



Lasers in Manufacturing Conference 2023

Scan path optimization for laser additive manufacturing with quantum computing

Thomas Bussek^{a,*}, Annika Völl^a, Jochen Stollenwerk^{a,b}, Andrew Mitri^a, Anna Stollenwerk^a, Carlo Holly^{a,b}

^aRWTH Aachen University TOS - Chair for Technology of Optical Systems TOS, Steinbachstraße 15, 52074 Aachen, Germany ^bFraunhofer-Institute for Laser Technology ILT, Steinbachstraße 15, 52074 Aachen, Germany

Abstract

In laser additive manufacturing processes such as laser-based powder bed fusion (LPBF), standardized scan strategies are used in the layer-by-layer build-up of the workpieces. This non-optimized procedure results in heat accumulation and therefore in thermal stress as well as in large laser off times for multi-scanner systems. Optimizing the scan path for each layer is a computational expensive task that is difficult to solve on conventional computers within reasonable time. The recent rise of quantum computers promises to solve optimization problems in highly reduced computational time with increased solution quality in the future. To exploit these advantages for LPBF, an adaptation of the multi-vehicle routing problem is presented. This formulation allows for reducing the overall scan time while accounting for the interaction of multi-scanner systems, reducing heat accumulation, avoiding laser-plume interaction and accounting for the direction of the shield gas flow.

 $Keywords: LPBF; scan path \ optimization; \ multi-scanner \ systems; \ quantum \ computing; \ QUBO \ formulation$

1. Introduction

The laser-based powder bed fusion (LPBF) is an additive manufacturing technique that plays a crucial role in industrial additive manufacturing of metallic components. It enables the production of parts with diverse geometric designs, by building almost arbitrary geometries by layer-by-layer selective melting of metal powder and is especially promising for building prototypes and parts with small lot size within a short time scale. Within

* Corresponding author. Tel.: +49 241 89 06 81 96 E-mail address: thomas.bussek@tos.rwth-aachen.de. those build jobs, the scan path of the laser must be defined for each layer of the part to be manufactured, significantly influencing the heat input and any heat accumulation that may occur. The interaction between layers further complicates the process, as previously built regions are preheated and locally influence heat conduction and the melting process. This can lead to thermally induced stress, causing issues like local component distortion, cracks, and deviations in the final workpiece's dimensional and shape accuracy. The use of multi-scanner systems that promise to increase the relatively low productivity of current LPBF machines adds an additional aspect to finding suitable scan paths since an interaction of the individual lasers must be avoided. (Chowdhury et al. 2022)

Up to now, currently available build processors do not adequately account for these different requirements. The generation of the scan vectors is done primarily by using predefined scan strategies e.g., avoiding laser-laser interaction in a multi-scanner system by adding waiting times to the lasers or simply subdividing a 2D layer geometry into several slices that are each processed sequentially by single laser spots. Those predefined, non-optimized scan strategies are not capable of creating scan paths that are individually adapted to the specific manufacturing task associated with every layer of the build process. Consequently, users with expert knowledge must manually adjust the scan strategy which is a difficult and time-consuming task.

There are some approaches that adapt a predefined scan path according to the heat evolution within the workpiece to achieve a favorable temperature distribution during the build process (Boissier et al. 2020, 2022; Foteinopoulos et al. 2020). Nevertheless, those optimizations do not account for other aspects despite the heat evolution such as the difficulties of multi-scanner systems or the interaction with the shield gas. Furthermore, the computation time for a system of a few coupled layers within the build process is in the order of hours and therefore counteracting one of the main advantages of the LPBF of fast production of individual parts.

The recent rise of different quantum computer architectures (gate-based quantum computers as well as quantum annealers) promises to allow for solving certain optimization problems within shorter computation time while increasing the quality of the solution. This is done by exploiting different quantum mechanical properties such as the quantum tunnel effect, the superposition of quantum states and the adiabatic theorem of quantum mechanics. Those effects – in theory – allow for determining the global minimum of certain optimization problems. This may allow for individually optimizing the LPBF scan paths for each layer of a certain build job just-in-time without large computation times. Nevertheless, to do so, those problems have to be formulated in a certain way and it is a current research topic which kind of optimization problems are especially suitable to be solved on quantum computing hardware. (Symons et al. 2023)

Within this work two problem formulations that allow for optimizing the scan paths of laser manufacturing processes with different optimization criteria and constraints are derived and verified. In Section 2 those problem formulations are derived and in Section 3 the numerical setups to investigate the functionality of the derived problem formulations are presented. Section 4 discusses the obtained optimization results and compares them to predefined benchmark strategies while Section 5 concludes with a summary and an outlook for further optimization criteria that can be considered during the path optimization.

2. Problem formulation

To solve an optimization problem on quantum computing hardware it must be formulated as a Quadratic Unconstrained Binary Optimization (QUBO) problem of the form

$$\min_{\mathbf{x}} E(\mathbf{x}) = \min_{\mathbf{x}} \left(\sum_{n} Q_{n,n} x_n + \sum_{n \le m} Q_{n,m} x_n x_m \right) \tag{1}$$

with E the energy of the solution that shall be minimized, Q the matrix describing the biases ($Q_{n,n}$, diagonal entries) and coupler weights ($Q_{n,m}$, off-diagonal entries) and x_n and x_m the value of the n-th and m-th Qubit. (Symons et al. 2023)

Within this chapter the formulation of two optimization criteria for laser manufacturing processes as well as the required constraints are discussed: reduction of heat gradient for discretized paths and reduction of heat gradient and process time

2.1. Reduction of heat gradient for discretized paths

One of the main drawbacks of the use of non-optimized standard scan strategies is the potential of thermal build-up within the workpiece resulting in effects such as thermal cracks or distortion. In the following a QUBO formulation is presented that allows for optimizing the heat gradient within a single layer of the workpiece and an arbitrary number of lasers L working simultaneously.

Regardless of the concrete optimization criteria, to formulate a QUBO formulation the inherent continuous path optimization problem must be discretized both spatially and temporal. This is done similarly to several approaches to the traveling salesperson problem (Lucas 2014) or the multi-vehicle routing problem (Xu et al. 2022):

For the spatial discretization, the region of the layer of the workpiece is discretized using an equidistant Cartesian coordinate grid where each cell which shall be processed within the current layer is assigned to one of N grid points (cf. Figure 1). The time scale is also discretized by T equidistantly chosen time steps (cf. Figure 1). Then, each qubit x_{itl} is assigned the following meaning: If qubit x_{itl} takes the value 1 (0), then grid point i is (not) visited by laser l at time t.

From this, the necessary number of qubits $N_{\rm qubits}$ can be calculated to $N_{\rm qubits} = N \cdot T \cdot L$, where the number of time steps T must be at least equal to the number of grid points N to be visited divided by the number of lasers L used so that each point can be visited once by one of the different lasers. A lower bound on the problem size is thus obtained as $N_{\rm qubits} \geq N^2$.

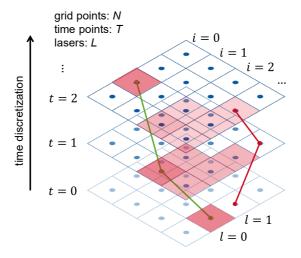


Fig. 1. Discretization of path optimization problem in space and time for two laser beams.

To enable a reduction of the heat gradient in the workpiece in the QUBO formulation, the heat input of the corresponding laser beams is simulated. It is assumed that the visit of a location i at time t yields a temperature increase ΔT which occurs after a laser pulse modelled by a point heat source. Using the heat kernel of a 2-dimensional Euclidian space (Alexander Grigor'yan 1999), the temperature increase is given by the equation

$$\Delta T(\Delta t, \Delta s, l) = \begin{cases} q_{0,l} \cdot \frac{1}{4\pi\sigma\Delta t} \exp\left(-\frac{\Delta s^2}{4\sigma\Delta t}\right) & \text{for } \Delta t \ge 0\\ 0, & \text{otherwise} \end{cases}$$
 (2)

where $q_{0,l}$ is a factor accounting for the heat source applied by laser l and σ is the thermal diffusivity of the material. Δt denotes the time difference t-t' between the time t' at which there was a heat input at a certain point and the current time point t under consideration. Δs describes the spatial distance $|s_i-s_j|$ between the node j of the heat source and the node i under consideration with coordinates s_i and s_j , respectively. To calculate the temperature of node i at time t, all previous temperature increases at all nodes by all lasers multiplied with the qubit $x_{jt,l}$ are summed up so that only the heat inputs of previously visited nodes are considered. The temperature is given by

$$T_{it} = \sum_{l=0}^{L-1} \sum_{t'=0}^{t} \sum_{j=0}^{N-1} \Delta T(t-t', |\mathbf{s}_i - \mathbf{s}_j|, l) \, x_{jt'l} \,. \tag{3}$$

The QUBO formulation for the reduction of the heat gradient in the workpiece at all times t consists of a term to be optimized and several hard constraints. The term to be optimized is given by

$$\Lambda_0 \sum_{i \in \mathcal{N}_t} \left(\frac{T_{it} - T_{jt}}{|\mathbf{s}_i - \mathbf{s}_j|} \right)^2 \, \forall \, t, i. \tag{4}$$

Here Λ_0 is the weight factor of the heat gradient criterium and \mathcal{N}_i denotes the neighbors of point i, so that at all times t and for all points i the sum of the squared deviations of the temperature at the point i to the temperatures of the immediate neighbors \mathcal{N}_i divided by the corresponding distance should be minimized. The necessary constraints multiplied by their weight factors λ are:

1. Each node must be visited exactly once:

Since the nodes correspond to the locations that shall be processed, it must be ensured that each node is visited and therefore molten. At the same time, nodes should not be visited more than once since this would yield an unnecessary energy input. Therefore, the sum of all x_{itl} over all lasers and all time points should be exactly 1 for each node i which is ensured by the weight factor λ_0

$$\lambda_0 \left(\left(\sum_{t=0}^{T-1} \sum_{l=0}^{L-1} x_{itl} \right) - 1 \right)^2 \, \forall \, i. \tag{5}$$

2. A laser can only be in one place at a time:

A laser cannot be at more than one location at a time. Therefore, it should be energetical favorable when a laser is visiting up to one node at a certain time. There should be no difference between both cases when a laser is visiting one point or no point at all at a certain time. This can be ensured by the following formulation with the weight factor λ_1

$$\lambda_1 \sum_{i=0}^{N-1} \sum_{j=i+1}^{N-1} x_{jtl} \, x_{itl} \, \forall \, t, l, \tag{6}$$

that adds a penalty for each additional point visited by the same laser at the same time that exceeds the limit of 1.

The total QUBO formulation is given by adding the optimization criteria and both constraints with their respective weights Λ_0 , λ_0 and λ_1 while also substituting the temperature variable in Equation 4 with the expression shown in Equation 3 resulting in

$$\min_{\mathbf{x}} \left(\Lambda_{0} \sum_{t=0}^{T-1} \sum_{i=0}^{N-1} \sum_{j \in \mathcal{N}_{i}} \left(\sum_{l=0}^{L-1} \sum_{t'=0}^{t} \sum_{k=0}^{N-1} \frac{1}{|\mathbf{s}_{i} - \mathbf{s}_{j}|} \left(\Delta T(t - t', |\mathbf{s}_{i} - \mathbf{s}_{k}|, l) - \Delta T(t - t', |\mathbf{s}_{j} - \mathbf{s}_{k}|, l) \right) \right) + \lambda_{0} \sum_{i=0}^{N-1} \left(\left(\sum_{t=0}^{T-1} \sum_{l=0}^{L-1} x_{itl} \right) - 1 \right)^{2} + \lambda_{1} \sum_{l=0}^{L-1} \sum_{t=0}^{T-1} \sum_{j=i+1}^{N-1} x_{jtl} x_{itl} \right). \tag{7}$$

Equation 7 contains only linear and quadratic terms with respect to the binary qubit variables x, so that this equation is of the form of a QUBO problem as shown in Equation 1.

2.2. Process time & heat gradient minimization for continuous paths

The formulation presented above allows the optimization of the order in which the grid nodes are traversed but does not produce a continuous path as required in the LPBF framework. Furthermore, an optimization of the total processing time per layer which is of special interest in the case of multi-scanner systems is not possible. To ensure this, the problem formulation as well as the assignment of the qubits must be extended.

In addition to the qubit assignment discussed in Section 2.1 additional qubits have to be used to monitor the total processing time for an arbitrary number of lasers. For this purpose, each possible time t is assigned a qubit x_t , which should be 1 (0) if the respective time is (not) the last time a point of the current layer is visited by any laser. The total solution vector \boldsymbol{x} is thus given by $\boldsymbol{x}=(x_{itl},x_t)$ where the first part x_{itl} describes the path discretization discussed in Section 2.1 and x_t the time discretization discussed in this chapter. This adds T additional qubits to the problem size discussed in Section 2.1 so that the total problem size is described by $N_{\text{qubits}} = N \cdot T \cdot L + T$.

The additional qubit x_t is used to minimize the total processing time by minimizing

$$\Lambda_1 \sum_{t=0}^{T-1} x_t t \tag{8}$$

with the weight factor Λ_1 .

It is important for this modeling to ensure that the qubits x_t correctly represent the end time of the respective process considering all laser sources. This is done by using several constraints:

1. There must be exactly one $x_t = 1$

For the optimization, exactly one time step must be identified as the end point of the scan path. This can be ensured by minimizing

$$\lambda_2 \left(\sum_{t=0}^{T-1} x_t - 1 \right)^2 \tag{9}$$

which means that the sum of all x_t has to be exactly 1. A violation of this constraint would be penalized at least with the weight factor λ_2 .

2. No point is visited after the last time point t:

If $x_t=1$ and the time point is thus identified as the last time step t, it must be ensured that none of the lasers visit any of the nodes at a later time. This is done by applying a penalty λ_3 for any node that is visited by any laser at time t' after the identified last time step t which can be expressed by

$$\lambda_3 x_t \sum_{i=0}^{N-1} \sum_{l=0}^{L-1} \sum_{t'=t+1}^{T-1} x_{it'l} \ \forall \ t. \tag{10}$$

Another constraint that is not related to the definition of time qubits x_t has to be added to ensure that the scan path optimization respects the maximal scanning velocity of the laser:

3. The scanning speed v_l of the laser is limited:

In the context of path planning in LPBF, the scanning speeds v_l of the lasers are limited meaning that when a laser visits a certain point i the same laser cannot visit another point j until the time $d_{ij} = |s_i - s_j|/v_l$ has passed. To this extend for each point i that is visited by laser l at a certain time t a penalty λ_4 is applied for each point that is visited by the same laser without respecting the time this laser would have required to move from spot i to j (meaning it is visited at least one time step dt before the waiting time d_{ij} have passed). This penalty is equal to the time benefit that the system would get by ignoring the waiting time, resulting in

$$\lambda_4 x_{itl} \sum_{j=0}^{N-1} \sum_{t'=t}^{t+d_{ij}-dt} \left(d_{ij} - (t'-t) \right) x_{jt'l} \ \forall l, t, i.$$
 (11)

Adding the optimization criterium and all three constraints discussed in this section to the QUBO formulation of Section 2.1 shown in Equation 7 yield the total problem formulation required for the simultaneous optimization of heat gradient and total processing time while considering maximal scanning speeds of the lasers as

$$\min_{x} \left(\Lambda_{0} \sum_{t=0}^{T-1} \sum_{i=0}^{N-1} \sum_{j \in \mathcal{N}_{i}} \frac{1}{|s_{i} - s_{j}|} \left(\sum_{l=0}^{L-1} \sum_{t'=0}^{t} \sum_{k=0}^{N-1} \left(\Delta T(t - t', |s_{i} - s_{k}|, l) - \Delta T(t - t', |s_{j} - s_{k}|, l) \right) \right) + \Lambda_{1} \sum_{l=0}^{T-1} x_{t} t + \lambda_{0} \sum_{i=0}^{N-1} \left(\left(\sum_{t=0}^{T-1} \sum_{l=0}^{L-1} x_{itl} \right) - 1 \right)^{2} + \lambda_{1} \sum_{l=0}^{L-1} \sum_{t=0}^{T-1} \sum_{i=0}^{N-1} \sum_{j=i+1}^{N-1} x_{jtl} x_{itl} + \lambda_{2} \left(\sum_{t=0}^{T-1} x_{t} - 1 \right)^{2} + \lambda_{3} \sum_{t=0}^{T-1} x_{t} \sum_{l=0}^{N-1} \sum_{t=0}^{L-1} \sum_{t'=t+1}^{T-1} x_{it'l} + \lambda_{4} \sum_{l=0}^{L-1} \sum_{t=0}^{T-1} \sum_{t=0}^{N-1} \sum_{i=0}^{N-1} x_{itl} \sum_{j} \sum_{t'=t}^{N-1} \left(d_{ij} - (t' - t) \right) x_{jt'l} \right).$$
(12)

This formulation consists of only linear and quadratic terms of the solution vector $\mathbf{x} = (x_{itl}, x_t)$, meaning it is of the form of a QUBO formulation.

3. Numerical setup

Two benchmark problems are used to verify the suitability of both presented QUBO problems for the path optimization of laser manufacturing processes such as LPBF. The corresponding problem sizes are chosen relatively small to account for the current limitations of classical and quantum computers to solve discrete optimization problems while in theory the presented problem formulations can be scaled to larger problem sizes without restrictions.

For the verification of the first QUBO formulation (cf. Section 2.1) a single laser is considered that shall scan a quadratic 3x3 grid with the number of time steps T equal to the number of grid points N=9. For the second QUBO formulation (cf. Section 2.2) which optimizes the heat gradient and the total processing time while considering the maximal scan speed of the lasers a system of two lasers is investigated. The corresponding scan area is defined by a quadratic 4x4 grid with the scanning speed of both lasers equal to one element size per time step. The number of time steps T is set to T=N/L+1 and thus allows for a potential violation of the time minimization since finishing the process in time step 9 counteracts the energy minimization given by Equation 8. Those and some other numerical parameters such as the heat amplitude $q_{0,l}$, the thermal diffusivity σ and the different weight factors Λ and λ are listed in Table 1 in Appendix A.

For the optimization of both presented QUBO formulations the Hybrid quantum-classical Solver Service (HSS) provided by D-Wave is used (D-Wave Inc. 2020). The only hyperparameter that can be adjusted for this solver is the time limit of the total computing time $t_{\rm limit}$. Within this solver the problem is internally subdivided into parts that are solved on a D-Wave Advantage quantum annealer and parts that are solved on classical high-performance computers. The obtained solutions are compared to predefined, problem specific scan strategies that are commonly used within laser materials processing (cf. Figure 2).

4. Results

For both QUBO formulations a solution is found that has a smaller energy value than the corresponding benchmark scan strategy.

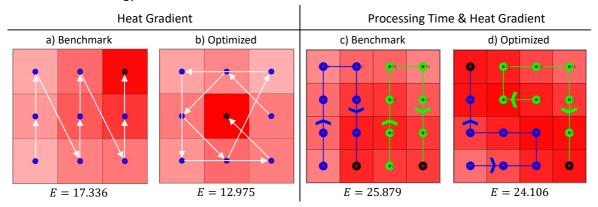


Fig. 2. Benchmark scan strategies and optimized paths for the heat gradient formulation (a, b) and the formulation for the minimization of processing time and heat gradient (c, d). The shown temperature distributions (visualized in red) correspond to the last time step.

The solution found for the heat gradient optimization (cf. Figure 2 b) shows a systematic behavior of first scanning the points in the middle of the outer frame counterclockwise before jumping to one of the most distant corners and continuing with the counterclockwise iteration of the corners of the simulation domain. The last point visited is the center of the simulation domain. This results in a smaller energy value compared to the benchmark scan strategy (cf. Figure 2 a), which is defined by the unidirectional scanning from left to right. The QUBO formulation does not consider a certain scanning speed of the laser and therefore allows scanner jumps.

The scan path optimization considering the processing time and heat gradient (cf. Figure 2 d) shows a different behavior which is mainly reasoned in the additional constraint of a maximal scan speed which yields it to be energetically favorable to always visit one of the nearest neighbors of the point visited in the previous time step. The benchmark scan strategy (cf. Figure 2 c) is defined by subdividing the scan area in two 4x2 grids and scanning those subdomains with two meander-like scan paths along the long axis of the subdomains (the unidirectional scanning used for the previous benchmark is not suitable for this problem since it contains scanner jumps). In contrast to the benchmark scan path, the optimized scan paths end in opposite corners of the simulation domain while also yielding an almost rotationally symmetrical scan path. To avoid heat accumulation in the middle of the scan paths, the green laser starts near the middle of the simulation domain and moves towards a corner while the blue laser starts in a corner and moves towards the middle of the layer. This ensures that both laser spots are at least two element sizes apart from each other for every time step and therefore avoids heat accumulation due to simultaneous heating of scanning neighbored points. Furthermore, the last time step is ignored for the optimized scan paths resulting in the lowest possible total processing time as well.

5. Conclusion & outlook

It is shown that the continuous path optimization problem can be described as a discrete QUBO problem that can be solved on quantum computing hardware. For both benchmark problems the hybrid quantum-

classical HSS finds scan paths with smaller energy values compared to the default scan strategies. Nevertheless, the problem sizes for which suitable scan paths that outperform the standardized scan strategies could be found are well below the size of state-of-the-art LPBF build jobs which consists of up to thousands of scan vectors per layer. This drawback could be addressed in the future by the ongoing development and performance increase of quantum computing hardware as well as subdividing the overall problem in spatial and temporal less dependent subproblems.

In the next steps, the presented QUBO formulations will be extended to account for more aspects that have to be considered within the framework of laser-based additive manufacturing. Those extensions can include the consideration of the shield gas flow or avoiding laser-plume interaction.

Acknowledgements

Thomas Bussek is part of the Max Planck School of Photonics supported by the German Federal Ministry of Education and Research (BMBF), the Max Planck Society and the Fraunhofer Society.

This research is funded by the Digital Photonic Production DPP Research Campus as part of the "Research Campus Public-Private Partnership for Innovation" research funding initiative of the German Federal Ministry of Education and Research (BMBF). As part of the German government's high-tech strategy, the BMBF is using this initiative to promote strategic and long-term cooperation between science and industry "under one roof" (Funding number: 13N15423).

The authors gratefully acknowledge the Jülich Supercomputing Centre (https://www.fzjuelich.de/ias/jsc) for funding this project by providing computing time through the Jülich UNified Infrastructure for Quantum computing (JUNIQ).

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Appendix A. Numerical parameter for QUBO verification

Table 1: Numerical parameters used for the investigation of the presented QUBO formulations.

	Heat Gradient	Processing Time & Heat Gradient
Spatial grid <i>N</i>	3 x 3 = 9	4 x 4 = 16
Total size of spatial grid	12 x 12 (a.u.)	12 x 12 (a.u.)
Number of time steps T	9	9
Time step dt	1	1
Number of lasers L	1	2
Scanning speed v_l	-	3 (a.u.) / time step
Heat source amplitude $q_{0,l}$	3000π	6000π
Thermal diffusivity σ	2.5	5
Weight factor Λ_0	$1.37 \cdot 10^{-5}$	$4.34 \cdot 10^{-6}$
Weight factor Λ_1	-	2
Weight factor λ_0	1	9
Weight factor λ_1	1	9
Weight factor λ_2	-	20
Weight factor λ_3	-	20
Weight factor λ_4	-	2
Time limit $t_{ m limit}$	3 s	40 s