

EFFICIENT REDUCED MODELS FOR PARAMETRIZED DYNAMICAL SYSTEMS BY OFFLINE/ONLINE DECOMPOSITION

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Abstract. Reduced basis (RB) methods are effective methods for model reduction of parametrized partial differential equations (P²DEs). During the last years various types of stationary and time-dependent, linear and nonlinear P²DEs have been treated. In the field of dynamical systems' order reduction, these methods are largely unknown, but the interest in reduction of parametrized systems is increasing. In the current presentation, we show that some characteristic components of RB-methods can be transferred to model reduction of parametrized dynamical systems. We exemplify this for linear systems with output estimation. A so called offline/online decomposition is the key for efficient simulation: In the offline phase, one prepares the reduced basis and auxiliary parameter-independent quantities. These preparations allow rapid online simulations for varying parameters. The possibly extensive offline phase pays off in case of a multi-query context, where sufficiently many reduced simulations with different parameter constellations are to be expected. In addition to the effective reduced simulation schemes, error control is possible by a posteriori error estimators. These are based on residual analysis and can also be effectively decomposed in an offline/online fashion and hence allow fast and rigorous error guarantees.

1 Introduction

Reduced basis (RB) methods are effective methods for model reduction of parametrized partial differential equations (P²DEs). This are partial differential equations, where parameters characterize the system, e.g. geometry, material, boundary-value, initial-value or control parameters. The need for parametrized reduced models can result from multi-query scenarios, where many simulations have to be performed for varying parameters such as parameter studies, parameter optimization, inverse problems, etc. Similarly, real-time requirements can be a motivation for parametrized model reduction, e.g. control, interactive simulation environments, etc. In addition to parametrized reduced models, a fast rigorous parameter-dependent quantification of the model error is required. This is provided by RB-methods. During the last years various types of stationary and time-dependent, linear and nonlinear P²DEs have been treated with this technique [12, 5, 6, 8, 14]. An overview with many further recent references is given by [11]. In the field of dynamical systems' order reduction, these methods are partially unknown, but the interest in reduction of parametrized systems is increasing. For example, [2] already considers solution of parametrized systems by concatenating projection bases of special parameter choices. Parametrized systems are tackled with moment matching techniques in [13] and [4].

In the current presentation, we show that some characteristic components of RB-methods can be transferred to model reduction of parametrized dynamical systems. We exemplify this for linear systems with output estimation. A so called offline/online decomposition is the key for efficient simulation. In the offline phase, one prepares the reduced basis and auxiliary parameter-independent quantities. These preparations allow rapid online simulations for varying parameters with complexity independent of the original state dimension. The possibly extensive offline phase pays off in case of a multi-query context, where sufficiently many reduced simulations with different parameter constellations are to be expected. In addition to the effective reduced simulation schemes, error control is possible by a posteriori error estimators. These are based on residual analysis and can also be effectively decomposed in an offline/online fashion and hence allow fast and rigorous error guarantees. In contrast to global-in-time a priori estimates in classical MOR of dynamical systems, these a posteriori error estimates provide error bounds for the state variable or output variable point-wise in time.

In the following section, we introduce the reduced basis simulation scheme for parametrized problems. Sec. 3 is devoted to the algorithmical decomposition into an offline and online phase. For the current formulation a posteriori error estimation is demonstrated in Sec. 4 including a full offline-online decomposition. We conclude in Sec. 5. We refrain from presenting experiments in this paper, but refer to RB schemes for linear instationary P²DEs, as these are particular instances of the presented reduced simulation scheme after simple time discretization, [6, 8].

2 Parametrized Reduced Simulation Scheme

We assume the following parametrized linear dynamical system for a state variable $x(t) \in \mathbb{R}^n$, input $u(t) \in \mathbb{R}^m$ and output variable $y(t) \in \mathbb{R}^p$ for $t \in [0, \infty)$

$$\frac{d}{dt}x(t) = \mathbf{A}(t, \mu)x(t) + \mathbf{B}(t, \mu)u(t) \quad (1)$$

$$y(t) = \mathbf{C}(t, \mu)x(t) + \mathbf{D}(t, \mu)u(t). \quad (2)$$

The system matrices $\mathbf{A}(t, \mu) \in \mathbb{R}^{n \times n}$, $\mathbf{B}(t, \mu) \in \mathbb{R}^{n \times m}$, $\mathbf{C}(t, \mu) \in \mathbb{R}^{p \times n}$, $\mathbf{D}(t, \mu) \in \mathbb{R}^{p \times m}$ depend on a parameter $\mu \in \mathcal{P} \subset \mathbb{R}^d$ from a bounded parameter domain \mathcal{P} . The parameter μ is assumed to be fixed during a single simulation of the dynamical system. Occasionally, the solution and output will be denoted as $x(t, \mu), y(t, \mu)$ to emphasize their parameter dependence. Given a projection matrix $\mathbf{V} \in \mathbb{R}^{n \times k}$ with reduced model order $k \ll n$ and $\mathbf{W} \in \mathbb{R}^{n \times k}$ biorthogonal, i.e. $\mathbf{W}^T \mathbf{V} = \mathbf{I}_{k \times k}$, the reduced system reads as usual [1]

$$\frac{d}{dt}\hat{x}(t) = \hat{\mathbf{A}}(t, \mu)\hat{x}(t) + \hat{\mathbf{B}}(t, \mu)u(t) \quad (3)$$

$$\hat{y}(t) = \hat{\mathbf{C}}(t, \mu)\hat{x}(t) + \hat{\mathbf{D}}(t, \mu)u(t) \quad (4)$$

with reduced system matrices

$$\hat{\mathbf{A}}(t, \mu) := \mathbf{W}^T \mathbf{A}(t, \mu) \mathbf{V}, \quad \hat{\mathbf{B}}(t, \mu) := \mathbf{W}^T \mathbf{B}(t, \mu) \quad (5)$$

$$\hat{\mathbf{C}}(t, \mu) := \mathbf{C}(t, \mu) \mathbf{V}, \quad \hat{\mathbf{D}}(t, \mu) := \mathbf{D}(t, \mu) \quad (6)$$

and initial condition

$$\hat{x}(0) = \hat{x}_0 := \mathbf{W}^T x(0). \quad (7)$$

In reduced basis methods, the projection basis \mathbf{V} is constructed in a simulation-based way such that $\text{colspan} \mathbf{V} \subset \text{span}\{x(t_i, \mu_i)\}_{i \in I}$. Here t_i, μ_i are suitably selected time instants and parameters and $x(t_i, \mu_i)$ so called snapshots of the solution. The basis matrix \mathbf{V} is commonly orthonormalized with respect to a certain problem specific inner product, such that the reduced system is numerically more stable. For more details on basis generation in RB-methods, we refer to [11, 7, 8, 6]. In the following, however, we do not put any assumption on the reduced basis apart from biorthogonality of \mathbf{V} and \mathbf{W} . Hence in particular, the method and results are as well valid for Krylov-subspace bases, bases obtained from balanced truncation, POD, etc.

3 Offline-Online Decomposition

For efficient computation, we put some assumptions on the matrices and initial data, such that the system matrices can be decomposed as a weighted sum of parameter-independent parts, where the weights are parameter dependent. Note that the basic idea of linear superposition of systems has also been used in [2]. Here we perform a refined argumentation, which results in an online simulation scheme, the complexity of which is completely independent of n .

For the system matrices we assume the following separable parameter dependence

$$\mathbf{A}(t, \mu) = \sum_{q=1}^{Q_A} \sigma_A^q(t, \mu) \mathbf{A}^q, \quad \mathbf{B}(t, \mu) = \sum_{q=1}^{Q_B} \sigma_B^q(t, \mu) \mathbf{B}^q, \quad \mathbf{C}(t, \mu) = \sum_{q=1}^{Q_C} \sigma_C^q(t, \mu) \mathbf{C}^q. \quad (8)$$

with scalar parameter- and time-dependent coefficient functions $\sigma_A^q, \sigma_B^q, \sigma_C^q$ and parameter- and time-independent matrices $\mathbf{A}^q, \mathbf{B}^q, \mathbf{C}^q$ of suitable dimensions and small number of components Q_A, Q_B, Q_C . We assume, that the initial data variations of the system are not arbitrary, but can similarly be described by parameter variations, i.e. $x(0) = x_0(\mu)$ with

$$x_0(\mu) = \sum_{q=1}^{Q_{x_0}} \sigma_{x_0}^q(\mu) x_0^q. \quad (9)$$

Making use of the assumed parameter dependence, the reduced simulation can be performed rapidly in a complexity, which is completely independent of n . This is obtained by an offline/online decomposition.

In the offline phase, the parameter-independent quantities of the reduction scheme are computed. This phase may be arbitrary time consuming, as it will pay off in view of sufficiently many online simulations. First, the biorthogonal projection matrices \mathbf{V} and \mathbf{W} may be generated by any algorithm. Then the following parameter independent components are computed:

$$\hat{\mathbf{A}}^q := \mathbf{W}^T \mathbf{A}^q \mathbf{V}, \quad \hat{\mathbf{B}}^q := \mathbf{W}^T \mathbf{B}^q, \quad \hat{\mathbf{C}}^q := \mathbf{A}^q \mathbf{V}, \quad \hat{x}_0^q := \mathbf{W}^T x_0^q. \quad (10)$$

In the online phase, the parameter μ is known and the reduced simulation matrices can be assembled in complexity independent of n . In particular we obtain from (8)–(9) and (10).

$$\hat{\mathbf{A}}(t, \mu) = \sum_{q=1}^{Q_A} \sigma_A^q(t, \mu) \hat{\mathbf{A}}^q, \quad \hat{\mathbf{B}}(t, \mu) = \sum_{q=1}^{Q_B} \sigma_B^q(t, \mu) \hat{\mathbf{B}}^q, \quad (11)$$

$$\hat{\mathbf{C}}(t, \mu) = \sum_{q=1}^{Q_C} \sigma_C^q(t, \mu) \hat{\mathbf{C}}^q, \quad \hat{\mathbf{D}}(t, \mu) = \mathbf{D}(t, \mu), \quad \hat{x}_0(\mu) = \sum_{q=1}^{Q_{x_0}} \sigma_{x_0}^q(\mu) \hat{x}_0^q. \quad (12)$$

The separable parameter dependence of the components is not a strong assumption, as there are several methods to obtain such exact or approximate decompositions. First, if the dynamical system results from a discretization of a physical problem, the physical parameters can frequently be tracked through the discretization and hereby explicitly give such a desired decomposition, as e.g. done for finite volume discretizations [8]. This clearly requires full control over the discretization, which is realizable (and a good argument) for own development of discretization code instead of using black-box discretization packages. If there is some algebraic model knowledge about the parameter dependence, e.g. the number of components and the coefficient functions are known, but the component matrices not, these matrices can be constructed by setting up matrix equations from sample matrices and solving for the matrix components [10]. If the matrices are given as explicit functions $\mathbf{A}(\mu, t)$ or can be obtained from a black-box discretization software-package, approximation methods can be used to produce finite-sum representations, e.g. polynomial, modal or empirical interpolation [3].

4 A Posteriori Error Estimation

A further attractive aspect of RB-methods is rigorous error analysis. In particular a posteriori error estimates can be obtained. For this we define the error and residual

$$e(t, \mu) := x(t, \mu) - \mathbf{V}\hat{x}(t, \mu), \quad R(t, \mu) := \mathbf{A}(t, \mu)\mathbf{V}\hat{x}(t) + \mathbf{B}(t, \mu)u(t) - \mathbf{V}\frac{d}{dt}\hat{x}(t). \quad (13)$$

This residual has the notable property, that it is zero, if the exact solution $x(t)$ evolves in the column-span of \mathbf{V} , i.e. the reduced system reproduces the exact system's solution without approximation. Further, it satisfies a so called *Galerkin orthogonality* $\mathbf{W}^T R(t, \mu) = 0$ due to (3) and the biorthogonality of \mathbf{W} and \mathbf{V} . The error in particular satisfies

$$e(0, \mu) = x_0(\mu) - \mathbf{V}\hat{x}_0(\mu) = (\mathbf{I}_{n \times n} - \mathbf{V}\mathbf{W}^T)x_0(\mu). \quad (14)$$

For deriving a posteriori error estimators, suitable norms must be chosen. We assume, that some positive definite inner matrix $\mathbf{G} \in \mathbb{R}^{n \times n}$ is given and denote $\langle x, x' \rangle_{\mathbf{G}} := x^T \mathbf{G} x'$ as the corresponding inner product. This induces a vector norm $\|x\|_{\mathbf{G}} := \sqrt{\langle x, x \rangle_{\mathbf{G}}}$ on \mathbb{R}^n and a matrix-norm $\|\mathbf{A}\|_{\mathbf{G}} := \sup_{\|x\|_{\mathbf{G}}=1} \|\mathbf{A}x\|_{\mathbf{G}}$ for $\mathbf{A} \in \mathbb{R}^{n \times n}$. For the output, we will consider the simple 2-norm, hence define the induced matrix norm $\|\mathbf{C}\|_{\mathbf{G}} := \sup_{\|x\|_{\mathbf{G}}=1} \|\mathbf{C}x\|$ for $\mathbf{C} \in \mathbb{R}^{p \times n}$. The matrix \mathbf{G} can be chosen trivially $\mathbf{G} = \mathbf{I}_{n \times n}$ in the following, which then reproduces the usual 2-norm $\|\cdot\|$ for vectors and matrices. However, other choices of \mathbf{G} are possible in a problem-dependent way, which may improve the error estimator. For demonstrating the error estimation technique, we propose the following a posteriori error estimators for the state variable and output:

Proposition 4.1 (A Posteriori Error Estimate). *We assume that $\mathbf{A}(t, \mu) = \mathbf{A}(\mu)$ is time-invariant and has eigenvalues with nonpositive real part for all μ . Hence, the solutions are bounded and we assume to have a computable constant $C_1(\mu)$ with*

$$C_1(\mu) \geq \sup_t \|\exp(\mathbf{A}(\mu)t)\|_{\mathbf{G}}. \quad (15)$$

Then for the state variable the following error estimate holds:

$$\|x(t, \mu) - \mathbf{V}\hat{x}(t, \mu)\|_{\mathbf{G}} \leq \Delta_x(t, \mu) := C_1(\mu) \|e(0, \mu)\|_{\mathbf{G}} + C_1(\mu) \int_0^t \|R(\tau, \mu)\|_{\mathbf{G}} d\tau. \quad (16)$$

If we additionally assume to have an upper bound $C_2(\mu) \geq \sup_t \|\mathbf{C}(t, \mu)\|_{\mathbf{G}}$, then the following output error estimate holds:

$$\|y(t, \mu) - \hat{y}(t, \mu)\| \leq \Delta_y(t, \mu) := C_2(\mu) \Delta_x(t, \mu). \quad (17)$$

Proof. From the definition of the residual (13) we see that

$$\mathbf{V}\frac{d}{dt}\hat{x}(t) = \mathbf{A}(\mu)\mathbf{V}\hat{x}(t) + \mathbf{B}(t, \mu)u(t) - R(t, \mu). \quad (18)$$

Subtracting this from the original system yields the error evolution equation

$$\frac{d}{dt}e(t) = \mathbf{A}(\mu)e + R(t, \mu) \quad (19)$$

with initial condition (14). This linear system has the explicit solution

$$e(t, \mu) = \exp(\mathbf{A}(\mu)t)e(0) + \int_0^t R(\tau) \exp(\mathbf{A}(\mu)(t - \tau))d\tau. \quad (20)$$

Due to the assumed boundedness of $\|\exp(\mathbf{A}(\mu)s)\|_{\mathbf{G}} \leq C_1(\mu)$ for $s \in \mathbb{R}^+$ we obtain the claimed bound Eqn. (16). For the second statement, we observe that

$$y(t, \mu) - \hat{y}(t, \mu) = \mathbf{C}(t, \mu)x(t, \mu) + \mathbf{D}(t, \mu)u(t) - \mathbf{C}(t, \mu)\mathbf{V}\hat{x}(t, \mu) - \mathbf{D}(t, \mu)u(t) \quad (21)$$

$$= \mathbf{C}(t, \mu)(x(t, \mu) - \mathbf{V}\hat{x}(t, \mu)). \quad (22)$$

which yields Eqn. (17) and concludes the proof. \square

Note, that similar statements for non-stable systems are possible, if only finite times $t \in [0, T]$ are considered. We remark, that the matrix \mathbf{G} in the above formulation is a degree of freedom, which can be used to keep the constants C_1 and C_2 small. Let $\mathbf{A} = \mathbf{U}\mathbf{J}\mathbf{U}^{-1}$ be an eigendecomposition of \mathbf{A} with unitary $\mathbf{U} \in \mathbb{C}^{n \times n}$ and Jordan-block matrix \mathbf{J} . Hence (after extending the $\|\cdot\|_{\mathbf{G}}$ on complex matrices) we have

$$\|\exp(\mathbf{A}t)\|_{\mathbf{G}} = \|\mathbf{U}\exp(\mathbf{J}t)\mathbf{U}^{-1}\|_{\mathbf{G}} \leq \|\mathbf{U}\|_{\mathbf{G}} \|\exp(\mathbf{J}t)\|_{\mathbf{G}} \|\mathbf{U}^{-1}\|_{\mathbf{G}}. \quad (23)$$

If, for example, \mathbf{A} is symmetric, \mathbf{J} is a real diagonal matrix with negative entries. By choosing \mathbf{G} as (a multiple of) the identity matrix, the product remains upper bounded by 1 and $C_1 = 1$ is a proper choice. In dynamical systems obtained from PDE discretizations, the matrix \mathbf{G} is usually chosen as the Gram-Matrix of the finite element / finite volume basis. Then, $\|e\|_{\mathbf{G}}$ is the real function space norm of the error in the finite element / finite volume function space.

The above simple result is practically relevant, as a full offline/online decomposition of the error bound is possible which enables fast and rigorous error estimation during the reduced simulation. This is based on the fact, that residual norms can be determined exactly based on (13). We omit time and parameter dependency in the following notation:

$$\|R\|_{\mathbf{G}}^2 = R^T \mathbf{G} R = \hat{x}^T \mathbf{V}^T \mathbf{A}^T \mathbf{G} \mathbf{A} \mathbf{V} \hat{x} + u^T \mathbf{B}^T \mathbf{G} \mathbf{B} u + \left(\frac{d}{dt}\hat{x}\right)^T \mathbf{V}^T \mathbf{G} \mathbf{V} \left(\frac{d}{dt}\hat{x}\right) \quad (24)$$

$$+ 2u^T \mathbf{B}^T \mathbf{G} \mathbf{A} \mathbf{V} \hat{x} - 2\left(\frac{d}{dt}\hat{x}\right)^T \mathbf{V}^T \mathbf{G} \mathbf{A} \mathbf{V} \hat{x} - 2\left(\frac{d}{dt}\hat{x}\right)^T \mathbf{V}^T \mathbf{G} \mathbf{B} u \quad (25)$$

$$= \hat{x}^T \mathbf{M}_1 \hat{x} + u^T \mathbf{M}_2 u + \left(\frac{d}{dt}\hat{x}\right)^T \mathbf{M}_3 \left(\frac{d}{dt}\hat{x}\right) + \quad (26)$$

$$2u^T \mathbf{M}_4 \hat{x} - 2\left(\frac{d}{dt}\hat{x}\right)^T \mathbf{M}_5 \hat{x} - 2\left(\frac{d}{dt}\hat{x}\right)^T \mathbf{M}_6 u \quad (27)$$

where the matrices \mathbf{M}_1 – \mathbf{M}_6 are introduced as abbreviations for the matrices in (24)–(25).

$$\mathbf{M}_1(t, \mu) = \mathbf{V}^T \mathbf{A}(t, \mu)^T \mathbf{G} \mathbf{A}(t, \mu) \mathbf{V}, \quad \mathbf{M}_2(t, \mu) = \mathbf{B}(t, \mu)^T \mathbf{G} \mathbf{B}(t, \mu), \quad \mathbf{M}_3 := \mathbf{V}^T \mathbf{G} \mathbf{V} \quad (28)$$

$$\mathbf{M}_4(t, \mu) = \mathbf{B}(t, \mu)^T \mathbf{G} \mathbf{A}(t, \mu) \mathbf{V}, \quad \mathbf{M}_5(t, \mu) = \mathbf{V}^T \mathbf{G} \mathbf{A}(t, \mu) \mathbf{V}, \quad \mathbf{M}_6(t, \mu) = \mathbf{V}^T \mathbf{G} \mathbf{B}(t, \mu). \quad (29)$$

In the offline phase, we can compute time- and parameter-independent component matrices, i.e.

$$\mathbf{M}_1^{q, q'} := \mathbf{V}^T (\mathbf{A}^q)^T \mathbf{G} \mathbf{A}^{q'} \mathbf{V} \quad (30)$$

for $q, q' = 1, \dots, Q_A$ and similarly for $\mathbf{M}_2^{q, q'}$, \mathbf{M}_3 (not parameter dependent), $\mathbf{M}_4^{q, q'}$, \mathbf{M}_5^q and \mathbf{M}_6^q . In the online phase, these matrices can be combined and we assemble the matrices of (28)–(29), i.e.

$$\mathbf{M}_1(t, \mu) := \sum_{q, q'} \sigma_A^q(t, \mu) \sigma_A^{q'}(t, \mu) \mathbf{M}_1^{q, q'} \quad (31)$$

and similarly $\mathbf{M}_2, \mathbf{M}_4, \mathbf{M}_5, \mathbf{M}_6$. Note again, that \mathbf{M}_3 is already available from the offline phase. The quantities $\hat{x}(t)$, $\frac{d}{dt}\hat{x}(t)$ and $u(t)$ are available during the reduced simulation, hence the error bound can be computed online.

The initial error in the above estimate (16) can easily be set to 0 by ensuring, that the components of the initial data are in the reduced space, i.e. $x_0^q \in \text{colspan} \mathbf{V}$. For more general basis \mathbf{V} , the norm of the initial error is required for the error estimator in (16)

$$\|e(0, \mu)\|_{\mathbf{G}}^2 = x_0(\mu)^T (\mathbf{I}_{n \times n} - \mathbf{V}\mathbf{W}^T)^T \mathbf{G} (\mathbf{I}_{n \times n} - \mathbf{V}\mathbf{W}^T) x_0(\mu). \quad (32)$$

This can similarly be decomposed in an offline/online fashion. In the offline phase we compute the parameter independent components

$$m^{q,q'} := (x_0^q)^T (\mathbf{I}_{n \times n} - \mathbf{V}\mathbf{W}^T)^T \mathbf{G} (\mathbf{I}_{n \times n} - \mathbf{V}\mathbf{W}^T) x_0^{q'} \quad (33)$$

for $q, q' = 1, \dots, Q_{x_0}$. In the online phase the error norm is assembled by

$$\|e(0, \mu)\|_{\mathbf{G}}^2 = \sum_{q,q'=1}^{Q_{x_0}} \sigma_{x_0}^q(\mu) \sigma_{x_0}^{q'}(\mu) m^{q,q'}. \quad (34)$$

Note, that this error estimator was chosen for simple presentation of the approach. For computation of the above error bound, the exact integral cannot be determined but must be approximated by some quadrature rule. Further, the presented RB-method still is continuous in time and results in a real simulation scheme after suitable time discretization by ordinary differential equation solvers. These steps introduce additional (but controllable) numerical errors in the above analysis. To prevent these additional approximation issues, a posteriori error bounds can be derived, which are suited to specific time integration schemes [8, 6].

Better output-error estimates are possible by considering and computing a suitable dual problem and corresponding dual error estimator [9]. In the linear time-invariant case, this dual problem only has to be computed once. In the linear variant case, however, the dual problem must be solved once for each error estimator evaluation in time, i.e. once for each time t that the estimator is to be evaluated [6].

5 Conclusions

We presented a method for obtaining fast reduced models for parametrized dynamical systems, which is motivated by RB-methods. In view of a multi-query context the resulting offline/online decomposition is an effective algorithmic approach. In particular, the reduced basis is constructed in the offline phase, which relaxes time-constraints. For example time-extensive greedy searches for determining suitable basis vectors can be performed [11]. We presented an example of a posteriori error estimation for state variable and system outputs. The error estimators also allow a full offline/online decomposition. This means, that the reduced simulation not only produces the fast reduced solution, but also a fast and rigorous estimate of the error. These are provided in an online complexity, which is completely independent of the dimensionality n .

If the dimension m of the input variable $u(t)$ is too large, the reduced scheme still may be expensive to simulate. An additional parametrization and assumption of separable decomposition of u may be beneficial, i.e. $u(t, \mu) = \sum_{q=1}^{Q_u} \sigma_u^q(t, \mu) u^q$. By choosing 'typical' input signals u^q , which may be available in practice, this equation (5) then allows to model arbitrary linear combinations of the components u^q over time by suitable choice of coefficient function σ_u^q .

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7 References

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