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	Summary: We present a brief survey of the current MOR methods, and propose the most appropriate methods for the models considered in Task T1.3. Next, mathematical modelling of coupled problems is introduced. Finally, the accuracy and efficiency of the proposed MOR methods are checked by the models provided by partner MAGWEL.
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D1.1 Intermediate report on pMOR for linear and nonlinear coupled problems

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In this Deliverable D1.1, we first present a brief review of the current MOR methods, and propose the most appropriate methods for the models considered in Task T1.3. Afterwards, mathematical modelling of electric or thermal problems, as well as electro-thermal coupled problems is introduced. Finally, preliminary results of the proposed MOR methods applied to different models are presented.

1 Introduction

Model Order Reduction (MOR) is an increasingly popular approach to overcome the obstacles posed by the computational demands in a many-query context. By MOR, a small dimensional approximate system, the so-called Reduced Order Model (ROM) can be derived, so that it can reliably replace the original system during the simulation. This can often save much simulation time and computer memory.

1.1 Motivation of MOR for coupled problems

Electro-thermal simulation at system level is a joint simulation of electrical and thermal parts of the system (as schematically shown in Fig. 1). The circuit dissipates energy and therefore leads to variation of the temperature. Temperature in their turn influence the circuit parameters, e.g., the electrical conductivity with the final result being bi-directional coupling.
The thermal model in Fig. 1 is a simple, lumped-element model.

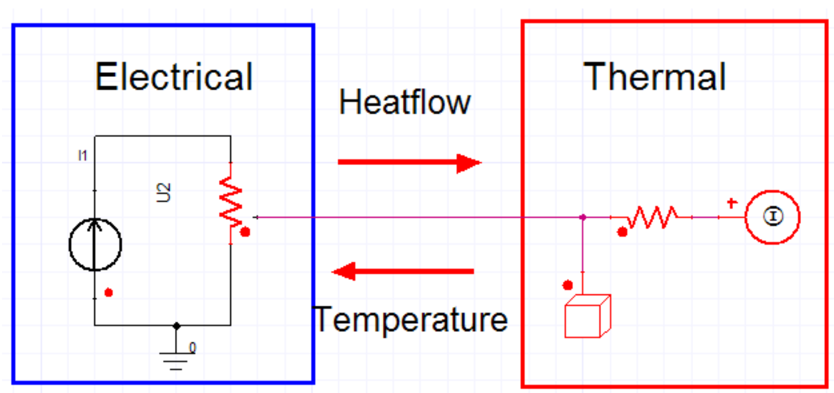

Figure 1: Simple electrothermal simulation [4].

For general complex geometries, a more accurate, physical model in the form of heat transfer partial differential equations is required. To be more precise: The electrical transport is controlled by Ohm's law and the current continuity equation in conductive material

$$\nabla \cdot \vec{J} = 0, \qquad \vec{J} = \sigma(T)\, \vec{E}. \tag{1}$$

The generated-energy transport is controlled by Joule's law

$$\partial U_t = -\nabla \cdot \vec{Q} + \Sigma \qquad \vec{Q} = -\kappa(T)\nabla T, \qquad U = C_V(T - T^*). \tag{2}$$

Of particular interest is the local heat generation, which is given by

$$\Sigma = \vec{E} \cdot \vec{J} = \sigma(T)\,(\nabla V)^2\,. \tag{3}$$

Here C_V is the constant-volume heat capacitance of the material, which is also T-dependent and T^* is a reference or ambient temperature. The latter expression results in a non-linear relation between the variables V, the electrical voltages, and the temperature variables, T.
Spatial discretization (using the finite-element method, or finite volume method, like Finite Integration) of (1) and (2) results in a large-scale system of ODEs in the form of

$$E\tfrac{dx(t)}{dt} = Ax(t) + x(t)^T F x(t) + Bu(t), \tag{4}$$

where x is the state vector including the nodal voltages and nodal temperatures varying with time. The dyadic F represents the non-linear character of the heat source Σ. The matrix E is a capacity matrix for both the electrical and the thermal part, and the matrix A is the conductivity matrix for both the electrical and the thermal part.
In both cases, (4) is not compatible with system level simulation, as the vector x usually contains several hundred thousands of degrees of freedom. The remedy is to apply the technique of MOR, which enables a formal transformation of (4), to a system in the same form but with much less equations. The basic idea of MOR can be described as below.
Apart in using MOR in applications in its own merit, MOR now also finds applications in improving co-simulation (or dynamic iteration), which is also a point of interest in our project nanoCOPS (Task T1.4) [34, 24, 26]. For nonlinear MOR we refer to [5, 10, 44, 27]. IN [9] extensions have been proposed to port-Hamiltonian systems: this offers a way to guarantee passive, reduced subsystems.

1.2 Basic idea of MOR

The general idea of almost all the MOR methods is to find a subspace S_1 which approximates the manifold where the state vector $x(t)$ resides. Afterwards, $x(t)$ is approximated by its projection $\tilde{x}(t) \in S_1$. The reduced model is produced by Petrov-Galerkin projection onto another subspace S_2, or by Galerkin projection onto the same subspace S_1.
Assuming that an orthonormal basis $V = (v_1, v_2, \ldots, v_q)$ of the subspace S_1 has been found, then the projection $\tilde{x}(t) \in S_1$ can be represented by the basis as $\tilde{x}(t) = Vz(t)$. Therefore, $x(t)$ can be approximated by $x(t) \approx Vz(t)$. Here z is a vector of length $q \ll n$.
Once $z(t)$ is computed, we can get an approximate solution $\tilde{x}(t) = Vz(t)$ for $x(t)$. The vector $z(t)$ can be computed from the ROM, which is derived by the following two steps.

1. By replacing x in (4) with Vz, we get

$$\begin{array}{rcl} E\frac{dVz}{dt} & = & AVz + z^T V^T F V z + Bu(t) + e(t), \\ \hat{y}(t) & = & CVz, \end{array} \tag{5}$$

where $e(t)$ is the error caused by the approximation.

2. Forcing $e(t)$ to be zero in a properly chosen subspace S_2 of $\mathbb{R}^n$, by some Galerkin procedure, we get the reduced model

$$\begin{aligned} W^T E V \tfrac{dz}{dt} &= W^T A V z + W^T z^T V^T F V z + W^T B u(t), \\ \hat{y}(t) &= C V z, \end{aligned} \tag{6}$$

where the columns of W are an orthonormal basis of S_2.

1.3 A review of (p)MOR methods

The technique of MOR can be traced back to the 1980s or even earlier. Till now, MOR has already been applied to various research areas, due to its great potential in accelerating simulation in various applications. There are different kinds of MOR methods in the literature. The modal truncation methods [12, 29] are among the earliest developed methods and are mainly applied in structural dynamics. In electronics enhancements have been developed as well [36, 35]. The Gramian-based MOR methods are mostly used in the area of electrical and control engineering [30, 2]. Reduced basis methods [32, 38] are known in mechanical engineering, computational fluid dynamics. Proper Orthogonal Decomposition (POD) is widely used in fluid dynamics [37, 41, 34] and has found applications on a much broader scale [28, 42]. The moment matching MOR methods for linear and bilinear systems [15, 31, 22, 23], and the MOR methods based on Volterra series expansion [33] for nonlinear systems are popular in simulation of micro- & nano- electrical systems and micro- & nano- electromechanical systems. For good overviews, see [2, 39, 8].

Parametric model order reduction(pMOR) targets the broad class of problems for which the equations governing the system behavior depend on a set of parameters. The goal of parametric model reduction is to generate low cost but accurate models that characterize system response for different values of the parameters. Thus, a change in parameters does not require computing a new reduced-order model, but simply the evaluation of the reduced-order model for the new parameter values. If the error in the whole feasible parameter domain can be proven to satisfy an acceptable error tolerance, design and optimization of systems and devices can be significantly accelerated.

First attempts at deriving pMOR methods for parametric systems were based on extending the popular moment-matching methods (aka Padé approximation, rational interpolation, Krylov subspace based MOR methods) to parametric systems by multivariate power series expansions around appropriate interpolation points. We call them multi-moment-matching pMOR methods or Krylov subspace based pMOR methods, which can be found in the early literature [43, 11, 20], and the very recent one [6]. Later, other variants of (rational) interpolation techniques were derived, combining, e.g., by employing $\mathcal{H}_2$-optimal interpolation techniques [3], or using matrix and manifold interpolation techniques (e.g., [1]). For recent papers, see [7, 19]. Another large class of pMOR techniques is based on the Reduced Basis Method (RBM) [32, 38, 13, 25], originating in the fast approximation of parametric partial differential equations.

The (multi-)moment-matching (p)MOR methods for linear (non)parametric systems and the MOR methods based on Volterra series expansion for nonlinear systems have the following advantages which make them still the most popular approach used in practical applications,

- They are easy to implement and require almost no assumptions on system properties.
- Their cost is limited to a few (according to the number of employed expansion points) factorizations of sparse matrices and forward/backward solves using the computed factors. The computation is much cheaper than the methods based on balanced truncation and interpolation, where full-sized matrix equations need to be solved. They do not require generation of trajectories and are therefore called ”simulation-free” (in contrast to RBM and proper orthogonal decomposition (POD) methods). As a consequence, the ”offline-phase” for computing the reduced-order model is cheap compared to RBM and POD, and it is often possible to achieve the goal encountered in practical industrial engineering design.
- As they are simulation-free, no training inputs u(t) need to be chosen so that the approximation quality is usually good for all feasible input signals, not only close to training inputs as in RBM and POD methods.

Furthermore, we have proposed an error estimation for linear parametric systems [17, 18, 16], which provides a way of automatically generating reliable reduced models.

The models in Task T1.3 include linear electrical or thermal models, coupled nonlinear (parametric) systems. Based on the above general review and the detailed analysis of the models, we plan to use the following methods to solve different systems:

- Moment-matching methods for linear electrical or thermal models.
- MOR methods based on Volterra-series expansion for coupled nonlinear non-parametric systems.
- Combination of multi-moment-matching MOR methods and methods based on Volterra-series expansion for coupled parametric nonlinear systems.

2 Mathematical modelling of coupled problems (MAG, TUD)

We define some testcases. All ROMs are used in the time domain. A more detailed description for the test cases 1 to 3, can be found in Deliverable D1.2.

2.1 Test Case 1: Transient simulation, linear non-parametric model (MAG)

In order to realize the interfacing of the electro-thermal field solver and the ROM libraries, we propose a series of applications with increasing level of complexity. Linear non-parametric models are realized by considering electric-only systems or thermal-only systems with fixed heat sources.
After spatial discretization we end up with a (long) state-space vector x in (4) that represents all grid voltages $\{V_1, V_2, ...V_n\}$, or in the other case the grid temperatures $\{T_1, T_2, ..., T_m\}$. For the same grid the number of voltages (n) may differ from the number of temperatures (m), since this number depends on the specific boundary

conditions. The stimuli vector $\mathbf{u}$ is given by the time-dependent applied voltages at the contacts $\{u_1, u_2, u_k\}$. Finally, the output vector $\mathbf{y}$ are the electrical and thermal fluxes at the contacts $\{I_1, I_2, ..I_k, Q_1, Q_2, ...Q_k\}$. For this linear case, the dyadic F in (4) is zero.

2.2 Test Case 2: Transient simulation, coupled models (MAG)

The electro-thermal problem represents a complete transient coupled model but we may gradually increase the complexity again by considering fixed heat sources and turn off the Joule heating, i.e., the term Σ, but maintaining the temperature dependence of the electrical conductance. In general, the T-dependence is non-linear but we may apply a Taylor expansion around the environment temperature T^* and arrive at a coupling that is 3^{rd} order in the state-space variables $\mathbf{X} = \{V_1, V_2, ...V_n, T_1, T_2, ..., T_m\}$. The first coupled model for test is in the form of (4), but again with $F = 0$.

2.3 Test Case 3: Transient simulation, parametric coupled models (MAG)

Based on the coupled model in Test case 2, if we further consider the variation of p, the thickness of the top layer of the package, then the resulting coupled problem is a parametric system with nonlinear coupling. For the moment, we assume that in the system (4), $E(p)$ has the form $E(p) = E_0 + pE_1 + \frac{1}{p}E_2$. Also for $A(p)$, $B(p)$ we use similar formulations as for $E(p)$.

2.4 Test Case 4: A fast and reliable model for bond-wire heating (TUD)

This test case deals with the development and validation of fast and reliable model for the calculation of the temperature distribution in bond-wires, and thus the determination of the maximum allowable current for its posterior dimensioning as requested by our partner ON Semiconductors (ONN) [14]. The model will permit to take into account the parameters, i.e., moulding compound material and dimensions, bond-wire characteristics, etc., that geometrically define a package. To validate our model, results will be compared with those obtained through high-fidelity computer simulations of a realistic configuration, as illustrated in Fig 2.3 in [40], and measurement data, if available.

3 Preliminary results on (p)MOR (MPG)

3.1 Results for Test Case 1: Transient simulation, linear non-parametric model

The first test case is a linear non-parametric model with 242 differential equations, i.e. $n = 242$. There are 2 inputs, and 4 outputs. We use the moment-matching method to compute the reduced model, and there are only $r = 13$ equations in the reduced model. The maximal error of the outputs computed by the reduced model is around $O(10^{-13})$. We have achieved a speed-up factor of 10 for the simulation. In Figure 2, we plot the output responses of the original system and the reduced model at node 2 and node 3. Here and below, node i means the output produced by the ith row of the output matrix C.

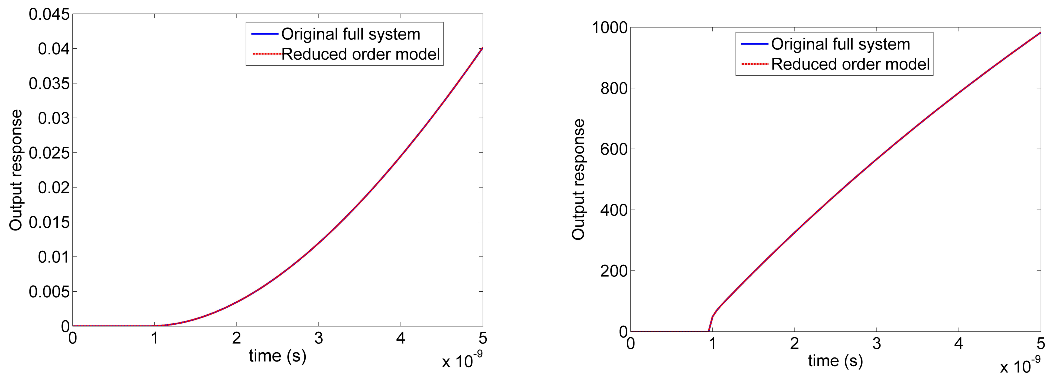

Figure 2: Output response comparison for Test Case 3.1: FOM $n = 242$, ROM $r = 13$, error $||y - y_r||_2/||y||_2 \leq O(10^{-13})$. Factor of speed up 10.

3.2 Results for Test Case 1: Transient simulation, linear non-parametric model

The structure of this model is basically the same as the previous one. The only difference is that there are many more differential equations, $n = 21760$, and more inputs and more outputs. It has 11 inputs and 22 outputs. We still use moment-matching methods to compute the reduced model of size $r = 66$, which preserves the inputs and the outputs. The maximum output error among all the outputs is 6.25×10^{-11}. The simulation time is largely reduced and the factor of speed up is 2100. The output responses of the original system and those of the reduced model at node 16 and node 22 are presented in Figure 3.

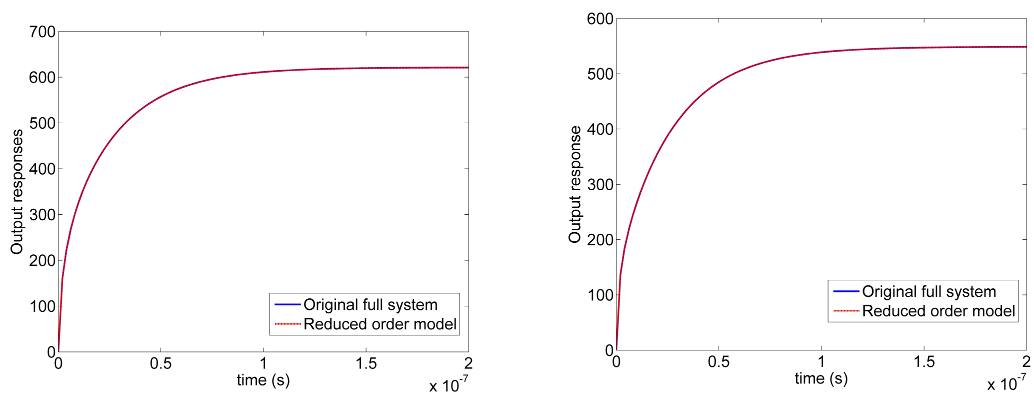

Figure 3: Output response comparison for Test Case 3.2: FOM $n = 21760$, ROM $r = 66$, output error $||y - y_r||_2/||y||_2 \leq 6.25 \times 10^{-11}$. Factor of speed up 2100.

3.3 Results for Test Case 2: Transient simulation, coupled models

This test concerns a nonlinear system of 76 degrees of freedom, $n = 76$. The nonlinear model in (4) can be written into the following form,

$$\begin{aligned} \frac{dx(t)}{dt} &= Ax(t) + x(t)^T \mathcal{W} x(t) + Bu(t) + f(0), \\ y(t) &= Cx(t), \end{aligned} \tag{7}$$

where the nonlinear term $x(t)^T \mathcal{W} x(t)$ is quadratic. Here $\mathcal{W} = [W_1, \ldots, W_n]$ is a tensor. Each W_i, $i = 1, \ldots, n$ is a matrix. It is desired that the reduced model preserves the structure of the original system. It is observed that the matrix A has block form

$$A = \begin{bmatrix} A_1 & \\ & A_2 \end{bmatrix}.$$

Here $A_1 \in \mathbb{R}^{n_1 \times n_1}$, $A_2 \in \mathbb{R}^{n_2 \times n_2}$, and $n_1 + n_2 = n$. Furthermore $W_1, \ldots, W_{n1}$ are all zero matrices. Hence, the tensor can be written as $\mathcal{W} = [\mathbf{0}, \mathcal{W}_2]$. Taking use of the block form of A, and the block form of the tensor, structure preserving MOR can be realized by applying MOR to the linear part and the nonlinear part separately. I.e. Computing two projection matrices $V_1 \in \mathbb{R}^{n_1 \times r_1}$ and $V_2 \in \mathbb{R}^{n_2 \times r_2}$, the reduced model is obtained as

$$\begin{aligned} \frac{dz_1(t)}{dt} &= V_1^T A_1 V_1 z_1(t) + V_1^T B_1 u(t), \\ \frac{dz_2(t)}{dt} &= V_2^T A_2 V_2 z_2(t) + V_2^T z(t)^T V^T \mathcal{W}_2 V z(t) + V_2^T B_2 u(t), \\ y(t) &= C[V_1, V_2] z(t), \end{aligned} \tag{8}$$

where the dimensions of B_1 and B_2 in B

$$B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$$

are the same as A_1 and A_2 respectively, and

$$z(t) = \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix}$$

is the state vector of the reduced model. It can be easily seen that the reduced model has the same block structure as the original system.

According to the preliminary implementation of MOR, it is shown that if using moment-matching method to compute V_1, then $V_1 z_1(t)$ approximates the first part of $x(t)$ very well. However, if using moment-matching method and ignoring the information of the quadratic part to compute V_2, the resulting V_2 is not accurate enough to approximate the second part of $x(t)$, i.e. there is a big error between $x_2(t)$ and $V_2 z_2(t)$. Here

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}.$$

In Table 3, we have listed the static solutions computed by simulating the original full system, and by solving the reduced order model. The outputs at node 5 and node 6

Table 3: Output response comparison for Test Case 3.3: Static output of the original full system and the reduced model.

Output	node 1	node 2	node 3	node 4	node 5	node 6	node 7	node 8
y	-33.33	33.33	10	0	150	150	0	0
y_r	-33.33	33.33	10	0	-30.53	-4.95	0	0

depend on $V_2 z_2(t)$ and it is obvious that they are very different from those of the full model. The outputs at node 1-node 4 only depends on the input and $V_1 z_1(t)$. The outputs y and y_r are exactly the same at those nodes, showing that MOR for the linear part is accurate enough. The inaccuracy is caused by MOR for the nonlinear part.

Therefore, we plan to use more accurate MOR method for nonlinear systems. The method based on Volterra series expansion [33, 21] is the first choice. From our experience of MOR for nonlinear systems, they are expected to achieve much better accuracy. In order to preserve the structure of the original system, the Volterra series based MOR methods are good candidates to achieve the goal.

3.4 Results for Test Case 3: Transient simulation, parametric coupled models

The implementation is in progress. We plan to use the error bound proposed in[16, 17, 18], and combined with the multi-moment-matching pMOR method in [6] to adaptively select the parameters so as to automatically compute the reduced model.
In the first stage, we ignore the nonlinear part and consider only a linear parametric system. Once good results can be obtained, we combine the MOR method based on Volterra series expansion with the pMOR method [6] to compute the reduced model of the nonlinear parametric system.

4 Future work

We plan the following steps

- Use the reduced-order models, generated for Test Case 1 and Test Case 2 for the preliminary implementation of Task T1.4: MOR based compact netlist generation for electro-thermal circuits (MPG, HUB, MAG, ONN).
- Use more accurate nonlinear MOR methods for the coupled model of Test Case 3. The method based on Volterra series expansion [33, 21] is the first choice. Propose and implement suitable pMOR methods for the parametrized coupled models of Test Case 3.
- Propose and implement suitable pMOR methods for the parametrized coupled models of Test Case 4.
- Once the reduced-order models are constructed for coupled problems and parametrized coupled problems, they are expected to be further be used within Task T1.4, as well as in Task T1.1.

For the next nanoCOPS Workshop in Berlin, October 6, 2014, preparations will be made for making decisions on the best methods to be implemented.

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