Project Summary

Optimization problems with constraints given by partial differential equations (PDEs) and systems thereof frequently occur in real-life applications such as the structural optimization of technological devices and systems and the identification of physical quantities in atmospheric and geophysical processes.

After an appropriate discretization by, e.g., finite elements with respect to a triangulation of the computational domain, the problems typically emerge as large-scale equality and inequality constrained nonlinear programming problems whose efficient and reliable numerical solution represents a challenging task. The state-of-the-art in PDE-constrained optimization are so-called ‘all-at-once’ methods where in contrast to more traditional optimization strategies the numerical solution of the PDEs is an integral part of the optimization routine, thus often saving a considerable amount of computational work. Typical representatives of this approach are sequential quadratic programming (SQP) and reduced SQP (RSQP) methods. Whereas SQP and RSQP methods typically use quasi-Newton updates of the Hessian, it can often be advantageous to use a Newton method instead, applied to the first order optimality system, known as the Karush-Kuhn-Tucker (KKT) conditions. When taking care of the inequality constraints by either interior-point methods or active set strategies, this results in Newton type interior-point methods and Newton type active set strategies.

In this proposal, the aim is to provide multilevel iterative solvers for PDE constrained optimization problems. Multilevel techniques provide efficient solvers with regard to algorithmic complexity. Moreover, we believe that they also offer the possibility to extract an adequate amount of structural information from the originally infinite dimensional problem which cannot be achieved when only relying on a single grid. In particular, the main focus of this proposal is on the development, analysis and implementation of multilevel path-following continuation methods for primal-dual Newton interior-point methods and for primal-dual Newton type active set strategies. As applications, we will consider the shape optimization of electrorheological devices and the identification of different phases in atmospheric aerosol modeling.

The scientific merit of the proposal is to provide efficient algorithmic tools for a challenging problem in nonlinear optimization and to demonstrate their performance by the application to real-life problems that have a significant impact on materials and life science.

The educational merit of the proposal will be to educate graduate students in an important area of optimization. The results of the proposal will be used in regularly offered courses on optimization as well as in special courses and seminars that focus on PDE-constrained optimization.
1. PDE constrained optimization

On an abstract level, an optimization problem with constraints given by partial differential equations (PDE) can be written as follows

\[(1.1a) \minimize J(y, u) \over (y, u) \in K_1 \times K_2 , \]

subject to:

\[(1.1b) e(y, u) = 0 . \]

Here, \( J(\cdot, \cdot) : Y \times U \rightarrow \mathbb{R} \) stands for the objective functional depending on the state variables \( y \) in the state space \( Y \) and the design variables \( u \) in the design space \( U \). The equation \((1.1b)\) corresponds to the PDE, and \( K_1 \subset Y , K_2 \subset U \) refer to the sets of admissible states and design variables, respectively.

The numerical solution of such PDE constrained optimization problems is an area of research that is still in its infancy. It faces a series of theoretically and practically relevant challenges:

- The structural interaction between the optimization issue and the underlying PDE and the impact of the discretization processes have to be taken into account. For instance, following the principle "discretize first, then optimize", the granularity of the discretizations is a critical issue, since the discretization goes along with a certain loss of the inherent structure of the infinite dimensional problem. On the other hand, the principle "optimize first, then discretize" conserves the structure of the problem, but the optimality conditions in terms of derivatives can only be realized approximately. Is there a best compromise?

- Optimization problems with special structures arise from parameter identification issues associated with PDEs. They require the development and analysis of specific algorithmic tools (cf., e.g., [13, 14, 138]).

- In contrast to more traditional optimization methodologies that rely on a separate treatment of the optimization issue and the solution of the state equation, recent interest is on so-called "all-at-once" approaches. Here, the numerical solution of the state equation is an integral part of the optimization routine which may result in a considerable savings of computational time (cf., e.g., [27, 28, 76, 118, 122, 140, 162]).

- The numerical approaches typically lead to large-scale nonlinear programming problems. With regard to algorithmic complexity, their numerical solution requires the use of efficient iterative schemes such as multilevel techniques.

In this proposal, we will address these issues with strong emphasis on the development, analysis, and implementation of multilevel iterative solvers for the optimality system.

As far as applications are concerned, we will concentrate on structural optimization in materials science and parameter identification in atmospheric processes.

The optimization of the shape and the topology of technologically relevant devices and systems by means of a systematic, physically consistent design methodology is
referred to as structural optimization. Simplified problems in structural optimization have already been addressed by Bernoulli, Euler, Lagrange and Saint-Venant. However, it became its own discipline during the second half of the last century when the rapidly growing performance of computing platforms and the simultaneously achieved significant improvement of algorithmic tools enabled the appropriate treatment of complex problems (cf. [4, 19, 20, 47, 55, 89, 144, 154, 158, 167] and the references therein). The design criteria in structural optimization are determined by a goal oriented operational behavior of the devices and systems under consideration and typically occur as a nonlinear, often non convex, objective functionals which depend on the state variables describing the operational mode and the design variables determining the shape and the topology. The state variables have to satisfy differential equations or systems thereof representing the underlying physical laws. Technological aspects are taken into account by constraints on the state and design variables which may occur both as equality and inequality constraints in the model. In particular, we will consider the shape optimization of electrorheological shock absorbers [30, 61, 66, 73, 74, 110, 111, 112, 113, 153, 156, 159, 168].

Anthropogenic emissions leading to atmospheric aerosols have increased dramatically over the past century. Atmospheric aerosols have been implicated in human health effects, visibility reduction in urban and regional areas, acidic deposition, and alteration of the earth’s radiation balance [164]. At present, the knowledge and understanding of aerosol composition, physiochemical properties, sources and transformation is very limited, and estimates of their actual environmental effects are highly uncertain [128]. A major goal of environmental research for the last twenty years has been the development of the necessary models, using first principles, that can be used in order to predict the physical and chemical properties of atmospheric aerosols [38] . With a few exceptions, current aerosol models often fail to predict the phase state and composition and the multistage growth phenomena of atmospheric aerosols [11, 12]. On the other hand, there is a growing need for reliable micro-physically consistent models in assessment of radiative and health effects of atmospheric aerosols and their impact on climate [141]. This is driven, in part, by new advances in the technology for particle measurement [48, 131]. The need for efficient microphysical-based models that can be run in real time and compared with these new kinds of measurements has motivated our proposed research in modeling of the physical state of atmospheric aerosol particles. In particular, we will consider the identification of different phases in atmospheric aerosol modeling.

2. **Equality and inequality constrained nonlinear programming problems**

The discretization of PDE constrained optimization problems typically gives rise ro large-scale, equality and inequality constrained nonlinear programming problems
of the form
\[ \begin{align*}
(2.1a) & \quad \text{minimize} & f(x_1, x_2) \\
& \text{over} & (x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}, \\
(2.1b) & \quad \text{subject to:} & h(x_1, x_2) = 0, \\
(2.1c) & \quad & g(x_1, x_2) \geq 0,
\end{align*} \]

where \( f : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R} \) is the discretized objective functional depending on the discrete state variables \( x_1 \in \mathbb{R}^{n_1} \) and design variables \( x_2 \in \mathbb{R}^{n_2} \), (2.1b) with \( h = (h_1, h_2)^T : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R}^m, \ m \geq n_1 \), comprises the discretized state equation \( h_1 : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R}^{n_1} \) and possibly further equality constraints \( h_2 : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R}^{m-n_1} \), whereas (2.1c) with \( g : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R}^p \) represents inequality constraints on the state and design variables.

If we define the feasible set \( \mathcal{F} \) according to
\[\mathcal{F} := \{(x_1, x_2) \mid h(x_1, x_2) = 0, \ g(x_1, x_2) \geq 0\},\]
then (2.1a)-(2.1c) can be written more concisely as
\[ (2.2) \quad \min_{(x_1, x_2) \in \mathcal{F}} f(x_1, x_2). \]

Coupling the constraints by Lagrangian multipliers \( \lambda \in \mathbb{R}^m \) and \( \mu \in \mathbb{R}^p_+ \), we are led to the saddle point problem
\[ (2.3) \quad \min_{(x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}} \max_{(\lambda, \mu) \in \mathbb{R}^m \times \mathbb{R}^p_+} L(x_1, x_2, \lambda, \mu), \]
where \( L \) stands for the Lagrangian
\[ (2.4) \quad L(x_1, x_2, \lambda, \mu) := f(x_1, x_2) + \lambda^T h(x_1, x_2) - \mu^T g(x_1, x_2). \]

The Karush-Kuhn-Tucker (KKT) conditions give rise to the nonlinear system
\[ (2.5) \quad \begin{bmatrix}
\nabla f(x) + \nabla h(x) \lambda + \nabla g(x) \mu \\
h(x) \\
g(x) - z \\
D_z D_\mu e
\end{bmatrix} = 0. \]

Here, \( z \in \mathbb{R}^p_+ \) is the vector of slack variables, \( D_z = \text{diag}(z_1, ..., z_p) \), \( D_\mu = \text{diag}(\mu_1, ..., \mu_p) \) and \( e = (1, ..., 1)^T \). If Newton’s method is applied to the KKT conditions, each Newton step requires the solution of a linear algebraic system representing the optimality conditions of a related quadratic programming (QP) problem. Hence, Newton methods can be interpreted in the framework of sequential quadratic programming (SQP) which is the most successful method for solving constrained nonlinear optimization problems [31, 148].

As far as the appropriate treatment of the inequality constraints is concerned, a local optimum can be approximated from within the feasible set, which is the idea behind interior-point methods [68, 178, 179, 180], or by using active set strategies where the iterates are not necessarily restricted to feasibility (cf., e.g., [21, 102] for recent work in the context of constrained optimal control problems).
2.1. **Interior point methods.** The so-called interior-point revolution in continuous optimization started in the eighties of the last century with Karmarkar’s polynomial-time linear programming algorithm [133]. It was immediately found [82] that there is a close relationship to barrier functions which had been used long time before for inequality constrained nonlinear programming problems. Nowadays, interior-point methods are well established tools for constrained nonlinear optimization problems (cf., e.g., [16, 40, 67, 68, 69, 75, 79, 82, 170, 171, 173, 178, 179, 180]). Barrier methods are used to transform constrained problems to unconstrained ones and typically give rise to parametrized families of approximate subproblems. In particular, coupling the inequality constraints (2.1c) by classical logarithmic barrier functions

\[ B^{(\beta)}(x_1, x_2) := f(x_1, x_2) - \beta \sum_{i=1}^{p} \log(g_i(x_1, x_2)), \]

where \( \beta > 0 \) stands for the barrier parameter [65, 68, 178], leads to the consideration of the following parametrized family of minimization subproblems

\[
\begin{align*}
\text{(2.7a)} & \quad \text{minimize} \quad B^{(\beta)}(x_1, x_2) \\
& \quad \text{over} \quad (x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}, \\
\text{(2.7b)} & \quad \text{subject to:} \quad h(x_1, x_2) = 0.
\end{align*}
\]

Under standard assumptions on the NLP, for sufficiently small \( \beta > 0 \) there exist local minima \((x_1^{(\beta)}, x_2^{(\beta)})\) of (2.7a), (2.7b) which converge along centered pathes to an isolated local minimum of (2.1a)-(2.1c) as \( \beta \to 0 \) (cf., e.g., [65].

Taking care of the equality constraint (2.7b) by a Lagrangian multiplier \( \lambda = (\lambda_1, \lambda_2)^T, \lambda_1 \in \mathbb{R}^{n_1}, \lambda_2 \in \mathbb{R}^{m - n_1} \), leads to the saddle point problem

\[
\begin{align*}
\min_{(x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}} \max_{\lambda \in \mathbb{R}^m} L^{(\beta)}(x_1, x_2, \lambda),
\end{align*}
\]

where \( L^{(\beta)} \) refers to the Lagrangian

\[
L^{(\beta)}(x_1, x_2, \lambda) := B^{(\beta)}(x_1, x_2) + \lambda^T h(x_1, x_2).
\]

Considering the KKT-conditions for (2.8), introducing the slack variable \( z \in \mathbb{R}^{q} \) (approximate complementarity) according to

\[
z_i := \frac{\beta}{g_i(x_1, x_2)}, \quad 1 \leq i \leq p,
\]

and applying Newton’s method with respect to \( \varphi = (x_1, x_2, \lambda, z) \), we arrive at the primal-dual system

\[
K \delta_\varphi = -F^{(\beta)}(\varphi)
\]

for the Newton increments \( \delta_\varphi := (\delta_{x_1}, \delta_{x_2}, \delta_\lambda, \delta_z)^T \). Here, the right-hand side is the residual with respect to the KKT conditions and the primal-dual matrix \( K \) is given
by

\[
K = \begin{pmatrix}
\nabla^2 x_1 L^{(\beta)} & \nabla^2 x_2 L^{(\beta)} & (\nabla x_1 h)^T & -(\nabla x_1 g)^T \\
\nabla^2 x_2 L^{(\beta)} & \nabla^2 x_2 L^{(\beta)} & (\nabla x_2 h)^T & -(\nabla x_2 g)^T \\
\nabla x_1 h & \nabla x_2 h & 0 & 0 \\
\nabla x_1 g & \nabla x_2 g & 0 & D_z^{-1} D_g
\end{pmatrix}
\]

with \(D_g := \text{diag}(g_i(x_1, x_2))_{i=1}^p\) and \(D_z := \text{diag}(z_i)_{i=1}^p\).

Since \(D_g, D_z\) are diagonal matrices, it is easy to perform block Gauss elimination of the approximate complementarity \( z \) which leads to the condensed primal-dual system in \( \delta_{\varphi(C)} = (\delta x_1, \delta x_2, \delta \lambda)^T \) (2.11)

\[
K^{(C)} \delta_{\varphi(C)} = -F^{(C)}(\varphi^{(C)})
\]

with the condensed primal-dual matrix

(2.12)

\[
K^{(C)} = \begin{pmatrix}
\nabla^2 x_1 L^{(\beta)} & \nabla^2 x_2 L^{(\beta)} & (\nabla x_1 h)^T & -(\nabla x_1 g)^T \\
\nabla x_2 L^{(\beta)} & \nabla x_2 L^{(\beta)} & (\nabla x_2 h)^T & -(\nabla x_2 g)^T \\
\nabla x_1 h & \nabla x_2 h & 0 & 0 \\
\nabla x_1 g & \nabla x_2 g & 0 & D_z^{-1} D_g
\end{pmatrix}
\]

Note that for \(1 \leq i, j \leq 2\)

\[
\nabla^2 x_i x_j L^{(\beta)} = \nabla^2 x_i x_j L^{(\beta)} + (\nabla x_i g)^T D_g^{-1} D_z \nabla x_j g ,
\]

and that the right-hand side in (2.11) is given by

\[
F_{x_i}^{(C)}(\varphi^{(C)}) = \nabla x_i f + \nabla x_i h - \beta (\nabla x_i g)^T D_g^{-1} e ,
\]

\[
F_{\lambda}^{(C)}(\varphi^{(C)}) = h , \quad \text{where } e = (1, ... , 1)^T \in \mathbb{R}^p .
\]

Multilevel iterative solvers for the condensed primal-dual system (2.11) have been considered in [117, 118, 140] using a heuristically motivated decreasing sequence of barrier parameters and a step-length selection to ensure feasibility of the iterates.

Following [75], global convergence issues have been addressed by means of a watchdog strategy relying on a hierarchy of two merit functions.

It is the aim of this proposal to develop, analyze and implement theoretically supported multilevel path-following continuation methods with an adaptive trust-region approach featuring a multilevel predictor-corrector strategy. We note that for parameter dependent nonlinear PDEs and variational inequalities, multilevel continuation methods have been suggested in [15, 88] and [114], but have not yet been studied in the context of barrier methods for PDE constrained optimization problems.

In particular, we will study the

- sensitivity of the multigrid scheme with respect to the barrier parameters, since it is well-known that the Hessian gets ill-conditioned when the barrier parameter approaches zero (cf., e.g., [69]),
- detection of negative curvature by using computationally inexpensive information from coarser grids [37],
- appropriate specification of termination criteria for the multilevel iterative solver within an affine invariant framework (cf., e.g., [57]).
2.2. **Active set strategies.** Active set strategies are iterative schemes for the solution of inequality constrained optimization problems, where at each iteration step the solution of an equality constrained subproblem is required by identifying a set of active constraints (cf., e.g., [148] and the references therein). In case of bilateral box constraints on the design variables

\[ c_i \leq x_{2,i} \leq d_i , \quad i \in I := \{1, ..., n_2\} , \]

we define \(A\) as the active set, i.e., the set where the inequality constraints are active, according to

\[ A = A_1 \cup A_2 , \]

\[ A_1 := \{ i \in I \mid x_{2,i} = c_i \} , \quad A_2 := \{ i \in I \mid x_{2,i} = d_i \} . \]

The set

\[ I := I \setminus A \]

is referred to as the set of inactive constraints. In this case, the KKT conditions associated with the saddle point problem (2.3) take the form

\[ \nabla_{x_1} L(x_1, x_2, \lambda, \mu) = \nabla_{x_1} f(x_1, x_2) + \nabla_{x_1} h(x_1, x_2) = 0 , \]

(2.13a)

\[ \nabla_{x_2} L(x_1, x_2, \lambda, \mu) = \nabla_{x_2} f(x_1, x_2) + \nabla_{x_2} h(x_1, x_2) - \sum_{i \in A} \mu_i = 0 , \]

(2.13b)

\[ \nabla_{\lambda} L(x_1, x_2, \lambda, \mu) = h(x_1, x_2) = 0 , \]

(2.13c)

\[ c_i^{\min} \leq x_{2,i} \leq d_i^{\max} , \quad i \in I , \]

(2.13d)

\[ \mu_{|A_1} \leq 0 , \quad \mu_{|A_2} \geq 0 , \quad \mu_{|I} = 0 , \]

(2.13e)

where \(\mu_{|S}\) denotes the restriction of \(\mu\) to \(S \subset I\).

The complementarity conditions (2.13d)-(2.13e) can be stated as

\[ \mu \in \partial I_K(x_2) , \]

(2.14)

where \(\partial I_K\) denotes the subdifferential of the indicator function \(I_K\) of the convex set

\[ K := \{ x_2 \in \mathbb{R}^{n_2} \mid c_i \leq x_{2,i} \leq d_i , 1 \leq i \leq n_2 \} . \]

Following [21, 102] and using the generalized Moreau-Yosida approximation

\[ (\partial I_K)_\sigma(v) := \frac{1}{\sigma} (I - J_{\sigma I}^{\partial I_K}) = ((\partial I_K)^{-1} + \sigma I)^{-1} , \quad \sigma > 0 , \]

of the indicator function \(I_K\), (2.14) can be replaced by the computationally more feasible condition

\[ \mu = \sigma \left[ x_2 + \sigma^{-1} \mu - P_K(x_2 + \sigma^{-1} \mu) \right] , \]

(2.15)

where \(P_K\) denotes the projection onto \(K\) as given by

\[ P_K(w) := \begin{cases} 
  c_i , & w_i < c_i , \\
  w_i , & c_i \leq w_i \leq d_i , \\
  d_i , & w_i > d_i 
\end{cases} , \quad i \in I . \]
The active set method proceeds as follows: Given start iterates $x_1^{(0)}, x_2^{(0)}, \lambda^{(0)}, \mu^{(0)}$, for $\nu \geq 1$ we determine the set $A^{(\nu)}$ of active constraints according to

$$A^{(\nu)} = A^{(\nu)}_1 \bigcup A^{(\nu)}_2,$$

where

$$A^{(\nu)}_1 := \{ i \in I | x_2^{(\nu-1)} + \sigma^{-1} \mu_i^{(\nu-1)} < c_i \}, \quad A^{(\nu)}_2 := \{ i \in I | x_2^{(\nu-1)} + \sigma^{-1} \mu_i^{(\nu-1)} > d_i \},$$

and define $T^{(\nu)} := I \setminus A^{(\nu)}$. We set

$$(2.16) \quad x_{2,i}^{(\nu)} := c_i, \quad x_1^{(\nu)} := \tilde{x}_1, \quad x_2^{(\nu)} := d_i, \quad \mu_i^{(\nu)} := 0, \quad i \in T^{(\nu)}.$$

Taking (2.17) into account, for $\tilde{x}_2 := (x_{2,i})_{i \in T^{(\nu)}}$ we define $f : \mathbb{R}^{n_1} \times \mathbb{R}^{n_3} \to \mathbb{R}^{n_1}$, $(x_1, \tilde{x}_2) \mapsto f(x_1, x_2^{(\nu-1)/2})$, and $\hat{h} : \mathbb{R}^{n_1} \times \mathbb{R}^{n_3} \to \mathbb{R}^m$, $(x_1, \tilde{x}_2) \mapsto \hat{h}(x_1, \tilde{x}_2) := h(x_1, x_2^{(\nu-1/2)})$, where $n_3 := \text{card } T^{(\nu)}$ and

$$x_{2,i}^{(\nu-1/2)} := \begin{cases} x_{2,i}^{(\nu)}, & i \in T^{(\nu)} \\ x_{2,i}^{(\nu)}, & i \in A^{(\nu)} \end{cases}. $$

We compute $(x_1^{(\nu)}, \tilde{x}_2^{(\nu)}, \lambda^{(\nu)}) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_3} \times \mathbb{R}^m$ as the solution of

$$(2.17) \quad \min_{(x_1, \tilde{x}_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_3}} \max_{\lambda \in \mathbb{R}^m} \tilde{L}(x_1, \tilde{x}_2, \lambda),$$

where the Lagrangian is given by

$$\tilde{L}(x_1, \tilde{x}_2, \lambda) := f(x_1, \tilde{x}_2) + \lambda^T \hat{h}(x_1, \tilde{x}_2).$$

Finally, setting $x_2^{(\nu)} := \tilde{x}_2^{(\nu)}, i \in T^{(\nu)}$, results in the new iterate $x_2^{(\nu)}$ for the design variable.

The KKT conditions for (2.17) are given by

$$\nabla_{x_1} \tilde{L}(x_1, \tilde{x}_2, \lambda) = \nabla_{x_1} f(x_1, \tilde{x}_2) + \nabla_{x_1} \hat{h}(x_1, \tilde{x}_2) = 0,$$

$$\nabla_{\tilde{x}_2} \tilde{L}(x_1, \tilde{x}_2, \lambda) = \nabla_{\tilde{x}_2} f(x_1, \tilde{x}_2) + \nabla_{\tilde{x}_2} \hat{h}(x_1, \tilde{x}_2) = 0,$$

$$\nabla_\lambda \tilde{L}(x_1, \tilde{x}_2, \lambda) = \hat{h}(x_1, \tilde{x}_2) = 0.$$

The iteration is stopped when the active set becomes stationary, i.e., $A^{(\nu)} = A^{(\nu-1)}$.

Applying Newton’s method to the KKT conditions, we arrive at a block-structured linear system of much the same form as (2.12).

In view of (2.15), the active set strategy can be interpreted as the discrete version of a semismooth Newton method in function space [103, 169]. Based on this interpretation, it is the aim of the proposal to develop, analyze and implement Newton multigrid methods as well as full nonlinear multigrid methods. Specific issues that will be addressed include the

- synopsis of the continuous and discrete Newton methods with regard to a mesh independence principle (cf., e.g., [175] for elliptic PDEs),
- specification of appropriate termination criteria for the inner multilevel iterative solvers within a Newton multilevel approach (cf., e.g., [58, 59] for nonlinear elliptic PDEs),
• design of suitable transfer operators ('fine-to-coarse' and 'coarse-to-fine') in a full nonlinear multilevel approach, when the transfer effects active and inactive nodal points at subsequent levels of the hierarchy of grids (cf., e.g., [109, 134] in case of obstacle problems for elliptic PDEs).

3. Applications in materials science and atmospheric research

3.1. Materials science. We will apply the algorithmic tools, developed in this proposal, to the shape optimization of electrorheological devices whose operational behavior strongly takes advantage of the rheological properties of such fluids. In fact, electrorheological fluids are concentrated suspensions of small electrically polarizable particles with diameters in the range of micrometers dissolved in nonconducting silicon oils. The rheological effect is based on the fact that under the influence of an outer electric field the particles form chains along the field lines and then aggregate to form larger and larger columns. The impact on the macroscopic scale consists in rapid change of the rheological properties which happens within a few milliseconds. Therefore, electrorheological fluids are used in all technological processes where a controlled power transmission plays a significant role. The field of applications ranges from automotive shock absorbers and actuators in hydraulic systems to tactile devices for virtual reality [66].

In this proposal, we will be concerned with the optimization of the shape of the walls of an ERF shock absorber (cf. Figure 1 (left)) in a vicinity of the inlet and outlet boundary of the ERF transfer ducts. A schematic diagram of such a shock absorber is shown in Figure 1 (left). The absorber contains two chambers filled with an ERF, a piston with two transfer ducts connecting the chambers, and a third gas-filled chamber separated from the others by a floating piston. The inner walls of the transfer ducts serve as electrodes and counter-electrodes, respectively. The electrodes are connected with an outer power source by a high voltage lead within the piston rod. As the piston moves, the fluid passes through the ducts from one chamber to the other.

In contrast to conventional shock absorbers, where the fluid chambers are filled with hydraulic oils, ERF shock absorbers have a much wider characteristics (damper force as a function of the velocity of the piston). Therefore, ERF shock absorbers offer the best compromise between safety and comfort for a wide spectrum of road conditions. The performance of the shock absorber does not only depend on the applied voltage and the velocity of the piston, but also on the geometry of the device. In particular, the geometry of the inlet and outlet boundaries of the ducts play a decisive role. In extreme cases, cavitation due to high pressure variations may occur which negatively effects the damper characteristics. Therefore, given a prescribed pressure profile \( p_d \), the optimization issue is to design the geometry in such a way that pressure variations are minimized. Due to axisymmetry, the computational domain \( \Omega \) reduces to the right part of the fluid chamber. The inlet and outlet boundaries are represented by B-splines using the de Boor control points \( \alpha = (\alpha_1, ..., \alpha_m) \) as design variables (cf. Figure 1 (right)). Consequently, the computational domain depends on the choice of the design variables, i.e., \( \Omega = \Omega(\alpha) \).
In the stationary case, the fluid flow is described by the equations

\begin{align}
- \nabla \cdot \sigma(u) &= f \quad \text{in } \Omega(\alpha), \\
\nabla \cdot u &= 0 \quad \text{in } \Omega(\alpha)
\end{align}

along with appropriate boundary conditions. Here, \( u = (u_1, u_2) \) is the velocity vector, \( \sigma \) refers to the stress tensor and \( f \) describes exterior forces acting on the fluid. The stress tensor \( \sigma \) is related to the rate of deformation tensor \( D(u) \) with \( (D(u))_{ij} := (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2 \), \( 1 \leq i, j \leq 2 \), by a constitutive equation where the electric field \( E \) enters as a parameter. Most constitutive equations are of extended Bingham fluid type \( [61, 156] \) and use some sort of power law dependence \( [159] \). Here, we use a constitutive equation developed in \( [110] \)

\begin{equation}
\sigma = -p I + 2 \varphi(I(u), |E|, \mu(u, E)) D(u),
\end{equation}

where \( \varphi \) is a viscosity function depending on the shear rate \( I(u) \), the electric field strength \( |E| \), and the angle \( \mu(u, E) \) between the velocity field \( u \) and the electric field \( E \). In particular, the viscosity function \( \varphi \) is assumed to be of the form

\[ \varphi(I(u), |E|, \mu(u, E)) = b(|E|, \mu(u, E)) (\varepsilon + I(u))^{-\frac{1}{2}} + \psi(I(u), |E|, \mu(u, E)), \]

where \( \varepsilon > 0 \) is a regularization parameter. In practice, the functions \( b \) and \( \psi \) are approximated by splines fitted to rheometrical data obtained for different electric field strengths.
The shape optimization problem can be stated as follows

$$\inf_{(u,p,\alpha)} J(u,p,\alpha), \ J(u,p,\alpha) := \int_{\Omega(\alpha)} |\nabla p - \nabla p_d|^2 dx$$

subject to the state equations (3.18),(3.19) and the inequality constraints

$$\alpha_i^{\min} \leq \alpha_i \leq \alpha_i^{\max}, \ 1 \leq i \leq m$$

on the design variables which are motivated by technological constraints on the shape of the inlet and outlet boundaries.

Assuming a known angle $\mu(u,E)$ between the velocity vector and the exterior electric field, the flow model (3.18)-(3.20) will be discretized in space by $Q_2 - P_1$ Taylor-Hood elements with respect to a simplicial triangulation of a reference computational domain $\Omega(\hat{\alpha})$, where $\hat{\alpha} \in \mathbb{R}^m$ is chosen within the set of feasible design parameters such that $\Omega(\alpha) = \Phi(\Omega(\hat{\alpha}))$. The resulting nonlinear programming problem will be solved by the primal-dual Newton interior point methods and the primal-dual active set strategies to be developed in this proposal.

3.2. Atmospheric research. Atmospheric aerosols are airborne particles that are composed of water, inorganic salts, insoluble materials (dust, crustal material), organics (soot, VOC) and trace metals [150, 157, 165]. Knowledge of the physical state and chemical composition of these particles is of great importance because of the role they play in important atmospheric processes. The atmosphere subjects aerosol particles to an array of transport and transformation processes that alter their size, number, and composition. The transformation processes include condensation and evaporation, homogeneous nucleation, coagulation, and chemical reactions. A major goal of our research has been to use first principles to gain a predictive understanding of the physical and chemical processes that govern the dynamics, size, and chemical composition of atmospheric aerosols.

The physical state and chemical composition of aerosol particles is governed by the mass transfer between the bulk gas phase and the surface of the particles and the phase transition at the surface. Let $b(r, x, t) = (b_1(r, x, t), ..., b_{m_e}(r, x, t))^T$ be the species mass density function of particles having particle (mass) size $r$ at space $x$ and time $t$ and let $b_s(r, x, t) = \sum_{i=1}^{m_e} b_i(r, x, t)$. The general dynamic equation governing $b_i(r, x, t)$ is

$$\frac{\partial}{\partial t} b_i(r, x, t) + (u_t(x, t) - u_d(r)e_z) \cdot \nabla_x b_i(r, x, t) -$$

$$\nabla_x \cdot (K(x,t)\nabla_x b_i(r, x, t)) + \frac{\partial}{\partial r} (I_s(r, x, t)b_i(r, x, t)) - \frac{I_i(r, x, t)}{r} b_s(r, x, t)$$

$$= \int_0^r \beta(r - r', x, t) \frac{b_s(r - r', x, t)}{r - r'} b_i(r', x, t) dr'$$

$$- b_i(r, x, t) \int_0^\infty \beta(r, r') \frac{b_s(r', x, t)}{r'} dr' + S_i(r, x, t),$$

\[11\]
where $\mathbf{u}$ is the resolved wind vector, $\mathbf{K}$ is the eddy-diffusivity tensor, $u_{d,i}$ is the vertical deposition velocity that includes gravitational settling, $\beta(r, r')$ is the coagulation coefficient between particles of sizes $r$ and $r'$, $I_i(r, \mathbf{x}, t), 1 \leq i \leq m_e$, is the rate of species mass transfer of of particle of size $r$ as a result of condensation and evaporation processes, $I_i(r, \mathbf{x}, t) = \sum_{i=1}^{m_e} I_i(r, \mathbf{x}, t)$, and $S_i(r, \mathbf{x}, t)$ represents any source of particles of size $r$ (e.g., nucleation, emission). Let $\mathbf{c}(\mathbf{x}, t) = (c_1(\mathbf{x}, t), ..., c_{m_g}(\mathbf{x}, t))^T$ be the gas species concentration at space $\mathbf{x}$ and time $t$. The equation of conservation governing $c_i(\mathbf{x}, t)$ is

$$
\frac{\partial}{\partial t} c_i(\mathbf{x}, t) + (\mathbf{u}(\mathbf{x}, t) - u_{d,i} \mathbf{e}_z) \cdot \nabla_x c_i(\mathbf{x}, t) - \nabla_x \cdot (\mathbf{K}(\mathbf{x}, t) \nabla_x c_i(\mathbf{x}, t))
$$

$$
+ \int_0^\infty \frac{b_i(r, \mathbf{x}, t)}{r} I_i(r, \mathbf{x}, t) dr = f_i(\mathbf{c}(\mathbf{x}, t)) + E_i(\mathbf{x}, t),
$$

where $f_i(\mathbf{c}(\mathbf{x}, t))$ is the rate of chemical reactions in the the bulk gas phase and $E_i(\mathbf{x}, t)$ is the emission rate of gas species $i$.

The coupling of equations (3.23) and (3.24) is a result of condensation and evaporation processes, which depends strongly on the composition at thermodynamic equilibrium between the bulk gas phase and the particles. Driven by the difference of the concentrations of species in the bulk gas phase and at the particle surface, the mass transfer rate $I_i$ is is defined by [176]

$$
I_i(r, \mathbf{x}, t) = h_i(r) \left( c_i(\mathbf{x}, t) - \eta(r) c_{i,\text{surf}}(r, \mathbf{x}, t) \right),
$$

where $\eta(r)$ is the Kelvin constant of particle size $r$, and $c_{i,\text{surf}}(r, \mathbf{x}, t)$ is the gas concentration at the surface of particle size $r$ at space $\mathbf{x}$ and time $t$. Let $p_i^{\text{equil}}(r, \mathbf{x}, t)$ be the fugacity of gas species $i$ that is in equilibrium with the particle of size $r$ at space $\mathbf{x}$ and time $t$. The surface gas concentration is then given by $c_{i,\text{surf}}(r, \mathbf{x}, t) = \frac{1}{RH_{100}^2} p_i^{\text{equil}}(r, \mathbf{x}, t)$.

For the calculation of $p_i^{\text{equil}}(r, \mathbf{x}, t)$, one needs first to solve a multiphase and multi-reaction chemical equilibrium problem (CEP). Assuming constant temperature, pressure, and specific relative humidity $R_{H_{100}}$, the CEP is modeled by the following inequality constrained minimization problem:

Find $(y_{a1}, x_{a1}, n_1, n_2, n_g, n_{H_2O(pm)}) \in L^2_+(\Omega) \times L^2_+(\Omega)^{2m_1 + m_s + m_g} \times L^2_+(\Omega)$ such that

$$
\min G(y_{a1}, x_{a1}, n_1, n_2, n_g, n_{H_2O(pm)})
$$

where $G$ stands for the Gibbs free energy

$$
G(y_{a1}, x_{a1}, n_1, n_2, n_g, n_{H_2O(pm)}) = \int_\Omega \left( \sum_{a=1}^p y_{a1} x_{a1} \ln a_{a,l} + n_l \ln k_l 
$$

$$
+ n_{g} \cdot (\ln a_{g} + \ln k_{g}) + n_s \cdot \ln k_s - n_{H_2O(pm)} \ln RH_{100} \right) dx,
$$

subject to the constraints

$$
(3.27) \ b \text{ and } c \text{ satisfy the state equations (3.23), (3.24), and (3.25),}
$$
\( \mathbf{A}_l \mathbf{n}_l + \mathbf{A}_g \mathbf{n}_g + \mathbf{A}_s \mathbf{n}_s - n_{H_2O(p)} \mathbf{a}_{H_2O} = \mathbf{b} , \)

\[
\sum_{\alpha=1}^{p} y_{\alpha} x_{\alpha} - \mathbf{n}_l = 0 , \quad \sum_{\alpha=1}^{p} x_{\alpha} = 1 .
\]

Here, \( \mathbf{n}_k, \mathbf{a}_k, \mathbf{k}_k \) and \( \mathbf{A}_k \in \mathbb{R}^{m_k \times m_k} \) are the concentration vector, the chemical activity vector, the canonical equilibrium constant vector, and the component-based formula matrix for the species set \( k = l, g, s \) respectively. The subscripts \( l, g, s \) denote the liquid, gas and solid phases respectively.

Once the equilibrium solution of the CEP is known, the gas fugacity \( p_{g}^{\text{equil}}(r, \mathbf{x}, t) \) is given by the activities of gas species that is in equilibrium with the particle of size \( r \) at space \( \mathbf{x} \) and time \( t \).

Over the last two decades, a succession of thermodynamic models \([17, 129, 130, 132, 136, 137, 135, 143, 145, 146, 155, 161]\) has been developed to predict the phase transition and multistage growth phenomena of inorganic aerosols. These modules calculate the composition of atmospheric aerosols by solving a set of nonlinear algebraic equations derived from chemical equilibrium relations. One of the most challenging parts for them is the prediction of the partitioning of the inorganic aerosol components between aqueous and solid phases. A major weakness in these modules lies in the way they treat the transition between aqueous and solid aerosol phases. By relying on a priori and often incomplete knowledge of the presence of solid phases at a certain relative humidity and overall composition, these modules often fail to accurately predict the phase state and composition and the multistage growth phenomena of inorganic aerosols \([11, 12]\).

While considerable progress has been made in understanding the physical and chemical properties of inorganic aerosols, relatively less attention has been given to atmospheric particles containing both inorganic and organic compounds. Furthermore, less emphasis has been put on liquid-liquid equilibria (LLE) and solid-liquid equilibria (SLE) than vapor-liquid equilibria (VLE) in water-organic electrolyte systems \([151, 152, 165]\). An accurate and consistent representation of VLE, LLE and SLE in water-organic electrolyte systems is one of the challenging research fields in atmospheric aerosol modeling \([64]\).

Recently, we developed a primal-dual active set algorithm for the efficient and accurate prediction of the phase transition and multistage growth phenomena of inorganic aerosols \([7, 8]\). The mathematical framework for modeling solid-liquid equilibrium reactions is based on the canonical stoichiometry of inorganic aerosols \([181]\).

The primal-dual active set algorithm is implemented in UHAERO, a general aerosol model which uses the Extended UNIQUAC model (ExUNIQUAC), a multicomponent mole-fraction-based thermodynamic model, to represent aqueous phase activities and solid-liquid-vapor equilibrium in the system \( H^+ - NH_4^+ - SO_4^{2-} - NO_3^- - Na^+ - Cl^- - H_2O \). Figure 2 shows the simulation results about the multi-stage growth and phase diagram of sulfate aerosols. The accuracy of the model prediction compared well with available measurements.
We also developed a primal-dual interior-point algorithm for the efficient solution of the phase equilibrium problem (PEP) in organic aerosols [9, 10] where the PEP is reformulated as a problem of constructing the convex hull of the molar Gibbs free energy.

Figure 3 shows the simulation results on the mixture of water (1) - n-propanol(2) - n-hexane (3). This example was given in Appendix 2 of Fredenslund et al. [70] as an example of liquid-liquid phase equilibrium calculations. Floudas et al. [142] applied a global optimization approach to the problem and obtained the global minimum of three liquid phases in 10990 iterations. The fact that our model finds the global liquid-liquid-liquid (LLL) equilibrium solution in less than 30 iterations from general starting points in convex regions of the molar Gibbs free energy function illustrates the efficiency of our primal-dual interior-point method in predicting phase equilibria of mixed water-organic systems.

The proposed atmospheric research will center on the development of a comprehensive mathematical computational model for mixed inorganic-organic atmospheric aerosols. We will develop primal-dual Newton methods for the numerical solution of the CEP (3.26).

The computational model to be developed in this project is intended to be incorporated in 3D air quality models such as the U.S. EPA Models3/CMAQ model [38] and the Harvard GEOS-CHEM model for the prediction of the effects of the
physical state of tropospheric particles on gas/particle partitioning and on global aerosol direct radiative forcing.

4. Research Plan and Outreach

The detailed research plan for this proposal is as follows:

First Year: Development and analysis of multilevel iterative solvers for PDE constrained optimization problems based on Newton interior-point methods.

Second Year: Development and analysis of multilevel iterative solvers for PDE constrained optimization problems based on active set strategies.

Third Year: Application of the algorithmic tools to shape optimization in CFD and phase identification in atmospheric research.

The research teams of the principal investigators have substantial experiences in the development, analysis, and implementation of advanced numerical techniques for

- partial differential equations and systems thereof [62, 63, 87, 104, 105, 106, 107, 109, 114, 124, 125, 126, 127],

They have also intensively worked on the mathematical modeling, simulation, and optimization of

- Newtonian and non-Newtonian fluid flows, [1, 2, 3, 30, 50, 51, 52, 53, 61, 110, 111, 166],
- reaction-diffusion-advection processes in atmospheric research and air-quality control.

We think that this background provides a solid basis for the successful realization of the research plan.

The University of Houston and Rice University are only 20min apart. This geographic proximity will further facilitate the collaboration between the PIs. The PIs plan to conduct a weekly research seminar to promote interaction among their groups. This seminar will be held at the University of Houston and at Rice University in alternating weeks.

The PIs maintain active co-operations with a number of academic researchers, Sandia Nat. Labs, the Fraunhofer Institute for Research on Silicates (Würzburg), the Center for Environmental Simulations (University of Augsburg), the Institute for Atmospheric Research (Garmisch-Partenkirchen), and with industrial partners (Fluidicon, Porsche AG, SGL Carbon). These collaborations will be useful to facilitate dissemination of our research results into the optimization and application communities.
The PIs have been and will be involved in the organization of international workshops, conferences and minisymposia on topics in the numerical analysis of partial differential equations and in PDE constrained optimization (e.g., Conferences at the Math. Research Center Oberwolfach (Oberwolfach, Germany 2003,2006), GAMM Annual Meeting 2004, ECCOMAS 2004 (Jyväskylä, Finland), ECCOMAS 2008 (Venice, Italy), ENUMATH 2003 (Prague, Czech Republic), ENUMATH 2005 (Santiago de Compostela, Spain), International Conference on Domain Decomposition Methods (2003 (Berlin, Germany), 2005 (New York, USA), 2006 (Strobl, Austria)), Sandia Workshops on PDE Constrained Optimization (Santa Fe 2001,2004), CIM Workshop on PDE Constrained Optimization (Tomar, Portugal, 2005). One goal of these activities is to facilitate interactions among researchers in numerical PDEs, in numerical optimization, and in application areas. Additionally, they will be useful to promote dissemination of our research results.
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