

Asymptotic and Discrete Concepts for Optimal Control in Radiative Transfer

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Abstract

Optimal control problems for radiative transfer and for approximate models are considered. Following the approach *first discretize, then optimize*, the discrete SP_N approximations are for the first time derived exactly, which can be used to study optimal control on reduced order models. Combining asymptotic analysis and the adjoint calculus yields diffusive-type approximations for the adjoint radiative transport equation in the spirit of the approach *first optimize, then discretize*.

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1 Introduction

The simulation and optimization of radiation dominated heat transfer processes, e.g. in the field of glass cooling processes or the design of combustion chambers, pose several challenging problems for applied mathematicians and engineers and have been extensively studied during the last years [3, 21, 16, 2, 1, 6, 13]. Due to the high numerical complexity of the model equations which are given by the radiative heat transfer system for the radiative intensity, there is a strong need for sophisticated reduced order models. This led to the development of a whole hierarchy of approximate equations, ranging from moment expansions to diffusive type models, like the SP_N -systems [9, 8, 4]. Other recent developments discuss the coupling of radiative transfer and heat equations, see for example [7, 10], and efficient numerical schemes for resolving the arising systems [17, 19, 18]. In this work, we are interested in the study of *optimal control problems* of tracking-type in radiative transfer. The general problem we are considering is formulated as follows:

$$\min_{\varphi, Q} \mathcal{F}(\varphi, Q) \text{ subject to (1.3),} \tag{1.1}$$

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where φ is the mean intensity,

$$\varphi(\mathbf{x}) := \int_{S^{d-1}} I(\mathbf{x}, \omega) d\omega, \quad (1.2)$$

S^{d-1} the unit sphere in \mathbb{R}^d , and $I = I(\mathbf{x}, \omega)$, the intensity at position \mathbf{x} propagating along direction ω . We assume, I satisfies the scaled radiative transfer equation

$$\begin{aligned} \varepsilon \omega \cdot \nabla I + (\sigma + \kappa) I &= \frac{\sigma}{4\pi} \int_{S^{d-1}} I d\omega + Q, \\ I(\omega, \mathbf{x}) &= A, \quad \mathbf{n} \cdot \omega < 0, \end{aligned} \quad (1.3)$$

for given boundary data $A = A(\omega)$ and source term $Q = Q(\mathbf{x})$. Further, $\kappa = \kappa(\mathbf{x})$ is the absorption coefficient and $\sigma = \sigma(\mathbf{x})$ is the scattering coefficient. By $n = n(\mathbf{x})$ we denote the outer normal at a boundary point \mathbf{x} . We consider an optically thick medium, where the opacity or the scattering cross section are large and therefore the radiation is conveyed in a diffusive way. Hence, the scaled equation contain the asymptotic parameter $\varepsilon = 1/((\kappa_{ref} + \sigma_{ref})\mathbf{x}_{ref})$ which tends to 0.

Finally, the objective functional is of tracking-type,

$$\mathcal{F}(\varphi, Q) := \frac{\alpha_1}{2} \int_D (\varphi - \bar{\varphi})^2 d\mathbf{x} + \frac{\alpha_2}{2} \int_D (Q - \bar{Q})^2 d\mathbf{x}, \quad (1.4)$$

for a domain $D \in \mathbb{R}^d$ and positive constants α_1, α_2 and given (desired) states and controls $\bar{\varphi}(\mathbf{x})$ and $\bar{Q}(\mathbf{x})$, respectively.

This work extends recently published results [5, 14] on such optimal control problems (1.1). Here, we essentially focus on the well-known SP_N approximations for (1.3) (see e.g. [9, 8] and the references therein). We employ techniques from asymptotic analysis to derive approximate models and adjoints which are more suitable for optimization purposes than the full transport equation. Essentially, we follow the two common approaches *first discretize, then optimize*, or, vice versa, *first optimize, then discretize*.

Our motivation is two-fold: First, we are interested in a thorough derivation of the SP_N approximations by starting from a discretization of the radiative transfer equations and using von Neumann's series to invert the arising matrices of the discrete system. This procedure parallels the derivation of the SP_N approximations in the continuous case and leads to discretizations of the corresponding diffusion equations, c.f. Section 2.

Second, we apply the adjoint calculus to the RHT equation and use the continuous SP_N approximation procedure to derive the SP_N system for the adjoint problem, see Section 3. In combination with the results of [5, 14] we finally establish the following diagram (Figure 1) for general tracking-type optimal control problems in radiative transfer.

We collect some references concerning already discussed connections in Figure 1:

- 'Continuous RTE' \rightarrow ' SP_N approximations': The continuous SP_N approximations for the continuous RT equation are well-known, see for example [20, 9]. But they can be only derived in a *formal* manner due the usage of the von Neumann series for unbounded operators.
- 'Continuous RTE' \rightarrow 'Continuous Adjoints of the RTE': This connection has been established in [5]. The result, which will be used later, is as follows [5, Theorem 1]: Given

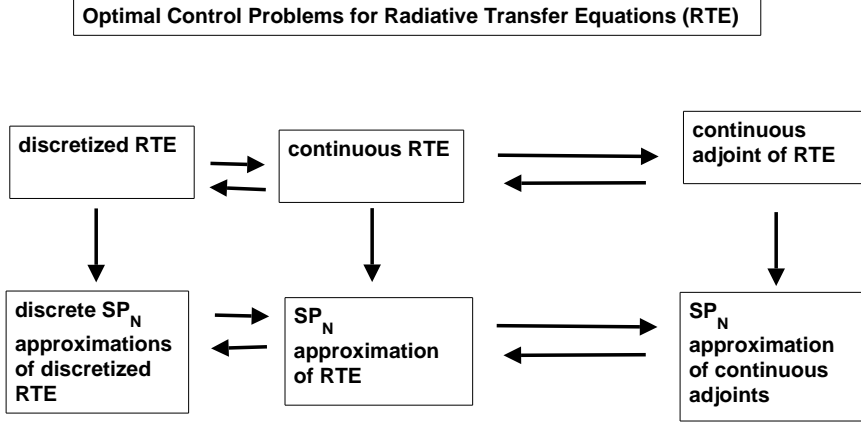


Figure 1: Diagram of the interplay of discrete, adjoint and SP_N approximations in radiative transfer.

a sufficiently regular, bounded domain $D \in \mathbb{R}^{2,3}$ and $\bar{\varphi}, \bar{Q} \in L^2(D)$. Then, there exists a function $\lambda \in L^2(D)$, such that the necessary and sufficient first-order optimality conditions for (1.1). Moreover, λ could be obtained from the formal adjoints to (1.3), i.e., λ depends on the solution J to

$$\begin{aligned}
 -\varepsilon \boldsymbol{\omega} \cdot \nabla J + (\sigma + \kappa)J &= \frac{\sigma}{4\pi} \int_{S^{d-1}} J d\boldsymbol{\omega} + \alpha_1 (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})), \\
 J(\boldsymbol{\omega}, \mathbf{x}) &= 0, \quad \mathbf{n} \cdot \boldsymbol{\omega} > 0,
 \end{aligned} \tag{1.5}$$

and the following (gradient) equation holds:

$$\alpha_2 (Q(\mathbf{x}) - \bar{Q}(\mathbf{x})) + \int_{S^{d-1}} J d\boldsymbol{\omega} = 0. \tag{1.6}$$

- ' SP_N approximations of RTE' \rightarrow ' SP_N of adjoints of the RTE' as been discussed in [14, 15]. Here, the adjoint calculus was used for the derivation of first- and second-order optimality conditions for minimization problems constrained by the continuous SP_N system coupled with a nonlinear heat equation.

In this work, we discuss the remaining links, being 'discretized RTE' \rightarrow 'discrete SP_N ', 'discrete SP_N ' \rightarrow ' SP_N of continuous RTE' (both in Section 2) and finally, 'adjoints of RTE' \rightarrow ' SP_N of adjoints' (see Section 3).

Remark 1 In general, radiative transfer equations have the form [12, 11]

$$\varepsilon\omega \cdot \nabla \mathbf{I} + (\sigma + \kappa)\mathbf{I} = \frac{\sigma}{4\pi} \int_{S^{d-1}} \mathbf{I} d\omega + \kappa B(\theta). \quad (1.7)$$

In (1.7), θ is the temperature, and $B(\theta)$ is the intensity of the black-body radiation given by the Stefan-Boltzmann law, compare [11] for further physical details. The equations (1.7) are solved subject to the boundary condition

$$\mathbf{I}(t\omega, \mathbf{x}) = \varrho(\mathbf{n} \cdot \omega)\mathbf{I}(t, \omega', \mathbf{x}) + (1 - \varrho(\mathbf{n} \cdot \omega)) B(\theta_b), \quad \mathbf{n} \cdot \omega < 0, \quad (1.8)$$

where $\varrho \in [0, 1]$ is the reflectivity: $\varrho = 1$ for total reflection and $\varrho = 0$ for Dirichlet type boundary conditions. The temperature θ_b is a fixed boundary function, \mathbf{n} is the outward normal on the boundary and $\omega' = \omega - 2(\mathbf{n} \cdot \omega)\mathbf{n}$ is the specular reflection of ω on the boundary.

For the sake of simplicity, we shall consider the radiative transfer model (1.3). Although we assume several simplifications, these equations are still reasonable in many applications, e.g. when dealing with a grey medium and if the mean free path of the radiation is small compared to a characteristic length.

2 Discrete derivation of the SP_N approximations

In this section we follow the approach *first discretize, then optimize* to derive a reduced order model valid in the diffusive limit on the discrete level. Due to the special, symmetric structure of the discretizations these can then be directly used for the implementation of the corresponding discrete adjoints.

Starting from a discretization of the radiative transfer equations, we use Neumann's series to invert the matrices of the discrete system and derive a discrete version of the SP_N approximations. The procedure closely resembles the derivation of the SP_N approximations in the continuous case and results in valid discretizations of the corresponding diffusion equations. This substantiates the construction of the continuous SP_N equations in the framework of an asymptotic analysis where Neumann's series has been formally applied to invert the transport operator, which contains the unbounded space derivative operator [8].

The medium is assumed to be optically thick, i.e. κ or σ are large such that the mean free path is small. For notational convenience we define the source term

$$\kappa B := Q. \quad (2.1)$$

The continuous SP_1 , SP_2 and SP_3 approximations of (1.3) are given, respectively, by

$$-\frac{\varepsilon^2}{3(\sigma + \kappa)} \nabla^2 \varphi + \kappa \varphi = 4\pi \kappa B, \quad (2.2)$$

and

$$-\varepsilon^2 \frac{5(\sigma + \kappa) + 4\kappa}{15(\sigma + \kappa)} \nabla^2 \xi + \kappa \xi = 4\pi \kappa B, \quad (2.3)$$

where $\xi = \varphi + \frac{4\kappa}{5(\sigma + \kappa)}(\varphi - 4\pi B)$, and

$$-\frac{\varepsilon^2}{3(\sigma + \kappa)} \nabla^2 (\varphi + 2\varphi_2) + \kappa \varphi = 4\pi \kappa B, \quad (2.4a)$$

$$-\frac{9\varepsilon^2}{35(\sigma + \kappa)} \nabla^2 \varphi_2 + (\sigma + \kappa)\varphi_2 - \frac{2}{5}\kappa\varphi = -\frac{2}{5} 4\pi \kappa B. \quad (2.4b)$$

Remark 2 Hence we have the condition $\varepsilon = O(h)$ for the applicability of the first step in the derivation of the SP_N equations. This reflects the fact that the onesided differences above discretize the unbounded space derivative operator, and the norms of the corresponding matrices grow with order $O(1/h)$ as h tends to zero.

From the Neumann series representation of the intensity

$$\begin{aligned} I_m &= \left(Id + \frac{\varepsilon|\mu_m|}{\bar{\kappa}h} D_m \right)^{-1} c_m \\ &= \left(Id - \frac{\varepsilon|\mu_m|}{\bar{\kappa}h} D_m + \left(\frac{\varepsilon|\mu_m|}{\bar{\kappa}h} D_m \right)^2 - \left(\frac{\varepsilon|\mu_m|}{\bar{\kappa}h} D_m \right)^3 \pm \dots \right) c_m \end{aligned}$$

we compute the mean intensity $\varphi = (\varphi_k)_{k=0,\dots,K}$

$$\begin{aligned} \varphi &= 2\pi \sum_m w_m I_m \tag{2.6} \\ &= 2\pi \sum_m w_m \left(Id + \frac{\varepsilon|\mu_m|}{\bar{\kappa}h} D_m \right)^{-1} c_m \\ &= 2\pi \left(\sum_m w_m c_m - \frac{\varepsilon h}{\bar{\kappa}} \sum_m w_m |\mu_m| \frac{D_m c_m}{h^2} + \frac{\varepsilon^2}{\bar{\kappa}^2} \sum_m w_m \mu_m^2 \frac{D_m^2 c_m}{h^2} \pm \dots \right) \\ &= \left(Id + \frac{\varepsilon}{2\bar{\kappa}} h H_1 + \frac{\varepsilon^2}{3\bar{\kappa}^2} H_2 + \frac{\varepsilon^3}{4\bar{\kappa}^3} h H_3 + \dots \right) \cdot \frac{\kappa}{\bar{\kappa}} \left(\frac{\sigma}{\kappa} \varphi + 4\pi B \right) + R. \end{aligned}$$

In R we collect the contributions of boundary terms. Here, odd and even order matrices are defined via

$$H_{2n-1} = -n \sum_{m=1}^M w_m |\mu_m|^{2n-1} \frac{D_m^{2n-1}}{h^{2n}}, \quad H_{2n} = \frac{2n+1}{2} \sum_{m=1}^M w_m \mu_m^{2n} \frac{D_m^{2n}}{h^{2n}},$$

(the detailed form can be found in appendix A).

Remark 3 It may be observed that H_2, H_4, \dots are $O(h^2)$ consistent approximations to the second, fourth and higher even space derivatives, respectively. However, since they are based on onesided differences, their stencil is twice as large as corresponding stencils of standard finite difference approximations. Moreover, it can be verified that also the matrices H_1, H_3, \dots are second order approximations to even space derivatives of increasing order. In this form the expansion for the flux strongly resembles the continuous flux equation. However, in the discrete case the odd order sums do not vanish as the continuous integrals do. Instead there remain terms of order h ; but these terms can be made arbitrarily small by choosing the grid size appropriately.

We proceed by inverting the operator on the right using Neumann's series once more. This, in turn, is justified by the following argument. In the maximum norm we have $\|D_m\| = 2$, and hence, by choosing ε such that $q = \frac{2\varepsilon}{\bar{\kappa}h} < 1$, we can show the uniform boundedness with

respect to ε of the matrix series:

$$\begin{aligned} \left\| \sum_{n=1}^{\infty} (-1)^n \frac{n+1}{2} \sum_m w_m \left(\frac{\varepsilon |\mu_m|}{\bar{\kappa} h} \right)^n D_m^n \right\| &\leq \sum_{n=1}^{\infty} \frac{n+1}{2} \sum_m w_m \left(\frac{\varepsilon |\mu_m|}{\bar{\kappa} h} \right)^n \|D_m^n\|^n \\ &= \sum_{n=1}^{\infty} \frac{n+1}{2} \left(\frac{2\varepsilon}{\bar{\kappa} h} \right)^n \sum_m w_m |\mu_m|^n \\ &\leq \frac{1}{q} \sum_{n=0}^{\infty} n q^n < \infty \end{aligned}$$

Then the Neumann series

$$\begin{aligned} \frac{\kappa}{\bar{\kappa}} \left(\frac{\sigma}{\kappa} \varphi + 4\pi B \right) &= \left[Id - \left(\frac{\varepsilon}{2\bar{\kappa}} h H_1 + \frac{\varepsilon^2}{3\bar{\kappa}^2} H_2 + \dots \right) \right. \\ &\quad + \left(\frac{\varepsilon}{2\bar{\kappa}} h H_1 + \frac{\varepsilon^2}{3\bar{\kappa}^2} H_2 + \dots \right)^2 \\ &\quad \left. - \left(\frac{\varepsilon}{2\bar{\kappa}} h H_1 + \frac{\varepsilon^2}{3\bar{\kappa}^2} H_2 + \dots \right)^3 \pm \dots \right] (\varphi - R) \end{aligned}$$

eventually yields the sought-for asymptotic expansion

$$\frac{\kappa}{\bar{\kappa}} 4\pi B = \left[\frac{\kappa}{\bar{\kappa}} - \frac{\varepsilon}{2\bar{\kappa}} h H_1 + \frac{\varepsilon^2}{\bar{\kappa}^2} \left(-\frac{1}{3} H_2 + \frac{h^2}{4} H_1^2 \right) + \dots \right] \varphi + \tilde{R}. \quad (2.7)$$

2.1 The discrete SP_1 approximation

When we keep only terms up to second order in ε , the asymptotic expansion (2.7) suggests the following approximation to the radiative transfer equations

$$\frac{\kappa}{\bar{\kappa}} 4\pi B = \frac{\kappa}{\bar{\kappa}} \varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2} H_2 \varphi + \left[-\frac{\varepsilon h}{2\bar{\kappa}} H_1 \varphi + \frac{\varepsilon^2 h^2}{4\bar{\kappa}^2} H_1^2 \varphi \right] + O(\varepsilon^3). \quad (2.8)$$

This system is no standard discretization of the continuous SP_1 equation, but it is nevertheless consistent up to second order in h with this PDE. For points x_k in the interior of the domain which are sufficiently far from the boundary such that perturbations owing to boundary values can be neglected, we have

$$(H_2 \varphi)_k = \partial_x^2 \varphi_k + \frac{7}{12} h^2 \partial_x^4 \varphi_k + O(h^4)$$

and, furthermore,

$$(H_1 \varphi)_k = \partial_x^2 \varphi_k + \frac{1}{12} h^2 \partial_x^4 \varphi_k + O(h^4)$$

$$(H_1^2 \varphi)_k = \partial_x^4 \varphi_k + \frac{1}{6} h^2 \partial_x^6 \varphi_k + O(h^4),$$

(see appendix A) such that the approximation above is consistent to

$$\kappa 4\pi B_k = \kappa \varphi_k - \frac{\varepsilon^2}{3(\sigma + \kappa)} \partial_x^2 \varphi_k + O(\varepsilon h) + O(\varepsilon^3). \quad (2.9)$$

Remark 4 *Up to additional terms of order εh this limit equation coincides with the SP_1 equation. Since the underlying asymptotic expansion is only valid when $\varepsilon \leq Ch$, the discrepancy is at most of order h^2 , which is comparable with the consistency error of standard finite difference approximations of the equation using e.g. central differences.*

2.2 The discrete SP_2 approximation

For the SP_2 approximation we consider terms up to fourth order in expansion (2.7)

$$\begin{aligned} \frac{\kappa}{\bar{\kappa}}4\pi B &= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi - \frac{\varepsilon^4}{5\bar{\kappa}^4}H_4\varphi + \frac{\varepsilon^4}{9\bar{\kappa}^4}H_2^2\varphi \\ &+ \left[-\frac{\varepsilon h}{2\bar{\kappa}}H_1\varphi + \frac{\varepsilon^2 h^2}{4\bar{\kappa}^2}H_1^2\varphi - \frac{\varepsilon^3 h}{4\bar{\kappa}^3}H_3\varphi + \frac{\varepsilon^3 h}{3\bar{\kappa}^3}H_1H_2\varphi \right. \\ &\quad \left. - \frac{\varepsilon^3 h^3}{8\bar{\kappa}^3}H_1^3\varphi + \frac{\varepsilon^4 h^2}{4\bar{\kappa}^4}H_1H_3\varphi + \frac{\varepsilon^4 h^4}{16\bar{\kappa}^4}H_1^4\varphi \right] + O(\varepsilon^5). \end{aligned} \quad (2.10)$$

Since $H_4\varphi = H_2^2\varphi + O(h^2)$, we replace H_4 in the equation above. Furthermore, we can use (2.8) to express $H_2^2\varphi$ in terms of $H_2\varphi$

$$\begin{aligned} \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2^2\varphi &= H_2\left(\frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi\right) \\ &= H_2\left(\frac{\kappa}{\bar{\kappa}}(\varphi - 4\pi B) - \frac{\varepsilon h}{2\bar{\kappa}}H_1\varphi + \frac{\varepsilon^2 h^2}{4\bar{\kappa}^2}H_1^2\varphi + O(\varepsilon^3)\right), \end{aligned}$$

which leads to the equation

$$\begin{aligned} \frac{\kappa}{\bar{\kappa}}4\pi B &= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\left(\varphi + \frac{4\kappa}{5\bar{\kappa}}(\varphi - 4\pi B)\right) \\ &+ \left[-\frac{\varepsilon h}{2\bar{\kappa}}H_1\varphi + \frac{\varepsilon^2 h^2}{4\bar{\kappa}^2}H_1^2\varphi - \frac{\varepsilon^3 h}{4\bar{\kappa}^3}H_3\varphi + \frac{\varepsilon^3 h}{6\bar{\kappa}^3}H_1H_2\varphi \right. \\ &\quad \left. - \frac{\varepsilon^3 h^3}{8\bar{\kappa}^3}H_1^3\varphi + \frac{\varepsilon^4 h^2}{4\bar{\kappa}^4}H_1H_3\varphi + \frac{\varepsilon^4 h^4}{12\bar{\kappa}^4}H_1^2H_2\varphi \right] + O(\varepsilon^5). \end{aligned}$$

This expression can be rewritten by introducing the variable $\xi = \varphi + \frac{4\kappa}{5\bar{\kappa}}(\varphi - 4\pi B)$:

$$\begin{aligned} \kappa 4\pi B &= \kappa \xi - \varepsilon^2 \frac{5\bar{\kappa} + 4\kappa}{15\bar{\kappa}} H_2 \xi \\ &+ \varepsilon h \left[-\frac{1}{2} H_1 + \frac{\varepsilon h}{4\bar{\kappa}} H_1^2 - \frac{\varepsilon^2}{4\bar{\kappa}^2} H_3 \right. \\ &\quad \left. + \frac{\varepsilon^2}{3\bar{\kappa}^2} H_1 H_2 - \frac{\varepsilon^2 h^2}{8\bar{\kappa}^2} H_1^3 + \frac{\varepsilon^3 h}{4\bar{\kappa}^3} H_1 H_3 + \frac{\varepsilon^3 h^3}{16\bar{\kappa}^3} H_1^4 \right] \\ &\quad \left(\frac{5\bar{\kappa}}{5\bar{\kappa} + 4\kappa} \xi + \frac{4\kappa}{5\bar{\kappa} + 4\kappa} 4\pi B \right) + O(\varepsilon^5). \end{aligned} \quad (2.11)$$

Remark 5 Up to $O(\varepsilon h)$ this is a discretization of the continuous SP_2 equation. As in the SP_1 case above, since the asymptotics is only valid when $\varepsilon \leq Ch$, the discrete system is second order consistent.

2.3 The discrete SP_3 approximation

The SP_3 approximation is derived from expansion (2.7) by skipping terms of order seven.

$$\begin{aligned}
\frac{\kappa}{\bar{\kappa}}4\pi B &= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi - \frac{\varepsilon^4}{5\bar{\kappa}^4}H_4\varphi + \frac{\varepsilon^4}{9\bar{\kappa}^4}H_2^2\varphi \\
&\quad - \frac{\varepsilon^6}{7\bar{\kappa}^4}H_6\varphi + \frac{2\varepsilon^6}{15\bar{\kappa}^6}H_2H_4\varphi - \frac{\varepsilon^6}{27\bar{\kappa}^4}H_2^3\varphi \\
&\quad + \left[-\frac{\varepsilon h}{2\bar{\kappa}}H_1\varphi - \frac{\varepsilon^3 h}{4\bar{\kappa}^3}H_3\varphi - \frac{\varepsilon^5 h}{6\bar{\kappa}}H_5\varphi \right. \\
&\quad + \frac{\varepsilon^2 h^2}{4\bar{\kappa}^2}H_1^2\varphi + \frac{\varepsilon^3 h}{3\bar{\kappa}^3}H_1H_2\varphi + \frac{\varepsilon^4 h^2}{4\bar{\kappa}^4}H_1H_3\varphi + \frac{\varepsilon^5 h}{5\bar{\kappa}^5}H_1H_4\varphi \\
&\quad + \frac{\varepsilon^5 h}{6\bar{\kappa}^5}H_2H_3\varphi + \frac{\varepsilon^6 h^2}{6\bar{\kappa}^6}H_1H_5\varphi + \frac{\varepsilon^6 h^2}{16\bar{\kappa}^6}H_3^2\varphi \\
&\quad - \frac{\varepsilon^3 h^3}{8\bar{\kappa}^3}H_1^3\varphi - \frac{\varepsilon^4 h^2}{4\bar{\kappa}^4}H_1^2H_2\varphi - \frac{\varepsilon^5 h}{6\bar{\kappa}^5}H_1H_2^2\varphi - \frac{3\varepsilon^6 h^2}{20\bar{\kappa}^6}H_1^2H_4\varphi \\
&\quad - \frac{\varepsilon^6 h^2}{4\bar{\kappa}^6}H_1H_2H_3\varphi - \frac{3\varepsilon^5 h^2}{16\bar{\kappa}}H_1^2H_3\varphi \\
&\quad + \frac{\varepsilon^4 h^4}{16\bar{\kappa}^4}H_1^4\varphi + \frac{\varepsilon^5 h^3}{6\bar{\kappa}^5}H_1^3H_2\varphi + \frac{\varepsilon^6 h^2}{6\bar{\kappa}^6}H_1^2H_2^2\varphi + \frac{\varepsilon^6 h^3}{8\bar{\kappa}^6}H_1^3H_3\varphi \\
&\quad \left. - \frac{\varepsilon^5 h^5}{32\bar{\kappa}^5}H_1^5\varphi + \frac{\varepsilon^6 h^6}{64\bar{\kappa}^6}H_1^6\varphi \right] + O(\varepsilon^7). \tag{2.12}
\end{aligned}$$

Using the relations $H_4\varphi = H_2^2\varphi + O(h^2)$ and $H_6\varphi = H_2^3\varphi + O(h^2)$, which are valid in the grid interior, we can rewrite the equation

$$\begin{aligned}
\frac{\kappa}{\bar{\kappa}}4\pi B &= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi - \frac{4\varepsilon^4}{45\bar{\kappa}^4}H_2^2\varphi - \frac{44\varepsilon^6}{945\bar{\kappa}^6}H_2^3\varphi + O(\varepsilon h) + O(\varepsilon^7) \\
&= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2 \left[Id + \frac{4\varepsilon^2}{15\bar{\kappa}^2}H_2 + \frac{44\varepsilon^4}{315\bar{\kappa}^4}H_2^2 \right] \varphi + O(\varepsilon h) + O(\varepsilon^7) \\
&= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2 \left[Id + 2 \left(Id + \frac{11\varepsilon^2}{21\bar{\kappa}^2}H_2^2 \right) \frac{2\varepsilon^2}{15\bar{\kappa}^2}H_2 \right] \varphi + O(\varepsilon h) + O(\varepsilon^7) \\
&= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2 \left[Id + 2 \left(Id - \frac{11\varepsilon^2}{21\bar{\kappa}^2}H_2^2 \right)^{-1} \frac{2\varepsilon^2}{15\bar{\kappa}^2}H_2 \right] \varphi + O(\varepsilon h) + O(\varepsilon^7) \\
&= \frac{\kappa}{\bar{\kappa}}\varphi - \frac{\varepsilon^2}{3\bar{\kappa}^2}H_2(\varphi + 2\varphi_2) + O(\varepsilon h) + O(\varepsilon^7). \tag{2.13a}
\end{aligned}$$

Here, the variable φ_2 is defined via an additional equation

$$-\frac{11\varepsilon^2}{21\bar{\kappa}^2}H_2^2\varphi_2 + \varphi_2 = \frac{2\varepsilon^2}{15\bar{\kappa}^2}H_2\varphi = \frac{2}{5} \left(\frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi \right).$$

From the expansion above we may also conclude that the right side of the auxiliary equation can be modified according to

$$\frac{\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi = \frac{\kappa}{\bar{\kappa}}(\varphi - 4\pi B) - \frac{2\varepsilon^2}{3\bar{\kappa}^2}H_2\varphi_2 + O(\varepsilon h),$$

and therefore the equation is equivalent to

$$-\frac{9\varepsilon^2}{35\bar{\kappa}^2}H_2^2\varphi_2 + \varphi_2 = \frac{2}{5\bar{\kappa}}(\kappa\varphi - 4\pi\kappa B) + O(\varepsilon h). \tag{2.13b}$$

Remark 6 Equations (2.13a) and (2.13b) can be regarded as discretizations of the continuous SP_3 equations up to terms of $O(\varepsilon h)$ in the interior of the domain. As before, they are second order consistent with respect to the grid size h .

3 SP_N approximations for the Adjoint Radiative Transfer Equation

In this section we follow the approach *first optimize, then discretize* and discuss the remaining link, namely, deriving formally the SP_N approximations for the adjoint radiative transfer equation in \mathbb{R}^3 . As discussed in Section 1 and [5], the adjoint equations for the (continuous) optimal control problem (1.1) can be obtained by equation (1.5).

In order to apply the SP_N approximations to (1.5) we consider an optically thick medium, where the opacity κ is large and therefore the radiation is conveyed in a diffusive way. Hence, we consider the rescaled equation for small value of $\varepsilon = 1/((\kappa_{ref} + \sigma_{ref})\mathbf{x}_{ref})$:

$$-\varepsilon\omega\nabla J + (\sigma + \kappa)J = (\sigma + \kappa)G, \quad (3.1)$$

for some function

$$G(\mathbf{x}) = \frac{\alpha_1}{\sigma + \kappa}(\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})) + \frac{\sigma}{4\pi(\sigma + \kappa)} \int_{S^2} Jd\omega. \quad (3.2)$$

As for the radiative transfer equation, Neumann's series is applied to formally compute the inverse of the transport operator:

$$\left(1 - \frac{\varepsilon}{\sigma + \kappa}\omega \cdot \nabla\right)^{-1} = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{(\sigma + \kappa)^n}(\omega \cdot \nabla)^n. \quad (3.3)$$

Now, integrating (3.1) over ω and using (3.3) yields

$$\psi := \int_{S^3} Jd\omega = 4\pi \left(1 + \frac{\varepsilon^2}{3(\sigma + \kappa)^2}\nabla^2 + \frac{\varepsilon^4}{5(\sigma + \kappa)^4}\nabla^4 + \frac{\varepsilon^6}{7(\sigma + \kappa)^6}\nabla^6\right) G + O(\varepsilon^8) \quad (3.4)$$

This yields the following asymptotic expansion for the variable ψ ,

$$\left(1 - \frac{\varepsilon^2}{3(\sigma + \kappa)^2}\nabla^2 - \frac{4\varepsilon^4}{45(\sigma + \kappa)^4}\nabla^4 - \frac{44\varepsilon^6}{945(\sigma + \kappa)^6}\nabla^6\right) \psi + O(\varepsilon^8), \quad (3.5)$$

and finally the SP_N , $N = 1, 2, 3$ by neglecting terms of order $O(\varepsilon^4)$, $O(\varepsilon^6)$ and $O(\varepsilon^8)$, respectively.

Summarizing, the SP_1 approximation for the adjoint equation (3.1) in the case of a optically thick medium is given by

$$\psi - \frac{\varepsilon^2}{3(\sigma + \kappa)^2}\nabla^2\psi = \frac{4\pi}{\sigma + \kappa}\alpha_1(\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})) + \frac{\sigma}{\sigma + \kappa}\psi, \quad (3.6)$$

or equivalently

$$\kappa\psi - \frac{\varepsilon^2}{3(\sigma + \kappa)}\nabla^2\psi = 4\pi\alpha_1(\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})), \quad (3.7)$$

for the mean intensity $\psi := \int J d\omega$. Similarly, the SP_2 and SP_3 approximations are given by

$$\kappa\xi - \varepsilon^2 \frac{5\sigma + 9\kappa}{15(\sigma + \kappa)} \nabla^2 \xi = 4\pi\alpha_1 (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})), \quad (3.8)$$

where $\xi = \psi + \frac{4\kappa}{5(\sigma + \kappa)} (\psi - 4\pi \frac{\alpha_1}{\kappa} (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})))$, and

$$\kappa\psi - \frac{\varepsilon^2}{3(\sigma + \kappa)} \nabla^2 (\psi + 2\psi_2) = 4\pi\alpha_1 (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})), \quad (3.9)$$

$$(\sigma + \kappa)\psi_2 - \frac{9\varepsilon^2}{35(\sigma + \kappa)} \nabla^2 \psi_2 - \frac{2}{5} \kappa\psi = -\frac{2}{5} 4\pi\alpha_1 (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x})), \quad (3.10)$$

respectively.

Moreover, for any SP_N approximation, the optimality condition (1.6) reads,

$$\alpha_2 (Q(\mathbf{x}) - \bar{Q}(\mathbf{x})) + \psi = 0, \quad (3.11)$$

where ψ is the mean intensity given by the SP_N approximations.

Remark 7 *Similarly to [14], let us now consider the optimal control problem subject to the (forward) SP_1 approximation of the radiative transfer equation, i.e.,*

$$\min \mathcal{F}_{SP}(\phi, q) \text{ subject to } \kappa\phi - \frac{\varepsilon^2}{3(\sigma + \kappa)} \nabla^2 \phi = q(\mathbf{x}). \quad (3.12)$$

Then, the first-order optimality conditions for (3.12) for \mathcal{F}_{SP} ,

$$\mathcal{F}_{SP}(\phi, q) = \mathcal{F}(\phi, q/4\pi), \quad (3.13)$$

state ϕ , control q and adjoint variable λ are

$$\begin{aligned} \kappa\phi - \frac{\varepsilon^2}{3(\sigma + \kappa)} \nabla^2 \phi &= q(\mathbf{x}), \\ \kappa\lambda - \frac{\varepsilon^2}{3(\sigma + \kappa)} \nabla^2 \lambda &= \alpha_1 (\phi - \bar{\phi}), \\ \alpha_2 (q - \bar{q}) + \lambda &= 0. \end{aligned}$$

Obviously, the adjoint and gradient equation of above coincide with (3.11) and (3.6) for the rescaled control $4\pi Q = q$ and Lagrange multiplier $\psi = \lambda$. Moreover, a similar discussion holds true for the SP_2 and SP_3 equations. For theoretical results on the optimality system we refer to [14].

The previous remark and the previous discussion show that – figuratively speaking – deriving the adjoint equations *commutes* with constructing the SP_N approximations.

4 Conclusions

The overall performance of optimization algorithms in radiative transfer relies crucially on the number of degrees of freedom, which is general large due to the angular and frequency dependence of the radiative intensity. Here, we used asymptotic methods in the diffusive regime to reduce the discrete phase space. Future work will focus on moment methods yielding approximate optimization problems via maximum entropy closures.

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