Reduced order modelling for wafer heating with the Method of Freezing

E.J.I. Hoeijmakers, H. Bansal, T.M. van Opstal, and P.A. Bobbert

Abstract Accurate and real-time temperature control for wafer heating is one of the main challenges in semiconductor manufacturing processes. With reduced-order modelling (ROM), the computational complexity of the mathematical model can be decreased in order to solve the model quickly at a low computational cost, while still maintaining the computational accuracy. However, the translating temperature profile, due to moving sources, render the standard reduction approaches to be ineffective. We propose to invoke the concept of the "Method of Freezing" and use it in conjunction with the standard ROM approaches to obtain an effective low-complexity model. We finally assess the effectiveness of the proposed approach on the 2-dimensional heat equation with moving heat loads. Numerical results clearly show the potential of the proposed approach over the standard one in terms of computational accuracy and the dimension of the resulting reduced-order model.

1 Introduction

In photolithography, feature sizes are decreasing in effort for manufacturers to keep up with Moore's law. This has prompted the use of higher energy lasers, leading to more wafer heating and, therefore, more thermal expansion. Accurate and real-time prediction of the temperature distribution around the moving laser beam is a necessity as this facilitates to correct the laser beam trajectory and to create the desired

E.J.I. Hoeijmakers, P.A. Bobbert
Department of Applied Physics, Technical University of Eindhoven, e-mail: eviehoeijmakers@outlook.com, p.a.bobbert@tue.nl

H. Bansal
Department of Mathematics and Computer Science, Technical University of Eindhoven, e-mail: h.bansal@tue.nl

T.M. van Opstal
Sioux Mathware, e-mail: timo.van.opstal@sioux.eu

temperature at every place on the wafer [1]. However, this remains a challenge since standard numerical methods take a lot of computational time, and the increased resolution requirements due to the reduced feature sizes slow the model down.

Reduced-order modelling (ROM) reduces the model complexity and aids in real-time prediction of the quantity of interest. Translating temperature profiles, due to moving sources, render the standard ROM approaches ineffective [2]. Hence, we propose to invoke the "Method of Freezing" along with standard ROM approaches in order to obtain an effective low-complexity model computable in real-time.

The concept of the "Method of Freezing" has been applied on parabolic and hyperbolic problems in the past [3]. However, [4] is the only work which so far exploits the "Method of Freezing" for non-linear reduced basis approximations. This work considers a numerical experiment, which falls in the realm of hyperbolic problems, namely the parameterized Burgers-type problem in 2D (without source terms).

The main contribution of this work is to use the "Method of Freezing" in conjunction with standard ROM approaches to facilitate accurate and real-time prediction of the temperature. The "Method of Freezing" relies on an ansatz that decomposes the original dynamics into shape and travelling dynamics. The resulting shape dynamics is amenable for an efficient basis generation. We then use these generated bases to apply Proper Orthogonal Decomposition (POD) on the shape dynamics and, ultimately, obtain a reduced-order model. We finally assess the performance of the combined approach of the "Method of Freezing" and reduced basis approximations on a test-case of practical relevance, and discuss the computational merits of the proposed ROM approach over the standard one.

The paper is organized as follows. In Section 2.1, we introduce the 2-dimensional heat equation and discuss the numerical method for its discretization. We invoke the idea of the "Method of Freezing", reformulate the model problem and present the corresponding discretized representation in Section 2.2. A Galerkin-type projection-based ROM is performed on a semi-discrete model representation in Section 3. A numerical case-study is presented in Section 4 to showcase the effectiveness of the proposed approach. Finally, Section 5 ends with conclusions and future works.

2 Theory

In this section, we first introduce the model and the numerical method employed for the spatio-temporal discretization. We then introduce the idea of the "Method of Freezing" and present a model reformulation and its discrete representation.

2.1 Model introduction

To model the wafer heating, we use the well-known heat equation in two-dimensions. As the height of the wafer is one order of magnitude less than the length and the width of the wafer, the temperature gradient along the thickness of the wafer is very small. This makes the 2-dimensional heat equation a good approximation of the real situation. The 2-dimensional heat equation is governed by:

$$\frac{\partial u}{\partial t} - \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = Q(x,y,t), \quad (x,y) \in \Omega, \quad t \in [0,t_f], \tag{1}$$

$$u(x,y,t=0) = u_0, \tag{2}$$

$$n_x \frac{\partial u}{\partial x} + n_y \frac{\partial u}{\partial y} = 0 \text{ on } \partial\Omega, \tag{3}$$

where u represents the wafer temperature, u_0 stands for a constant initial temperature, Ω stands for the spatial domain of interest, $n = (n_x, n_y)$ denotes the normal to the boundary $\partial\Omega$, t_f indicates the final simulation time, and α is the thermal diffusivity constant. The thermal diffusivity constant can be expressed with the thermal conductivity k, the specific heat capacity C_p and the density ρ of the wafer in the form $\alpha = \frac{k}{\rho C_p}$. Here, a moving heat load $Q(x,y,t)$ is assumed to be of the non-affine form:

$$Q(x,y,t) = e^{-\frac{1}{2}\left(\frac{x-c_x t}{\sigma_x}\right)^2 - \frac{1}{2}\left(\frac{y-c_y t}{\sigma_y}\right)^2}, \tag{4}$$

where c_x and c_y are the speeds of the heat load in the $x-$ and $y-$direction, respectively and, the variance of the Gaussian distribution along the $x-$ and the $y-$direction is given by σ_x^2 and σ_y^2, respectively.

After multiplying (1) by a smooth test-function w, integrating over the domain and invoking Green's theorem, a weak formulation of the 2-dimensional heat equation can be constructed, resulting in:

$$\int_\Omega \frac{\partial u}{\partial t} w dA + \alpha \left(\int_\Omega \frac{\partial u}{\partial x}\frac{\partial w}{\partial x} dA + \int_\Omega \frac{\partial u}{\partial y}\frac{\partial w}{\partial y} dA \right) - \alpha \int_{\partial\Omega} \frac{\partial u}{\partial n} w ds = \int_\Omega Q w dA, \tag{5}$$

where $dA = dxdy$ and ds is a boundary surface element. Using (3), the fourth term on the left-hand-side of (5) cancels out [5].

In order to solve (5) numerically, discretization in space and time is necessary. We discretize the domain such that the structured mesh aligns with the orientation of the features which need to be printed. We then employ a finite element method to discretize in space. We approximate the solution with a summation over B-spline basis-functions ϕ_i, $u = \sum_{i=1}^N u_i(t)\phi_i(x)$ [6]. Here, N is the number of finite elements used in the domain discretization and u_i is the weight of every basis function. To discretize in time, the first-order backwards Euler method is applied as is also used in Chapter 8 of [5]. Discretizing in both space and time results in the following equation:

$$Mu^{k+1} + \Delta t \alpha D u^{k+1} - \Delta t \tilde{Q}^{k+1} = Mu^k, \tag{6}$$

where M is the mass matrix, D is the diffusion matrix, $\tilde{Q}$ is the source vector representative of the moving heat loads and Δt indicates the time-step. Equation (6) needs to be solved for every time instant $k+1$.

The numerical solution will be at most first-order accurate if the first-order backwards Euler method is applied in conjunction with the higher-order spatial discretization. However, in this paper, we are not concerned about the order of accuracy of the numerical solution, but intend to show the potential of the "Method of Freezing". To this end, the first-order temporal discretization is representative enough for quantifying the numerical performance, while being simple to implement. The implementation of a higher-order temporal discretization is deferred to future works.

We will now discuss a change of coordinates or so-called "Method of Freezing" that we propose to use in conjunction with standard ROM techniques to obtain an effective complexity reduction for problems with moving heat load(s).

2.2 Model reformulation: Method of Freezing

The "Method of Freezing" maps all symmetry-related solutions to a single class of solutions. This method separates the dynamics in the group direction from the dynamics in the remaining directions of the phase space. The general idea of this method is to perform a coordinate transformation of the form:

$$u(x,y,t) = v(x - c_x t, y - c_y t, t) = v(\xi_x, \xi_y, t), \tag{7}$$

Incorporating (7) in (1) results in the following modified heat equation:

$$\frac{\partial v}{\partial t} - c_x \frac{\partial v}{\partial \xi_x} - c_y \frac{\partial v}{\partial \xi_y} - \alpha \left(\frac{\partial^2 v}{\partial \xi_x^2} + \frac{\partial^2 v}{\partial \xi_y^2} \right) = Q(\xi_x, \xi_y). \tag{8}$$

This modified heat equation is quite similar to the original equation given in (1), except the additional second and third term on the left-hand side which represent an extra convection term. The weak formulation of (8) under zero Neumann boundary conditions is given by:

$$\begin{aligned} &\int_\Sigma \frac{\partial v}{\partial t} w d\xi_x d\xi_y - c_x \int_\Sigma \frac{\partial v}{\partial \xi_x} w d\xi_x d\xi_y - c_y \int_\Sigma \frac{\partial v}{\partial \xi_y} w d\xi_x d\xi_y \\ &- \alpha \left(\int_\Sigma \frac{\partial v}{\partial \xi_x} \frac{\partial w}{\partial \xi_x} d\xi_x d\xi_y + \int_\Sigma \frac{\partial v}{\partial \xi_y} \frac{\partial w}{\partial \xi_y} d\xi_x d\xi_y \right) = \int_\Sigma Q(\xi_x, \xi_y) w d\xi_x d\xi_y, \end{aligned} \tag{9}$$

where Σ represents the transformed domain as per the coordinate transformation.

Discretizing (9) in space and time yields:

$$M v^{k+1} + \alpha \Delta t D v^{k+1} - \Delta t C v^{k+1} - \Delta t \tilde{Q}^{k+1} = M v^k, \tag{10}$$

where M and D are, respectively, the mass and diffusion matrix, and C is the convection matrix.

Although we consider constant c_x and c_y, the "Method of Freezing" can handle time-dependent speeds by adding an ingredient known as phase conditions; see [3].

3 Reduced order modelling

In this section, we build a reduced-order model both via the standard and the proposed ROM approach. The standard and the proposed ROM approach, built upon a Galerkin type projection-based ROM methodology [7], is discussed in Section 3.1 and Section 3.2, respectively.

3.1 Standard reduced order modelling approach

The numerical solution of the 2-dimensional heat equation can be written as a u-snapshot matrix, where every column k represents the solution at the k-th time-step. Upon performing singular value decomposition (SVD) on the snapshot matrix composed of u, a projector $P^T : U_h \to U_r$ is obtained and further used to build a reduced-order model. Here, U_h is a h-dimensional high-fidelity space and U_r is a r-dimensional reduced space spanned by the functions obtained from a truncated singular value decomposition of the u snapshot matrix. The standard reduced-order model is given by:

$$M_{red} u_{red}^{k+1} + \alpha \Delta t D_{red} u_{red}^{k+1} - P^T \Delta t \tilde{Q}^{k+1} = M_{red} u_{red}^{k}, \tag{11}$$

where $D_{red} = P^T DP$ and $M_{red} = P^T MP$ are the reduced diffusion and mass matrices, respectively.

3.2 Proposed reduced order modelling approach

The proposed novel ROM approach employs the "Method of Freezing" in conjunction with standard projection-based reduction techniques. We again employ SVD. However, in this proposed framework, the SVD is performed on the v snapshot matrix, instead of the u snapshot matrix. We now obtain a projector $L^T : V_h \to V_r$ where V_h is a h-dimensional high-fidelity space and V_r is a r-dimensional reduced space spanned by the functions obtained from a truncated singular value decomposition of the v snapshot matrix. Finally, the proposed (frozen) reduced-order model is:

$$M_{red,p} v_{red}^{k+1} + \alpha \Delta t D_{red,p} v_{red}^{k+1} - \Delta t C_{red,p} v_{red}^{k+1} - L^T \Delta t \tilde{Q}^{k+1} = M_{red,p} v_{red}^{k}, \tag{12}$$

where $C_{red,p} = L^T CL$ represents the reduced matrix corresponding to the extra convection term, and, $M_{red,p} = L^T ML$ and $D_{red,p} = L^T DL$, respectively, represent the reduced mass and diffusion matrices.

4 Numerical results

In this section, we numerically test the proposed (Freezing-POD) approach and show its effectiveness as a reduced-order modelling technique.

Let the domain of the wafer be given by $\Omega_d = [-0.01, 0.02]\text{m} \times [-0.02, 0.04]\text{m}$. The wafer is subdivided into 9 smaller rectangular sub-domains and each sub-domain has the dimensions 1 by 2 cm. The heat load will move around one of these sub-domains in practice. In order to not consider the boundary conditions close to the boundary edges of the wafer, we consider that the laser only moves over the middle sub-domain Ω, i.e., $\Omega = [0, 0.01]\text{m} \times [0, 0.02]\text{m}$. Motivated by the application, we consider u_0 in (2) to be equal to the room temperature, i.e., $u_0 = 298K$. Furthermore, we spatially discretize a rectangular sub-domain by a 20×20 mesh, i.e., 400 finite-elements. Moreover, we consider a silicon wafer with thermal diffusivity constant $\alpha = 8.8 \cdot 10^{-5}$ m^2/s [8]. Additionally, we assume that the laser has a surface of approximately 2 by 20 mm. As a result, the variance in the x-direction, σ_x^2, is 0.002 m, and the variance in the y-direction, σ_y^2, is 0.02 m. We take 50 steps in time for the scenario under consideration, i.e., $t \in [0, 0.05]$s with a time step of 0.001s. A laser is considered to move along the x-direction with a speed of 0.2 m/s for first 25 time steps, i.e., $c_x = 0.2$ m/s and $c_y = 0$ m/s for $t = [0, 0.025]$s and along the y-direction with a speed of 0.2 m/s for next 25 time steps, i.e., $c_x = 0$ m/s and $c_y = 0.2$ m/s for $t = (0.025, 0.05]$s.

We build the snapshot matrix composed of solution u obtained in (6) and another snapshot matrix composed of shape dynamics v obtained in (10). We then perform SVD on these snapshot matrices to obtain the corresponding singular values, whose decay behavior is known to give a good expectation about the possible reduction in the dimensionality of the full-order model. In Figure 1, the singular value decay behavior for the proposed and the standard ROM approach is shown. It can be observed that incrementing the number of POD modes by one yields a sharp initial decrease in the singular values both for the proposed and the standard ROM approach. However, post the sharp decay, we can see that the singular values corresponding to the proposed approach decay faster than the one corresponding to the standard approach. An initial sharp decrease is attributed to the fact that only a single mode is representative enough to capture the mean temperature on the silicon wafer. Other modes are required to accurately determine the change (with respect to the mean) in the temperature due to the moving heat loads. The observed decay behavior clearly indicates a possibility of an effective dimensionality reduction if the “Method of Freezing” is used together with the standard ROM techniques.

Further computational benefits of the proposed approach over the standard one can be clearly seen in Figure 2, which shows the behavior of the reduced-order modelling (ROM) error for increasing dimensions of the reduced-order model. We assess the error of the standard and proposed approaches in the (absolute) L^2-norm in space and time. The error via the standard approach corresponds to the difference between the finite-element based numerical solution u and the reconstructed solution obtained by lifting the standard reduced-order solution u_{red}, obtained in (11), to the high-dimensional problem space. And, the error via the proposed approach

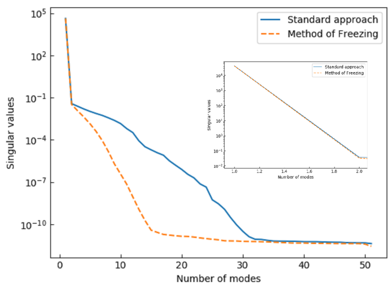

Fig. 1: Singular value decay behavior for the proposed and the standard approach.

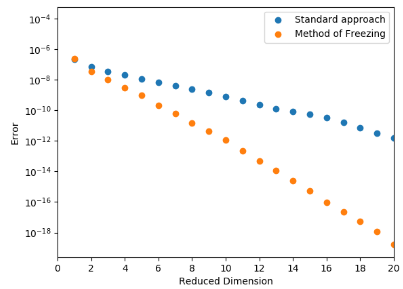

Fig. 2: ROM error for the proposed and the standard approach versus varying dimensions of the reduced-order model.

corresponds to the difference between the finite-element based numerical solution u and the reconstructed solution obtained by lifting and shifting the reduced-order solution v_{red} obtained in (12). It is clearly observable that the (absolute) ROM error incurred upon using the proposed approach for varying dimensions of the reduced-order model is lower than the error incurred while using the standard approach. The proposed approach is expected to give a lower ROM error as the shape dynamics is essentially localized around the initial configuration. In principle, the ROM error is a function of the spatial and the temporal discretization error. Given the fact that the shape dynamics is essentially localized in the proposed approach, the amount of temporal discretization error is significantly less than that obtained in the standard approach. We also claim that the larger time-step size can be used to advance the reduced-order model built using the "Method of Freezing" compared to the admissible time-step size in the standard ROM framework. This claim is supported by the fact that the time-step size is generally controlled by the CFL restrictions, which are dictated by the time-scale of the problem. As a consequence of localized shape dynamics, the time-step size is not too severely restricted in the proposed approach as in the standard approach, which also eventually aids in temporal complexity reduction. As a result, the dimension of the reduced-order model obtained by using the proposed approach will be much smaller than the counterpart obtained using the standard reduction approach in order to have the same accuracy.

5 Conclusion and future outlook

We have proposed to employ the concept of the "Method of Freezing" in conjunction with a Galerkin-type projection based methodology in order to overcome the limitation of the standard projection-based reduced-order modelling (ROM) techniques in dealing with moving heat loads. We have demonstrated the performance of the proposed approach on a test-case of practical relevance that encompasses the movement of the laser beam along both dimensions of the wafer.

This work focused on reproducing the results of the time-dependent heat equation via standard and proposed ROM approaches. This *reproduction* step is essential before attempting to develop a parametric reduced-order model as we cannot hope to have an effective low-complexity reduced-order model if the numerical approach does not fare well in the *reproduction* step. Furthermore, it should be emphasized that the considered model is non-affine due to the nature of the moving heat load(s), and that the projection alone is not sufficient to reduce the costs of constructing a reduced-order model for such non-affine (and non-linear) problems. Moreover, there might be other sources of non-affine and/or non-linear nature, such as radiative heat fluxes, temperature-dependence of parameters, etc. These non-affine and non-linear problems can be effectively dealt with the proposed ROM approach by using an additional concept of hyper-reduction introduced in [9].

Future works will deal with a modification to the idea of the “Method of Freezing” to eventually obtain a suitable decomposition ansatz that accounts for the physical boundary conditions. In addition, the effectiveness of the proposed approach will be investigated in terms of the computational speed-up. Moreover, the “Method of Freezing” in conjunction with standard projection-based ROM approaches and hyper-reduction will be used to develop a framework for parametric ROM.

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