

# Transformed Primal-Dual Methods for Smooth Nonlinear Saddle Point Systems

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Interplay of discretization and algebraic solvers: a posteriori error estimates and adaptivity.  
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# Overview

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$$\min_{u \in \mathbb{R}^m} \max_{p \in \mathbb{R}^n} \mathcal{L}(u, p)$$

- How to design iterative methods for solving saddle point systems?
- How to analyze the convergence (rate) of the numerical method?  
Linear convergence and inexact inner solvers etc.
- **Goal:** set up a systematic framework to design and analyze iterative methods for nonlinear saddle point systems.

# Outline

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## 1. Lyapunov Analysis for Convex Optimization

## 2. Transformed Primal-Dual Flow

## 3. Algorithms

## 4. Convergence Analysis

## 5. Numerical Results

## 6. Conclusions

# Convex Optimization

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Consider

$$\min_{x \in \mathcal{V}} f(x)$$

where  $\mathcal{V}$  is a Hilbert space, and  $f : \mathcal{V} \rightarrow \mathbb{R}$  is a convex function.

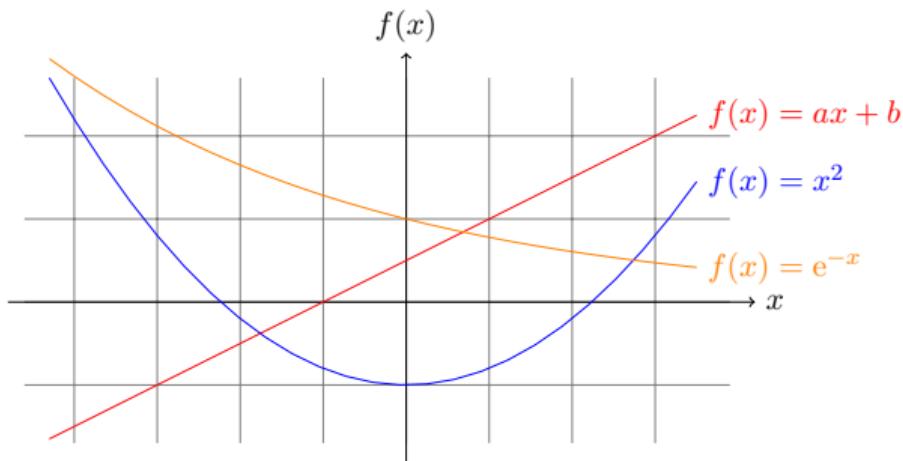


Figure: Examples of convex functions.

## Assumptions

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- **Smoothness:**  $f$  is differentiable;  $\nabla f$  is Lipschitz continuous with  $L$ .
- **Convexity:** for all  $x, y \in \mathcal{V}$ , for all  $\lambda \in [0, 1]$ ,

$$\lambda f(x) + (1 - \lambda)f(y) \geq f(\lambda x + (1 - \lambda)y),$$

or for all  $x, y \in \mathcal{V}$ ,

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle,$$

or if  $f \in \mathcal{C}^2$ ,  $\nabla^2 f \succeq 0$ .

- **Strong convexity:** there exists  $\mu > 0$ , for all  $x, y \in \mathcal{V}$ ,

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{\mu}{2} \|y - x\|^2.$$

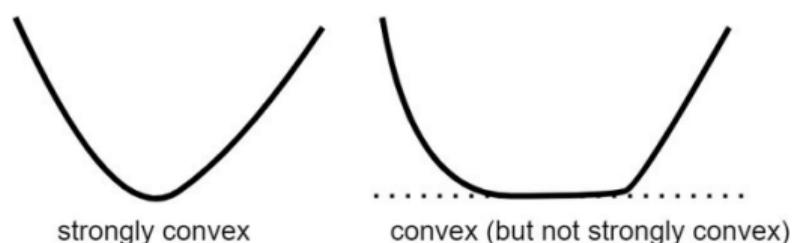
- **Coercivity:**  $f(x) \rightarrow +\infty$ , as  $\|x\| \rightarrow +\infty$ .

# Existence and Uniqueness

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$$x^* = \arg \min_{x \in \mathcal{V}} f(x)$$

- Convexity + coercivity  $\implies x^*$  exists
- Strong convexity  $\implies x^*$  exists and is unique



# Gradient Flow

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Consider the ODE system:

$$x'(t) = -\nabla f(x(t))$$

- $x^*$  is an equilibrium point of the system, i.e.,  $\nabla f(x^*) = 0$ .
- Function decay is obvious:

$$\frac{d}{dt}f(x(t)) = \langle \nabla f(x(t)), x'(t) \rangle = -\|\nabla f(x(t))\|^2 < 0$$

if  $x(t)$  is not an equilibrium point and thus  $f(x(t)) \rightarrow f(x^*)$ .

- Strong convexity

$$\|x - x^*\|^2 \leq \frac{1}{\mu}(f(x) - f(x^*))$$

implies

$$\|x - x^*\| \rightarrow 0.$$

# Lyapunov Analysis

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$$x' = \mathcal{G}(x).$$

Lyapunov function:  $\mathcal{E}(x) \geq 0$ ,  $\mathcal{E}(x^*) = 0$  and  $-\nabla \mathcal{E}(x) \cdot \mathcal{G}(x) > 0$  near  $x^*$ .

**Theorem (Strong Lyapunov Property [Chen and Luo, 2021])**

*Suppose  $\mathcal{E}(x)$  is a Lyapunov function and there exist constant  $q \geq 1$ , strictly positive function  $c(x)$  and function  $p(x)$  such that*

$$-\nabla \mathcal{E}(x) \cdot \mathcal{G}(x) \geq c(x) \mathcal{E}^q(x) + p^2(x).$$

*Then*

- $q = 1 \implies \frac{d}{dt} \mathcal{E}(x(t)) \leq -c \mathcal{E}(x(t)) \implies \mathcal{E}(x(t)) = O(e^{-ct})$ .
- $q > 1 \implies \mathcal{E}(x(t)) = O\left(t^{-\frac{1}{q-1}}\right)$ .

# Lyapunov Analysis: Gradient Flow

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$$x' = -\nabla f(x).$$

Choices of strong Lyapunov functions [Chen and Luo, 2021]:

- $\mathcal{E}(x) = f(x) - f(x^*)$

$$-\nabla \mathcal{E}(x) \cdot \mathcal{G}(x) \geq \mu \mathcal{E}(x) + \frac{1}{2} \|\nabla f(x)\|^2.$$

- $\mathcal{E}(x) = \frac{1}{2} \|x - x^*\|^2$

$$-\nabla \mathcal{E}(x) \cdot \mathcal{G}(x) \geq \frac{2\mu L}{L + \mu} \mathcal{E}(x) + \frac{1}{L + \mu} \|\nabla f(x)\|^2.$$

- $\mathcal{E}(x) = f(x) - f(x^*) + \frac{\mu}{2} \|x - x^*\|^2$

$$-\nabla \mathcal{E}(x) \cdot \mathcal{G}(x) \geq \mu \mathcal{E}(x) + \|\nabla f(x)\|^2.$$

## Lyapunov Analysis: Iterations

Theorem (Strong Lyapunov Property for Iterations [Chen and Luo, 2021])

Let  $q \geq 1$  and  $\{\mathcal{E}_k = \mathcal{E}(x_k) : k \geq k_0\}$  be any positive sequence. If

$$\mathcal{E}_{k+1} - \mathcal{E}_k \leq -\alpha_k \mathcal{E}_k^q, \quad k \geq k_0,$$

for some  $0 \leq \alpha_k < 1$ , then for all  $k \geq k_0$

$$\mathcal{E}_k \leq \begin{cases} \mathcal{E}_{k_0} \times \prod_{i=k_0}^{k-1} (1 - \alpha_i) & \text{if } q = 1, \\ \left( (q-1) \sum_{i=k_0}^{k-1} \alpha_i + \mathcal{E}_{k_0}^{1-q} \right)^{-1/(q-1)} & \text{if } q > 1. \end{cases}$$

- $k_0 = 0, q = 1, \alpha_k \geq \alpha \implies \mathcal{E}_{k+1} \leq (1 - \alpha)^k \mathcal{E}_0$

# Lyapunov Analysis for First Order Methods

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Consider discretization of the gradient flow

$$x' = -\nabla f(x).$$

- **Explicit Euler method (Gradient descent methods):**

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$$

For  $0 < \alpha_k \leq 2/(L + \mu)$ ,

$$\mathcal{E}_{k+1} \leq (1 - \mu\alpha_k) \mathcal{E}_k, \quad \text{when } \alpha_k = 1/L, \quad \mathcal{E}_{k+1} \leq \left(1 - \frac{\mu}{L}\right) \mathcal{E}_k.$$

- **Implicit Euler method (Proximal methods):**

$$x_{k+1} = x_k - \alpha_k \nabla f(x_{k+1}) = \text{prox}_{f,\alpha_k}(x_k)$$

where  $\text{prox}_{f,\alpha_k}(x_k) = \arg \min_x f(x) + \frac{1}{2\alpha_k} \|x - x_k\|^2$ .

For  $\alpha_k > 0$ ,

$$\mathcal{E}_{k+1} \leq \frac{1}{1 + \mu\alpha_k} \mathcal{E}_k.$$

## IMEX or Proximal Gradient Methods

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$$x' = -(\nabla h(x) + \nabla g(x))$$

- **IMEX or Proximal Gradient Methods**

$$\frac{x_{k+1} - x_k}{\alpha_k} \in -\nabla h(x_k) - \partial g(x_{k+1}),$$

$$x_{k+1} = \text{prox}_{\alpha_k g}(x_k - \alpha_k \nabla h(x_k)).$$

For  $\mathcal{E}_k = f(x_k) - f(x^*)$ :

$$\mathcal{E}_k \leqslant \begin{cases} \mathcal{E}_0(1 + \mu/L)^{-k} & \text{if } \mu > 0, \\ \left(1 + \frac{\mathcal{E}_0}{1 + 2R_0^2\mathcal{E}_0}\right) \frac{\mathcal{E}_0}{2R_0^2 + \mathcal{E}_0 k} & \text{if } \mu = 0. \end{cases}$$

# ODE to OPT

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$$\min_{x \in V} f(x),$$

$$x_t = -\nabla f(x)$$

- Gradient descent
- Proximal
- Proximal gradient
- Explicit Euler
- Implicit Euler
- IMEX

# ODE to OPT

---

$$\min_{x \in V} f(x),$$

$$x_t = -\nabla f(x)$$

- Gradient descent
- Proximal
- Proximal gradient
- Momentum
- Nesterov Acceleration
- FISTA
- Explicit Euler
- Implicit Euler
- IMEX
- ?
- ?
- ?

## References

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- H. Luo and L. Chen. From Differential Equation Solvers to Accelerated First-Order Methods for Convex Optimization. *Mathematical Programming*. 2021.
- L. Chen and H. Luo. A Unified Convergence Analysis of First Order Convex Optimization Methods via Strong Lyapunov Functions. *arXiv*. 2021.

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2. **Transformed Primal-Dual Flow**
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# Saddle Point Systems

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$$\min_{u \in \mathbb{R}^m} \max_{p \in \mathbb{R}^n} \mathcal{L}(u, p) = f(u) - h(p) + (Bu, p)$$

- $f(u), h(p)$  are smooth convex functions.
- $\nabla f(u), \nabla h(p)$  are Lipschitz continuous.
- $B$  is a  $n \times m$  matrix,  $n \leq m$ , with full row rank.

The saddle point  $(u^*, p^*)$  satisfies

$$\mathcal{L}(u^*, p) \leq \mathcal{L}(u^*, p^*) \leq \mathcal{L}(u, p^*), \quad \forall (u, p) \in \mathbb{R}^m \times \mathbb{R}^n.$$

# Saddle Point Systems

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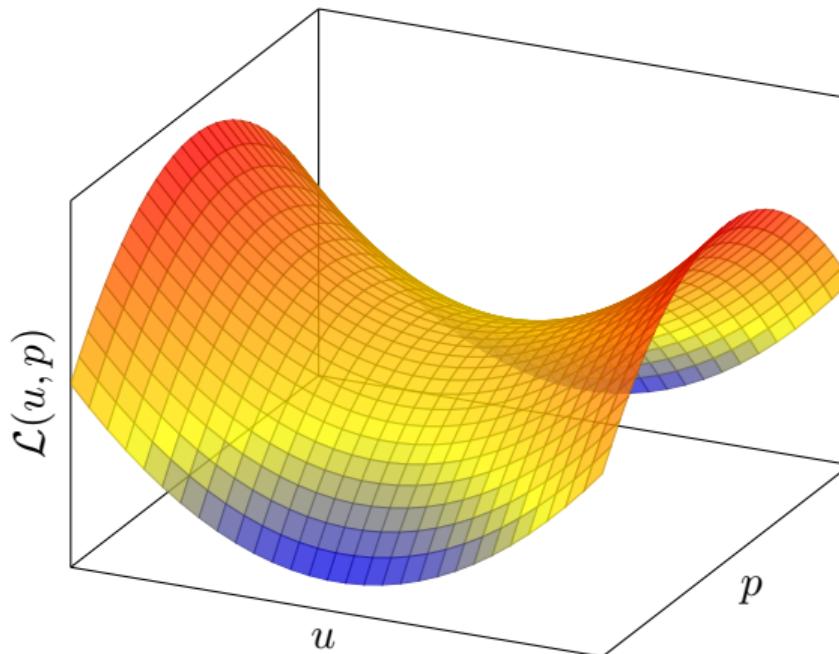


Figure:  $(0, 0)$  is a saddle point.

## Examples: Stokes and Darcy-Forchheimer Equations

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- Stokes equation:

$$\begin{cases} -\mu \Delta u + \nabla p = f & \text{in } \Omega \\ -\operatorname{div} u = 0 & \text{in } \Omega \end{cases}$$

In the operator form:

$$\begin{pmatrix} A & B^\top \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

where  $A = -\mu \Delta$ ,  $B = -\operatorname{div}$ .

- Darcy-Forchheimer equation:

$$\frac{\mu}{\rho} K^{-1} u + \frac{\beta}{\rho} |u| u + \nabla p = f \quad \text{in } \Omega,$$

with the divergence constraint

$$\operatorname{div} u = g \quad \text{in } \Omega.$$

## Examples: Constrained Optimization

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- Convex optimization with affined equality constraints:

$$\min_{u \in \mathbb{R}^m} f(u) \quad \text{subject to} \quad Bu = b.$$

$\mathcal{L}(u, p)$  is the Lagrangian:

$$\min_{u \in \mathbb{R}^m} \max_{p \in \mathbb{R}^n} \mathcal{L}(u, p) = f(u) + (p, Bu - b),$$

with  $h(p) = (p, b)$  and  $p$  is the Lagrange multiplier.

# Primal-Dual Methods

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'Natural' primal-dual gradient flow:

$$\begin{cases} u' = -\partial_u \mathcal{L}(u, p) = -\nabla f(u) - B^\top p \\ p' = \partial_p \mathcal{L}(u, p) = Bu - \nabla h(p) \end{cases},$$

- **Explicit schemes:** the extragradient algorithm [Korpelevich, 1976] and the optimistic gradient descent-ascent method [Popov, 1980]
- **Implicit schemes:** the proximal point algorithm [Rockafellar, 1976]
- Only **sub-linear** convergence for (non-strongly) convex  $f$  and  $h$  [Nemirovski, 2004, Mokhtari et al., 2020, Song et al., 2020, Jiang and Mokhtari, 2022].

# Primal-Dual Methods

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Lyapunov function  $\mathcal{E}(u, p) = \frac{1}{2}\|u - u^*\|^2 + \frac{1}{2}\|p - p^*\|^2$ .

## Primal-Dual Flow

Assume  $f(u)$  is  $\mu_f$ -strongly convex and  $h(p)$   $\mu_h$ -strongly convex with  $\mu_f > 0$ ,  $\mu_h \geq 0$ . Then it holds that

$$-\nabla \mathcal{E}(u, p) \cdot \begin{pmatrix} -\partial_u \mathcal{L}(u, p) \\ \partial_p \mathcal{L}(u, p) \end{pmatrix} \geq \mu_f \|u - u^*\|^2 + \mu_h \|p - p^*\|^2.$$

- No strong Lyapunov property if  $\mu_h = 0$ .

## Block Factorization for Linear Case

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$$\begin{pmatrix} A & B^\top \\ B & -C \end{pmatrix} = \begin{pmatrix} I & 0 \\ BA^{-1} & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & -S \end{pmatrix} \begin{pmatrix} I & A^{-1}B^\top \\ 0 & I \end{pmatrix}$$

- $A$  is symmetric positive definite (SPD).
- $B$  is surjective,  $C$  is symmetric semi-positive definite.
- $S = BA^{-1}B^\top + C$  is the Schur complement of  $A$ .

# Uzawa Methods

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Consider linear saddle point system:

$$\begin{pmatrix} A & B^\top \\ B & -C \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

Uzawa method [Uzawa, 1958]

Given  $u_k, p_k$ , compute

$$u_{k+1} = A^{-1} \left( f - B^\top p_k \right),$$
$$p_{k+1} = p_k + \alpha (B u_{k+1} - C p_k).$$

## Uzawa Methods

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Elimination of  $u_{k+1}$  gives the iteration

$$p_{k+1} = p_k + \alpha \left( BA^{-1}f - \left( BA^{-1}B^\top + C \right) p_k \right).$$

This is a Richardson iteration applied to the system

$$Sp = BA^{-1}f$$

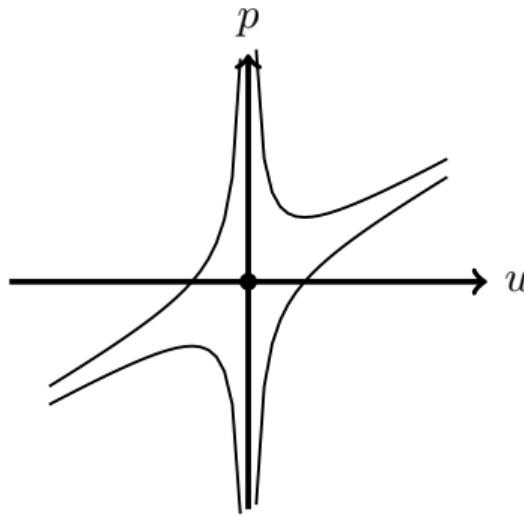
where  $S = (BA^{-1}B^\top + C)$  is called the Schur complement.

- Preconditioning and inexact Uzawa methods [Elman and Golub, 1994]
- Generalized to some nonlinear systems: [Chen, 1998, Hu and Zou, 2006]

# Change of Coordinate

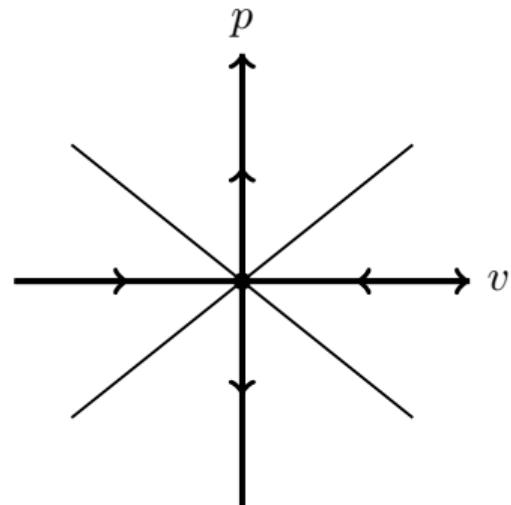
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- Coordinate:  $(u, p)$



$\Rightarrow$

- Coordinate:  $(v, p)$ ,  
 $v = u + A^{-1}B^\top p$



- $\mathcal{L}(u, p) = u^2 - 2up$

- $L(v, p) = v^2 - p^2$

## Approximated Schur Complement

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When  $A^{-1}$  is expensive to compute, approximate by  $\mathcal{I}_V^{-1}$ :

$$\begin{pmatrix} A & B^\top \\ B & -C \end{pmatrix} \approx \begin{pmatrix} I & 0 \\ B\mathcal{I}_V^{-1} & I \end{pmatrix} \begin{pmatrix} A & (I - A\mathcal{I}_V^{-1})B^\top \\ B(I - \mathcal{I}_V^{-1}A) & -\tilde{S} \end{pmatrix} \begin{pmatrix} I & \mathcal{I}_V^{-1}B^\top \\ 0 & I \end{pmatrix}$$

where  $\tilde{S} = B(2I - \mathcal{I}_V^{-1}A)\mathcal{I}_V^{-1}B^\top + C$  [Bank et al., 1989].

Inexact Uzawa iteration [Elman and Golub, 1994, Bramble et al., 1997, Hu and Zou, 2006]

Given  $u_k, p_k$ , compute

$$u_{k+1} = u_k + \mathcal{I}_V^{-1} \left( f - Au_k B^\top p_k \right),$$

$$p_{k+1} = p_k + \mathcal{I}_Q^{-1} (Bu_{k+1} - Cp_k).$$

## Flow for Uzawa Iteration

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Gradient descent methods

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$$

is the explicit Euler method for the gradient flow

$$x' = -\nabla f(x).$$

# Flow for Uzawa Iteration

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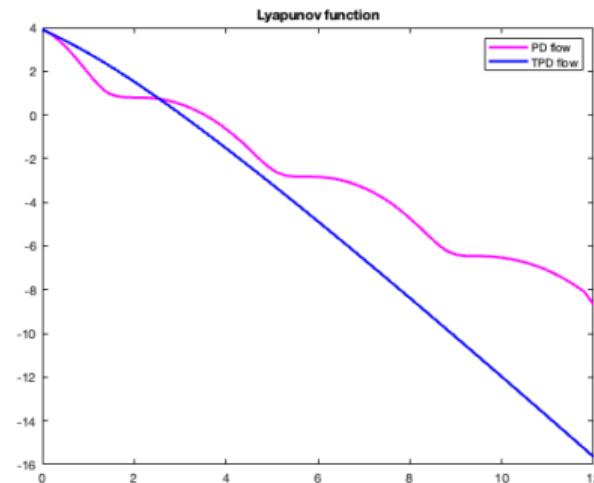
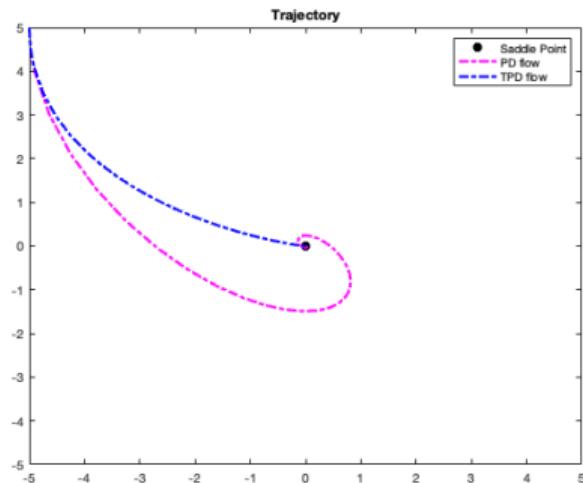
## Question

Can we find a flow (an ODE system) for (inexact) Uzawa Iteration?

# A Toy Problem

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$$(\text{PD}) \quad \begin{pmatrix} u' \\ p' \end{pmatrix} = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} \quad \begin{pmatrix} u' \\ p' \end{pmatrix} = \begin{pmatrix} -1 & -1 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} \quad (\text{TPD})$$



## Transformed Primal-Dual Flow

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$$\begin{cases} u' = \mathcal{G}^u(u, p) \\ p' = \mathcal{G}^p(u, p) \end{cases}$$

with

$$\begin{aligned}\mathcal{G}^u(u, p) &= -\mathcal{I}_{\mathcal{V}}^{-1} \partial_u \mathcal{L}(u, p) = -\mathcal{I}_{\mathcal{V}}^{-1} (\nabla f(u) + B^\top p), \\ \mathcal{G}^p(u, p) &= \mathcal{I}_{\mathcal{Q}}^{-1} (\partial_p \mathcal{L}(u, p) - B \mathcal{I}_{\mathcal{V}}^{-1} \partial_u \mathcal{L}(u, p)) \\ &= -\mathcal{I}_{\mathcal{Q}}^{-1} \left( \nabla h(p) + B \mathcal{I}_{\mathcal{V}}^{-1} B^\top p - Bu + B \mathcal{I}_{\mathcal{V}}^{-1} \nabla f(u) \right).\end{aligned}$$

- $\mathcal{I}_{\mathcal{V}}, \mathcal{I}_{\mathcal{Q}}$ : SPD matrices.
- $f(u)$  is strongly convex.
- $h_B(p) = h(p) + \frac{1}{2}(B \mathcal{I}_{\mathcal{V}}^{-1} B^\top p, p)$  is strongly convex:  $\mu_{h_B} > 0, \mu_h = 0$ .

# Exponential Stability

Theorem (C. and Wei 2022)

Suppose  $f(u) \in \mathcal{S}_{\mu_{f,\mathcal{I}_V}, L_{f,\mathcal{I}_V}}^{1,1}$  with  $\mu_{f,\mathcal{I}_V} > 0$  and  $e(u)$  is a contraction map, i.e.,  $L_{e,\mathcal{I}_V} < 1$ . Let  $\mathcal{E}(u, p) = \frac{1}{2}\|u - u^*\|_{\mathcal{I}_V}^2 + \frac{1}{2}\|p - p^*\|_{\mathcal{I}_Q}^2$ . Then for the transformed primal-dual (TPD) flow, the strong Lyapunov property holds

$$-\nabla \mathcal{E}(u, p) \cdot \mathcal{G}(u, p) \geq \mu \mathcal{E}(u, p) + \frac{\mu_{f,\mathcal{I}_V}}{2} \|v - v^*\|_{\mathcal{I}_V}^2,$$

where  $0 < \mu = \min \{\mu_V, \mu_Q\}$ . Consequently if  $(u(t), p(t))$  solves the TPD flow, we have the exponential decay

$$\mathcal{E}(u(t), p(t)) \leq e^{-\mu t} \mathcal{E}(u(0), p(0))$$

for  $0 \leq t < \infty$ .

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# TPD Flow: Implicit Euler Method

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## Algorithm 1: TPD - Implicit Scheme

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**Input:**  $u_0 \in \mathbb{R}^m, p_0 \in \mathbb{R}^n, \alpha > 0, \mathcal{I}_{\mathcal{V}} \in \mathbb{R}^{m \times m}, \mathcal{I}_{\mathcal{Q}} \in \mathbb{R}^{n \times n}$

**for**  $k = 0, 1, 2, \dots$  **do**

$$\begin{aligned} u_{k+1} &= u_k - \alpha_k \mathcal{G}^u(u_{k+1}, p_{k+1}) \\ p_{k+1} &= p_k - \alpha_k \mathcal{G}^p(u_{k+1}, p_{k+1}) \end{aligned}$$

**end**

---

- No restriction on step size  $\Rightarrow$  super-linear convergence.
- Choose  $\mathcal{I}_{\mathcal{V}} = L_f I_m$  and solve a nonlinear equation [Li et al., 2018]

$$\begin{cases} p_{k+1} = p_k + \mathcal{I}_{\mathcal{Q}}^{-1} \left[ \alpha_k \nabla h(p_{k+1}) + Bu_k - (1 + \alpha_k)B \text{prox}_{f, \alpha_k / L_f} \left( u_k - \frac{\alpha_k}{L_f} B^\top p_{k+1} \right) \right] \\ u_{k+1} = \text{prox}_{f, \alpha_k / L_f} \left( u_k - \frac{\alpha_k}{L_f} B^\top p_{k+1} \right) \end{cases}$$

## TPD Flow: Explicit Euler Method

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**Algorithm 2:** TPD - Explicit Scheme

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**Input:**  $u_0 \in \mathbb{R}^m, p_0 \in \mathbb{R}^n, \alpha \in (0, 1], \mathcal{I}_{\mathcal{V}} \in \mathbb{R}^{m \times m}, \mathcal{I}_{\mathcal{Q}} \in \mathbb{R}^{n \times n}$

**for**  $k = 0, 1, 2, \dots$  **do**

$$\begin{cases} u_{k+\frac{1}{2}} = u_k - \mathcal{I}_{\mathcal{V}}^{-1}(\nabla f(u_k) + B^\top p_k) \\ p_{k+1} = p_k - \alpha \mathcal{I}_{\mathcal{Q}}^{-1} \left( \nabla h(p_k) - Bu_{k+\frac{1}{2}} \right) \\ u_{k+1} = (1 - \alpha)u_k + \alpha u_{k+\frac{1}{2}} \end{cases}$$

**end**

---

$$p_{k+1} = p_k - \alpha_k \mathcal{G}^p(u_k, p_k),$$

$$u_{k+1} = u_k - \alpha_k \mathcal{G}^u(u_k, p_k).$$

- A relaxation of inexact Uzawa methods.

# TPD Flow: Implicit-Explicit (IMEX) Method

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## Algorithm 3: TPD - IMEX scheme

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**Input:**  $u_0 \in \mathbb{R}^m, p_0 \in \mathbb{R}^n, \alpha \in (0, 1], \mathcal{I}_V \in \mathbb{R}^{m \times m}, \mathcal{I}_Q \in \mathbb{R}^{n \times n}$

**for**  $k = 0, 1, 2, \dots$  **do**

$$u_{k+\frac{1}{2}} = u_k - \mathcal{I}_V^{-1}(\nabla f(u_k) + B^\top p_k)$$

$$p_{k+1} = p_k - \alpha \mathcal{I}_Q^{-1} \left( \nabla h(p_k) - Bu_{k+\frac{1}{2}} \right) \quad \text{Explicit}$$

$$u_{k+1} = \arg \min_{u \in \mathbb{R}^m} f(u) + \frac{1}{2\alpha} \|u - u_k + \alpha \mathcal{I}_V^{-1} B^\top p_{k+1}\|_{\mathcal{I}_V}^2 \quad \text{Implicit}$$

**end**

---

- For  $\mathcal{I}_V^{-1} = \frac{1}{L} I_m$ , the last step is one proximal iteration:

$$u_{k+1} = \text{prox}_{f, \frac{\alpha}{L}}(u_k - \frac{\alpha_k}{L_f} B^\top p_{k+1}).$$

# TPD Flow: IMEX with Inexact Inner Solvers

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## Algorithm 4: TPD - inexact IMEX scheme

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**Input:**  $u_0 \in \mathbb{R}^m, p_0 \in \mathbb{R}^n, \alpha \in (0, 1], \mathcal{I}_V \in \mathbb{R}^{m \times m}, \mathcal{I}_Q \in \mathbb{R}^{n \times n}$

**for**  $k = 0, 1, 2, \dots$  **do**

$$u_{k+\frac{1}{2}} = u_k - \mathcal{I}_V^{-1}(\nabla f(u_k) + B^\top p_k)$$

$$p_{k+1} = p_k - \alpha \mathcal{I}_Q^{-1} \left( \nabla h(p_k) - Bu_{k+\frac{1}{2}} \right)$$

$$u_{k+1} \approx \arg \min_{u \in \mathbb{R}^m} \tilde{f}(u) = f(u) + \frac{1}{2\alpha} \|u - u_k + \alpha \mathcal{I}_V^{-1} B^\top p_{k+1}\|_{\mathcal{I}_V}^2$$

**end**

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### Inexact solver

The inexact inner solver returns  $u_{k+1}$  satisfying  $\|\nabla \tilde{f}(u_{k+1})\|_{\mathcal{I}_V^{-1}}^2 \leq \epsilon_k$  for some small enough  $\epsilon_k, k = 1, 2, \dots$

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## Convergence Analysis: Preliminary

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- Define inner product

$$(u, v)_{\mathcal{I}_{\mathcal{V}}} := (\mathcal{I}_{\mathcal{V}}u, v) = (u, \mathcal{I}_{\mathcal{V}}v), \quad \forall u, v \in \mathbb{R}^m$$

and associated norm  $\|\cdot\|_{\mathcal{I}_{\mathcal{V}}}$ :

$$\|u\|_{\mathcal{I}_{\mathcal{V}}} = (u, u)_{\mathcal{I}_{\mathcal{V}}}^{1/2}.$$

- Denote  $f \in \mathcal{S}_{\mu_{f,\mathcal{I}_{\mathcal{V}}}, L_{f,\mathcal{I}_{\mathcal{V}}}}^{1,1}$  with  $\mu_{f,\mathcal{I}_{\mathcal{V}}} \geq 0$ , if  $f$  is differentiable and for all  $u, v \in \text{dom}(f)$ ,

$$f(v) - f(u) - \langle \nabla f(u), v - u \rangle \geq \frac{\mu_{f,\mathcal{I}_{\mathcal{V}}}}{2} \|u - v\|_{\mathcal{I}_{\mathcal{V}}}^2,$$

$$f(v) - f(u) - \langle \nabla f(u), v - u \rangle \leq \frac{L_{f,\mathcal{I}_{\mathcal{V}}}}{2} \|u - v\|_{\mathcal{I}_{\mathcal{V}}}^2.$$

## Preliminary

---

- Define inner product

$$(p, q)_{\mathcal{I}_{\mathcal{Q}}} := (\mathcal{I}_{\mathcal{Q}} p, q) = (p, \mathcal{I}_{\mathcal{Q}} q), \quad \forall p, q \in \mathbb{R}^n$$

and associated norm  $\|\cdot\|_{\mathcal{I}_{\mathcal{Q}}}$ :

$$\|p\|_{\mathcal{I}_{\mathcal{Q}}} = (p, p)_{\mathcal{I}_{\mathcal{Q}}}^{1/2}.$$

- Denote  $h \in \mathcal{S}_{\mu_{h, \mathcal{I}_{\mathcal{Q}}}, L_{h, \mathcal{I}_{\mathcal{Q}}}}^{1,1}$  with  $\mu_{h, \mathcal{I}_{\mathcal{Q}}} \geq 0$ , if  $h$  is differentiable and for all  $p, q \in \text{dom}(h)$ ,

$$h(q) - h(p) - \langle \nabla h(p), p - q \rangle \geq \frac{\mu_{h, \mathcal{I}_{\mathcal{Q}}}}{2} \|p - q\|_{\mathcal{I}_{\mathcal{Q}}}^2,$$

$$h(q) - h(p) - \langle \nabla h(p), q - p \rangle \leq \frac{L_{h, \mathcal{I}_{\mathcal{Q}}}}{2} \|p - q\|_{\mathcal{I}_{\mathcal{Q}}}^2.$$

# Preliminary

---

- Define function

$$e(u) = u - \mathcal{I}_{\mathcal{V}}^{-1} \nabla f(u)$$

Lemma (C. and Wei 2022)

Suppose  $f \in \mathcal{S}_{\mu_f, \mathcal{I}_{\mathcal{V}}}^{1,1} L_{f, \mathcal{I}_{\mathcal{V}}}$ , then  $e(u)$  is Lipschitz continuous with  $L_{e, \mathcal{I}_{\mathcal{V}}}$ .  $L_{e, \mathcal{I}_{\mathcal{V}}} < 1$  if and only if  $L_{f, \mathcal{I}_{\mathcal{V}}} < 2$ .

- Define Lyapunov function

$$\mathcal{E}(u, p) = \frac{1}{2} \|u - u^*\|_{\mathcal{I}_{\mathcal{V}}}^2 + \frac{1}{2} \|p - p^*\|_{\mathcal{I}_{\mathcal{Q}}}^2$$

where  $(u^*, p^*)$  is the saddle point of  $\mathcal{L}(u, p)$ .

# Constants

---

$\mu$	$L$
	$L_S^2 = \lambda_{\max} (\mathcal{I}_Q^{-1} B \mathcal{I}_V^{-1} B^\top)$
$\mu_V = \mu_{f, \mathcal{I}_V}$	$L_V^2 = 2 \left( L_{f, \mathcal{I}_V}^2 + L_{e, \mathcal{I}_V}^2 L_S^2 \right)$
$\mu_Q = (2 - L_{f, \mathcal{I}_V}) \mu_{h_B, \mathcal{I}_Q}$	$L_Q^2 = 2 \left( L_{h_B, \mathcal{I}_Q}^2 + L_{e, \mathcal{I}_V}^2 L_S^2 \right)$

Table: Derived convexity constants and Lipschitz constants for  $f \in \mathcal{S}_{\mu_{f, \mathcal{I}_V}, L_{f, \mathcal{I}_V}}^{1,1}$ ,  
 $h \in \mathcal{S}_{\mu_h, \mathcal{I}_Q, L_{h, \mathcal{I}_Q}}^{1,1}$ , and  $e(u)$  is Lipschitz continuous with constant  $L_{e, \mathcal{I}_V}$ .

# Exponential Stability

Theorem (Exponential decay C. and Wei 2022)

Suppose  $f(u) \in \mathcal{S}_{\mu_{f,\mathcal{I}_V}, L_{f,\mathcal{I}_V}}^{1,1}$  with  $\mu_{f,\mathcal{I}_V} > 0$  and  $e(u)$  is a contraction map, i.e.,  $L_{e,\mathcal{I}_V} < 1$ . Let  $\mathcal{E}(u, p) = \frac{1}{2}\|u - u^*\|_{\mathcal{I}_V}^2 + \frac{1}{2}\|p - p^*\|_{\mathcal{I}_Q}^2$ . Then for the transformed primal-dual (TPD) flow, the strong Lyapunov property holds

$$-\nabla \mathcal{E}(u, p) \cdot \mathcal{G}(u, p) \geq \mu \mathcal{E}(u, p) + \frac{\mu_{f,\mathcal{I}_V}}{2} \|v - v^*\|_{\mathcal{I}_V}^2,$$

where  $0 < \mu = \min \{\mu_V, \mu_Q\}$ . Consequently if  $(u(t), p(t))$  solves the TPD flow, we have the exponential decay

$$\mathcal{E}(u(t), p(t)) \leq e^{-\mu t} \mathcal{E}(u(0), p(0))$$

for  $0 \leq t < \infty$ .

## Discrete Level: Linear Convergence

Theorem (Linear convergence for IMEX scheme C. and Wei 2022)

Suppose  $f(u) \in \mathcal{S}_{\mu_{f,\mathcal{I}_V}, L_{f,\mathcal{I}_V}}^{1,1}$  with  $\mu_{f,\mathcal{I}_V} > 0$  and  $e(u)$  is a contraction map, i.e.,  $L_{e,\mathcal{I}_V} < 1$ . For  $0 < \alpha < \mu_Q/L_Q^2$  in Algorithm 3, it holds that

$$\mathcal{E}(u_{k+1}, p_{k+1}) \leq \frac{1}{1 + \alpha\mu} \mathcal{E}(u_k, p_k),$$

and  $\mu = \min \{\mu_V, \mu_Q - \alpha L_Q^2/2\}$ . In particular, for  $\alpha = \mu_Q/L_Q^2$ , we have

$$\mathcal{E}(u_{k+1}, p_{k+1}) \leq \frac{1}{1 + \alpha \min\{\mu_V, \mu_Q/2\}} \mathcal{E}(u_k, p_k).$$

- If  $\mu_Q$  is  $\mathcal{O}(1)$ , the convergence rate is determined by  $\mu_V$ , i.e, the condition number of  $f(u)$ .

# Augmented Lagrangian Method

---

Consider the convex optimization problems with affined equality constraints:

$$\min_{u \in \mathbb{R}^m} f(u) \quad \text{subject to} \quad Bu = b.$$

The augmented Lagrangian

$$\min_{u \in \mathcal{V}} \max_{p \in \mathcal{Q}} \mathcal{L}_\beta(u, p) = f(u) + \frac{\beta}{2} \|Bu - b\|^2 + (p, Bu - b),$$

where  $\beta \geq 0$ . Effect of the augmented Lagrangian

- $f_\beta(u) = f(u) + \frac{\beta}{2} \|Bu - b\|^2$  is strongly convex:  $\mu_{f_B} > 0$  v.s.  $\mu_f = 0$ .
- Precondition the Schur complement.

## Example: Maxwell Equations

---

- Maxwell equations with divergence-free constraint:

$$\begin{cases} \operatorname{curl} \operatorname{curl} u = f & \text{in } \Omega \\ \operatorname{div} u = 0 & \text{in } \Omega \\ u \times n = 0 & \text{on } \partial\Omega \end{cases}$$

- In the operator form:

$$\begin{pmatrix} C^\top C & B^\top \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

where  $C = \operatorname{curl}$ ,  $B = -\operatorname{div}$ .

- The augmented Lagrangian formulation:

$$\begin{pmatrix} C^\top C + B^\top B & B^\top \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f + B^\top g \\ g \end{pmatrix}.$$

# TPD Flow: Augmented Lagrangian Methods (ALM)

---

## Algorithm 5: TPD - ALM - IMEX scheme

---

**Input:**  $u_0 \in \mathbb{R}^m, p_0 \in \mathbb{R}^n, \alpha \in (0, 1], \beta > 0, \mathcal{I}_{\mathcal{V}} \in \mathbb{R}^{m \times m}$

**for**  $k = 0, 1, 2, \dots$  **do**

$$u_{k+\frac{1}{2}} = u_k - \mathcal{I}_{\mathcal{V}}^{-1}(\nabla f(u_k) + \beta B^\top(Bu_k - b) + B^\top p_k)$$

$$p_{k+1} = p_k - \alpha\beta \left( b - Bu_{k+\frac{1}{2}} \right)$$

$$u_{k+1} = \arg \min_{u \in \mathcal{V}} f(u) + \frac{\beta}{2} \|Bu - b\|^2 + \frac{1}{2\alpha} \|u - u_k + \alpha \mathcal{I}_{\mathcal{V}}^{-1} B^\top p_{k+1}\|_{\mathcal{I}_{\mathcal{V}}}^2$$

**end**

---

- When  $\alpha = 1$ , this scheme recovers the proximal ALM [He et al., 2020].
- Other specific IMEX schemes and choices of parameters recover a class of augmented Lagrangian methods [Chambolle and Pock, 2011, He and Yuan, 2021].

# Preconditioning Effect

Theorem (Preconditioned Schur complement C. and Wei 2022)

Let  $A$  be an SPD matrix and define  $A_\beta = A + \beta B^\top B$ . Assume  $f(u) \in \mathcal{S}_{\mu_{f,A}, L_{f,A}}^{1,1}$ . Choose

$$\mathcal{I}_V^{-1} = A_\beta^{-1} = \left( A + \beta B^\top B \right)^{-1}, \quad \mathcal{I}_Q^{-1} = \beta I_n.$$

Then

$$\min\{\mu_{f,A}, 1\} \leq \mu_{f_\beta, \mathcal{I}_V} \leq L_{f_\beta, \mathcal{I}_V} \leq \max\{L_{f,A}, 1\},$$

and

$$\frac{\mu_{S_0}}{1 + \beta \mu_{S_0}} \leq \lambda_{\min} \left( BA_\beta^{-1} B^\top \right) \leq \lambda_{\max} \left( BA_\beta^{-1} B^\top \right) \leq \frac{1}{\beta},$$

where  $\mu_{S_0} = \lambda_{\min}(BA^{-1}B^\top)$ . Consequently

$$\kappa_{\mathcal{I}_V}(f_\beta) \leq \kappa_A(f), \quad \kappa(\mathcal{I}_Q^{-1} B \mathcal{I}_V^{-1} B^\top) \leq 1 + \frac{1}{\beta \mu_{S_0}}.$$

# Convergence Rates

---

Table: Examples of  $\mathcal{I}_{\mathcal{V}}^{-1}$  and  $\mathcal{I}_{\mathcal{Q}}^{-1}$  for  $f \in \mathcal{S}_{\mu_f, L_f}^{1,1}$  or  $f \in \mathcal{S}_{\mu_{f,A}, L_{f,A}}^{1,1}$  and  $h(p) = (b, p)$ .  $A$  is an SPD matrix with  $L_{f,A} \leq 1$  and  $\kappa_A(f) = L_{f,A}/\mu_{f,A}$ .

	Linear inner solvers		Rate
	$\mathcal{I}_{\mathcal{V}}^{-1}$	$\mathcal{I}_{\mathcal{Q}}^{-1}$	$\beta \gg 1$
TPD-Explicit	$A^{-1}$	$(BA^{-1}B^\top)^{-1}$	$1 - 1/\kappa_A^2(f)$
TPD-IMEX	$A^{-1}$	$(BA^{-1}B^\top)^{-1}$	$(1 + 1/\kappa_A(f))^{-1}$
TPD-ALM-Explicit	$(L_f I_m + \beta B^\top B)^{-1}$	$\beta I_n$	$1 - 1/\kappa^2(f)$
TPD-ALM-IMEX	$(A + \beta B^\top B)^{-1}$	$\beta I_n$	$(1 + 1/\kappa_A(f))^{-1}$

## Symmetric Transformed Primal-Dual Gradient Flow

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$$\begin{cases} u' = \mathcal{G}^u(u, p) \\ p' = \mathcal{G}^p(u, p) \end{cases}$$

with

$$\begin{aligned}\mathcal{G}^u(u, p) &= -\mathcal{I}_{\mathcal{V}}^{-1}(\partial_u \mathcal{L}(u, p) + B^\top \mathcal{I}_{\mathcal{Q}}^{-1} \partial_p \mathcal{L}(u, p)), \\ &= -\mathcal{I}_{\mathcal{V}}^{-1} (\nabla f(u) + B^\top \mathcal{I}_{\mathcal{Q}}^{-1} Bu + B^\top p - B^\top \mathcal{I}_{\mathcal{Q}}^{-1} \nabla h(p)), \\ \mathcal{G}^p(u, p) &= \mathcal{I}_{\mathcal{Q}}^{-1} (\partial_p \mathcal{L}(u, p) - B \mathcal{I}_{\mathcal{V}}^{-1} \partial_u \mathcal{L}(u, p)) \\ &= -\mathcal{I}_{\mathcal{Q}}^{-1} (\nabla h(p) + B \mathcal{I}_{\mathcal{V}}^{-1} B^\top p - Bu + B \mathcal{I}_{\mathcal{V}}^{-1} \nabla f(u)).\end{aligned}$$

Generalization of [Zulehner, 2011] to nonlinear saddle point system

- $f_B(u) = f(u) + \frac{1}{2}(B^\top \mathcal{I}_{\mathcal{Q}}^{-1} Bu, u)$  is strongly convex:  $\mu_{f_B} > 0, \mu_f = 0$ .
- $h_B(p) = h(p) + \frac{1}{2}(B \mathcal{I}_{\mathcal{V}}^{-1} B^\top p, p)$  is strongly convex:  $\mu_{h_B} > 0, \mu_h = 0$ .

# Strong Lyapunov Property

Theorem (C. and Wei 2022)

Assume  $f_B(u) \in \mathcal{S}_{\mu_{f_B, \mathcal{I}_V}, L_{f_B, \mathcal{I}_V}}^{1,1}$  with  $\mu_{f_B, \mathcal{I}_V} > 0$  and  $e_V(u)$  and  $e_Q(p)$  are contraction maps. Suppose  $(u, p)$  solves the symmetric TPD flow. Then for the Lyapunov function  $\mathcal{E}(u, p) = \frac{1}{2}\|u - u^*\|_{\mathcal{I}_V}^2 + \frac{1}{2}\|p - p^*\|_{\mathcal{I}_Q}^2$ ,

$$-\nabla \mathcal{E}(u, p) \cdot \mathcal{G}(u, p) \geq \mu \mathcal{E}(u, p) + \frac{\mu_{f, \mathcal{I}_V}}{2} \|v - v^*\|_{\mathcal{I}_V}^2 + \frac{\mu_{h, \mathcal{I}_Q}}{2} \|q - q^*\|_{\mathcal{I}_Q}^2$$

where  $\mu = \min\{\mu_{f_B, \mathcal{I}_V}, \mu_{h_B, \mathcal{I}_Q}\}$  and the transformed variables are

$$v = u + \mathcal{I}_V^{-1} B^\top p, \quad q = p - \mathcal{I}_Q^{-1} B u.$$

Consequently

$$\mathcal{E}(u(t), p(t)) \leq e^{-\mu t} \mathcal{E}(u(0), p(0)), \quad t > 0.$$

# Symmetric Transformed Primal-Dual Iterations

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**Algorithm 6:** Symmetric TPD - IMEX Scheme

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**Input:**  $u_0 \in \mathbb{R}^m, p_0 \in \mathbb{R}^n, \alpha \in (0, 1], \mathcal{I}_{\mathcal{V}} \in \mathbb{R}^{m \times m}, \mathcal{I}_{\mathcal{Q}} \in \mathbb{R}^{n \times n}$

**for**  $k = 0, 1, 2, \dots$  **do**

$$u_{k+\frac{1}{2}} = u_k - \mathcal{I}_{\mathcal{V}}^{-1}(\nabla f(u_k) + B^\top p_k)$$

$$p_{k+1} = p_k - \alpha \mathcal{I}_{\mathcal{Q}}^{-1} \left( \nabla h(p_k) - Bu_{k+\frac{1}{2}} \right)$$

$$u_{k+1} =$$

$$\arg \min_{u \in \mathbb{R}^m} f_B(u) + \frac{1}{2\alpha} \|u - u_k + \alpha \mathcal{I}_{\mathcal{V}}^{-1} B^\top (p_{k+1} - \mathcal{I}_{\mathcal{Q}}^{-1} \nabla h(p_{k+1}))\|_{\mathcal{I}_{\mathcal{V}}}^2$$

**end**

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# Outline

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1. Lyapunov Analysis for Convex Optimization
2. Transformed Primal-Dual Flow
3. Algorithms
4. Convergence Analysis
- 5. Numerical Results**
6. Conclusions

## Example: Cahn-Hilliard Equation

---

Minimizing a non-convex free-energy functional:

$$\min_u E(u) = \int_{\Omega} \left( \frac{\epsilon^2}{2} |\nabla u|^2 + F(u) \right) dx.$$

$H^{-1}$ -gradient flow:

$$\partial_t u(x, t) = (-\Delta) (\epsilon^2 \Delta u - F'(u)), \quad (x, t) \in \Omega$$

with Neumann boundary condition and initial condition.

## Example: Cahn-Hilliard Equation

---

- Let  $w = (\epsilon^2 \Delta u - F'(u))$  and discretize implicitly in time.
- Convex splitting scheme [Eyre, 1998] gives a saddle point system:

Given  $(u_h^{n-1}, w_h^{n-1})$ , each time step  $(u_h^n, w_h^n)$  solves

$$\begin{aligned} \min_{u_h \in V_h} \max_{w_h \in V_h} & \left\{ \frac{\epsilon^2}{2} \|u_h\|_A^2 + \int_{\Omega} F_+(u_h) - \hat{F}_-(u_h; u_h^{n-1}) \, dx \right. \\ & \left. - \frac{k_n}{2} \|w_h\|_A^2 - (w_h, u_h^{n-1}) + (w_h, u_h) \right\}. \end{aligned}$$

where  $A = -\Delta$ ,  $F$  is splitted into the difference between two convex functions  $F(u) = F_+(u) - F_-(u)$  and  $\hat{F}_-(\cdot; u_h^{n-1})$  is the linearization of  $F_-(\cdot)$  at  $u_h^{n-1}$ .

## Example: Cahn-Hilliard Equation

---

- Set  $\Omega = (0, 1)^2$ ,  $F = u^2(1 - u)^2$ ,  $\epsilon = 0.01$  and time step size  $k_n = 5e - 6$  and a random initial value around 0.63 is chosen. The mesh grid  $h = 1/64$ .
- Let  $M$  be the mass matrix and  $H_+$  is the Hessian of  $F_+$ .  $M, H_+$  are diagonal matrices. Set

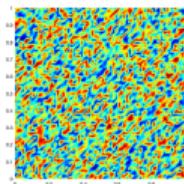
$$\mathcal{I}_{\mathcal{V}}^{-1} = (\epsilon^2 A + H_+(u_{n-1}))^{-1}$$

$$\mathcal{I}_{\mathcal{Q}}^{-1} = (k_n H_+(u_{n-1}) A + M)^{-1} H_+(u_{n-1}) (\epsilon^2 A + H_+(u_{n-1}))^{-1} M \mathcal{I}_{\mathcal{V}} M^{-1}.$$

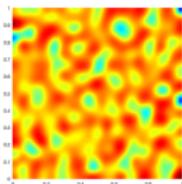
- For TPD-Explicit scheme,  $\alpha = 1$  and the saddle point system is solved exactly with relative residual less than  $1e - 6$ . Each time step converges within 10 iterations.

# Example: Cahn-Hilliard Equation

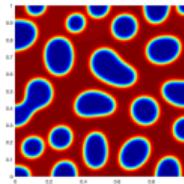
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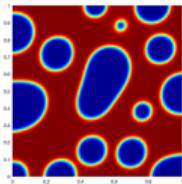
(a)  $t = 0.$



(b)  $t = 5e - 5.$



(c)  $t = 1.5e - 3.$



(d)  $t = 5e - 3.$

Figure: Spinodal decomposition

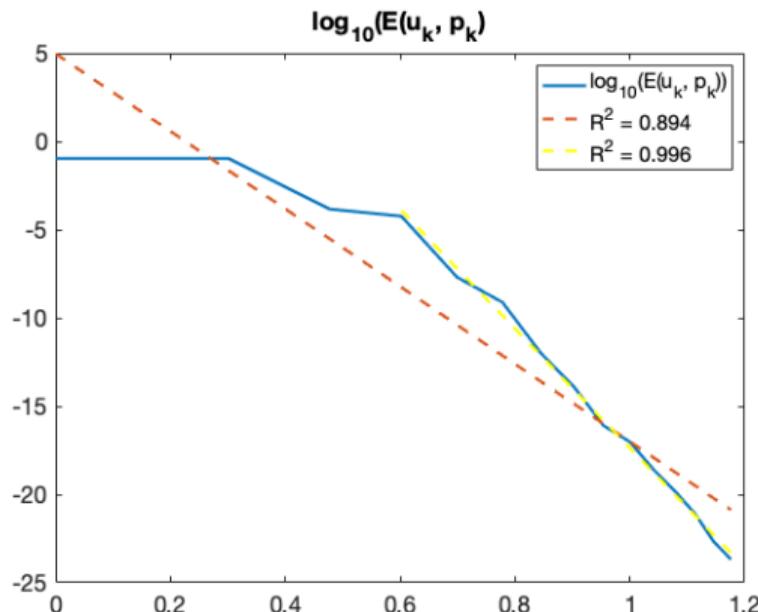


Figure: Lyapunov function.

# Outline

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# Conclusions

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- A systematic framework to design and analyze iterative methods for smooth nonlinear saddle point systems.
- A novel transformed primal-dual (TPD) flow is proposed and exponential decay of a Lyapunov function is obtained.
- Several TPD iterations as implicit, explicit or IMEX scheme of TPD flow are proposed. All the schemes achieve the state-of-the-art convergence rates.
- Linear convergence rate is possible even  $\mu_f = 0$  and  $\mu_h = 0$ .

## Future Work

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- Derive nonlinear multigrid-type scheme for saddle point systems. TPD iterations can be used as the smoother.
- Time-dependent  $\mathcal{I}_V, \mathcal{I}_Q$  might be more appropriate, but the convergence analysis will be harder.
- Extend this framework to tackle more general nonlinear saddle point systems, such as non-smooth objective function  $f$ , variables  $(u, p)$  restricted in convex sets and nonlinear bicoupling terms.

**THANK YOU FOR YOUR ATTENTION!**



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