# Exploiting pHS when Preconditioning SPPs

Building Preconditioners for Saddle Point Problems
in port-Hamiltonian Systems

René H. P. Noffke

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CRC 1701 PORT-HAMILTONIAN SYSTEMS

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# A port-Hamiltonian Aperitif

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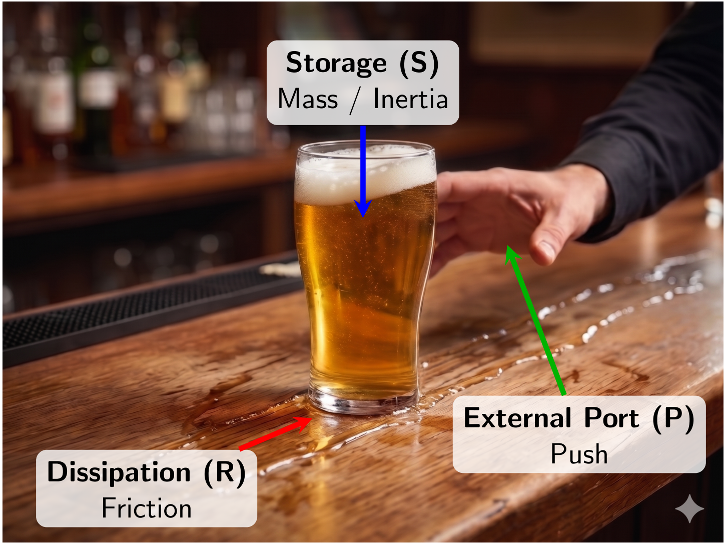


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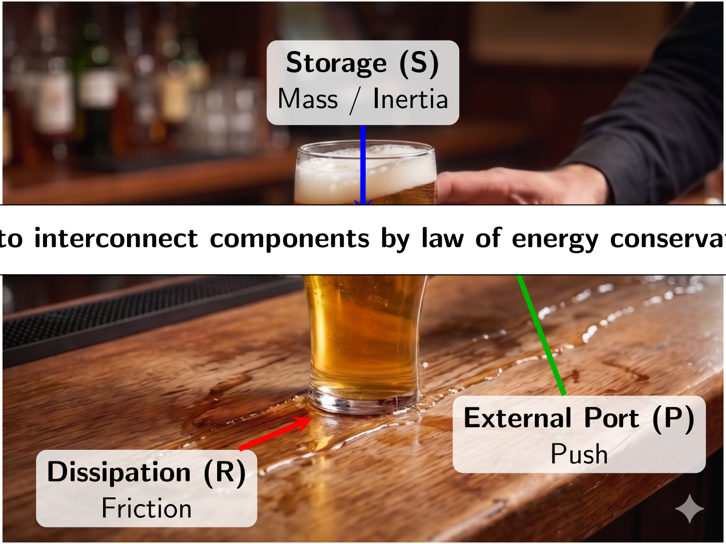
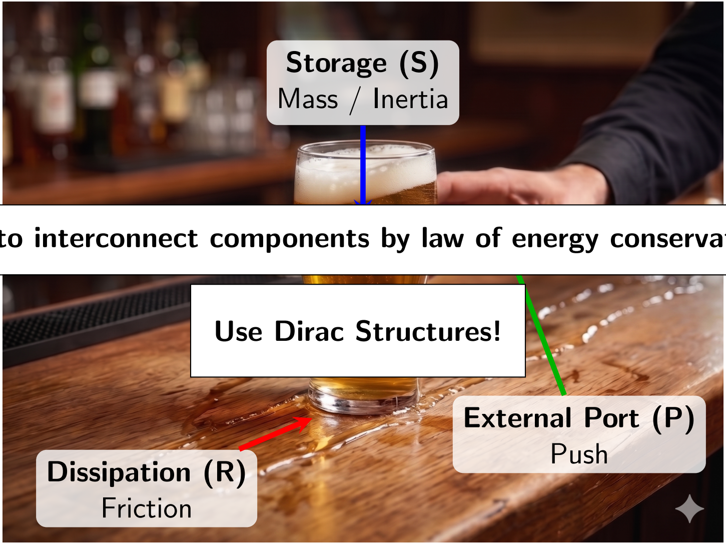



**How to interconnect components by law of energy conservation?**

# A port-Hamiltonian Aperitif






**How to interconnect components by law of energy conservation?**

**Use Dirac Structures!**

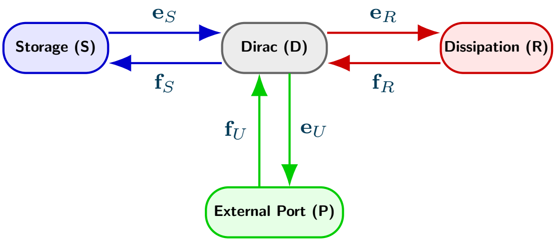
# Today's Journey

**What? Foundations of pHS**
What defines a port-Hamiltonian System (pHS) mathematically and physically?

**Why? Connecting pHS and SPP**
Why and when do port-Hamiltonian Systems translate into Saddle Point Problems (SPP)?

**How? Preconditioning Strategies**
How can we exploit the pHS structure to construct efficient SPP preconditioners?

- Well-established framework in control engineering and mechatronics
- Deeply rooted in differential geometry (Dirac structures) and functional analysis
- *Relatively* new research area in numerical linear algebra and scientific computing



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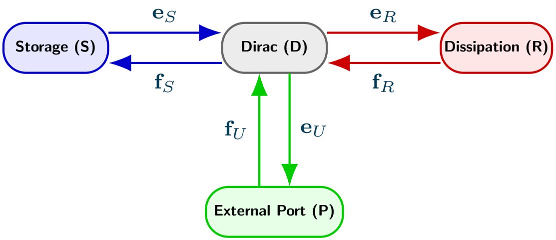

### Dirac Structure

$\mathcal{D} \subset \mathcal{F} \times \mathcal{F}^*$ with $\dim \mathcal{D} = \dim \mathcal{F} < \infty$ is called **Dirac structure**, iff for duality product $\langle \cdot, \cdot \rangle$ it holds that

$$\langle e, f \rangle = 0 \quad \text{for all } (e, f) \in \mathcal{D}\,.$$

### Duality Product for $\mathcal{F} = \mathbb{R}^k$

For $\mathcal{F} = \mathbb{R}^k$, we get

$$\langle e, f \rangle = e^\top f\,.$$

For a pHS with $e = (e_R, e_S, e_P)^\top$ and $f = (f_R, f_S, f_P)^\top$, we get

$$\langle e, f \rangle = e_R f_R + e_S f_S + e_P f_P \stackrel{!}{=} 0\,.$$

**Linear port-Hamiltonian System:**
Linear differential equation system

$$M\dot{x}(t) = (J - R)x(t) + Bu(t)$$

with

- coupling matrix $J$ **skew symmetric**,
- resistive matrix $R$, s.t. $R + R^\top \succeq 0$,
- material matrix $M = M^\top \succeq 0$ and
- external port $Bu(t)$.

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# port-Hamiltonian Systems (pHS)

## Why should we use pHS?

- **Physical Energy Conservation**
  Energy changes only through internal dissipation or exchange via ports
- **Structure-Preserving Interconnection**
  Modular coupling of multi-physical domains results in new pHS
- **Natural Stability**
  Physical energy bounds naturally prevent unbounded system growth

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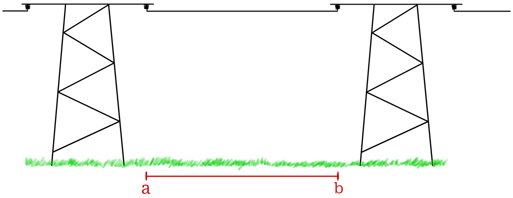
**Continuous Formulation:**




**Telegrapher's Equations**

$$R'i(z,t) + L'\frac{\partial i(z,t)}{\partial t} + \frac{\partial u(z,t)}{\partial z} = 0,$$
$$\frac{\partial i(z,t)}{\partial z} + G'u(z,t) + C'\frac{\partial u(z,t)}{\partial t} = 0\,,$$

with suitable boundary and initial conditions.

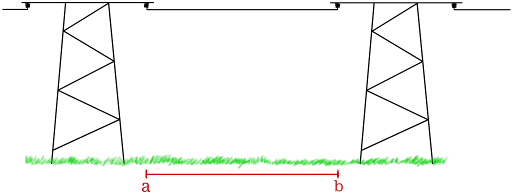
**Properties:**

- Describes voltage $u(z,t)$ and current $i(z,t)$ in space $z \in [a,b]$ and time $t \in [0,T]$
- Can be formulated as an infinite-dimensional port-Hamiltonian System

# A port-Hamiltonian Example

## The 1D Transmission Line Model I

**Continuous Formulation:**

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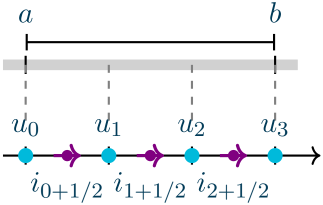
Need a discretization that keeps pHS structure as well as energy properties!

# A port-Hamiltonian Example

## The 1D Transmission Line Model II

### Space Discretization:




$$\mathbf{u} = (u_1, \dots, u_N)^\top, \ \mathbf{i} = (i_{1/2}, \dots, i_{N+1/2})^\top, B\mathbf{v} = (0_N, u_0, 0_N, u_{N+1})^\top$$

$$\frac{\partial}{\partial t} \underbrace{\begin{bmatrix} C' & 0 \\ 0 & L' \end{bmatrix}}_{M} \underbrace{\begin{bmatrix} \mathbf{u} \\ \mathbf{i} \end{bmatrix}}_{\mathbf{x}} = \left( \underbrace{\begin{bmatrix} 0 & -D \\ D^\top & 0 \end{bmatrix}}_{J} - \underbrace{\begin{bmatrix} G' & 0 \\ 0 & R' \end{bmatrix}}_{R} \right) \underbrace{\begin{bmatrix} \mathbf{u} \\ \mathbf{i} \end{bmatrix}}_{\mathbf{x}} + B\mathbf{v}$$

---

### Time Discretization:

For $\mathbf{x}_k = \mathbf{x}(t_k)$, $t_k = k\tau$ and $\Gamma = \operatorname{diag}(\mathbf{I}_N, -\mathbf{I}_{N+1})$, implicit midpoint rule yields

$$\Gamma \mathcal{A} \mathbf{x}_{k+1} = \begin{bmatrix} \mathbf{I}_N (C' + \frac{\tau}{2} G') & \frac{\tau}{2} D \\ \frac{\tau}{2} D^\top & -\mathbf{I}_{N+1} (L' + \frac{\tau}{2} R') \end{bmatrix} \mathbf{x}_{k+1} = \Gamma b(\mathbf{x}_k)$$

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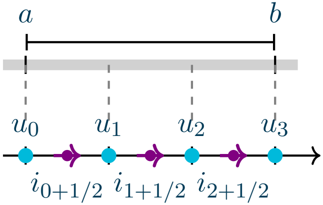


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**We get a Saddle Point Problem! – Coincidence? –**

# From pHS to SPP

- A space discrete port-Hamiltonian System **always** gives $M\dot{x}(t) = (J - R)x(t) + Bu(t)$, with

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} = M^\top \succeq 0, \quad J = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} = -J^\top, \quad R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}$$

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- Need for symplectic and locally and globally energy consistent time discretization
  $\rightarrow$ Implicit Midpoint Rule

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# From pHS to SPP



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**Proposition:**
Applying implicit midpoint rule to a real valued linear pHS always yields

$$\mathcal{A} = M - \frac{\tau}{2}(J - R) = \begin{bmatrix} M_{11} - \frac{\tau}{2}J_{11} + \frac{\tau}{2}R_{11} & M_{12} - \frac{\tau}{2}J_{12} + \frac{\tau}{2}R_{12} \\ M_{12}^\top + \frac{\tau}{2}J_{12}^\top + \frac{\tau}{2}R_{21} & M_{22} - \frac{\tau}{2}J_{22} + \frac{\tau}{2}R_{22} \end{bmatrix}.$$

This fits the definition of a **generalized Saddle Point Problem** w.l.o.g.

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**What we have:**

- $2 \times 2$ block-structure in the system matrix
- Generalized Saddle Point Problem
  $\rightarrow$ Under reasonable assumptions, even classic SPP

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- $2 \times 2$ block-structure in the system matrix
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**What we want:**

- Apply well known preconditioners for Saddle Point Problems on pHS
- Develop new preconditioners exploiting the pHS properties

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# A novel pH-Constraint Preconditioner

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**Classic Constraint Preconditioner:**
Solve

$$\mathcal{A}v = b \quad \Leftrightarrow \quad \begin{bmatrix} A & B_1 \\ B_2 & -C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

in two steps:

1. $y = (C + B_2 A^{-1} B_1)^{-1}(B_2 A^{-1} f - g)$
2. $x = A^{-1}(f - B_1 y)$

**Implicit Midpoint Formulation:**
For a linear pHS we always get

$$\mathcal{A} = \begin{bmatrix} M_{11} - \frac{\tau}{2} J_{11} + \frac{\tau}{2} R_{11} & M_{12} - \frac{\tau}{2} J_{12} + \frac{\tau}{2} R_{12} \\ M_{12}^\top + \frac{\tau}{2} J_{12}^\top + \frac{\tau}{2} R_{21} & M_{22} - \frac{\tau}{2} J_{22} + \frac{\tau}{2} R_{22} \end{bmatrix}$$

**Proposition:**
Writing the Schur Complement as

$$S = C + B_2 A^{-1} B_1 =: S_1 + S_2,$$

we see that for an underlying pHS

$$-S_1 = \underbrace{M_{22} + \frac{\tau}{2} R_{22}^{\text{sym}}}_{S_1^{\text{sym}}} + \underbrace{\frac{\tau}{2}\left(R_{22}^{\text{skew}} - J_{22}\right)}_{S_1^{\text{skew}}}$$

with $R_{22}^{\text{skew/sym}} = \frac{1}{2}(R_{22} \pm R_{22}^\top)$.

**Unique HSS Splitting:**
No explicit $J, M, R$ needed!

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# A novel pH-Constraint Preconditioner



**We have to solve:**

1. $y = (C + B_2 A^{-1} B_1)^{-1} (B_2 A^{-1} f - g)$
2. $x = A^{-1}(f - B_1 y)$

**Outer Solver:**

Take e.g. AMG solver to approximate $A^{-1}$

**Inner Solver:**

- Approximate just $S_1$ instead of $S$
- **Widlund method** to approximate $S_1^{-1}$
- Use e.g. AMG to approximate $(S_1^{\mathrm{sym}})^{-1}$

**Algorithm:**

1. **Inner Solve I (AMG):**
   $\tilde{f} = \texttt{AMG}(A)\texttt{.matvec}(f)$
2. **Schur RHS:**
   $r_S = B_2 \tilde{f} - g$
3. **Inner Solve II (Widlund):**
   $y = \texttt{Widlund}(S_1, r_S)$
4. **Outer Solve (AMG):**
   $x = \texttt{AMG}(A)\texttt{.matvec}(f - B_1 y)$

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# Preconditioning port-Hamiltonian Systems

## Considered Candidates

**Baselines & General-Purpose:**

- No Preconditioner – Pure GMRES
- Incomplete LU Decomposition

**SPP related:**

- SIMPLE Block-Triangular
- Constraint (AMG/ILU inner solver)

**pHS related:**

- Widlund
- Rapoport

**pHS & SPP related:**

- Novel constraint preconditioning approach

# Preconditioning port-Hamiltonian Systems

## Test Problems

### Stabilized Stokes Problem

(cf. Güdücü et al., 2022)

- Discretization of unsteady incompressible Stokes equations yields $\mathcal{A} = H + S$
- The Hermitian part $H = H^\top \succeq 0$ and skew-Hermitian part $S = -S^\top$

$$\mathcal{A} = \begin{bmatrix} M - \frac{\tau}{2} A_H & -\frac{\tau}{2} B \\ \frac{\tau}{2} B^* & -\frac{\tau}{2} C \end{bmatrix}$$

with $C$ stabilization term

### Transmission Line & Maxwell pHS

(cf. Kasolis et al., in prep.)

- Discrete pH-coupling of Transmission Line Model and Maxwell's equations
- With impl. midpoint rule pH-System $M\dot{x} = (J - R)x + Bf$ yields

$$\mathcal{A} = \begin{bmatrix} M^L + \frac{\tau}{2} M^R & -\frac{\tau}{2}\Theta & 0 \\ \frac{\tau}{2}\Theta^\top & M^\varepsilon + \frac{\tau}{2}(M^\sigma + Z^\eta) & -\frac{\tau}{2} K^\top \\ 0 & \frac{\tau}{2} K & M^\mu \end{bmatrix}$$

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# A novel pH-Constraint Preconditioner

## Numerical Results – Stabilized Stokes I

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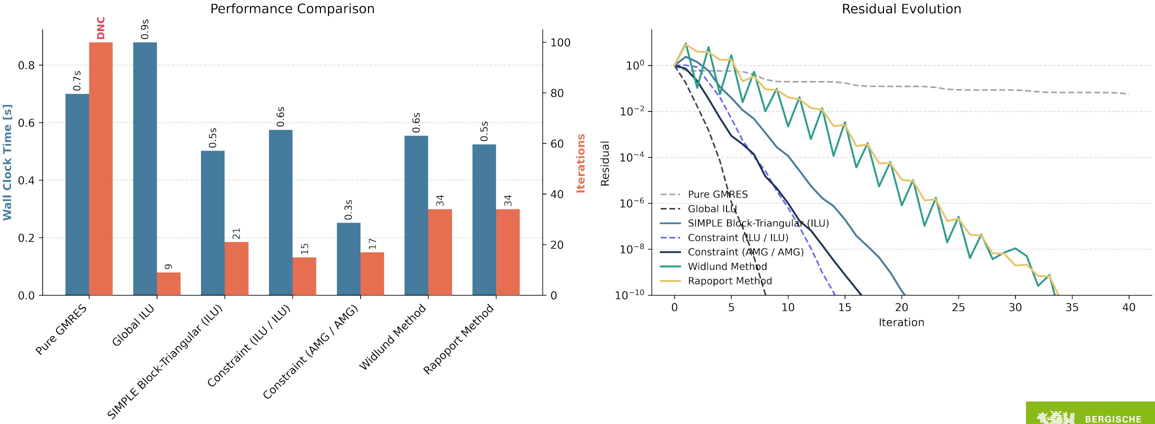
**Stabilized Stokes (49923 x 49923) Acc. 1.0e-10**

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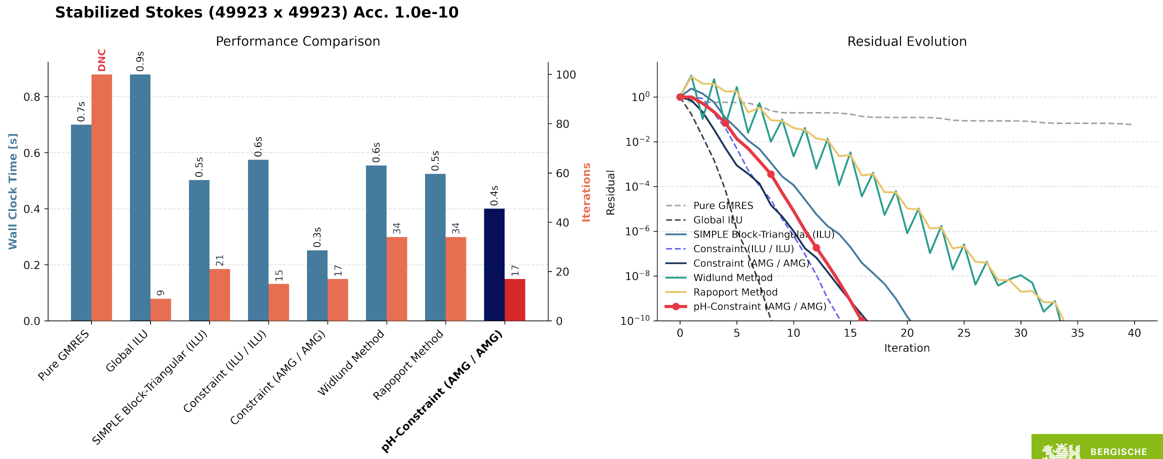

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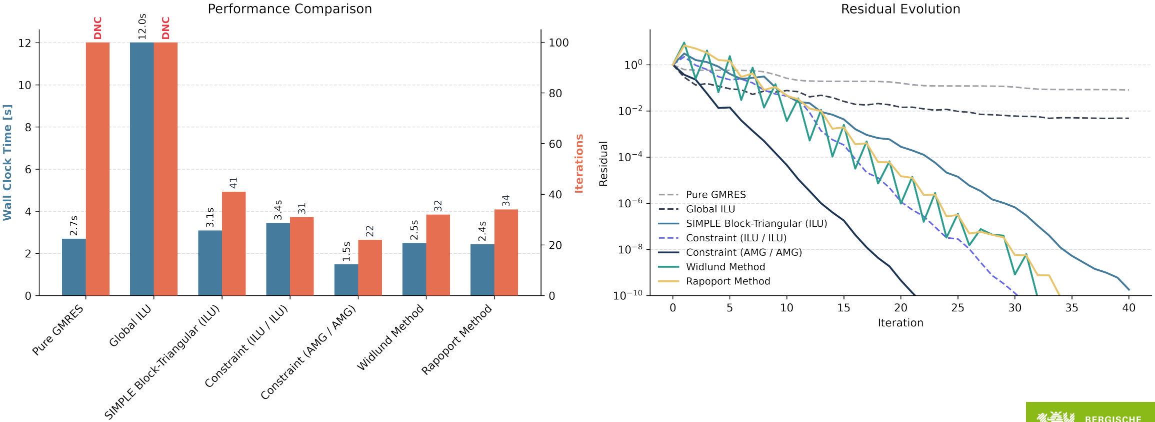
## Numerical Results – Stabilized Stokes II

**Stabilized Stokes (198147 x 198147) Acc. 1.0e-10**



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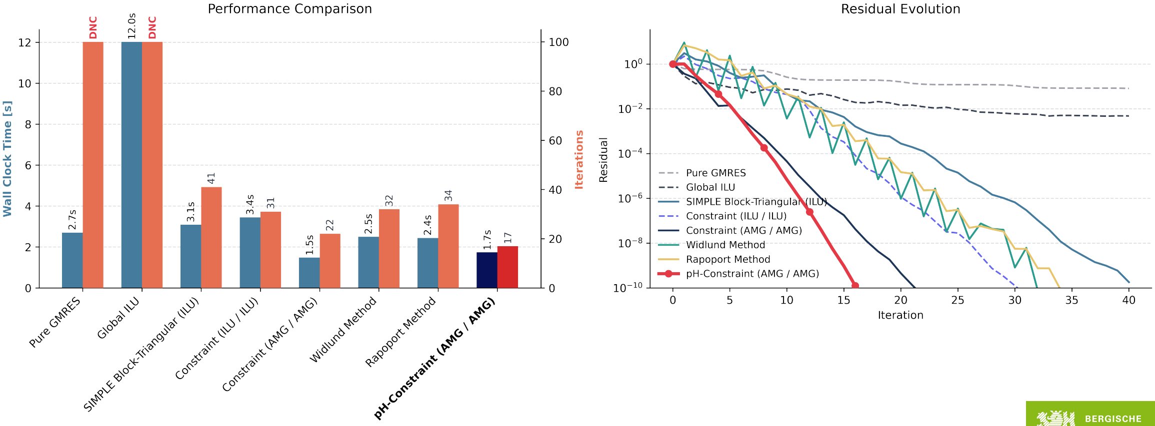

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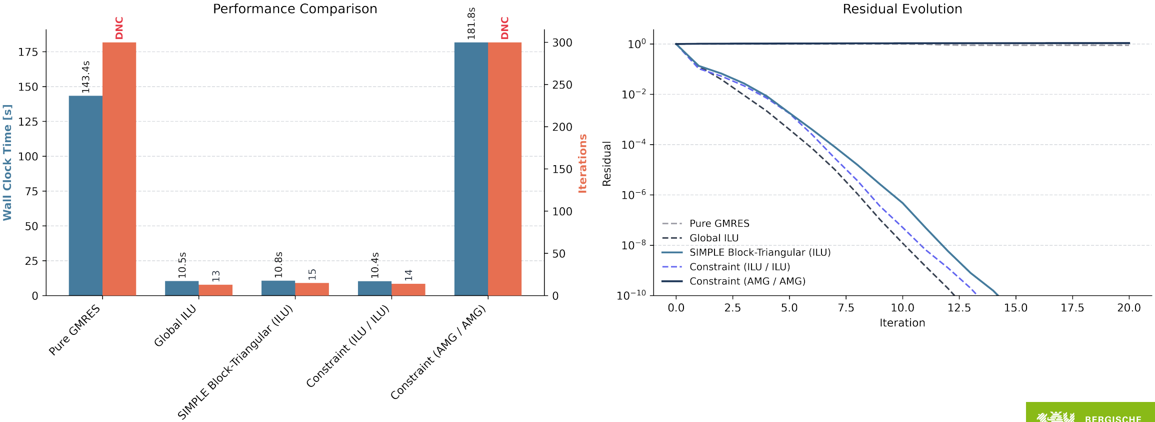
# A novel pH-Constraint Preconditioner

## Numerical Results – Coupled Transmission Line

**Antenna 2D (1203424 x 1203424) Acc. 1.0e-10**



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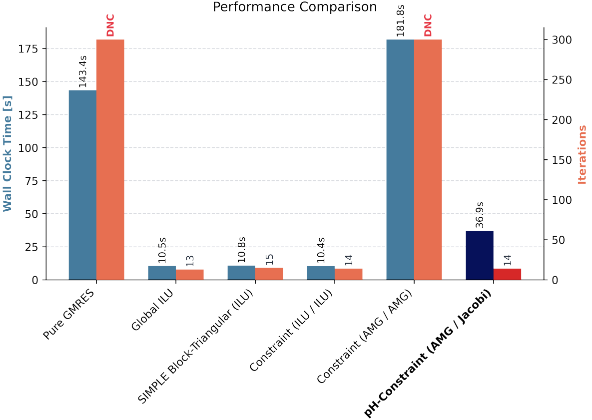


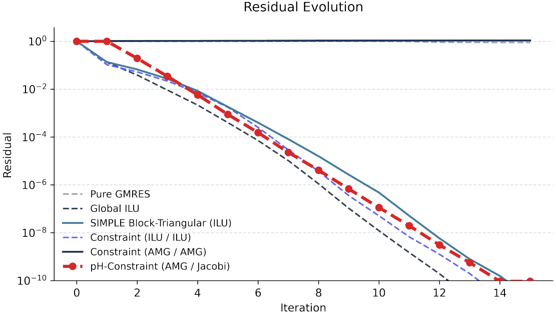

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# Conclusion

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- Implicit midpoint rule transforms any linear port-Hamiltonian System into a generalized Saddle Point Problem
- Established preconditioners for Saddle Point Problems also work for port-Hamiltonian Systems
- Novel pH-Constraint preconditioner exploits both SPP and pHS structures, overcoming the non-scalability and null-space issues of standard approaches

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# Thanks for your Attention!



**Slides and Contact:**

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(CRC 1701)

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**There's More!**

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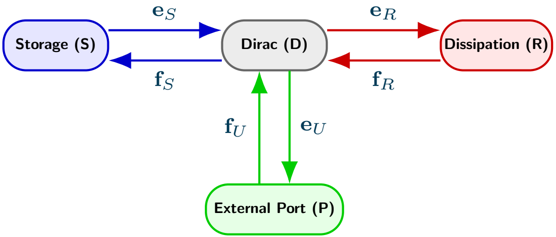
## Definition Dirac Structure

Let there be:

- A finite-dimensional linear space $\mathcal{F}$,
- its dual space $\mathcal{E} = \mathcal{F}^*$ and
- the duality product $\langle e, f \rangle$ for $(e, f) \in \mathcal{E} \times \mathcal{F}$.

Then, $\mathcal{D} \subset \mathcal{F} \times \mathcal{E}$ with $\dim \mathcal{D} = \dim \mathcal{F}$ is called **Dirac structure**, iff

$$\langle e, f \rangle = 0 \quad \text{for all } (e, f) \in \mathcal{D} \, .$$

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# From pHS to SPP
## Proof I



We know that for a real valued linear pHS implicit midpoint rule gives

$$\mathcal{A} = M - \frac{\tau}{2}(J - R) = \begin{bmatrix} M_{11} - \frac{\tau}{2}J_{11} + \frac{\tau}{2}R_{11} & M_{12} - \frac{\tau}{2}J_{12} + \frac{\tau}{2}R_{12} \\ M_{12}^\top + \frac{\tau}{2}J_{12}^\top + \frac{\tau}{2}R_{21} & M_{22} - \frac{\tau}{2}J_{22} + \frac{\tau}{2}R_{22} \end{bmatrix}.$$

A **generalized Saddle Point Problem**, requires at least one of the following conditions to hold:

C1 $A$ is symmetric.

C2 The symmetric part $H = \frac{1}{2}(A + A^\top)$ is positive semidefinite.

C3 $B_1 = B_2 = B$.

C4 $C$ is symmetric positive definite.

C5 $C = 0$.

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# From pHS to SPP
## Proof II

We use C2. We have

$$A = M_{11} - \frac{\tau}{2} J_{11} + \frac{\tau}{2} R_{11}\,.$$

This gives

$$\frac{1}{2}(A + A^\top) = \frac{1}{2}\left((M_{11} - \frac{\tau}{2} J_{11} + \frac{\tau}{2} R_{11}) + (M_{11}^\top - \frac{\tau}{2} J_{11}^\top + \frac{\tau}{2} R_{11}^\top)\right)$$

due to symmetry of $M$ and skew symmetry of $J$

$$= \frac{1}{2}\left((M_{11} - \frac{\tau}{2} J_{11} + \frac{\tau}{2} R_{11}) + (M_{11} + \frac{\tau}{2} J_{11} + \frac{\tau}{2} R_{11}^\top)\right)$$
$$= M_{11} + \frac{\tau}{4}(R_{11} + R_{11}^\top)\,.$$

Since $M \succeq 0$ and $R + R^\top \succeq 0$ this is also positive semi-definite.

# Motivation for Approximation of $S$



We have

$$S = \underbrace{C}_{S_1} + \underbrace{B_2 A^{-1} B_1}_{S_2} .$$

From the pHS structure, we know that:

$$S_1 = C = \frac{\tau}{2}(J_{22} - R_{22}) - M_{22}$$
$$S_2 = B_2 A^{-1} B_1 = \left[M_{21} - \frac{\tau}{2}(J_{21} - R_{21})\right]\left[M_{11} - \frac{\tau}{2}(J_{11} - R_{11})\right]^{-1}\left[M_{12} - \frac{\tau}{2}(J_{12} - R_{12})\right]$$

Making the reasonable assumption that the non-diagonal blocks of $M$ are zero, we get:

$$S_1 \sim -M_{22} + \mathcal{O}(\tau), \qquad S_2 \sim \mathcal{O}(\tau^2)$$

$\rightarrow$ **For small $\tau$ $S_2$ becomes neglectable!**

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# Used Solvers/Preconditioners

## Global Preconditioners/Solvers

**GMRES:**

- Custom implementation of Full GMRES
- Computes $x$ explicitly in each iteration to determine the residual exactly

**Jacobi:**

- **Jacobi:** Diagonal inverse applied to the whole system $\mathcal{A}$

**Global ILU:**

- BlackBox `SciPy` implementation of sparse ILU decomposition applied to whole $\mathcal{A}$

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**SIMPLE Diagonal:**

- Approximation of $A$-block by inverse diagonal
- Approximation of Schur complement $S \approx C + B_2(\mathrm{diag}(A))^{-1}B_1$ by `SciPy` implementation of sparse ILU decomposition

**SIMPLE Tridiagonal:**

- SIMPLE diagonal approach with substitution step for $x$
- Schur complement approximation by `SciPy` implementation of sparse ILU decomposition

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**Constraint ILU / ILU:**

- $A^{-1}$ approximation by `SciPy` implementation of sparse ILU decomposition
- Approximation of inverse Schur complement $S^{-1}$ by `SciPy` implementation of sparse ILU decomposition

**Constraint AMG / AMG:**

- $A^{-1}$ approximation by `pyAMG` implementation of smoothed aggregation AMG
- Approximation of inverse Schur complement $S^{-1}$ by `pyAMG` implementation of smoothed aggregation AMG

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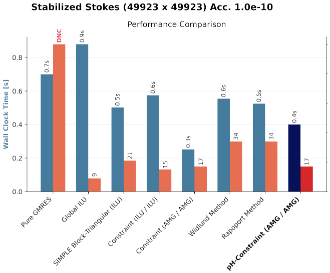
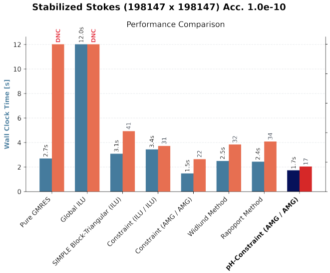
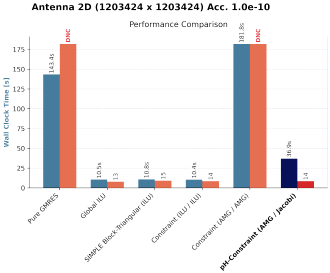
# Performance Comparison




- Global ILU scales poorly and fails to converge for large-scale SPPs
- AMG struggles with large null spaces $\rightarrow$ pH-Constraint + Jacobi does not

$\longrightarrow$ New solver is scalable and addresses the AMG problem with exchangeable inner solvers!