# Numerical Methods for Optimization-Constrained Differential Equations with Discontinuities.

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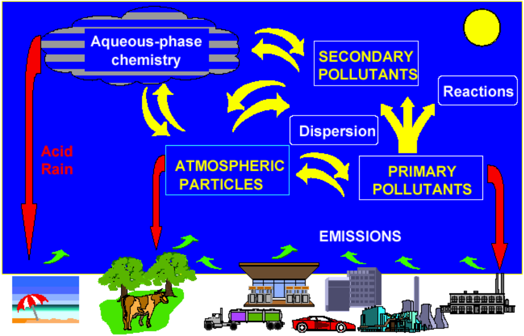
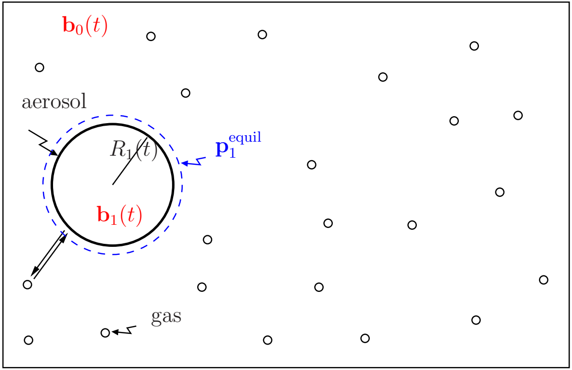
# Motivation : Atmospheric Aerosol Particles




- Aerosols particles have effects on human health, visibility reduction in urban and regional areas, acid rain, alteration of the earth's radiation balance, oxidation due to aqueous droplets, cloud and ozone formation, etc.

# Motivations

- Modeling and computation of the physical state and chemical composition of a population of atmospheric aerosol particles.



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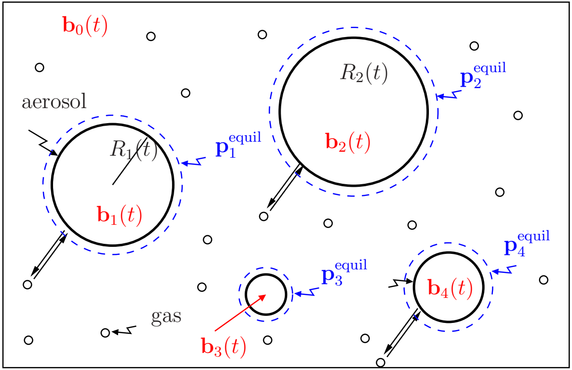

# Modeling of a Population of Subsystems

- Coupling between optimization problems and differential equations . For one subsystem/particle ($i = 1, \ldots, N$):

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

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

- Differential equation for the evolution of the concentration in the common medium:

$$\frac{d}{dt}\mathbf{b}_0(t) = -\sum_{i=1}^{N} f(t, \mathbf{b}_i(t), \mathbf{b}_0(t), \mathbf{z}_i(t), r_i), \quad \mathbf{b}_0(0) = \mathbf{b}_{0,0}.$$

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# System of Differential-Algebraic Equations

- Replace the optimization problem by the first order optimality conditions (KKT conditions), and search for stationary points.

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&\frac{d}{dt}\mathbf{b}_i(t) = f(t, \mathbf{b}_i(t), \mathbf{b}_0(t), \mathbf{z}_i(t), r_i), \quad \mathbf{b}_i(0) = \mathbf{b}_{i,0},\\
&\nabla g(\mathbf{z}_i(t)) + A^T \boldsymbol{\lambda}_i(t) - \boldsymbol{\theta}_i(t) = 0,\\
&A\mathbf{z}_i(t) = \mathbf{b}_i(t), \qquad\qquad i = 1, \ldots, N\\
&\boldsymbol{\theta}_i(t)\mathbf{z}_i(t) = 0, \quad \boldsymbol{\theta}_i(t) \geq 0, \quad \mathbf{z}_i(t) \geq 0.
\end{aligned}
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$\boldsymbol{\lambda}_i(t)$ is the Lagrange multiplier related to the equality constraint, $\boldsymbol{\theta}_i(t)$ is the Kuhn-Tucker multiplier related to the inequality constraint.

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# Model Problem

## System of Differential-Algebraic Equations

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- Stiff differential-algebraic equations.
- The global non-convex optimization implies that $G(\mathbf{z}, \mathbf{b}, \lambda, \theta) = 0$ does not admit a unique solution.
- The inequality constraints imply that the variables $\mathbf{z}_i(t), \theta_i(t)$ are truncated and non-smooth.

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# Time Discretization

- Consider $h > 0$, $t^n = nh$. An implicit first order discretization reads, for all $n \geq 0$:

$$\frac{\mathbf{b}_0^{n+1} - \mathbf{b}_0^n}{h} = -\sum_{i=1}^{N} f(t^{n+1}, \mathbf{b}_i^{n+1}, \mathbf{b}_0^{n+1}, \mathbf{z}_i^{n+1}, r_i), \quad \mathbf{b}_0^0 = \mathbf{b}_{0,0},$$

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- Large system of nonlinear algebraic equations, to solve with a Newton method.
- How to handle the inequality constraints?

# Interior-Point Method

- Relax the inequality constraints, by introducing $\nu > 0$:

$$\frac{\mathbf{b}_0^{n+1} - \mathbf{b}_0^n}{h} = -\sum_{i=1}^{N} f(t^{n+1}, \mathbf{b}_i^{n+1}, \mathbf{b}_0^{n+1}, \mathbf{z}_i^{n+1}, r_i), \quad \mathbf{b}^0 = \mathbf{b}_{0,0},$$

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- Penalty parameter $\nu$ tends to zero **at each time step.**
- The solution of the relaxed problem of nonlinear equations tends to the exact solution of the initial problem when $\nu$ tends to zero.

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$$\boldsymbol{\theta}_i^{n+1}\mathbf{z}_i^{n+1} = \nu, \quad \boldsymbol{\theta}_i^{n+1} > 0, \quad \mathbf{z}_i^{n+1} > 0.$$

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# Newton System

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

$$
\left[\begin{array}{cc|cc|cc|c}
H_1 & B_1 & 0 & 0 & \dots & \dots & C_1 \\
E_1 & O_1(\nu) & 0 & 0 & & & 0 \\
\hline
0 & 0 & H_2 & B_2 & & & C_2 \\
0 & 0 & E_2 & O_2(\nu) & & & 0 \\
\hline
\vdots & & & & \ddots & & \vdots \\
\vdots & & & & & \ddots & \vdots \\
\hline
0 & D_1 & 0 & D_2 & \dots & \dots & H_0
\end{array}\right]
\left[\begin{array}{c}
p_{\mathbf{b}_1} \\ p_{\mathbf{x}_1} \\ \hline p_{\mathbf{b}_2} \\ p_{\mathbf{x}_2} \\ \hline \vdots \\ \vdots \\ \hline p_{\mathbf{b}_0}
\end{array}\right]
=
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r_{\mathbf{b}_1} \\ r_{\mathbf{x}_1} \\ \hline r_{\mathbf{b}_2} \\ r_{\mathbf{x}_2} \\ \hline \vdots \\ \vdots \\ \hline r_{\mathbf{b}_0}
\end{array}\right]
$$

- Newton method incorporated in the interior-point iterations (decreasing values of the parameter $\nu$).

# Schur Complement Techniques

- Construct and solve the Schur complement system

$$\mathcal{S} p_{\mathbf{b}_0} = \mathcal{R}$$

$$\mathcal{S} = H_0 - \sum_{i=1}^{N} \begin{pmatrix} 0 & D_i \end{pmatrix} \begin{pmatrix} H_i & B_i \\ E_i & O_i \end{pmatrix}^{-1} \begin{pmatrix} C_i \\ 0 \end{pmatrix}$$

$$\mathcal{R} = r_{\mathbf{b}_0} - \sum_{i=1}^{N} \begin{pmatrix} 0 & D_i \end{pmatrix} \begin{pmatrix} H_i & B_i \\ E_i & O_i \end{pmatrix}^{-1} \begin{pmatrix} r_{\mathbf{b}_i} \\ r_{\mathbf{x}_i} \end{pmatrix}$$

- Solve, $i = 1, \ldots, N$

$$\begin{pmatrix} H_i & B_i \\ E_i & O_i \end{pmatrix} \begin{pmatrix} p_{\mathbf{b}_i} \\ p_{\mathbf{x}_i} \end{pmatrix} = \begin{pmatrix} r_{\mathbf{b}} \\ r_{\mathbf{x}} \end{pmatrix} - \begin{pmatrix} C_i \\ 0 \end{pmatrix} p_{\mathbf{b}_0}$$

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# Hierarchic Structure

- Linear systems related to one particle:

$$\begin{pmatrix} H_i & B_i \\ E_i & O_i \end{pmatrix} \begin{pmatrix} p_{\mathbf{b}} \\ p_{\mathbf{x}} \end{pmatrix} = \begin{pmatrix} r_{\mathbf{b}} \\ r_{\mathbf{x}} \end{pmatrix}$$

- Resolution by LU decomposition:

$$\begin{pmatrix} H_i & B_i \\ E_i & O_i \end{pmatrix} = \begin{pmatrix} H_i & 0 \\ E_i & V_i \end{pmatrix} \begin{pmatrix} I & H_i^{-1} B_i \\ 0 & I \end{pmatrix}$$

where

$$V_i = O_i - E_i H_i^{-1} B_i$$

corresponds to an optimization problem.

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# Application to Atmospheric Chemistry

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

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

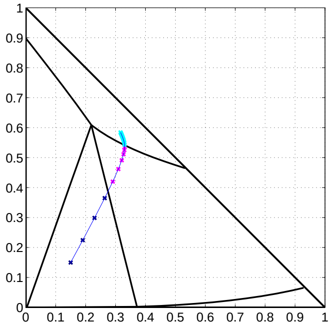
$$\text{s. t.} \quad \sum_{\alpha=1}^{N+1} y_\alpha \mathbf{x}_\alpha = \mathbf{b}_i,$$

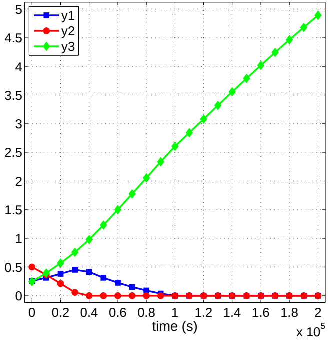
$$y_\alpha \geq 0,\ \mathbf{e}^T \mathbf{x}_\alpha = 1,\ \mathbf{x}_\alpha > 0,\ \alpha = 1, \ldots, N+1.$$

- $y_\alpha$ is the total number of moles in phase $\alpha$ 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.

# Single Particle

- Trajectory of the (normalized) feed vector $\mathbf{b}_1(t)$.




- Discontinuities when the trajectories crosses the black lines.
- Accurate detection of the phase separations when $G(\mathbf{z}, \mathbf{b}, \boldsymbol{\lambda}, \boldsymbol{\theta}) = 0$ has a unique solution.
- What happens if $G(\mathbf{z}, \mathbf{b}, \boldsymbol{\lambda}, \boldsymbol{\theta})$ admits multiple roots?

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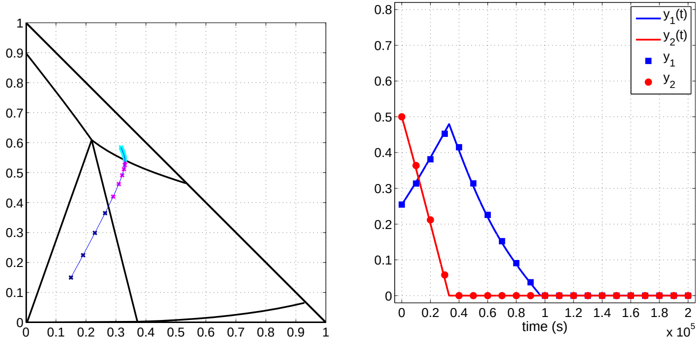


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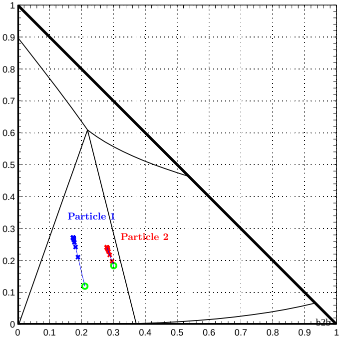
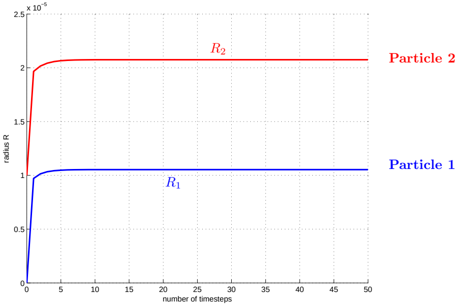
# Multiple Particles without Discontinuities

- Two particles without tracking of discontinuities.

Trajectories $\mathbf{b}_i$

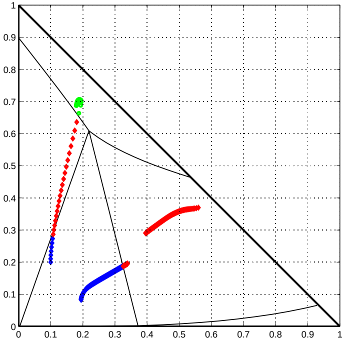



Radii $R_i$



# Multiple Particles without Discontinuities

- Three particles without tracking of discontinuities.

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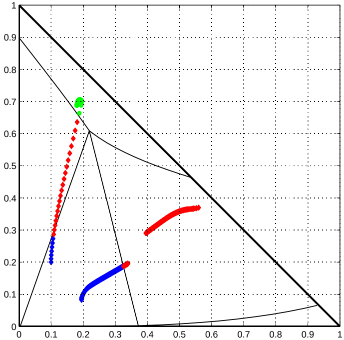

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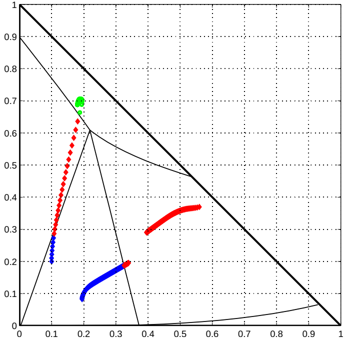


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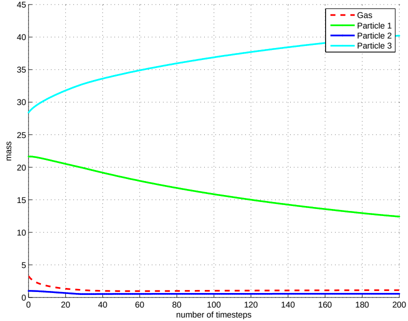


Mass

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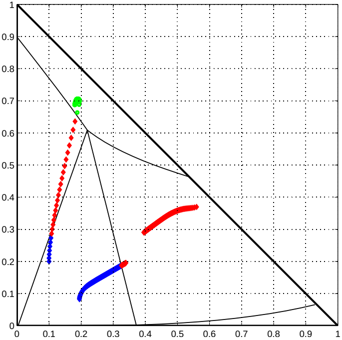


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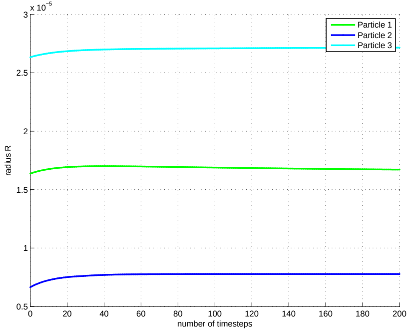


Radii

# Discontinuities and Bifurcation

- When $G(\mathbf{z}, \mathbf{b}, \boldsymbol{\lambda}, \theta)$ has multiple roots, the solution depends on the initial guess of the Newton method. This induces a bifurcation effects (local minima vs. global minima).
- When the objective function is non-convex, the algebraic part $G(\mathbf{z}, \mathbf{b}, \lambda, \theta) = 0$ may admit multiple solutions (correspond to many stationary points).
- The solution will depend strongly on the initial guess of the Newton method and the size of the time step.
- Bifurcation to branches of local minima and activation/deactivation of inequality constraints can be missed!
- Tracking techniques for the time of activation/deactivation of the constraints $\mathbf{z} \geq 0$ are required!

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# Event Location Techniques

- One particle model problem: DAE with discontinuous right-hand sides $\Rightarrow$ event in $(t^n, t^{n+1})$:

$$\frac{\mathbf{b}_1^{n+1} - \mathbf{b}_1^n}{h} = f(t^{n+1}, \mathbf{b}_1^{n+1}, \mathbf{b}_0^{n+1}, \mathbf{z}_1^{n+1}),$$
$$0 = G(t, \mathbf{b}_1^{n+1}, \mathbf{z}_1^{n+1}, \boldsymbol{\lambda}_1^{n+1}, \boldsymbol{\theta}_1^{n+1}).$$

(In that case : $\mathbf{b}_0^{n+1} = \mathbf{b}^{tot} - \mathbf{b}_1^{n+1}$ and one equation can be removed.)

- One additional equation describes the *event*:

$$w(t^n + h^\star, \mathbf{b}_1^{n+1}(t^n + h^\star), \mathbf{z}_1^{n+1}(t^n + h^\star)) = 0$$

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# Two Kinds of Events for Inequality Constraints

## Activation

$$\mathbf{z}_i(t) > 0 \longrightarrow \mathbf{z}_i(t) = 0.$$

## Deactivation

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- In both cases, the event detection function $w$ is not known explicitly. Difficult/expensive to evaluate the function $w$ or its derivatives.
- Once $h^\star$ is known, **multistep methods.**

# Tracking of Activations: $\mathbf{z}_i(t) > 0 \rightarrow \mathbf{z}_i(t) = 0$

- In the activation case, we look for $h^\star$ such that $\mathbf{z}_i(t^n + h^\star) = 0$.
- Extrapolation method and Taylor expansion

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

- Truncation of the Taylor expansion:

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

- Approximation of $\frac{d\mathbf{z}_i}{dt}(t^n)$ with **sensitivity analysis**.

# Tracking of Deactivations: $\mathbf{z}_i(t) = 0 \rightarrow \mathbf{z}_i(t) > 0$

- In the deactivation case, we look for $h^\star$ such that

$$\boldsymbol{\theta}(t^n + h^\star) = \nabla g(\mathbf{z}(t^n + h^\star)) + A^T \boldsymbol{\lambda}(t^n + h^\star) = 0.$$

- Evaluation of $\theta(t)$ requires to solve this nonlinear equation, that admits multiple solutions (local/global minima).
- If $\theta(t)$ is positive, no event yet, if $\theta(t)$ is negative, the contact has already happened. Implementation of a bisection method.

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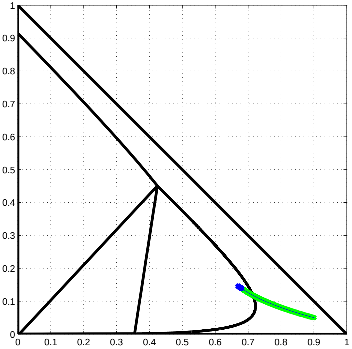
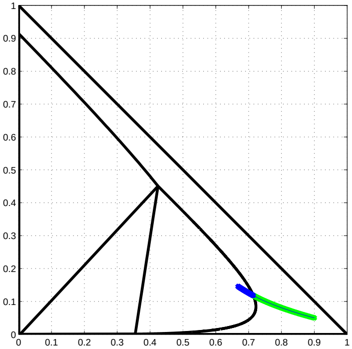
# Comparison of Tracking Results

- Evolution of $\mathbf{b}(t)$:



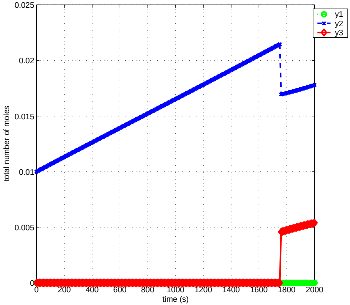

Warm-start




Warm-start with detection

# Comparison of Tracking Results

- Evolution of $y_\alpha(t)$:

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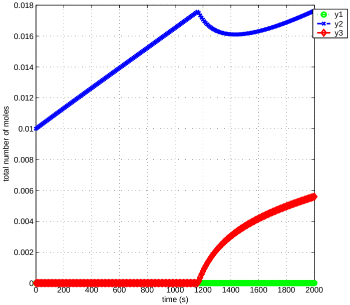


Warm-start with detection

# Conclusions and Perspectives

- Coupling optimization problems with differential equations.
- Numerical linear algebra techniques for large linear systems.
- Numerical techniques for the tracking of discontinuities.

- Multiscale analysis of the population of particles.
- Fast/slow decompositions.