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Exact linear lumping in abstract spaces*

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Abstract

Exact linear lumping has earlier been defined for a finite dimensional space, that is, for the system of ordinary differential equations $y' = f \circ y$ as a linear transformation M for which there exists a function $\hat{f}$ such that $\hat{y} := My$ itself obeys a differential equation $\hat{y}' = \hat{f} \circ \hat{y}$. Here we extend the idea for the case when the values of y are taken in a Banach space. The investigations are restricted to the case when f is linear.

Many theorems hold for the generalization of exact lumping, such as necessary and sufficient conditions for lumpability, and relations between the qualitative properties of the original and the transformed equations.

The motivation behind the generalization of exact lumping is to apply the theory to reaction-diffusion systems, to an infinite number of chemical species, to continuous components, or to stochastic models as well.

Keywords: reduction of the number of variables, lumping, reaction-diffusion equations, differential equations in abstract spaces, qualitative properties
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1 Introduction

Mathematical models of chemical reaction kinetics are used in many fields such as in basic research in physical chemistry and biochemistry and in the design and control of chemical reactors, in combustion, in atmospheric chemistry, in pharmacokinetics, etc. The use of these models is often restricted because of the large number of dependent variables, which usually are the species' concentrations. There is a technique in finite dimensional real spaces, called *lumping:* reduction of the number of variables by grouping them via a linear or nonlinear function. This approach was initiated by [Wei and Kuo, 1969], and extended to exact linear [Li, G. and Rabitz, H., 1989],[Li, G. and Rabitz, H., 1991a], [Li, G. and Rabitz, H., 1991b] and exact nonlinear [Li, G. et al., 1994] lumping

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of arbitrary nonlinear differential equations, and these methods have also been applied to practical problems arising in petroleum cracking, catalytic reforming, biochemistry, combustion, see the reference list of [Tóth et al., 1997], toxicology [Verhaar et al., 1997] etc.

Similar reduction methods have been investigated in many areas such as control theory, econometrics, biology, and ecology [Luenberger, 1964], [Łos and Łos, 1974], [Iwasa et al., 1987], [Iwasa et al., 1989], [Luckyanov et al., 1983].

In the present paper our goal is to extend the theory of lumping to infinite dimensional abstract spaces, so as to be able to apply it to systems of partial differential equations, such as reaction-diffusion systems, to an infinite number of chemical species (occuring e.g. in petroleum cracking), to continuous components (where the species are parameterized by the value of some physical quantity), or to stochastic models as well. Let us mention that reaction diffusion systems have been treated earlier by covering also the case when the reaction is not necessarily linear ([Li, G. and Rabitz, H., 1991b]).

The application of lumping to abstract differential equations will also be useful for stochastic models and difference equations. We have to use some notions and theorems from the theory of functional analysis, but beyond these, the paper is self-contained.

In Section 2 we introduce some notions we will use in the rest of the paper. In Section 3 we establish and prove some necessary and sufficient conditions on exact linear lumpability. Section 4 treats the behavior of periodic solutions and equilibria under lumping. Next, relation between stability of the original and the lumped model is investigated. Finally, applying the theory presented we do lump a simple, and a slightly more complicated equation in Section 6, and discuss the possible further developments.

2 Basic notions

Let X and $\widehat{X}$ be Hilbert-spaces, such that X has a closed subspace W for which $W \cong \widehat{X}$. $K \in \mathcal{L}(X)$ is a (*not necessarily bounded*) linear transformation of X, $\mathbf{u} : \mathbb{R} \to X$ is a solution of

$$\dot{\mathbf{u}} = K\mathbf{u}. \tag{1}$$

Lemma 1 Suppose that $\mathbf{k} \circ \mathbf{u}_\alpha = \mathbf{l} \circ \mathbf{u}_\alpha$ holds for the functions $\mathbf{k}, \mathbf{l} : X \to \widehat{X}$ with some functions $\mathbf{u}_\alpha : \mathbf{R} \to X$ ($\alpha \in A$, where A is a set of indices) for which $\cup_\alpha \mathrm{Range}(\mathbf{u}_\alpha) = X$ holds. Then $\mathbf{k} = \mathbf{l}$ is also true.

The proof is straightforward, so we omit it.

Definition 1 Let $M : X \to \widehat{X}$ be a bounded linear operator such that $\mathrm{Range}(M) = \widehat{X}$. If for all solutions $\mathbf{u}$ to (1)

$$\widehat{\mathbf{u}} := M\mathbf{u} \tag{2}$$

obeys a differential equation

$$\dot{\widehat{\mathbf{u}}} = \widehat{K}\widehat{\mathbf{u}} \tag{3}$$

with some linear transformation $\widehat{K} \in \mathcal{L}(\widehat{X})$, then (1) is said to be exactly lumpable to (3) by M.

3 Lumpability

For the finite dimensional case of the statements below see [Tóth et al., 1996]

Theorem 1 Equation (1) is exactly linearly lumpable to (3) by M if and only if

$$MK = \widehat{K}M \tag{4}$$

holds.

Proof. A) Suppose (1) is exactly lumpable to (3). Then $\dot{\widehat{\mathbf{u}}} = (M\mathbf{u})^{\cdot} = M\dot{\mathbf{u}} = MK\mathbf{u}$ and $\dot{\widehat{\mathbf{u}}} = \widehat{K}\widehat{\mathbf{u}} = \widehat{K}M\mathbf{u}$ shows the necessity through Lemma 1.
B) Suppose $\mathbf{u}$ is a solution of (1) and $MK = \widehat{K}M$ holds. Then

$$\dot{\widehat{\mathbf{u}}} = (M\mathbf{u})^{\cdot} = M\dot{\mathbf{u}} = MK\mathbf{u} = \widehat{K}M\mathbf{u} = \widehat{K}\widehat{\mathbf{u}}$$

shows that (3) also holds.

Remark 1 Li and Rabitz [Li, G. and Rabitz, H., 1991b] investigated reaction-diffusion systems of the form

$$\dot{\mathbf{u}} = \mathcal{K}\mathbf{u} + \mathcal{D}\Delta\mathbf{u}, \tag{5}$$

where $\mathcal{K}$ and $\mathcal{D}$ are operators induced by matrices K and D. They tried to lump it to another reaction-diffusion system

$$\dot{\widehat{\mathbf{u}}} = \widehat{\mathcal{K}}\widehat{\mathbf{u}} + \widehat{\mathcal{D}}\Delta\widehat{\mathbf{u}} \tag{6}$$

by $\mathcal{M}$, so that $\widehat{\mathbf{u}} = \mathcal{M}\mathbf{u}$, where $\mathcal{M}$ is induced by the matrix M. In this special case they found that (5) is exactly linearly lumpable to (6) if and only if both of the requirements

$$MK = \widehat{K}M \tag{7}$$

and

$$MD = \widehat{D}M \tag{8}$$

are fulfilled. Multiplying (8) by Δ from the right and adding it to (7) we get

$$M(K + D\Delta) = (\widehat{K} + \widehat{D}\Delta)M, \tag{9}$$

which shows that the case treated by Li and Rabitz is a special case of ours.

Nevertheless our last example in Section (6) is a reaction-diffusion system, and we also lump it to another reaction-diffusion system in that special case, when $D = d \cdot I$, d is a positive constant.

Definition 2 ([Luenberger, 1969], p. 163) Let X and $\widehat{X}$ be Hilbert spaces, $M \in \mathcal{L}(X, \widehat{X})$ continuous and $\mathrm{Range}(M)$ closed. Let $\widehat{\mathbf{x}} \in \widehat{X}$ be fixed and denote by $\widehat{\mathbf{y}} \in \mathrm{Range}(M)$ the element for which $\|\widehat{\mathbf{x}} - \widehat{\mathbf{y}}\| \leq \|\widehat{\mathbf{x}} - \widetilde{\mathbf{y}}\|$ for all $\widetilde{\mathbf{y}} \in \mathrm{Range}(M)$. Let $Y \subset X, \quad Y := \{\mathbf{x} \in X | M\mathbf{x} = \widehat{\mathbf{y}}\}$ and denote by $\overline{\mathbf{y}} \in Y$ that element for which $\|\overline{\mathbf{y}}\|_X \leq \|\mathbf{y}\|_X$ holds for all $\mathbf{y} \in Y$. Let us define the operator $\overline{M} \in \mathcal{L}(\widehat{X}, X)$ by $\overline{M}\widehat{\mathbf{x}} := \overline{\mathbf{y}}$. This operator is referred to as *the pseudoinverse* of M, and can be shown to be continuous.

Definition 3 Suppose for a linear operator $M : X \to \widehat{X}$ there exists another linear operator $\overline{M} : \widehat{X} \to X$ such that $M\overline{M} = I_{\widehat{X}}$. This will be referred to as a *generalized (right) inverse* of M.

Remark 2 The pseudoinverse of a continuous linear operator is not always a generalized inverse as well.

Lemma 2 ([Luenberger, 1969], p. 165) Suppose $M : X \to \widehat{X}$ is a continuous linear operator, such that $\mathrm{Range}(M) = \widehat{X}$. Then the pseudoinverse $\overline{M}$ of M, can be calculated as $M^*(MM^*)^{-1}$, where M^* is the adjoint of M and this pseudoinverse is also a generalized inverse.

Theorem 2 Let $\overline{M}$ be a generalized inverse of M. Then (1) is exactly linearly lumpable to (3) by M if and only if $MK = MK\overline{M}M$ holds.

Proof. A) Suppose (1) is exactly linearly lumpable to (3). Then, Theorem 1 implies that, $MK = \widehat{K}M$. Composing both sides with $\overline{M}$ from the right we get $MK\overline{M} = \widehat{K}$, and this again with M from the right $MK\overline{M}M = \widehat{K}M = MK$, where the last equality also comes from Theorem 1.
B) To prove sufficiency, let $\widehat{K} := MK\overline{M}$ and use the assumption to obtain $\widehat{K}M = MK\overline{M}M = MK$, which is known to be a sufficient condition to exact lumpability by Theorem 1.

Theorem 3 If (1) is exactly linearly lumpable to (3) by M, then the right hand side $\widehat{K}$ does not depend on the specific choice of the generalized inverse of M.

Proof. Let $\overline{M}$ and $\widetilde{M}$ be two generalized inverses of M. Then by Theorem 2 $(MK)\overline{M} = (MK\widetilde{M}M)\overline{M} = MK\widetilde{M}(M\overline{M}) = MK\widetilde{M}$.

Theorem 4 Equation (1) is exactly linearly lumpable to (3) with M if and only if $\mathrm{Ker}(M)$ is invariant for K.

Proof. A) We need to prove that for any $\mathbf{x} \in X$ such that $M\mathbf{x} = \widehat{\mathbf{0}} \in \widehat{X}$, $MK\mathbf{x} = \widehat{\mathbf{0}}$ is also valid. Suppose $\mathbf{x} \in X$, such that $M\mathbf{x} = \widehat{\mathbf{0}}$, and use Theorem 1 to get $MK\mathbf{x} = \widehat{K}M\mathbf{x} = \widehat{K}\widehat{\mathbf{0}} = \widehat{\mathbf{0}}$.

B) Conversely, let $\mathbf{x} \in X$. $M\mathbf{x} = M\overline{M}M\mathbf{x}$, so $M(\mathbf{x} - \overline{M}M\mathbf{x}) = \widehat{\mathbf{0}}$, that is, $\mathbf{x} - \overline{M}M\mathbf{x} \in \mathrm{Ker}(M)$, so using our assumption we have $MK(\mathbf{x} - \overline{M}M\mathbf{x}) = \widehat{\mathbf{0}}$, which means that $MK\mathbf{x} = MK\overline{M}M\mathbf{x}$. Now Theorem 2 proves sufficiency.

Remark 3 The theorem above implies that for all linear systems there exists a linear lumping operator. The analogous statement is not true for nonlinear systems.

Remark 4 This means that to construct a lumping operator M, it is enough to search for invariant subspaces of X for a given linear transformation.

We shall also use the statement (which is easy to prove) below.

Lemma 3 Let $W \subset X$ be a linear subspace, and let $K \in \mathcal{L}(X)$ be a linear operator on X. W is invariant for K if and only if $W^{\perp}$ is invariant for K^*, where K^* is the adjoint of K.

Corollary 1 Equation (1) is exactly linearly lumpable to (3) with M if and only if $\mathrm{Ker}(M)^{\perp}$ is invariant for K^*

Definition 4 (1) is said to induce the *dynamical system* (or: *characterisitc function*) $\psi : \mathbf{R} \times X \to X$, where $\psi(t, \mathbf{u}_0)$ is the solution of (1) with the initial condition $\mathbf{u}(0) = \mathbf{u}_0$ at time $t \in \mathbf{R}$. We also use the notation $\psi_t := \psi(t, .)$ to denote *the flow* induced by (1).

Theorem 5 The flow induced by (3) is the function $\widehat{\psi}_t := M\psi_t \circ \overline{M}$. Furthermore, $\widehat{\psi}_t \circ M = M\psi_t$ also holds.

Proof. Let $\widehat{\mathbf{u}}_0 := M\mathbf{u}_0$ and let us show that $t \mapsto \widehat{\psi}_t(\widehat{\mathbf{u}}_0)$ is *the* solution of the differential equation (3) with the initial condition $\widehat{\mathbf{u}}(0) = \widehat{\mathbf{u}}_0$. Let us start with the initial condition $M\psi_0(\overline{M}\widehat{\mathbf{u}}_0) = M\overline{M}\widehat{\mathbf{u}}_0 = \widehat{\mathbf{u}}_0$. Now let us calculate the time derivative of $t \mapsto \widehat{\psi}_t(\widehat{\mathbf{u}}_0)$:

$$
\begin{aligned}
(\widehat{\psi}_t)^{\cdot}(\widehat{\mathbf{u}}_0) = M\dot{\psi}_t(\overline{M}\widehat{\mathbf{u}}_0) = MK\psi_t(\overline{M}\widehat{\mathbf{u}}_0) = \\
= \widehat{K}M\psi_t(\overline{M}\widehat{\mathbf{u}}_0) = \widehat{K}\widehat{\psi}_t(\widehat{\mathbf{u}}_0)
\end{aligned}
$$

The proof of the second statement is similar.

Remark 5 The relation between $\widehat{\psi}_t$ and ψ_t is a generalized conjugacy [Godbillon, 1969].

4 Invariant sets

Definition 5 A set $S \subset X$ is said to be *invariant under the flow* ψ_t, if $\psi_t(S) \subset S$ for all $t \in \mathbf{R}$.

Theorem 6 Invariant sets under the flow generated by (1) are transformed by a lumping operator into invariant sets of (3).

Proof. Let S be an invariant set of (1), and let $\widehat{S}$ be defined as the set obtained from S by lumping: $\widehat{S} := \{M\mathbf{u}|\mathbf{u} \in S\}$. Let us denote the flow generated by (1) by ψ_t. Let $\widehat{\mathbf{u}} \in \widehat{S}$ be an arbitrary vector. By definition, there exists $\mathbf{u} \in S$ such that $\widehat{\mathbf{u}} = M\mathbf{u}$ holds. By Theorem 5, $\widehat{\psi}_t(\widehat{\mathbf{u}}) = \widehat{\psi}_t(M\mathbf{u}) = M\psi_t(\mathbf{u})$. However, $\psi_t(\mathbf{u}) \in S$ because S is invariant; thus $M\psi_t(\mathbf{u}) \in \widehat{S}$ as it is a result of applying the mapping M to an element of S.

Definition 6 Let $K \in \mathcal{L}(X)$. The vector $\mathbf{u}^* \in X$ for which $K\mathbf{u}^* = \mathbf{0}$ holds is an *equilibrium.*

Theorem 7 Equilibria are lumped into equilibria.

Proof. Let $\mathbf{u}^*$ be an equilibrium of the original system: $K\mathbf{u}^* = \mathbf{0}$, and let $\widehat{\mathbf{u}}^* := M\mathbf{u}^*$. Then

$$\widehat{K}\widehat{\mathbf{u}}^* = \widehat{K}M\mathbf{u}^* = MK\mathbf{u}^* = \widehat{\mathbf{0}}.$$

Theorem 8 Periodic solutions of (1) are lumped into periodic solutions of (3).

Proof. Let $\mathbf{u}$ be a periodic solution of (1) with the fundamental period $T \in \mathbf{R}^+ : \mathbf{u}(t+T) = \mathbf{u}(t)$ for all $t \in \mathbf{R}$. Then $\widehat{\mathbf{u}} := M\mathbf{u}$ is a periodic solution to (3) as well, since $\widehat{\mathbf{u}}(t+T) = M\mathbf{u}(t+T) = M\mathbf{u}(t) = \widehat{\mathbf{u}}(t)$ shows, and the fundamental period of $\widehat{\mathbf{u}}$ can easily be seen not to be larger than T.

The finite dimensional version of the statement below has been proved in [Tóth et al., 1997]. Here we give the proof by Prof. Z. Sebestyén for the infinite dimensional case.

Theorem 9 Let $X, \widehat{X}$ Hilbert-spaces, $\widehat{X} \subset X$, $M \in \mathcal{L}(X, \widehat{X})$, Range$(M) = \widehat{X}$, $A \in \mathcal{L}(\widehat{X})$, $B \in \mathcal{L}(X)$. If the relation $AM = MB$ holds, then the spectrum of A is a subset of the spectrum of B, i.e.: $\sigma(A) \subset \sigma(B)$.

Proof. Let us show that $(A-\lambda I_{\widehat{X}})$ is not invertible for any $\lambda \in \mathbf{C}$ implies $(B-\lambda I_X)$ is not invertible for the same λ either, that is $\sigma(A) \subset \sigma(B)$. Nevertheless, if we can prove that, if $(B-\lambda I_X)$ is invertible, then $(A-\lambda I_{\widehat{X}})$ is invertible too, that is the resolvent of B is a subset of the resolvent of $A : \rho(B) \subset \rho(A)$, this statement is equivalent to the original one.
Now, suppose for $\lambda \in \mathbf{C}$ there exists $(B-\lambda I_X)^{-1}$. We show that in this case there exists $(A-\lambda I_{\widehat{X}})^{-1}$, as well. Because of the assumption Range$(M) = \widehat{X}$, by Lemma 2 there exists a generalised inverse $\overline{M}$ of M. The only thing we have to do is to check that $M(B-\lambda I_X)^{-1}\overline{M}$ gives us the inverse of $(A-\lambda I_{\widehat{X}})^{-1}$.

$$\begin{aligned}(A-\lambda I_{\widehat{X}})(M(B-\lambda I_X)^{-1}\overline{M}) &= (AM-\lambda M)(B-\lambda I_X)^{-1}\overline{M}\\ = (MB-\lambda M)(B-\lambda I_X)^{-1}\overline{M} &= M(B-\lambda I_X)(B-\lambda I_X)^{-1}\overline{M}\\ &= M\overline{M} = I_{\widehat{X}}.\end{aligned}$$

5 Stability

For the investigation of stability we use standard notions and a statement. For the case of linear systems, it is enough to study the stability of the zero solution.

Definition 7 Let A be the generator the generator of a strongly continuous semigroup $(T(t))_{t\geq 0}$ on a Banach space E. Then

1. $\omega(f) := \inf\{w : \|T(t)f\| \leq Me^{wt} \textit{for some } M \textit{ and every } t \geq 0\}$ is called the *(exponential) growth bound of* $T(\cdot)f$.

2. $\omega_1(A) := \sup\{\omega(f) : f \in D(A)\}$ is called the *(exponential) growth bound of the solutions* of the Cauchy problem $\dot{\mathbf{u}}(t) = A\mathbf{u}(t)$.

3. $\omega(A) = \sup\{\omega(f) : f \in E\}$ is called the *(exponential) growth bound of the mild solutions* of the Cauchy problem $\dot{\mathbf{u}}(t) = A\mathbf{u}(t)$.

Definition 8 The semigroup $(T(t))_{t\geq 0}$ is called

1. *uniformly exponentially stable* if $\omega(A) < 0$;

2. *exponentially stable* if $\omega_1(A) < 0$;

3. *uniformly stable* if $\|T(t)f\| \to 0$ (as $t \to +\infty$) for every $f \in E$;

4. *stable* if $\|T(t)f\| \to 0$ as $t \to +\infty$) for every $f \in D(A)$.

Definition 9 The semigroup $(T(t))_{t\geq 0}$ is called *eventually norm continuous* if there exists $t' \geq 0$ such that the function $t \to T(t)$ from $(t', +\infty)$ into $\mathcal{L}(E)$ is norm continuous.

Remark 6 In the equation

$$\dot{\mathbf{u}} = \mathcal{K}\mathbf{u} + \mathcal{D}\Delta\mathbf{u}, \tag{10}$$

where $\mathcal{K}$ and $\mathcal{D}$ are operators induced by matrices K and D, the operator $\mathcal{K}+\mathcal{D}\Delta$ is eventually norm continuous with all $t' > 0$.

Theorem 10 [Engel and Nagel, 2000, p. 302] An eventually norm-continuous semigroup $(T(t))_{t\geq 0}$ is uniformly exponentially stable if and only if the spectral abscissa $\beta := \sup\{\mathrm{Re}(\lambda); \lambda \in \sigma(\mathcal{A})\}$ of its generator A satisfies $\beta < 0$.

Corollary 2 Consider the abstract differential equation (1) $\dot{\mathbf{u}} = K\mathbf{u}$ which can be exactly linearly lumped to (3) $\dot{\widehat{\mathbf{u}}} = \widehat{K}\widehat{\mathbf{u}}$, and consider also one of the equilibria $\mathbf{u}^* \in X$ of (1). By Theorem 7 $\widehat{\mathbf{u}}^* := M\mathbf{u}^*$ is an equilibrium of (3).

1. If the spectral abscissa of the operator on the right hand side of the original equation (1) is negative, then both the equilibrium $\mathbf{0}$ of the original equation and $\widehat{\mathbf{0}}$ of the lumped equation are globally stable.

2. If the spectral abscissa of the operator on the right hand side of the lumped equation (3) is positive, then both the equilibrium of the lumped equation $\widehat{\mathbf{u}}^*$ and the original equation $\mathbf{u}^*$ are unstable.

Proof.

1. First of all note that, if the spectral abscissa of an operator on the right hand side of an equation is negative, then 0 is not an eigenvalue of the operator, so the kernel of the operator consists only of $\mathbf{0}$.

   By Theorem 9, which says $\sigma(\widehat{K}) \subset \sigma(K)$, the spectral abscissa of $\widehat{K} \leq$ the spectral abscissa of K.

   (These also mean that the equilibrium points $\mathbf{u}^*$ and $\widehat{\mathbf{u}}^*$ in the assumption of the theorem must be $\mathbf{0} \in X$ and $\widehat{\mathbf{0}} \in \widehat{X}$, respectively.)

2. Again, we use the fact that $\sigma(\widehat{K}) \subset \sigma(K)$, the spectral abscissa of $\widehat{K} \leq$ the spectral abscissa of K, and also Theorem 10.

6 Examples

The first example shows that our framework is a generalization of the finite dimensional theory.

Example 1 The usual mass action type deterministic model of the formal chemical reaction $\mathcal{A}+\mathcal{U} \longrightarrow 2\mathcal{U}+2\mathcal{V} \quad \mathcal{V} \longrightarrow \mathcal{U}$, where $\mathcal{A}$ is an external species of constant concentration is the ordinary differential equation

$$\dot{c}_u = c_u + c_v, \quad \dot{c}_v = 2c_u - c_v$$

for the concentrations $t \mapsto c_u(t), t \mapsto c_v(t)$ of the species $\mathcal{U}$ and $\mathcal{V}$ [Érdi and Tóth, 1989]. In the present case $X = \mathbf{R}^2; K = \begin{pmatrix} 1 & 1 \\ 2 & -1 \end{pmatrix}$, and all the invariant subspaces under K^* can be obtained by calculating its eigenvectors and putting them into the matrix M as rows. (Multiplications with nonsingular matrices from the left are also allowed, because the same subspace will be generated.) The eigenvectors of K^* being $\begin{pmatrix} 1+\sqrt{3} \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1-\sqrt{3} \\ 1 \end{pmatrix}$ (corresponding to the eigenvalues $\sqrt{3}$ and $-\sqrt{3}$, respectively) the possible choices for M are:

$$\begin{pmatrix} n(1+\sqrt{3}) & n \end{pmatrix} \quad (n \in \mathbf{R} \setminus \{0\}), \tag{11}$$

$$\begin{pmatrix} n(1-\sqrt{3}) & n \end{pmatrix} \quad (n \in \mathbf{R} \setminus \{0\}), \tag{12}$$

$$\begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix} \begin{pmatrix} 1+\sqrt{3} & 1 \\ 1-\sqrt{3} & 1 \end{pmatrix}$$

$$(n_{ij} \in \mathbf{R}; i,j \in \{1,2\}, \quad n_{11}n_{22} - n_{12}n_{21} \neq 0). \tag{13}$$

Using the first possibility with $n := 1$ we obtain for $\widehat{c} := (1+\sqrt{3})c_u + c_v$ the lumped differential equation

$$\dot{\widehat{c}} = \sqrt{3}\widehat{c}$$

in accordance with the classical finite dimensional theory [Li, 1984], [Li, G. and Rabitz, H., 1989].

The second example shows the obviously expected fact that elimination of diffusion leads to the original kinetic differential equation.

Example 2 Now let us have the previous reaction system with diffusion, that is, we are given a partial differential equation system, where the operator Δ represents the diffusion, and assume that Neumann boundary conditions hold true:

$$\begin{aligned} \partial_0 u(t,x) &= \Delta u(t,x) + u(t,x) + v(t,x), \qquad & \partial_0 v(t,x) &= \Delta v(t,x) + 2u(t,x) - v(t,x) \\ \partial_1 u(t,-\pi) &= 0, \partial_1 u(t,\pi) = 0 & \partial_1 v(t,-\pi) &= 0, \partial_1 v(t,\pi) = 0, \end{aligned} \tag{14}$$

with $\Delta := \partial_1^2$. It is convenient to introduce the following Hilbert spaces:

$$X := H^2([-\pi,\pi]) \times H^2([-\pi,\pi]),$$

where $H^2([-\pi,\pi])$ is the Sobolev space of distributions which are twice differentiable and square integrable together with their second derivative on $[-\pi,\pi]$, with the scalar product

$$\left\langle \begin{pmatrix} u_1 \\ v_1 \end{pmatrix}, \begin{pmatrix} u_2 \\ v_2 \end{pmatrix} \right\rangle := \int_{-\pi}^{\pi} u_1 v_1 + \int_{-\pi}^{\pi} u_2 v_2;$$

and $\widehat{X} := \mathbb{R}^2$ with the usual scalar product in $\mathbf{R}^2$.

The right hand side of (14) is obtained by applying the operator K to the elements of X, where K is defined in the following way:

$$\left(K\begin{pmatrix} u \\ v \end{pmatrix}\right)(t,x) := \begin{pmatrix} \Delta u(t,x) + u(t,x) + v(t,x) \\ \Delta v(t,x) + 2u(t,x) - v(t,x) \end{pmatrix}.$$

(One question is: how to find all the nontrivial invariant subspaces of the linear operator K. Here we choose only one possibility.)

We shall show that the kernel of the operator $M : X \longrightarrow \widehat{X}$ defined by $\left(M\begin{pmatrix} u \\ v \end{pmatrix}\right)(t) := \int_{-\pi}^{\pi} \begin{pmatrix} u(t,x) \\ v(t,x) \end{pmatrix} \mathrm{d}x$ is invariant to K.

Let $\begin{pmatrix} u \\ v \end{pmatrix} \in X$ be an element of the kernel of M. Then, applying K we have to prove that $\begin{pmatrix} \Delta u + u + v \\ \Delta v + 2u - v \end{pmatrix}$ is also in the kernel of M. Let's apply M :

$$\begin{aligned} \int_{-\pi}^{\pi} \begin{pmatrix} \Delta u(t,x) + u(t,x) + v(t,x) \\ \Delta v(t,x) + 2u(t,x) - v(t,x) \end{pmatrix} \mathrm{d}x &= \\ \begin{pmatrix} \int_{-\pi}^{\pi} \Delta u(t,x)\mathrm{d}x + \int_{-\pi}^{\pi} u(t,x)\mathrm{d}x + \int_{-\pi}^{\pi} v(t,x)\mathrm{d}x \\ \int_{-\pi}^{\pi} \Delta v(t,x)\mathrm{d}x + 2\int_{-\pi}^{\pi} u(t,x)\mathrm{d}x - \int_{-\pi}^{\pi} v(t,x)\mathrm{d}x \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \end{aligned}$$

taking into consideration that, $\Delta u = \operatorname{div}\operatorname{grad} u$, so by *Gauss–Ostrogradski theorem* or *divergence theorem* (to think of the multidimensional case) $\int_{[-\pi,\pi]} \Delta u = \int_{[-\pi,\pi]} \operatorname{div}\operatorname{grad} u = \operatorname{grad} u(t,\pi) - \operatorname{grad} u(t,-\pi) = 0$, for every u or v in X. By this, the operator M is a lumping operator.

Let's look for an appropriate $\widehat{K}$.

$$
\begin{aligned}
\dot{\widehat{\begin{pmatrix} u \\ v \end{pmatrix}}}(t) &= \left(M\begin{pmatrix} u \\ v \end{pmatrix}\right)^{\cdot}(t) = M\partial_0\begin{pmatrix} u \\ v \end{pmatrix}(t) = \int_{-\pi}^{\pi}\begin{pmatrix} \partial_0 u(t,x) \\ \partial_0 v(t,x) \end{pmatrix}\mathrm{d}x \\
&= \int_{-\pi}^{\pi}\begin{pmatrix} \Delta u(t,x) + u(t,x) + v(t,x) \\ \Delta v(t,x) + 2u(t,x) - v(t,x) \end{pmatrix}\mathrm{d}x \\
&= \begin{pmatrix} \int_{-\pi}^{\pi}\Delta u(t,x)\mathrm{d}x + \int_{-\pi}^{\pi}u(t,x)\mathrm{d}x + \int_{-\pi}^{\pi}v(t,x)\mathrm{d}x \\ \int_{-\pi}^{\pi}\Delta v(t,x)\mathrm{d}x + 2\int_{-\pi}^{\pi}u(t,x)\mathrm{d}x - \int_{-\pi}^{\pi}v(t,x)\mathrm{d}x \end{pmatrix} \\
&= \begin{pmatrix} \int_{-\pi}^{\pi}u(t,x)\mathrm{d}x + \int_{-\pi}^{\pi}v(t,x)\mathrm{d}x \\ 2\int_{-\pi}^{\pi}u(t,x)\mathrm{d}x - \int_{-\pi}^{\pi}v(t,x)\mathrm{d}x \end{pmatrix} \\
&= \widehat{K}\widehat{\begin{pmatrix} u \\ v \end{pmatrix}}(t),
\end{aligned} \tag{15}
$$

where $\widehat{K}$ acts on the space $\widehat{X}$ as $\widehat{K}\begin{pmatrix} d_u \\ d_v \end{pmatrix}(t) = \widehat{\mathcal{K}}\begin{pmatrix} d_u(t) \\ d_v(t) \end{pmatrix}$ and $\widehat{\mathcal{K}} = \begin{pmatrix} 1 & 1 \\ 2 & -1 \end{pmatrix}$.

Upon denoting $d_u(t) := \int_{-\pi}^{\pi} u(t,x)\mathrm{d}x, \quad d_v(t) := \int_{-\pi}^{\pi} v(t,x)\mathrm{d}x$, by lumping we have obtained from the original PDE this ODE:

$$d_u'(t) = d_u(t) + d_v(t), \quad d_v'(t) = 2d_u(t) - d_v(t). \tag{16}$$

Although the above two examples might be instructive, the structure of the next one is much closer to real life applications.

Example 3 Now let us have the same partial differential equation system, as above. Now our aim is to simplify it, but not necessarily eliminate diffusion.

$$\partial_0 u = \Delta u + u + v, \quad \partial_0 v = \Delta v + 2u - v.$$

If we define the operator

$$\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \mathbf{w} \mapsto K\mathbf{w} := (\Delta w_1 + w_1 + w_2, \Delta w_2 + 2w_1 - w_2)$$

on pairs of analytic functions, we get the abstract form of the above partial differential equation system:

$$\dot{\mathbf{w}} = K\mathbf{w}.$$

First, we try to solve this equation. Let us represent the values of the solutions of the two above examples in $L^2[-\pi,\pi]\times L^2[-\pi,\pi]$ using the orthogonal basis: $\{\cos(nx), \sin(nx)\}\quad (n \in \mathbf{N})$. Now we are looking for solutions in the form:

$$\mathbf{w}(t) = x \mapsto \begin{pmatrix} a_0(t) + \sum_{n=1}^{+\infty} \big(a_n(t)\cos(nx) + b_n(t)\sin(nx)\big) \\ c_0(t) + \sum_{n=1}^{+\infty} \big(c_n(t)\cos(nx) + d_n(t)\sin(nx)\big) \end{pmatrix} \tag{17}$$

with differentiable functions a_n, b_n, c_n, d_n, for $n \in \mathbf{N}_0$. What does it mean that the function (17) is the solution of the original equation $\dot{\mathbf{w}} = K\mathbf{w}$? Calculating the time derivative term by term we get

$$(\dot{\mathbf{w}}(t))(x) = \begin{pmatrix} a_0'(t) + \sum_{n=1}^{+\infty} \big(a_n'(t)\cos(nx) + b_n'(t)\sin(nx)\big) \\ c_0'(t) + \sum_{n=1}^{+\infty} \big(c_n'(t)\cos(nx) + d_n'(t)\sin(nx)\big) \end{pmatrix}.$$

On the other hand, applying the operator K we obtain

$$((K\mathbf{w})(t))(x) = \left(\begin{matrix} a_0(t) + c_0(t) + \sum_{n=1}^{+\infty} \big(a_n(t) + c_n(t) - n^2 a_n(t)\big)\cos(nx) + \\ 2a_0(t) - c_0(t) + \sum_{n=1}^{+\infty} \big(2a_n(t) - c_n(t) - n^2 c_n(t)\big)\cos(nx) + \end{matrix} \right. \\ \left. \begin{matrix} + \sum_{n=1}^{+\infty} \big(b_n(t) + d_n(t) - n^2 b_n(t)\big)\sin(nx) \\ + \sum_{n=1}^{+\infty} \big(2b_n(t) - d_n(t) - n^2 d_n(t)\big)\sin(nx) \end{matrix} \right),$$

and comparing the coefficients we get

$$a_0'(t) = a_0(t) + c_0(t) \quad c_0'(t) = 2a_0(t) - c_0(t),$$

and the infinite system of linear constant coefficient differential equations

$$\begin{aligned} a_n'(t) &= a_n(t) + c_n(t) - n^2 a_n(t) \quad c_n'(t) = 2a_n(t) - c_n(t) - n^2 c_n(t), \\ b_n'(t) &= b_n(t) + d_n(t) - n^2 b_n(t) \quad d_n'(t) = 2b_n(t) - d_n(t) - n^2 d_n(t), \end{aligned}$$

$(n = 1, 2, \ldots)$ consisting of 2×2 blocks, which is therefore easily solvable.

If we would like to lump our system, we have to find if not all, but at least one of the nontrivial invariant subspaces of the linear operator K, if we wish to lump the equation by the method described above.

Now, it is obvious, that with respect to the operator K, the closed linear subspace:

$$V := \left\{ \mathbf{v} | \mathbf{v} = \begin{pmatrix} x \mapsto a_0 + \sum_{k=1}^{+\infty} \big(a_{2k}\cos(2kx) + b_{2k}\sin(2kx)\big) \\ x \mapsto c_0 + \sum_{k=1}^{+\infty} \big(c_{2k}\cos(2kx) + d_{2k}\sin(2kx)\big) \end{pmatrix}, \right. \\ \left. \sum_{k=1}^{+\infty} k^2(|a_k|^2 + |b_k|^2 + |c_k|^2 + |d_k|^2) < +\infty \right\}$$

(actually, H^2 again) is invariant: $KV \subset V$. Let us define the linear operator $M : V \times V \to V$ by

$$\begin{aligned} (M\mathbf{w})(x) &:= M \begin{pmatrix} a_0 + \sum_{n=1}^{+\infty} \big(a_n\cos(nx) + b_n\sin(nx)\big) \\ c_0 + \sum_{n=1}^{+\infty} \big(c_n\cos(nx) + d_n\sin(nx)\big) \end{pmatrix} \\ &= c_1 + a_1\cos(x) + b_1\sin(x) + \sum_{k=1}^{+\infty} \big(c_{2k+1}\cos(2kx) + d_{2k+1}\sin(2kx) \\ &+ a_{2k+1}\cos((2k+1)x) + b_{2k+1}\sin((2k+1)x)\big). \end{aligned}$$

Lemma 4 With the above definitions we have $V = \mathrm{Ker}(M)$.

Proof. A) It is obvious that $V \subset \mathrm{Ker}(M)$.

B) Now let us take an element from $\mathrm{Ker}(M)$, and let us show that it should be of the form which can be found in the definition of the subspace V. $(M\mathbf{w})(x) = 0$ means that that for all $x \in [-\pi, \pi]$ we have

$$\begin{aligned}(c_1 + a_1 \cos(x) + b_1 \sin(x) + \sum_{k=1}^{+\infty} \big(c_{2k+1} \cos(2kx) + d_{2k+1} \sin(2kx)\\ + a_{2k+1} \cos((2k+1)x) + b_{2k+1} \sin((2k+1)x)\big) = 0.\end{aligned}$$

This, however, implies that all the coefficients with odd indices are zero, therefore $\mathbf{w} \in V$.

The next step is to find a generalized inverse $\overline{M}$ of M, because knowing it will give us $\widehat{K} = MK\overline{M}$. To do this, we shall construct M^* first, and then $\overline{M}$ comes (according to Lemma 2) from the equation $\overline{M} = M^*(MM^*)^{-1}$.

By straightforward, although lengthy calculations M^* is derived:

$$M^* \left(a_0 + \sum_{n=1}^{+\infty} a_n \cos(nx) + b_n \sin(nx) \right) =$$

$$\begin{pmatrix} \sum_{k=1}^{+\infty} \big(a_{2k-1} \cos((2k-1)x) + b_{2k-1} \sin((2k-1)x)\big) \\ 2a_0 \cos(x) + \sum_{k=1}^{+\infty} \big(a_{2k} \cos((2k+1)x) + b_{2k} \sin((2k+1)x)\big) \end{pmatrix}$$

and then,

$$\overline{M} \left(a_0 + \sum_{n=1}^{+\infty} a_n \cos(nx) + b_n \sin(nx) \right) =$$

$$M^*(MM^*)^{-1} \left(a_0 + \sum_{n=1}^{+\infty} a_n \cos(nx) + b_n \sin(nx) \right) =$$

$$\begin{pmatrix} \sum_{k=1}^{+\infty} \big(a_{2k-1} \cos((2k-1)x) + b_{2k-1} \sin((2k-1)x)\big) \\ a_0 \cos(x) + \sum_{k=1}^{+\infty} \big(a_{2k} \cos((2k+1)x) + b_{2k} \sin((2k+1)x)\big) \end{pmatrix}$$

Now, denoting $\widehat{\mathbf{u}}(x) := a_0 + \sum_{n=1}^{+\infty} a_n \cos(nx) + b_n \sin(nx)$, we have

$$\widehat{K}\widehat{\mathbf{u}} = MK\overline{M}\widehat{\mathbf{u}} =$$

$$\begin{aligned}\Big(-2a_0 + 2a_1 + a_0 \cos(x) + \sum_{k=1}^{+\infty} \alpha_{2k} \cos(2kx) + \beta_{2k} \sin(2kx) +\\ \alpha_{2k+1} \cos((2k+1)x) + \beta_{2k+1} \sin((2k+1)x)\Big)\end{aligned}$$

where

$$\begin{aligned}\alpha_{2k} &:= 2a_{2k+1} - a_{2k} - (2k+1)^2 a_{2k}\\ \beta_{2k} &:= 2b_{2k+1} - b_{2k} - (2k+1)^2 b_{2k}\\ \alpha_{2k+1} &:= a_{2k} + a_{2k+1} - (2k+1)^2 a_{2k+1}\\ \beta_{2k+1} &:= b_{2k} + b_{2k+1} - (2k+1)^2 b_{2k+1}\end{aligned}$$

Comparing the derivative

$$\dot{\widehat{\mathbf{u}}} = \left(a_0'(t) + \sum_{n=1}^{+\infty} a_n'(t)\cos(nx) + b_n'(t)\sin(nx) \right),$$

and the right hand side

$$\widehat{K}\widehat{\mathbf{u}} = \Big(-2a_0(t) + 2a_1(t) + a_0(t)\cos(x) + \sum_{k=1}^{+\infty} \alpha_{2k}(t)\cos(2kx) + \\ \beta_{2k}(t)\sin(2kx) + \alpha_{2k+1}(t)\cos((2k+1)x) + \\ \beta_{2k+1}(t)\sin((2k+1)x)\Big)$$

the lumped equation $\dot{\widehat{\mathbf{u}}} = \widehat{K}\widehat{\mathbf{u}}$ takes the form

$$\begin{aligned}
a_0'(t) &= -2a_0(t) + 2a_1(t)\\
a_1'(t) &= a_0(t)\\
b_1'(t) &= 0\\
a_{2k}'(t) &= 2a_{2k+1}(t) - a_{2k}(t) - (2k+1)^2 a_{2k}(t)\\
a_{2k+1}'(t) &= a_{2k}(t) + a_{2k+1}(t) - (2k+1)^2 a_{2k+1}(t)\\
b_{2k}'(t) &= 2b_{2k+1}(t) - b_{2k}(t) - (2k+1)^2 b_{2k}(t)\\
b_{2k+1}'(t) &= b_{2k}(t) + b_{2k+1}(t) - (2k+1)^2 b_{2k+1}(t)
\end{aligned}$$

(k=1,2,...). Again we have a 2×2 blocks, but now we only have 2 one-parameter families of functions, instead of the original 4 families.

As for a remark of the stability of the original partial differential equation system. Take that equation (14) with Neumann boundary condition and with a special initial condition:

$$\begin{aligned}
\partial_0 u(t,x) = \Delta u(t,x) + u(t,x) + v(t,x), &\qquad \partial_0 v(t,x) = \Delta v(t,x) + 2u(t,x) - v(t,x)\\
\partial_1 u(t,-\pi) = 0, \partial_1 u(t,\pi) = 0 &\qquad \partial_1 v(t,-\pi) = 0, \partial_1 v(t,\pi) = 0\\
u(0,x) = v(0,x) = (x-\pi)^2(x+\pi)^2. &
\end{aligned} \tag{18}$$

Solving this numerically with a computer, the solution shows instability of the zero solution, as the figures show below.

The plots and solutions were generated by *Mathematica.* They suggest that there must be at least one eigenvalue with positive real part of the operator K.

Let's look for the spectrum of operator K. $\alpha \in \sigma(K)$ if and only if $K - \alpha I$ is not invertible, that is,

$$\begin{pmatrix} \Delta u + u + v - \alpha u \\ \Delta v + 2u - v - \alpha v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

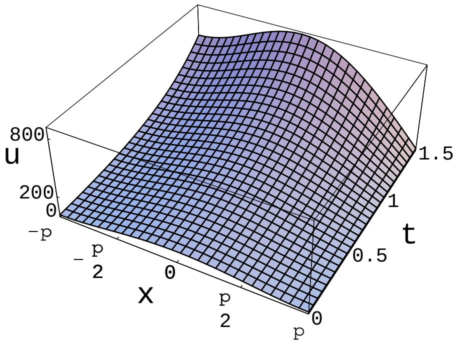

Figure 1: Concentration of species $\mathcal{U}$ at location x at time t

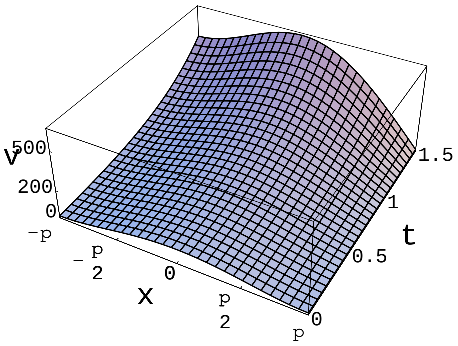

Figure 2: Concentration of species $\mathcal{V}$ at location x at time t

with Neumann boundary condition has a nontrivial pair of solutions $(u,v)^T$. This means, for any $x \in [-\pi,\pi]$

$$\begin{pmatrix} u''(x)+u(x)+v(x)-\alpha u(x) \\ v''(x)+2u(x)-v(x)-\alpha v(x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and

$$u'(-\pi)=u'(\pi)=v'(-\pi)=v'(\pi)=0$$

simultaneously hold, with the assertion that there is at least one $x \in [-\pi,\pi]$, for which $(u(x))^2+(v(x))^2>0$ holds. Reformulate our claim. When does the system

$$\begin{array}{rcl} y' & = & (\alpha-1)u - v \\ z' & = & -2u + (\alpha v+1)v \\ u' & = & y \\ v' & = & z \end{array}$$

$$u'(-\pi) = u'(\pi) = v'(-\pi) = v'(\pi) = 0$$

have a solution other than the trivial one. It is well known that it is true if and only if the determinant of the coefficient matrix of this system equals to zero. Let us check it.

$$\begin{vmatrix} 0 & 0 & \alpha-1 & -1 \\ 0 & 0 & -2 & \alpha+1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{vmatrix} = \begin{vmatrix} \alpha-1 & -1 \\ -2 & \alpha+1 \end{vmatrix} = \alpha^2 - 3 = 0,$$

for $\alpha = \pm\sqrt{3}$. We could say the $\sqrt{3}$ eigenvalue of operator K has positive real part. This, together with Theorem 10 verifies our guess suggested by the two figures above, that the zero solution of our special, numerically calculated system is unstable.

Example 4 We introduce here a concept. Take an arbitrary function space of real valued functions H, and take the vector space H^n $(n \in \mathbb{N})$. Let $\mathbf{u} = (u_1, \dots, u_n) \in V := H^n$. Let K be an $n \times n$ matrix. We define the operator $\mathcal{K}$ on V induced by the matrix K: $\mathcal{K}\mathbf{u} := K \cdot (u_1, \dots, u_n)^T$, in the same way we can define the operator $\mathcal{M} : V \to H^m$ induced by the matrix $M^{m \times n}$ for arbitrary $m \in \mathbb{N}$.

Let $\mathcal{A} := \{a^i | i = 1, \dots, k\}$ (for some $k \in \mathbb{N}$ and $a^i \in \mathbb{R}^n$) be a vector-system. We define a subset of V with them: $S := \{\sum_{i=1}^k a^i u_i\}$ where $u_i \in H$. It is easy to check that S is a subspace of V. If $\mathcal{A}$ is an eigensystem of K, then S is invariant for $\mathcal{K}$. If $\mathcal{A}$ spans $\ker M$, then $S = \ker \mathcal{M}$. Take one of the Laplacians Δ. This is linear, thus $\Delta \sum_{i=1}^k a_i u_i = \sum_{i=1}^k a_i \Delta u_i$. That is S is invariant for Δ. A diagonal matrix D will only have eigenvectors from the standard base. Therefore S is not invariant for an arbitrary $\mathcal{D}$, only if it is $d\mathcal{I}$, (induced by dI); the unit operator multiplied with at most a scalar $d \in \mathbb{R}$.

Now here is a partial differential equation system derived from a genetical system of ten coupled genes. [Yeung, Tegnér, Collins, 2002] (This paper considers a genetical system near steady state, therefore approximates it by a linear system. For simplicity we omitted external stimuli, noise and decaying of the species.)

$$\begin{aligned}
\partial_0 u_1 &= -u_2 + u_3 + d_1 \Delta u_1 \\
\partial_0 u_2 &= u_1 - u_3 + d_2 \Delta u_2 \\
\partial_0 u_3 &= u_1 + d_3 \Delta u_3 \\
\partial_0 u_4 &= u_3 + u_5 - u_7 + d_4 \Delta u_4 \\
\partial_0 u_5 &= u_7 + u_9 + d_5 \Delta u_5 \\
\partial_0 u_6 &= -u_4 + u_8 - u_9 + d_6 \Delta u_6 \\
\partial_0 u_7 &= u_4 + u_6 + u_8 - u_9 + d_7 \Delta u_7 \\
\partial_0 u_8 &= -u_7 + u_{10} + d_8 \Delta u_8 \\
\partial_0 u_9 &= u_8 + d_9 \Delta u_9 \\
\partial_0 u_{10} &= -u_4 + u_5 + u_7 - u_8 + d_{10} \Delta u_{10}
\end{aligned}$$

Translate it to an Abstract Cauchy Problem. Introduce the matrix

$$K := \begin{pmatrix} 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 1 & -1 & 0 & 0 \end{pmatrix}$$

and the diagonal matrix $D := \mathrm{diag}\{d_1, \ldots, d_{10}\}$. Let $\mathcal{K}$ and $\mathcal{D}$ be the operators induced by K and D. The new equation is $\dot{\mathbf{u}} = \mathcal{K}\mathbf{u} + \mathcal{D}\Delta\mathbf{u}$. Linear lumping won't work unless $D = dI$, that is $D := \mathrm{diag}\{d, \ldots, d\}$.

We compute the eigenvectors of the transpose of K, choose two, and arrange them into rows. These make M.

$$M = \begin{pmatrix} 1 & -1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.25 & 0.28 & -0.5 & 0.48 & -1.66 & -0.3 & 0.27 & -0.89 & 1.83 & 1 \end{pmatrix}$$

$\ker M$ consists of the eigenvectors of K. Our statements mentioned above guarantees that the S subspace of V made from these eigenvectors is invariant for $\mathcal{K} + d\mathcal{I}\Delta$ and $S = \ker \mathcal{M}$. Let's compute $\widehat{\mathcal{K}}$.

$$\begin{aligned} M(K + dI\Delta)\overline{M} &= MK\overline{M} + MdI\Delta\overline{M} = \\ &= MK\overline{M} + dMI\Delta\overline{M} = \\ &= MK\overline{M} + dM\Delta\overline{M} = \\ &= MK\overline{M} + dM\overline{M}\Delta = \\ &= MK\overline{M} + d\widehat{I}\Delta = \\ &= \widehat{K} + d\widehat{I}\Delta \end{aligned}$$

$$\widehat{K} = \begin{pmatrix} 1 & 0 \\ 0.002 & -0.9 \end{pmatrix}$$

The new system of partial differential equation $\dot{\widehat{\mathbf{u}}} = \widehat{\mathcal{K}}\widehat{\mathbf{u}} + d\Delta\widehat{\mathbf{u}}$.

$$\begin{aligned} \partial_0\widehat{u}_1 &= \widehat{u}_1 + d\Delta\widehat{u}_1 \\ \partial_0\widehat{u}_2 &= 0.002\widehat{u}_1 - 0.9\widehat{u}_1 + d\Delta\widehat{u}_2. \end{aligned}$$

7 Discussion and perspectives

Some of the calculations on the examples would have been a bit more complicated if we included different diffusion coefficients before the individual Laplacians.

The main differences between our approach and the one presented in [Li, G. and Rabitz, H., 1991b] are as follows. Li and Rabitz allows higher than first order reactions and a positive definite diagonal matrix different from the identity in the concrete applications. We exclude higher order reactions but do not exclude the presence of a positive definite diagonal matrix of diffusion coefficients, although it didn't play any role in the examples. They only treat reaction-diffusion equations and use a very strict requirement: they want to have a reaction diffusion equation as the lumped model. The lumping operator can only be generated by a matrix in the natural way. We allow a very broad class of linear equations and also a very broad class of lumping operators (which gives greater flexibility) and only require that the lumped equation be linear.

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8 Notation

a_n, b_n, c_n, d_n	real numbers or functions like: $a_n : \mathbf{R} \to \mathbf{R}$
A, B	$A \in \mathcal{L}(\widehat{X}), B \in \mathcal{L}(X)$
$\mathcal{A}, \mathcal{U}, \mathcal{V}$	formal signs of chemical species
c_u, c_v	concentrations of species $\mathcal{U}, \mathcal{V}$, respectively, also they are $\mathbf{R} \to \mathbf{R}$ functions
$\widehat{c}$	concentration of a fictive species, $\mathbf{R} \to \mathbf{R}$ function
d_u, d_v	concentrations of species $\mathcal{U}, \mathcal{V}$, respectively, also they are $\mathbf{R} \to \mathbf{R}$ functions
$I_{\widehat{X}}$	the identity operator of space $\widehat{X}$
$\mathbf{k}, \mathbf{l}$	$\mathbf{k}, \mathbf{l} : X \to \widehat{X}$
K	$K \in \mathcal{L}(X)$
$\widehat{K}$	$\widehat{K} \in \mathcal{L}(\widehat{X})$
$\widehat{\mathcal{K}}$	$n \times n$ matrix
M	$M \in \mathcal{L}(X, \widehat{X})$
M^*	the adjoint of M
$\overline{M}, \widetilde{M}$	the generalized inverses of M
n	$n \in \mathbf{N}$, within theoretical sections, $n \in \mathbf{R} \setminus \{0\}$, within Examples
$n_{11}, n_{12}, n_{21}, n_{22},$	real numbers
S	$S \subset X$, an invariant subspace of X under the flow ψ_t
t	$t \in \mathbf{R}$, time
T	$T \in \mathbf{R}^+$, fundamental period
$\mathbf{u}$	$\mathbf{u} : \mathbf{R} \to X$
$\mathbf{u}^*, \widehat{\mathbf{u}}^*$	$\mathbf{u}^* \in X, \widehat{\mathbf{u}}^* \in \widehat{X}$ equilibrium points
$\mathbf{u}_0, \widehat{\mathbf{u}}_0$	$\mathbf{u}_0 \in X, \widehat{\mathbf{u}}_0 \in \widehat{X}, \mathbf{u}_0 = \mathbf{u}(0), \widehat{\mathbf{u}}_0 = \widehat{\mathbf{u}}(0)$
$\mathbf{w}$	$\mathbf{w} : \mathbf{R} \to X$
$\widehat{\mathbf{w}}$	$\widehat{\mathbf{w}} : \mathbf{R} \to \widehat{X}$ means $\widehat{\mathbf{w}} = M\mathbf{w}$
W	$W \subset X$, $\widehat{X} \cong W$
$W^\perp$	orthogonal complement of W
x	n-dimensional space vector, specially in this paper $n = 1$, i.e. $x \in \mathbf{R}$
$\mathbf{x}$	$\mathbf{x} \in X$
$\widehat{\mathbf{x}}$	$\widehat{\mathbf{x}} \in \widehat{X}$
X	Hilbert space
$\widehat{X}$	Hilbert space
$\mathbf{y}, \overline{\mathbf{y}}$	$\mathbf{y} \in X, \overline{\mathbf{y}} \in X$
$\widehat{\mathbf{y}}, \widetilde{\mathbf{y}}$	$\widehat{\mathbf{y}} \in \widehat{X}, \widetilde{\mathbf{y}} \in \widehat{X}$
Y	$Y \subset X$

α	$\alpha \in \mathbf{C}$
α_n, β_n	real numbers, in particular constant coefficients
β	the sepctral abscissa of an operator, i.e. $\sup\{\mathrm{Re}(\lambda); \lambda \in \sigma(K)\}$
δ	$\delta \in \mathbf{R}^+$
ε	$\varepsilon \in \mathbf{R}^+$
λ	$\lambda \in \mathbf{C}$, an eigenvalue of an operator
ψ	$\psi : \mathbf{R} \times X \to X$ the dynamical system, induced by (1)
ψ_t	$\psi_t = \psi(t, .)$
ρ	the resolvent set of an operator
σ	the spectrum of an operator
$0, \mathbf{0}, \widehat{\mathbf{0}}$	the zero element of the vector space $\mathbf{R}, X, \widehat{X}$, respectively
$\dot{}$	$\dot{} = \frac{d}{\mathrm{d}t}$, i.e. the time derivative of
Δ	the Laplacian operator, i.e. $\Delta = \nabla^2$
∂_0	time derivative of
∂_n	partial derivative of a function in the n-th variable

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