Model Hierarchies and Optimal Control of Radiative Transfer

R. Pinnau[1] and G. Thömmes[2]

[1] TU Kaiserslautern, Department of Mathematics, Kaiserslautern, Germany, pinnau@mathematik.uni-kl.de
[2] Fraunhofer ITWM, Kaiserslautern, Germany

Summary. Optimal control problems in radiative transfer are solved by means of the space mapping technique. Exploiting a hierarchy of approximate models, this allows for the construction of fast numerical algorithms. The performance of the algorithms is underlined by numerical experiments.

1 Introduction

We consider an optimal control problem in the realm of radiative transfer with a tracking-type cost functional for given functions $\bar{\varphi}, \bar{Q} : D \to \mathbb{R}$,

$$F(\varphi, Q) = \frac{\alpha_1}{2} \int_D (\varphi - \bar{\varphi})^2 dx + \frac{\alpha_2}{2} \int_D (Q - \bar{Q})^2 dx. \tag{1}$$

Here, $\varphi(x) = \int_{S^2} I(x,\omega) d\omega$ denotes total flux corresponding to the space and direction dependent intensity I.

The intensity $I(x,\omega) : \mathbb{R}^d \times S^2 \to \mathbb{R}$ is computed by solving the radiative transfer equation,

$$\varepsilon\omega \cdot \nabla I + (\sigma_s + \sigma_a) I = \frac{\sigma_s}{4\pi} \int_{S^2} I \, d\omega' + Q(x), \tag{2a}$$

where d is the space dimension of the underlying domain, S^2 is the sphere in $\mathbb{R}^3$ and σ_s and σ_a are problem dependent scattering and absorption parameters and ε is a scaling factor of the equation, i.e. $\varepsilon = x^{ref}/(\sigma_a^{ref} + \sigma_s^{ref})$. This equation is supplemented with appropriate Dirichlet data

$$I(x,\omega) = A, \qquad n \cdot \omega < 0, \tag{2b}$$

for ingoing directions. The equation contains the source term $Q(x)$, which can be interpreted as an exterior source or sink of radiation energy. This external source is the control variable of our problem.

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The corresponding optimisation problem for determining a distributed control $Q(x)$ reads

$$\min_{\varphi,Q} F(\varphi, Q) \text{ subject to (2).} \tag{3}$$

This optimisation problem was first analysed in [4], where the existence and uniqueness of an optimal control Q is proved. Here, we exploit the approximate SP_N model hierarchy [6] and the space mapping technique [2, 3] to construct a fast optimisation algorithm. This model hierarchy was already used studied in the context of optimal control in radiative transfer in [5], where an asymptotic analysis of the first order optimality system is performed.

In the following we describe the approximate model hierarchy and the space mapping technique and discuss some numerical results.

2 The SP_N Models

The SP_N approximations for the radiative transfer equation (2) are derived in a formal manner applying the Neumann series to an unbounded operator when the medium is assumed to be optically thick, i.e. the mean free path ϵ is small (for a detailed derivation see [8]). The continuous SP_1 approximation of (2) is given by

$$-\frac{\varepsilon^2}{3(\sigma+\kappa)}\nabla^2\phi + \kappa\phi = 4\pi Q, \tag{4a}$$

and the corresponding SP_2 approximation is

$$-\varepsilon^2\frac{5(\sigma+\kappa)+4\kappa}{15(\sigma+\kappa)}\nabla^2\xi + \kappa\xi = 4\pi Q, \tag{4b}$$

where $\xi = \phi + \frac{4\kappa}{5(\sigma+\kappa)}(\phi - 4\pi Q/\kappa)$, and the SP_3 equations are

$$-\frac{\varepsilon^2}{3(\sigma+\kappa)}\nabla^2(\phi + 2\phi_2) + \kappa\phi = 4\pi Q, \tag{4c}$$

$$-\frac{9\varepsilon^2}{35(\sigma+\kappa)}\nabla^2\phi_2 + (\sigma+\kappa)\phi_2 - \frac{2}{5}\kappa\phi = -\frac{2}{5}\,4\pi Q. \tag{4d}$$

In all cases, ϕ approximates the mean intensity given by (2). For the validity of the SP_N approximations we refer to [8]. This model hierarchy yields the so-called coarse models, which are used in the setup of the following space mapping algorithm.

3 Aggressive Space Mapping

The solution of the full optimisation problem (3) is rather time consuming, since it requires the discretisation of the spatial and of the angular variable.

Now, we want to define a algorithm which only requires solves of the *fine* radiative transfer problem (2) and not the solution of the full optimisation problem. Instead, we will only solve optimisation problems based on the *coarse* SP_N models, for which one can easily implement an optimisation algorithm using the adjoint information for the computation of descent directions (for details we refer to [5]).

In particular, we want to approximate the solution of the fine model by an appropriate solution of the coarse model for which we define the misalignment function (here we follow [3])

$$r(R, Q) = \|\phi(R) - \varphi(Q)\|,$$

where $\phi(R)$ is the coarse model output of a SP_N model for a given source R and $\varphi(Q)$ is fine model output computed by (2) for a given source Q. For a given Q we look for R such that $r(R, Q)$ is minimal, i.e., we define the space mapping function

$$p(Q) = \operatorname{argmin}_R r(R, Q).$$

Since we want to evaluate p only a few times, we assume $\varphi(Q^*) \approx \phi(R^*)$, such that

$$p(Q^*) = \operatorname{argmin}_R r(R, Q^*) \approx R^*.$$

Hence, we first determine R^* and then solve for $p(Q^*) = R^*$. But in general it holds $p(Q^*) \neq R^*$, such that we solve instead for

$$Q^* = \operatorname{argmin}_Q \|p(Q) - Q^*\|.$$

This is done iteratively and the space mapping p is updated using a Broyden–rank–1 update yielding the so–called ASM (aggressive space mapping) algorithm (for details we refer to [3]):

1. Evaluate $Q_0 = R^* = \operatorname{argmin}_R \|c(R)\|^2$ and let B_0 be the identity matrix.
2. While $\|p(Q_k) - R^*\| / \|\zeta^*\| >$ tolerance
   a) Evaluate $\varphi(Q_k)$ by solving the fine model (2)
   b) Determine $R_k = p(Q_k) = \operatorname{argmin}_R \|c(R) - f(Q)\|^2$
   c) Solve $B_k h_k = -(p(Q_k) - R^*)$ for h_k
   d) Set $Q_{k+1} = Q_k + h_k$
   e) Update $B_{k+1} = B_k + \frac{(p(Q_{k+1}) - R^*) h_k^T}{h_k^T h_k}$
   f) Set $k \to k + 1$.

Here, we have rewritten the cost functional (1) by defining

$$c(R) = \begin{pmatrix} \sqrt{\frac{\alpha_1}{2}}(\varphi(R) - \bar{\varphi}) \\ \sqrt{\frac{\alpha_2}{2}}(R - \bar{Q}) \end{pmatrix}, \quad \text{and} \quad f(Q) = \begin{pmatrix} \sqrt{\frac{\alpha_1}{2}}(\phi(Q) - \bar{\varphi}) \\ \sqrt{\frac{\alpha_2}{2}}(Q - \bar{Q}) \end{pmatrix}.$$

Remark 1. On each iteration level we need one evaluation of the fine model and one solve of the optimal control problem for the coarse model. That is, it is sufficient to implement an adjoint code for the coarse model [5].

4 Numerical Results

We implemented test cases in 1D using the DSA iterative scheme for the transport equations of the forward and adjoint equations on the *fine* level [1,7]. The radiative transfer equation was discretised on an equidistant space grid using the diamond differencing scheme by evaluating intensity I and source q at the nodes $x_i = i\Delta x,\ i = 0, \dots, M$ and using averages $I_{i+\frac{1}{2}} = (I_{i+1} + I_i)/2$ and $q_{i+\frac{1}{2}} = (q_{i+1} + q_i)/2$. The iteration is started by choosing an initial iterate I_{ij}^0 and computing the flux $\varphi_i^0 = \sum_{j=1}^N I_{ij}^0 w_j$. Then, for $k \geq 0$, the iteration proceeds in two substeps. First, the following transport equation with given right side is solved for the intermediate intensity $I_{ij}^{k+\frac{1}{2}}$

$$\varepsilon\mu_j \frac{I_{i+1,j}^{k+\frac{1}{2}} - I_{ij}^{k+\frac{1}{2}}}{\Delta x} + \sigma_t I_{i+\frac{1}{2},j}^{k+\frac{1}{2}} = \frac{\sigma_s}{2}\varphi_{i+\frac{1}{2}}^k + q_{i+\frac{1}{2}},$$

$$\text{with b.c.} \quad I_{0,j}^{k+\frac{1}{2}} = A,\ \mu_j > 0, \quad I_{M,j}^{k+\frac{1}{2}} = A,\ \mu_j < 0.$$

This corresponds to the transport sweep in the source iteration method. Note that the sweep is done from left to right when $\mu_j > 0$, and from right to left when $\mu_j < 0$. Then the flux difference $\varphi_i^{k+\frac{1}{2}} = \sum_{j=1}^N (I_{ij}^{k+\frac{1}{2}} - I_{ij}^k) w_j$ is taken as source term for the computation of the correction $\delta\varphi^{k+\frac{1}{2}}$:

$$-\frac{\varepsilon^2}{3\sigma_t}\frac{\delta\varphi_{i+1}^{k+\frac{1}{2}} - 2\delta\varphi_i^{k+\frac{1}{2}} + \delta\varphi_{i-1}^{k+\frac{1}{2}}}{\Delta x^2} + \sigma_a \frac{\delta\varphi_{i+1}^{k+\frac{1}{2}} + 2\delta\varphi_i^{k+\frac{1}{2}} + \delta\varphi_{i-1}^{k+\frac{1}{2}}}{4}$$
$$= \sigma_s \frac{\varphi_{i+1}^{k+\frac{1}{2}} - \varphi_{i+1}^k}{2} + \sigma_s \frac{\varphi_i^{k+\frac{1}{2}} - \varphi_i^k}{2},$$

with homogeneous boundary conditions on the left and right of the interval. The new iterate for the flux is eventually updated

$$\varphi_i^{k+1} = \varphi_i^{k+\frac{1}{2}} + \delta\varphi_i^{k+\frac{1}{2}}.$$

After the iteration has stopped, we obtain a numerical solution for the intensity by performing an additional sweep with the final flux. The coarse level SP_N approximations corresponding to the one-dimensional transfer equation were discretised using standard finite differences.

In the examples presented in the following, the radiative transfer problem had an absorption cross section $\sigma_a = 1$ and a scattering cross section $\sigma_s = 1$, and the non-dimensional parameter $\varepsilon = 1$ was used. The equation was discretised with $N_x = 51$ nodes $x_i = i/N_x$ in space. For the angular variable, $N_g = 32$ nodes given by the quadrature points of double Gaussian quadrature on $[-1, +1]$ were used. The RTE equation was solved for homogeneous Dirichlet boundary conditions $A = 0$ for ingoing directions at the left and right, respectively. The tracking part of the functional had the weight $\alpha_1 = 1$

Table 1. Comparison of the optimisation methods

	Iterations	Evals	Runtime $[s]$	F_{End}
Gradient	12	44	0.7	$5.3540 \cdot 10^{-8}$
Trust region	14	15	0.5	$7.5886 \cdot 10^{-6}$
ASM	3	3(40)	0.3	$2.9682 \cdot 10^{-6}$

Table 2. Comparison of the optimisation methods

	Iterations	Evals	Runtime $[s]$	F_{End}
Gradient	11	42	0.8	$7.2731 \cdot 10^{-3}$
Trust region	4	5	0.2	$7.2733 \cdot 10^{-3}$
ASM	2	2(14)	0.2	$7.4130 \cdot 10^{-3}$

and the regularisation the weight $\alpha_2 = 1$. The same functional was also used for the coarse model.

The performance of a classical gradient and a trust region algorithm for the fine model was compared with aggressive space mapping based on the SP_1 model. The space mapping $p(Q)$ was evaluated using a trust region method for the coarse functional optimisations [3]. We used a stopping criterion based on the functional values and the size of the gradient of the functional. These parameters were also used for the standard trust region method. The standard gradient method included an Armijo line search.

4.1 Box-Shaped Source

In the first numerical test we use a prescribed reference source q_{ref} as shown in Fig. 1, for which φ_{ref} is computed. Then, we seek the optimiser starting from a vanishing source. The performance of the algorithms can be seen from Table 1 and the corresponding final results are depicted in Fig. 1. The aggressive space mapping needs just three evaluations of the fine model and 40 function evaluations on the coarse level. Hence, we get comparable results with less numerical effort.

4.2 Unknown Reference Source

In the second test case we want to reconstruct an unknown source and set $q_{ref} = 0$. The reference intensity belongs to a Gaussian source term (center 0.5, std. dev. 0.1) and we start the algorithms again from a vanishing source. The performance of the algorithms can be seen from Table 2. Again, the aggressive space mapping needs just very few evaluations of the fine model and yields results comparable to the full optimisation.

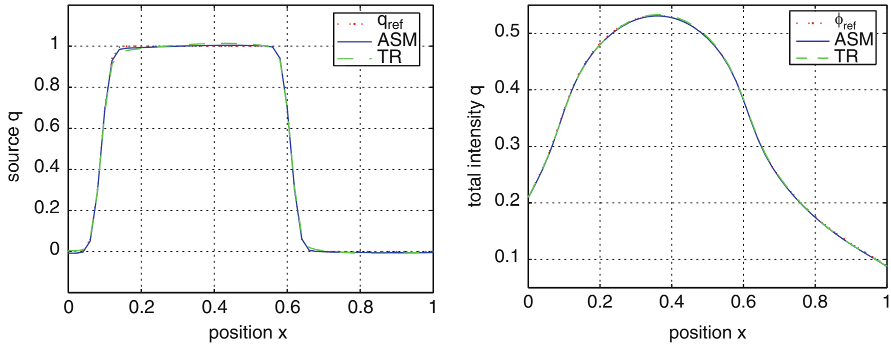

Fig. 1. *Left*: Control after optimisation using space mapping. The results of aggressive space mapping and a trust region solve are compared with the reference solution *Right*: The corresponding state given by the flux, i.e., the angle-integrated intensity

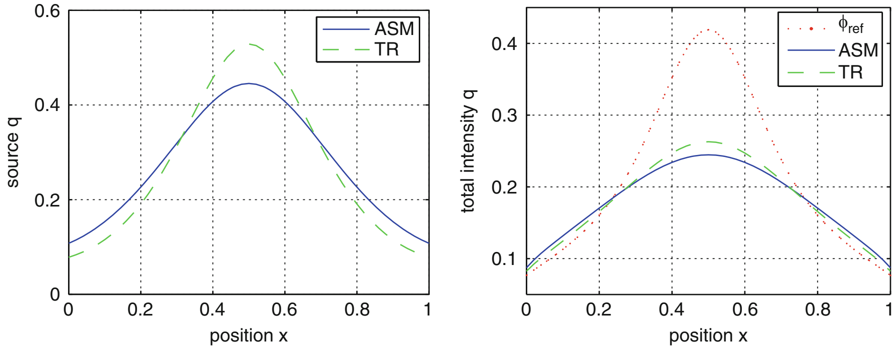

Fig. 2. *Left*: Control after optimisation using space mapping. The results of aggressive space mapping and a trust region solution are compared. *Right*: The corresponding state given by the flux, i.e., the angle-integrated intensity and the reference intensity

References

1. Alcouffe, R.E.: Nucl. Sci. Eng. **64**, 344–355 (1977)
2. Bandler, J.W., Biernacki, R.M., Chen, S.H., Grobelny, P.A., Hemmers, R.H.: IEEE Trans. Microw. Theory Tech. **43**, 2874–288 (1995)
3. Echeverría, D., Hemker, P.W.: Comput. Methods Appl. Math. **5**(2), 107–136 (2005)
4. Herty, M., Pinnau, R., Seaid, M.: OMS **22**(6), 917–936 (2007)
5. Herty, M., Pinnau, R., Thömmes, G.: ZAMM **87**(5), 333–347 (2007)
6. Larsen, E.W., Thömmes, G., Klar, A., Seaid, M., Götz, T.: JCP **183** (2002)
7. Lewis, E.E., Miller, W.F. Jr.: Comput. Methods of Neutron Transport, Wiley New York (1984)
8. Thömmes, G.: Radioactive Heat Transfer for Glass Cooling Problems, PhD Thesis, Tu Darmstadt (2002)