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Numerical Solution of Integral Equations in Solidification and Laser Melting

Elizabeth Case
Southern Methodist University, ekaram@mail.smu.edu

Johannes Tausch
Southern Methodist University, tausch@mail.smu.edu

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Elizabeth Case & Johannes Tausch
Department of Mathematics, Southern Methodist University
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Abstract

Many applications in solidifcation or melting are described by a two-phase Stefan problem with elliptical geometry. Here, we model a scanning laser as it heats and melts a metal surface and compute the evolution of the boundary between the solid and liquid material. Using Green's representation theorem, the heat equation is reformulated as a system of nonlinear integro-differential equations in time. The unknown fluxes and radius of the solid-liquid interface are determined from this system and the Stefan condition. The integral equation is discretized with the Nyström method which leads to an efficient time stepping scheme to determine the position and velocity of the interface with given melting temperature and material properties. We first tested this method with the assumption of spherical symmetry on a problem with a known analytical solution, and are currently extending it to general geometries. Examples and numerical results are presented that demonstrate the effectiveness of the method.

Introduction

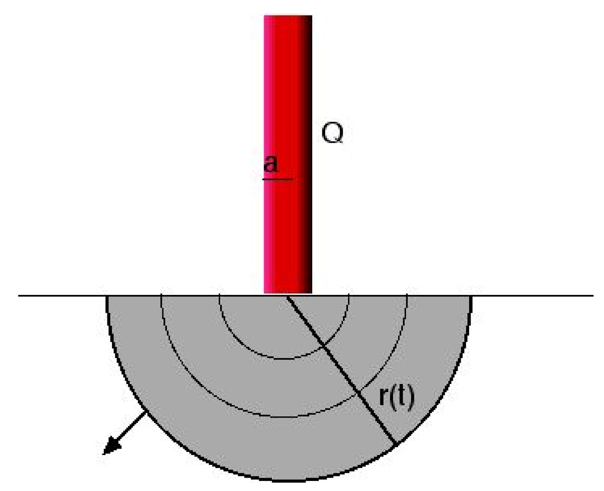
Laser heat sources are used in many methods of material production. A laser source can be easily controlled and has a concentrated heating area. Some applications include:

- Laser Engraving: used to develop metal plated for printing
- Welding
- Laser Cutting: used for manufacturing
- Ablation: converts solid material into vapor for removing excess material
- Laser Annealing: a method of strengthening a sheet of metal by scanning a laser evenly over the surface

Geometry of Problem

We consider a material which occupies all of $\mathbb{R}^3$, where the solid and liquid phase are separated by a smooth interface $\Gamma(t)$, whose size and location depend on time.
We assume that the problem is governed by the heat equation where u is the interface temperature:

$$\begin{aligned} \partial_t u &= \alpha\Delta u + q_v, \\ \frac{\partial u}{\partial n} &= f \text{ on } \Gamma_0, \\ u_0 = u_l &= u_s \text{ on } \Gamma(t) \\ v &= k_s\tfrac{\partial u_s}{\partial n} - k_l\tfrac{\partial u_l}{\partial n} = 0. \end{aligned} \tag{1}$$



The variables are defined as:

- q_v: Volume heat source,
- u_0: Initial condition,
- f: Boundary condition,
- v: Velocity of the interface.

The constant α is the thermal diffusivity, k is conductivity, and the subscripts 's' and 'l' indicate the solid and liquid phase.

Integral Equation Formulation

Green's representation formula for (1) can be derived and a solution of (1) satisfies

$$\frac{1}{2}u(x,t) = -\alpha\mathcal{K}u(x,t) + \alpha\mathcal{V}\left(\frac{\partial u}{\partial n} + \frac{uv}{\alpha}\right)(x,t) + \mathcal{A}u_0(x,t) + \mathcal{N}q(x,t), \tag{2}$$

where $\mathcal{V}$ and $\mathcal{K}$ are the single and double layer potentials defined by

$$\begin{aligned} \mathcal{V}g(x,t) &= \int_0^t\int_\Gamma G(x-y,t-\tau)g(y,\tau)dyd\tau, \\ \mathcal{K}g(x,t) &= \int_0^t\int_\Gamma \frac{\partial G}{\partial n}(x-y,t-\tau)g(y,\tau)dyd\tau, \\ \mathcal{A}u_0(x,t) &= \int_{\Gamma_0} G(x-y,t)u_0(y)dy, \\ \mathcal{N}q(x,t) &= \int_0^t\int_{\Gamma_0} G(x-y,t-\tau)q(y,\tau)dyd\tau, \end{aligned}$$

where $\mathcal{A}$ and $\mathcal{N}$ are contributions from the source terms.

Spherical Symmetry

In this simplified problem we assume the interface and source terms have spherical symmetry, and

$$\begin{aligned} q_s &= 0, u_0 = 0, \\ q_v(x) &= \exp\left(-\tfrac{r^2}{a}\right). \end{aligned}$$

Because of the symmetry the heat equation can be written in spherical coordinates as

$$u_t - \frac{\alpha}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial u}{\partial\rho}\right) = q. \tag{3}$$

$\Gamma(t)$ is spherical with r as its radius. The surface integrals for the single and double layer operators are done analytically. We obtain an integral equation in time for the unknown radius. The time integrals are replaced by a singularity corrected quadrature rule, and we solve equation (2) in the solid and liquid phase for each time step. We discretize the operators with the Nyström Method, using a singularity corrected version of the quadrature rule.

$$\begin{aligned} V_h[g_a(t_i)] &= \sum_{j=0}^{i-1}\frac{h_t}{\sqrt{t_i-t_j}}k^d(t_i,t_j)g_a(t_j) + \mu_i k^d(t_i,t_i)f(t_i) \\ K_h[g_a(t_i)] &= \sum_{j=0}^{i-1}\frac{h_t}{\sqrt{t_i-t_j}}k^v(t_i,t_j)g_a(t_j) + \mu_i k^v(t_i,t_i)f(t_i) \end{aligned}$$

The μ_i are determined to correct the singularities at $t=\tau$ and $t=\tau=0$. Some of these corrective weights can be computed in advance for efficiency since they do not depend on the radius of the interface.
Applying these quadrature rules to (2) leads to a lower triangular system. At each time step we compute $v_{n,i}$ and then $x(i+1)$ using a singularity corrected Euler approximation.

Gibbs-Thompson Equation

The effects of surface tension are modeled through the Gibbs-Thompson equation, given by

$$u(t) = 1 + \frac{\gamma}{r(t)}.$$

The system of equations from (2) involves a Newton potential which increases the numerical complexity. The free-space solution of the inhomogeneous equation in closed form is

$$w_a(\rho,t) = Q\frac{a^{\frac{3}{2}}}{4\alpha_s}\frac{\sqrt{\pi}}{\rho}\left[\operatorname{erf}\left(\frac{\rho}{\sqrt{a}}\right) - \operatorname{erf}\left(\frac{\rho}{\sqrt{a+4\alpha_s t}}\right)\right], \quad a \in \{s,l\}.$$

We define $\tilde{u}_a$ as

$$u_a = \tilde{u}_a + w_a,$$

which satisfies the homogeneous heat equation. Then our system becomes

$$\begin{aligned} \frac{1}{2}\tilde{u}_l &= -\alpha_l\mathcal{K}_l u_l + \alpha_l\mathcal{V}_l g_l + \mathcal{A}_l u_{l0}, \\ \frac{1}{2}\tilde{u}_s &= \alpha_s\mathcal{K}_s u_s - \alpha_s\mathcal{V}_s g_s + \mathcal{A}_s u_{s0}, \end{aligned}$$

where

$$\begin{aligned} \tilde{u}_{a0} &= u_0 - w_a, \quad \tilde{u}_a = u - w_a \\ g_a &= \tfrac{\partial\tilde{u}_a}{\partial\rho} + \tfrac{\tilde{u}_a}{\alpha_a}r'. \end{aligned}$$

The propagation of the interface is now

$$v = k_s g_s - k_l g_l + k_s\frac{\partial w_s}{\partial\rho} - k_l\frac{\partial w_l}{\partial\rho}.$$

Results

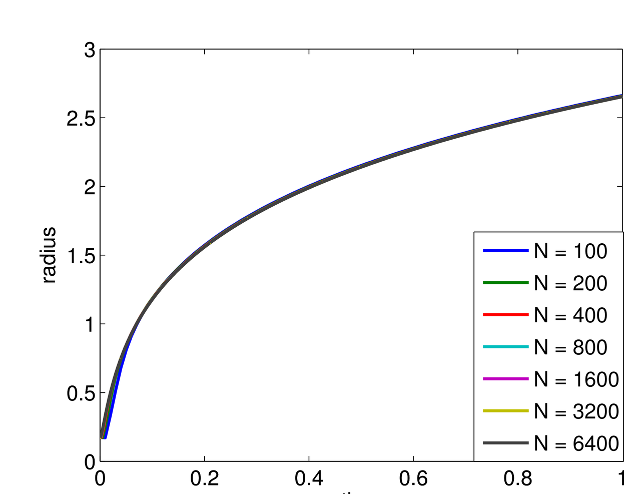


Figure: The computed radius using $N=100$ up to $N=6400$ time steps. Note that the curves for different time step sizes overlap.

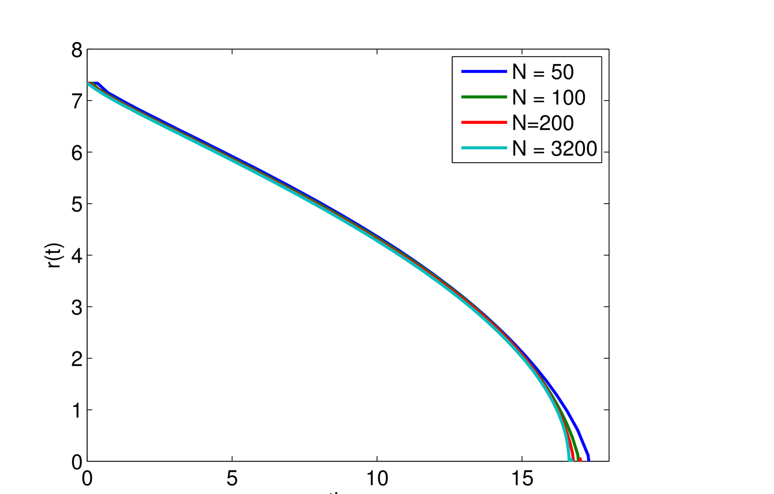


Figure: The computed radius after the laser is turned off. Here, N denotes the number of time steps.

Discretization of the 2D Integral Equation

We are currently looking at this problem in two dimensions, without the assumption of spherical symmetry. Before we can address the complications of a moving heat source, we must first look at a moving geometry. We developed a method to discretize an evolving surface of a general geometry over time and solve the heat equation for either u or $\frac{\partial u_h}{\partial n}$.
The base of the surface is discretized with points

$$\{x_{t,0}, x_{t,1}, ..., x_{t,l-1}, x_{t,l}, ..., x_{t,N-1}, x_{t,N}\}$$

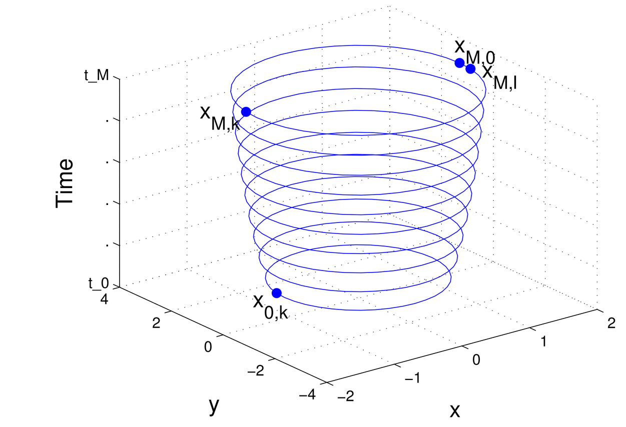
at each time t, where N is the spatial mesh size. To test the accuracy of the method we use a prescribed geometry and omit the initial conditions and source terms. Equation (2) becomes

$$\frac{1}{2}u_h(x_l,t_k) = -\alpha\mathcal{K}_h u_h(x_l,t_k) + \alpha\mathcal{V}_h\left(\frac{\partial u_h}{\partial n} + \frac{u_h v}{\alpha}\right)(x_l,t_k)$$

The discretized single layer operator is now

$$V_h[g(x_k,t_i)] = h_t\sum_{j=0}^{i-1}\sum_{l=1}^{N}G(t_i-t_j, x_k-x_l)w_l(t_j)g_a(x_l,t_j) + \mu_i g(x_k,t_i)$$

and the double layer operator is similarly defined.



The spatial discritization is illustrated above. At each time step i, each point x is determined with information from all other points at t_i and all previous times.

Results and Errors

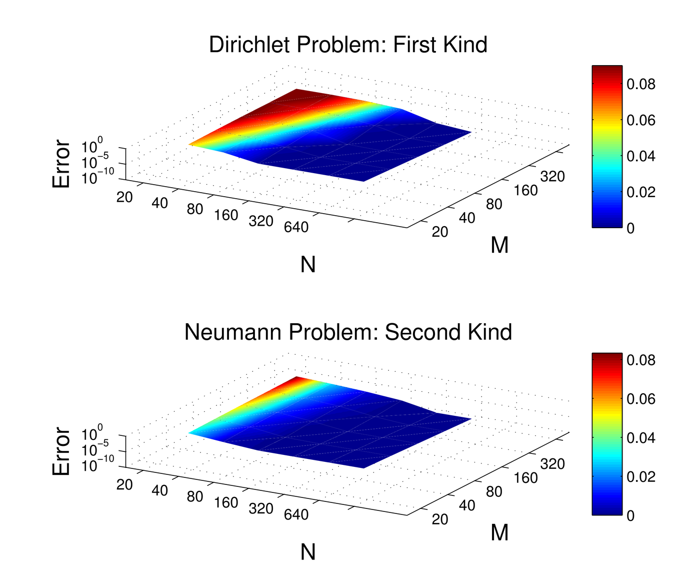


Figure: The plots display errors of the 2D method for various discretizations of time and space. The Neumann problem relates to our Laser problem.

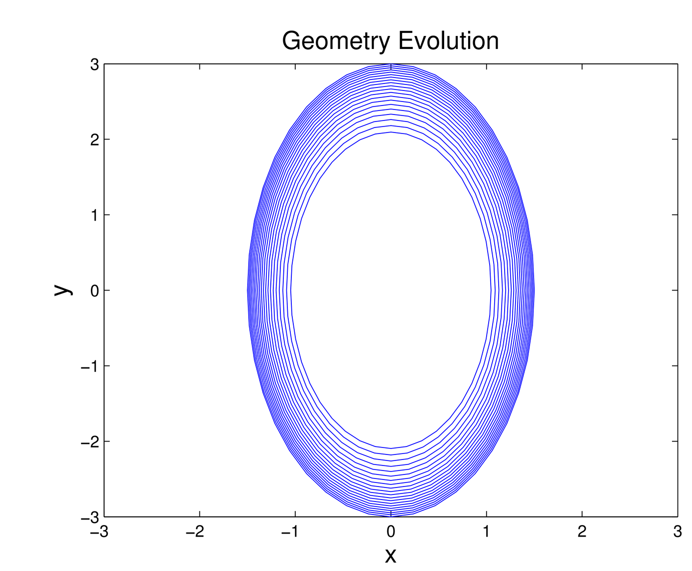


Figure: The above plot is the prescribed geometry of the test problem, evolving in time.

Current Work

We are currently extending this problem to solve for an unknown surface of general geometry in three dimensions with a moving laser heat source. We plan to use the Boundary Element Method on this 3D parabolic problem.

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Southern Methodist University, Dallas, Texas
Mail: ekaram@smu.edu
WWW: http://smu.edu/math