# Optimal Locally-Constrained Basis-Dependent Projection-Based Model Reduction

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One popular category of model reduction techniques is projection-based model reduction [1]. This class of techniques takes the right-hand side of an ODE (1)

$$\dot{\mathbf{y}}(t) = \mathbf{\Gamma}(\mathbf{y}(t)) \tag{1}$$

and determines a projection matrix $\mathbf{P}$ from this right-hand side and some additional data (typically reference values of state variables and error tolerances). This right-hand side is called the original model. The reduced model (2) constructed by the technique is the right-hand side of the ODE, premultiplied by the projection matrix determined by the technique:

$$\dot{\mathbf{y}}(t) = \mathbf{P}\mathbf{\Gamma}(\mathbf{y}(t)). \tag{2}$$

However, despite the popularity of projection-based model reduction techniques, for the case of nonlinear ODEs, there exists no practical procedure to bound the approximation error in the solution of the reduced model ODE constructed by one of these techniques, relative to the solution of the original model ODE, given comparable initial conditions for both ODEs.

The projection-based model reduction technique with the most developed theory for bounding the approximation error is proper orthogonal decomposition [2]. A classical result on error bounds exists for linear systems [3], [4]. Rathinam and Petzold [5] proved a result on error bounds for nonlinear systems; their result requires bounds on the logarithmic norm of the Jacobian of the right-hand side of the reduced model ODE and bounds on the Lipschitz constant of the right-hand side of the reduced model ODE. Homescu, *et al.* [6] also suggest using a small sample statistical condition to estimate the bounds on the approximation error with a known probability that these bounds are valid.

Other projection-based model reduction techniques have much less well-developed theories for bounding the approximation error due to model reduction. Computational singular perturbation [7], [8] bounds the approximation error in the right-hand side of the reduced model at a single point. The method of reaction invariants [9] yields an exact reduced model (no approximation error), where the rank of the projection matrix obtained from the reduced model is equal to the rank of the stoichiometry matrix in the right-hand side of the original model ODE. The methods of linear species lumping first proposed by Wei and Kuo [10] and later expanded upon by Li and Rabitz [11], [12] (and others) also yield exact reduced models under certain conditions. For the remainder of techniques, although many authors have proposed error control heuristics, rigorous error bounds of any sort are not usually available. Li and Rabitz [13] also developed error metrics for the case where linear species lumping does not yield an exact reduced model. The linearized quasi-steady state approximation [14] uses error tolerances that resemble relative approximation error in the right-hand side of the reduced model relative to the right-hand side of the original model. Gorban and Karlin state that the method of invariant manifolds yields a reduced model whose solution is attracted to the solution of the corresponding original model [15], [16].

The contribution of this work will be to propose a new projection-based model reduction technique that, given a set of basis vectors, determines a minimum rank projector satisfying local error constraints on the time derivatives of state variables. This technique will be extended in subsequent work to yield the first projection-based model reduction technique that can be used to construct bounds on the approximation error in the solution of the reduced model ODE it constructs, relative to the solution of the original model ODE, given comparable initial conditions for both ODEs. It can also be used to compare the efficiency of basis sets (such as the CSP basis vectors) from different model reduction techniques subject to the same local error constraints; here, the projector rank is one proposed metric for efficiency (discounting bases with pathologically low rank). Finally, to the knowledge of the authors, this formulation is the first projection-based model reduction technique determined using optimization.

Given an original model with $n$ state variables, the proposed algorithm takes a basis set of vectors in $n$-dimensional Euclidean space, a collection of reference values for state variables, and error tolerances as input. From these inputs, an integer linear program (ILP) is constructed. This ILP determines the minimum rank projector satisfying local error constraints such that the basis set can be partitioned into vectors that are either in the range of the projector or its nullspace.

To formulate a projection-based model reduction technique by solving an optimization problem, both an objective function to be optimized and constraints must be defined. An intuitive objective function to be minimized is the rank of the projector, since it is a linear function of the elements of a projection matrix (the rank of a projection matrix is its trace), and the rank of a projection matrix

corresponds to the number of lumped species (similar to CSP modes) required in a lumped model representation of the reduced model. Since the computational effort required to integrate the chemistry term in a reacting flow simulation scales roughly quadratically with the number of species, minimizing the number of lumped species also corresponds to minimizing the CPU time needed to solve the reduced model. Furthermore, the rank of the projection matrix corresponds to the maximum number of nonzero eigenvalues of the Jacobian matrix of the reduced model, so minimizing the rank of the projection matrix is likely to yield a less stiff reduced model, which will also decrease its solution time.

Two types of constraints are necessary for an optimization problem governing a projection-based model reduction technique to be well posed. The first constraint is obvious: the formulation must determine a projection matrix, so if $\mathbf{P}$ is the projection matrix determined by the formulation, then $\mathbf{P}^2 = \mathbf{P}$. Note that $\mathbf{P}$ is not required to be symmetric, allowing the possibility of skew projectors. The second constraint follows from previous work on reaction-elimination and species elimination: the approximation error incurred by model reduction must be limited.

The combination of the proposed objective function and constraints suggests an optimization formulation of the form:

$$\min_{\mathbf{P}} \sum_{j=1}^{n} p_{jj} \tag{3a}$$

$$\text{s.t. } \mathbf{P}^2 = \mathbf{P} \tag{3b}$$

$$G[\mathbf{y}_{\text{ref}}(t), \mathbf{y}(t, \mathbf{P})] \leq 0 \tag{3c}$$

$$\mathbf{P} \in \mathbb{R}^{n \times n},$$

where $\mathbf{y}_{\text{ref}}$ is a reference solution of (1) (a collection of reference points also suffices) and $G$ is a user-defined functional describing the approximation error incurred by model reduction. For reasons detailed in [17], $G$ will be chosen to limit the difference between the time derivative of the solution of the original model and the solution of the detailed model at user-specified reference points:

$$|((\mathbf{I} - \mathbf{P})\mathbf{\Gamma}(\mathbf{y}_{\text{ref},i}))_j| \leq (atol)_j + (rtol)_j |\Gamma_j(\mathbf{y}_{\text{ref},i})|, \quad j = 1, \ldots, n; i = 1, \ldots, N_R, \tag{4}$$

where $\mathbf{y}_{\text{ref},i} \in \mathbb{R}^n$, $i = 1, \ldots, N_R$ is a collection of $N_R$ reference points, and $(atol)_j$ and $(rtol)_j$ are user-specified absolute and relative error tolerances, respectively, for state variable $j = 1, \ldots, n$. This form for $G$ yields linear constraints that ease significantly the solution of an optimization formulation.

The constraint $\mathbf{P}^2 = \mathbf{P}$ poses considerable difficulty from an optimization standpoint because it is a nonlinear, nonconvex constraint. The only way to enforce this constraint in such a way that it yields a tractable formulation for large-scale problems is to make assumptions about the structure of the projection matrix $\mathbf{P}$. One such assumption follows by noting that the Jordan decomposition of any projection matrix has the form:

$$\mathbf{P} = \mathbf{B}\mathbf{W}\mathbf{B}^{-1}, \tag{5}$$

where $\mathbf{B}$ is an invertible matrix, and $\mathbf{W}$ is a diagonal matrix consisting of ones and zeroes. If $\mathbf{w}$ is the vector of diagonal elements of $\mathbf{W}$, then such a projection matrix has the property that its range is the span of the set of vectors $\{\mathbf{b}_j : w_j = 1\}$, and its nullspace is the span of the set of vectors $\{\mathbf{b}_j : w_j = 0\}$; these mathematical properties of the projector also determine the physical behavior of the reduced model. The relationship between the projector $\mathbf{P}$ and the matrix $\mathbf{B}$ indicates that $\mathbf{B}$ is a basis matrix; in conjunction with the constraint (4), this relationship gives rise to the name "optimal locally-constrained basis-dependent projection-based model reduction".

Combining (3), (4), and (5) yields the formulation:

$$\min_{\mathbf{w}} \sum_{j=1}^{n} w_j \tag{6a}$$

$$|((\mathbf{I} - \mathbf{B}\mathbf{W}\mathbf{B}^{-1})\mathbf{\Gamma}(\mathbf{y}_{\text{ref},i}))_j| \leq (atol)_j + (rtol)_j |\Gamma_j(\mathbf{y}_{\text{ref},i})|, \quad j = 1, \ldots, n; i = 1, \ldots, N_R, \tag{6b}$$

$$\mathbf{w} \in \{0, 1\}^n,$$

where $\mathbf{B}$ is a constant, user-supplied, and invertible basis matrix. This formulation is an ILP, and can be solved quite efficiently for large case studies, as evidenced by similar ILP formulations shown in [17], [18], [19].

Using this newly proposed technique, model reduction case studies are carried out to demonstrate that this technique is practical by showing that the computations are feasible, and can be carried out in a reasonable amount of time, even on large case studies.

Both the theory and the numerical experiments show that the proposed technique reliably bounds the approximation error in the right-hand side of the reduced model ODE relative to the right-hand side of the original model ODE at the reference values of the state variables specified by the user.

In the future, the ILP formulation in this work will be extended using interval arithmetic [20] to bound the approximation error in the right-hand side of the reduced model ODE relative to the right-hand side of the original model ODE over a range of reference values of the state variables specified by the user. This extension parallels the extension of point-constrained reaction elimination [17] to range-constrained reaction elimination [18] and the extension of point-constrained simultaneous reaction and species elimination [19] to range-constrained simultaneous reaction and species elimination [21]. Bounding the approximation error for a range of reference values of state variables enables the construction of error bounds on the solution of the reduced model ODE relative to the solution of the original model ODE. By constructing these bounds, it will be possible to reduce the computational

costs of combustion simulations for practical applications and guarantee the accuracy of these simulation results to within known tolerances.

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