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# Reduced Order Models for Thermal Analysis

# Final Report: LDRD Project No. 137807

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**Abstract**

This LDRD Senior's Council Project is focused on the development, implementation and evaluation of Reduced Order Models (ROM) for application in the thermal analysis of complex engineering problems. Two basic approaches to developing a ROM for combined thermal conduction and enclosure radiation problems are considered. As a prerequisite to a ROM a fully coupled solution method for conduction/radiation models is required; a parallel implementation is explored for this class of problems.

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# CONTENTS



# FIGURES

# 1. INTRODUCTION

## 1.1. Reduced Order Models

High-fidelity models of large, complex systems are now used routinely to verify design and performance. However, there are applications where the high-fidelity model is too large to be used repetitively in a design mode. One such application is the design of a control system that oversees the functioning of the complex, high-fidelity model. Examples include control systems for manufacturing processes such as brazing and annealing furnaces as well as control systems for the thermal management of optical systems.

A reduced order model (ROM) seeks to reduce the number of degrees of freedom needed to represent the overall behavior of the large system without a significant loss in accuracy. The reduction in the number of degrees of freedom of the ROM leads to immediate increases in computational efficiency and allows many design parameters and perturbations to be quickly and effectively evaluated. Reduced order models are routinely used in solid mechanics where techniques such as modal analysis have reached a high state of refinement. Similar techniques have recently been applied in standard thermal conduction problems *e.g.* [1-5] though the general use of ROM for heat transfer is not yet widespread. One major difficulty with the development of ROM for general thermal analysis is the need to include the very nonlinear effects of enclosure radiation in many applications. Many ROM methods have considered only linear or mildly nonlinear problems.

## 1.2 Present Study

In the present study a reduced order model is considered for application to the combined problem of thermal conduction and enclosure radiation. The main objective is to develop a procedure that can be implemented in an existing thermal analysis code. The main analysis objective is to allow thermal controller software to be used in the design of a control system for a large optical system that resides with a complex radiation dominated enclosure.

In the remainder of this section a brief outline of ROM methods is provided. The following chapter describes the fully coupled conduction /radiation method that is required prior to considering a ROM approach. Considerable effort was expended to implement and test the combined solution method; the ROM project ended shortly after the completion of this milestone and thus the ROM results are incomplete.  The report concludes with some observations and recommendations.

## 1.3 Overview of ROM

The general theory and some applications of ROM to several typical problems in mechanics have been well described in a number of research publications, *e.g.* [1-6]. Here a simple sketch of the attributes and procedure is provided to introduce the method for the particular applications of interest. This is not a formal mathematical derivation and many technical details are omitted.

Consideration is given to methods for extracting a reduced order model from a high-fidelity, finite element representation of a heat transfer system of interest. The resulting ROM is required to be small enough to run effectively on a single processor computer. This implies that the ROM must have significantly fewer degrees of freedom than the original finite element model which may be usable only on a parallel computer. The ROM must also be sufficiently accurate to represent all of the relevant physical processes in the original system. In the present case this is primarily thermal conduction and enclosure radiation; both processes being generally nonlinear and time dependent. The reduced model must be flexible enough to account for changes in boundary conditions because this is the primary avenue for design studies. Finally, the ROM must be compatible with standard controller design software.

Two main approaches to ROM have been considered. The first is modal analysis that has been very successful in solid mechanics for generally linear problems. In finite element form the combined transient conduction /radiation problem can be expressed as (see next section for derivation)

$$\mathbf{M}\dot{\mathbf{U}} + \mathbf{K}\mathbf{U} = \mathbf{F} \quad (1.1)$$

where $\mathbf{K}$ is the general diffusion (matrix) operator, $\mathbf{M}$ is the general (matrix) capacitance, $\mathbf{F}$ is the forcing function (vector) and $\mathbf{U}$ is the vector of unknown thermal degrees of freedom. To proceed with a modal analysis of this system, the generalized eigenvalue problem for the unforced system must be solved. That is

$$\mathbf{K}\mathbf{\Phi} - \mathbf{\Lambda}\mathbf{M}\mathbf{\Phi} = \mathbf{0} \quad (1.2)$$

where $\mathbf{\Phi}$ is a matrix of eigenvectors corresponding to the eigenvalues in the matrix $\mathbf{\Lambda}$. When this is solved for the eigenvalues and eigenvectors a change of basis is performed to the generalized coordinates $\mathbf{X}$ which is defined by

$$\mathbf{U} = \mathbf{\Phi}\mathbf{X} \quad (1.3)$$

When change of basis is substituted into the original conduction/radiation matrix problem and the system is premultiplied by $\mathbf{\Phi}^{\mathbf{T}}$, the resulting uncoupled ordinary differential equation system for the generalized coordinates is

$$\dot{\mathbf{X}} + \mathbf{\Lambda}\mathbf{X} = \mathbf{\Phi}^{\mathbf{T}}\mathbf{F} \quad (1.4)$$

In deriving the ODE’s the orthogonality of the eigenvectors has been used to simplify the equations.

If only the first *p* eigenvectors contain a significant portion of the energy in the system, then a ROM of order p can be produced by computing and using only the first *p* eigenvectors. Note that the ODE’s may be integrated in time, either analytically or numerically, depending on the complexity of the forcing function $\mathbf{\Phi}^{\mathbf{T}}\mathbf{F}$. Once the first *p* generalized coordinates have been computed, the approximation to the thermal field may be constructed from the change of basis relation.

The utility of the modal method requires that the eigenvalue problem be limited to the computation of only a few modes as the generalized eigenproblem can be computationally expensive for large finite element models. For application as a ROM, the modal approach would depend on the ability to "linearize" the original system, *i.e.* find an average temperature field for the simulation such that properties and enclosure radiation may be approximated. Alternatively, a series of eigenvalues problems could be computed as a function of time though this would be relatively expensive.

The second approach considered for generating a reduced order model utilized Proper Orthogonal Decomposition or POD. This method has a long history dating to the early 1900's and has been used in a wide variety of applications. The basic method goes by a variety of names including Karhunen-Loeve decomposition, principal component analysis and singular value decomposition (SVD). Proper orthogonal decomposition has recently become a very active area of research in computational mechanics because it has none of the drawbacks of modal analysis and is readily applicable to complex, nonlinear systems. The method is not limited to numerical models but may also be used with experimental data. POD is a procedure for optimizing the solution basis (functions) so that they are close to the solution. Eigenfunctions are extracted from the vector space of the solution rather than the vector space of the differential operators as in the modal analysis case.

The POD method is initiated by generating a series of *L* solution vectors or snapshots from the high-fidelity model which has, in general, *N* degrees of freedom. From this solution a matrix is constructed

$$\mathbf{U} = \left[\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3 \quad \cdots \quad \mathbf{u}_L\right] \quad (1.5)$$

A covariance matrix is then constructed by premultiplying by the transpose of the snapshots or

$$\mathbf{C} = \mathbf{U}^{\mathrm{T}}\,\mathbf{U} \quad (1.6)$$

An orthonormal basis for the covariance matrix can be constructed by solving the standard eigenvalue problem associated with $\mathbf{\Lambda}$. That is, solve

$$\mathbf{C}\,\mathbf{\Phi} = \mathbf{\Lambda}\,\mathbf{\Phi} \quad (1.7)$$

The complete basis is truncated (not solved) to the first *K* eigenvectors such that the snapshots (solutions) are approximated by the basis

$$\mathbf{U} = \tilde{\mathbf{\Phi}}\,\tilde{\mathbf{a}} \quad (1.8)$$

It can be shown that this basis is optimal in the sense that it contains the most energy from the system. With the truncated basis, a coordinate transformation may again be defined for the original high-fidelity system. Let the global trial functions and weighting functions be defined by

$$\tilde{\mathbf{N}}^{\mathrm{T}} = \mathbf{N}^{\mathrm{T}}\,\tilde{\mathbf{\Phi}} \qquad ; \qquad \mathbf{w} = \tilde{\mathbf{\Phi}}^{\mathrm{T}}\,\mathbf{N} \qquad ; \qquad \mathbf{U} = \mathbf{N}^{\mathrm{T}}\,\tilde{\mathbf{\Phi}}\,\tilde{\mathbf{U}} \quad (1.9)$$

where $N$ is the original finite element basis. The original finite element model may then be transformed to a *K x K* ROM system as

$$\tilde{\mathbf{\Phi}}^{\mathrm{T}}\mathbf{M}\tilde{\mathbf{\Phi}}\dot{\tilde{\mathbf{U}}} + \tilde{\mathbf{\Phi}}^{\mathrm{T}}\mathbf{K}\tilde{\mathbf{\Phi}}\tilde{\mathbf{U}} = \tilde{\mathbf{\Phi}}^{\mathrm{T}}\mathbf{F} \quad (1.10)$$

or

$$\tilde{\mathbf{M}}\dot{\tilde{\mathbf{U}}} + \tilde{\mathbf{K}}\tilde{\mathbf{U}} = \tilde{\mathbf{F}} \quad (1.11)$$

This last matrix system may be solved by standard methods such as direct time integration.

# 2. GENERAL HEAT TRANSFER PROBLEM

## 2.1 Heat Transfer Boundary Value Problem

Complete details of this formulation for the conduction/enclosure radiation problem can be found in [7]. Heat conduction in homogeneous materials is described by the standard nonlinear, diffusion equation

$$\rho C \frac{\partial T}{\partial t} + \frac{\partial}{\partial x_i}\left(-k_{ij}\frac{\partial T}{\partial x_j}\right) = S \quad (2.1)$$

where $T$ is the temperature, $t$ is the time, $x_i$ are the coordinate directions, $\rho$ is the material density, $C$ is the specific heat, $k_{ij}$ is the conductivity tensor and $S$ is the volumetric heat source. The general boundary value problem is completed through specification of boundary conditions

$$T = T_{spec}\left(s_i, t\right) \qquad \text{over} \quad \Gamma_T \quad (2.2)$$

$$\left(-k_{ij}\frac{\partial T}{\partial x_j}\right)n_i = q_{spec}\left(s_i, t\right) + q_{conv} + q_{rad} + q_{enc} \qquad \text{over} \quad \Gamma_q + \Gamma_{enc} \quad (2.3)$$

In the boundary conditions $T_{spec}$ and $q_{spec}$ are specified values of the boundary temperature and heat fluxes; surface-to-surface radiative transfer is represented by $q_{enc}$. Also, $n_i$ is the outward normal to the boundary, $s_i$ are coordinates defined on the boundary, and $q_{conv}$ and $q_{rad}$ refer to the convective and far-field radiative components of the boundary heat flux. These last two quantities are defined by

$$q_{conv} = h_c\left(s_i, T, t\right)\left(T - T_c\right) \quad (2.4)$$

$$q_{rad} = \mathcal{F}\left(\varepsilon\right)\sigma\varepsilon\left(T^4 - T_r^4\right) \quad (2.5)$$

where $h_c$ is the convective heat transfer coefficient, $\varepsilon$ is the surface emissivity, $\mathcal{F}\left(\varepsilon\right)$ is the radiation form factor, $\sigma$ is the Stefan-Boltzmann constant and $T_c$ and $T_r$ are the equilibrium temperatures for which no convection or far-field radiation occur.

The enclosure radiation part of the boundary condition is provided by the radiative energy balance for an enclosure (with *N* surfaces) and is described by

$$\sum_{j=1}^{N}\left[\frac{\delta_{kj}}{\varepsilon_j} - F_{k-j}\left(\frac{1-\varepsilon_j}{\varepsilon_j}\right)\right]\frac{\bar{Q}_j}{A_j} = \sum_{j=1}^{N}\left(\delta_{kj} - F_{k-j}\right)\sigma\,\bar{T}_j^4 \quad (2.6)$$

This relation is written assuming that the surfaces in the enclosure are diffuse and gray; each individual surface is isothermal with a uniform net flux. In the above relation, $\bar{Q}_j$ is the net energy loss, $\bar{T}_j$ is the surface temperature, $\delta_{ij}$ is the unit tensor and $F_{k-j}$ are radiative view factors (configuration factors). The view factors for surfaces with finite area are defined by

$$F_{k-j} = \frac{1}{A_j}\int_{A_k}\int_{A_j}\frac{\cos\theta_k \cos\theta_j}{\pi S^2}\,dA_j\,dA_k \quad (2.7)$$

where the quantities in the equation are defined in Figure 1.

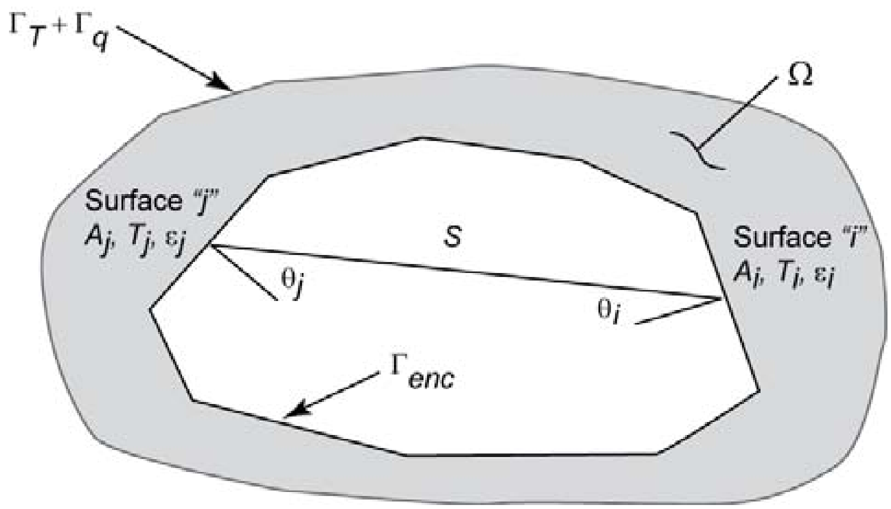


**Figure 1. Sketch of enclosure radiation geometry**

For purposes of computation the above surface energy balance is more conveniently written as

$$\sum_{j=1}^{N}\left[\delta_{kj} - \left(1-\varepsilon_k\right)F_{k-j}\right]\bar{q}_j^{\,o} = \varepsilon_k\,\sigma\,\bar{T}_k^4 \quad (2.8)$$

and

$$\bar{q}_k = \bar{q}_k^o - \sum_{j=1}^{N} F_{k-j}\bar{q}_j^o \quad (2.9)$$

Equations (2.8) and (2.9) are expressed in terms of the outgoing radiative flux for each surface, $\bar{q}_k^o$, and the net flux from each surface, $\bar{q}_k$. For known surface temperatures in the enclosure, Equation (2.8) can be solved for the outgoing radiative flux at each surface. Equation (2.9) then allows the net flux to be evaluated and applied to the conduction problem as a known flux boundary condition $q_{enc}$. This procedure basically defines the standard sequential solution procedure used for coupled conduction, enclosure radiation problems.

## 2.2 Finite Element Models

The reduced order models of interest are those that are derived from high-fidelity, finite element models of the conduction and radiation transfer processes. A standard form of the Galerkin finite element method (GFEM) is used to transform the above continuum problem to a numerical model. The GFEM method is detailed in [7] and need not be repeated here.

The nonlinear heat conduction problem (Equations (2.1) - (2.5)) when reduced to a finite element model may be written in matrix form as

$$\mathbf{K}(\mathbf{T})\mathbf{T} + \mathbf{B}\bar{\mathbf{q}} = \mathbf{F} \quad (2.10)$$

Here, $\mathbf{K}$ represents the global "stiffness" matrix which includes the diffusion operator and contributions from the capacitance term in the time-dependent case. The $\mathbf{F}$ vector represents boundary fluxes, source terms and contributions from the capacitance term when an implicit integration method is used. In all of the present work a second-order, predictor-corrector (Adams-Bashforth/trapezoid rule) algorithm has been employed. Complete details of these numerical methods are available in [7]. The entries in $\mathbf{B}$ are from the weak form of the boundary integral for the applied enclosure radiation fluxes denoted by $\bar{q}$.

The discrete form of the enclosure radiation problem (Equations (2.8) - (2.9)) can be expressed in matrix form as

$$\left(\mathbf{I} - \boldsymbol{\rho}\mathbf{F}_{\mathrm{vf}}\right)\bar{\mathbf{q}} = \left(\mathbf{I} - \mathbf{F}_{\mathrm{vf}}\right)\boldsymbol{\varepsilon}\boldsymbol{\sigma}\bar{\mathbf{T}}^4 = \left(\mathbf{I} - \mathbf{F}_{\mathrm{vf}}\right)\boldsymbol{\varepsilon}\boldsymbol{\sigma}\mathbf{E}_{\mathrm{b}} \quad (2.11)$$

or in a compact form

$$\mathbf{A}(\bar{\mathbf{T}})\bar{\mathbf{q}} = \mathbf{D}(\bar{\mathbf{T}})\bar{\mathbf{T}} \quad (2.12)$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{F}_{\mathrm{vf}}$ is the matrix of view factors, $\boldsymbol{\rho}$ and $\boldsymbol{\varepsilon}$ are diagonal matrices of reflectances and emittances and $\mathbf{E}_{\mathrm{b}}$ is a vector representing the black-body emissive power. Also, $\mathbf{A}$ is the radiative flux coefficient matrix with a temperature dependence due only to surface properties and $\mathbf{D}$ is the surface temperature coefficient matrix with a cubic dependence on temperature. The vector $\bar{q}$ is the net radiative flux on each surface and $\bar{\mathbf{T}}$ is the vector of uniform temperatures on each surface.

## 2.3 Computation Technique for Fully Coupled Method

Most combined heat conduction and enclosure radiation problems are solved in some type of decoupled algorithm in which each type of thermal transport is solved in sequence and iteratively coupled at the boundary of the domains. This type of method was alluded to in a previous section. A prerequisite to reduced order modeling for general problems is the ability to solve conduction and radiation in a fully coupled manner. This is a requirement because global basis functions are utilized and separate functions for the conduction and radiation parts are not very useful.

Previous work on fully coupled methods [8] has shown the effectiveness of the approach in terms of computational efficiency and rate of convergence. The previous implementation was limited to small problems as the algorithm was constructed using methods appropriate for single processor applications. To be useful for ROM work, a fully coupled, parallel algorithm needed to be designed and implemented. To comment further on the implementation difficulties of a parallel, fully coupled solution method, some details of the algorithm and matrix problem are required.

Following the description in [8], the fully coupled solution method first combines the finite element form of the conduction equation (2.10) with the discrete form of the enclosure radiation equation (2.12) to form the matrix system

$$\begin{bmatrix} \mathbf{K}(\mathbf{T}) & \mathbf{B} \\ -\bar{\mathbf{D}}(\mathbf{T}) & \mathbf{A} \end{bmatrix} \begin{Bmatrix} \mathbf{T} \\ \bar{\mathbf{q}} \end{Bmatrix} = \begin{Bmatrix} \mathbf{F}(\mathbf{T}) \\ \mathbf{0} \end{Bmatrix} \quad (2.13)$$

The unknowns in this system are the nodal point temperatures in the conduction regions and the net radiative flux on each surface of the enclosure. Manipulations to transform (uniform) surface temperatures in the enclosure to nodal point temperatures are not detailed here but may be found in [8]. Note that the conduction portions of the problem lead to sparse, symmetric matrices; the matrix associated with enclosure radiation is fully populated and unsymmetric.

The combined system in (2.13) is a nonlinear algebraic system that could be solved with any fixed point iterative method. The method of choice is Newton's method because of the polynomial dependence of the radiation equation on temperature. A Newton iteration for (2.13) may be written as

$$\begin{bmatrix} \mathbf{K}(\mathbf{T}^n) & \mathbf{B} \\ -4\bar{\mathbf{D}}(\mathbf{T}^n) & \mathbf{A} \end{bmatrix} \begin{Bmatrix} \Delta\mathbf{T} \\ \Delta\bar{\mathbf{q}} \end{Bmatrix} = \begin{Bmatrix} -\mathbf{K}(\mathbf{T}^n)\mathbf{T}^n - \mathbf{B}\bar{\mathbf{q}}^n + \mathbf{F}(\mathbf{T}) \\ -\mathbf{A}\bar{\mathbf{q}}^n + \bar{\mathbf{D}}(\mathbf{T}^n)\mathbf{T}^n \end{Bmatrix} \quad (2.14)$$

Note that for time dependent problems the solution of (2.14) provides the field solution at a given time plane; predictor, multiple corrector methods at a time plane can provide a robust and accurate solution to the high-fidelity model.

The solution of the matrix problem given in (2.14) is amenable to iterative solvers, such as GMRES [9]. At Sandia, access to the various libraries of matrix solvers is usually provided by a software library called the Finite Element Interface (FEI) [10]. This interface provides the utilities for assembling the coefficient matrices in standard finite element models, implementation of boundary conditions, solver processing and returning of the solution values. The construction and assembly of the equation coefficients for each element degree of freedom is normally done on an element by element basis. The relation between the local element degrees of freedom and the global degrees of freedom is contained in a connectivity array which is a relatively short list of node numbers. The length of the connectivity vector is determined by how many degrees of freedom are in an element. This type of assembly works extremely well for standard finite element equations such as found in the conduction part of the problem.

The assembly of the equations for the enclosure radiation part of the problem and the coupling terms with the conduction problem is more problematic using the FEI approach. While a temperature degree of freedom (in the conducting region) is connected to relatively few other temperature degrees of freedom, a surface flux or surface temperature may be connected to every other surface in the enclosure. Most finite element mesh generators do not construct a connectivity array relating all exposed surfaces and exposed surfaces to the nodes on those surfaces. Basically, the FEI was not designed to handle enclosure radiation type equations. Note that the connectivity problem is compounded when a parallel implementation is considered and processor to processor communication of surface data is required.

The limitations of the standard FEI were overcome by using a combination of MPI [11] routines to generate an internal enclosure connectivity and some low-level, FEI routines to manipulate individual equations within the global matrix. Unfortunately, this implementation took considerable time and compromised the original timeline for the ROM project. The result however, was a parallel solution capability for fully coupled conduction and enclosure radiation problems. This is a capability unique to Sandia software. The legacy code COYOTE [12] contains this coupled capability and will be made available in an open source format. Note that newer versions of the FEI may allow this type of assembly to be performed directly. This path was not pursued because access to the newer FEI would have required a very significant amount of legacy code modification.

## 2.4 Fully Coupled Example

A number of coupled conduction/radiation problems have been used as test problems to demonstrate the efficiency of the fully coupled algorithm. These problems were used in [8] to test various solution strategies and were all run on a single processor with a research version of the finite element thermal analysis software. These tests were rerun with the new version of the parallel code and found to produce the same results. Details of these solutions are available in [8] and need not be repeated here. In the present study, the fully coupled algorithm was implemented to ensure the ability to perform large, high-fidelity simulations as a precursor to the ROM.

# 3. REDUCED ORDER MODELS

## 3.1 Introduction

As noted in Section 1.3, two basic approaches to reduced order models were initially considered; modal analysis and proper orthogonal decomposition. Looking first at the modal analysis approach, we were unable to determine a useful method for linearizing the system for a general transient problem. This implied that a series of eigensolutions would have to be generated during the course of a transient analysis. A study of the form of the generalized eigenvalue problem corresponding to (2.14) revealed other potential difficulties. The availability of an eigensolver that would run in parallel and handle the large dense unsymmetric radiation part of the system was questionable. It was also unknown if the dominant transport would be contained in only the few lowest modes of the system. To our knowledge no one has looked at the eigen-structure of a radiation problem much less a combined system. For these reasons and a diminished timeline, the modal approach was dropped from further consideration.

The POD method appeared to have none of the drawbacks of the modal approach and was selected for further investigation. As a standard eigenvalue problem would be part of this method we obtained a version of the ARPACK [13] library for eventual use in our implementation. A software implementation of the POD method was initiated using the legacy code COYOTE [12]. The thermal analysis code was first modified to run a fully coupled, high-fidelity model and record a number of user defined snapshots. These snapshots (solutions) would be used in a subsequent run to generate the covariance matrix and ultimately the reduced order model. Unfortunately, at this point project funding expired and the investigation was terminated.

# 4. SUMMARY AND SUGGESTIONS FOR FURTHER WORK

This late start LDRD program focused on the development and implementation of a Reduced Order Model for combined heat conduction and enclosure radiation problems. Though ROM of heat conduction problems have been generated and used successfully, no combined conduction and radiation models have been considered. These types of problems are of some importance to a number of applications at Sandia. The project first constructed a parallel, fully coupled conduction/enclosure radiation solution method. This algorithm was essential to generating a ROM and also provided a unique capability in thermal analysis. Unfortunately, this implementation was very time consuming because of the special nature of the matrix assembly process for the combined system and the lack of functionality in various software libraries.

Of the various methods for ROM generation we believe that Proper Orthogonal Decomposition (POD) holds the most promise for combined conduction/radiation problems. This study should be continued as the need for ROM of thermal systems will only increase in future projects.

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