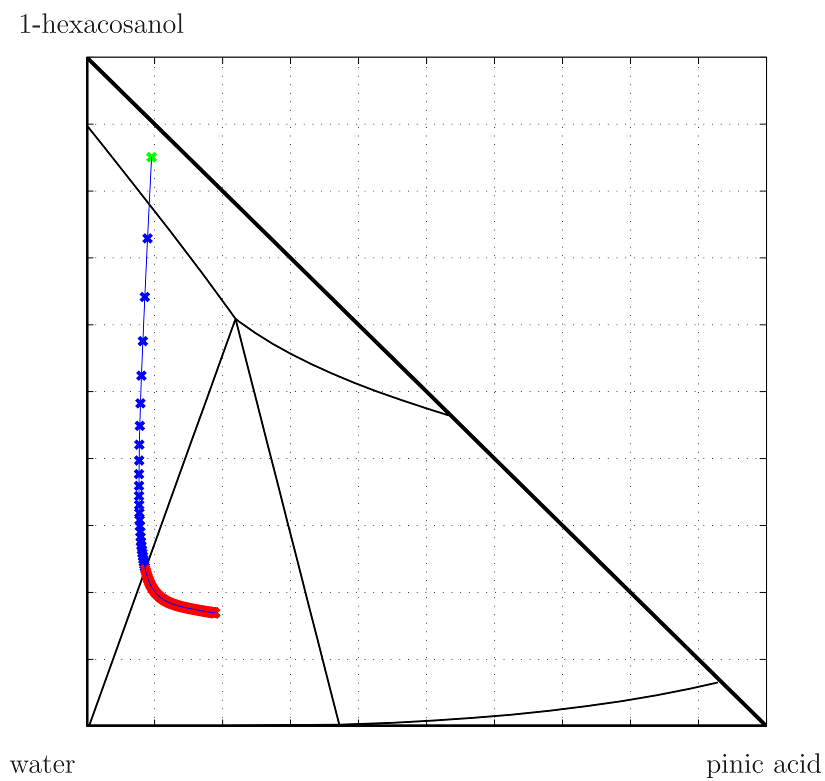
- The KKT system can be expressed as the convex problem:

$$\min_{\mathbf{p_b}} \left\{ \frac{1}{2} \mathbf{p_b}^T \mathbf{H_b} \mathbf{p_b} + \tilde{\mathbf{r}}_{\mathbf{b}}^T \mathbf{p_b} + \mathcal{G}(\mathbf{p_b}) \right\},$$

- The displacements $\mathbf{p}_g$ are solution of an unconstrained convex minimization problem that admits a unique global minimizer, due to the positiveness of $\mathbf{H}_g$.
- Once the displacements $\mathbf{p}_g$ are known, the other increments are computed independently of the addition of the variables $\mathbf{b}$.

Numerical Results

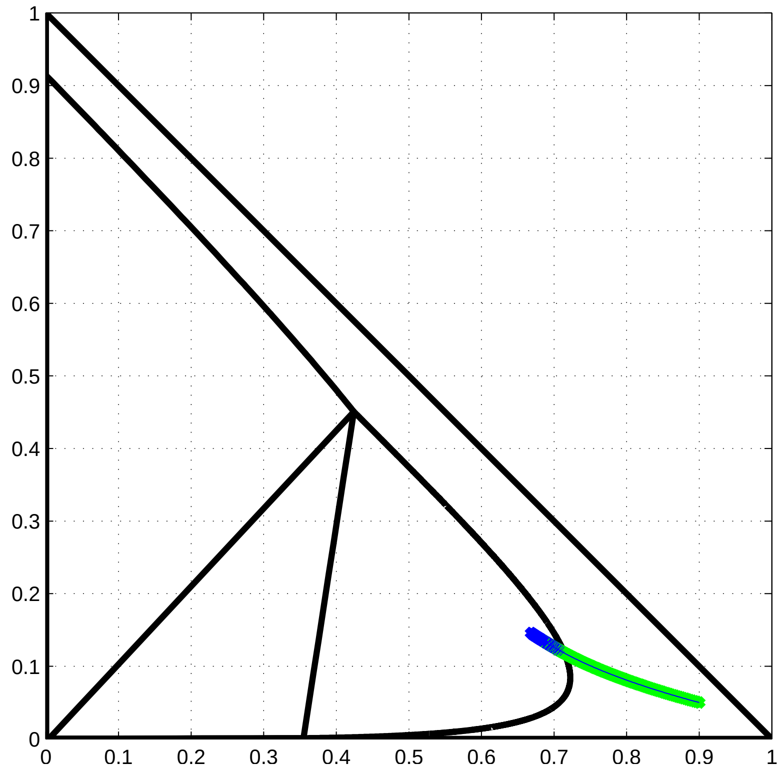
- Trajectory of the (normalized) feed vector $\mathbf{b}(t)$ (mixing inside the particle). Convergence to a stationary solution.



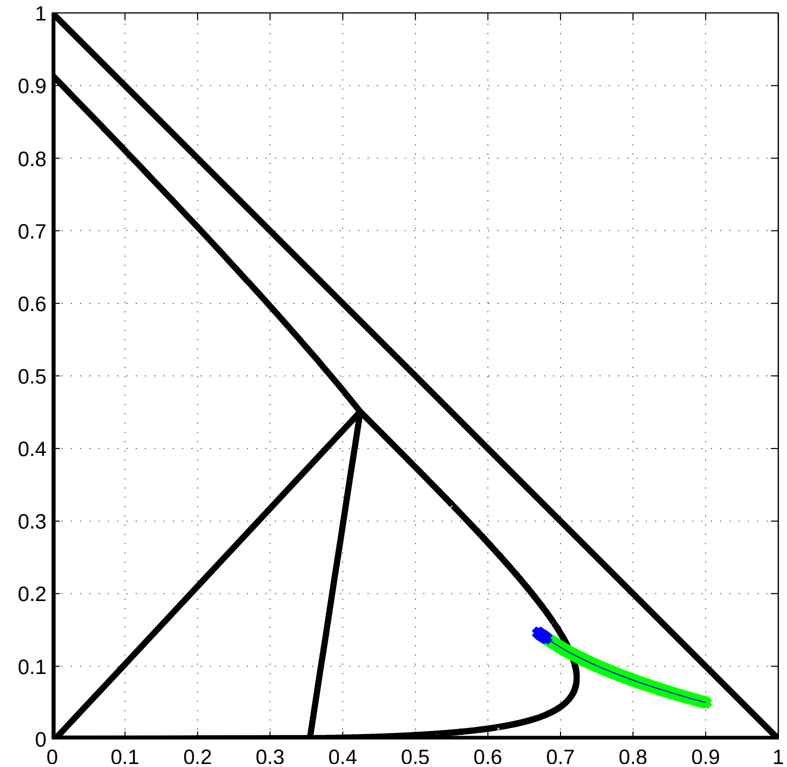
- Detection of the phase separations with cold starts.
- What happens with warm starts ??

Warm-Start Effect

- Influence of warm-start approach when computing the trajectory.



Cold-starts



Warm-starts

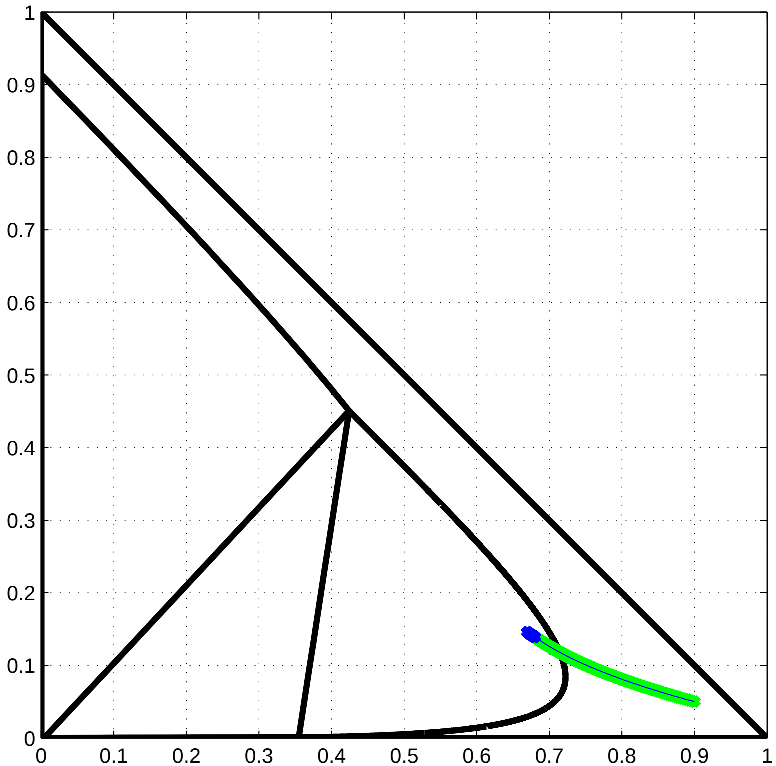
- Various warm-starts allow the speed-up, but miss the time of activation/deactivation!

Tracking Effect

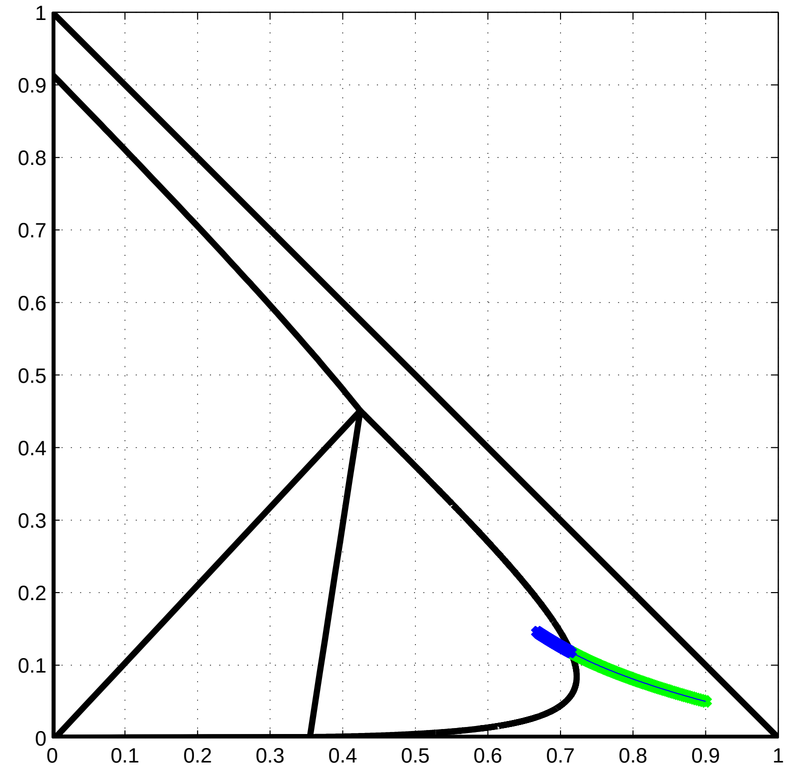
- Warm-start techniques with backtracking and detection procedure.
- **Algorithm:**
  - Perform the algorithm with warm-start techniques.
  - Once the error is detected (*e.g.* loss of second order conditions, ill-conditioning, wrong convergence properties, ...), backtrack on the trajectory, with cold-starts.
  - Once the time interval $[t^n, t^{n+1}]$ where the activation/deactivation happens is detected, use tracking techniques to determine $h^\star$ and the point of impact.
  - Restart with warm-start techniques from the point of impact.

Tracking Effect

- Warm-start techniques with backtracking and detection procedure.
- Evolution of $\mathbf{b}(t)$:



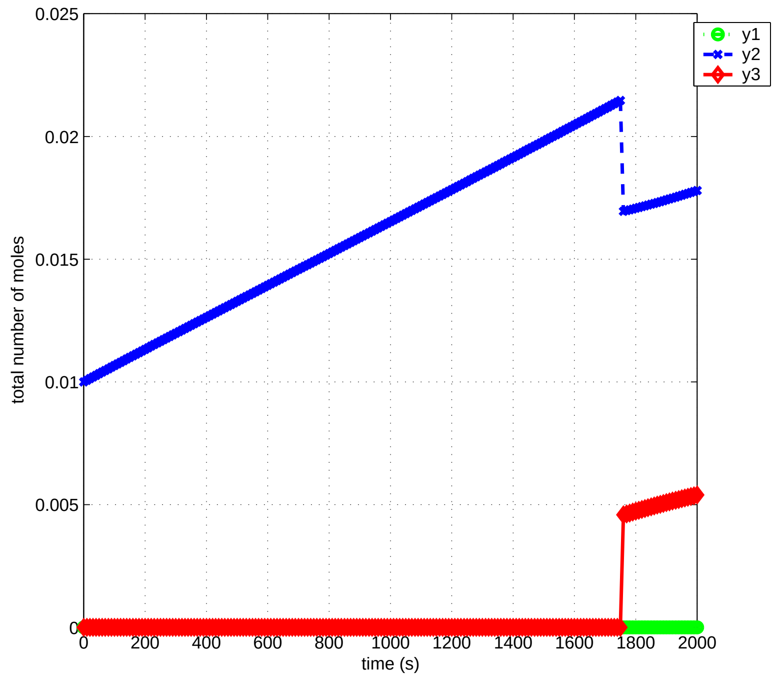
Warm-start



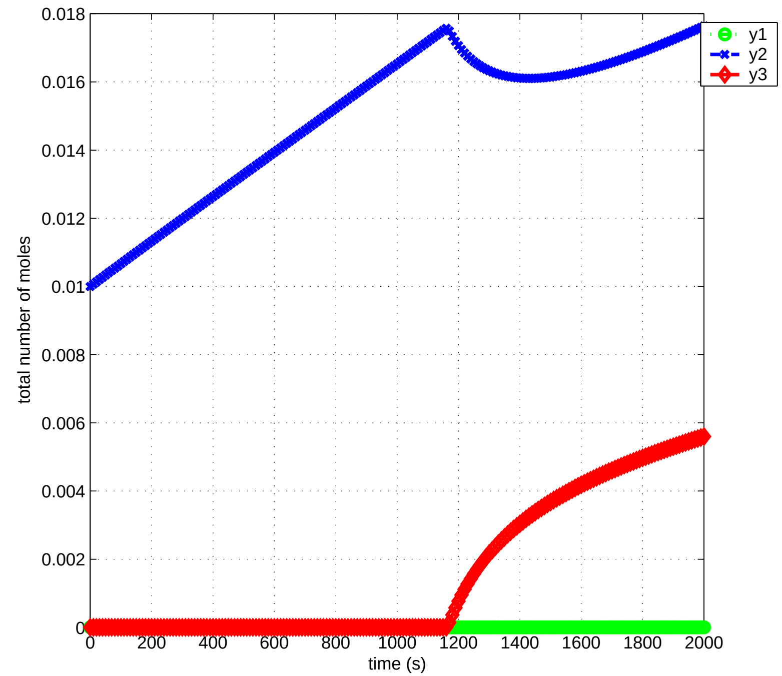
Warm-start with detection

Tracking Effect

- Warm-start techniques with backtracking and detection procedure.
- Evolution of $y_\alpha(t)$:



Warm-start

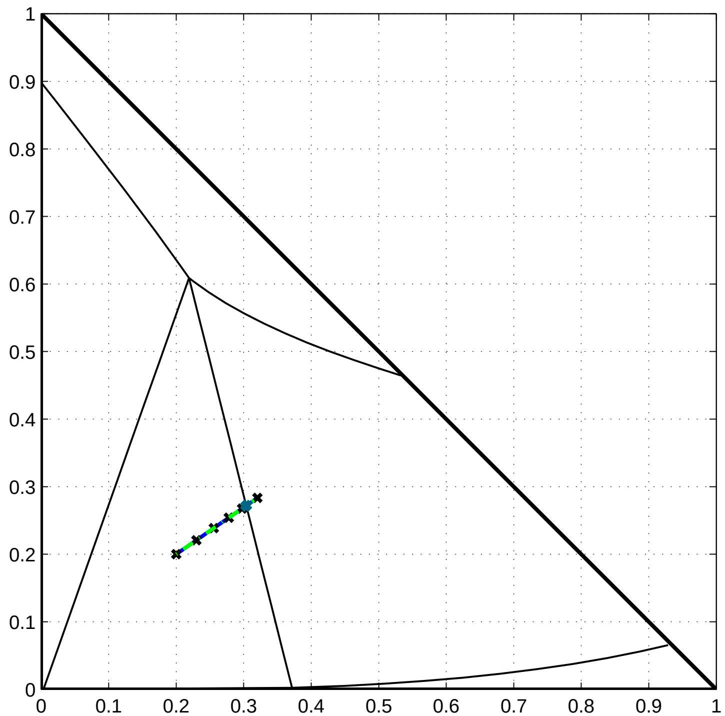


Warm-start with detection

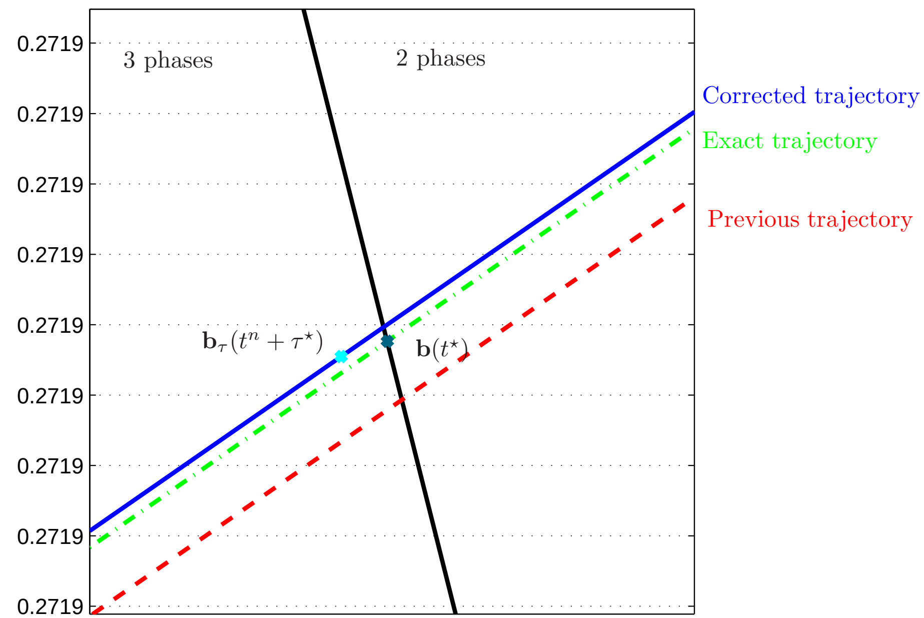
- Consistent with partial theoretical results.

Constraint Deactivation

- Time of impact $t^\star$ when $y_\alpha = 0$. Transition from 3 to 2 phases.



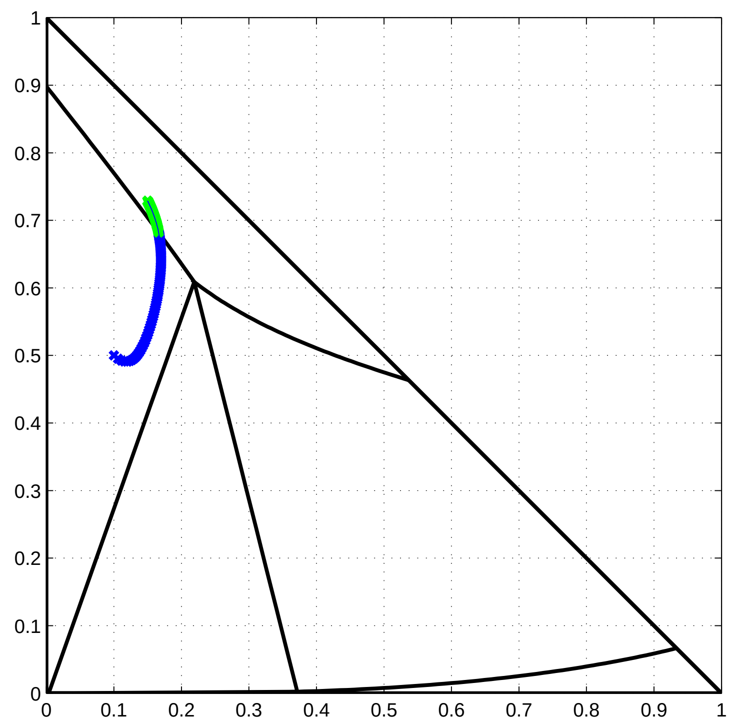
Trajectory



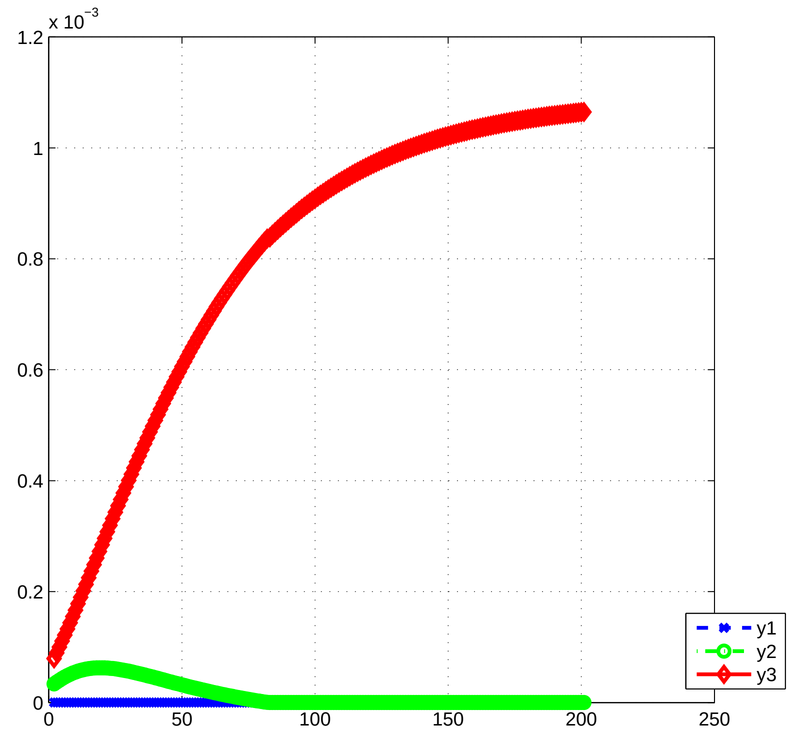
Trajectory (zoom)

Constraint Deactivation

- Time of impact $t^\star$ when $y_\alpha = 0$.Transition from 2 phases to 1 phase.



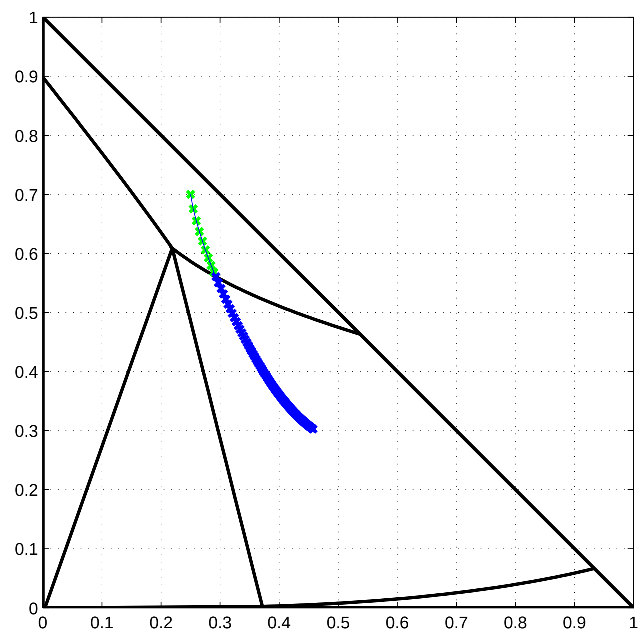
Trajectory



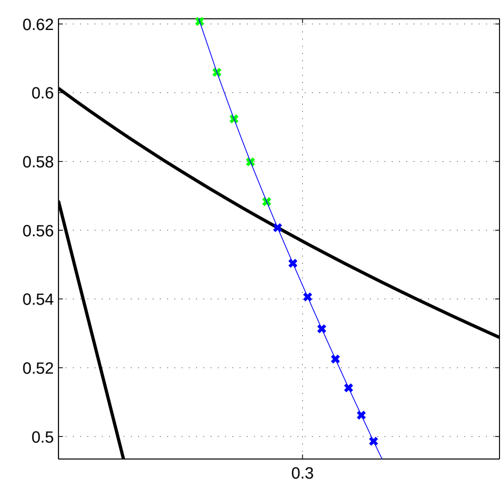
Values of y_α

Constraint Activation

- No dual variables available to replace y_α (high oscillation of dual variables).
- Geometric reconstruction of the interface with least-squares, interpolation, etc.
- Computation of intersection point of the trajectory with given reconstructed interface.



Trajectory



Trajectory (zoom)

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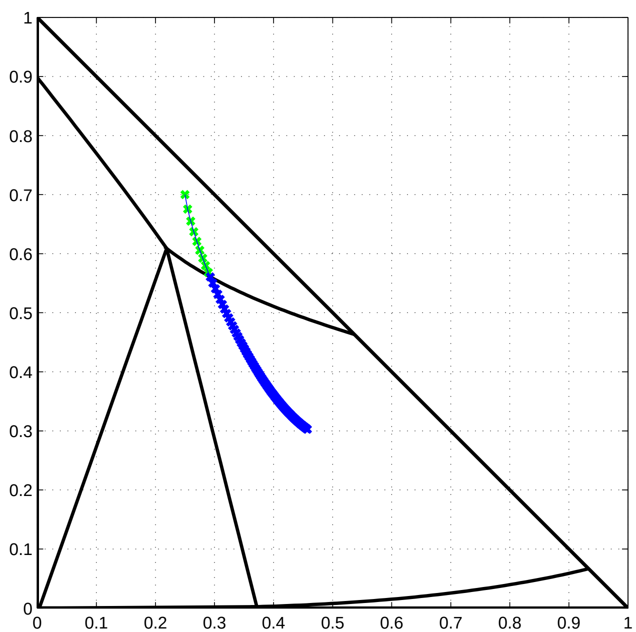
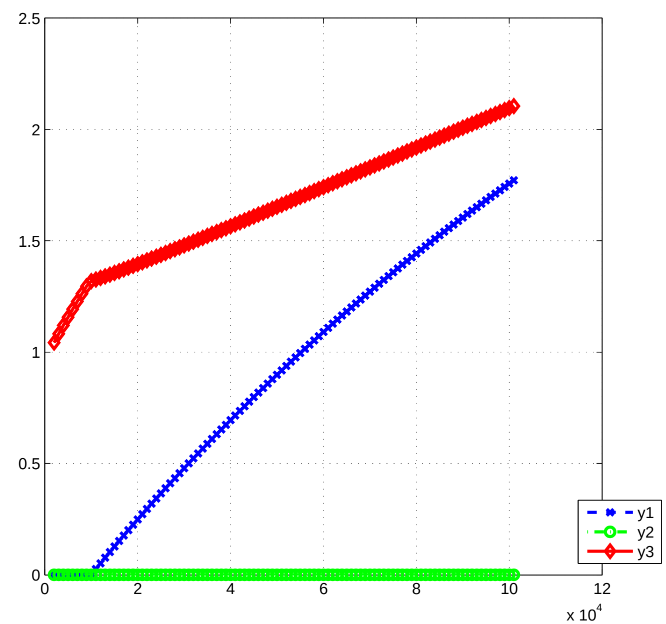


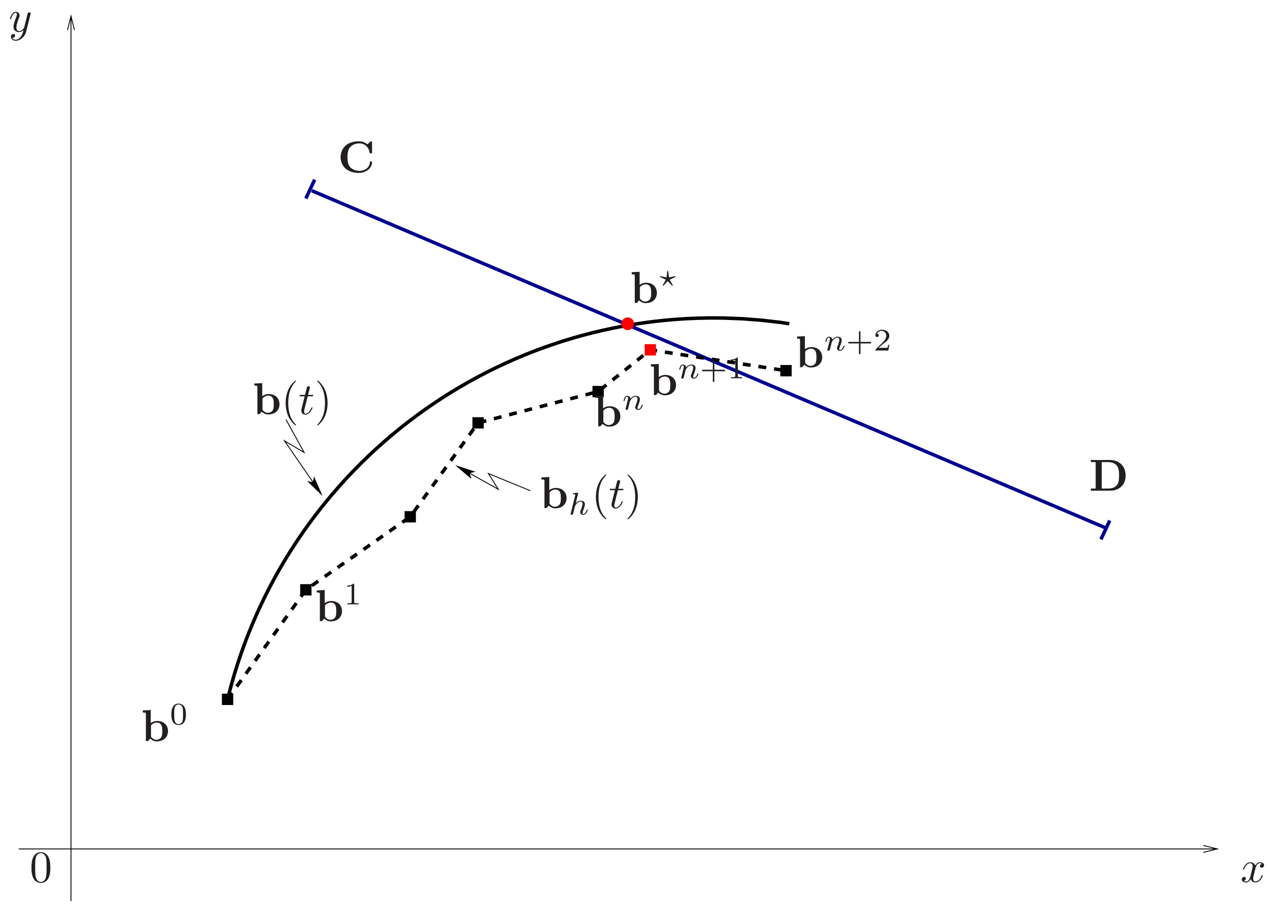
Trajectory



Values of y_α

Validation and Convergence Results

- Intersection of trajectories with one known boundary (segment). Time of impact $t^{\star}$:



Theoretical Results

If $\alpha + \lambda\beta = 0$ is the interface equation and $u = (t^\star, \lambda^\star)$

$$F(u) = \mathbf{b}(t) - (\alpha + \lambda\beta), \quad F_h(u) = \mathbf{b}_h(t) - (\alpha + \lambda\beta)$$

- Linear spline interpolation $\mathbf{b}_h(t)$ of $\mathbf{b}(t)$ satisfies:

$$\lim_{h \to 0} \mathbf{b}_h(t^\star) = \mathbf{b}(t^\star).$$

- **Consistency :**

$$\lim_{h \to 0} ||F_h(u)||_\infty = 0.$$

- **Convergence :** If $u = (t^\star, \lambda^\star)$ is solution to $F(u) = 0$, there exists u_h in a neighborhood of u such that $F_h(u) = 0$ and

$$||u - u_h||_\infty \leq C \, ||F_h(u)||_\infty \, .$$

[Handbook of Numerical Analysis, Caloz, Rappaz (1997)]

Conclusions and Perspectives

- Coupling optimization problem with differential equations.
- Use of both differential equations and optimization features.
- Numerical techniques for the tracking of discontinuities in the trajectories.
- Warm-starting heuristics.
- Existence results in simple cases.
- Extension to sequences of optimization problems.