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# Optimal control of the gradient systems

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## Abstract

In this paper we consider the optimal control problems governed by the gradient systems

$$\frac{\partial y}{\partial t} = -\frac{\delta E}{\delta y}, \quad \Omega \in R^d, d = 1, 2,$$

for the Ginzburg-Landau free energy

$$E(u) = \int_\Omega \left( \frac{\epsilon}{2} |\nabla y|^2 - F(y) \right) d\Omega,$$

where $F(y)$ denotes a potential function and ε is the diffusivity. One example of gradient systems are the Schlögl equation arising in chemical waves with a quartic potential function F(y). Gradient systems are characterized by energy decreasing property $E(y(t)) \leq E(y(s)), s > t$. Numerical integrators that preserve the energy decreasing property in the discrete setting are called energy or gradient stable. It is known that the implicit Euler method is first order unconditionally energy stable method. The only second order unconditionally energy stable method is the average vector field (AVF) method. We discretize the gradients systems by discontinuous Galerkin method in space and by AVF integrator in time. We solve optimal control problems for the Schlögl equation with traveling and spiraling waves using sparse and $H_1$ regularized controls .

**Keywords:** Gradient system; Optimal control; Average vector field; Schlögl equation; Discontinuous Galerkin method

## 1. Introduction

Gradient systems are a class of dynamical systems that evolve over time to minimize a certain potential, often governed by a Lyapunov-like function. These systems play a significant role in various scientific fields, including physics, chemistry, biology, and economics, where they model phenomena such as diffusion, phase transitions, and optimization processes. The study of gradient systems is crucial for understanding stability, pattern formation, and the dynamics of nonequilibrium systems. In particular, the Schlögl equation is one of the prototypical models used to describe autocatalytic reactions in chemical systems, capturing essential features such as bistability, instability, and pattern formation.

The Schlögl equation is a system of nonlinear differential equations that models the evolution of a chemical reaction network with feedback mechanisms. It has been widely studied due to its rich dynamics, which include the potential for oscillatory behavior, bifurcations, and the emergence of spatially heterogeneous states. Given the complexity and nonlinearity of the Schlögl system, controlling its dynamics to achieve specific behavior is of great interest in both

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theoretical and applied contexts. The ability to steer the system to desired states using minimal control efforts is a key challenge.

In this paper, we consider the optimal control problems for gradient system, namely Schlögl equation [1, 2, 3, 5]. For gradient systems, the energy decreases along solutions as fast as possible. Schlögl equation describes the auto-catalytic chemical reaction mechanism.

In the following we consider the minimization of an objective function given by

$$J(y,u)=\frac{c_D}{2}\int_Q (y(x,t)-y_D(x,t))^2 dx\,dt+\frac{c_T}{2}\int_\Omega (y(x,T)-y_T(x))^2 dx+\frac{\lambda}{2}\int_Q u(x,t)^2 dx\,dt \tag{1}$$

subject to

$$\begin{aligned} y_t(x,t)-\varepsilon y_{xx}(x,t)+f(y) &= u(x,t) && \text{in} \quad Q=\Omega\times(0,T] \\ y(x,0) &= y_0(x) && \text{in} \quad \Omega \\ y_x(0,t)=y_x(L,t) &= 0 && \text{in} \quad (0,T] \end{aligned} \tag{2}$$

where $\Omega=(a,b), \varepsilon > 0$. In addition, $u, yD \in L^2(0,T;L^2(\Omega)), y_0(x) \in L^2(\Omega)$ are given source function, desired state and initial condition, resp. There can be also box constraints on the control: $u_a \leq u(x,t) \leq u_b$. The nonlinearity $f(y)$ is the differential of the potential function $F(y)$, i.e., $f(y) = F'(y)$. Here, $y$ and $u$ are state and control variables, resp. The aim is finding a control u to minimize the difference between the state y and the desired state $y_D$ with $c_D = 1, c_T = 0$ or to minimize the difference between the final state $y(T)$ and the desired final state $y_T$ with $c_D = 0, c_T = 1$. There are two approach for solving the above given optimization problem (1)-(2), namely discretize–then–optimize and optimize–then–discretize. Here we use the second case, optimize–then–discretize procedure which means that we first derive the first order necessary optimality conditions established on the continuous level and then we continue with the discretization of the problem. For the optimization, the nonlinear conjugate gradient method equipped with the line search algorithm using the strong Wolfe-Powell conditions and approximate Wolfe conditions is used. For the space discretization, discontinuous Galerkin finite elements (DG) [6], for the time discretization average vector field (AVF) method preserving the energy of the Hamiltonian systems and energy dissipation of the gradient systems are used [4].

## 2. First order optimality conditions

In order to derive the first order necessary optimality conditions, we first set the Lagrangian function as

$$\begin{aligned} L(y,u,p) &= J(y,u)-\iint_Q p\,(y_t-\varepsilon y_{xx}+f(y)-u)\,dx\,dt \\ &= \frac{c_D}{2}\iint_Q (y(x,t)-y_D(x,t))^2\,dx\,dt+\frac{c_T}{2}\int_\Omega (y(x,t)-y_T(x))^2\,dx+\frac{\lambda}{2}\iint_Q u^2\,dx\,dt \\ &\quad -\iint_Q p\,y_t\,dx\,dt+\iint_Q p\,\varepsilon\Delta y\,dx\,dt-\iint_Q p\,f(y)\,dx\,dt+\iint_Q p\,u\,dx\,dt \end{aligned}$$

Derivative of the Lagrangian $L(y,u,p)$ w.r.t. the adjoint variable $p$ gives the state equation (2).

Derivative of the Lagrangian $L(y,u,p)$ w.r.t. the state variable y gives the following adjoint equation:

$$\begin{aligned} -p_t-\varepsilon p_{xx}+f'(y)\,p &= c_D\,(y-y_D) && \text{in} \quad \Omega\times[0,T), \\ p(x,T) &= c_T(y(x,T)-y_T(x)) && \text{in} \quad \Omega, \\ p_x(0,t)=p_x(L,t) &= 0 && \text{in} \quad [0,T). \end{aligned} \tag{3}$$

The initial condition of this equation is given at the final time T, so it has to be solved backward in time. Lastly, the derivative of the Lagrangian $L(y,u,p)$ w.r.t. the control variable $u$ leads to the gradient equation:

$$\lambda u + p = 0 \qquad a.e.\ in\ Q. \tag{4}$$

## 3. Discontinuous Galerkin method

In this section, semi-discrete form of the first order optimality conditions consisting of state, adjoint and gradient equations will be given. As we have pointed out, for the space discretization we use piecewise linear discontinuous finite elements [6]. The classical weak formulation of the state equation (2) reads: for fixed control $u$, find $y(t) \in H_0^1(\Omega)$ s.t.

$$\begin{aligned} (y_t, v) + a(y, v) + (f(y), v) &= (u, v) \qquad \forall v \in H_0^1(\Omega), \quad t \in (0, T] \\ (y(0), v) &= (y_0, v) \qquad \forall v \in H_0^1(\Omega) \end{aligned}$$

where $(\cdot,\cdot)$ denotes the usual $L^2$-inner product over the domain Ω and $a(u, v) = \varepsilon(\nabla u, \nabla v)$ is the bilinear form over the domain Ω. Let εh be the disjoint partition of the domain Ω with elements $\{E_i\}_{i=1}^N \in \epsilon_h$, where $N$ is the number of elements in the partition. On $\epsilon_h$, set the discrete solution and test function space as

$$D_k = D_k(\varepsilon_h) := \{v \in L^2(\Omega) : v_E \in \mathbb{P}_k(E)\ \forall E \in \varepsilon_h\},$$

where $P_k(E)$ is the space of polynomials of degree at most k on $E \in \epsilon_h$. In our problem we choose k = 1. We split the set of all edges $\Gamma_h$ into the set $\Gamma_h^0$ of interior edges and the set $\Gamma_h^\partial$ of boundary edges so that $\Gamma_h = \Gamma_h^0 \cup \Gamma_h^\partial$. Let $E_1^e$ and $E_2^e$ be the two elements sharing the common edge $e$. Then, since the functions in $D_k$ are allowed to be discontinuous along the interior edges, any scalar function $v \in D_k$ has two traces along the edge $e$, denoted by $v|\_E_1^e$ and $v|\_|\_E_2^e$. Then the jump and average of $v$ across the edge e are defined by

$$[v]_e = v|_{E_1^e}\mathbf{n}_{E_1} + v|_{E_2^e}\mathbf{n}_{E_2}, \quad \{v\}_e = \frac{1}{2}(v|_{E_1^e} + v|_{E_2^e}),$$

where $n_{E_1}$ and $n_{E_2}$ denote the outward unit normal vectors to the edge $e$ from $E_1$ and $E_2$, respectively. Similarly, the jump and average terms for a piecewise continuous vector valued function $\nabla y$ on the edge $e$ are defined by

$$[\nabla y]_e = \nabla y|_{E_1^e} \cdot \mathbf{n}_{E_1} + \nabla y|_{E_2^e} \cdot \mathbf{n}_{E_2}, \quad \{\nabla y\}_e = \frac{1}{2}(\nabla yq|_{E_1^e} + \nabla yq|_{E_2^e}).$$

From now on, for convenient, we omit the subscript notation in the formulations and we write as $[\cdot]$ and $\{\cdot\}$. Then, (SIPG) DG formulation of the state equation (2) is written as follows:

$$\left(\frac{\partial y_h}{\partial t}, v_h\right) + a_h(\varepsilon; y_h, v_h) + (f(y_h), v_h) = (u_h, v_h), \quad \forall v_h \in D_k, \quad t \in (0, T]) \tag{5}$$

where the DG bilinear form $a_h(\varepsilon; y_h, v_h)$ is given by

$$\begin{aligned} a_h(\varepsilon; y_h, v_h) &= \sum_{E \in \varepsilon_h} \int_E \varepsilon \nabla y_h \cdot \nabla v_h - \sum_{e \in \Gamma_h^0} \int_e \{d \nabla y_h\} \cdot [v_h] \mathrm{d}s \\ &\quad - \sum_{e \in \Gamma_h^0} \int_e \{\varepsilon \nabla v_h\} \cdot [y_h] \mathrm{d}s + \sum_{e \in \Gamma_h^0} \frac{\sigma \varepsilon}{h_e} \int_e \{\nabla y_h\} \cdot [v_h] \mathrm{d}s. \end{aligned} \tag{6}$$

Here σ >0 is called the penalty parameter and it should be sufficiently large to ensure the stability of the DG discretization. Also he denotes the length of the edge e.

Hence, the semi-discretized form of the first order optimality conditions (2)-(3)-(4) is written as follows

$$\begin{aligned}
\left(\frac{\partial y_h}{\partial t}, v_h\right) + a_h(\varepsilon; y_h, v_h) + (f(y_h), v_h) &= (u_h, v_h) && \forall v_h \text{ in } D_k, \quad \forall t \in (0,T], \\
-\left(\frac{\partial p_h}{\partial t}, q_h\right) + a_h(\varepsilon; p_h, q_h) + (f'(y_h)p_h, q_h) &= (c_D; y_h - (y_h)_D, q_h) && \forall p_h \text{ in } D_k, \quad \forall t \in (0,T], \\
\lambda u_h + p_h &= 0 && \forall t \in (0,T].
\end{aligned}$$

Now, let us write (7) in matrix-vector form. The semi-discrete solutions of (7) are written using the global basis functions of $D_k$. For instance, the solution of the state and adjoint equations are of the form

$$\begin{aligned}
\mathbf{y}_h(t) &= \sum_{n=1}^{N} \sum_{i=1}^{N_{loc}} y_i^n(t)\phi_i^n(x), && \forall x \in \Omega, \quad \forall t \in (0,T], \\
\mathbf{p}_h(t) &= \sum_{n=1}^{N} \sum_{i=1}^{N_{loc}} p_i^n(t)\phi_i^n(x), && \forall x \in \Omega, \quad \forall t \in (0,T].
\end{aligned}$$

Here, $\phi_i^n, i = 1,\cdots, N_{loc}, n = 1,\cdots, N$, are the basis functions of $D_k$, and $N$ denotes the number of elements, $N_{loc}$ is the local dimension. $y_i^n$ and $p_i^n$ are the unknown coefficients of $y$ and $p$.

When we substitute (7) into the semi-discretized form (7), we obtain the following semi linear system of ordinary differential equations

$$\begin{aligned}
\mathbf{M}\frac{\mathrm{d}\mathbf{y}_h(t)}{\mathrm{d}t} + \mathbf{S}\mathbf{y}_h + \mathbf{F}(t) &= \mathbf{M}\mathbf{u}_h(t) \\
M\mathbf{y}_h(0) &= (\mathbf{y_h})_0 \\
\\
-\mathbf{M}\frac{\mathrm{d}\mathbf{y}_h(t)}{\mathrm{d}t} + \mathbf{S}\mathbf{p}_h + \mathbf{F}(t) &= c_D\mathbf{M}(\mathbf{y}_h - (\mathbf{y}_h)_D) \\
\mathbf{M}\mathbf{p}_h(T) &= c_T\mathbf{M}(\mathbf{y}_h(T) - (\mathbf{y_h})_T) \\
\\
\lambda\mathbf{M}\mathbf{u}_h + \mathbf{M}\mathbf{p}_h &= 0
\end{aligned}$$

where $M$ and $S$ denote mass and stiffness matrices, resp. In a similar way, we can discretize our objective functional as

$$\begin{aligned}
J(\mathbf{y}_h, \mathbf{u}_h) &= \frac{c_D}{2}\int_0^T (\mathbf{y}_h(t) - (\mathbf{y}_h)_D(t))^T\mathbf{M}(\mathbf{y}_h(t) - (\mathbf{y}_h)_D(t))\,\mathrm{d}t \\
&+ \frac{c_T}{2}(\mathbf{y}_h(T) - (\mathbf{y}_h)_T)^T\mathbf{M}(\mathbf{y}_h(T) - (\mathbf{y}_h)_T) \\
&+ \frac{\lambda}{2}\int_0^T \mathbf{u}_h(t)\mathbf{M}\mathbf{u}_h(t)\,\mathrm{d}t \qquad (7)
\end{aligned}$$

## 4. Time discretization methods

Let $0 = t_0 < t_1 < \cdots < t_j = T$ be the uniform partition of the time interval $I = [0,T]$ into $J$ time-steps $[t_{j-1}, t_j]$, $j = 1,\ldots,J$,with the step size $\Delta t = \frac{T}{J-1}$. Let us denote the approximate coefficients vector $\boldsymbol{y}(t)$ of (7) at the time $t = t_j$ by $\boldsymbol{y}_j$,and similarly approximate solution by $\boldsymbol{y}^j \approx \boldsymbol{y}_h(t_j)$. Then, the fully discrete forms of the semi-discrete state and adjoint equations in (7) read as: for all $j = 1,\ldots,J$, find $\boldsymbol{y}_j, \boldsymbol{p}_j$ such that with backward Euler

$$M\left(\frac{\mathbf{y}^j-\mathbf{y}^{j-1}}{\Delta t}\right)+S\mathbf{y}^j+F(\mathbf{y}^j)=M\mathbf{u}^j,\quad j=1,\cdots,n \tag{8}$$

$$-M\left(\frac{\mathbf{p}^j-\mathbf{p}^{j-1}}{\Delta t}\right)+S\mathbf{p}^j+F'(\mathbf{y}^j)\mathbf{p}^j=c_DM(\mathbf{y}^j-\mathbf{y}_D),\qquad j=n,\cdots,1, \tag{9}$$

with semi-implicit Euler

$$M\left(\frac{\mathbf{y}^j-\mathbf{y}^{j-1}}{\Delta t}\right)+S\mathbf{y}^j+F(\mathbf{y}^{j-1})=M\mathbf{u}^j,\quad j=1,\cdots,n \tag{10}$$

$$-M\left(\frac{\mathbf{y}^j-\mathbf{y}^{j-1}}{\Delta t}\right)+S\mathbf{y}^j+F'(\mathbf{y}^{j-1})p^j=c_DM(\mathbf{y}^j-\mathbf{y}_D),\quad j=n,\cdots,1, \tag{11}$$

with average vector field [4]

$$\left(M+S\frac{\mathrm{d}t}{2}\right)\mathbf{y}^{j+1}-\left(M-S\frac{dt}{2}\right)\mathbf{y}^j+d\mathrm{t}\int_0^1F(\xi\mathbf{y}^{j+1}+(1-\xi)\mathbf{y}^j)\mathrm{d}\xi=M\mathbf{u}^j,\quad j=1,\cdots,n \tag{12}$$

$$\left(-M+S\frac{\mathrm{d}t}{2}\right)\mathbf{y}^{j+1}+\left(M+S\frac{\mathrm{d}t}{2}\right)\mathbf{y}^j+\frac{\mathrm{d}t}{2}F'(\mathbf{y}^j)(\mathbf{p}^j+\mathbf{p}^{j+1})=c_DM(\mathbf{y}^j-\mathbf{y}_D),\quad j=n,\cdots,1. \tag{13}$$

Except semi-implicit-Euler method, they are solved by Newton method.

## 5. Numerical results

### 5.1. 1D Schlögl equation (reach to zero state)

For the 1D Schlögl equation, we consider a gradient system with the nonlinearity $F'(y)=f(y)=\frac{1}{3}y^3(x,t)-y(x,t)$ where $y\in\{-1,1\}$ are stable fixed points whereas $y=0$ is the unstable fixed point. We use the regularization parameter $\lambda=10^{-6}$. We consider as space time domain $x\in[0,20]$ with $\Delta x=0.2$ and $t\in[0,5]$ with $\Delta t=0.05$. Our aim is to reach zero state at the final time $t=5$ through the parameters $c_Q=0, c_T=1$. The initial condition is taken as

$$y_0(x)=\begin{cases}-1.2\sqrt{3} & x<9\\ 1.2\sqrt{3}(x-10) & x\in[9,11]\\ 1.2\sqrt{3} & x>11\end{cases}$$

**Table 1** Result for the ID schlogl model (control in the whole domain)

| Method | Objective Value | #NCG it. | # Line Search | # Newton it | CPU Time |
|---|---|---|---|---|---|
| **BE** | 4.06e-05 | 23 | 1.5 | 1.0 | 39.1 |
| **AVF** | 4.46e-05 | 23 | 1.4 | 1.0 | 80.2 |
| **SIE** | 3.83e-05 | 23 | 1.4 | - | 31.5 |

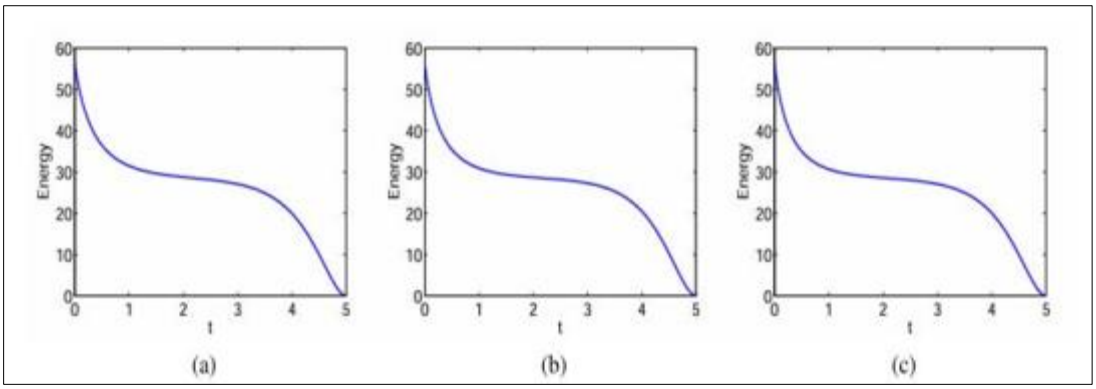


**Figure 1** Energies of the states though the time integrators backword Euler, average vector field and semi-implicit Euler time integrators from left or right for the ID Schlögl model (reach to zero state)

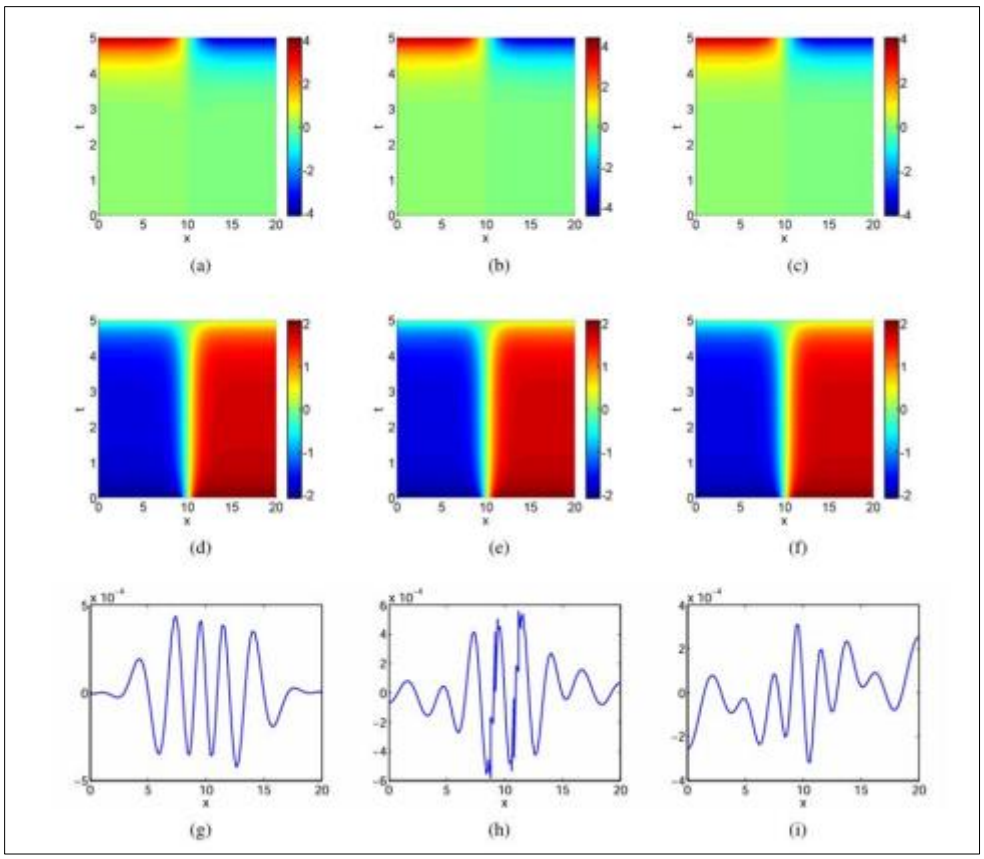


**Figure 2** Optimal control profiles (top row), optimal state profile (middle row) and optimal state at the final time (bottom row) solved by backword Euler, average vector field and semi-implicit Euler time integrators from left or right for the ID Schlögl model (reach to zero state)

### 5.2. 1D Schlögl equation (with desired state)

We consider again the 1D Schlögl equation with the regularization parameter $\lambda = 10^{-6}$, and space-time domain $x \in [0, 20]$ with $\Delta x = 0.2$ and $t \in [0, 5]$ with $\Delta t = 0.05$. Our aim is now to impose a desired state through the parameters $c_Q = 1, c_T = 0$ and with the initial condition

$$y_0(x) = \begin{cases} -1.2\sqrt{3} & x < 9 \\ 1.2\sqrt{3}(x-10) & x \in [9,11] \\ 1.2\sqrt{3} & x > 11 \end{cases}$$

The desired state is chosen as the natural solution $u^*$(solution of the uncontrolled model) until the time $t = 2.5$ and zero after

$$y_D(x,t) = \begin{cases} u^*(x,t) & t \in [0,2.5] \\ 0 & t \in (2.5,5] \end{cases}$$

**Table 2** Result for the ID Schlögl model (control in the whole domain)

| Method | Objective Value | #NCG it. | # Line Search | # Newton it | CPU Time |
|---|---|---|---|---|---|
| BE | 3.55e-01 | 200 | 2.3 | 1.0 | 738.7 |
| AVF | 3.87e-01 | 200 | 2.3 | 1.0 | 1717.4 |
| SIE | 3.76e-01 | 200 | 2.5 | - | 661.5 |

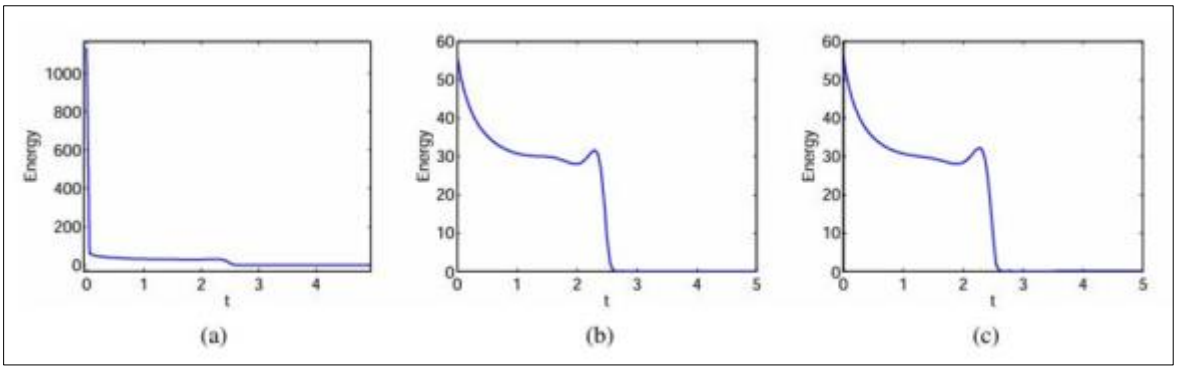


**Figure 3** Energies of the states though the time integrators backword Euler, average vector field and semi-implicit Euler from left or right for the ID Schlögl model (with desired state)

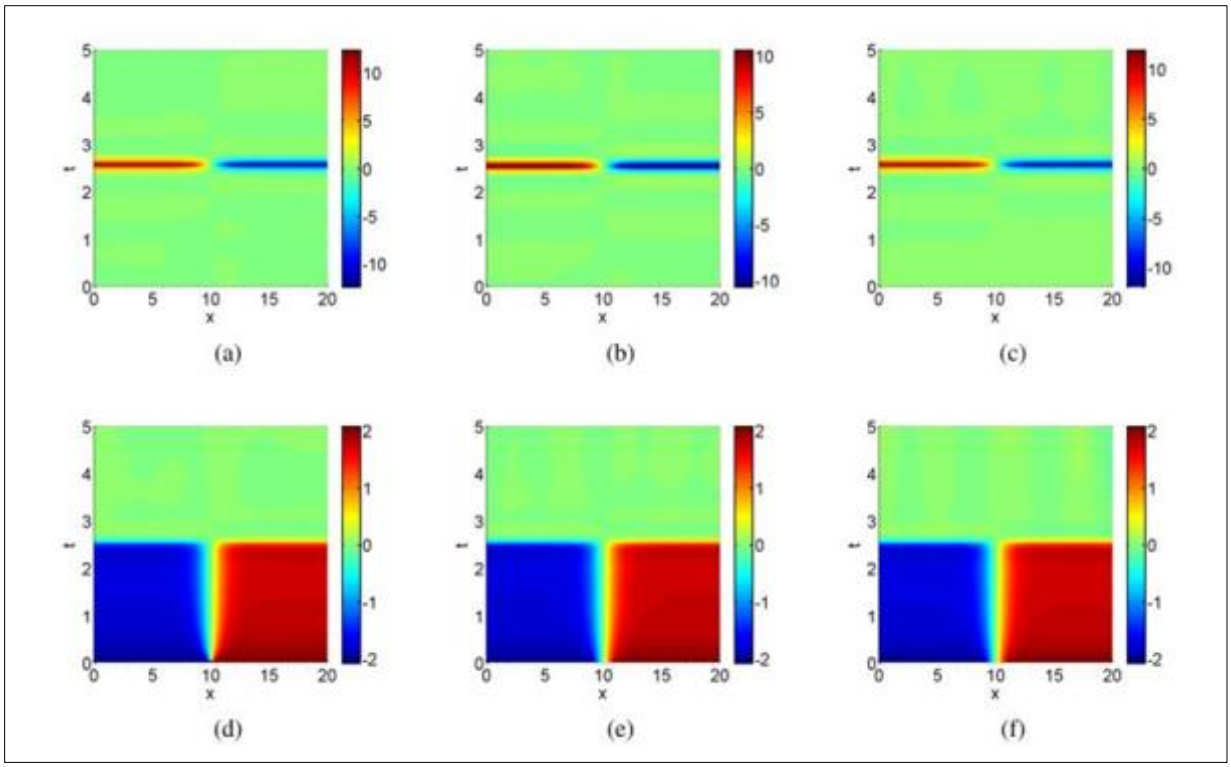


**Figure 4** Optimal control profiles ( top row), optimal state profile (bottom row) solved by backword Euler , average vector field and semi-implicit Euler time integrators from left or right for the ID Schlögl model (with desired state)

### 5.3. 2D Schlögl equation (reach to zero state)

For the 2D Schlögl equation, we consider a gradient system the nonlinearity $F'(y) = f(y) = y(y - 0.25)(y + 1)$. We use the regularization parameter $\lambda = 10^{-10}$. We consider as space-time domain $(x, t) = [0, 70]^2 \times [0, 20]$ with the spatial and temporal mesh sizes $\Delta x_1 = \Delta x_2 = \frac{35}{8}$ and $\Delta t = 0.5$, resp. Our aim is to reach zero state at the final time $T = 20$ through the parameters $c_Q = 0, c_T = 1$ and the box constraint $-1 \leq u(x, t) \leq 1$. The initial condition is taken as

$$y_0(x) = \left(1 + \exp\left(\frac{\frac{70}{3} - x_1}{\sqrt{2}}\right)\right)^{-1} + \left(1 + \exp\left(\frac{x_1 - \frac{140}{3}}{\sqrt{2}}\right)\right)^{-1} - 1$$

**Table 3** Result for the 2D Schlögl model (reach to zero state)

| Method | Objective Value | #NCG it. | # Line Search | # Newton it | CPU Time |
|---|---|---|---|---|---|
| BE | 9.26e-06 | 22 | 2.5 | 1.0 | 66.1 |
| AVF | 5.64e-06 | 55 | 8.0 | 1.0 | 843.9 |
| SIE | 5.88e-06 | 31 | 5.3 | - | 134.7 |

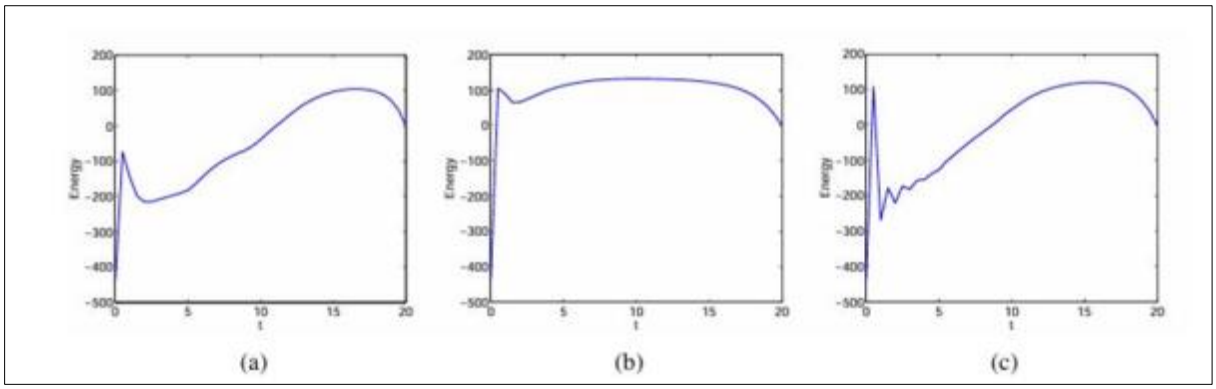


**Figure 5** Energies of the states though the time integrators backword Euler, average vector field and semi-implicit Euler time integrators from left or right for the 2D Schlögl model (reach to zero state)

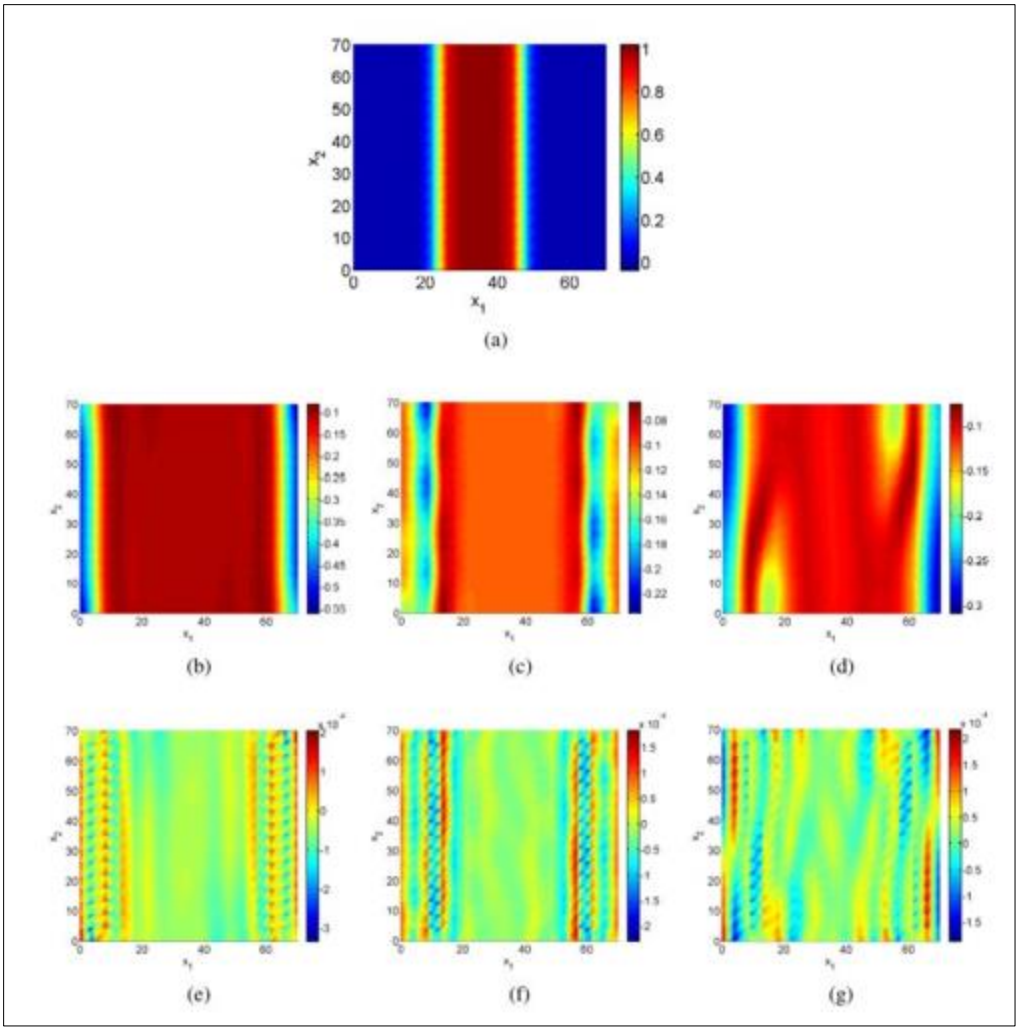


**Figure 6** Initial state (top row) optimal control (middle row) and optimal state (bottom row) at the final time T=20 solved by backword Euler, average vector field and semi-implicit Euler time integrators from left or right for the 2D Schlögl model (reach to zero state)

## 6. Conclusion

In this study, we have successfully applied optimal control theory to the Schlögl equation, demonstrating how control inputs can be used to stabilize unstable equilibria and guide the system toward desired states. By deriving the necessary conditions for optimality and using numerical simulations, we showed that effective control strategies can significantly reduce control effort while maintaining the system's dynamics. Additionally, model order reduction techniques were employed to further decrease the computational cost, making the control problem more efficient and scalable. Our findings highlight the potential of optimal control for managing complex, nonlinear gradient systems and offer insights into its practical applications in fields such as chemical engineering and biochemistry. Future work will focus on addressing computational challenges and extending these techniques to more complex systems, further enhancing their real-world applicability.

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