Solving the Heat Equation in Connection with Electron Beam Melting

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Abstract

In this thesis we study the time dependent heat equation in $\mathbb{R}^2 \times \mathbb{R}_-$ subject to an inhomogeneous Neumann boundary condition, for the use in process control in Electron Beam Melting. We derive a solution formula that is valid for certain boundedness assumptions on the boundary condition. The solution formula is then applied in the specific case where the boundary condition describes a Gaussian distributed heat source with a centre moving along the boundary $\mathbb{R}^2 \times \{0\}$. By discretising the solution, using an adaptive quadrature method, we derive a numerical solution scheme. Using Newton's method, characteristics of the discretised solution, such as maximum temperature, are found. Numerical procedures are tested in one particular case with positive results. By an application of Banach's fixed point theorem, we indicate the possibility of finding and approximating a solution if radiative heat transfer by the Stefan-Boltzmann law is included in the boundary condition.

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1 Introduction

Arcam is a company that develops and manufactures machines that utilise Electron Beam Melting (EBM) to produce metal parts from metal powder. In the EBM process, parts of a thin layer of metal powder is melted by an electron beam, and cooled to form a solid structure. Then a new layer of powder is added on top of the previous one and is in turn melted together with its underlying regions. This procedure is repeated until a complete three dimensional metal structure is formed. This allows a production of components of highly complex geometries and high mechanical and chemical quality.

In order to control the melting process, the movement, focus and power of the electron beam (herein referred to as 'beam parameters') must be adjusted so that only the desired regions of each layer of powder is melted. It is not possible to measure the temperature of the material during the melting process and so a model for predicting the correct choice of beam parameters for a given melting pattern is required.

Arcam has developed such a model, but, as the optimisation problem of choosing the correct beam parameters requires repeated solution of the heat equation for the temperature distribution in the material, the model cannot be used to control the electron beam in real time. Instead, the optimisation problem is solved in advance for a large number of standard situations. For each situation, the correct choice of beam parameters and the resulting temperature profile are stored in a database for use in real time beam control.

When optimising the beam parameters, the temperature distribution in the material is found by solving the heat equation for an initial guess of parameters. On the basis of the results, a new set of parameters is found and the heat equation is solved again for the new set. The process is repeated until a choice of parameters that produces the desired temperature profile is found. The desired temperature distribution is characterised by two main criteria:

1. the maximum width of the region along the path of the electron beam that has attained a temperature at least as high as the melting temperature, herein referred to as 'maximum melted width', should have a prescribed value at a given depth, and

2. the global maximum temperature should not exceed a given highest acceptable temperature.

The general differential equation for the temperature distribution is

$$
\begin{aligned}
&\rho c_\mathrm{p} D_t T - \lambda \Delta T = 0 && \text{in } \Omega \times \mathbb{R}_+, \\
&\lambda D_\mathbf{n} T = F + k_\mathrm{r}(T^4 - T_\mathrm{s}^4) && \text{on } \Gamma_1 \times \mathbb{R}_+, \\
&\mathscr{B}(T, D_\mathbf{n} T) = 0 && \text{on } \Gamma_2 \times \mathbb{R}_+, \\
&T = T_0 && \text{in } \Omega \times \{0\},
\end{aligned}
\tag{1.1}
$$

where $F = F(\mathbf{x}, t)$ is the heat flux from the electron beam, which depends on the beam parameters, Ω is the geometry of the bulk of the material, Γ_1 is the part of the boundary of Ω where the beam is operating, Γ_2 is the rest of the boundary of Ω. $T = T(\mathbf{x}, t) = T(x, y, z, t)$, λ, ρ, c_p are temperature, heat conductivity, density and heat capacity of the metal. k_r is the coefficient of radiative heat transfer at the boundary Γ_1, T_s is the temperature of the surrounding of the boundary Γ_1. $\mathscr{B}(T, D_\mathbf{n} T, \mathbf{x}, t)$, with $D_\mathbf{n} T$ representing the directional derivative in the direction of the outward normal of the boundary, describes some boundary condition on Γ_2. $T_0(\mathbf{x})$ is a given initial temperature.

For Arcam's purposes the problem (1.1) has been simplified by only considering the case where the material occupies the lower half space, $z \leq 0$, and the electron beam is operating on the surface $z = 0$, that is, $\Omega = \mathbb{R}^2 \times \mathbb{R}_-$, $\Gamma_1 = \mathbb{R}^2 \times \{0\}$, $\Gamma_2 = \emptyset$. The power of the electron beam is assumed to have a Gaussian distribution with centre at a moving point at Γ_1. This leads to

$$(1.2)\qquad \begin{aligned} &\rho c_{\mathrm{p}} D_t T(\mathbf{x}, t) - \lambda \Delta T(\mathbf{x}, t) = 0, && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-,\ t \in \mathbb{R}_+, \\ &\lambda D_z T(\mathbf{x}, t) = \Pi(x, y, t) + k_{\mathrm{r}}(T^4(\mathbf{x}, t) - T_{\mathrm{s}}^4), && \mathbf{x} \in \mathbb{R}^2 \times \{0\},\ t \in \mathbb{R}_+, \\ &T(\mathbf{x}, 0) = T_0(\mathbf{x}), && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-, \\ &T(\mathbf{x}, t) \to T_\infty, && |\mathbf{x}| \to \infty,\ z < 0,\ t \in \mathbb{R}_+, \end{aligned}$$

where $\Pi(x, y, t) = (P_{\mathrm{in}}(t)/2\pi\sigma(t)^2) \exp(-((x - x_{\mathrm{c}}(t))^2 + (y - y_{\mathrm{c}}(t))^2)/2\sigma(t)^2)$, $P_{\mathrm{in}}(t)$ is the total power, $\sigma(t)$ describes the focus and $x_{\mathrm{c}}(t)$ and $y_{\mathrm{c}}(t)$ are the coordinates of the centre of the beam. This model is further simplified by neglecting the non-linear radiative heat transfer term, that is, assuming $k_{\mathrm{r}} = 0$. In addition, the beam parameters P_{in} and σ are assumed to be constant, while $x_{\mathrm{c}}(t) = v_x t$ for some constant speed v_x, and $y_{\mathrm{c}}(t) = 0$. This yields

$$(1.3)\qquad \begin{aligned} &\rho c_{\mathrm{p}} D_t T(\mathbf{x}, t) - \lambda \Delta T(\mathbf{x}, t) = 0, && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-,\ t \in \mathbb{R}_+, \\ &\lambda D_z T(\mathbf{x}, t) = \frac{P_{\mathrm{in}}}{2\pi\sigma^2} e^{-\frac{(x - v_x t)^2 + y^2}{2\sigma^2}}, && \mathbf{x} \in \mathbb{R}^2 \times \{0\},\ t \in \mathbb{R}_+, \\ &T(\mathbf{x}, 0) = T_0(\mathbf{x}), && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-, \\ &T(\mathbf{x}, t) \to T_\infty, && |\mathbf{x}| \to \infty,\ z < 0,\ t \in \mathbb{R}_+, \end{aligned}$$

The assumptions on the beam parameters are justified by the fact that if a solution T to (1.3) is found, it may be introduced as a new initial condition $T_0(\mathbf{x}) = T(\mathbf{x}, t_0)$ by the change of variables $t \to t - t_0$. (1.3) can then be solved with this new initial condition and new values of the beam parameters.

Arcam's current solution procedure involves a quasi-stationary assumption where the temperature distribution remains constant around the moving centre. That is, after the change of variables $x \to x - v_x t$, the assumption $D_t T = 0$ is used to get

$$(1.4)\qquad \begin{aligned} &-\rho c_{\mathrm{p}} v_x D_x T(\mathbf{x}) - \lambda \Delta T(\mathbf{x}) = 0, && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-, \\ &\lambda D_z T(\mathbf{x}) = \frac{P_{\mathrm{in}}}{2\pi\sigma^2} e^{-\frac{x^2 + y^2}{2\sigma^2}}, && \mathbf{x} \in \mathbb{R}^2 \times \{0\}, \\ &T(\mathbf{x}) \to T_\infty, && |\mathbf{x}| \to \infty,\ z < 0, \end{aligned}$$

which is solved with a finite element method. The width of the melted zone is determined by an interpolation procedure based on the finite element mesh. Once optimal beam parameters are found the solution is projected onto a set of special basis functions by the method of least squares.

In order to be able to control the electron beam for any melting pattern, a large number of optimisations of beam parameters needs to be carried out. Because of this, the process of creating the database of optimal parameter values and corresponding temperature profiles is very time consuming. Moreover, the quasi-stationary assumption used in (1.4) and the neglect of radiative heat transfer can not be expected to be valid in general.

In this thesis we seek to solve these problems by deriving a solution formula to an initial-boundary value problem of the same type as (1.2) and (1.3). We then use this formula together with a simple adaptive quadrature algorithm to generate approximations to the solution to (1.3) at any given time. For approximations of this type we develop a scheme based on Newton's method for finding the maximum temperature and the maximum melted width. This procedure is tested for a typical set of parameter values.

By using the solution formula together with Banach's fixed point theorem we explore the possibility of similarly generating approximate solutions to (1.2).

2 Solution formula for the heat equation

In this section we derive a solution formula to the heat equation in the half-space $\mathbb{R}^2 \times \mathbb{R}_-$, subject to a general boundary condition of the Neumann type. We then use the result to derive an explicit solution to the problem (1.3) and a method to solve (1.2) by means of a fixed point iteration.

2.1 Solution with general boundary condition

We consider the problem

$$\begin{aligned} & aD_t u(\mathbf{x},t) - b\Delta u(\mathbf{x},t) = 0, && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-,\ t \in [0,\tau], \\ & bD_z u(\mathbf{x},t) = f(x,y,t), && \mathbf{x} \in \mathbb{R}^2 \times \{0\},\ t \in [0,\tau], \\ & u(\mathbf{x},0) = u_0(\mathbf{x}), && \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}_-. \end{aligned} \tag{2.1}$$

We assume that a and b are positive constants and that u_0 and f are bounded continuous functions, f satisfying

$$|f(x,y,t)| \le M_1, \qquad (x,y) \in \mathbb{R}^2,\ t \in [0,\tau], \tag{2.2}$$

$$|D_t f(x,y,t)| \le M_2, \qquad (x,y) \in \mathbb{R}^2,\ t \in [0,\tau], \tag{2.3}$$

for some positive constants M_1 and M_2. Intuitively (2.1), as interpreted in a sense of heat distribution, seems to be equivalent to the problem where twice as much heat is added at $z = 0$ in the whole space $\mathbb{R}^3$, that is,

$$\begin{aligned} & aD_t u(\mathbf{x},t) - b\Delta u(\mathbf{x},t) = 2f(x,y,t)\delta(z), && \mathbf{x} \in \mathbb{R}^3,\ t \in [0,\tau], \\ & u(\mathbf{x},0) = u_0(\mathbf{x}), && \mathbf{x} \in \mathbb{R}^3, \end{aligned} \tag{2.4}$$

where δ is the Dirac delta and $u_0(x,y,z) = u_0(x,y,-|z|)$. Applying the Fourier transform to (2.4) yields

$$\begin{aligned} & aD_t \hat{u}(\boldsymbol{\xi},t) + b|\boldsymbol{\xi}|^2 \hat{u}(\boldsymbol{\xi},t) = 2(\hat{f}(\cdot,t) * \hat{\delta})(\boldsymbol{\xi}), && \boldsymbol{\xi} \in \mathbb{R}^3,\ t \in [0,\tau], \\ & \hat{u}(\boldsymbol{\xi},0) = \hat{u}(\boldsymbol{\xi}), && \boldsymbol{\xi} \in \mathbb{R}^3. \end{aligned} \tag{2.5}$$

(2.5) has the solution [11, p. 200]

$$\hat{u}(\boldsymbol{\xi},t) = a^{-1}\hat{u}_0(\boldsymbol{\xi})e^{-\frac{b}{a}|\boldsymbol{\xi}|^2 t} + 2a^{-1}\int_0^t e^{-\frac{b}{a}|\boldsymbol{\xi}|^2(t-s)}(\hat{f}(\cdot,s) * \hat{\delta})(\boldsymbol{\xi})\,ds, \tag{2.6}$$

With the *Gauss kernel* $U(\mathbf{x},t) := \sqrt{a}(4\pi bt)^{-3/2}e^{-a|\mathbf{x}|^2/4bt}$, applying the inverse Fourier transform to (2.6) yields

$$u(\mathbf{x},t) = (U(\cdot,t) * u_0)(\mathbf{x}) + 2\int_0^t (U(\cdot,t-s) * (f(\cdot,s)\delta))(\mathbf{x})\,ds =: u_\mathrm{i}(\mathbf{x},t) + u_\mathrm{s}(\mathbf{x},t), \tag{2.7}$$

It can be shown that u_i satisfies the differential equation and the initial condition in (2.1) [9, pp.109-111]. Moreover, it satisfies a homogenous Neumann boundary condition at $z = 0$ because

$$\begin{aligned} D_z u_\mathrm{i}(\mathbf{x},t)|_{z=0} &= \int_{\mathbb{R}^3} D_z U(x-\bar{x}, y-\bar{y}, -\bar{z}, t)u_0(\bar{\mathbf{x}})\,d\bar{x}\,d\bar{y}\,d\bar{z} \\ &= \int_{\mathbb{R}^3} \frac{a\bar{z}}{2bt} U(x-\bar{x}, y-\bar{y}, -\bar{z}, t)u_0(\bar{\mathbf{x}})\,d\bar{x}\,d\bar{y}\,d\bar{z} = 0, \end{aligned}$$

and U and u_0 are even functions of $\bar{z}$ while $\bar{z}$ is odd. For u_s we note

$$u_\mathrm{s}(\mathbf{x},t) = 2\int_0^t \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s) f(\bar{x},\bar{y},s)\, d\bar{x}\, d\bar{y}\, ds. \tag{2.8}$$

Differentiating u_s with respect to t by the chain rule yields

$$\begin{aligned} D_t u_\mathrm{s}(\mathbf{x},t) &= 2\int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, 0) f(\bar{x},\bar{y},t)\, d\bar{x}\, d\bar{y} \\ &\quad + 2\int_0^t \int_{\mathbb{R}^2} D_t U(x-\bar{x}, y-\bar{y}, z, t-s) f(\bar{x},\bar{y},s)\, ds. \end{aligned} \tag{2.9}$$

Here the first term vanishes as for fixed $z \neq 0$

$$\begin{aligned} &\lim_{s\to t} \left| \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s) f(\bar{x},\bar{y},s)\, d\bar{x}\, d\bar{y} \right| \\ &\quad \leq \lim_{s\to t} \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s) |f(\bar{x},\bar{y},s)|\, d\bar{x}\, d\bar{y} \\ &\quad \leq \frac{\sqrt{a}M_1}{(4\pi b)^{3/2}} \lim_{s\to t} (t-s)^{-3/2} \int_{\mathbb{R}^2} e^{-a((x-\bar{x})^2+(y-\bar{y})^2+z^2)/4b(t-s)}\, d\bar{x}\, d\bar{y} \\ &\quad = \frac{M_1}{\sqrt{4\pi ab}} \lim_{s\to t} (t-s)^{-1/2} e^{-az^2/4b(t-s)} = \frac{M_1}{\sqrt{4\pi ab}} \lim_{p\to\infty} \sqrt{p} e^{-az^2 p/4b} = 0. \end{aligned}$$

Applying the Laplace operator to u_s, differentiating under the time integral and using the differentiation property $D(v*w) = (Dv)*w$ of the convolution we get

$$\Delta u_\mathrm{s}(\mathbf{x},t) = 2\int_0^t \int_{\mathbb{R}^2} \Delta U(x-\bar{x}, y-\bar{y}, z, t-s) f(\bar{x},\bar{y},s)\, d\bar{x}\, d\bar{y}\, ds. \tag{2.10}$$

It is easily verified that U satisfies the differential equation in (2.1), and so by combining the results (2.9) and (2.10) we see that u_s satisfies the equation provided that the derivatives exist. But this is so as, for $z \neq 0$ and using the notation $C = 2a^{5/2}/\pi^{3/2}(4b)^{7/2} + 2a^{3/2}/\pi^{3/2}(4b)^{5/2}$

$$\begin{aligned} \int_0^t \int_{-\infty}^{\infty} \left| D_x^2 U(\mathbf{x},s) \right| \, dx\, ds &\leq C \int_0^t \int_{-\infty}^{\infty} \left(\frac{x^2}{s^{7/2}} + \frac{1}{s^{5/2}} \right) e^{-a(x^2+z^2)/4bs}\, dx\, ds \\ &= C\sqrt{\frac{4\pi b}{a}} \int_0^t s^{-2} e^{-az^2/4bs}\, ds = \frac{C}{z^2} \left(\frac{4\pi b}{a} \right)^{3/2} e^{-az^2/4bt} < \infty, \end{aligned}$$

and the same is true for y. This, together with the boundedness of f implies the existence of the derivatives whenever $z \neq 0$. Furthermore we have

$$\begin{aligned} &\lim_{t\to 0} \left| \int_0^t \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s) f(\bar{x},\bar{y},s)\, d\bar{x}\, d\bar{y}\, ds \right| \\ &\quad \leq \lim_{t\to 0} \frac{\sqrt{a}M_1}{(4\pi b)^{3/2}} \int_0^t (t-s)^{-3/2} \int_{\mathbb{R}^2} e^{-a((x-\bar{x})^2+(y-\bar{y})^2+z^2)/4b(t-s)}\, d\bar{x}\, d\bar{y}\, ds \\ &\quad \leq \lim_{t\to 0} \frac{M_1}{\sqrt{4\pi ab}} \int_0^t (t-s)^{-1/2} e^{-az^2/4b(t-s)}\, ds \leq M_1 \lim_{t\to 0} \sqrt{\frac{t}{\pi ab}} = 0, \end{aligned}$$

that is, $u_{\mathrm{s}}(\mathbf{x},t) \to 0$ as $t \to 0$. Finally, differentiating under the integral, we have

$$bD_z u_{\mathrm{s}}(\mathbf{x},t) = -\int_0^t \int_{\mathbb{R}^2} \frac{a^{3/2} z f(\bar{x},\bar{y},s)}{(4\pi b)^{3/2}(t-s)^{5/2}} e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2+z^2}{4b(t-s)}} \, d\bar{x}\, d\bar{y}\, ds$$
$$= -\int_0^t \int_{\mathbb{R}^2} \frac{a f(\bar{x},\bar{y},s)}{4\pi b(t-s)} e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}} D_s \mathrm{erf}\left(z\sqrt{\frac{a}{4b(t-s)}}\right) d\bar{x}\, d\bar{y}\, ds, \tag{2.11}$$

where erf is the *error function* [1]. Changing the order of integration in (2.11) and integrating by parts gives

$$bD_z u_{\mathrm{s}}(\mathbf{x},t) = -\int_{\mathbb{R}^2} \left\{ \left[\frac{a f(\bar{x},\bar{y},s)}{4\pi b(t-s)} e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}} \mathrm{erf}\left(z\sqrt{\frac{a}{4b(t-s)}}\right)\right]_{s=0}^{t} \right.$$
$$\left. - \int_0^t D_s \left(\frac{a f(\bar{x},\bar{y},s)}{4\pi b(t-s)} e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}} \right) \mathrm{erf}\left(z\sqrt{\frac{a}{4b(t-s)}}\right) ds \right\} d\bar{x}\, d\bar{y}. \tag{2.12}$$

Let $\epsilon = \sqrt{4b(t-s)/a}$ and note that $\lim_{\epsilon\to 0}(\epsilon\sqrt{\pi})^{-1}e^{-\beta^2/\epsilon^2} = \delta(\beta)$ in the sense of distributions [6, pp. 34-37] and $\lim_{\epsilon\to 0}\mathrm{erf}(\beta/\epsilon) = \mathrm{sgn}(\beta)$ and so

$$\lim_{s\to t} \int_{\mathbb{R}^2} \frac{a f(\bar{x},\bar{y},s)}{4\pi b(t-s)} e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}} \mathrm{erf}\left(z\sqrt{\frac{a}{4b(t-s)}}\right) d\bar{x}\, d\bar{y} = \tag{2.13}$$
$$= \int_{\mathbb{R}^2} \lim_{\epsilon\to 0} f(\bar{x},\bar{y},t-a\epsilon^2/4b) \frac{e^{-(x-\bar{x})^2/\epsilon^2}}{\sqrt{\pi}\epsilon} \frac{e^{-(y-\bar{y})^2/\epsilon^2}}{\sqrt{\pi}\epsilon} \mathrm{erf}(z/\epsilon)\, d\bar{x}\, d\bar{y}$$
$$= \int_{\mathbb{R}^2} f(\bar{x},\bar{y},t)\delta(x-\bar{x})\delta(y-\bar{y})\mathrm{sgn}(z)\, d\bar{x}\, d\bar{y} = \mathrm{sgn}(z) f(x,y,t).$$

We also have

$$\left| \int_{\mathbb{R}^2} \frac{a f(\bar{x},\bar{y},0)}{4\pi bt} e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4bt}} \mathrm{erf}\left(z\sqrt{\frac{a}{4bt}}\right) d\bar{x}\, d\bar{y} \right| \tag{2.14}$$
$$\le \frac{a}{4\pi bt} M_1 \mathrm{erf}\left(z\sqrt{\frac{a}{4bt}}\right) \int_{\mathbb{R}^2} e^{-\frac{a((x-\bar{x})^2+(y-\bar{y})^2)}{4bt}} \, d\bar{x}\, d\bar{y}$$
$$= M_1 \mathrm{erf}\left(z\sqrt{\frac{a}{4bt}}\right) \to 0,\ z \to 0.$$

Changing the orders of integration and differentiation in the remaining term of (2.12) gives, with the notation $Z := z\sqrt{a/4b}$

$$\left|\int_{\mathbb{R}^2}\int_0^t D_s\left(\frac{af(\bar{x},\bar{y},s)}{4\pi b(t-s)}e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}}\right)\operatorname{erf}\left(\frac{Z}{\sqrt{t-s}}\right)ds\,d\bar{x}\,d\bar{y}\right| \tag{2.15}$$

$$\begin{aligned}
&= \left|\int_0^t\int_{\mathbb{R}^2} D_s\left(\frac{af(\bar{x},\bar{y},s)}{4\pi b(t-s)}e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}}\right)d\bar{x}\,d\bar{y}\operatorname{erf}\left(\frac{Z}{\sqrt{t-s}}\right)ds\right| \\
&\le \int_0^t\int_{\mathbb{R}^2}\frac{(4b(t-s)+1)M_1+4(t-s)^2M_2}{16\pi a^{-1}b(t-s)^3}e^{-a\frac{(x-\bar{x})^2+(y-\bar{y})^2}{4b(t-s)}}d\bar{x}\,d\bar{y}\operatorname{erf}\left(\frac{|Z|}{\sqrt{t-s}}\right)ds \\
&= \int_0^t\left(\frac{M_1}{t-s}+\frac{aM_1}{4b(t-s)^2}+M_2\right)\operatorname{erf}\left(\frac{|Z|}{\sqrt{t-s}}\right)ds \\
&\le \left(M_1+M_2+\frac{aM_1}{4b}\right)\lim_{l\to t}\int_0^t(1+(t-s)^{-1}+(t-s)^{-2})\operatorname{erf}\left(\frac{|Z|}{\sqrt{t-s}}\right)ds \\
&\le \left(M_1+M_2+\frac{aM_1}{4b}\right)\lim_{l\to t} l(1+(t-l)^{-1}+(t-l)^{-2})\operatorname{erf}\left(\frac{|Z|}{\sqrt{t-l}}\right) \\
&\le \left(M_1+M_2+\frac{aM_1}{4b}\right)t\lim_{q\to 0}(1+q^{-1}+q^{-2})\operatorname{erf}\left(\frac{|Z|}{\sqrt{q}}\right),
\end{aligned}$$

where the last expression tends to zero when z, and hence $|Z|$, tends to zero and we let $q = |Z|^{1/3} \to 0$. In the calculations above (from (2.11) and on), finiteness of the results justifies the changes of order of integration. Combining the results from (2.12), (2.13), (2.14) and (2.15) we get

$$\lim_{z\to 0-} bD_z u_{\mathrm{s}}(\mathbf{x},t) = \lim_{z\to 0-} -\operatorname{sgn}(z)f(x,y,t) = f(x,y,t). \tag{2.16}$$

The results above may be summarised in the following proposition:

Proposition 1. *For positive constants a, b, continuous and bounded u_0 and f satisfying* (2.2) *and* (2.3) *the formula* (2.7) *is a solution to* (2.1) *in the sense that*

- *it satisfies the differential equation for fixed $z < 0$ and $t > 0$,*
- *it tends to the initial data u_0 as t tends to zero for fixed $z < 0$, and*
- *its directional derivative in the z-direction tends to the boundary data f as z tends to zero from below for fixed $t > 0$.*

2.2 Solution in the case of negligible radiative heat transfer

Having developed a solution formula to the general Neumann problem, we now seek to employ it for solving (1.3). Let $T = u + T_\infty$ and $T_0 = u_0 + T_\infty$, yielding

$$\begin{aligned}
&\rho c_{\mathrm{p}} D_t u(\mathbf{x},t) - \lambda\Delta u(\mathbf{x},t) = 0, && \mathbf{x}\in\mathbb{R}^2\times\mathbb{R}_-,\ t\in\mathbb{R}_+, \\
&\lambda D_z u(\mathbf{x},t) = \Pi(x,y,t), && \mathbf{x}\in\mathbb{R}^2\times\{0\},\ t\in\mathbb{R}_+, \\
&u(\mathbf{x},0) = u_0(\mathbf{x}), && \mathbf{x}\in\mathbb{R}^2\times\mathbb{R}_-.
\end{aligned} \tag{2.17}$$

Noting that

$$\begin{aligned}
|\Pi(x,y,t)| &= \left|\frac{P_{\mathrm{in}}}{2\pi\sigma^2}e^{-\frac{(x-v_xt)^2+y^2}{2\sigma^2}}\right| \le \frac{P_{\mathrm{in}}}{2\pi\sigma^2}, \\
|D_t\Pi(x,y,t)| &= \frac{P_{\mathrm{in}}|x-v_xt|}{2\pi\sigma^4}e^{-\frac{(x-v_xt)^2+y^2}{2\sigma^2}} \le \frac{P_{\mathrm{in}}}{\sqrt{2e}\pi\sigma^2},
\end{aligned}$$

we may use Proposition 1 to get a solution where

$$u_{\rm s}(\mathbf{x},t) = 2\int_0^t \left(\frac{\sqrt{\rho c_{\rm p}}}{(4\pi\lambda(t-s))^{3/2}} e^{-\frac{|x|^2}{4\kappa^2(t-s)}} * (\delta(z)\frac{P_{\rm in}}{2\pi\sigma^2} e^{-\frac{(x-v_x s)^2+y^2}{2\sigma^2}}\right)(x)\,ds \tag{2.18}$$
$$= 2\int_0^t \frac{\sqrt{\rho c_{\rm p}}}{(4\pi\lambda(t-s))^{3/2}} \frac{P_{\rm in}}{2\pi\sigma^2}\int_{\mathbb{R}^2} e^{-\frac{(x-\bar{x})^2+(y-\bar{y})^2+z^2}{4\kappa^2(t-s)}} e^{-\frac{(\bar{x}-v_x s)^2+\bar{y}^2}{2\sigma^2}}\,d\bar{x}\,d\bar{y}\,ds$$
$$= \int_0^t \frac{P_{\rm in}}{2\pi^{3/2}\kappa\rho c_{\rm p}(t-s)^{1/2}(\sigma^2+2\kappa^2(t-s))} e^{-\frac{(x-v_x s)^2+y^2}{2\sigma^2+4\kappa^2(t-s)}-\frac{z^2}{4\kappa^2(t-s)}}\,ds,$$

by using (2.7). Typically for Arcam's purposes u_0 is constant, whence $u_{\rm i}(\mathbf{x},t) = u_0$.

With

$$\kappa^2 = \lambda/\rho c_{\rm p},$$
$$T^* = P_{\rm in}/\sqrt{2}\pi^{3/2}\lambda\sigma,$$
$$V = v_x\sigma/2\sqrt{2}\kappa^2,$$

we make the substitutions

$$s \to 2\kappa^2 s^2/\sigma^2,$$
$$x \to (x - v_x t)/\sqrt{2}\sigma,$$
$$y \to y/\sqrt{2}\sigma,$$
$$z \to z/\sqrt{2}\sigma,$$
$$t \to \sqrt{2t}\kappa/\sigma.$$

These new variables will be referred to as dimensionless. We get

$$u_{\rm s}(\mathbf{x},t) = T^*\int_0^t \frac{1}{1+s^2} e^{-\frac{(x+Vs^2)^2+y^2}{1+s^2}-\frac{z^2}{s^2}}\,ds, \tag{2.19}$$

which we will approximate in Subsection 4.1.

2.3 Solution in the case with radiative heat transfer

Given $v\colon \mathbb{R}^3\times[0,\tau] \to \mathbb{R}$ let in the formula (2.7) $f(x,y,t) = \Pi(x,y,t) - k_{\rm r}((v(x,y,0,t)+T_{\rm s})^4 - T_{\rm s}^4)$. We then define

$$u(\mathbf{x},t) = (U(\cdot,t) * u_0)(\mathbf{x}) + \int_0^t\int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s)\Pi(\bar{x},\bar{y},0,s)\,d\bar{x}\,d\bar{y}\,ds \tag{2.20}$$
$$- k_{\rm r}\int_0^t\int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s)((v(\bar{x},\bar{y},0,s)+T_{\rm s})^4 - T_{\rm s}^4)\,d\bar{x}\,d\bar{y}\,ds$$
$$=: u_{\rm i}(\mathbf{x},t) + \bar{u}_{\rm s}(\mathbf{x},t) - \mathscr{A}v(\mathbf{x},t) =: \mathscr{S}v(\mathbf{x},t).$$

Define $\|v\| := \max_{(\mathbf{x},t)\in\mathbb{R}^3\times[0,\tau]} |v(\mathbf{x},t)|$ and let $\mathcal{C}_B := \{v \in \mathcal{C}(\mathbb{R}^3\times[0,\tau]) : \|v\| \le B\}$ be a closed subset of $\mathcal{C}(\mathbb{R}^3\times[0,\tau])$, which is a Banach space with respect to $\|\cdot\|$ by a generalisation of Example 1.4.7 of [3]. Choose $B = 2\|u_{\rm i}\| + 2\|\bar{u}_{\rm s}\|$. Then for sufficiently small τ we have $\mathscr{S}\colon \mathcal{C}_B \to \mathcal{C}_B$ as by the triangle inequality

$$\|\mathscr{S}v(\mathbf{x},t)\| = \|u_{\rm i}(\mathbf{x},t) + \bar{u}_{\rm s}(\mathbf{x},t) - \mathscr{A}v(\mathbf{x},t)\| \le \|u_{\rm i}\| + \|\bar{u}_{\rm s}\| + \|\mathscr{A}v\|,$$

where the last expression is no greater than B if $\|\mathscr{A}v\| \le \frac{1}{2}B$. For $v \in \mathcal{C}_B$ we have

$$
\begin{aligned}
|\mathscr{A}v(\mathbf{x},t)| &= \left| k_\mathrm{r} \int_0^t \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s)((v(\bar{x},\bar{y},0,s)+T_\mathrm{s})^4 - T_\mathrm{s}^4)\, d\bar{x}\, d\bar{y}\, ds \right| \\
&\le k_\mathrm{r} \|(v+T_\mathrm{s})^4 - T_\mathrm{s}^4\| \int_0^t \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s)\, d\bar{x}\, d\bar{y}\, ds \\
&\le \frac{k_\mathrm{r}((B+T_\mathrm{s})^4 - T_\mathrm{s}^4)\sqrt{\tau}}{\sqrt{\pi ab}} \le \frac{B}{2} \iff \tau \le \frac{\pi ab B^2}{4k_\mathrm{r}^2((B+T_\mathrm{s})^4 - T_\mathrm{s}^4)^2}.
\end{aligned}
$$

Let v_1, $v_2 \in \mathcal{C}_B$. Then with $V_i = v_i + T_\mathrm{s}$ for $i = 1, 2$ and using $p^4 - q^4 = (p-q)(p^3+p^2q+pq^2+q^3)$

$$
\begin{aligned}
|\mathscr{S}v_1(\mathbf{x},t) - \mathscr{S}v_2(\mathbf{x},t)| &= |\mathscr{A}v_1(\mathbf{x},t) - \mathscr{A}v_2(\mathbf{x},t)| \\
&= \left| k_\mathrm{r} \int_0^t \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s)(V_1(\bar{x},\bar{y},0,s)^4 - V_2(\bar{x},\bar{y},0,s)^4)\, d\bar{x}\, d\bar{y}\, ds \right| \\
&\le 4k_\mathrm{r}\|v_1 - v_2\| |B + T_\mathrm{s}|^3 \int_0^t \int_{\mathbb{R}^2} U(x-\bar{x}, y-\bar{y}, z, t-s)\, d\bar{x}\, d\bar{y}\, ds \\
&\le \frac{4k_\mathrm{r}(B+T_\mathrm{s})^3\sqrt{\tau}}{\sqrt{\pi ab}} \|v_1 - v_2\|,
\end{aligned}
\tag{2.21}
$$

from which we see that whenever

$$
\tau < \min\left\{ \frac{\pi ab}{16k_\mathrm{r}^2(B+T_\mathrm{s})^6}, \frac{\pi ab B^2}{4k_\mathrm{r}^2\left((B+T_\mathrm{s})^4 - T_\mathrm{s}^4\right)^2} \right\},
\tag{2.22}
$$

$\mathscr{S}\colon \mathcal{C}_B \to \mathcal{C}_B$ and there exists a constant $\alpha = 4k_\mathrm{r}(B+T_\mathrm{s})^3\sqrt{\tau}/\sqrt{\pi ab} < 1$ such that $\|\mathscr{S}v_1 - \mathscr{S}v_2\| \le \alpha\|v_1 - v_2\|$ for any v_1, v_2 in $\mathcal{C}_B$. Thus, assuming that (2.22) holds, we can apply Banach's fixed point theorem [3, Theorem 1.6.4] to find $u = \lim_{n\to\infty} \mathscr{S}^n v_0$, for any $v_0 \in \mathcal{C}_B$, such that $u = \mathscr{S}u$, being in this sense a solution to the problem with radiative heat transfer.

3 Basic adaptive quadrature

The integral in (2.19) cannot, to the authors' knowledge, be computed analytically. Thus, in order to use (2.19) the integral must be approximated. In this section we present an outline of the basic concepts of adaptive quadrature for that purpose.

An adaptive quadrature method for approximating an integral $I_{[a,b]}(f) = \int_a^b f(s)\,ds$ in its simplest form consists of a quadrature rule $Q_{[a,b]}(f)$ approximating the integral over a given (sub-) interval, a method for estimating the error $E_{[a,b]}(f) = |I_{[a,b]}(f) - Q_{[a,b]}(f)|$ or the relative error $E^{\text{rel}}_{[a,b]}(f) = |I_{[a,b]}(f) - Q_{[a,b]}(f)|/|I_{[a,b]}(f)|$, a method of dividing the integration interval into subintervals and an termination criterion. The termination criterion typically states that if the sum of error estimates over all subintervals is small enough, then the approximation is accepted [5], [7].

An algorithm employing this kind of adaptive quadrature typically starts out with some initial partition of the interval of integration (possibly the whole interval). It then applies the quadrature rule Q to each subinterval and estimates the error over each such interval, and goes on by further subdivision of the intervals until the termination criterion is met [5].

3.1 Quadrature rules

Many quadrature rules approximate an integral by a sum of weighted evaluations of the integrand and may be written as

$$I_{[a,b]}(f) \approx Q_{[a,b]}(f) = \sum_{k=1}^{N} w_k f(s_k). \tag{3.1}$$

The choice of N, the weights $\{w_k\}_{k=1}^N$ and evaluation points $\{s_k\}_{k=1}^N \subset [a,b]$ characterises the rule.

One of the simplest quadrature rules is the midpoint rule, where $N = 1$, $w_1 = b - a$ and $s_1 = (a+b)/2$. Several more advanced rules exists, some of which involve reformulations of the integrand. Examples of other rules are Simpson's rule where $N = 3$, $w_1 = w_3 = (b-a)/6$, $w_2 = 2(b-a)/3$, $s_1 = a$, $s_2 = (a+b)/2$ and $s_3 = b$ and the Gauss quadrature formula which uses N points and where $s_k = ((b-a)r_k + b + a)/2$, $w_k = (b-a)/((1-r_k^2)(P_N'(r_k))^2)$ and r_k is the k:th root of the N:th Legendre polynomial P_N [11, pp. 404-407].

3.2 Error estimates

The quadrature rules are, for sufficiently smooth integrands, associated to some local *a priori* error estimate in terms of derivatives of the integrand. Usually on the form

$$E_{[a,b]}(f) \leq C(b-a)^{n+1} \sup_{s\in[a,b]} |D_s^n f(s)|. \tag{3.2}$$

Estimates of this type are

$$E_{[a,b]}(f) \leq \frac{(b-a)^3}{24} \sup_{s\in[a,b]} |D_s^2 f(s)|,$$

for the midpoint rule,

$$E_{[a,b]}(f) \leq \frac{(b-a)^5}{2880} \sup_{s\in[a,b]} |D_s^4 f(s)|,$$

for Simpson's rule and

$$E_{[a,b]}(f) \leq \frac{(N!)^4(b-a)^{2N+1}}{(2N+1)((2N)!)^3} \sup_{s\in[a,b]} |D_s^{2N} f(s)|,$$

for the Gauss quadrature formula [11, pp. 404-407].

These estimates, while important for theoretical results concerning rates of convergence, are usually of little practical importance as higher order derivatives seldom are available and difficult to estimate [12, p. 159]. Many adaptive quadrature schemes use instead one or several more accurate approximations (for example using a greater number of evaluation points) [5], [7] or special rules based on such approximations [4] for estimating the error. However, if explicit numerical evaluations of the integrand are unavailable, such as when the integrand depends on some undetermined parameter $p \in \mathscr{P}$ (where $\mathscr{P}$ is the set of parameter values), that is, $f(s) = f(s,p)$, then theoretical error estimates based on (3.2) makes a 'semi-numerical' treatment of the integral possible. We would then have an estimate of the type

$$E_{[a,b]}(f) \leq C(b-a)^{n+1} \sup_{s\in[a,b],p\in\mathscr{P}} |D_s^n f(s,p)|. \tag{3.3}$$

3.3 Interval subdivision

The simplest and quickest method of dividing the integration intervals is bisection of the interval where the error is the greatest. That is, if the interval of integration, $[A,B]$ is partitioned into subintervals $\{[a_k,b_k]\}_{k=1}^{M}$ and $k^* \in \arg\max_{1\leq k\leq M} E_{[a_k,b_k]}(f)$, then $[a_{k^*}, b_{k^*}]$ is replaced by $[a_{k^*}, c]$ and $[c, b_{k^*}]$ where $c = (a_{k^*} + b_{k^*})/2$. This method has got the benefit of refining the integration grid very quickly but does not in general yield an optimal integration grid in a sense of using a minimum number of evaluation points for given error tolerances.

3.4 Termination criteria

Assuming that the integrand is 'well-behaved' enough for the quadrature algorithm to converge, we need to define conditions where the result should be accepted as a sufficiently good approximation of the integral. Often such conditions are described by tolerances of the errors, such as

$$\sum_{k=1}^{M} E_{[a_k,b_k]}(f) < TOL, \tag{3.4}$$

where the sum in the left-hand side gives a bound of the global quadrature error $E_{[A,B]}(f)$ and TOL is some decided tolerance.

In general we can not guarantee convergence of the quadrature algorithm to any given error tolerance, and so conditions for termination due to failure of the quadrature should also be included. These conditions can involve a maximum number of integrand evaluations or a minimum interval length [5].

4 Implementation

The results of Subsections 2.2 and 2.3 give solutions to the temperature distribution problems of Section 1. To use these results in the optimisation of beam parameters we need to develop numerical approximations of these solutions. Here, we start by employing the concepts of Section 3 to create an algorithm for the quadrature of the integral in (2.19). We then investigate the possibility of discretising the solution operator from Subsection 2.3, and show a convergence result for this operator, under the assumption that sufficiently good quadrature rules can be found.

4.1 Quadrature of the solution formula without radiative heat transfer

We now turn to approximating the integral in (2.19) using the principles of Section 3, where we consider the spatial coordinates as parameters. In order to control the error we need to use error estimates of the type (3.3). We note that differentiation of the integrand with respect to s yields increasingly complicated expressions (ee Appendix B). Moreover, due to terms of the form z^2/s^n, where $n \in \mathbb{Z}_+$, appearing in the derivatives these are singular at $s = 0$. Thus, in order to get a manageable error analysis we will employ the midpoint rule with error estimates in terms of the integral itself and its first derivative as well as the standard error estimate for the midpoint rule as given in Subsection 3.2. For each integration interval we use the estimate that give the lowest bound on the error.

In the case where $t = \infty$ we also need an estimate of the error derived from integration over only a finite interval $[0, b] \subset [0, \infty]$. The error estimates used are shown in Appendix A.

For speed we use bisection of the interval with the largest error when refining the integration grid. The termination criterion should describe a bound of the maximum error and so we use a criterion of the type (3.4). The procedure of the integration is outlined in Algorithm 1. With

Algorithm 1 Adaptive quadrature

$V \leftarrow$ dimensionless speed {See Subsection 2.2}
$\mathbf{s} \leftarrow \mathbf{s}_0$ {Vector with initial endpoints of integration intervals}
$TOL \leftarrow$ absolute error tolerance
$\mathbf{e} \leftarrow \mathit{error\_estimate}(\mathbf{s}_0, V)$ {Gives av vector of local error estimates}
while $\mathit{sum}(\mathbf{e}) > TOL$ **do**
  $k \leftarrow$ index of greatest element of $\mathbf{e}$
  if $s_{k+1} = \infty$ **then**
    $\mathbf{s} \leftarrow [\mathbf{s}_{1:k-1} | \tan(\pi/2 - TOL/\#\text{elements in } \mathbf{s}) | \infty]$ {Add interval}
  else
    $\mathbf{s} \leftarrow [\mathbf{s}_{1:k} | (s_k + s_{k+1})/2 | \mathbf{s}_{k+1:end}]$ {Bisect interval}
  end if
  $\mathbf{e} \leftarrow [\mathbf{e}_{1:k-1} | \mathit{error\_estimate}(\mathbf{s}_{k:k+2}, V) | \mathbf{e}_{k+1:end}]$ {Update error}
end while
return $\mathbf{s}$

this method the numerical approximation of (2.19) will be written as

$$u_{s,h}(\mathbf{x}, t) = T^* \sum_{i=1}^{N-1} \frac{k_i}{1 + m_i^2} e^{-\frac{(x+Vm_i^2)^2+y^2}{1+m_i^2} - \frac{z^2}{m_i^2}}, \tag{4.1}$$

where $k_i = s_{i+1} - s_i$, $m_i = (s_i + s_{i+1})/2$, $i = 1, \ldots, N-1$ and N is the number of elements in $\mathbf{s}$.

4.2 Discretisation of the solution operator with radiative heat transfer

We have the solution operator $\mathscr{S}v = u_\mathrm{i} + \bar{u}_\mathrm{s} - \mathscr{A}v$ as defined in (2.20). We define the corresponding discrete operator $\mathscr{S}_h v = u_{\mathrm{i},h} + \bar{u}_{\mathrm{s},h} - \mathscr{A}_h v$ for some (small) discretisation parameter h, where $u_{\mathrm{i},h}$, $\bar{u}_{\mathrm{s},h}$ are discrete approximations of u_i and $\bar{u}_\mathrm{s}$, and

$$\mathscr{A}_h v(\mathbf{x}, t) = k_\mathrm{r} Q_{h,[0,t]} \int_{\mathbb{R}^2} U(x - \bar{x}, y - \bar{y}, z, t - s)((v(\bar{x}, \bar{y}, 0, s) + T_\mathrm{s})^4 - T_\mathrm{s}^4)\, d\bar{x}\, d\bar{y},$$

where $Q_{h,[0,t]}$ denotes some quadrature rule in the variable s over the interval $[0, t]$, characterised by h.

We consider $u = \lim_{n\to\infty} \mathscr{S}^n v_0$ for appropriate $v_0 \in \mathcal{C}_B$ to be a solution to the heat distribution problem with radiative heat transfer and seek an estimate of how well u can be approximated by a finite number of applications of the discrete operator $\mathscr{S}_h$ to v_0. In particular we seek conditions such that there is a convergence $\|\mathscr{S}_h^N v_0 - u\| \to 0$ as $h \to 0$ and $N \to \infty$. First, note that the error can be split into one part corresponding to discretisation and one part corresponding to finite application of the solution operator as by the triangle inequality

$$\begin{aligned} \|\mathscr{S}_h^N v_0 - u\| &= \|\mathscr{S}_h^N v_0 - \mathscr{S}^N v_0 + \mathscr{S}^N v_0 - u\| \\ &\le \|\mathscr{S}_h^N v_0 - \mathscr{S}^N v_0\| + \|\mathscr{S}^N v_0 - u\|. \end{aligned} \tag{4.2}$$

By the same argument as in the proof of Theorem 4.34 (a) of [2] but in the context of the Banach space $(\mathcal{C}(\mathbb{R}^3 \times [0, \tau]), \|\cdot\|)$ rather than $(\mathbb{R}^N, |\cdot|)$ and as $v_0, u \in \mathcal{C}_B$ we have

$$\|\mathscr{S}^N v_0 - u\| \le \alpha^N \|v_0 - u\| \le 2B\alpha^N, \tag{4.3}$$

with $\alpha < 1$ for sufficiently small τ (cf. Section 2.3). Let $\mathscr{E}_h^m v_0 = \mathscr{S}_h^m v_0 - \mathscr{S}^m v_0$ for $m = 0,\ 1,\ 2, ...$ with $\mathscr{S}_h^0 = \mathscr{S}^0 = \mathscr{I}$, the identity operator. Further, let $R(p, q) = (p + q)^4 - p^4$ and

$$\mathscr{R}_h(v, w)(\mathbf{x}, t) = Q_{h,[0,t]} \int_{\mathbb{R}^2} U(x - \bar{x}, y - \bar{y}, z, t - s) R(v(\bar{x}, \bar{y}, 0, s), w(\bar{x}, \bar{y}, 0, s))\, d\bar{x}\, d\bar{y}.$$

Then by the triangle inequality

$$\begin{aligned} \|\mathscr{E}_h^N v_0\| &\le \|u_\mathrm{i} - u_{\mathrm{i},h}\| + \|\bar{u}_\mathrm{s} - \bar{u}_{\mathrm{s},h}\| + \|\mathscr{A}_h \mathscr{S}_h^{N-1} v_0 - \mathscr{A}\mathscr{S}^{N-1} v_0\| \\ &= \|u_\mathrm{i} - u_{\mathrm{i},h}\| + \|\bar{u}_\mathrm{s} - \bar{u}_{\mathrm{s},h}\| + \|\mathscr{A}_h(\mathscr{S}^{N-1} v_0 + \mathscr{E}_h^{N-1} v_0) - \mathscr{A}\mathscr{S}^{N-1} v_0\| \\ &\le \|u_\mathrm{i} - u_{\mathrm{i},h}\| + \|\bar{u}_\mathrm{s} - \bar{u}_{\mathrm{s},h}\| + \|\mathscr{A}_h \mathscr{S}^{N-1} v_0 - \mathscr{A}\mathscr{S}^{N-1} v_0\| \\ &\quad + \|\mathscr{R}_h(\mathscr{S}^{N-1} v_0 + T_\mathrm{s}, \mathscr{E}_h^{N-1} v_0)\|. \end{aligned} \tag{4.4}$$

We have demonstrated (see Appendix C) that it is possible to find an approximation $\bar{u}_{\mathrm{s},h}$ of $\bar{u}_s$ that can be made arbitrarily accurate with respect to the maximum norm, by appropriate application of the midpoint rule. In other words, there exists $\epsilon_\mathrm{s} = \epsilon_\mathrm{s}(h)$ tending to zero as h tends to zero and such that $\|\bar{u}_{\mathrm{s},h} - \bar{u}_\mathrm{s}\| \le \epsilon_\mathrm{s}(h)$ holds. We assume that there exists a similar bound $\epsilon_\mathrm{i}(h)$ for $\|u_\mathrm{i} - u_{\mathrm{i},h}\|$, that the quadrature rule Q_h can be constructed so that there exists $\epsilon_\mathrm{q}(h)$ so that$\|\mathscr{A}_h \mathscr{S}^m v_0 - \mathscr{A}\mathscr{S}^m v_0\| \le \epsilon_\mathrm{q}(h)$ for appropriate choice of $v_0 \in \mathcal{C}_B$ and for any $m \in \mathbb{Z}_+$ and that Q_h integrates $(t - s)^{-1/2}$ over the interval $[0, t] \subseteq [0, \tau]$ with a finite maximum error d. Then because $\mathscr{S}^m v_0 \in \mathcal{C}_B$

$$|\mathscr{R}_h(\mathscr{S}^m v_0 + T_\mathrm{s}, w)(\mathbf{x}, t)| \le R(B + T_\mathrm{s}, \|w\|) \left(\sqrt{\frac{\tau}{\pi ab}} + d \right),$$

indicating that there exists a constant K such that

$$\|\mathscr{R}_h(\mathscr{S}^m v_0 + T_{\mathrm{s}}, w)\| \leq K(\|w\| + \|w\|^2 + \|w\|^3 + \|w\|^4). \tag{4.5}$$

Under these assumptions, using (4.4) and (4.5) we get

$$\|\mathscr{E}_h^N v_0\| \leq \epsilon_{\mathrm{i}}(h) + \epsilon_{\mathrm{s}}(h) + \epsilon_{\mathrm{q}}(h) + K \sum_{p=1}^{4} \|\mathscr{E}_h^{N-1} v_0\|^p =: E_N(h).$$

This gives rise to a sequence of error estimates $\{E_n(h)\}_{n=0}^N$ by

$$\begin{aligned} E_{n+1}(h) &= \epsilon(h) + K \sum_{p=1}^{4} E_n(h)^p, \quad n = 0, 1, \dots, \\ E_0(h) &= \|\mathscr{S}_h^0 v_0 - \mathscr{S}^0 v_0\| = 0, \end{aligned}$$

where we have used the notation $\epsilon(h) = \epsilon_{\mathrm{i}}(h) + \epsilon_{\mathrm{s}}(h) + \epsilon_{\mathrm{q}}(h)$. Define the sequence $\{a_n\}_{n=0}^\infty$ by $a_{n+1} = 4Ka_n + 1$, $a_0 = 0$. We then have

$$\begin{aligned} &E_0(h) = 0, \\ &E_1(h) = \epsilon(h), \\ &E_2(h) = \epsilon(h) + K \sum_{p=1}^{4} \epsilon(h)^p \leq (4K+1)\epsilon(h) && \text{if } \epsilon(h) \leq 1, \\ &E_3(h) \leq \epsilon(h) + K \sum_{p=1}^{4} (4K+1)^p \epsilon(h)^p \leq (4K(4K+1)+1)\epsilon(h) && \text{if } (4K+1)\epsilon(h) \leq 1, \\ &\quad \dots \\ &E_N(h) \leq a_N \epsilon(h) && \text{if } a_{N-1}\epsilon(h) \leq 1. \end{aligned}$$

By assumption $\epsilon(h)$ can be made arbitrarily small by choosing small enough h. Thus, if we pick $h(N)$ so that $\epsilon(h(N)) \leq (Na_N)^{-1} \leq a_{N-1}^{-1}$ and use the sequence of error estimates above together with (4.2) and (4.3) we arrive at the following result

$$\|\mathscr{S}_h^N v_0 - u\| \leq E_N(h(N)) + 2B\alpha^N \leq N^{-1} + 2B\alpha^N \to 0,\ N \to \infty, \tag{4.6}$$

and so we may conclude that under the assumption that sufficiently good quadrature rules may be found for appropriate choice of v_0, the result from N applications of the discrete operator $\mathscr{S}_h$ tends to u as N tends to infinity, provided that the discretisation parameter h tends to zero fast enough.

5 Characterising the melted zone

In the optimisation of beam parameters there are two important characteristics of the melted zone, maximum temperature and maximum width at given depth, as stated in Section 1. For a temperature profile $T(x, y, z, t)$ being a solution to (1.2) or (1.3) with constant initial temperature T_0 the maximum temperature $T_{\max}$ and maximum width y_z at depth z are formally defined as

$$T_{\max}(t) := \sup_{\mathbf{x}\in\mathbb{R}^2\times\mathbb{R}_-} T(\mathbf{x}, t), \tag{5.1}$$

and

$$y_z(t) := \sup\{y \in \mathbb{R} : \exists x \in \mathbb{R} : T(x, y, z, t) = T_{\mathrm{m}}\}, \tag{5.2}$$

where T_{m} is the melting temperature of the material. In order to determine for which values of z y_z is defined, we also need to find the maximum depth $z_{\max}$ defined as

$$z_{\max}(t) := \inf\{z \in \mathbb{R}_- : \exists(x, y) \in \mathbb{R}^2 : T(x, y, z, t) = T_{\mathrm{m}}\}. \tag{5.3}$$

In this section we develop a scheme for finding $T_{\max}$ and y_z at any given time t for an approximate solution $T(\mathbf{x}, t) \approx T_0 + u_{\mathrm{s},h}(\mathbf{x}, t)$ with $u_{\mathrm{s},h}$ as in (4.1).

5.1 Approximate maximum temperature

Denoting the approximate maximum temperature $T_{\max,h}$ and using the approximate solution into the definition (5.1) we get

$$T_{\max,h}(t) = T_0 + \sup_{\mathbf{x}\in\mathbb{R}^2\times\mathbb{R}_-} u_{\mathrm{s},h}(\mathbf{x}, t). \tag{5.4}$$

By continuity and boundedness of $u_{\mathrm{s},h}$, we have that if $T_0 + u_{\mathrm{s},h}(\mathbf{x}^*, t) = T_{\max,h}(t)$ then $\nabla u_{\mathrm{s},h}(\mathbf{x}^*, t) = \mathbf{0}$. It is easily verified that derivatives of $u_{\mathrm{s},h}$ in the y- and z-directions take the value zero if and only if y and z take the value zero, thus if we define $X(t) := \{x \in \mathbb{R} : D_x u_{\mathrm{s},h}(x, 0, 0, t) = 0\} \neq \emptyset$ then

$$T_{\max,h}(t) = T_0 + \max_{x\in X(t)} u_{\mathrm{s},h}(x, 0, 0, t). \tag{5.5}$$

For fixed t, we can find an approximation of $x \in X(t)$ by Newton's method, Algorithm 2, using $f(x) = D_x u_{\mathrm{s},h}(x, 0, 0, t)$. We note that, from (4.1), exact expressions for the spatial derivatives of $u_{\mathrm{s},h}$ can be found, and thus equation vectors and inverse Jacobi matrices can be given by exact formulae.

Let $X_h(t) = \{-V m_i\}_{i=1}^N$ with V, $\{m_i\}_{i=1}^N$ and N as in Subsection 4.1. Then we get a starting approximation by choosing $x \in X_h(t)$ maximising $u_{\mathrm{s},h}(x, 0, 0, t)$ over $X_h(t)$.

It is possible that the set $X(t)$ contains more than one element, and so, once an approximate x is found it must be checked for global optimality. Assume that we have a candidate for an optimal point, $\tilde{x}$, we then try to solve the equation

$$u_{\mathrm{s},h}(x, 0, 0, t) = u_{\mathrm{s},h}(\tilde{x}, 0, 0, t) + T_{\mathrm{d}}, \tag{5.6}$$

for some (small) temperature step T_{d}, by Newtons method. If no new solution is found, $\tilde{x}$ is accepted as an approximation the globally optimal point, otherwise, the solution x is used as a starting approximation for a new Newton iteration, and procedure is repeated until no further new solutions are found. This process ensures that, for the accepted x, $|T_{\max,h}(t) - T_0 - u_{\mathrm{s},h}(x, 0, 0, t)| \leq T_{\mathrm{d}}$.

Algorithm 2 Newton's method for the system of equations $f(\mathbf{x}) = \mathbf{0}$

$f(\mathbf{x}) \leftarrow N$-vector of equations in the variable $\mathbf{x} \in \mathbb{R}^N$
$J_{\text{inv}}(\mathbf{x}) \leftarrow$ inverse of Jacobi matrix of f
$TOL \leftarrow$ relative error tolerance
$MaxItr \leftarrow$ maximum number of iterations
$n \leftarrow 0$ {Number of performed iterations}
$\mathbf{x}_{n+1} \leftarrow$ starting approximation
$\mathbf{x}_n \leftarrow \mathbf{x}_{n+1}(2 + TOL)$ {To enter the loop}
while $\|\mathbf{x}_{n+1} - \mathbf{x}_n\|_2 > TOL \cdot \|\mathbf{x}_n\|_2$ & $n < MaxItr$ **do**
  $\mathbf{x}_n \leftarrow \mathbf{x}_{n+1}$ {Old approximation}
  $\mathbf{x}_{n+1} \leftarrow \mathbf{x}_{n+1} - J_{\text{inv}}(\mathbf{x}_{n+1}) f(\mathbf{x}_{n+1})$ {Update approximation}
  $n \leftarrow n + 1$ {Update number of performed iterations}
end while
return $\mathbf{x}_{n+1}$ {Accepted approximation}

5.2 Approximate depth and width

Assuming that $T_{\max,h} \geq T_m \geq T_0$, by the continuity of $u_{\mathrm{s},h}$ and decrease of $u_{\mathrm{s},h}$ in the negative z-direction[1] we are assured that there exists an approximate maximum depth $z_{\max,h}$, defined by

$$z_{\max,h}(t) := \inf\{z \in \mathbb{R}_- : \exists (x, y) \in \mathbb{R}^2 : T_0 + u_{\mathrm{s},h}(x, y, z, t) = T_{\mathrm{m}}\}, \tag{5.7}$$

and that for any $z \in [z_{\max,h}(t), 0]$ there exists an approximate maximum width $y_{z,h}$ defined by

$$y_{z,h}(t) := \sup\{y \in \mathbb{R} : \exists x \in \mathbb{R} : T_0 + u_{\mathrm{s},h}(x, y, z, t) = T_{\mathrm{m}}\}. \tag{5.8}$$

For the maximum depth, we note that, by the same continuity arguments as for the maximum temperature, with fixed t, for some $x \in \mathbb{R}$, $z_{\max,h}(t)$ satisfies

$$D_x u_{\mathrm{s},h}(x, 0, z_{\max,h}(t), t) = 0, \tag{5.9}$$

and, by definition,

$$T_0 + u_{\mathrm{s},h}(x, 0, z_{\max,h}(t), t) = T_{\mathrm{m}}. \tag{5.10}$$

The two equations above form a system that can be solved by Newton's method, starting, for instance, at a point $(x, z) \in \mathbb{R} \times \mathbb{R}_-$ with $T_0 + u_{\mathrm{s},h}(x, 0, 0, t) = T_{\max,h}$ and $T_0 + u_{\mathrm{s},h}(x, 0, z, t) \approx T_{\mathrm{m}}$ that may be found by a simple line-search once $T_{\max,h}$ is located.

Again, it may be possible to find a point where this system is satisfied while not being at the maximum depth. Similarly to the procedure used for the maximum temperature, given one solution $(\tilde{x}, \tilde{z})$ to the system of equations, we seek a solution $x \in \mathbb{R}$ to

$$T_0 + u_{\mathrm{s},h}(x, 0, \tilde{z} - z_{\mathrm{d}}, t) = T_{\mathrm{m}}, \tag{5.11}$$

for some (small) step z_{d}. The procedure is repeated in the same manner as for the maximum temperature, until no further solutions are found, whence the last approximation is accepted.

For given $z \in [z_{\max,h}(t), 0]$, $y_{z,h}(t)$ can be found in the same manner as $z_{\max,h}(t)$, by instead noting that for some $x \in \mathbb{R}$, $y_{z,h}(t)$ satisfies the equations

$$D_x u_{\mathrm{s},h}(x, y_{z,h}(t), z, t) = 0, \tag{5.12}$$

[1] As $D_z u_{\mathrm{s},h}(x, y, z, t) > 0$ whenever $z < 0$.

and

$$T_0 + u_{\mathrm{s},h}(x, y_{z,h}(t), z, t) = T_{\mathrm{m}}, \tag{5.13}$$

and for the global optimality check attempt to solve

$$T_0 + u_{\mathrm{s},h}(x, \tilde{y} + y_{\mathrm{d}}, z, t) = T_{\mathrm{m}}, \tag{5.14}$$

with a current approximation $\tilde{y}$ and some (small) step y_{d}.

5.3 The depth-width curve

It has been observed by Arcam that for fixed t, the graph of $(y_z(t), z)$ for $z \in [z_{\max}(t), 0]$ appears to be 'roughly' parabolic. Therefore, after calculating $z_{\max,h}(t)$ and $y_{z,h}(t)$ at a number $N \geq 2$ of points $\{z_i\}_{i=1}^N \subset [z_{\max,h}(t), 0]$ we use the method of linear least squares to fit a curve on the form

$$z = \beta_1 + \beta_2 y_{z,h}(t)^2, \tag{5.15}$$

with β_1, $\beta_2 \in \mathbb{R}$, to the data points $\{(y_{z_i,h}(t), z_i)\}_{i=1}^N$.

6 Testing of the algorithms for the problem with no radiative heat transfer

In this section we present the results from temperature simulations using the principles of Subsection 4.1 and Section 5, implemented in Matlab. The results are for a 'typical' set of parameters as presented to us by Arcam:

$$\begin{array}{ll} P_{\text{in}}{=}120\ \texttt{W}, & T_{\text{m}}{=}1873\ \texttt{K}, \\ v_x{=}0.2337\ \texttt{m/s}, & \lambda{=}7\ \texttt{W/m K}, \\ \sigma = 3.8263 \cdot 10^{-4}\ \texttt{m}, & \rho{=}4430\ \texttt{kg/m}^3, \\ T_0{=}973\ \texttt{K}, & c_{\text{p}}{=}526\ \texttt{J/kg K}. \end{array}$$

With these parameters and for times $t = 0.001$, 0.002, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1 and ∞, in seconds, we use Algorithm 1, with absolute error tolerance 10 K, to describe the temperature profiles, and the procedures in Section 5, with relative tolerance 0.01 in Algorithm 2 and using 10 data points uniformly distributed in the z-direction between $z_{\max}$ and 0, to find $T_{\max,h}$, β_1 and β_2 for each time. In the optimality checks we use $T_{\text{d}} = 10$ K, while y_{d} and z_{d} are taken as one percent of the current candidate. When running Algorithm 1 we notice that the error estimate (A.2) is never used, while (A.1) is used only in the interval including zero.

To study the error in Algorithm 2 and we create a reference lattice $\mathbb{V}$ with dimensionless spatial coordinates (cf. Subsection 2.2) x, y and z uniformly distributed in $[-6, 2]$, $[0, 3]$ and $[-0.5, 0]$ with 100 points respectively. At each point $\mathbf{x}$ in the lattice we compute a reference temperature $T_{\text{ref}}(\mathbf{x})$ using Matlab's `quadgk` on (2.19), with an absolute error tolerance of 10^{-15} as termination criterion. For our purposes we consider $T_{\text{ref}}(\mathbf{x})$ to be exact in every point $\mathbf{x} \in \mathbb{V}$. The reference temperatures are compared to those given by (4.1). We see from Figures 1 and 2 that the errors as well as the approximation quickly decays outside the reference lattice except in the case $t = \infty$ where the error is small everywhere. The largest error over the lattice,

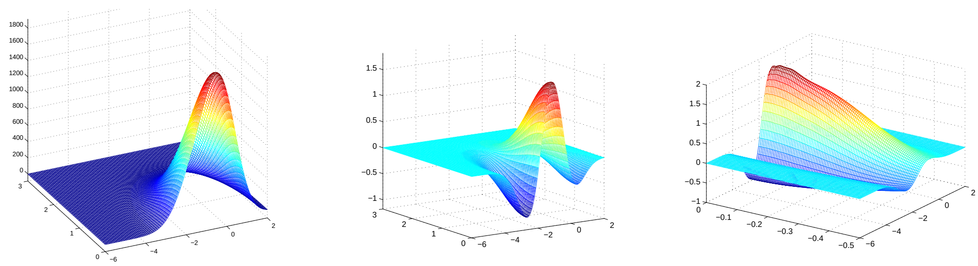

Figure 1: Temperature [K] (left), error [K] in the xy-plane with $z = 0$ (centre), and error in the xz-plane with $y = 0$ (right) for $t = 0.005$ s.

$d(t) = \max_{\mathbf{x}\in\mathbb{V}} |T_{\text{ref}}(\mathbf{x}) - T_0 - u_{\text{s},h}(\mathbf{x}, t)|$ is shown for each time t in Table 1 along with the number of points, N, used to approximate the integral (2.19) with Algorithm 1, the approximate maximum temperature $T_{\max,h}$ and parameters β_1 and β_2.

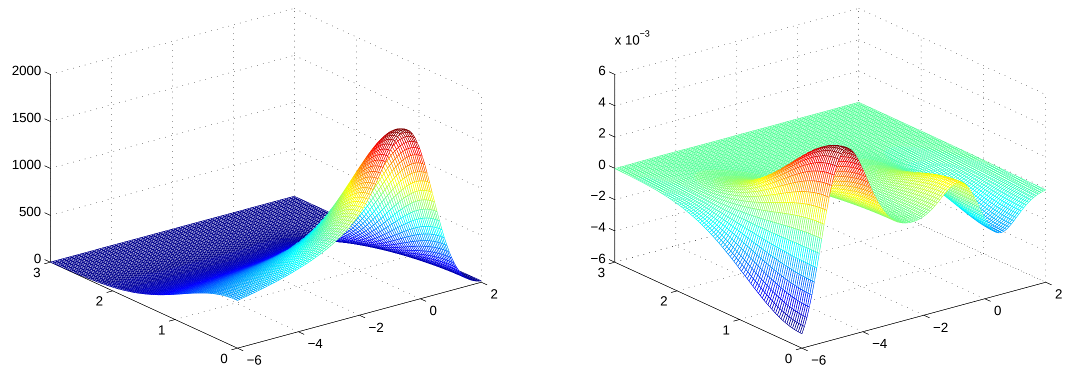

Figure 2: Temperature [K] (left) and error [K] (right) in the xy-plane with $z = 0$ for $t = \infty$

For each value of z in the lattice, we find (if possible) the lattice point with the largest value of y at which $T_{\mathrm{ref}} \geq T_{\mathrm{m}}$. Assuming that y_i has this property for some z, then the true value of $y_z \in [y_i, y_{i+1}]$, thus we get an upper and lower bound for the true width. The results are shown in Appendix D.

t [s]	N	$T_{\max,h}$ [K]	β_1	β_2	d [K]
0.001	24	2093	-0.0241	0.1080	1.2111
0.002	29	2468	-0.0761	0.1442	1.5839
0.005	41	2799	-0.1615	0.2152	1.7333
0.01	58	2814	-0.1807	0.2404	0.5978
0.02	84	2814	-0.1806	0.2404	0.4018
0.05	150	2814	-0.1806	0.2404	0.2579
0.1	249	2814	-0.1807	0.2405	0.3439
0.2	379	2814	-0.1806	0.2404	0.1588
0.5	595	2814	-0.1806	0.2404	0.0898
1	808	2814	-0.1806	0.2404	0.0792
∞	45845	2814	-0.1806	0.2404	0.0060

Table 1: Results

7 Discussion

Here we discuss the performance of the methods of Sections 4 and 5. In the case of negligible radiation we base our discussion on the results presented in Section 6.

7.1 Performance of the procedure in the case of negligible radiative heat transfer

We see from Table 1 that the number of points produced by Algorithm 1 increases, as expected, with increasing time, while the largest detected error d remains small compared to the used tolerance. In particular, we note that for $t = \infty$, the number of points used is very large, while the detected maximum error is less than one thousandth of the used tolerance. We can see three main reasons for this. Firstly, it is possible that our error estimates (cf. Appendix A), in particular the one used for truncating the integration interval in the case of $t = \infty$, are overly pessimistic. Secondly, the routine of bisection of the interval with the largest estimated local error used in Algorithm 1 is likely to produce a non-optimal distribution of points, thus requiring a larger number of points to meet the required tolerance. Thirdly, we note that, although the temperature far back along the path of the electron beam (that is, for large negative x in dimensionless coordinates) is of less interest when considering maximum temperature and melted width, we still demand that it is calculated as accurately as the temperature close to the current position of the electron beam, thus requiring more points.

For the error estimates, as noted in Section 6, only the second order estimate is used, except for the interval including zero, where the derivatives of the integrand are singular. This could indicate that higher order quadrature rules, such as the Gauss quadrature rules, with associated error estimates, might meet the error tolerance with fewer interval subdivisions than the midpoint rule, provided that the higher order derivatives of the integrand in (2.19) can be estimated in an efficient manner.

Optimising the positions of points, as opposed to interval bisection, in Algorithm 1 is likely to make the algorithm very slow, as the optimisation problem would involve a combination of integer programming, in the description of the number of points used, and continuous non-linear programming, for the positioning of the points, in a large number of variables.

Introducing error tolerances varying in space would involve finding error estimates depending on the spatial coordinates. It is possible that this, while involving a larger number of error estimations to be carried out, nevertheless could improve the overall performance of Algorithm 1 by focusing only on the regions of interest. This would be especially useful for large values of t. On the other hand, we see from Table 1 that, for purposes of calculating maximum temperature and widths, small values of t are, at least for the used values of the parameters, sufficient, as $T_{\max,h}$, β_1 and β_2 have reached equilibrium values after 0.01 seconds.

The data of Appendix D suggests that the depth-width curve on the form (5.15) describes the maximum melted width well, if slightly less so before equilibrium is reached. This can be accepted as an empirical result in itself, but as such it would require further validation than the test performed for this thesis. Otherwise it would be useful to find a mathematical justification for this observation.

7.2 Considerations with radiative heat transfer

In Subsection 2.3 we state that $u = \lim_{n\to\infty} \mathscr{S}^n v_0$ for $v_0 \in \mathcal{C}_B$ is a solution to (1.2) in the sense that it is a fixed point to the solution operator $\mathscr{S}$. This does not in itself imply that u is a solution in the sense of Proposition 1. To satisfy the hypothesis of Proposition 1, we must show that $\Pi(x,y,t) - k_\mathrm{r}((u(x,y,0,t)+T_\mathrm{s})^4 - T_\mathrm{s}^4)$ satisfies (2.2) and (2.3). As $u \in \mathcal{C}_B$ it is easy to show that the first statement holds, while the second requires that there is a constant C such that $|D_t u(x,y,0,t)| \leq C$ whenever $(x,y) \in \mathbb{R}^2$ and $t \in [0,\tau]$, and this is yet to be shown.

When we show that $\mathscr{S}$ is a contraction on $\mathcal{C}_B$ we assume that the stopping time τ is small enough. If we, for instance, use the parameter values from Section 6, the Stefan-Boltzmann constant [10, pp. 14, 344] for k_r (which underestimates τ) and $T_\mathrm{s} = 400$ K we would get $\tau \approx 1$ second, about 100 times as long as the time to reach equilibrium, if radiative heat transfer is neglected. This implies that the requirement on τ is not necessarily a severe limitation. Moreover, once the solution is found at $t = \tau$ it can be introduced as a new initial condition in (1.2) whereupon the solution procedure can be repeated with a new stopping time τ_1. Proceeding inductively in this manner gives a sequence of stopping times $\{\tau_i\}_{i=1}^{\infty}$. If this sequence does *not* converge to zero then the solution to (1.2) could be calculated in this manner for any time $t > 0$. From (2.22) we see that $\tau > 0$ as long as $B < \infty$ which in turn implies that the sequence $\{\tau_i\}_{i=1}^{\infty}$ does not converge to zero if the solution to (1.2) is bounded for any time $t > 0$. From a physical point of view and comparing to the case of negligible radiation, we would expect this to be true, but mathematical proof of this remains to be done.

In Subsection 4.2 we assume that converging quadrature methods can be found for the use in the discretised solution operator $\mathscr{S}_h$ and we show in Appendix C that such a rule exists for part of the operator. Continuity of the integrands, except possibly at a finite set of points in $[0,\tau]$ would suggest that satisfactory quadrature rules may indeed be constructed.

In the definition of $\mathscr{S}_h$ we have assumed that the spatial convolution involved in $\mathscr{A}_h$ may be calculated analytically. Thus an appropriate choice of v_0 should ensure that this is fulfilled. If such a v_0 is not used, then the convolution operation must be discretised as well as the time integral,using some convergent scheme.

7.3 Suggested topics for further study

On the basis of the discussion above we here suggest some topics for further study. In the case of negligible radiation we propose:

- further empirical testing of the same type as in Section 6 using a wider range of parameter values,
- investigation of efficiency of higher order quadrature rules in Algorithm 1,
- finding an analytical justification or further empirical evidence for (5.15), or a reason to reject it, such as an example where it is not a valid approximation.

In the case of radiative heat transfer we suggest:

- investigation of whether the fixed point to the solution operator is a solution to (1.2) in the sense of Proposition 1,
- finding a mathematical proof that the solution to (1.2) is bounded for any positive time,
- finding, if possible, convergent quadrature rules for the use in $\mathscr{S}_h$.

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A Error estimates for the midpoint rule

Apart from the standard error estimate for the midpoint rule we use the following additional estimates

$$E_{[a,b]}(f) \le \max\left\{ \int_a^b |f(s)|\, ds, (b-a)\left| f\left(\frac{a+b}{2}\right)\right| \right\}, \tag{A.1}$$

and

$$E_{[a,b]}(f) \le \frac{(b-a)^2}{2} \sup_{s\in[a,b]} |D_s f(s)|. \tag{A.2}$$

(A.1) follows directly from the definition of the error for an integrand of constant sign. To show (A.2) we write the integrand as the integral of its derivative to get

$$\begin{aligned}
E_{[a,b]}(f) &= \left| \int_a^b f(x)\, dx - (b-a) f\left(\frac{a+b}{2}\right)\right| \\
&= \left| \int_a^b \left(f\left(\frac{a+b}{2}\right) + \int_{(a+b)/2}^s D_t f(t)\, dt \right) ds - (b-a) f\left(\frac{a+b}{2}\right)\right| \\
&= \left| \int_a^b \int_{(a+b)/2}^s D_t f(t)\, dt\, ds \right| \le \int_a^b \int_{(a+b)/2}^s |D_t f(t)|\, dt\, ds \\
&\le \int_a^b \left| \int_{(a+b)/2}^s dt \right| ds \sup_{s\in[a,b]} |D_s f(s)|.
\end{aligned}$$

Noting that $|s-(a+b)/2| \le (b-a)/2$ gives the desired result.

In the case of $t=\infty$ we estimate the remaining integral by

$$\int_b^\infty \frac{1}{1+s^2} e^{-\frac{(x+Vs^2)^2+y^2}{1+s^2} - \frac{z^2}{s^2}}\, ds \le \frac{\pi}{2} - \arctan(b). \tag{A.3}$$

We continue by giving estimates of $\sup_{\mathbf{x}\in\mathbb{R}^3} |D^k h(\mathbf{x}, s)|$ for the integrand h in (2.19) for $k = 1,\ 2$. Let

$$\begin{aligned}
f &= \frac{1}{1+s^2}, \\
g &= \frac{(x+Vs^2)^2+y^2}{1+s^2} + \frac{z^2}{s^2}, \\
h(s) &= f \cdot \exp(-g),
\end{aligned}$$

and $h'(s) = D_s h(s)$. If we in the following omit the time variable, that is $f = f(s)$, then the derivatives can be written as

$$
\begin{aligned}
f' &= \frac{-2s}{(1+s^2)^2} = -2sf^2 \\
f'' &= -2f^2 - 2s(2f'f) = -2f^2 + 8s^2 f^3 \\
g' &= \frac{4Vs(x+Vs^2)}{1+s^2} - \frac{2s((x+Vs^2)^2+y^2)}{(1+s^2)^2} - \frac{2z^2}{s^3} \\
&= 4Vs(x+Vs^2)f - 2s((x+Vs^2)^2+y^2)f^2 - 2z^2 s^{-3} \\
g'' &= 4V(x+Vs^2)f + 8V^2s^2 f + 4Vs(x+Vs^2)f' - 2((x+Vs^2)^2+y^2)f^2 - 2s(4Vs(x+Vs^2))f^2 \\
&\quad - 2s((x+Vs^2)^2+y^2)\cdot 2ff' + 6z^2 s^{-4} \\
&= 4V(x+Vs^2)f + 8V^2s^2 f + 4Vs(x+Vs^2)(-2sf^2) - 2((x+Vs^2)^2+y^2)f^2 \\
&\quad - 2s(4Vs(x+Vs^2))f^2 - 4s((x+Vs^2)^2+y^2)f(-2sf^2) + 6z^2 s^{-4} \\
&= 4V(x+Vs^2)f + 8V^2s^2 f - 8Vs^2(x+Vs^2)f^2 - 2((x+Vs^2)^2+y^2)f^2 \\
&\quad - 8Vs^2(x+Vs^2)f^2 + 8s^2((x+Vs^2)^2+y^2)f^3 + 6z^2 s^{-4} \\
&= 4V(x+Vs^2)f + 8V^2s^2 f - 16Vs^2(x+Vs^2)f^2 - 2((x+Vs^2)^2+y^2)f^2 \\
&\quad + 8s^2((x+Vs^2)^2+y^2)f^3 + 6z^2 s^{-4}
\end{aligned}
$$

$$
\begin{aligned}
(g')^2 &= (4Vs(x+Vs^2)f - 2s((x+Vs^2)^2+y^2)f^2 - 2z^2s^{-3})^2 \\
&= 16V^2s^2f^2(x+Vs^2)^2 + 4s^2f^4((x+Vs^2)^2+y^2)^2 + 4z^4s^{-6} - 16Vs^2f^3(x+Vs^2)((x+Vs^2)^2+y^2) \\
&\quad - 16Vf(x+Vs^2)z^2s^{-2} + 8f^2((x+Vs^2)^2+y^2)z^2s^{-2} \\
h' &= (f' - fg')\exp(-g) \\
&= (-2sf^2 - f(4Vs(x+Vs^2)f - 2s((x+Vs^2)^2+y^2)f^2 - 2z^2s^{-3}))\exp(-g) \\
&= (-\underbrace{2sf^2}_{\varphi_{\mathrm{n},1}} + \underbrace{2s((x+Vs^2)^2+y^2)f^3 + 2z^2s^{-3}f}_{\varphi_{\mathrm{p},1}} - \underbrace{4Vs(x+Vs^2)f^2}_{\varphi_{\mathrm{u},1}})\exp(-g),
\end{aligned}
$$

where $\varphi_{\mathrm{n},1}$, $\varphi_{\mathrm{p},1}$, $\varphi_{\mathrm{u},1}$ represent the negative and positive terms and terms of undetermined sign of h' respectively. Continuing with

$$
\begin{aligned}
h'' &= (f'' - f'g' - fg'' - g'(f' - fg'))\exp(-g) \\
&= (f'' - 2f'g' - fg'' + fg'g')\exp(-g) \\
&= \exp(-g)\big[-2f^2 + 8s^2f^3 - 2(-2sf^2)(4Vs(x+Vs^2)f - 2s((x+Vs^2)^2+y^2)f^2 - 2z^2s^{-3}) \\
&\quad -f\{4V(x+Vs^2)f + 8V^2s^2f - 16Vs^2(x+Vs^2)f^2 - 2((x+Vs^2)^2+y^2)f^2 \\
&\quad +8s^2((x+Vs^2)^2+y^2)f^3 + 6z^2s^{-4}\} + f\{16V^2s^2f^2(x+Vs^2)^2 + 4s^2f^4((x+Vs^2)^2+y^2)^2 \\
&\quad +4z^4s^{-6} - 16Vs^2f^3(x+Vs^2)((x+Vs^2)^2+y^2) - 16Vf(x+Vs^2)z^2s^{-2} \\
&\quad +8f^2((x+Vs^2)^2+y^2)z^2s^{-2}\}\big] \\
&= \exp(-g)\big[-2f^2 + 8s^2f^3 + 16Vs^2(x+Vs^2)f^3 - 8s^2((x+Vs^2)^2+y^2)f^4 - 8f^2z^2s^{-2} \\
&\quad -4V(x+Vs^2)f^2 - 8V^2s^2f^2 + 16Vs^2(x+Vs^2)f^3 + 2((x+Vs^2)^2+y^2)f^3 \\
&\quad -8s^2((x+Vs^2)^2+y^2)f^4 - 6fz^2s^{-4} + 16V^2s^2f^3(x+Vs^2)^2 + 4s^2f^5((x+Vs^2)^2+y^2)^2 \\
&\quad +4fz^4s^{-6} - 16Vs^2f^4(x+Vs^2)((x+Vs^2)^2+y^2) - 16Vf^2(x+Vs^2)z^2s^{-2} \\
&\quad +8f^3((x+Vs^2)^2+y^2)z^2s^{-2}\big] \\
&= \exp(-g)[\varphi_{\mathrm{n},2} + \varphi_{\mathrm{p},2} + \varphi_{\mathrm{u},2,V} + \varphi_{\mathrm{u},2,V^2}]
\end{aligned}
$$

where $\varphi_{\mathrm{n},2}$, $\varphi_{\mathrm{p},2}$ are the negative and positive parts of the second derivative of h, while $\varphi_{\mathrm{u},2,V}$ and $\varphi_{\mathrm{u},2,V^2}$ represent the terms of undecided sign having V and V^2 dependency respectively.

$$\begin{aligned}
\varphi_{\mathrm{n},2} &= -2f^2 - 8s^2((x+Vs^2)^2+y^2)f^4 - 8f^2z^2s^{-2} - 8s^2((x+Vs^2)^2+y^2)f^4 - 6fz^2s^{-4} \\
&= -2f^2 - 16s^2((x+Vs^2)^2+y^2)f^4 - 8f^2z^2s^{-2} - 6fz^2s^{-4} \\
\varphi_{\mathrm{p},2} &= 8s^2f^3 + 2((x+Vs^2)^2+y^2)f^3 + 4s^2f^5((x+Vs^2)^2+y^2)^2 + 8f^3((x+Vs^2)^2+y^2)z^2s^{-2} \\
&\quad + 4fz^4s^{-6} \\
\varphi_{\mathrm{u},2,V} &= 16Vs^2(x+Vs^2)f^3 - 4V(x+Vs^2)f^2 + 16Vs^2(x+Vs^2)f^3 \\
&\quad - 16Vs^2f^4(x+Vs^2)((x+Vs^2)^2+y^2) - 16Vf^2(x+Vs^2)z^2s^{-2} \\
&= 32Vs^2(x+Vs^2)f^3 - 4V(x+Vs^2)f^2 \\
&\quad - 16Vs^2f^4(x+Vs^2)((x+Vs^2)^2+y^2) - 16Vf^2(x+Vs^2)z^2s^{-2} \\
&= (x+Vs^2)\left[32Vs^2f^3 - 4Vf^2 - 16Vs^2f^4((x+Vs^2)^2+y^2) - 16Vf^2z^2s^{-2}\right] \\
\varphi_{\mathrm{u},2,V^2} &= 16V^2s^2f^3(x+Vs^2)^2 - 8V^2s^2f^2
\end{aligned}$$

Below we will frequently use the estimate $|\alpha|^n e^{-\alpha^2} \leq \left(\frac{n}{2e}\right)^{n/2}$ $\forall \alpha \in \mathbb{R}$ when we establish the bounds of the derivatives.

$$\begin{aligned}
|\varphi_{\mathrm{n},1}| &= 2sf^2\exp(-g) \leq 2sf^2 \\
|\varphi_{\mathrm{p},1}| &= 2sf^3((x+Vs^2)^2+y^2)\exp(-g) + 2z^2s^{-3}f\exp(-g) \\
&\leq 2sf^2 \underbrace{((x+Vs^2)^2+y^2)f\exp(-((x+Vs^2)^2+y^2)f)}_{\leq e^{-1}} + 2s^{-1}f \underbrace{(z^2s^{-2})\exp(-z^2s^{-2})}_{\leq e^{-1}} \\
&\leq 2sf^2e^{-1} + 2s^{-1}fe^{-1} \\
|\varphi_{\mathrm{u},1}| &= 4V|s(x+Vs^2)f^2|\exp(-g) \\
&\leq 4Vsf^{3/2}\underbrace{|(x+Vs^2)f^{1/2}|\exp(-(x+Vs^2)^2f)}_{\leq(2e)^{-1/2}} \\
&\leq \sqrt{8}Vsf^{3/2}e^{-1/2} \\
|\varphi_{\mathrm{n},2}| &= \exp(-g)\left[2f^2 + 16s^2((x+Vs^2)^2+y^2)f^4 + 8f^2z^2s^{-2} + 6fz^2s^{-4}\right] \\
&\leq 2f^2 + 16s^2f^3((x+Vs^2)^2+y^2)f\exp(-((x+Vs^2)^2+y^2)f) + 8f^2z^2s^{-2}\exp(-z^2s^{-2}) \\
&\quad + 6fs^{-2}z^2s^{-2}\exp(-z^2s^{-2}) \\
&\leq 2f^2 + 16s^2f^3e^{-1} + 8f^2e^{-1} + 6fs^{-2}e^{-1} \\
|\varphi_{\mathrm{p},2}| &= \exp(-g)\left[8s^2f^3 + 2((x+Vs^2)^2+y^2)f^3 + 4s^2f^5((x+Vs^2)^2+y^2)^2\right. \\
&\quad \left.+8f^3((x+Vs^2)^2+y^2)z^2s^{-2} + 4fz^4s^{-6}\right] \\
&\leq 8s^2f^3 + 2f^2((x+Vs^2)^2+y^2)f\exp(-((x+Vs^2)^2+y^2)f) \\
&\quad + 4s^2f^3((x+Vs^2)^2+y^2)^2f^2\exp(-((x+Vs^2)^2+y^2)f) \\
&\quad + 8f^2((x+Vs^2)^2+y^2)f\exp(-((x+Vs^2)^2+y^2)f)z^2s^{-2}\exp(-z^2s^{-2}) \\
&\quad + 4s^{-2}fz^4s^{-4}\exp(-z^2s^{-2}) \\
&\leq 8s^2f^3 + 2f^2e^{-1} + 4s^2f^3\cdot 4e^{-2} + 8f^2e^{-1}e^{-1} + 4s^{-2}f\cdot 4e^{-2} \\
&= 8s^2f^3 + 2e^{-1}f^2 + 16e^{-2}s^2f^3 + 8e^{-2}f^2 + 16e^{-2}s^{-2}f
\end{aligned}$$

Since the difference of the positive and negative terms is no greater than the maximum of their respective absolute values we get by the triangle inequality

$$\begin{aligned}
|\varphi_{\mathrm{u},2,V}| &= V\cdot\exp(-g)\left|(x+Vs^2)\left[32s^2f^3-4f^2-16s^2f^4((x+Vs^2)^2+y^2)-16f^2z^2s^{-2}\right]\right| \\
&\le V\cdot\exp(-g)\left|(x+Vs^2)\max\left\{32s^2f^3,4f^2+16s^2f^4((x+Vs^2)^2+y^2)+16f^2z^2s^{-2}\right\}\right| \\
&\le V\cdot\max\left\{32s^2f^3|(x+Vs^2)|\exp(-g),\right. \\
&\quad \left.(4f^2+16s^2f^4((x+Vs^2)^2+y^2)+16f^2z^2s^{-2})|(x+Vs^2)|\exp(-g)\right\} \\
&\le V\cdot\max\left\{32s^2f^{5/2}|(x+Vs^2)|f^{1/2}\exp(-(x+Vs^2)^2f),\right. \\
&\quad 4f^{3/2}|(x+Vs^2)|f^{1/2}\exp(-(x+Vs^2)^2f)+ \\
&\quad +16s^2f^{5/2}\sqrt{8}\frac{((x+Vs^2)^2+y^2)f}{2}\frac{|(x+Vs^2)|f^{1/2}}{\sqrt{2}}\exp\left(-\frac{1}{2}((x+Vs^2)^2+y^2)f\right. \\
&\quad \left.\left.-\frac{1}{2}(x+Vs^2)^2f\right)+16f^{3/2}z^2s^{-2}|(x+Vs^2)|f^{1/2}\exp(-(x+Vs^2)^2f-z^2s^{-2})\right\} \\
&\le V\cdot\max\left\{32s^2f^{5/2}(2e)^{-1/2},\right. \\
&\quad \left.4f^{3/2}(2e)^{-1/2}+16s^2f^{5/2}\sqrt{8}e^{-1}(2e)^{-1/2}+16f^{3/2}e^{-1}(2e)^{-1/2}\right\} \\
&\le V(2e)^{-1/2}f^{3/2}\cdot\begin{cases}4+32\sqrt{2}s^2fe^{-1}+16e^{-1}, & s<1.34491\\ 32s^2f, & s>1.34491\end{cases} \\
|\varphi_{\mathrm{u},2,V^2}| &= \exp(-g)|16V^2s^2f^3(x+Vs^2)^2-8V^2s^2f^2| \\
&\le \max\{16V^2s^2f^3(x+Vs^2)^2\exp(-g),8V^2s^2f^2\exp(-g)\} \\
&\le \max\{16V^2s^2f^2(x+Vs^2)^2f\exp(-(x+Vs^2)^2f),8V^2s^2f^2\exp(-g)\} \\
&\le \max\{16V^2s^2f^2e^{-1},8V^2s^2f^2\} \\
&\le 8V^2s^2f^2\max\{2e^{-1},1\} \\
&\le 8V^2s^2f^2
\end{aligned}$$

$$\begin{aligned}
\text{(A.4)}\qquad |h''(s)| &= \left|\exp(-g)[\varphi_{\mathrm{p},2}+\varphi_{\mathrm{n},2}+\varphi_{\mathrm{u},2,V}+\varphi_{\mathrm{u},2,V^2}]\right| \\
&\le \exp(-g)\left[\max\{\varphi_{\mathrm{p},2},|\varphi_{\mathrm{n},2}|\}+|\varphi_{\mathrm{u},2,V}|+|\varphi_{\mathrm{u},2,V^2}|\right] \\
&\le \max\{8s^2f^3+2e^{-1}f^2+16e^{-2}s^2f^3+8e^{-2}f^2+16e^{-2}s^{-2}f, \\
&\quad 2f^2+16s^2f^3e^{-1}+8f^2e^{-1}+6fs^{-2}e^{-1}\} \\
&\quad +V(2e)^{-1/2}f^{3/2}\cdot\max\left\{32s^2f,4+32\sqrt{2}s^2fe^{-1}+16e^{-1}\right\} \\
&\quad +8V^2s^2f^2 \\
&\le 2f\begin{cases}4s^2f^2+e^{-1}f+8e^{-2}s^2f^2+4e^{-2}f+8e^{-2}s^{-2} & \text{if } s>1.7018321\\ f+8s^2f^2e^{-1}+4fe^{-1}+3s^{-2}e^{-1} & \text{if } s\le 1.7018321\end{cases} \\
&\quad +V(2e)^{-1/2}f^{3/2}\cdot\begin{cases}32s^2f & \text{if } s>\sqrt{\frac{4+e}{7e-4-8\sqrt{2}}}\\ 4+32\sqrt{2}s^2fe^{-1}+16e^{-1} & \text{if } s\le\sqrt{\frac{4+e}{7e-4-8\sqrt{2}}}\end{cases} \\
&\quad +8V^2s^2f^2
\end{aligned}$$

$$
\text{(A.5)} \qquad \begin{aligned} |h'(s)| &\leq \sqrt{8} V s f^{3/2} e^{-1/2} + \max\{2sf^2, 2sf^2 e^{-1} + 2s^{-1} f e^{-1}\} \\ &\leq \sqrt{8} V s f^{3/2} e^{-1/2} + f \begin{cases} 2sf & \text{if } s > \frac{1}{\sqrt{e-2}} \\ 2sfe^{-1} + 2s^{-1}e^{-1} & \text{if } s \leq \frac{1}{\sqrt{e-2}} \end{cases} \end{aligned}
$$

Now we have established bounds for the first derivative of the integrand (2.19) expressed in (A.5) and for the second derivative in (A.4).

B Higher order derivatives of the integrand in (2.19)

For the possible use in error analysis for higher order quadrature methods we here derive a formula for the n:th derivative of the integrand in (2.19). Following the notation in Appendix A we write $h(\mathbf{x}, s) = f(s)e^{-g(\mathbf{x},s)}$. By Leibniz's formula [11, p. 305] we have

$$D_s^n h(\mathbf{x}, s) = D_s^n \left(f(s)e^{-g(\mathbf{x},s)} \right) = \sum_{k=0}^{n} \binom{n}{k} D_s^{n-k} f(s) D_s^k e^{-g(\mathbf{x},s)}. \tag{B.1}$$

For derivatives of f, using Leibniz's formula again and the formula for the sum of a geometric progression, we have

$$\begin{aligned} D_s^n f(s) = D_s^n \frac{1}{1+s^2} &= D_s^n \left(\frac{1}{1+is} \frac{1}{1-is} \right) = \sum_{k=0}^{n} \binom{n}{k} \frac{(-1)^k i^k k!}{(1+is)^{k+1}} \frac{i^{n-k}(n-k!)}{(1-is)^{n-k+1}} \\ &= \frac{i^n n!}{(1+s^2)(1-is)^n} \sum_{k=0}^{n} \left(-\frac{1-is}{1+is} \right)^k = \frac{i^n n!}{(1+s^2)(1-is)^n} \frac{\left(-\frac{1-is}{1+is}\right)^n - 1}{-\frac{1-is}{1+is} - 1} \\ &= \frac{i^n n!}{2(1+s^2)^{n+1}} ((-1)^n (1-is)^{n+1} + (1+is)^{n+1}) \\ &= \frac{n!}{2(1+s^2)^{n+1}} \sum_{k=0}^{n+1} \binom{n+1}{k} (1 + (-1)^{n+k}) i^{n+k} s^k. \end{aligned} \tag{B.2}$$

By an application of Faa di Bruno's formula for derivatives of compositions [8, Example 2] we can express the derivatives of the exponential terms in (B.1) as

$$D_s^n e^{-g(\mathbf{x},s)} = Y_n(-D_s g(\mathbf{x}, s), -D_s^2 g(\mathbf{x}, s), \ldots, -D_s^n g(\mathbf{x}, s)) e^{-g(\mathbf{x},s)}, \tag{B.3}$$

where $Y_n(\chi_1, \chi_2, \ldots, \chi_n)$ is defined as the determinant of the matrix $M = (m_{ij}(\chi_{j-i+1}))$ with

$$m_{ij}(\chi_{j-i+1}) = \begin{cases} \binom{n-i}{j-i} \chi_{j-i+1}, & j \geq i \\ -1, & j = i-1, \\ 0, & \text{otherwise.} \end{cases}$$

We apply Leibniz's formula one last time in order to compute the derivatives of g

$$\begin{aligned} D_s^n g(\mathbf{x}, s) &= D^n[((x+vs^2)^2 + y^2) f(s)] + D_s^n \frac{z^2}{s^2} \\ &= \sum_{k=0}^{\min\{n,4\}} \binom{n}{k} D_s^k [((x+Vs^2)^2 + y^2)] D_s^{n-k} f(s) + \frac{(-1)^n (n+1)! z^2}{s^{n+2}}. \end{aligned} \tag{B.4}$$

Combining (B.1), (B.2), (B.3) and (B.4) gives the formula for the n:th derivative of the integrand in (2.19).

C Convergence of the midpoint rule

Here we show that the integral (2.19) can by approximated arbitrarily well by adaptive application of the midpoint rule.

By applying the 0:th and 1:st order error bounds from appendix A we get

$$
\begin{aligned}
E_{[0,t]}(h(\mathbf{x})) &\leq \max\left\{\arctan(s_1), \frac{4s_1}{4+s_1^2}\right\} + \sum_{i=2}^{N} \frac{k_i^2}{2} \sup_{\mathbf{x}\in\mathbb{R}^2\times\mathbb{R}_-} \sup_{s\in[s_i,s_{i+1}]} |D_s h(\mathbf{x},s)| \\
&\leq \arctan(s_1) + \frac{4s_1}{4+s_1^2} + \frac{t}{2}k \sup_{\mathbf{x}\in\mathbb{R}^2\times\mathbb{R}_-} \sup_{s\in[s_1,t]} |D_s h(\mathbf{x},s)| \\
&\leq \arctan(s_1) + \frac{4s_1}{4+s_1^2} + \frac{t}{2}k(C_1 + C_2 s_1^{-1}),
\end{aligned}
$$

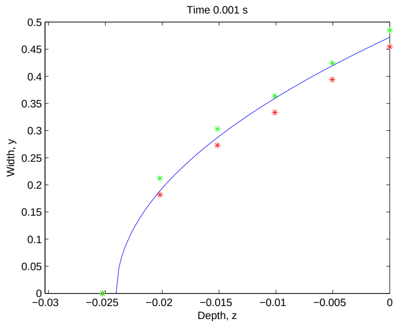
where $k = \max_{2\leq i\leq N} k_i$ and C_1, C_2 are constants. Let now $N \to \infty$ in such a manner that $k \to 0$ and $s_1 = C_3 k^p$ for C_3 constant and some p such that there exists constants $\alpha, \beta > 0$ so that $0 < \alpha \leq p \leq \beta < 1$. Then

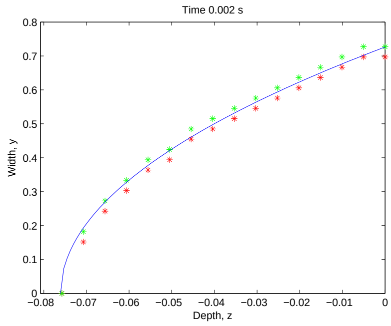
$$
E_{[0,t]}(h(\mathbf{x})) \leq \arctan(C_3 k^p) + \frac{4C_3 k^p}{4 + C_3^2 k^{2p}} + \frac{t}{2}(C_1 k + \frac{C_2}{C_3} k^{1-p}) \to 0,
$$

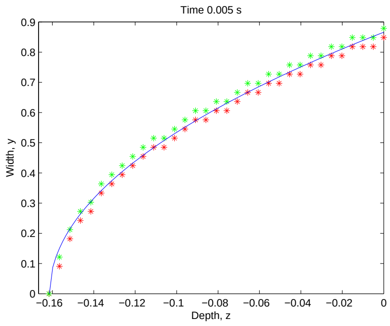
as $k \to 0$, which show the desired result.

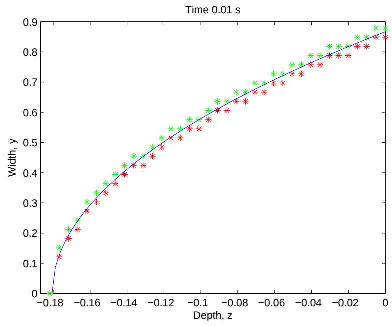
D Depth-width curves

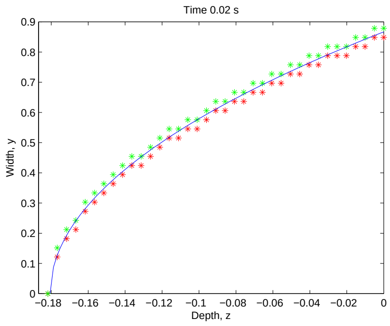
Below we show the plots of the depth-width curves from Section 6. In the plots the solid line represents the result of (5.15) and stars represent upper and lower bounds on the widths as estimated from the reference lattice.

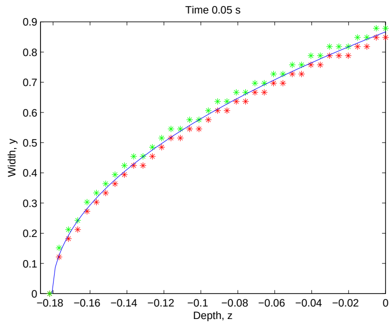


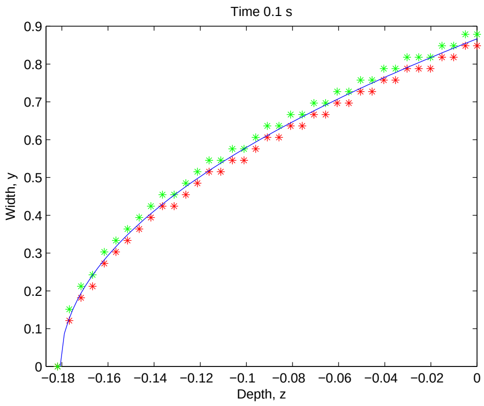


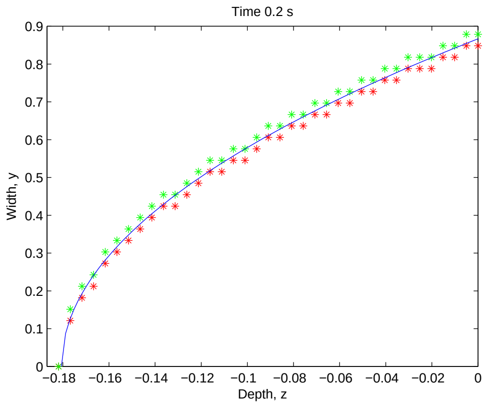


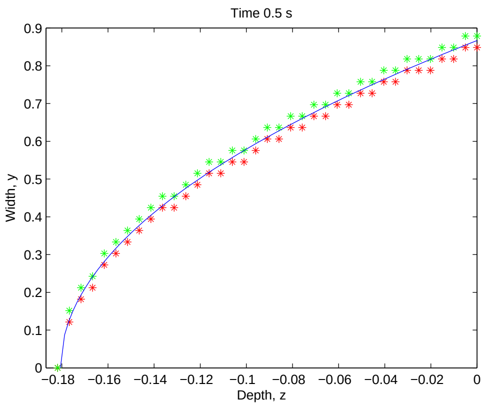


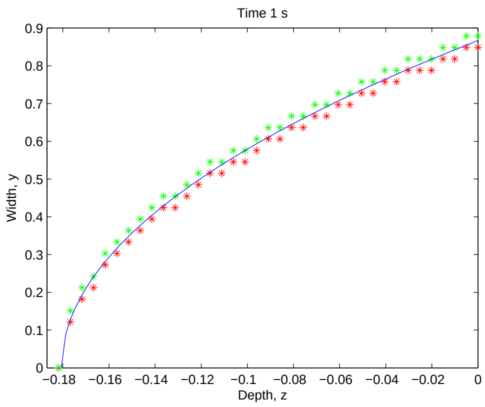


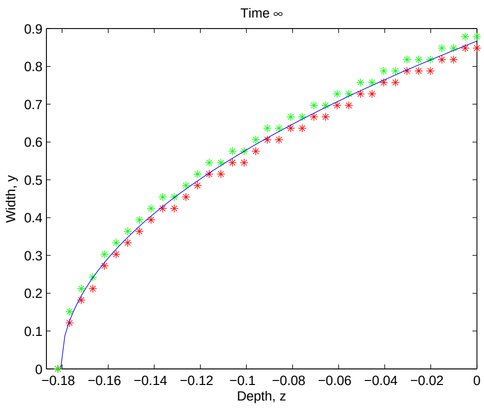



Time 0.1 s
Width, y
Depth, z


Time 0.2 s
Width, y
Depth, z


Time 0.5 s
Width, y
Depth, z


Time 1 s
Width, y
Depth, z


Time ∞
Width, y
Depth, z