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# Local Defect Correction in Numerical Simulation of Surface Remelting

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**Abstract**

We study the efficient numerical simulation of laser surface remelting, a process to improve the surface quality of steel components. To this end we use adaptive grids, which are well-suited for problems with moving heat sources. To account for the local high activity due to the heat source, we introduce local uniform grids and couple the solutions on the global coarse and local fine grids using local defect correction (LDC). LDC is based on simple data structures and simple discretization stencils on uniform or tensor-product grids.

**Key words:** local defect correction, heat treatment, surface remelting

## 1 Introduction

Partial differential equations (PDEs) with solutions that have highly localized properties appear in many application areas. Such problems require a fine grid only in the region(s) of high activity, whereas elsewhere a coarser grid suffices. We consider the local defect correction (LDC) method, in which the discretization on the composite grid is based on a combination of standard discretizations on uniform grids with different spacings that cover different parts of the domain. The coarse grid must cover the entire domain, and its spacing is chosen in agreement with the relatively smooth behavior of the solution outside the high activity areas. Additionally one or more local fine grids are used that are also uniform, each of which covers only a (small) part of the domain and contains a high activity region. The grid spacings of the local grids are chosen in agreement with the local behavior of the solution. The local problems can be solved in parallel.

The LDC method is an iterative process: the basic global discretization is improved by the local discretizations defined in subdomains. The update of the coarse grid solution is achieved by adding a defect correction term to the right hand side of the coarse grid problem. At each iteration step, the process yields a discrete approximation of the continuous solution on the composite grid. The discrete problem that is actually being solved is an implicit result

of the iterative process. Therefore, the LDC method is both a discretization method and an iterative solution method.

LDC is related to methods like the *multi-level adaptive techniques* (MLAT) [7]; the *fast adaptive composite grid* (FAC) method [13]; *adaptive mesh refinement* (AMR) [6]; *local rectangular refinement* (LRR) [5] and *local uniform grid refinement* (LUGR) [18]. MLAT uses a multigrid-like hierarchy of (local) grids and uses coarser grids as correction grids for accelerating convergence. The finer grids are used as correction grids to improve accuracy, because the fine grid solution is used to approximate the coarse grid discretization error [10]. An important difference of e.g. FAC and LRR with LDC is that these methods propose an explicit discretization scheme for the composite grid, in which special difference stars near the grid interfaces are used. This is a crucial difference with the LDC method, which combines standard discretizations on uniform grids only and does not use an a priori given composite grid discretization. One of the distinctive features of the LDC method is the two-way coupling between grids. It is common in local refinement techniques that the coarse grid solution is used to define boundary conditions for the local fine grid. While this one-way communication suffices for hyperbolic problems [6], it is essential for elliptic problems to transfer information from the fine to the coarse grid, too. As is noted in e.g. [12], the naive approach of only coarse-to-fine communication gives the accuracy of the coarse grid alone.

An analysis of LDC in combination with finite difference discretizations is presented in [8]. The method is combined with finite volume discretizations in [4] and with finite elements in [19]. So-called high order compact difference schemes can be used in an LDC technique too [16]. In [9, 17] LDC is studied with different grid types. The method is successfully applied to a combustion problem in [1]. A generalization to time-dependent problem is presented in [15] for finite difference discretizations and in [14] for finite volume schemes.

This paper is organized as follows. In Section 2 we formulate the mathematical model for surface hardening of steel. In Section 3 we outline the LDC method as used in our simulations; the results of the latter are presented in Section 4. We list conclusions and propose possibilities for future work in Section 5.

## 2 Problem formulation

We study a technique to increase the strength of the surface of mechanical parts such as cutting tools, gears, machine parts etc. There are several ways to alter the properties of a given part. The techniques include laser cladding, laser surface alloying, and laser heat treatment. So-called laser heat treatment covers both hardening and surface remelting. These methods improve mechanical properties through microstructural changes. The typical depth of the hardened layer is 0.1–0.2 mm. In this paper we will model and simulate remelting. Figure 1 sketches the process.

In this paper, we will use the following model for laser surface remelting. We consider a rectangular domain $\Omega = (0, X) \times (0, Y)$ and solve the heat equation in the space-time domain $\Omega \times (0, t_E)$ with end-time $t_E$ viz.

$$\rho c(T) \frac{\partial T}{\partial t} - \operatorname{div}(k(T) \operatorname{grad} T) = -\rho L \frac{da}{dt} \qquad \text{in } \Omega \times (0, t_E), \tag{1}$$

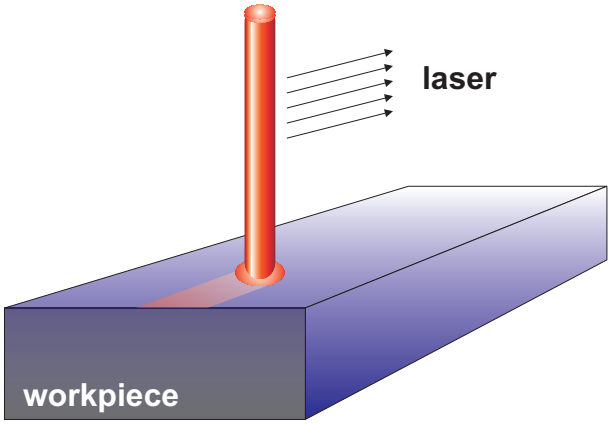


Figure 1: Laser surface remelting.

$$\frac{da}{dt} = \frac{1}{\tau(T)} \left( a_{\text{eq}}(T) - a \right). \tag{2}$$

In (1), $\rho$ is the density, $c$ is the specific heat, $T$ is the temperature, $k$ is the heat conductivity, $L$ is the latent heat of the liquid phase, and $a$ is the liquid phase. The function $a_{\text{eq}}$ in (2) is defined by

$$a_{\text{eq}}(T) = \begin{cases} 0, & \text{for } T < T_s \text{ ($T_s$: only solid in equilibrium),} \\ \text{linear}, & \text{for } T_s < T < T_l, \\ 1, & \text{for } T < T_l \text{ ($T_l$: only liquid in equilibrium).} \end{cases}$$

We model the laser via the boundary condition at the top of the domain, see also Figure 2; the boundary conditions for the system of differential equations (1)–(2) are:

$$-k\frac{\partial T}{\partial n} = \begin{cases} \kappa P F(x - vt), & \text{at the top of the domain,} \\ \mu(T - T_0), & \text{at the bottom,} \\ 0, & \text{at the left and at the right.} \end{cases} \tag{3}$$

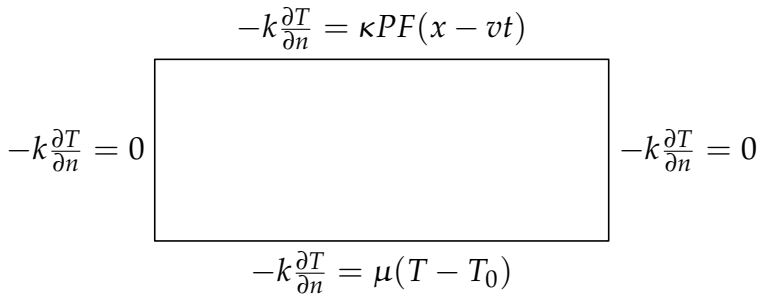


Figure 2: Boundary conditions for the model problem.

Here, $\kappa$ is the absorption coefficient, $P$ is the radiation power, and $F$ is the radiation flux defined by $F(x) = \alpha_1 \exp(-\alpha_2 x^2)$. The velocity $v$ of the laser

beam is assumed to be constant during the simulation. The initial condition for the problem is $T = T_0$ and $a = 0$ at $t = 0$. A typical solution of the initial value problem will have large differences in geometric scales: the temperature is very high near the spot at the surface where the laser beam is located and will drop sharply and be almost constant in the larger part of the computational domain. It is evident, that a computational grid for a problem of this type should reflect the solution behavior, i.e., it should have many grid points with fine spacing near the laser, and it may be (much) coarser elsewhere. In the next section we present a method for solving the problem on a composite grid with local refinement.

# 3 Local defect correction

Adaptive grid methods for time-dependent problems may be divided in so-called dynamic-regridding and static-regridding methods. In the first category nodes are moving in the space-time domain and the discretization of the PDEs is coupled with the motion of the grid. Several strategies have been proposed to govern the movement of the grids; all of them lead to a nonuniform grid where the number of nodes is constant in time. Special care should be taken to maintain a good quality of the grid. Also, due to the nonuniformity of the grid, they may require tedious programming.

The idea in static-regridding techniques is to add grid points when a high activity occurs and to remove them when they are no longer needed. This process is controlled by error estimates or by measuring characteristics of the solution such as its gradients (cf. [1]). In static-regridding methods the number of grid points is not constant in time. By choosing local uniform grids to cover areas of high activity, a composite grid can be formed that is built up of grids with a simple structure.

In this paper we effectively transform the initial value problem (1)–(2) into a series of boundary value problems and apply LDC on each of them. Since we choose the area of refinement per time step, this leads to a static-regridding technique. In [15] Local Uniform Grid Refinement (LUGR) is compared with an LDC technique adapted for time-dependent problems. In both LDC and LUGR, the problem is first solved on a global uniform coarse grid at each time step. The coarse grid solution provides approximate boundary conditions on a local uniform fine grid and the problem is then solved locally. In LUGR, the fine grid values are used to replace the coarse grid values in the region of refinement. This technique relies on the fact that the coarse grid solution provides sufficiently accurate artificial boundary conditions for the local problem. The main advantage is the possibility of working with uniform grids and uniform grid solvers. LDC shares this advantage, but it also uses the fine grid solution to overall improve the coarse grid approximation. The improved coarse grid approximation defines new artificial boundary conditions for a new local problem, which in turn can correct the global solution. LDC is thus an iterative process at each time step. In this way, LDC does not have to rely on the accuracy of the artificial boundary condition of the *first* coarse grid approximation and turns out to be more robust than LUGR. This is illustrated for a model problem in [15]. The approach outlined in [15] is more advanced than the LDC technique used here since the defect includes an estimate of the error due to

time discretization. Here, we use the same time step on coarse and fine grids and we actually solve a boundary value problem at each time step.

We now briefly outline the basic version of the LDC technique that is used at each time step. Consider to that end the elliptic boundary value problem

$$\begin{cases} Lu = f, & \text{in } \Omega, \\ u = g, & \text{on } \partial\Omega. \end{cases} \tag{4}$$

In (4), $L$ is a linear elliptic differential operator, and $f$ and $g$ are the source term and Dirichlet boundary condition, respectively. Other types of boundary conditions can be used as well, but for ease of presentation we formulate the method for (4). To discretize (4), we first choose a global coarse grid (grid spacing $H$), which we denote by $\Omega^H$. An initial approximation $u_0^H$ on $\Omega^H$ can be found by solving the system

$$L^H u_0^H = f^H, \tag{5}$$

which is a discretization of (4). In (5), the right-hand side $f^H$ incorporates the source term $f$ as well as the Dirichlet boundary condition $g$. We assume $L^H$ to be invertible.

Assume that the continuous solution $u$ of (4) has a high activity region in some (small) part of the domain. We select a subdomain $\Omega_l \subset \Omega$ such that the high activity region of $u$ is contained in $\Omega_l$. In $\Omega_l$, we choose a local fine grid (grid spacing $h$), which we denote by $\Omega_l^h$, such that grid points of the global coarse grid that lie in the area of refinement also belong to the local fine grid. In order to formulate a discrete problem on $\Omega_l^h$, we define artificial boundary conditions on $\Gamma$, the interface between $\Omega_l$ and $\Omega \setminus \Omega_l$. We apply an interpolation operator $P^{h,H}$ that maps function values at coarse grid points on the interface to function values at fine grid points on the interface. In the numerical simulations we use linear interpolation. In this way, we find the following approximation $u_{l,i}^h$, iteration $i = 0$, on $\Omega_l^h$:

$$L_l^h u_{l,i}^h = f_l^h - B_{l,\Gamma}^h P^{h,H} \left( u_i^H|_\Gamma \right). \tag{6}$$

In (6), matrix $L_l^h$ (assumed to be invertible) is a discrete approximation to $L$ on the subdomain $\Omega_l$. The first term on the right-hand side incorporates the source term $f$ as well as the Dirichlet boundary condition $g$ on $\partial\Omega_l \setminus \Gamma$ given in (4). In the second term, the operator $B_{l,\Gamma}^h$ represents the dependence of the fine grid points on the coarse grid solution at the artificial boundary $\Gamma$.

We now use the local fine grid solution to update the coarse grid approximation. If we were able to substitute the projection on $\Omega^H$ of the exact solution $u$ of boundary value problem (4) into the coarse grid discretization (5), we would find the local discretization error or *local defect* $d^H$, given by $L^H \left( u|_{\Omega^H} \right) = f^H + d^H$. We could then use $d^H$ within the right-hand side of (5) to find a better approximation on the coarse grid. However, as we do not know $u$, we instead use the fine grid approximation $u_{l,0}^h$ to estimate $d^H$ at the coarse grid points inside the area of refinement $(x, y) \in \Omega_l^H := \Omega^H \cap \Omega_l$. We define $w_0^H$ as the global coarse grid function of best approximations so far:

$$w_0^H(x, y) := \begin{cases} u_{l,0}^h(x, y), & (x, y) \in \Omega_l^H, \\ u_0^H(x, y), & (x, y) \in \Omega^H \setminus \Omega_l^H, \end{cases}$$

and estimate the defect by $d^H = L^H\left(u|_{\Omega^H}\right) - f^H \approx L^H w_0^H - f^H =: d_0^H$. Assuming that the stencil at grid point $(x, y)$ involves (at most) function values at $(x + iH, y + jH)$ with $i, j \in \{-1, 0, 1\}$, $d_0^H$ provides an estimate of the local discretization error of the coarse grid discretization at all points of $\Omega_l^H$. We apply the *coarse grid correction step* to find $u_i^H$, $i = 1$:

$$L^H u_{i+1}^H = \begin{cases} f^H(x,y) + d_i^H(x,y), & (x,y) \in \Omega_l^H, \\ f^H(x,y), & (x,y) \in \Omega^H \setminus \Omega_l^H. \end{cases} \tag{7}$$

Because (7) incorporates estimates of the local discretization error of the coarse grid discretization, $u_1^H$ is assumed to be more accurate than $u_0^H$. Hence it provides a better boundary condition on $\Gamma$, and a better solution on the local fine grid can be found by solving (6) with $i = 1$. This leads to an iterative method: we can solve a new updated coarse grid problem.

To summarize, we have outlined the following iterative method that is to be used at each time step.

**Algorithm 1.**
Two-grid LDC algorithm with area of refinement chosen a priori
*Initialization*

- Solve the basic coarse grid problem (5).
- Solve the local fine grid problem (6) with $i = 0$.

*Iteration*, $i = 1, 2, \ldots$

- Solve the updated coarse grid problem (7).
- Solve the local fine grid problem (6).

Often one or two LDC iterations will suffice to obtain a satisfactory approximation on the composite grid due to the high rate of convergence of the method. Typically, iteration errors are reduced by a factor of 10 to $1,000$ in each iteration step. A detailed analysis of the convergence behavior for diffusion equations is given in [3].

Algorithm 1 is a very basic LDC technique and allows for many generalizations, such as: usage of more than one local fine grid (note that the local problems are independent and can be treated simultaneously); refinement within refinement; usage of different discretization(s) on the local fine grid(s) and the global coarse grid; usage of local grids of a different type (e.g. polar grids instead of Cartesian; cf. [17]); solving a different system of equations on different grids (e.g. analytical expressions or equilibrium assumptions).

# 4 Simulations

To perform numerical simulation of the surface remelting process, we discretize the differential equations (1)–(2) in time using the $\theta$-method. By using this time discretization, we transform the continuous problem into a series of elliptic boundary value problems that we can solve using the LDC technique sketched in Section 3. For the space discretization, we use finite differences.

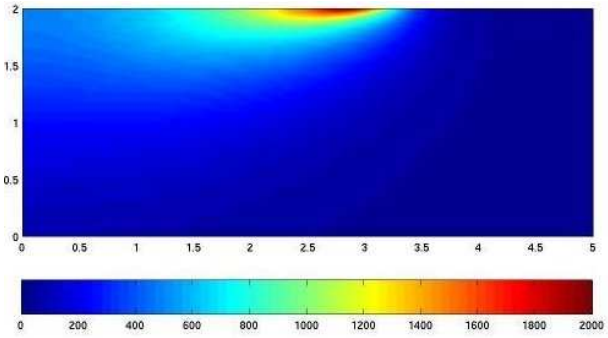


Figure 3: Temperature profile after 60 time steps calculated on a composite grid.

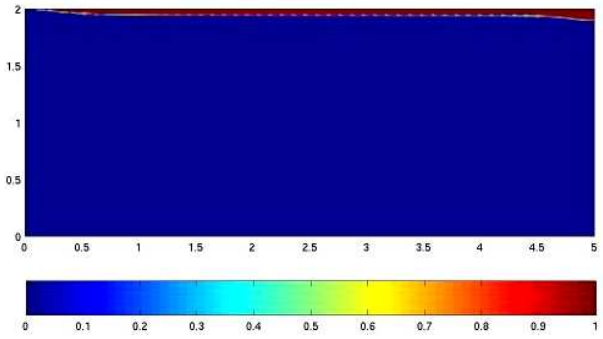


Figure 4: Hardening layer formed during the process.

The area of refinement is automatically chosen based on (smoothed) temperature values; this strategy is detailed in [1] where it is used for a combustion problem. To solve the resulting nonlinear problems on structured grids, we use a damped Newton solver in which the Jacobi matrix is found via numerical differentiation; the resulting linear systems are solved with BiCGSTAB.

We solve the initial value problem on the rectangular domain $\Omega = (0, 5) \times (0, 2)$. The global coarse grid is a structured grid with 50 grid points chosen equidistantly in horizontal, 40 grid points chosen with geometrical refinement in vertical direction. The grid sizes in vertical direction are smallest near the surface; from bottom to top they decrease with a factor of 0.975. We use one level of refinement and the grid sizes for the local grid are half those of the global. On both the coarse and the fine grids we employ a time step 0.1. We present a plot of the temperature field after 60 time steps, computed on the composite grid, in Figure 3; the hardening layer formed is given in Figure 4

When one observes the temperature field during the simulation, one notices that it takes some time for the workpiece to reach maximum surface temperature. Also, since the temperature drops due to self-cooling of the workpiece, it peaks near the right side of the domain, because it is more difficult to loose heat there. This is reflected in the resulting hardening layer (see Figure 4): it is shallow at the left, deeper at the right side of the domain. Naturally this is

undesirable in practice, where one wants the layer to be equally deep along the piece. This may be achieved by increasing the laser power at the left end of the part and decreasing it at the right. Simulations for more complicated geometries as well as involving PID control on the laser power to a achieve a uniform thickness of the layer can be found in [2, 11].

# 5 Conclusions and future work

We have successfully simulated the remelting process on locally refined grid using LDC. In this technique, PDEs need to be discretized on structured grids only. The resulting composite grid has far less grid points than a structured grid with comparable resolution. In future we would like to explore the following extensions of the current work. First we would like to perform refinement in time too, i.e., use smaller time steps on the fine grids, cf. [15]. It would be interesting to model the flow in the melted region—it may be necessary to perform 3D simulations to do so, as the convection takes place in a plane perpendicular to the plane in which the laser moves, cf. Figure 5.

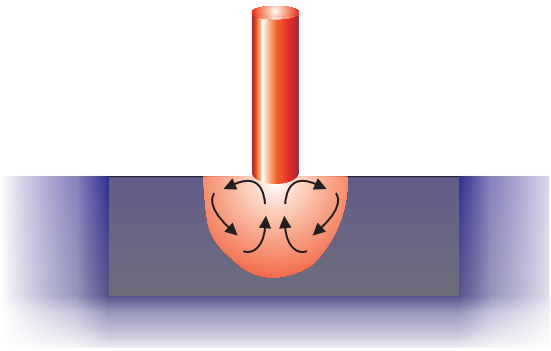

Figure 5: Convection in the melted region.

In the LDC method it is possible to use a different model in the local area than in the rest of the domain. This might be useful both for modelling the convection as well as modelling more complicated processes.

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