Operator splitting based dynamic iteration for linear differential-algebraic port-Hamiltonian systems

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Abstract
A dynamic iteration scheme for linear differential-algebraic port-Hamiltonian systems based on Lions–Mercier-type operator splitting methods is developed. The dynamic iteration is monotone in the sense that the error is decreasing and no stability conditions are required. The developed iteration scheme is even new for linear port-Hamiltonian systems governed by ODEs. The obtained algorithm is applied to a multibody system and an electrical network.

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1 Introduction

Dynamic iteration schemes for differential-algebraic equations (DAEs) have been widely used and discussed for multiphysics problems, which allow for an easy exploitation of the different properties of the subsystems [1–6]. In general, we consider an initial value problem for a (semi-explicit index-1) DAE of the form

\[
\begin{align}
\dot{v} &= f(t,v,w), \quad v(0) = v_0, \\
0 &= g(t,v,w),
\end{align}
\]
where \( \frac{\partial g(t, v, w)}{\partial w} \) is regular in a neighborhood of the solution \((v(t), w(t))\), \( t \in [0, T] \). A general dynamic iteration scheme is given by an initial guess \((v^{(0)}(t), w^{(0)}(t))^\top (t \in [0, T], \text{i.e., an initial waveform}) \) and the solution \((v^{(k)}(t), w^{(k)}(t))^\top \) of the DAE for integer \( k \geq 1 \)

\[
\begin{align*}
\dot{v}^{(k)} &= F(t, v^{(k)}, v^{(k-1)}, w^{(k)}, w^{(k-1)}), \quad v^{(k)}(0) = v_0, \\
0 &= G(t, v^{(k)}, v^{(k-1)}, w^{(k)}, w^{(k-1)})
\end{align*}
\]

with arbitrary splitting functions \( F, G \) fulfilling the compatibility conditions

\[
F(t, v, v, w, w) = f(t, v, w) \quad \text{and} \quad G(t, v, v, w, w) = g(t, v, w).
\]

Hence, a dynamic iteration defines as a mapping from the \((k-1)\)-st iterate to the \( k \)-th iterate:

\[
(v^{(k-1)}(t), w^{(k-1)}(t)) \mapsto (v^{(k)}(t), w^{(k)}(t)).
\]

Usually the integration interval \([0, T]\) is partitioned into sub intervals, so-called time windows, to speed up convergence or even allow for convergence. One drawback of such schemes for DAEs is given by the fact that stability conditions for a guaranteed convergence must hold in a twofold manner:

(a) Convergence within one time window has to be present [1, 7], and
(b) Stable error propagation from window to window is needed [1, 2].

If one of these conditions is not met choosing arbitrary small time windows will not help out (in general).

In the case of initial value problems of ordinary differential equations

\[
\dot{x} = f(t, x), \quad x(0) = x_0, \quad t \in [0, T],
\]

convergence of dynamic iteration schemes (analogously defined) is given for arbitrary long time windows \([0, T]\). However, the convergence might not be monotone, and the error might increase drastically in the beginning, causing an overflow in computer implementations, see chapter 3 for an example.

As an alternative, operator splitting is based not on splitting the ODE into subsystems componentwise, but on splitting the right-hand side of an ODE, which are solved one after the other, see [8] for an overview. Operator splitting cannot be easily generalized to DAEs, the splitting of the algebraic part poses convergence problems [9]. One way out is proposed in [10] for linear DAEs: there, the idea is to split the DAE into the underlying ODE and function evaluation of the algebraic components in terms of the differential components, which becomes computationally expensive for nonlinear systems, and destroys the structure of the respective DAE.

In this work, we show that an alternative iterative approach for linear DAEs can avoid the flaws of both dynamic iteration and operator splitting schemes described above if the DAE (1) is composed of coupled port-Hamiltonian (pH) systems. This
type of systems is motivated by physics, provides an energy balance and gives a sim-
ple framework for coupled systems, see [11, 12] for an introduction to pH systems.
Port-Hamiltonian DAEs are in particular investigated in [13–17]. Now, the alternative
iterative approach is based on an iteration scheme from Lions and Mercier [18]. The
convergence will be monotone, no stability conditions appear and the DAE structure
does not have to be changed.

The paper is organized as follows: in the subsequent chapter 2, the framework
of linear coupled port-Hamiltonian DAEs is set. Both, the perspective of an overall
coupled system and the perspective of a system composed of coupled port-Hamiltonian
differential-algebraic subsystems is given. Chapter 3 illustrates the limits of classical
dynamic iteration schemes such as the Jacobi iteration, which motivates the derivation
and analysis of operator splitting based dynamic iteration schemes in the following.
Chapter 4 recapitulates some basic facts on maximal monotone operators, which are
used in chapter 5 to derive the monotone convergence results of operator splitting
based dynamic iteration schemes. An estimate for the convergence rate can be given
in the case of systems governed by ODEs, or DAEs with strong enough dissipation.
Numerical results are discussed in chapter 6. The paper finishes with some concluding
remarks and an outlook.

2 The setting

We consider linear time-invariant initial value problems of DAE, which have the
following structure:

**Definition 1** For a final time \( T > 0 \), the descriptor variable \( x(t) \in \mathbb{R}^n \) and \( t \in [0, T] \), we consider

\[
\begin{align*}
\frac{d}{dt} Ex(t) &= (J - R) Q x(t) + Bu(t), \quad t \in [0, T], \quad Ex(0) = Ex_0, \quad (2a) \\
y(t) &= B^\top Q x(t), \quad (2b)
\end{align*}
\]

where \( E, J, R \) and \( Q \) are real \( n \times n \)-matrices, \( B \) is a \( n \times m \)-matrix, \( Ex_0 \in \mathbb{R}^n \) is a
given initial value, \( u \) is a given input and \( y \) is referred to as output. (The matrix \( E \)
may have no full rank.)

Proposition 3 Assume that a differential-algebraic system (2) is given with \( E, J, R, Q \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times m} \) satisfying \( E^\top Q = Q^\top E \geq 0 \), \( R = R^\top \geq 0 \) and \( J^\top = -J \).

Furthermore, let \( u \in L^2([0, T], \mathbb{R}^m) \), \( x_0 \in \mathbb{R}^n \), and let \( x \in L^2([0, T], \mathbb{R}^n) \) be a
solution of (2). Then the following statements hold:

(a) The function \( Ex \mapsto x^\top Q^\top Ex \) (mapping \( im E \to \mathbb{R} \)) is well-defined.
(b) The function \( t \mapsto x(t)\top Q\top E x(t) \) is weakly differentiable with
\[
\frac{d}{dt}(x\top Q\top E x) = 2x\top Q\top (\frac{d}{dt} E x) \in L^1([0, T], \mathbb{R}).
\]

(c) The following dissipation inequality holds for all \( t \in [0, T] \):
\[
\frac{1}{2}(x(t)\top Q\top E x(t)) - \frac{1}{2}(x_0\top Q\top E x_0) = -\int_0^t x(\tau)\top Q\top R Q x(\tau) d\tau + \int_0^t u(\tau)\top y(\tau) d\tau \leq \int_0^t u(\tau)\top y(\tau) d\tau.
\]

**Proof** (a) Assume that \( x_1, x_2 \in \mathbb{R}^n \) with \( E x_1 = E x_2 \). We have \( E\top Q = Q\top E \), and thus, for the Moore-Penrose inverse \( E^+ \) of \( E \), we have
\[
E\top Q = E\top (E^+)\top E\top Q = E\top (E^+)\top Q\top E.
\]
Consequently, for \( X = (E^+)\top Q\top \in \mathbb{R}^{n \times n} \), we have \( Q\top E = E\top X E \), and thus
\[
x_1\top Q\top E x_1 = (E x_1)\top X (E x_1) = (E x_2)\top X (E x_2) = x_2\top Q\top E x_2.
\]
Furthermore, it is easy to see that
\[
E\top X E = E\top X\top E. \quad (3)
\]

(b) By using that \( E x \in H^1([0, T], \mathbb{R}^n) \), the product rule for weak derivatives [19, Thm. 4.25] implies that, for \( X \) as in (a),
\[
x\top Q\top E x = (E x)\top X (E x) \in W^{1,1}([0, T], \mathbb{R})
\]
with
\[
\frac{d}{dt}(x\top Q\top E x) = \frac{d}{dt}((E x)\top X (E x)) = 2x\top E X \frac{d}{dt} (E x) = 2x\top \frac{d}{dt} (E\top X E x)
\]
\[
= 2x\top \frac{d}{dt} (Q\top E x) = 2x\top Q\top \frac{d}{dt} (E x).
\]
In the latter calculation we also used (3).

(c) The previous statement yields
\[
\frac{d}{dt} \frac{1}{2}(x\top Q\top E x) = x\top Q\top \frac{d}{dt} (E x) = x\top Q\top ((J - R)Q x + Bu)
\]
\[
= -(Q x)\top R (Q x) + x\top Q Bu \leq (B\top Q x)\top u = y\top u.
\]

Now an integration on \([0, t]\) leads to the dissipation inequality.

Thus, we investigate the following class of port-Hamiltonian DAE:

**Definition 4** (*pH DAE*) The system (2) with the assumptions of Proposition 3 is here referred as port-Hamiltonian DAE (*pH DAE*). 

\(\square\)

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2.1 Perspective as overall coupled system

We further assume that (2) is composed of several port-Hamiltonian systems which are coupled in an energy-preserving way. The assumptions are collected in the following.

**Assumption 5** *(Overall coupled pH DAE)* We consider the setting (2).

(a) The matrices in (2) are, for some $s, n_1, \ldots, n_s \in \mathbb{N}$, structured as

$$
E = \begin{bmatrix} E_1 & \cdots & E_s \end{bmatrix}, \quad R = \begin{bmatrix} R_1 & \cdots & R_s \end{bmatrix}, \quad Q = \begin{bmatrix} Q_1 & \cdots & Q_s \end{bmatrix},
$$

$$
J = \begin{bmatrix} J_1 & J_{12} & \cdots & J_{1s} \\
-J_{12}^T & \ddots & \cdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
-J_{1s}^T & \cdots & -J_{s-1,s}^T & J_s
\end{bmatrix}, \quad B = \begin{bmatrix} B_1 \\
\vdots \\
B_s
\end{bmatrix},
$$

with $n_1 + n_2 + \cdots + n_s = n$, where

(i) for $i = 1, \ldots, c, s$, $E_i, Q_i, J_i, R_i \in \mathbb{R}^{n_i \times n_i}$ with $R_i = R_i^T \geq 0$, $J_i^T = -J_i$,

$$
E_i^T Q_i = Q_i^T E_i \geq 0, \quad Q_i \text{ invertible and } B_i \in \mathbb{R}^{n_i \times m};
$$

(ii) $J_{ij} \in \mathbb{R}^{n_i \times n_j}$ for $i, j \in \{1, \ldots, s\}$ with $i < j$.

(b) $\text{rk} \left[ E R J \right] = n$.

(c) $T > 0, x_0 \in \mathbb{R}^n$ and $u \in L^2([0, T]; \mathbb{R}^m)$. Furthermore, for matrices $Z \in \mathbb{R}^{n \times r}$, $Z_1 \in \mathbb{R}^{r \times r_1}$, with full column rank and

$$
im Z = \ker E,$$

$$
im Z_1 = \ker R Q Z \cap \ker Z^T Q^T J Q Z,$$

the input $u$ and the initial value $E x_0$ fulfill

$$
Z_1^T Z^T Q^T B u \in H^1([0, T]; \mathbb{R}^{r_1}) \quad \text{with } Z_1^T Z^T Q^T (J Q x_0 + B u(0)) = 0.
$$

\[ \square \]

**Remark 6** Notice that with Assumption 5, we have for (2):

(a) $Q^T E = E^T Q \geq 0, \quad R = R^T \geq 0$, and $Q$ is invertible. Hence, the overall coupled pH DAE of Assumption 5 is a pH DAE (in the sense of Definition 4).

(b) As $Q^T E \geq 0$, we have that $E Q^{-1} = Q^{-T} (Q^T E) Q^{-1}$ is positive semi-definite as well, and therefore possesses a matrix square root $(E Q^{-1})^{1/2}$.

(c) The $i$th subsystem for the variable $x_i$ reads:

$$
E_i x_i = (J_i - R_i) Q_i x_i + B_i u - \sum_{j < i} J_{ji}^T Q_j x_j + \sum_{i < j} J_{ij} Q_j x_j.
$$
The coupling is facilitated by the off-diagonal terms within the matrix $J$. □

Remark 7 (Coupled linear pH DAEs) A pH DAE of type (2) with coupling structure (4) and (5) is naturally given in the case of $s$ coupled linear pH DAEs as follows: consider $s$ subsystems of pH DAEs

$$
\frac{d}{dt} E_i x_i(t) = (\tilde{J}_i - R_i) Q_i x_i(t) + B_i u_i(t), \quad y_i(t) = B_i^T Q_i x_i(t),
$$

$i = 1, \ldots, s$, with $\tilde{J}_i = -\tilde{J}_i^T$, $R_i = R_i^T \geq 0$, and $Q_i^T E_i = E_i^T Q_i \geq 0$. The input $u_i$, the output $y_i$ and $B_i$ are split into

$$
u_i(t) = \left( \begin{array}{c} \hat{u}_i(t) \\ \bar{u}_i(t) \end{array} \right), \quad y_i(t) = \left( \begin{array}{c} \hat{y}_i(t) \\ \bar{y}_i(t) \end{array} \right), \quad B_i = \left( \begin{array}{c} \hat{B}_i \\ \bar{B}_i \end{array} \right)$$

according to external and coupling quantities. The subsystems are coupled via external inputs and outputs by

$$
\begin{pmatrix} \hat{u}_1 \\ \vdots \\ \hat{u}_s \end{pmatrix} + \hat{C} \begin{pmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_s \end{pmatrix} = 0, \quad \hat{C} = -\hat{C}^T.
$$

These $s$ systems can be condensed to one large pH DAE [3]

$$
\frac{d}{dt} Ex = (J - R) Q x + \tilde{B} \bar{u},
$$

(6a)

$$
\bar{y} = B^T Q x
$$

(6b)

with $J = \tilde{J} - \hat{B} \hat{C} \hat{B}^T$ and the condensed quantities

$$v^T = (v_1^T, \ldots, v_s^T) \quad \text{for } v \in \{x, \hat{u}, \hat{y}\},
$$

$$F = \text{diag}(F_1, \ldots, F_s) \quad \text{for } F \in \{E, Q, \tilde{J}, R, \hat{B}, \bar{B}\}.$$

Equation (6) defines now a pH DAE of type (2) with structure given by (4) and (5): the matrices $\tilde{J}$ and $R$ are block-diagonal, and the Schur complement type matrix $-\hat{B} \hat{C} \hat{B}^T$ has only off-block diagonal entries. Note that the coupling has been shifted from the port matrices $B_i$ to the off-block diagonal part of $J$. □

Remark 8 As has been shown in Remark 7, all coupled linear subsystems of pH DAEs can be transformed into one pH DAE without port-coupling, i.e., the coupling of the different subsystems can always be given through $J$. Therefore the structure given in assumption 5 comprises the general case of a set of arbitrary linear pH DAEs which are coupled by a linear coupling condition for the inputs and outputs of the single systems.

Now we collect some properties of systems (2) satisfying Assumption 5. To this end, we note that a matrix pencil $sE - A \in \mathbb{R}[s]^{n \times n}$ is called regular if $\det(sE - A)$ is

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not the zero polynomial. Furthermore, for a regular pencil \( sE - A \), the index \( v \in \mathbb{N}_0 \) of the DAE \( \frac{d}{dt}Ex(t) = Ax(t) + f(t) \) is the smallest number for which the mapping \( \lambda \mapsto \lambda^{1-v}(vE - A)^{-1} \) is bounded outside a compact subset of \( \mathbb{C} \). Note that the index equals to the number of differentiations of the DAE needed to obtain an ordinary differential equation [20, Chap. 2].

**Proposition 9** Any system (2) fulfilling Assumption 5 has the following properties.

(a) The pencil \( sE - (J - R)Q \in \mathbb{R}[s]^{n \times n} \) is regular.

(b) There exists a unique solution \( x \) of (2).

(c) The index of the DAE (2) is at most two.

**Proof** (a) For \( \lambda \in \mathbb{C} \) with \( \text{Re} \lambda > 0 \), we show that \( C := \lambda E - (J - R)Q \) has a trivial kernel. Let \( z \in \mathbb{C}^n \) with \( Cz = 0 \). Then

\[
0 = \text{Re}(z^*Q^TCz) = \text{Re}(\lambda z^*Q^TEz) - \text{Re}(z^*Q^TJQx) + \text{Re}(z^*Q^TRQz).
\]

Invoking that \( J = -J^\top \), \( Q^TE = E^\top Q \geq 0 \) and \( R = R^\top \geq 0 \), we obtain

\[
\text{Re}(\lambda z^*Q^TEz) = \text{Re}(\lambda)z^*Q^TEz \geq 0,
\]

\[
\text{Re}(z^*Q^TJQz) = \text{Re}((Qz)^*J(Qz)) = 0,
\]

\[
\text{Re}(z^*Q^TRQz) = \text{Re}((Qz)^*R(Qz)) = (Qz)^*R(Qx) \geq 0,
\]

which leads to \( z^*Q^TEz = 0 \) and \( (Qz)^*R(Qz) = 0 \). The positive semi-definiteness of \( Q^TE \) and \( R \) implies that \( E^\top Qz = Q^TEz = 0 \) and \( RQz = 0 \). Using \( (\lambda E - (J - R)Q)z = 0 \), this yields \( JQz = 0 \). Hence, by \( R = R^\top \) and \( J = -J^\top \),

\[
Qz \in \ker [E R J]^\top.
\]

Assumption 5(b) now gives \( Qz = 0 \). Since \( Q \) is invertible, we are led to \( z = 0 \).

(b) By using that the pencil \( sE - (J - R)Q \) is regular, uniqueness of solutions of the initial value problem (2) follows from the considerations in [21, Sec. 1.1].

It remains to prove that a solution of (2) exists. Let \( Z \in \mathbb{R}^{n \times r} \), \( Z_1 \in \mathbb{R}^{r \times r_1} \) be as in Assumption 5(c). Furthermore, let \( Z' \in \mathbb{R}^{n \times (n-r)} \), \( Z'_1 \in \mathbb{R}^{r \times (r-r_1)} \) be matrices with \( \text{im} Z' = (\text{im} Z)^\perp \) and \( \text{im} Z'_1 = (\text{im} Z_1)^\perp \). Moreover, we introduce matrices \( Z_2 \in \mathbb{R}^{(n-r) \times r_1} \), \( Z'_2 \in \mathbb{R}^{(n-r) \times (n-r-r_1)} \) with full column rank and

\[
\text{im} Z_2 = \ker Z_1^\top Z_1^\top Q^\top (J - R)Z', \quad \text{im} Z'_2 = (\text{im} Z_2)^\perp.
\]

The construction of \( Z, Z', Z_1, Z'_1, Z_2, Z'_2 \) yields that the columns of the matrix

\[
V := [Z'Z'_2, Z'Z_2, ZZ'_1, ZZ_1]
\]

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are linearly independent, and thus, $V, V^\top Q^\top \in \mathbb{R}^{n \times n}$ are invertible matrices. Then we obtain

$$V^\top Q^\top (sE - (J - R)Q)V = \begin{bmatrix} sE_{11} - A_{11} & sE_{12} - A_{12} & -A_{13} & -A_{14} \\ sE_{12} - A_{21} & sE_{22} - A_{22} & -A_{23} & 0 \\ -A_{31} & -A_{32} & -A_{33} & 0 \\ A_{41} & 0 & 0 & 0 \end{bmatrix}, \quad (8)$$

where

$$E_{11} = (Z_2')^\top (Z')^\top Q^\top EZ'Z_2', \quad E_{12} = (Z_2')^\top (Z')^\top Q^\top (J - R)QZ'Z_2',$$

$$E_{22} = Z_2^2 (Z')^\top Q^\top EZ'Z_2, \quad A_{11} = (Z_2')^\top (Z')^\top Q^\top (J - R)QZ'Z_2',$$

$$A_{12} = (Z_2')^\top (Z')^\top Q^\top (J - R)QZ'Z_2, \quad A_{21} = Z_2^2 (Z')^\top Q^\top (J - R)QZ'Z_2',$$

$$A_{13} = (Z_2')^\top (Z')^\top Q^\top (J - R)QZ'Z_2, \quad A_{23} = (Z_1')^\top Z^\top Q^\top (J - R)QZ'Z_2',$$

$$A_{22} = Z_2^2 (Z')^\top Q^\top (J - R)QZ'Z_2, \quad A_{33} = (Z_1')^\top Z^\top Q^\top (J - R)QZ'Z_2,$$

$$A_{14} = (Z_2')^\top (Z')^\top Q^\top JQZZ_1,$$

$$B_1 = (Z_2')^\top (Z')^\top Q^\top B, \quad B_2 = Z_2^2 (Z')^\top Q^\top B,$$

$$B_3 = (Z_1')^\top Z^\top Q^\top B, \quad B_4 = Z_1^2 Z^\top Q^\top B.$$  

The construction of the matrices $Z, Z', Z_1, Z_1', Z_2, Z_2'$ yields that

- $\begin{bmatrix} E_{11} & E_{12} \\ E_{12} & E_{22} \end{bmatrix}$ is positive definite. In particular, $E_{22}$ is invertible,
- $A_{33}$ is invertible, and
- $A_{14}$ has full row rank.

The already proved regularity of $sE - (J - R)Q$, which implies regularity of the pencil $V^\top Q^\top (sE - (J - R)Q)QV$, which yields that $A_{14}$ has moreover full column rank. As a consequence, $A_{14}$ is square (i.e., $2r_1 = n - r$) and invertible. Set $z_0 = (z_{10}, z_{20}, z_{30}, z_{40}), z_{10} \in \mathbb{R}^{n-r}, z_{20} \in \mathbb{R}^{r}, z_{30} \in \mathbb{R}^{r}, z_{40} \in \mathbb{R}^{r}.$

By Assumption 5(c), we have $B_4u \in H^1([0, T]; \mathbb{R}^r)$ and

$$0 = Z_1^\top Z^\top Q^\top (JQx_0 + Bu(0)) = Z_1^\top Z^\top Q^\top JQx_0 + B_4u(0)$$

$$= Z_1^\top Z^\top Q^\top JQ(2z_2z_{10} + Z'Z_2z_{10} + ZZ_1z_{20} + ZZ_1z_{40}) + B_4u(0)$$

$$= Z_1^\top Z^\top Q^\top JQZ'Z_2z_{10} + B_4u(0) = -Z_1^\top Z^\top Q^\top JQZ'Z_2z_{10} + B_4u(0)$$

$$= -A_{14}z_{10} + B_4u(0).$$

Consequently, $z_1 = (A_{14}^{-1}B_4u)$ fulfills $z_1 \in H^1([0, T]; \mathbb{R}^r), -A_{14}z_1 + B_4u(t) = 0$ and $z_1(0) = z_{10}.$ Moreover, let $z_2 \in H^1([0, T]; \mathbb{R}^r)$ be the solution of the following ODE with initial value $z_2(0) = z_{20}$

$$\frac{dz_2}{dt} = E^{-1}_{22}(A_{22} - A_{23}A_{33}^{-1}A_{32})z_2(t)$$

$$+ E^{-1}_{22}(- \frac{d}{dt}E_{12}z_1(t) + A_{21}z_1(t) + B_2u(t) - A_{23}A_{33}^{-1}z_1(t) - A_{23}A_{33}^{-1}B_3u(t)).$$
and we successively define $z_3 \in L^2([0, T]; \mathbb{R}^{r-r_1})$, $z_4 \in L^2([0, T]; \mathbb{R}^{r_1})$ by

$$z_3(t) = -A_{33}^{-1}A_{23}z_2(t) - A_{33}^{-1}A_{13}z_1(t),$$
$$z_4(t) = -A_{14}^{-1}\left(\frac{d}{dt}E_{11}z_1(t) + \frac{d}{dt}E_{12}z_2(t) - A_{11}z_1(t) - A_{12}z_1(t) - A_{13}z_3(t)\right).$$

Altogether, we have that $z := (z_1^T, z_2^T, z_3^T, z_4^T)^T$ is a solution of the differential-algebraic equation

$$\frac{d}{dt} \begin{bmatrix} E_{11} & E_{12} & 0 & 0 \\ E_{12}^T & E_{22} & 0 & 0 \\ 0 & 0 & E_{33} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} z_1(t) \\ z_2(t) \\ z_3(t) \\ z_4(t) \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & 0 \\ A_{31} & A_{32} & A_{33} & 0 \\ -A_{14} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} z_1(t) \\ z_2(t) \\ z_3(t) \\ z_4(t) \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix} u(t),$$

(9)

Now setting

$$x(t) := (Q^T)^{-1}(V^T)^{-1}z(t),$$

we obtain from (8) and (9) that $x$ is a solution of (2).

(c) The result has been shown in [22, Thm. 4.3] and [16, Thm. 6.6]. Notice, this can also be seen from the proof of (b). □

**Remark 10** Assume that the DAE (2) fulfills Assumption 5(a) & (b). By using $V \in \mathbb{R}^{n \times n}$ as defined as in (7), we can transform (2) to an equivalent DAE (9). Consequently, the existence of a solution of (2) implies $z_1 \in H^1([0, T]; \mathbb{R}^{r_1})$ with, and thus $B_q u = (A_{14}^T)^{-1} \in H^1([0, T]; \mathbb{R}^{r_1})$. Invoking that $B_4 = Z_4^T Z^T Q^T B$, we obtain that $Z_4^T Z^T Q^T B u \in H^1([0, T]; \mathbb{R}^{r_1})$ with $Z_4^T Z^T Q^T (J Q x_0 + B u(0)) = 0$ has to be fulfilled. Consequently, under Assumption 5 (a) & (b), the conditions in Assumption 5(c) are also necessary for the existence of a solution of the DAE (2). □

### 2.2 Perspective as coupled pH-subsystems

We take the perspective of the paper [23] for the system (2) and its partitioning given in Rem. 6. To this end, we need to introduce the internal inputs $u_{ij}$, i.e., data stemming from the $j$th system being input for the $i$th system, and outputs $y_{ij}$ (i.e., data from the $i$th system to be transferred to the $j$th system). This reads for the $i$th subsystems ($i = 1, \ldots, s$):

$$\frac{d}{dt} E_i x_i(t) = (J_i - R_i) Q_i x_i(t) + \sum_{\substack{j=1 \\ j \neq i}}^s B_{ij} u_{ij}(t) + B_i u_i(t), \quad E_i x_i(0) = E x_{i0},$$
\[ y_{ij}(t) = B_{ij}^\top Q_i x_i(t), \quad j = 1, \ldots, s, \quad j \neq i, \]
\[ y_i(t) = B_i^\top Q_i x_i(t) \]

with matrices \( E_i, Q_i, J_i, R_i \in \mathbb{R}^{n_i \times n_i} \), and \( B_i \in \mathbb{R}^{n_i \times m} \) fulfilling the properties of Assumption 5(a), and \( B_{ij} \in \mathbb{R}^{n_i \times m_{ij}} \) for \( i = 1, \ldots, s, \quad j = 1, \ldots, s, \quad i \neq j \) with \( m_{ij} = m_{ji} \). The dissipation inequality for this subsystem reads

\[
\frac{1}{2} (x_i(t)^\top Q_i^\top E_i x_i(t)) - \frac{1}{2} (x_i(0)^\top Q_i^\top E_i x_i(0)) \leq \int_0^t u_i(\tau)^\top y_i(\tau) d\tau + \sum_{j=1}^s \int_0^t u_{ij}(\tau)^\top y_{ij}(\tau) d\tau \quad \forall t \in [0, T]
\]

The overall input \( u \) is composed of the inputs of the subsystems. By forming a suitable expansion of the input spaces of the subsystems, it is no loss of generality to assume that \( u = u_1 = \cdots = u_s \). The overall output is consequently given by the sum

\[ y = \sum_{j=1}^s y_i. \]

Coupling is done such that \( x \mapsto x^\top Q^\top E x \) with \( E \) and \( Q \) as in (4) is a storage function for the overall system [24]. This is for instance achieved by

\[
\forall i = 1, \ldots, s : \quad u_{ij} + y_{ji} = 0, \quad j = 1, \ldots, i - 1,
\]
\[
u_{ij} - y_{ji} = 0, \quad j = i + 1, \ldots, s,
\]

or equivalently

\[
\forall i = 1, \ldots, s \quad \forall j = 1, \ldots, i - 1 : \quad u_{ij} = -y_{ji}, \quad u_{ji} = y_{ij},
\]

since

\[
\frac{1}{2} (x(t)^\top Q^\top E x(t)) - \frac{1}{2} (x(0)^\top Q^\top E x(0)) = \sum_{i=1}^s \frac{1}{2} \left( (x_i(t)^\top Q_i^\top E_i x_i(t)) - \frac{1}{2} (x_i(0)^\top Q_i^\top E_i x_i(0)) \right) \\
\leq \sum_{i=1}^s \int_0^t u_i(\tau)^\top y_i(\tau) d\tau + \sum_{i=1}^s \sum_{j=1, j \neq i}^s \int_0^t u_{ij}(\tau)^\top y_{ij}(\tau) d\tau \\
= \int_0^t u(\tau)^\top y(\tau) d\tau + \sum_{i=1}^s \sum_{j=1}^{i-1} \int_0^t u_{ij}(\tau)^\top y_{ij}(\tau) d\tau + \sum_{i=1}^s \sum_{j=i+1}^s \int_0^t u_{ij}(\tau)^\top y_{ij}(\tau) d\tau \\
= \int_0^t u(\tau)^\top y(\tau) d\tau + \sum_{i=1}^s \sum_{j=1}^{i-1} \int_0^t -y_{ji}(\tau)^\top u_{ji}(\tau) d\tau + \sum_{i=1}^s \sum_{j=i+1}^s \int_0^t u_{ij}(\tau)^\top y_{ij}(\tau) d\tau
\]
\[ \int_0^t u(\tau) y(\tau) d\tau. \]

The overall system is given by (2) with \( E, Q \) and \( R \) as in (4), and \( J \) structured as in (5) with

\[ \forall i = 1, \ldots, s - 1, \ j = i + 1, \ldots, s : \ J_{ij} = B_{ij} B_{ji}^T. \]

**Remark 11** This coupling has the drawback that all variables enter the definition of the coupling. And we have as many outputs of a subsystem as the other subsystem has variables times the number of other subsystems. This will be treated differently in practice. An ‘essential’ coupling will be used (minimizing the number of coupling variables).

Before we investigate the Lions/Mercier based algorithm, we revisit the Jacobi dynamic iteration and discuss some limitations.

### 3 Failure of Jacobi dynamic iteration

To motivate the development of monotone operator splitting based dynamic iteration schemes in chapter 5, we remind that classical approaches such as the Jacobi or Gauss-Seidel iteration scheme may not always be feasible for a computer implementation. To this end, we address system (2) in the following ODE setting: assigning \( E = Q = I \), the initial value problem (2) reads

\[ \dot{x} = (J - R)x + Bu(t), \quad x(0) = x_0, \quad t \in [0, T]. \]  (10)

For this system, we recall that the dynamic iteration is based on a splitting \( J - R = M - N \) and an iteration count \( k \in \mathbb{N}_0 \). Now, let be an initial guess at \( k = 0 \) be given \( x^{(0)} \in C^0([0, T], \mathbb{R}^n) \) with \( x^{(0)}(0) = x_0 \) (e.g., \( x^{(0)}(t) = x_0 \)) for all \( t \in [0, T] \), the dynamic iteration scheme reads:

\[ x^{(k+1)} = Mx^{(k+1)} - Nx^{(k)} + Bu(t), \quad x^{(k+1)}(0) = x_0. \]  (11)

**Remark 12** Note that setting \( M = J_d - R \) and \( N = -J_o \) in the case of the pHS-ODE system (10) defines a block-Jacobi dynamic iteration scheme. Here \( J_d \) is a block diagonal matrix with diagonal elements \( J_i, i = 1, \ldots, s \), and \( J_o := J - J_d \).

If we restrict to \( u \in C^0([0, T], \mathbb{R}^m) \), we obtain from (11) \( x^{(k+1)} \in C^0([0, T], \mathbb{R}^n) \). Let \( x \in C^0([0, T], \mathbb{R}^n) \) denote the analytic solution of (10). Then, the recursion error is given by \( e^{(k)} := x^{(k)} - x \). Following Burrage [25], we can derive an exact error recursion for the dynamic iteration (11). Doing this, for the system (10) with

\[ R = \text{diag} (\tau, \ldots, \tau), \quad B = 0, \]  (12)
and setting $M = -R$, $N = -J_o = -J$, we get the error recursion on $t \in [0, T]$:

$$e^{(k)}(t) = \int_0^t e^{-(t-s_k-1)R} J e^{(k-1)}(s_{k-1}) ds_{k-1} = J \int_0^t e^{-\tau(t-s_k-1)} e^{(k-1)}(s_{k-1}) ds_{k-1}$$

$$= J^k \int_0^t e^{-\tau(t-s_k-1)} \int_0^{s_{k-1}} e^{-\tau(s_k-s_{k-2})} \cdots \int_0^{s_1} e^{-\tau(s_{1}-s_0)} e^{(0)}(s_0) ds_0 \cdots ds_{k-2} ds_{k-1}$$

$$= e^{-\tau T} J^k \int_0^t \int_0^{s_{k-1}} \cdots \int_0^{s_1} e^{\tau s_0} e^{(0)}(s_0) ds_0 \cdots ds_{k-2} ds_{k-1}.$$

Now, just for demonstration purposes and simplicity, let us assume that initial error has the format:

$$e^{(0)}(s_0) = D s_0 e^{-\tau s_0} \mathbb{1} \text{ with } \mathbb{1} = [1, \ldots, 1]^T \in \mathbb{R}^n$$

and $D > 0$. Using the maximum norm $\|f\|_T := \max_{t \in [0, T]} \|f(t)\|_2$ for $f \in C^0([0, T], \mathbb{R}^n)$, the error reads for all $k \geq \tau T - 1$ (maximal error at $T$):

$$\|e^{(k)}\|_T = \sqrt{2} D \|J\|_2^k \frac{e^{-\tau T} T^{k+1}}{(k+1)!} \Rightarrow \frac{\|e^{(k+1)}\|_T}{\|e^{(k)}\|_T} \frac{\|J\|_2 \cdot T}{k + 2}.$$

**Example 13** We analyse a $2 \times 2$ version of (10) with the restriction (12), which reads:

$$x' = (J - R)x, \quad x(0) = x_0 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}, \quad \text{with } J = \begin{bmatrix} 0 & v \\ -v & 0 \end{bmatrix}, \quad R = \begin{bmatrix} \tau & 0 \\ 0 & \tau \end{bmatrix} \quad (13)$$

and employing $\tau, v > 0$. The analytic solution and error evolution are given by:

$$x(t) = e^{-\tau t} \begin{bmatrix} \cos(vt) & \sin(vt) \\ -\sin(vt) & \cos(vt) \end{bmatrix} x_0, \quad \frac{\|e^{(k+1)}\|_T}{\|e^{(k)}\|_T} \frac{\|J\|_2 \cdot T}{k + 2} = \frac{v T}{k + 2} \forall k \geq \tau T - 1.$$

The error amplification factor $v T / (k + 2)$ is bounded by one for all $k > v T - 2$. For all $k < v T - 2$ the error is increasing. Hence, the convergence is monotone (for all $k$) only if $v T - 2 \leq 0$.

We remark that splitting the overall time window $[0, T]$ in several windows is always a solution to obtain (good) convergence.

To illustrate the below up, we present two configurations: an overflow in single precision for $T = 10$ in Fig. 1 (left) and a initial blow up and then decrease for $T = 0.5$ in Fig. 1 (right). Of course, decreasing the window size further will result in a monotone convergence. \hfill $\square$

### 4 Recap on maximal monotone operators

For $\omega \geq 0$, we introduce the weighted $L^2$-space

$$L^2_\omega([0, T], \mathbb{R}^n) := \{ f : [0, T] \to \mathbb{R}^n \mid t \mapsto e^{-t \omega} f(t) \in L^2([0, T], \mathbb{R}^n) \}.$$
Fig. 1 Jacobi iteration for system (13) with \( \nu = 15, \tau = 0.01, D = 1 \). Left: \( T = 10 \). The maximum error would be obtained at iteration \( k = 148: \sqrt{2} \cdot 150^{148} / 148! \) and error decrease from \( k = 149 \) on. Overflow in single precision at \( k = 40 \). Right: \( T = 0.5 \). Maximum error for \( k = 5 (\nu T - 2 = 5.5) \), then decrease. After \( k = 29 \), we achieve the solution (in single precision)

equipped with the norm \( \| \cdot \|_{2,\omega} \) defined as

\[
\| f \|_{2,\omega}^2 = \int_0^T e^{-2t\omega} \| f(t) \|^2 dt.
\]

Clearly, as \( T \in (0, \infty) \), we have \( L^2_{\omega}([0, T], \mathbb{R}^n) = L^2([0, T], \mathbb{R}^n) \) with equivalent norms. Furthermore, if \( \omega = 0 \), then the norms in \( L^2_{\omega}([0, T], \mathbb{R}^n) \) and \( L^2([0, T], \mathbb{R}^n) \) coincide.

**Definition 14** (Contraction) Let \( X \) be a Banach space space with norm \( \| \cdot \| \). A (possibly nonlinear) operator \( A: D(A) \subset X \to X \) is called contractive, if

\[
\| Ax - Ay \| \leq \| x - y \|, \quad \forall x, y \in X,
\]

and strictly contractive, if there exists some \( L < 1 \), such that

\[
\| Ax - Ay \| \leq L \| x - y \|, \quad \forall x, y \in X.
\]

**Definition 15** (Maximally monotone operator) Let \( X \) be a real Hilbert space with inner product \( \langle \cdot, \cdot \rangle \). A set \( Y \subset X \times X \) is called monotone, if

\[
\langle x - u, y - v \rangle \geq 0, \quad (x, y), (u, v) \in Y.
\]

Furthermore, \( Y \subset X \times X \) is called maximally monotone, if it is monotone and not a proper subset of a monotone subset of \( X \times X \).

A (possibly nonlinear) operator \( A: D(A) \subset X \to X \) is called (maximally) monotone, if the graph of \( A \), i.e., \( \{(x, Ax) : x \in D(A)\} \), is (maximally) monotone.
Remark 16 Let \( A : D(A) \subset X \rightarrow X \) be a monotone operator. It follows from the definition of monotonicity that \( I + \lambda A \) is injective for all \( \lambda > 0 \).

Moreover, by [26, Theorem 2.2], the following three statements are equivalent:

(i) \( A \) is maximally monotone,
(ii) \( I + \lambda A \) is surjective for some \( \lambda > 0 \),
(iii) \( I + \lambda A \) is surjective for all \( \lambda > 0 \).

Consequently, if \( A \) is maximally monotone, then \( I + \lambda A \) is bijective for all \( \lambda > 0 \).

The Cauchy-Schwarz inequality together with the given monotonicity yields that

\[
\| (I + \lambda A)x - (I + \lambda A)y \| \geq \| x - y \| \quad \forall x, y \in D(A),
\]

whence \( (I + \lambda A)^{-1} : X \rightarrow X \) is contractive.

Furthermore, \( (I - \lambda A)(I + \lambda A)^{-1} \) is contractive. This follows with \( \tilde{x} := (I + \lambda A)^{-1}x \) and \( \tilde{y} := (I + \lambda A)^{-1}y \) from

\[
\| x - y \|^2 - \| (I - \lambda A)(I + \lambda A)^{-1}x - (I - \lambda A)(I + \lambda A)^{-1}y \|^2
\]

\[
= \| \tilde{x} - \tilde{y} + \lambda A\tilde{x} - \lambda A\tilde{y} \|^2 - \| \tilde{x} - \tilde{y} - (\lambda A\tilde{x} - \lambda A\tilde{y}) \|^2
\]

\[
= 4\lambda \langle \tilde{x} - \tilde{y}, A\tilde{x} - A\tilde{y} \rangle \geq 0.
\]

\[\blacksquare\]

5 Dynamic iteration scheme

Now we develop a dynamic iteration scheme for the DAE (2) fulfilling Assumption 5. To facilitate the decoupling, we split \( J \) as follows

\[
J = \begin{bmatrix}
J_1 & 0 & \cdots & 0 \\
0 & \ddots & \cdots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & J_s
\end{bmatrix}
\]

\[
=: J_d
\]

and

\[
J = \begin{bmatrix}
0 & J_{12} & \cdots & J_{1s} \\
-\tilde{J}_{12} & \ddots & \cdots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
\tilde{J}_{1s} & \cdots & -\tilde{J}_{s-1,s} & 0
\end{bmatrix}
\]

\[
=: J_o
\] (14)

such that \( J_d = -J_d^\top \) and \( J_o = -J_o^\top \) (compare with Rem. 6 (c)).

Let \( \alpha \in [0, 1], \mu, \omega \in \mathbb{R} \) with \( 0 \leq \mu \leq \omega \). We introduce the affine-linear operator \( M \) by:

\[
M : \quad D(M) \subset L^2_\omega([0, T], \mathbb{R}^n) \rightarrow L^2_\omega([0, T], \mathbb{R}^n),
\]

\[
x \mapsto \frac{d}{dt}(Ex) - (J_d - \alpha R + \mu EQ^{-1})Qx - Bu
\]

(15b)

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with domain
\[
D(M) = \left\{ x \in L^2_\omega([0, T], \mathbb{R}^n) \mid Ex \in H^1([0, T], \mathbb{R}^n), \; Ex(0) = Ex_0 \right\},
\]
and the linear bounded multiplication operator \(N\) by
\[
N : L^2_\omega([0, T], \mathbb{R}^n) \to L^2_\omega([0, T], \mathbb{R}^n),
\]
\[
x \mapsto ((1 - \alpha)R + \mu EQ^{-1} - J_\omega)Qx.
\]

Remark 17 Notice that \(x\) is a solution of the DAE (2) if, and only if,
\[
Mx + Nx = 0
\]
holds. \(\square\)

In the following, we use \(\alpha \in [0, 1]\) in order to have both the contribution \((1 - \alpha)R\) to \(N\) and the contribution \(\alpha R\) to \(M\) positive semi-definite.

Lemma 18 Let \(\omega, \mu \in \mathbb{R}\) with \(0 \leq \mu \leq \omega\), and let \(\alpha \in [0, 1]\). Assume that the DAE (2) fulfills Assumption 5, and let the operator \(M\) be defined as in (15). Then \(MQ^{-1}\) is maximally monotone on \(L^2_\omega([0, T], \mathbb{R}^n)\). More precisely, \(MQ^{-1}\) satisfies
\[
\{MQ^{-1}v - MQ^{-1}w, \; v - w\}_{2,\omega} \\
= \frac{1}{2}e^{-2T\omega} \left( \|EQ^{-1}\|^{1/2}(v(T) - w(T))\|^2 \right) \\
(\omega - \mu)\|EQ^{-1}\|^{1/2}(v - w)\|^2_{2,\omega} + \alpha\|R^{1/2}(v - w)\|^2_{2,\omega} \geq 0
\]
for \(v, w \in QD(M)\), and \(I + \lambda MQ^{-1}\) is surjective for every \(\lambda > 0\).

Proof First of all, we have for \(v, w \in QD(M)\)
\[
\{MQ^{-1}v - MQ^{-1}w, \; v - w\}_{2,\omega} \\
= (\frac{d}{dt}EQ^{-1}(v - w), \; v - w)_{2,\omega} - ((J_d - \alpha R + \mu EQ^{-1})(v - w), \; v - w)_{2,\omega} \\
= (\frac{d}{dt}EQ^{-1}(v - w), \; v - w)_{2,\omega} - \mu((EQ^{-1}(v - w), \; v - w)_{2,\omega} + (\alpha R(v - w), \; v - w)_{2,\omega} \\
= \frac{1}{2}e^{-2T\omega} \left( \|EQ^{-1}\|^{1/2}(v(T) - w(T))\|^2 \right) \\
+ (\omega - \mu)\|EQ^{-1}\|^{1/2}(v - w)\|^2_{2,\omega} + (\alpha R(v - w), \; v - w)_{2,\omega} \geq 0,
\]
which shows that \(MQ^{-1}\) is monotone (thereby we also use integration by parts).

To prove that \(MQ^{-1}\) is maximally monotone, it suffices, by Remark 16, to prove that \(I + \lambda MQ^{-1}\) is surjective for some \(\lambda > 0\). Assume that \(y \in L^2_\omega([0, T], \mathbb{R}^n)\). Consider the matrices \(\tilde{E} = EQ^{-1}, \; \tilde{R} = \alpha R + \frac{1}{\lambda}I\) and \(\tilde{Q} = I\). Then the DAE
\[
\frac{d}{dt}\tilde{E}\tilde{v}(t) = (J_d - \tilde{R})\tilde{Q}\tilde{v}(t) + Be^{-\mu t}u(t) - \frac{1}{\lambda}e^{-\mu t}y(t), \; \tilde{E}\tilde{v}(0) = \tilde{E}Qx_0
\]
clearly fulfills Assumption 5(a)&(b). Moreover, by positive definiteness of \( \tilde{K} \), we obtain that any matrix \( Z \in \mathbb{R}^{n \times r} \) with full column rank and \( \mathrm{im} Z = \ker E \) fulfills \( \ker \tilde{R} Q Z = \{0\} \). This means that Assumption 5(c) is trivially fulfilled by (18), and Proposition 9 implies that (18) has a unique solution \( \tilde{v} \in L^2_\omega([0, T], \mathbb{R}^n) \) with \( \tilde{E} \tilde{v} \in H^1([0, T], \mathbb{R}^n) \). Now consider \( v \in L^2_\omega([0, T], \mathbb{R}^n) \) with \( v(t) = e^{\mu t} \tilde{v}(t) \). Then \( \tilde{E} \tilde{v}(0) = \tilde{E} \tilde{v}(0) = \tilde{E} Q x_0 \), and the product rule for weak derivatives [19, Thm. 4.25] yields \( \tilde{E} v \in H^1([0, T], \mathbb{R}^n) \) with

\[
\frac{d}{dt} \tilde{E} v = \frac{d}{dt} e^{\mu t} \tilde{E} \tilde{v} = e^{\mu t} \frac{d}{dt} \tilde{E} \tilde{v} + \mu e^{\mu t} \tilde{E} \tilde{v} = e^{\mu t} (J_d - \tilde{R}) \tilde{Q} \tilde{v} + e^{\mu t} B e^{-\mu t} u(t) - e^{\mu t} \frac{1}{\lambda} e^{-\mu t} y(t) + \mu e^{\mu t} \tilde{E} \tilde{v}
\]

and thus

\[
v + \lambda \left( \frac{d}{dt} E Q^{-1} v - (J_d - \alpha R + \mu E Q^{-1}) Q Q^{-1} v + Bu \right) = y.
\]

Since this means that \( (I + \lambda M Q^{-1}) v = y \), the result is shown. \( \square \)

**Lemma 19** Let \( \lambda > 0, \mu \geq 0, \alpha \in [0, 1] \), and let \( R, E, Q \in \mathbb{R}^{n \times n} \) with the properties as in Assumption 5. Then, for \( K := ((1 - \alpha) R + \mu E Q^{-1} - J_o) \)

\[
\| (I - \lambda K)(I + \lambda K)^{-1} x \|^2 - \| x \|^2 = -4\lambda \|(1 - \alpha) R + \mu E Q^{-1})^{1/2} (I + \lambda K)^{-1} x \|^2, \quad \forall x \in \mathbb{R}^n.
\]

Moreover, if

\[
\mathrm{rk} \left[ \mu E (1 - \alpha) R \right] = n,
\]

then \((1 - \alpha) R + \mu E Q^{-1} = K + J_o \in \mathbb{R}^{n \times n}\) is invertible, and

\[
\| (I - \lambda K)(I + \lambda K)^{-1} x \| \leq q \| x \|, \quad \forall x \in \mathbb{R}^n,
\]

where \( q \geq 0 \) with

\[
q^2 = 1 - \frac{4\lambda}{(1 + \lambda \| K \|)^2 \cdot \| (K + J_o)^{-1} \|} < 1.
\]

**Proof** By using that \( K + K^\top \geq 0 \), we see that \( I + \lambda K \) is an invertible matrix. Let \( x \in \mathbb{R}^n \) and \( y := (I + \lambda K)^{-1} x \). Then

\[
\| x \|^2 - \| (I - \lambda K)(I + \lambda K)^{-1} x \|^2 = \| y + \lambda K y \|^2 - \| y - \lambda K y \|^2 = 4\lambda \langle y, (K + K^\top) y \rangle = 4\lambda \langle y, ((1 - \alpha) R + \mu E Q^{-1}) y \rangle
\]
shows (19). To prove the remaining result, assume that (20) is fulfilled. Then it can be concluded from Assumption 5(a)(i) that \((1 - \alpha)R + \mu EQ^{-1}\) is positive definite. Furthermore, by

\[
\|x\| = \|(I + \lambda K)y\| \leq (1 + \lambda \|K\|)\|y\| = (1 + \lambda \|K\|)(I + \lambda K)^{-1}x,
\]

we have

\[
\|(I + \lambda K)^{-1}x\| \geq \frac{1}{1 + \lambda \|K\|} \|x\| \quad \forall x \in \mathbb{R}^n.
\]

Plugging this into (19), we obtain for all \(x \in \mathbb{R}^n\)

\[
\|(I - \lambda K)(I + \lambda K)^{-1}x\|^2 = \|x\|^2 - 4\lambda \|(I - \alpha)R + \mu EQ^{-1}\)^{1/2}(I + \lambda K)^{-1}x\|^2
\]

\[
\leq \|x\|^2 - 4\lambda \|(I - \alpha)R + \mu EQ^{-1}\)^{-1}\|\|\|1\|(I + \lambda K)^{-1}x\|^2
\]

\[
\leq \|x\|^2 - 4\lambda \|(I - \alpha)R + \mu EQ^{-1}\)^{-1}\|\|\|1\|(1 + \lambda \|K\|)^2 \|x\|^2.
\]

\[
= \left(1 - \frac{4\lambda}{\|(I - \alpha)R + \mu EQ^{-1}\)^{-1}\| \cdot (1 + \lambda \|K\|)^2}\right) \|x\|^2,
\]

which completes the proof. \(\square\)

**Remark 20** Condition (20) is equivalent to at least one of the following three statements being fulfilled:

(i) \(\text{rk} \left[ EQ \right] = n, \mu > 0\) and \(\alpha < 1\), or

(ii) \(\text{rk} E = n, \mu > 0,\) and \(\alpha \leq 1\), or

(iii) \(\text{rk} R = n, \mu \geq 0\) and \(\alpha < 1\). \(\square\)

As a direct conclusion of Lemma 19, we can draw the following result.

**Lemma 21** Let \(\lambda, \mu \geq 0, \alpha \in (0, 1]\), let \(R, E, Q \in \mathbb{R}^{n \times n}\) with the properties as in Assumption 5, and let the operator \(N\) be defined as in (16). The multiplication operator \(NQ^{-1}\) on \(L^2_\omega([0, T], \mathbb{R}^n)\) is linear, bounded and satisfies

\[
(x, NQ^{-1}x)_2,\omega \leq 0,
\]

i.e., \(NQ^{-1}\) is maximally monotone. Furthermore, the multiplication operator \(x \mapsto (I - \lambda NQ^{-1})(I + \lambda NQ^{-1})^{-1}x\) is a contraction on \(L^2_\omega([0, T], \mathbb{R}^n)\) for \(\lambda > 0\) satisfying

\[
\|(I - \lambda NQ^{-1})(I + \lambda NQ^{-1})^{-1}x\|_2,\omega \leq \|x\|_2,\omega \quad \forall x \in L^2_\omega([0, T], \mathbb{R}^n).
\]

Moreover, if \(\text{im} E + \text{im} R = \mathbb{R}^n\) and \(\alpha < 1\), then

\[
\|(I - \lambda NQ^{-1})(I + \lambda NQ^{-1})^{-1}x\|_2,\omega \leq q \|x\|_2,\omega \quad \forall x \in L^2_\omega([0, T], \mathbb{R}^n).
\]

for \(q < 1\) as in (22).
The first statement follows directly and the remaining statements are implied by Lemma 19. □

Our dynamic iteration scheme is built on Rem. 17. Following Lions and Mercier [18], we study the algorithms

\[ x^{k+1} := Q^{-1}(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}(I - \lambda M Q^{-1})Qx^k. \]  
(23)

with \( x^0 \in D(M) \) arbitrary.

**Remark 22** Note that equation (17) is equivalent to

\[ (I + \lambda N Q^{-1})(I + \lambda M Q^{-1})Qx = (I - \lambda N Q^{-1})(I - \lambda M Q^{-1})Qx, \]

or equivalently,

\[ x = Q^{-1}(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}(I - \lambda M Q^{-1})Qx. \]

□

**Remark 23** The iteration (23) is equivalent to

\[ x^{k+1} := (Q + \lambda M)^{-1}(Q - \lambda N)(Q + \lambda N)^{-1}(Q - \lambda M)x^k. \]  
(24)

**Theorem 24** Let \( \lambda > 0, \mu \geq 0, \) and let \( \alpha \in [0, 1] \). Assume that the DAE (2) fulfills Assumption 5, and let the operators \( M, N \) be defined as in (15) and (16). Let \( \lambda > 0 \) and \( x^0 \in D(M) \). Let the sequence \( (x^k)_k \) be defined by (23), and let \( x \) be the unique solution of (2). Then the following statements are fulfilled:

(a) \( (Ex^k)_k \) converges to \( Ex \) in \( L^2([0, T], \mathbb{R}^n) \),
(b) \( (Ex^k)_k \) converges uniformly to \( Ex \) on \([0, T]\),
(c) If \( \alpha > 0 \), then \( (RQx^k)_k \) converges to \( RQx \) in \( L^2([0, T], \mathbb{R}^n) \),
(d) For the sequence \( (z^k)_k \) given by

\[ \forall k \in \mathbb{N} : \ z^k := (I + \lambda M Q^{-1})Qx^k, \]

and the function \( z := (I + \lambda M Q^{-1})Qx \), the real sequence \( (\|z^k - z\|_{2,\omega})_k \) is monotonically decreasing, and

\[ \forall k \in \mathbb{N} : \ \|x^k - x\|_{2,\omega} \leq \|Q^{-1}\|\|z^k - z\|_{2,\omega}. \]  
(25)

**Proof** Let \( \omega \in \mathbb{R} \) with \( \mu < \omega \). We have

\[ z^{k+1} = (I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} (2I - (I + \lambda M Q^{-1}))(I + \lambda M Q^{-1})^{-1}z^k \]
\[ = (I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}[2Qx^k - z^k] \]  
(26)
and
\[ z = (I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}(2Qx - z). \]

We set
\[ \Delta x^k := x - x^k, \quad \Delta z^k := z - z^k. \]

Then using Lemmas 21 and 18 we calculate
\[
\|\Delta z^{k+1}\|_{2,\omega}^2 - \|\Delta z^k\|_{2,\omega}^2 = \|z - z^{k+1}\|_{2,\omega}^2 - \|\Delta z^k\|_{2,\omega}^2 \\
= \| (I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}[(2Qx - z) - (2Qx^k - z^k)]\|_{2,\omega}^2 - \|\Delta z^k\|_{2,\omega}^2 \\
\leq 2\|Q\Delta x^k - \Delta z^k\|_{2,\omega}^2 - \|\Delta z^k\|_{2,\omega}^2 \\
= 4\|Q\Delta x^k\|_{2,\omega}^2 - 4(Q\Delta x^k, \Delta z^k)_{2,\omega} \\
= 4\|Q\Delta x^k\|_{2,\omega}^2 - 4(Qx - Qx^k, (I + \lambda M Q^{-1})Qx - (I + \lambda M Q^{-1})Qx^k)_{2,\omega} \\
= -4\lambda\langle Qx - Qx^k, Mx - Mx^k \rangle_{2,\omega} \\
= -2\exp(-2T\omega)\| (E Q^{-1})^{1/2} Q\Delta x^k(T) \|^2 \\
- 4\lambda(\omega - \mu)\| (E Q^{-1})^{1/2} Q\Delta x^k \|_{2,\omega}^2 - 4\lambda\alpha\| R^{1/2} Q\Delta x^k \|_{2,\omega}^2. \tag{27}
\]

Thus the sequence \( (\|\Delta z^k\|_{2,\omega})_k \) monotonically decreasing, and therefore it converges. Inequality (25) follows from Remark 16, which completes the proof of (d). Furthermore, the latter inequality gives
\[
\|(E Q^{-1})^{1/2} Q\Delta x^k\|_{2,\omega}^2 \leq \frac{1}{4\lambda(\omega - \lambda)} (\|\Delta z^k\|_{2,\omega}^2 - \|\Delta z^{k+1}\|_{2,\omega}^2), \tag{28}
\]
\[
\|RQ\Delta x^k\|_{2,\omega}^2 \leq \|R^{1/2}\|^2 \cdot \|R^{1/2} Q\Delta x^k\|_{2,\omega}^2 \\
\leq \frac{\|R^{1/2}\|^2}{4\lambda\alpha} (\|\Delta z^k\|_{2,\omega}^2 - \|\Delta z^{k+1}\|_{2,\omega}^2). \tag{29}
\]

Combining (29) with the fact that the norms \( \| \cdot \|_{\omega,2} \) and \( \| \cdot \|_2 \) are equivalent, we are led to (c). In addition, (28) together with \( E = (E Q^{-1})^{1/2}(E Q^{-1})^{1/2} Q \)—and using that \( \|\Delta z^k\|_{2,\omega} \) is a convergent sequence—gives \( (\|E\Delta x^k\|_{2,\omega})_k \) converges to zero, and the equivalence between the norms \( \| \cdot \|_{\omega,2} \) and \( \| \cdot \|_2 \) now implies (a).

It remains to prove (b). We repeat the calculation (27) but with \( t \in (0, T] \) instead of \( T \) in the last step and obtain
\[
\|(E Q^{-1})^{1/2} Q\Delta x^k(t)\|^2 \leq \frac{e^{2\omega T}}{2\lambda} (\|\Delta z^k\|_{2,\omega}^2 - \|\Delta z^{k+1}\|_{2,\omega}^2),
\]
which shows that \( Ex^k(t) \to Ex(t) \) uniformly in \( t \in [0, T] \).
Lemma 18 and Lemma 21, we obtain, for (2)

Remark 25 Though the sequence \( \|\Delta x^k\|_{2,\omega} \) is usually not monotone decreasing, it is bounded by the monotone decreasing sequence \( \|Q^{-1}\|z^k - z\|_{2,\omega} \) due to (25).

Theorem 26 Let \( \lambda > 0, \mu \geq 0, \) and let \( \alpha \in [0, 1] \). Assume that the DAE (2) fulfills Assumption 5, and let the operators \( M, N \) be defined as in (15) and (16). Let \( x^0 \in D(M) \). Let the sequence \( (x^k) \) be defined by (23), and let \( x \) be the unique solution of (2). Then the following statements are fulfilled:

(a) If (20) holds, then the sequence \( z^k \) as defined in Theorem 24 (d) converges to

\[
\|\Delta x^k\|_{2,\omega} = \|(I - \lambda M Q^{-1})(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1}) (I + \lambda N Q^{-1})^{-1} z_k \|
\]

and we define \( \Delta z^k := z - z^k \). Assume that (20) holds. By invoking Remark 22, Lemma 18 and Lemma 21, we obtain, for \( q < 1 \) as in Lemma 19,

\[
\|\Delta x^k\|_{2,\omega} = \|((I - \lambda M Q^{-1})(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} z_k - ((I - \lambda M Q^{-1})(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} z_k)\|_{2,\omega}
\]

\[
\leq \|((I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}\Delta z^k\|_{2,\omega}
\]

\[
\leq q \|\Delta z^k\|_{2,\omega}.
\]

This implies that \( z^k \) converges in \( L^2([0, T], \mathbb{R}^n) \) to \( z \).

Next we prove that \( (Ex^k)_k \) converges to \( Ex \) in \( H^1([0, T], \mathbb{R}^n) \). We already know from Theorem 24 (a) that \( (Ex^k)_k \) converges to \( Ex \) in \( L^2([0, T], \mathbb{R}^n) \). Hence, it suffices to prove that \( \frac{d}{dt}Ex^k \) converges to \( \frac{d}{dt}Ex \) in \( L^2([0, T], \mathbb{R}^n) \). By invoking that \( (z^k) \) converges to \( z \) in \( L^2([0, T], \mathbb{R}^n) \), (25) yields that \( (x^k) \) converges to \( x \) in \( L^2([0, T], \mathbb{R}^n) \).

Now using the definition of \( x, z \) and \( M \), we have

\[
z_k = Qx^k + \lambda \left(\frac{d}{dt}(Ex^k) - (J_d - \alpha R + \mu Eq^{-1})Qx^k - Bu\right),
\]

\[
z = Qx + \lambda \left(\frac{d}{dt}(Ex) - (J_d - \alpha R + \mu Eq^{-1})Qx - Bu\right),
\]

which gives

\[
\frac{d}{dt}(Ex) - \frac{d}{dt}(Ex^k) = \frac{1}{\lambda}(z - z^k) + \frac{1}{\lambda}Q(x - x^k) + (J_d - \alpha R + \mu Eq^{-1})Q(x - x^k).
\]

Proof We start with the proof of (a): By (23) and Remark 22, we have

\[
z^{k+1} = (I - \lambda M Q^{-1})(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} z^k,
\]

\[
z = (I - \lambda M Q^{-1})Q(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} z,
\]

and we define \( \Delta z^k := z - z^k \). Assume that (20) holds. By invoking Remark 16, Lemma 18 and Lemma 21, we obtain, for \( q < 1 \) as in Lemma 19,

\[
\|\Delta z^{k+1}\|_{2,\omega} = \|(I - \lambda M Q^{-1})(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} z - (I - \lambda M Q^{-1})(I + \lambda M Q^{-1})^{-1}(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1} z^k\|_{2,\omega}
\]

\[
\leq \|(I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}\Delta z^k\|_{2,\omega}
\]

\[
\leq q \|\Delta z^k\|_{2,\omega}.
\]

This implies that \( z^k \) converges in \( L^2([0, T], \mathbb{R}^n) \) to \( z \).

Next we prove that \( (Ex^k)_k \) converges to \( Ex \) in \( H^1([0, T], \mathbb{R}^n) \). We already know from Theorem 24 (a) that \( (Ex^k)_k \) converges to \( Ex \) in \( L^2([0, T], \mathbb{R}^n) \). Hence, it suffices to prove that \( \frac{d}{dt}Ex^k \) converges to \( \frac{d}{dt}Ex \) in \( L^2([0, T], \mathbb{R}^n) \). By invoking that \( (z^k) \) converges to \( z \) in \( L^2([0, T], \mathbb{R}^n) \), (25) yields that \( (x^k) \) converges to \( x \) in \( L^2([0, T], \mathbb{R}^n) \). Now using the definition of \( x, z \) and \( M \), we have

\[
z_k = Qx^k + \lambda \left(\frac{d}{dt}(Ex^k) - (J_d - \alpha R + \mu Eq^{-1})Qx^k - Bu\right),
\]

\[
z = Qx + \lambda \left(\frac{d}{dt}(Ex) - (J_d - \alpha R + \mu Eq^{-1})Qx - Bu\right),
\]

which gives

\[
\frac{d}{dt}(Ex) - \frac{d}{dt}(Ex^k) = \frac{1}{\lambda}(z - z^k) + \frac{1}{\lambda}Q(x - x^k) + (J_d - \alpha R + \mu Eq^{-1})Q(x - x^k).
\]
Since \((x^k)\) converges to \(x\) in \(L^2([0, T], \mathbb{R}^n)\), and further, \((z^k)\) converges to \(z\) in \(L^2([0, T], \mathbb{R}^n)\), the above equation implies that \(\frac{d}{dt}(E \cdot x^k)\) converges in \(L^2([0, T], \mathbb{R}^n)\) to \(\frac{d}{dt}(E \cdot x)\). Altogether, this means that \((E \cdot x^k)\) converges to \(E \cdot x\) in \(H^1([0, T], \mathbb{R}^n)\).

Next we prove (b). The case where (20) is fulfilled, the result follows by a combination of (a) with (25).

Assume that (30) holds: Then, by invoking Assumption 5(a)(i), the matrix \(Q^\top E + \alpha Q^\top R Q\) is positive definite, and thus invertible. On the other hand, \(((Q^\top E + Q^\top R Q)x^k)\) converges to \((Q^\top E + \alpha Q^\top R Q)x\) in \(L^2([0, T], \mathbb{R}^n)\) by Theorem 24. Consequently, \((x^k)\) converges to \(x\) in \(L^2([0, T], \mathbb{R}^n)\).

Based on the results of the previous section, we present a respective dynamic iteration algorithm. We recall that we choose \(\omega > 0\) and we define

\[
x^{k+1} := (Q + \lambda M)^{-1}(Q - \lambda N)(Q + \lambda N)^{-1}(Q - \lambda M)x^k,
\]

with \(x^0 \in D(M)\) arbitrary, and

\[
z^k := (I + \lambda M Q^{-1})Qx^k.
\]

Using (26) we obtain

\[
z^{k+1} = (I - \lambda N Q^{-1})(I + \lambda N Q^{-1})^{-1}[2Qx^k - z^k].
\]

Furthermore, relation \(z^k = (Q + \lambda M)x^k\) corresponds to the DAE

\[
\frac{d}{dt}E_i x_i^k = (J_i - R_i + \mu E_i Q_i^{-1})Q_i x_i^k - \frac{1}{\lambda}Q_i x^k + B_i u + \frac{1}{\lambda}z_i^k, \quad i = 1, \ldots, s, \quad (A)
\]

with initial conditions \(E_i x_i^0(0) = E_ix_{0,i} (i = 1, \ldots, s)\). Given \(z_i^k\), we have \(s\) decoupled subsystems.

**Remark 27** (a) If \(\text{rk}\left[ E \quad R \right] < n\), then it is not possible to formulate any convergence results for \((x^k)\), in general. As an example, consider a system (2) with

\[
E = R = O_{2 \times 2}, \quad Q = I_2, \quad J = \left[ \begin{array}{c|c} 0 & 1 \\ \hline -1 & 0 \end{array} \right], \quad u = 0 \in L^2([0, T]; \mathbb{R}^2),
\]

which belongs to the class specified in Assumption 5 with \(s = 2\) and \(n_1 = n_2 = 1\). The unique solution of (2) is clearly given by \(x = 0\) (the specification of the initial value \(x_0\) is obsolete by \(E = 0\)).

The above choice of \(E, R\) and \(Q\) leads to \(M\) in (15) being the zero operator, whereas \(N\) as in (16) corresponds to the multiplication with the skew-Hermitian matrix \(-J\). Consequently, for \(\lambda > 0\), the iteration (24) now reads

\[
x^{k+1} := Ux^k, \quad \text{where} \quad U = (I + \lambda J)(I - \lambda J)^{-1}.
\]

By invoking Lemma 19, we see that \(U\) is a unitary matrix with \(U \neq I_2\). Therefore, \(\|x^{k+1}(t)\| = \|x^k(t)\|\) for all \(k \in \mathbb{N}, t \in [0, T]\), and thus \(\|x^{k+1}\|_2 = \|x^k\|_2\). It can
be concluded that the sequence \((x^k)\) does not converge in \(L^2([0, T], \mathbb{R}^2)\) to \(x = 0\). A closer look to the iteration yields that \((x^k)\) does not even have a subsequence which weakly converges in \(L^2([0, T], \mathbb{R}^2)\) to \(x = 0\).

(b) Under Assumption 5, (20) is equivalent to \(E\) and \(R\) fulfilling \(\text{rk} E = n\), or \(\text{rk} [E \quad R] = n\) and \(\alpha > 0\).

(c) In the case of ordinary differential equations, i.e., \(E = I\), then Theorem 26 simplifies to the following:

(i) If \(\mu > 0\), or \(\text{rk} R = n\) and \(\alpha < 1\), then \((z^k)\) converges to \(z\) in \(L^2([0, T], \mathbb{R}^n)\), and \((x^k)\) converges to \(x\) in \(H^1([0, T], \mathbb{R}^n)\).

(ii) \((x^k)\) converges to \(x\) in \(L^2([0, T], \mathbb{R}^n)\).

The above discussion results in a Lions–Mercier-type dynamic iteration for pH systems, which is summarized in Algorithm 1. Notice, we have different formulas for the iteration in \(x^k\); the algorithm is based on the decoupled formulation of subsystems \(A\).

**Algorithm 1** Lions–Mercier-type Dynamic Iteration for pH systems

**Require:** problem data: \(J_i, J_0, R_i, Q_i, E_i, B_i, u_i, x_{i,0} (i = 1, \ldots, s)\)

**Require:** choose for \(i = 1, \ldots, s\) \(z_i^0 \in L^2([0, T]; \mathbb{R}^{n_i})\) % initial guess

**Require:** choose parameters \(\alpha, \mu, \lambda\)

1: \(R \leftarrow \text{diag}(R_1, \ldots, R_s), E, Q\) analogously

2: \(K \leftarrow (1 - \alpha)R + \mu EQ^{-1} - J_0\)

3: \(z^0 \leftarrow [(z_1^0)^\top, \ldots, (z_s^0)^\top]^\top\)

4: for \(k = 0, 1, 2, \ldots\) do

5: for \(i = 1, 2, \ldots, s\) do

6: solve for \(x_i^k\)

\[
\frac{d}{dt} E_i x_i^k = (J_i - \alpha R_i + \mu E_i Q_i^{-1}) Q_i x_i^k - \frac{1}{K} Q_i x_i^k + B_i u + \frac{1}{K} z_i^k
\]

with initial value \(E_i x_i^k(0) = E_i x_{i,0}\)

7: end for

8: \(x^k \leftarrow [(x_1^k)^\top, \ldots, (x_s^k)^\top]^\top\)

9: \(z^{k+1} \leftarrow (I - \lambda K)(I + \lambda K)^{-1} \left(2Qx^k - z^k\right)\)

10: partition \(z^{k+1}\) into components \(z_1^{k+1}, \ldots, z_s^{k+1}\)

11: if error small then return

12: end if

13: end for

**6 Numerical results**

We analyse the convergence rates for the new type of monotonic dynamic iterations (Lions–Mercier-type iteration). Then, we show numerical convergence results for the promising monotone convergence algorithms developed here.
6.1 Convergence rate discussion

For $0 < \alpha < 1$ and $K = ((1 - \alpha)R + \mu EQ^{-1} - J_o)$ the convergence rate is given by the contraction factor (22)

$$q^2 = 1 - \frac{4\lambda}{(1 + \lambda\|K\|)^2\|K + J_o\|^{-1}}.$$ 

The optimal $\lambda^*$ will have the smallest error reduction factor. We find:

$$\lambda^*(\mu) = \frac{1}{\|K\|} \quad \text{and} \quad q^*(\mu, \lambda^*(\mu))^2 = 1 - \frac{1}{\|K\| \cdot \|K + J_o\|^{-1}}.$$ 

**Remark 28** (Decoupled setting) In the decoupled case, $J_o = 0$, hence, the optimal error reduction reads:

$$q^*(\mu, \lambda^*(\mu))^2 = 1 - \frac{1}{\text{cond}(K)},$$

which is only small for nearly equilibrated matrices $K$. This is in contrast to (e.g.) Jacobi dynamic iteration procedures, where we have immediate convergence. \hfill \Box

Considering ODEs with $E = I$ and setting $\alpha = 1$, we have $K = \mu Q^{-1} - J_o$.

**Remark 29** (ODE case)

(a) Transformation to $Q = I$: using the Cholesky factorization $Q = V^T V$, we multiply (2) with $V$, which yields

$$V \frac{d}{dt} x = V(J - R)(V^TV)x + VBu(t) \quad \Leftrightarrow \quad \frac{d}{dt} \tilde{x} = (\tilde{J} - \tilde{R})\tilde{x} + \tilde{B}u(t)$$

with $\tilde{x} = Vx$, $\tilde{J} = VJV^T$, $\tilde{R} = VRV^T$ and $\tilde{B} = VB$ provides a remedy. Correspondingly, $y = B^TQx$ is transformed into $\tilde{y} = \tilde{B}^T\tilde{x}$.

(b) Decoupled setting ($J_o = 0$): The reduction factor is $q^* = 1 - \frac{1}{\text{cond}(Q)}$. Again, this is only small for scaling matrices $Q$ with small condition number. The above transformation to $Q = I$ yields $q^* = 0$. An alternative is a shift with a matrix-valued $\lambda$ in Algorithm 1.

(c) Coupled setting: for $Q = I$ and the Euclidean norm this gives

$$\lambda^*(\mu) = \frac{1}{\sqrt{\mu^2 + \lambda_{\text{max}}(J_o^TJ_o)}} \quad \text{and} \quad q^*(\mu, \lambda^*(\mu))^2 = 1 - \frac{1}{\sqrt{1 + \lambda_{\text{max}}(J_o^TJ_o)/\mu^2}}. \quad (31)$$

6.2 Results for monotone Lions–Mercier-type algorithm

6.2.1 Example with Jacobi failure

For system (13) holds $Q = I$ and $\lambda_{\text{max}}(J_o^TJ_o) = v^2$. This gives the optimal contraction constant via (31): $(q^*)^2 = 1 - \frac{1}{\sqrt{1 + v^2/\mu^2}}$. We see the following:
(a) We have monotone convergence for the Lions–Mercier-type algorithm, Algorithm 1.
(b) In the limit of an undamped error bound $\omega \to 0^+$, the optimal convergence rate goes to one (for $\nu \neq 0$). This indicates an extremely slow convergence.
(c) One can get arbitrarily small convergence rates $q^*$ for $\mu \to \infty$. However, this corresponds to more and more damped error norms, which do not allow to estimate the numerically important undamped error.

$\square$

6.2.2 Simple $2 \times 2$ system with scaling

We introduce into the simple $2 \times 2$ example (13) a scaling matrix $Q$:

$$x' = (J - R)Qx, \quad x(0) = x_0, \quad \text{with } J - R = \begin{bmatrix} -\tau & \nu \\ -\nu & -\tau \end{bmatrix}, \quad Q = \begin{bmatrix} q_1 & 0 \\ 0 & q_2 \end{bmatrix},$$

(32)

where $\tau, \nu > 0$ and $q_1 \geq q_2 > 0$. In the decoupled case, $\nu = 0$, the optimal reduction factor is given by (see Rem. 29(b)):

$$q(\lambda^*) = 1 - \frac{1}{\operatorname{cond}(Q)} = 1 - \frac{q_2}{q_1}.$$

Figure 2 gives numerical results for the Lions–Mercier-type algorithm, showing that $Q$ not being a multiple of $I$ destroys the convergence in one step, although the system is fully decoupled.

6.2.3 Two masses and three springs example with damping

Now, we consider two masses $m_1, m_2 > 0$, which are connected via massless springs $K_1, K_2, K > 0$ to walls with damping $r_1, r_2 > 0$, see Fig. 3. To set up the system, we have positions $q_1, q_2$ and momenta $p_1, p_2$ for the masses $m_1, m_2$, respectively. Then, the system can be modeled by the following Hamiltonian equation of motion:

$$\dot{q}_1 = \frac{1}{m_1} p_1, \quad \dot{q}_2 = \frac{1}{m_2} p_2,$$

$$\dot{p}_1 = -(K + K_1)q_1 + Kq_2 - \frac{r_1}{m_1} p_1, \quad \dot{p}_2 = -(K + K_2)q_2 + Kq_1 - \frac{r_2}{m_2} p_2.$$

Notice, this is not yet given in our pH format (2) for the overall systems. Before we treat the overall system, we set up a description as coupled pH-subsystem as in Sec. 2.2, let $q = q_2$ denote the coupling variables, which we need for the first subsystem. Then, the two coupled pH systems read:

$$\dot{x}_1 = (J_1 - R_1)z_1 + B_1 u_1,$$

$$y_1 = B_1^\top z_1,$$

$$\dot{x}_2 = (J_2 - R_2)z_2 + B_2 u_2,$$

$$y_2 = B_2^\top z_2,$$

$$u = Cy,$$
Operator splitting based dynamic iteration...

Decoupled with optimal $\lambda$: the error reduced directly to zero (no logarithmic plot).

(a) decoupled, $Q = I$, non-optimal $\lambda$

(b) decoupled, $Q = I$, optimal $\lambda$

(c) decoupled, $Q \neq I$, optimal $\lambda$

$\nu_1 = 1.5$, $\nu_2 = 1$, $q(\lambda^*) \approx \frac{1}{3}$

(d) coupled, $Q = I$, non-optimal $\lambda$

(e) coupled, $Q = I$, optimal $\lambda$

(f) coupled, $Q \neq I$, optimal $\lambda$

$\nu_1 = 1.5$, $\nu_2 = 1$, $q(\lambda^*) \approx \frac{1}{3}$

Fig. 2 Lions–Mercier-type iteration with (32): number of iterations ($x$) versus scaled error in coupling term $\nu z$ for various settings. First column provide the decoupled case ($\nu = 0$), and the right column the coupled cases ($\nu = 1.5$). Always $\tau = -0.5$ and $\omega = 2.1$
Fig. 3 ODE two masses oscillator with damping. The coordinates $q_1$, $q_2$ describe the position of the masses

with quantities for the first subsystem: $x_1 = [p_1, q_1, q_1 - q]^{\top}$, $z_1 = Q_1 x_1$,

$$Q_1 = \begin{bmatrix} \frac{1}{m_1} & 0 & 0 \\ 0 & K_1 & 0 \\ 0 & 0 & K \end{bmatrix}, \quad J_1 = \begin{bmatrix} 0 & -1 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad R_1 = \begin{bmatrix} r_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad B_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

and for the second subsystem we have: $x_2 = [p_2, q_2]^{\top}$, $z_2 = Q_2 x_2$

$$Q_2 = \begin{bmatrix} \frac{1}{m_2} & 0 & 0 \\ 0 & K_2 & 0 \end{bmatrix}, \quad J_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad R_2 = \begin{bmatrix} r_2 & 0 \\ 0 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

and the coupling interface reads:

$$u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \quad C = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$  

Also the overall coupled system can be written in our pH-structure given in (2), with $F = \text{diag}(F_1, F_2)$ for $F \in \{J, R, Q, B\}$, cf. Rem. 7:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}' = \left( [J - BC B^{\top}] - R \right) \cdot Q \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}. \tag{33}$$

Numerical results for the Lions–Mercier-type Algorithm 1 are given in Fig. 4. These results show that the estimate $q^* \approx 0.975$ for the convergence rate (with an optimal choice leading to $q^* \approx 0.944$) is quite pessimistic in this case (for $\mu = 2$ – blue line with marker $\times$).

Remark 30 The index of linear pH DAEs does not exceed two, see Proposition 9(c). This might be confusing, especially since multibody systems are known to have index three, if holonomic position contraints are involved [6]. However, note that in the port-Hamiltonian formulation of multibody systems, the state is composed of forces and velocities; position constraints are here hidden in velocity contraints via differentiation. The latter causes an index drop.

Including coupling and output quantities as variables, i.e., $\tilde{x}_i = [x_i, u_i, y_i]^{\top}$ yields a DAE, which has no damping ($R$) in the coupling or output equations. Thus it does not fit into our framework.
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Fig. 4 Visualisation of the numerical error reduction for Lions–Mercier-type iteration of system (33) versus iteration count. Left in $x$, center in $z$, right in $z$ with scaled norm. Parameters of the benchmark: $K_i = 2$, $m_1 = m_2 = 2$, $K = 4$, $r_1 = 0.5$, $r_2 = 0.75$, and zero initial values apart from $p_{2,0} = 0.1$). And iteration parameters: $\omega = 2.2$, $\alpha = 0.5$, $\lambda = 1.5$ as well as $\mu = 2$ (blue line with marker $\times$), $\mu = 0.1$ (red line with bullet marker) (color figure online)

![Image](image_url)

Fig. 5 Example of a simple electric circuit; parameters for later simulation: $R_1 = R_2 = R_3 = R_4 = 0.5$, $R_5 = 5$, $C_1 = C_2 = 5 \cdot 10^{-4}$, $L = 20$, $i(t) = \sin(2\pi \cdot 50t) \cdot \sin(2\pi \cdot 500t)$

Finally, we like to discuss a DAE example. To have a DAE multibody system, a simple choice are holonomic constraints. However, such a constraint comes without dissipation. Hence $\text{rk}(E, R)$ is not full. Therefore, we change the field of applications.

6.3 Circuit example (DAE)

The electric circuit in Fig. 5 can be modelled as follows: for $x^\top = [u_1, u_2, u_3, j_1, u_4, u_5]$ and $E = \text{diag}(0, C_1, 0, L_1, 0, C_2)$ $B^\top = [1, 0, 0, 0, 0, 0]$

$$(Ex)' = B i(t) +$$

$$
\begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 1 \\
-1 & 0 & 0 \\
-1 & 0 & 0
\end{pmatrix}
- \begin{pmatrix}
\frac{1}{R_1} & \frac{1}{R_1} & \frac{1}{R_1} \\
\frac{1}{R_1} & \frac{1}{R_2} & \frac{1}{R_2} \\
\frac{1}{R_1} & \frac{1}{R_2} & \frac{1}{R_2}
\end{pmatrix}
\begin{pmatrix}
\frac{1}{R_4} & \frac{1}{R_4} \\
\frac{1}{R_4} & \frac{1}{R_5} \\
\frac{1}{R_4} & \frac{1}{R_5}
\end{pmatrix}

\begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix}
$$

$x$.

This example fulfills the rank condition $\text{rk}(E, R) = n = 6$ and has block-diagonal $R$.

Numerical results illustrating the Lions–Mercier-type Algorithm 1 are given in Fig. 6.
Fig. 6 Results for the circuit (Fig. 5): We depict the convergence in $x_3$ (first subsystem, first column) and in $x_5$ (second subsystem, second column) for various iterations; approximation in red with \( \circ \) marker, reference in blue with \( \times \) marker. (Lions–Mercier parameters: $\lambda = 1.2$, $\mu = 1$, $\omega = 2.2$, $\alpha = 0.2$.) (color figure online)
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Fig. 7 Error reduction for simple circuit (Fig. 5). We plot the achieved precision versus the iteration count for $x$ (left panel), $z$ (middle panel), scaled $z$ (right panel).

Fig. 8 Coupled mass-spring-damper chain with twice 25 links. We choose homogeneous parameters: $K_{i,j} = 50$, $K_{co} = 50$, $m_{i,j} = 0.3$, $r_{i,j} = 0.1$ for $i = 1, 2, j = 1, 2, \ldots, 25$.

Fig. 9 Error decay for MSD-chain with parameters given in Fig. 8. Left panel: error in the $x$-variable; right panel: error in the $z$ variable (scaled).

The respective error reduction is illustrated in Fig. 7. These results show that the estimate $q \approx 0.9998$ for the convergence rate (with an optimal choice leading to $q^* \approx 0.9980$) is quite pessimistic in this case, too.

**Remark 31** (Rank condition for circuits)

We discuss circuit equation modelled by modified nodal analysis.

i) Let a circuit include one voltage source. Then the model has a pure algebraic equation, which has no dissipation. Thus the rank condition is not satisfied.

ii) Electric circuits with current sources, capacitors, inductors and resistors can be made to fulfill the rank condition by adding sufficiently many resistors.

iii) The coupling—without auxiliary variables—can be facilitated via inductors.
Fig. 10  Results for the coupled MSD-chain (see Fig. 8). The reference solution (blue with × marker) is compared against the iterates (red with ◦ marker) for \( l = 10, 20, 30, 40 \) iterations (in the rows). Left panels: variable \( p_{1,2} \); right panels: variable \( q_{2,5} \) (color figure online)
6.4 Coupled MSD-Chain

A benchmark in port-Hamiltonian systems\(^1\) is the mass-spring-damper chain (MSD-chain), see [27]. We consider now two coupled MSD-chains, which consist of 25 mass-spring-damper elements each. The chains are coupled via a spring with stiffness \(K_{co}\), see Fig. 8. The mathematical model as pH system is given as follows. For both chains, we have

\[
\begin{align*}
\dot{x}_i &= (J - R_i) Q_i x_i + B_i u_i \quad i = 1, 2 \\
y_i &= B^T_i Q_i x_i
\end{align*}
\]

for variable \(x_i^\top = (q_{i,1}, p_{i,1}, \ldots, q_{i,25}, p_{i,25})\) for positions \(q_{i,j}\) and velocities \(p_{i,j}\) \((i = 1, 2, j = 1, \ldots, 25)\) with

\[
J = \begin{bmatrix}
0 & 1 \\
-1 & 0 \\
0 & 1 \\
-1 & 0 \\
& \ddots \\
0 & 1 \\
-1 & 0 \\
\end{bmatrix},
\]

\[
Q_i = \begin{bmatrix}
K_{i,1} & 0 & -K_{i,1} & 0 \\
0 & \frac{1}{m_{i,1}} & 0 & 0 \\
-K_{i,1} & 0 & K_{i,1} + K_{i,2} & 0 & -K_{i,2} & 0 \\
0 & 0 & 0 & \frac{1}{m_{i,2}} & 0 & 0 \\
& \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
& & & & -K_{i,24} & 0 \\
& & & & \ddots & \ddots & \ddots & \ddots \\
& & & & 0 & 0 \\
& & & & -K_{i,25} & 0 & K_{i,25} & 0 \\
& & & & 0 & 0 & 0 & \frac{1}{m_{i,25}}
\end{bmatrix}
\]

and \(R_i = \text{diag}(0, r_{i,1}, 0, r_{i,2}, \ldots, 0, r_{i,25})\) for \(i = 1, 2\). For the coupling, we introduce the additional scalar variable \(q\) or \(q_{1,1} - q\) (as in Sect. 6.2.3) and have the additional equation

\[0 = (q_{1,1} - q) - u_1,\]

which we put to subsystem \((i = 1)\) as:

\[
\frac{d}{dt} \tilde{x}_1 = (\tilde{J} - \tilde{R}_1) \tilde{Q}_1 \tilde{x}_1 + \tilde{B}_1 u_1 \quad \text{for} \quad \tilde{x}_1^\top = (x_1^\top, q_{1,1} - q),
\]

\(^1\) [URL](https://algopaul.github.io/PortHamiltonianBenchmarkSystems.jl/).
\[ \tilde{y}_1 = \tilde{B}_1^T \tilde{Q}_1 \tilde{x}_1 \]

with the enlarged matrices

\[
\begin{align*}
\tilde{J} &= \left[ \begin{array}{cc} J & -e_1 \\ e_1^T & 0 \end{array} \right], \\
\tilde{R}_1 &= \left[ \begin{array}{cc} R_1 & 0 \\ 0 & 0 \end{array} \right], \\
\tilde{Q}_1 &= \left[ \begin{array}{cc} Q_1 & 0 \\ 0 & K_{co} \end{array} \right] \in \mathbb{R}^{51 \times 51},
\end{align*}
\]

\[ \tilde{B}_1^T = (0, \ldots, 0, -1) \in \mathbb{R}^{51}, \quad B_2^T = (1, 0, \ldots, 0) \in \mathbb{R}^{50} \]

using \( e_1^T = (1, 0, \ldots, 0) \) and the coupling \( u_1 = y_2, \ u_2 = -y_1 \). Notice the overall unknowns \( (\tilde{x}_1^T(t), \ x_2^T(t)) \in \mathbb{R}^{101} \). As initial value at \( t = 0 \) we use zero, apart from \( \tilde{x}_{1,5} = q_{1,3}(0) = 0.1 \), we simulate for \( t \in [0, 2] \). Moreover, for the Lions–Mercier algorithm, we use the parameters: \( \lambda = 3.5, \ \alpha = 0.5, \ \mu = 2, \ \omega = 2.2 \). As reference solution, we use a standard time integration (Runge–Kutta of order five) with very small steps. We find that the error decays as expected. To illustrate the behavior, we show in Fig. 9 the overall error (\( L^2 \)-norm over all components summed over a discrete time grid).

To give further inside, we compare the reference solution (blue with \( \times \) marker) to the iterates (red with \( \circ \) marker) of the our Lions–Mercier-algorithm for various iteration counts in Fig. 10. This shows, how the algorithm converges. In the left column, we depict the variable \( \tilde{x}_{1,4} = p_{1,2} \) (of the first subsystem) and in the second column, we depict the variable \( \tilde{x}_{2,9} = q_{2,5} \).

### 7 Conclusions

For a general pH setting, we have shown existence and uniqueness of weak solutions. Furthermore, the perspective of coupled systems and coupling variables are treated. Then, it is demonstrated that Jacobi-type of dynamic iteration may fail in practice due to finite precision. To circumvent this, a Mercier-Lions-type dynamic iteration scheme is developed, which guarantees monotone convergence in a related variable. The proof is based on properties of the Cayley transform. Numerical results demonstrate the monotone convergence. As a drawback, we observe that the currently achieved optimal convergence rates still need some improvements in order to pave the way for a broader application.

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