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EINDHOVEN UNIVERSITY OF TECHNOLOGY
Department of Mathematics and Computing Science

RANA 98-17
August 1998

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Reports on Applied and Numerical Analysis
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P.O. Box 513
5600 MB Eindhoven, The Netherlands
ISSN: 0926-4507

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31st July 1998

Abstract

For the computation of three-dimensional heat flow in hot glass melts, an accurate model is needed that does not require an excess in computation time. Although the ray-trace method has been proven to give accurate results, its high computational consumption was prohibitive. In this article we study an algebraic formulation of the ray-trace method, which when implemented, eliminates most of the work needed for ray-tracing for certain applications.

1 Introduction

The mass character of glass production, implies that small improvements in the process, such as energy savings, have major benefits for the environment and the company's competitional position. One major field of research is the study of radiative heat transfer. This mechanism for transmitting energy is predominant in hot glass. For a proper treatment of radiation the Chemical Engineering, Mechanical Engineering and Mathematics Departments of the Eindhoven University have started a joint project with the industry under supervision of the Dutch Technology foundation STW[1] to gather and design material data, measurement equipment, and a computational model respectively.

In the present article we study the Method of Ray Tracing (RTM) which is used to solve the equations following from a Discrete Ordinate Method (DOM). The RTM can be elaborated algebraicly to a form where the actual process of ray tracing has to be performed only once, rather than at every time or iteration step. This means that for configurations satisfying suitable requirements an enormous saving in time can be achieved.

In the next section, we first look at the equations describing radiative heat transfer. Then the thought behind algebraic ray tracing and its theory is explained. Finally, we look at a simple application of the method.

2 Radiative heat transfer

Heat transfer by radiation cannot be described directly in terms of temperature. Because of the wave/particle nature of the transfer mechanism, thermal radiation is dependent on more variables than position alone. When the thermal light is unpolarised, radiation can be quantised by a sole direction dependent scalar variable: the *intensity* (see [1] and [6] for a detailed derivation); see Figure 1, where a small cone with spherical angle $d\Omega$ leaving a infinitesimal surface dA, is displayed. The intensity can now be defined as the radiative power travelling through this cone:

$$I(\mathbf{x},\mathbf{s}) := \frac{\text{radiative power}}{\Delta\Omega\Delta\nu\Delta A}\left[\frac{\mathrm{W}}{\mathrm{sr}\cdot\mathrm{Hz}\cdot\mathrm{m}^2}\right]$$

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[1]The project is listed under project number EWT55.3939

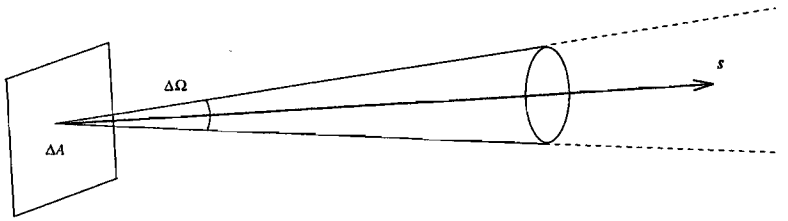

Figure 1: Definition of radiative intensity

As can be seen the intensity $I(\mathbf{x},\mathbf{s})$ is not only dependent on position $\mathbf{x}$ (three degrees of freedom), but also on direction $\mathbf{s}$(two degrees of freedom); adding up to a total of five degrees of freedom — we neglect the influence of time for the moment being as we do the influence of the frequency: a grey gas is considered. The behaviour of the intensity can be described by

$$\mathbf{s}\cdot\nabla I(\mathbf{x},\mathbf{s}) = \kappa(\mathbf{x})I_b(\mathbf{x}) - [\kappa(\mathbf{x})+\sigma_s(\mathbf{x})]\,I(\mathbf{x},\mathbf{s}) + \frac{\sigma_s(\mathbf{x})}{4\pi}\int_{4\pi} I(\mathbf{x},\mathbf{s}')\Phi(\mathbf{x};\mathbf{s}',\mathbf{s})d\Omega', \tag{1}$$

with boundary conditions

$$I(\mathbf{x}_w,\mathbf{s}) = \epsilon(\mathbf{x}_w)I_b(\mathbf{x}_w) + \frac{\rho(\mathbf{x}_w)}{\pi}\int_{|\mathbf{n}\cdot\mathbf{s}'|<0} I(\mathbf{x}_w,\mathbf{s}')\Psi(\mathbf{x};\mathbf{s}',\mathbf{s})d\Omega'. \tag{2}$$

(see [6]). Here $\kappa(\mathbf{x})$ is the *volumetric absorption coefficient* ($[\mathrm{m}^{-1}]$); $\sigma_s(\mathbf{x})$ is the *volumetric scattering coefficient.* Then, $\epsilon(\mathbf{x}_w)$ and $\rho(\mathbf{x}_w)$ respectively are the emissivity and the reflectivity of the boundary at position $\mathbf{x}_w$. The two *Hopf phase functions* $\Phi(\mathbf{x};\mathbf{s}',\mathbf{s})$ and $\Psi(\mathbf{x};\mathbf{s}',\mathbf{s})$ relate the scattering or reflection from radiation travelling in direction $\mathbf{s}'$ to that travelling in direction $\mathbf{s}$ respectively. For an isotropically scattering medium $\Phi(\mathbf{x};\mathbf{s}',\mathbf{s}) = 1$. Similarly, for a diffuse reflecting boundary we find $\Psi(\mathbf{x};\mathbf{s}',\mathbf{s}) = 1$, and for a specularly reflecting boundary $\Psi(\mathbf{x};\mathbf{s}',\mathbf{s}) = \delta(\mathbf{n}\cdot(\mathbf{s}-\mathbf{s}'))$, where $\delta(.)$ is the Dirac delta-function.

Finally, $I_b(\mathbf{x})$ is the black body intensity. Planck determined that a black body would emit radiation according to

$$I_b(T) = n^2\frac{\bar{\sigma}T^4}{\pi}, \tag{3}$$

in which n is the refractive index of the medium, T is the absolute temperature, and $\bar{\sigma}$ is the Stefan-Boltzmann constant.

3 Calculation of Radiative Heat Transfer

If we would know the temperature field in a certain domain, equations (1–3) allow us to compute the intensity. Because it it impossible to solve (1) for the an infinite number of directions $\mathbf{s}$, we have to find a way to treat this equation. One of the possible solutions is offered by the Discrete Ordinate Method. This method proposes to choose a finite set $\mathfrak{S}$ of directions $\mathbf{s}_i$ and replace the integrals in (1) and (2) by an appropriate quadrature using the directions $\mathbf{s}_i$ as base points. These equations then can be solved numerically, for example using a Finite Element Method code as proposed by Fiveland in [2].

A more generic approach is offered by the Ray Trace Method, where we solve equation (1) along a ray travelling in direction $\mathbf{s}$. Along this path, this equation simplifies to an ODE, albeit a coupled one because of the presence of the integral. The genericity of the method

comes forth from the the ease a ray of light can be followed across transitions in media with different refractive indices — there, after all, a ray changes direction abruptly but well defined by Snellius' law — and through complex geometries.

However, for most practical purposes we are not interested in the intensity itself. Only for measurements on hot glass, where we are able to measure the intensity from the outside, we need to know it. But then only at a certain point in a certain direction, not everywhere in all directions. These calculations are, however, often necessary as a by-product in the calculation of radiative heat. After all radiative heat flux is defined by

$$\mathbf{q}^r(\mathbf{x}) = \oint_{4\pi} \mathbf{s}\, I(\mathbf{x},\mathbf{s}) d\Omega;$$

so it seems we need to know the intensity before we can figure out the heat flux. Still, we realize that a lot of storage and computational costs, could be saved by by-passing the intensity calculations. After all, $\mathbf{q}^r(\mathbf{x})$ has a less degrees of freedom than $I(\mathbf{x},\mathbf{s})$.

That it is possible to by-pass the intensity calculations altogether is shown by the Rosseland approximation. Here, first the intensity equations are solved *formally* to obtain an expression in I_b. Then, the assumption of optical thickness of the problem is made, which simplifies the expressions significantly. It can be shown that in the one-dimensional case, the assumption of optical thickness is equivalent to following a discrete ordinate method using only two directions. For a detailed discussion of this approximation refer to [5] and [6]. Here we only state the result for a gray medium without scattering, as we use this expression later in this paper:

$$\mathbf{q}^r = -\frac{4\pi}{3\kappa}\nabla I_b =:= -k^r(T)\nabla T. \tag{4}$$

which is similar to the expression for the conductive heat flow, also called the diffusive term in heat calculations. Because the radiative 'conductivity' $k^r(T) \sim T^3$ the radiative diffusion term is highly non-linear, compared to the conductivity term. The major drawback of this method is the inaccuracy where the assumption optical thickness is violated: close to the boundaries and in case of steep temperature gradients. This makes the method unfit to study the behaviour of the heat transfer at the walls of a glass furnace, or the process of re-heating in the production of bottles. Recently, more accurate diffusion approximation have been derived, for example by Siedow in [4]. Like the method presented here, the numerical improvements cost additional computational effort. A comparison between these different techniques has not yet been made.

3.1 One-dimensional geometry

From studying the one-dimensional equations for radiative heat transfer, it becomes clear, that at some additional cost, the assumptions of optical thickness do not have to be made to come to a computationally affordable numerical model. The equations for one dimension in absence of scattering[2] are

$$\tilde{\mu}\frac{\partial I^+}{\partial \tau}(\tau,\tilde{\mu}) + I^+(\tau,\tilde{\mu}) = I_b(\tau),$$
$$-\tilde{\mu}\frac{\partial I^-}{\partial \tau}(\tau,\tilde{\mu}) + I^-(\tau,\tilde{\mu}) = I_b(\tau).$$

where the 'optical coordinate' τ is defined as $\tau := \kappa x$. Furthermore, $\tilde{\mu} := |\cos\vartheta|$ in which ϑ is the angle between the (three-dimensional) direction vector and the x-axis. I^+ stands for the intensities having directions with a positive x-component, and I^- for the intensities

[2] Glass is an amorphous material; scattering therefore can be neglected in absence of impurities as bubbles and batch products.

in the other directions. This equation can readily be solved formally, i.e. we pretend the unknown I_b is known and find that

$$I^+(\tau,\tilde{\mu}) = c_o e^{-\tau/\tilde{\mu}} + \frac{1}{\tilde{\mu}}\int_0^{\tau} e^{(s-\tau)/\tilde{\mu}}\, I_b(s)\, ds, \tag{5}$$

$$I^-(\tau,\tilde{\mu}) = c_1 e^{-\tau/\tilde{\mu}} + \frac{1}{\tilde{\mu}}\int_{\tau}^{\tau_1} e^{(\tau-s)/\tilde{\mu}}\, I_b(s)\, ds. \tag{6}$$

Remembering that the definition of q^r is

$$q^r(\tau) := \int_{-\pi}^{\pi} d\phi \int_0^1 d\tilde{\mu}\,\tilde{\mu}\left(I^+ - I^-\right) = 2\pi\int_0^1 \tilde{\mu}\left(I^+ - I^-\right) d\tilde{\mu}, \tag{7}$$

we can use the formal solutions (5) and (6) to obtain the following expression for the heat flux' gradient $\nabla\cdot\mathbf{q}^r = \kappa\frac{dq^r}{d\tau}q^r(\tau)$:

$$\frac{1}{\kappa}\nabla\cdot\mathbf{q}^r(\tau) = 4\pi I_b(\tau) - 2\pi I_{b_o}E_2(\tau) - 2\pi I_{b_1}E_2(\tau_1-\tau) - 2\pi\int_0^{\tau_1} E_2\left(|\tau-s|\right) I_b(s)ds \tag{8}$$

where we have assumed black boundaries on both sides with emitting intensities of I_{b_o} and I_{b_1} respectively. The domain was taken to be $0 \le \tau \le \tau_1$. Because we have assumed no scattering we can also express the radiative heat flux as (see [6]) as

$$\frac{1}{\kappa}\nabla\cdot\mathbf{q}^r(\tau) = 4\pi I_b(\tau) - G(\tau) \tag{9}$$

in which $G(\tau)$ is the *incident radiation* defined as $G(\tau) := \int_{4\pi} I(\tau,\mathbf{s})d\Omega$. From (8) and (9), we see immediately that

$$G(\tau) = 2\pi I_{b_o}E_2(\tau) + 2\pi I_{b_1}E_2(\tau_1-\tau) + 2\pi\int_0^{\tau_1} E_2\left(|\tau-s|\right) I_b(s)ds \tag{10}$$

Now, suppose we want to know the black body intensity at M points with coordinates $x_1, x_2, \ldots, x_M$ and corresponding optical coordinates $\tau_j := \kappa x_j$ and black body intensities $b_j := I_b(x_j)$. Discretising the integral in (10) in some manner allows us then to express $G(\tau)$ at chosen points as

$$g_j := G(\tau_j) = r_j + a_{jk}b_k \quad \text{or} \quad \mathbf{g} = \mathbf{r} + \mathbf{A}\mathbf{b},$$

with $\mathbf{r} := (r_j)$ in which $r_j := 2\pi I_{b_o}E_2(\tau_j) + 2\pi I_{b_1}E_2(\tau_1-\tau_j)$, and $\mathbf{A} := (a_{jk})$. The matrix elements a_{jk} are dependent on the way the integral is discretised. If we would, for example, estimate the function $I_b(\tau)$ by $I_b(\tau) \doteq \sum_i b_i\varphi_i(\tau)$ — where $\varphi_i(\tau)$ are appropriate hat functions — these coefficients would be $a_{jk} := 2\pi\int_{t_{k-1}}^{t_{k+1}} E_2(|s-t_j|)\phi_k(s)ds$.

With this notation we can estimate the heat flux' gradient with

$$\frac{1}{\kappa}\nabla\cdot\mathbf{q}^r \doteq (4\pi\mathbf{I} - \mathbf{A})\mathbf{b} - \mathbf{r} \tag{11}$$

which has a form similar to what the discretisation of (4) would be. So, by elaborating on the formal solution of the radiative transfer equation (1), we approximate more accurately without increasing the computational effort significantly. In Figure 2 we see the solution of a steady state radiation-only problem ($\frac{1}{\kappa}\nabla\cdot\mathbf{q}^r = 0$) solved by the present method (*"quasi-1d"*) and with the Rosseland approximation, both numerically (*"pure 1d"*) and analytically (*"exact 1d"*). The names stem from the notion that the one dimensional Rosseland approximation can be found by also limiting the directions radiation can travel to one dimension.

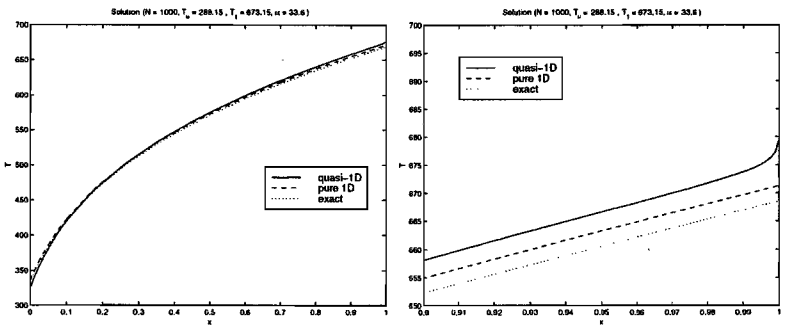

Figure 2: Temperature distribution in a thick glass rod (left) with detail close to the boundary (right)

3.2 Algebraic Ray Tracing

Suppose that we want to know the temperature at M positions in the set of points in the domain of interest $\mathfrak{M} := \{\mathbf{x}_j,\, j = 1, 2, \ldots, M\}$. Rather than at an infinite number of directions, we only look at N discrete directions from the set $\mathfrak{S} := \{\mathbf{s}_i | \mathbf{s}_i \in \mathbb{R}^3 \wedge \|\mathbf{s}_i\| = 1,\, i = 1, 2, \ldots, N\}$.

If we want to know the intensity at the j-th point (i.e. the point with coordinates $\mathbf{x}_j$) in the i-th direction (direction is $\mathbf{s}_i$), we trace the ray from that point back to the boundary (see Figure). On the line we construct, say P^{ij} points and interpolate at those points the value of the black body intensity using only the points in $\mathfrak{M}$. If we place the black body intensity at the M points in a vector $\mathbf{b}$ defined as $\mathbf{b} := (I_b(\mathbf{x}_1), I_b(\mathbf{x}_2), \ldots, I_b(\mathbf{x}_M))^T$ we can write black body intensity on the P^{ij} points on the ray as a vector $\mathbf{p}^{ij}$ described by

$$\mathbf{p}^{ij} = \mathbf{T}^{ij}\mathbf{b}, \tag{12}$$

in which $\mathbf{T}^{ij}$ is an $M \times P^{ij}$ matrix describing the interpolation coefficients at position j in direction i. For simple interpolations involving only a small subset (typically with two or three elements) $\mathbf{T}^{ij}$ is sparse. Furthermore, $\mathbf{T}^{ij}$ depends on the geometry and needs to be determined only once.

For simplicity we now assume scattering to be absent within the medium, so the inhomogeneous part of the radiative transfer equations is formed by the blackbody intensity only. Then the ODE can be solved to yield

$$I(s, \mathbf{s}_i) = \int_0^{\tau} e^{t-\tau} I_b(t) dt + r_{ij}, \tag{13}$$

with $\tau(s) := \int_0^s \kappa(\zeta) d\zeta$ and s is the distance along the ray from the boundary. Further, r_{ij} is given by the boundary condition. With a prescribed temperature on the boundary, r_{ij} is simply the black boundary intensity at the boundary. In case of reflections r_{ij} is more complicated. This case has not yet been considered.

If κ can be taken constant, s and τ are simply related, and (13) can be approximated by a numerical quadrature at point i:

$$I(\mathbf{x}_j, \mathbf{s}_i) \doteq \sum_{k=1}^{P^{ij}} w_k^{ij}\, p_k^{ij} = \mathbf{w}^{ij} \cdot \mathbf{p}^{ij} + r_{ij} =: \eta_{ij}, \tag{14}$$

where we used the notation η_{ij} for the approximation of the intensity at position j in direc-

tion i. We can rewrite this with (12) to

$$\begin{aligned} \eta_{ij} &= \mathbf{w}^{ij} \cdot \mathbf{T}^{ij}\mathbf{b} + r_{ij} && (15)\\ &= (\mathbf{T}^{ij})^T \mathbf{w}^{ij} \cdot \mathbf{b} + r_{ij} && (16)\\ &=: \sum_{k=1}^{M} a_{ijk} b_k + r_{ij}. && (17) \end{aligned}$$

We see that both the interpolation and the integration have been taken into the tensor $\mathfrak{A} := (a_{ijk})$. So for constant κ we do not need to store the matrices $\mathbf{T}^{ij}$ or the vectors $\mathbf{p}^{ij}$. In case κ cannot be taken constant, however, it is a function of the temperature, or $\kappa = \kappa(I_b)$ and in (14) $\mathbf{w}^{ij} = \mathbf{w}^{ij}(\mathbf{b})$. In that case it is wise to keep at least $\mathbf{T}^{ij}$ for every (i,j) in memory to facilitate the computation of the tensor $\mathfrak{A}$ according to (17). We call the tensor holding the intensity values $\mathbf{H}$, so $\mathbf{H} := (\eta_{ij})$, and the tensor holding the boundary conditions $\mathbf{R} := (r_{ij})$, so we can rewrite (17) as

$$\mathbf{H} = \mathfrak{A} \cdot \mathbf{b} + \mathbf{R}, \quad \text{or} \quad \eta_{ij} = a_{ijk} b_k + r_{ij}, \tag{18}$$

using tensor notation and Einstein's summation convention. This equation now allows us to express the intensity at the points in $\mathfrak{M}$ in terms of the black body intensity, and eliminate it from the heat equations. Equation (18) should be regarded as the higher-dimensional variant of the formal solution we used to solve the one-dimensional equation.

Now, if we want to express, for example, the incident radiative energy $G(\mathbf{x})$, defined by

$$G(\mathbf{x}) := \int_{4\pi} I(\mathbf{x}, \mathbf{\Omega}) d\mathbf{\Omega},$$

where 4π now indicates that we integrate over the whole unit sphere in $\mathbb{R}^3$ and a unit circle in $\mathbb{R}^2$. As in the discussion of the calculation of radiative intensity, we can replace this integral by a quadrature fit for our direction set $\mathfrak{S}$, or

$$G(\mathbf{x}) \doteq \sum_{i=1}^{N} w_i I(\mathbf{x}, \mathbf{s}_i).$$

Evaluated at the points in $\mathfrak{M}$, this can be written as

$$\mathbf{g} := (G(\mathbf{x}_1), G(\mathbf{x}_2), \ldots, G(\mathbf{x}_M))^T = \mathrm{H}^T \mathbf{w}, \quad \text{or} \quad g_j = \eta_{ij} w_i,$$

in tensor notation, which together with (18) leads to

$$g_j = a_{ijk} b_k w_i + r_{ij} w_i.$$

If we now define the matrix $\mathbf{A} = (\alpha_{ij})$ by $\alpha_{jk} := w_i\, a_{ijk}$ and the vector $\mathbf{f} = (f_j)$ by $f_j := r_{ij} w_i$, this is rewritten in the more readable form

$$\mathbf{g} = \mathbf{A}\mathbf{b} + \mathbf{f}, \quad \textit{or} \quad g_j = \alpha_{jk} b_k + f_j. \tag{19}$$

As said before, if radiation is the only mechanism for heat transfer, the heat flux' gradient can be written as

$$\nabla \cdot \mathbf{q}^r(\mathbf{x}) = 4\pi I_b(\mathbf{x}) - G(\mathbf{x})$$

which leads to an expression in the same form of (11), namely $\nabla \cdot \mathbf{q}^r(\mathbf{x}) = (4\pi\mathbf{I} - \mathbf{A})\mathbf{b} - \mathbf{f}$, which then can be applied for heat calculations. In Figure 3 ...

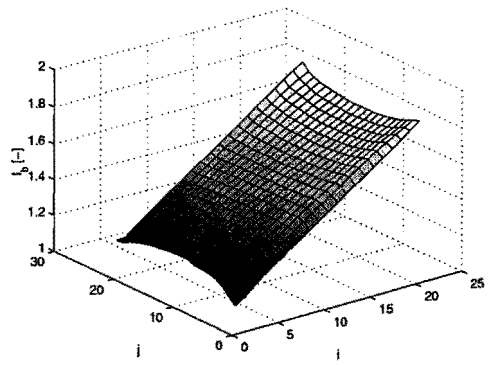

Figure 3: Radiative equilibrium on a square.

4 Conclusions and Further Research

Here we have presented a method of performing ray tracing, which replaces the ray tracing itself by a matrix multiplication. Especially in time dependent heat problems and in problems which also have convection and conduction present, this will lead to vast savings in time: These problems need the computation of $\nabla \cdot \mathbf{q}^r(\mathbf{x})$ for every time-step or iteration-step respectively. After the initial cost of performing an actual ray tracing and building the matrix $\mathbf{A}$, each time step will cost not more than a matrix multiplication.

Because the matrix $\mathbf{A}$ in general is a full matrix — with most elements close to zero, however — straightforward multiplication would still cost about M^2 flops, where M is the number of points, whereas Rosseland's method in its discretised form only costs about $3M$ flops. So, after all Rosseland remains cheaper to use. For geometries where Rosseland leads to unacceptable results — such as the region close to the boundary — the here presented method is the method of choice.

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