

EFFICIENT MODELLING AND SIMULATION OF 3D ELECTRO-THERMAL MODEL FOR A PYROTECHNICAL MICROTHRUSTER

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Abstract-In this paper we present a new modeling and simulation software for a pyrotechnical microthruster which includes an automatic, Krylov-subspace based order reduction of an electro-thermal model. Model order reduction is essential for achieving quickly evaluable, yet still accurate macromodel of the device, needed for design optimization or system-level simulation. We present numerical simulation results of the full-scale finite element model and the reduced order model describing the transient electro-thermal behavior. For the first time an order reduction of a large-3D device model has been successfully performed and implemented. Two different model reduction methods, based on Arnoldi algorithm have been compared and discussed.

I. INTRODUCTION

A new class of high energy MEMS actuator integrates solid fuel with three silicon micromachined wafers [1]. It delivers either an impulse-bit thrust or pressure waves within a sub millimeter volume of silicon, by producing a high amount of energy from an ignitable substance contained within the microsystem. The microthruster fuel is ignited by passing an electric current through a polysilicon resistor embedded in a dielectric membrane, as shown in Fig. 1. After the ignition

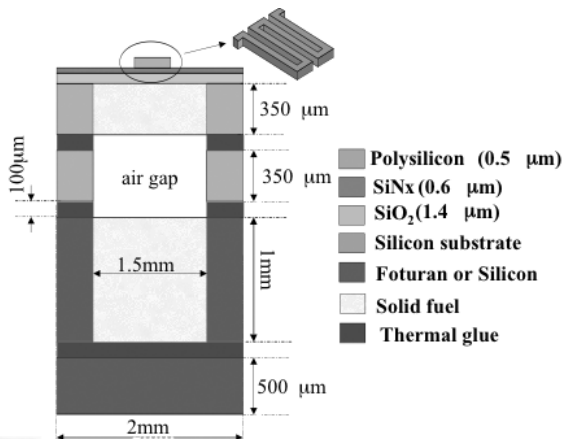


Fig. 1 Microthruster Structure.

phase, sustained combustion takes place and forms a high-pressure, high-temperature gas mixture. Under the pressure

of the gas the membrane ruptures, and an impulse is imparted to the carrier frame as the gas escapes from the tank. The device simulation is covered by four products, modeling different processes which take place within a microthruster, with a common graphic user interface (Fig. 1).

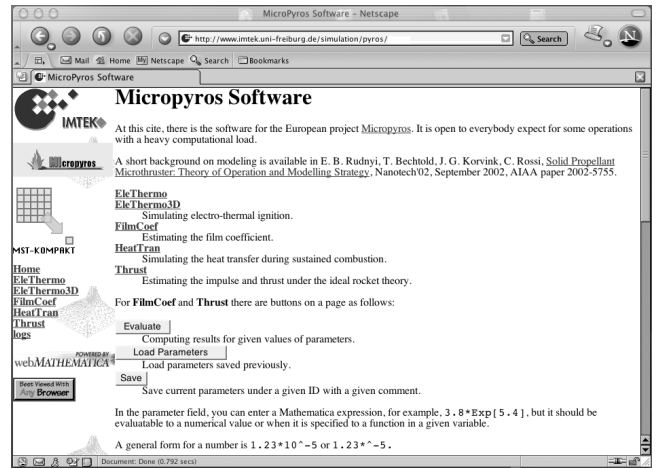


Fig. 2 MicroPyros simulation software - homepage.

Additionally a software tool *mor4ansys* has been developed, which allows automatic model order reduction of (electro)-thermal ANSYS models. All subsimulations are running on IMTEK's local system and are easily accessible via Internet for our project partners.

II. ELECTRO-THERMAL MODELING

The electro-thermal subsimulations are modeled through the following equations:

$$\nabla \cdot (\kappa \nabla T) + Q - \rho C_p \frac{\partial T}{\partial t} = 0, \quad Q = \frac{j^2}{\sigma} \quad (1)$$

where κ is the thermal conductivity, C_p is the specific heat capacity, ρ is the mass density, T is the temperature distribution, Q is the heat generation, j is the electric current density vector and σ is the specific electric conductivity. Because the Joule heating is a dominant heating mechanism, the heat generation in equation (1) can be replaced through the Joule heat. For the microthruster, as well as for the majority of MEMS devices, the assumption that κ and C_p around the operating point are temperature independent is acceptable. Another

important assumption is that the heat generation Q is uniformly distributed within the heating area. This leads after the spatial discretization of the governing equations (1) to a weak nonlinear ODE system of the form:

$$\begin{aligned} C\dot{T} + KT &= FI(t)^2R(T) \\ y &= E^T \cdot T \end{aligned} \quad (2)$$

where $K, C \in R^{n \times n}$ are the global heat conductivity and heat capacity matrix, $T(t), F \in R^n$ are the temperature (state), and the load vector respectively and n is the dimension of the system. The output parameter E could be either a vector or a matrix in dependence what states are required to be computed. In case when E is a unit matrix of the dimension n , the complete output (all the temperatures) are required. The electric current $I(t)$ through the heater with temperature dependant electric resistivity $R(T)$ is the input to the system. In the following it will be explained, why the resistor dependence on temperature doesn't influence the order reduction. A numerical simulation result of the full-3D finite element model is shown in Fig. 3.

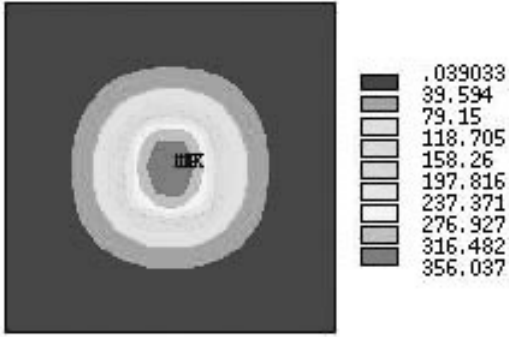


Fig. 3 Temperature distribution within the igniting wafer after 0.3s of heating with 80 mW power; $T_{ref} = 273 K$.

Now, the full-scale model contains over 79,000 degrees of freedom. As this number of equations is too large for repeated simulation corresponding to a possible design alteration or for an efficient system simulation, a reduced order model with much smaller dimension was generated.

III. MODEL ORDER REDUCTION

Conventionally, the reduction of thermo-electric models for MEMS devices is performed through a lumped-element decomposition of the model followed by parameter optimization [2]. Such a non-automatic approach requires the designer to choose the right reduced model structure without strict guidelines, and to perform a time-consuming parametrization including indispensable simulation of the full-scale model. We propose a different, automatic order reduction approach, suitable for the linear or weak nonlinear electro-thermal model of the microthruster device, and based on an Arnoldi algorithm [3], which transforms equation (2) into the following system:

$$\begin{aligned} C_r \dot{T}_r + K_r T_r &= F_r I(t)^2 R(T) \\ y_r &= E_r^T \cdot T_r \end{aligned} \quad (3)$$

with much smaller dimension $r \ll n$. Here T_r is a projection of the n -dimensional temperature vector to r -dimensional subspace, subjected to some error ε :

$$T = V \cdot T_r + \varepsilon, T_r \in R^r, r \ll n \quad (4)$$

and $y_r = E_r^T \cdot T_r$ is those linear combination of the reduced states which corresponds to the required states y in equation (2).

The matrix V in (4) is composed from r n -dimensional vectors that form a basis for the reduced subspace. When the subspace is found the whole equation (2) is projected onto it (by applying (4) and then multiplying (2) from the left side by V^T), and this projection process produces a reduced order system (3) according to the Pade or Pade-type approximation [4]:

$$C_r = V^T C V; K_r = V^T K V; F_r = V^T F; E_r = V^T E \quad (5)$$

For the large linear systems a transformation matrix V can be effectively computed as an orthogonal basis for the Krylov subspace of the dimension r . However, in order to compute this subspace it is necessary to change a system representation into the form:

$$\begin{aligned} A \dot{T} &= T + b I(t)^2 R(T) \\ y &= c^T \cdot T \end{aligned} \quad (6)$$

with $A = -K^{-1}C$, $b = -K^{-1}F$ and $c = E$. The new system matrix A and load vector b are the inputs to Arnoldi algorithm, and it's direct outputs are the matrix V and the matrix $A_r = V^T A V$. Consequently, the reduced order system originated from the representation (6) (by applying (4) and then multiplying the equation (6) from the left side by V^T) is automatically defined by Arnoldi algorithm itself as:

$$A_r = V^T A V; c_r = V^T c; b_r = \|b\| e_1 \quad (7)$$

with e_1 a first unit vector of the basis V . Note that the input term $I(t)^2 R(T)$, which causes the weak nonlinearity of the system, doesn't take part in the model order reduction. The reduced systems (5) and (7) are different and so are their solutions, as shown in the chapter V. The explanation lays in the very basic idea of Arnoldi algorithm, that is to write down the transfer function of (2) in the frequency domain using a Maclaurin expansion:

$$\{G(s)\} = - \sum_{i=0}^{\infty} \{m\}_i s^i \quad (8)$$

where $\{m\}_i = E^T (-C^{-1}K)^{-(i+1)} C^{-1}F$ is called the i th moment, and then to find a system (3) of the order r whose transfer function $\{G_r(s)\}$ has the first r moments same as $\{G(s)\}$. $\{G_r(s)\}$ is called Pade-type approximation of

$\{G(s)\}$. This system is however not unique, because only r out of $2r$ coefficients of it's transfer function are defined through the moments. The rest can be varied by changing the system representation like from equation (2) to equation (6). It is important to say, that the matrix V stays the same.

IV. IMPLEMENTATION

The software implementation is outlined in Table 1. The exchange of information between different types of software is made through text files and through ANSYS binary files. The subsimulations can be described as follows: Electro-thermal ignition (EleThermo) is modeled through heat transfer PDE (1) under assumption of homogeneous heat generation rate (lumped resistor model). Simulation's inputs are geometry, material properties, applied electrical power and initial and boundary conditions (BC). The outputs are time-dependant numerical results and/or system matrices for model

Our new tool *mor4ansys* allows automatic model order reduction of (electro)-thermal ANSYS models containing more then 100 000 degrees of freedom. The compact models can be easily used for a system-level simulation. The software forms equation system (2) directly out of ANSYS binary element matrix file, and performs Arnoldi algorithm to create a low dimensional system (3), either by using equation (5) or (7). The software expects the ANSYS model to be linear, this means that if material properties or film coefficients depend on temperature, an appropriate operation temperature should be chosen. Currently, it is still impossible to estimate the error between the full and reduced model different then to compare the both, i. e. to make full 3D simulation. How this can be circumvented is our current research topic.

Table 1: Software implementation for Micropyros project

Name	Description	Type	Inputs	Outputs
EleThermo	Simulation electro-thermal ignition	ANSYS script	Device specifications	System matrices or transient simulation results
FilmCoef	Estimating film coefficient	Mathematica notebook	Properties of the flow	Value of film coefficient
HeatTran	Simulating heat transfer during sustained combustion	ANSYS script	Device specifications	System matrices or transient simulation results
Thrust	Estimating impulse produced by the micro-thruster	Mathematica notebook	Properties of the solid fuel and the nozzle	Thrust and impulse produced by a microthruster device
mor4ansys	Performing model order reduction	Binary (executable) produced by C++ compiler	System matrices produced by EleThermo or HeatTran	Compact model for system-level simulations in HDL format

order reduction. Estimation of film coefficient (FilmCoef) is modeled through the convection BC for the estimation of heat transfer between the hot gases and the wafer, and the equation connecting Reynolds, Nusselt and Prundtl numbers. Simulation's inputs are diameter of the chamber, velocity, viscosity, heat capacity, heat conductivity and density, and the output is film coefficient. Heat transfer during sustained combustion (HeatTran) is modeled through (1) and convection BC. The inputs are the same as for EleThermo plus film coefficient, and the outputs are the same as well. The imparted impulse (Thrust) is modeled through the ideal rocket theory (stationary isentropic quasi-one-dimensional flow), and mass balance to estimate the chamber pressure. Simulation's inputs are atmospheric pressure, inlet temperature, areas of chamber, throat and outlet, heat capacity ratio and burning rate, and the outputs are outlet pressure, velocity, thrust and impulse.

V. RESULTS

By the means of Arnoldi algorithm we have reduced an equation system of 79.171 ODEs to only 20 ODEs, with the maximal absolute difference of only 5°C (Fig. 4 and 5). The reduction of the computation time allows the transient solution for the cost of the stationary one. The comparison between the reduced models (5) and (7) shows that the reduced system (7) is quicker to obtain, but the system (5) shows smaller differences (at least for the orders 5 to 13) to the original 3D model (Fig. 6). As the system order grows, both models show approximately the same deviation to the full-system.

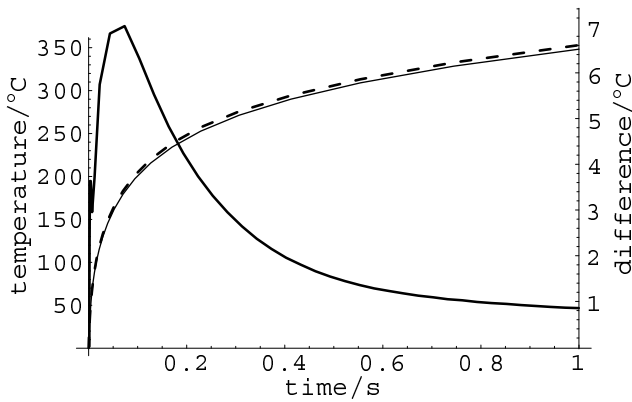


Fig. 4 Solution of the full 79. 171 order system(thin-straight) and of the reduced order 20 system (dashed) for node nr. 1; Difference between the both (thick-straight).

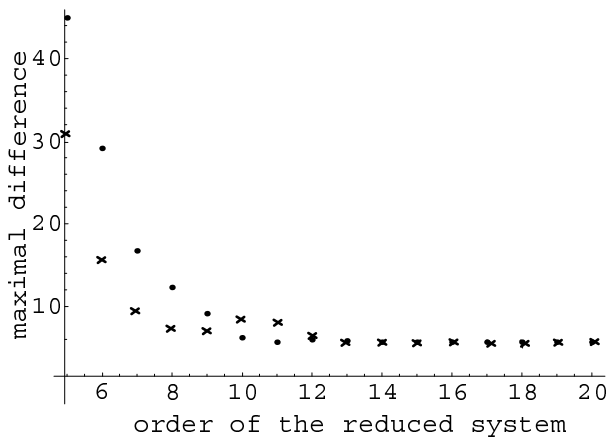


Fig. 5 Maximal difference over the defined output nodes for the reduced systems ((11) - dots and (9) - crosses).

VI. DISCUSSION

In this paper we have reported on the new efficient modeling and simulation software for the 3D pyrotechnical microthruster. For the fixed geometry, all the input data can be supplied from our project partner over internet. We have further developed a tool for the automatic model order reduction of electro-thermal models directly from ANSYS data files. The model order reduction is based on the Arnoldi algorithm and provides different low order models. It has been shown, that for the lower orders the model (5) provides higher accuracy, whereas the model (7) is more effective for reduction to higher orders. The apriori criterion to choose the right order of the reduced model, which fulfills the specified error bound is however still under development.

The weak nonlinearity of the system (2) caused by the resistor's dependence on temperature, can be overtaken within a reduced model, because the input function is not influenced

by reduction. This has been implemented through the back-coupling of the meander's resistivity, as shown in Fig. 6.

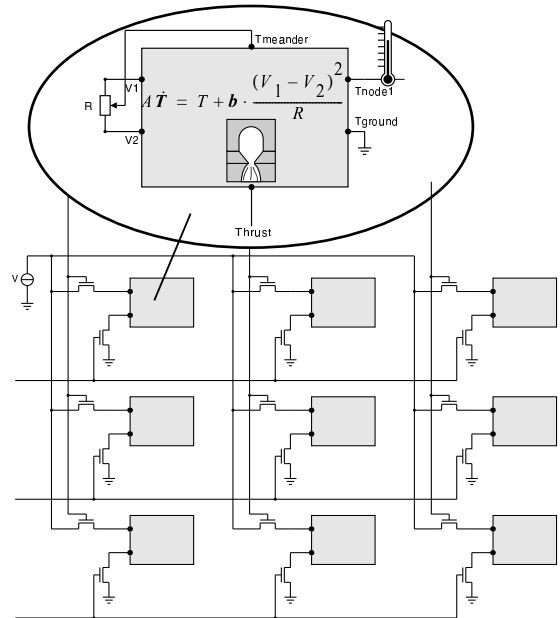


Fig. 6 Microthruster array structure without thermal coupling of the reduced models

As the microthruster device for space application is an array structure, the goal is to research the possibility of coupling the single reduced models within a system-level simulation. When the devices are to be fired independently, the thermal crosstalk between two neighboring devices can be neglected, and the structure as in Fig. 6 is sufficient. If this is not the case, the preheating of the nonfired devices must be taken into account, and some sort of thermal coupling between the reduced models is necessary. This is the current topic of the authors research.

VII. ACKNOWLEDGMENTS

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VIII. REFERENCES

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