DYNAMIC OPTIMIZATION OF DISSIPATIVE PDE SYSTEMS USING NONLINEAR ORDER REDUCTION

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MOTIVATION / BACKGROUND

- Optimization problems arising in distributed process systems.
  - ◇ Examples:
    - ▷ Chemical vapor deposition process design for deposition rate spatial uniformity.
    - ▷ Design of precursors' inflow time-profile to MOVPE reactor for deposition of desired heterostructures.
  - ◇ Main features:
    - ▷ Partial differential equation (PDE) equality constraints.
    - ▷ Nonlinear inequality constraints.
    - ▷ Steady-state / dynamic.
- Traditional spatial discretization approach for solution.
  - ◇ Discretization via finite-differences / finite-elements.
  - ◇ Computationally expensive approach!
- Spatial discretization using empirical eigenfunctions (e.g., Arian *et al*, NASA report, 2000; Bendersky and Christofides, CES, 2000).

PRESENT WORK

(Armaou and Christofides, CES, 2002)

- Objective: Computationally efficient methods for the solution of dynamic optimization problems involving highly dissipative PDE constraints.
  - ◇ Order reduction in the spatial domain via method of weighted residuals using global basis functions.
    - ▷ Analytical eigenfunctions / off-the-shelf sets of basis functions.
    - ▷ Empirical eigenfunctions from Karhunen-Loève expansion.
    - ▷ Accuracy and stability enhancement using the concept of approximate inertial manifolds.
  - ◇ Low-dimensional dynamic nonlinear programs.
    - ▷ Temporal discretization using finite differences.
    - ▷ Solution: Reduced gradient optimization methods.
- Application to diffusion-reaction processes and the Kuramoto-Sivashinsky equation.

DYNAMIC OPTIMIZATION PROBLEM

- Optimization objective:

$$min \int_0^{t_f} \int_\Omega G(x(z,t), d(t)) dz dt$$

- PDE equality constraints:

$$\frac{\partial x}{\partial t} = \mathcal{A}(x) + f(x, d(t)), \quad Cx + D\frac{dx}{d\eta}\bigg|_\Gamma = R, \quad x(z,0) = x_0(z)$$

$d(t)$: Vector of design variables.

$\mathcal{A}(x)$: Nonlinear spatial differential operator.

$f(x,d)$: Nonlinear function of state and design variables.

- Nonlinear inequality constraints:

$$g(x, d(t)) \leq 0$$

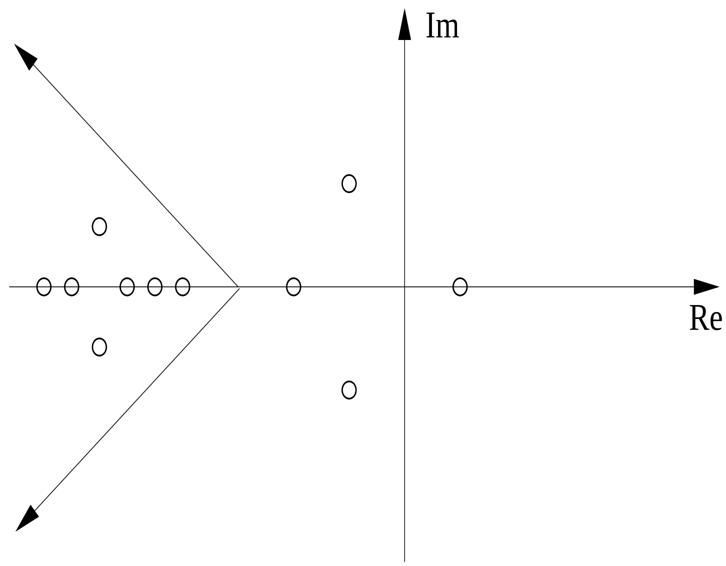
PROPERTIES OF HIGHLY DISSIPATIVE PDEs

- Eigenvalue problem of linearized spatial differential operator:

$$\mathcal{A}\phi_i(z) = \lambda_i \phi_i(z), \quad Cx + D\frac{dx}{d\eta}\bigg|_{\Gamma} = R$$

λ_i: eigenvalue; ϕ_i: eigenfunction.

- Typical structure of eigenspectrum:



- A finite number of dominant modes practically determines the system dynamics.

SPATIAL DISCRETIZATION USING WEIGHTED RESIDUALS

- State variable expansion ($n = 1$): $x(z,t) = \sum_{k=1}^{N} a_k(t)\phi_k(z)$,

  $a_k(t)$: time-varying coefficients, $\phi_k(z)$: global (analytical) basis functions.

- Resulting finite-dimensional approximate optimization program:

$$min \int_0^{t_f} \int_\Omega G(\sum_{k=1}^{N} a_{kN}(t)\phi_k(z), d) dz dt,$$

$$-\sum_{k=1}^{N} \dot{a}_{kN}(\int_\Omega \psi_\nu(z)\phi_k(z)dz) + \int_\Omega \psi_\nu(z)\mathcal{A}(\sum_{k=1}^{N} a_{kN}(t)\phi_k(z))dz$$

$$+\int_\Omega \psi_\nu(z) f(t, \sum_{k=1}^{N} a_{kN}(t)\phi_k(z), d)dz = 0$$

$$\int_\Omega \psi_\nu(z) g(\sum_{k=1}^{N} a_{kN}\phi_k(z), d)dz \leq 0$$

- When the basis functions and the weighted functions are identical:
  Galerkin's method.

SOLUTION OF DYNAMIC NONLINEAR PROGRAM

$$\begin{aligned}
&min \int_0^{t_f} G(a_N, d)dt \\
&s.t. \\
&\dot{a}_N = \tilde{f}(a_N, d) \\
&\tilde{g}(a_N, d) \leq 0
\end{aligned}$$

- Temporal discretization:
  - ◇ Finite-differences.
- Solution of reduced-order optimization problem:
  - ◇ Reduced gradient optimization method.
- Solution of reduced-order optimization problem for (N+1)-dimensional ODE system.
  - ◇ If $|J_{N+1} - J_N| < \theta_1$ and $|d_{N+1}(t) - d_N(t)| < \theta_2$ end, else repeat process for $N = N + 1$.
  - ◇ Gradient-based convergence criteria can be used (e.g., Alexandrov *et al*, Struct. Optim., 1998; Kelley and Sachs, SIAM JO, 1999).

DYNAMIC DIFFUSION-REACTION PROCESS

- Process dynamic model (constant coefficients):

$$\frac{\partial x}{\partial t} = k\frac{\partial^2 x}{\partial z^2} + \beta_T\left(e^{-\frac{\gamma}{1+x}} - e^{-\gamma}\right) + \beta_U\left(b(z)u(t) - x\right)$$

Process parameters: $k = 1, \quad \beta_T = 8.0 \quad \beta_U = 2.0 \quad \gamma = 2.0$

Boundary conditions: $x(0,t) = 0, \quad x(l,t) = 0$

Initial condition: $x(z,0) = x_0(z) = 0.5$

◇ The steady-state $x(z,t) = 0$ is unstable.

- Optimization objective:

$$min\left(\int_0^{t_f}\int_0^{l}(w_s x^2(z,t) + w_u u^2(t))dz\,dt\right)$$

REDUCED OPTIMIZATION PROBLEM

- Analytical Eigenfunctions: $\phi_j(z) = \sqrt{\frac{2}{l}} sin(j\pi\ z)$

- Applying Galerkin's method with 6 analytical eigenfunctions.

$$min \left(\int_0^{t_f} \int_0^{\pi} w_s (\sum_{i=1}^{6} a_i(t)\phi_i(z))^2 + w_u u^2(t) dz dt \right)$$

$$s.t.$$

$$\frac{da_i}{dt} = \sum_{j=1}^{6} \alpha_j \int_0^l \frac{d^2\phi_j(z)}{dz} \phi_i(z) dz - \beta_U a_i + \beta_U \int_0^l b(z)\phi_i(z) dz\ u(t)$$

$$+\beta_T \int_0^l \left(exp(-\gamma(\sum_{j=1}^{5} \alpha_j \phi_j(z) + 1)^{-1}) - exp(-\gamma) \right) \phi_i(z) dz,\ i = 1, ..., 6$$

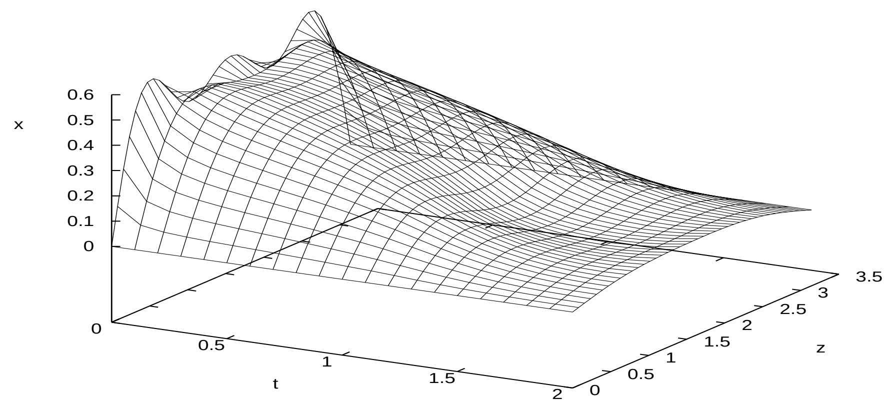
$$\|u(t)\| \leq 0.6, \qquad \forall (z,t) \in [0,l] \times [0,t_f]$$

- Temporal discretization using implicit Euler.

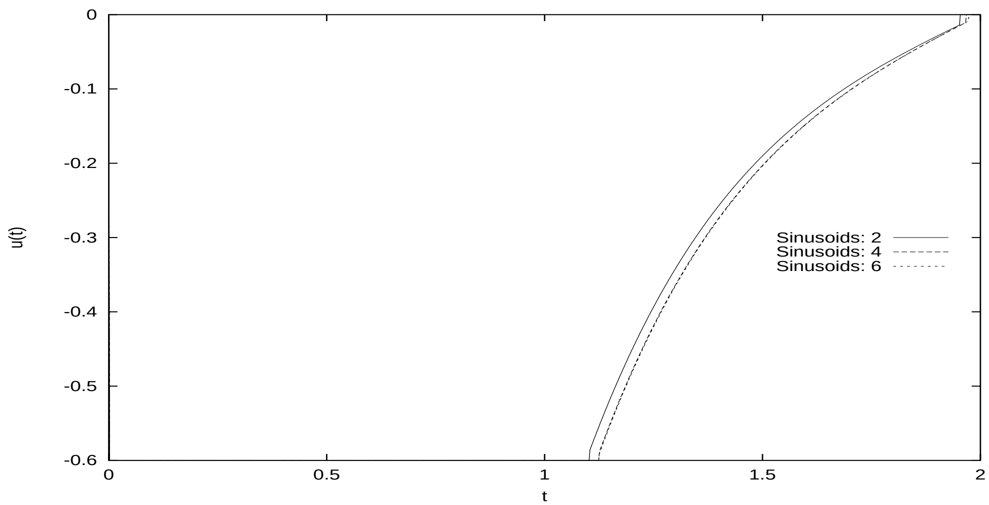
OPTIMIZATION RESULTS

Nominal conditions, $b(z) = H(z - 0.3l) - H(z - 0.7l)$

Spatiotemporal profile of solution $(N = 6)$.



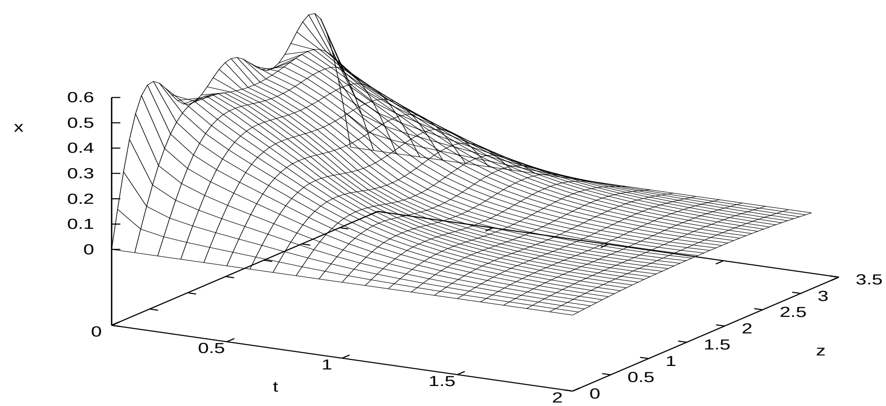
Design variable profile.



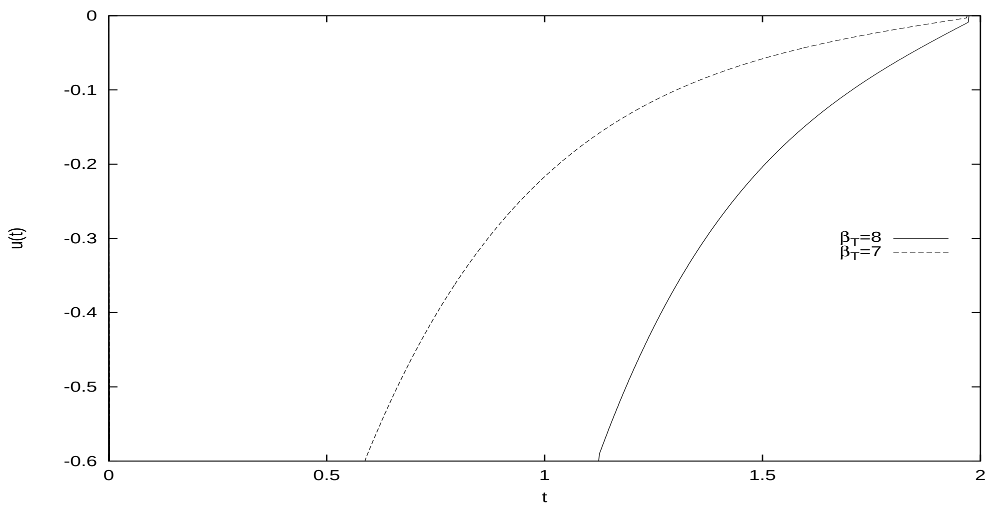
OPTIMIZATION RESULTS

-12.5% variation in β_T, $b(z) = H(z - 0.3l) - H(z - 0.7l)$

Spatiotemporal profile of solution ($N = 6$).



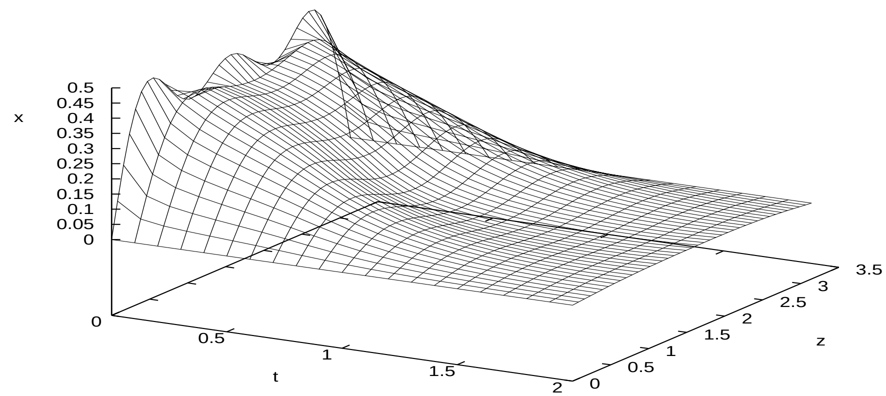
Design variable profile.



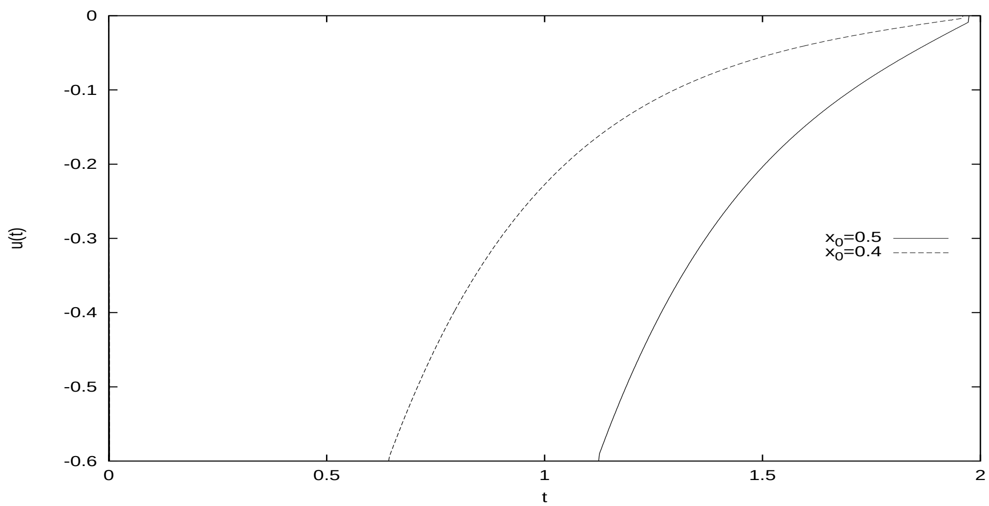
OPTIMIZATION RESULTS

-20% variation in $x_0(z)$, $b(z) = H(z - 0.3l) - H(z - 0.7l)$

Spatiotemporal profile of solution ($N = 6$).



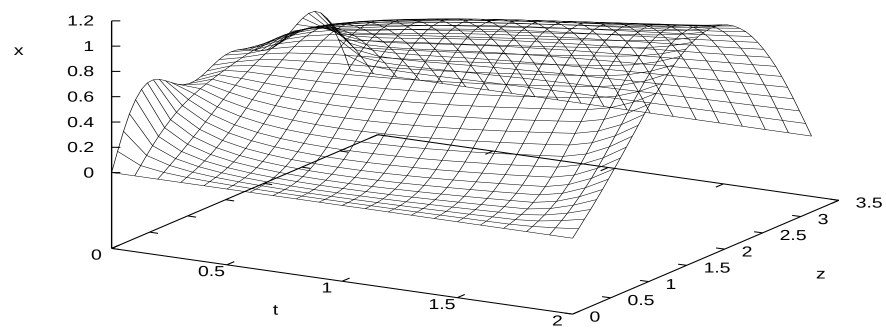
Independent variable profile.



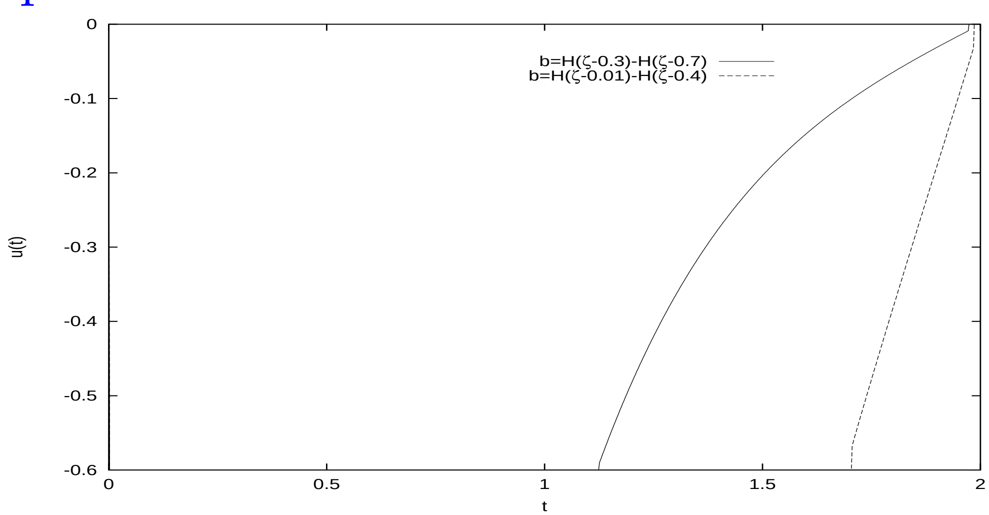
OPTIMIZATION RESULTS

Nominal conditions, $b(z) = H(z - 0.01l) - H(z - 0.4l)$

Spatiotemporal profile of solution ($N = 6$).



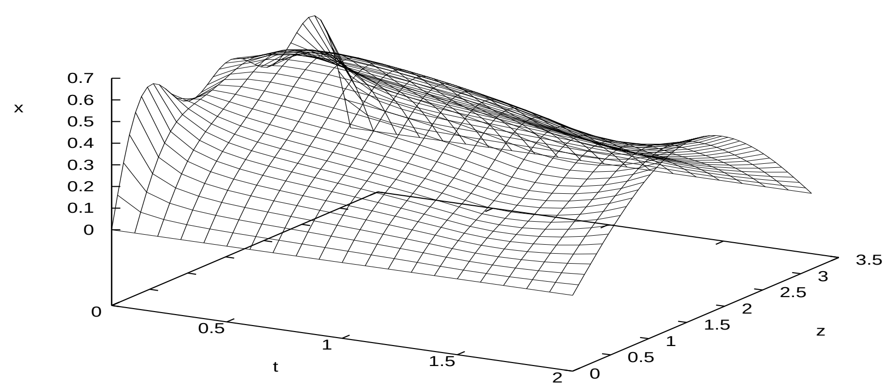
Design variable profile.



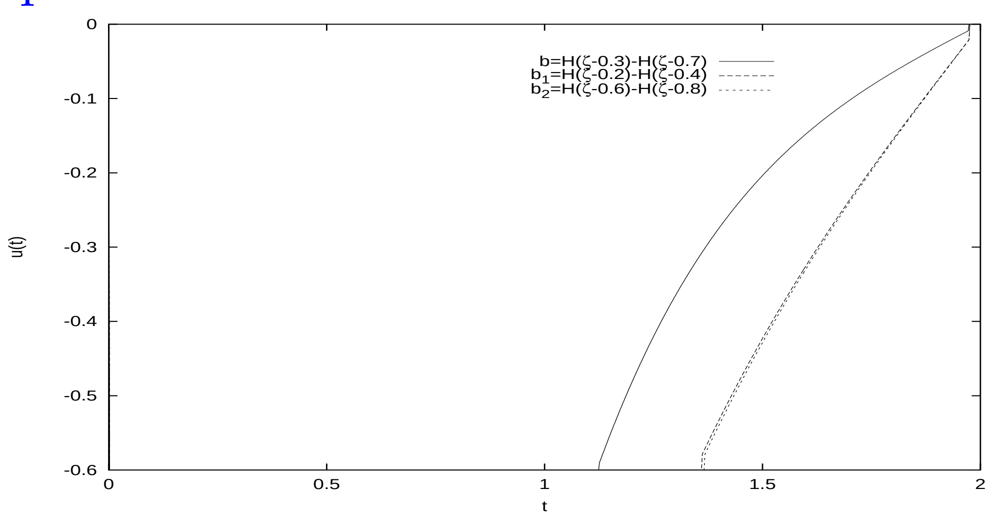
OPTIMIZATION RESULTS

Nominal, $b_1(z) = H(z - 0.2l) - H(z - 0.4l)$, $b_2(z) = H(z - 0.6l) - H(z - 0.8l)$

Spatiotemporal profile of solution ($N = 6$).



Design variable profiles.



DYNAMIC DIFFUSION-REACTION PROCESS

- Process dynamic model (nonlinear operator, spatially-varying parameters):

$$\frac{\partial x}{\partial t} = \frac{\partial}{\partial z}(k(x)\frac{\partial x}{\partial z}) + \beta_T(z)(e^{-\frac{\gamma}{1+x}} - e^{-\gamma}) + \beta_U(b(z)u(t) - x)$$

Process parameters: $k(x) = 0.5 + 0.7/(x+1)$, $\beta_T(z) = \beta_{T0}(cos(z) + 1)$

Boundary conditions: $x(0,t) = 0$, $x(l,t) = 0$

Initial condition: $x(z,0) = x_0(z) = 0.5$

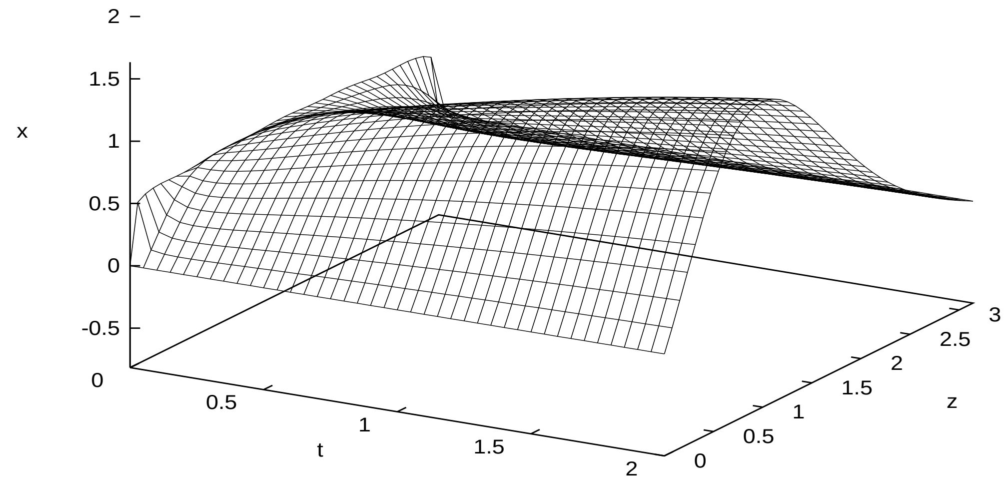
◇ The steady-state $x(z,t) = 0$ is unstable.

- Optimization objective:

$$min\left(\int_0^{t_f}\int_0^{l}(w_s x^2(z,t) + w_u u^2(z,t))dz\,dt\right)$$

DYNAMIC DIFFUSION-REACTION PROCESS

Spatiotemporal profile of solution for $u(t) = 0$.



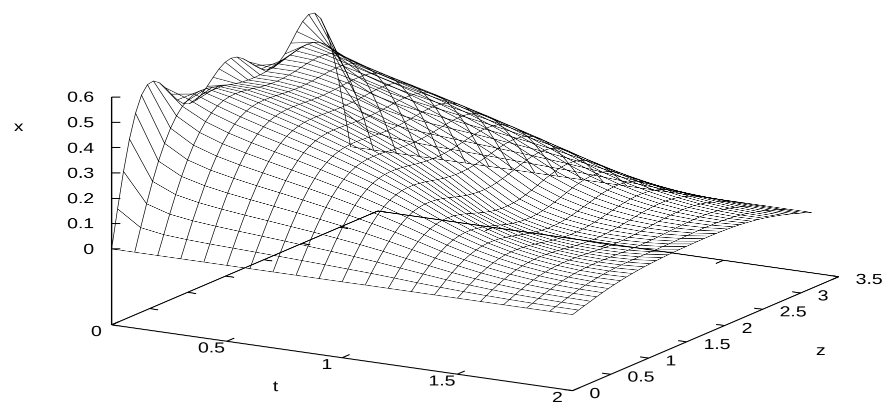
Available control actuators:

- Distributed actuator: $b_1(z) = H(z - 0.1l) - H(z - 0.5l)$.
- Point actuator: $b_2(z) = \delta(z - 0.3l)$.
- Distributed actuator: $b_3(z) = 1$.

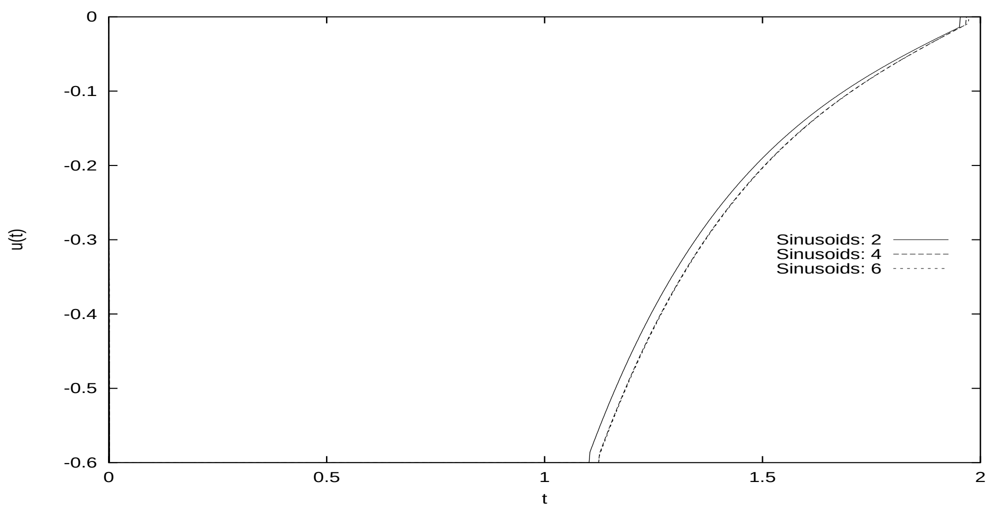
OPTIMIZATION RESULTS

Nominal conditions, sinusoidal basis functions

Spatiotemporal profile of solution ($N = 4$).



Design variable profile.



- Alternative approach to basis function construction?

OPTIMIZATION METHODOLOGY

- Spatial discretization:
  - ◇ Form an ensemble of solutions of the PDE system for different time profiles of the design variables.
    - ▷ Construction of a representative ensemble.
  - ◇ Apply Karhunen–Loève expansion to derive empirical eigenfunctions.
  - ◇ Discretization through Galerkin's method with empirical eigenfunctions.
    - ▷ Low-dimensional approximate ODE systems.
- Temporal discretization:
  - ◇ Finite-differences.
- Solution of reduced optimization problem:
  - ◇ Reduced gradient methods.
- Application to a diffusion-reaction process.

COMPUTATION OF EMPIRICAL EIGENFUNCTIONS USING PROCESS DATA

- Construction of an N-dimensional ensemble of solutions x_i.
  - ◇ Different initial conditions.
  - ◇ Excitation of system through variation of design variables.

- Karhunen-Loève expansion.
  - ◇ Calculation of C_i matrices: $C_i^{lm} = (x_i^l, x_i^m)$
    x_i^l: l-th snapshot of the i-th variable
  - ◇ Calculation of eigenvectors: $C_i A_{ik} = \lambda_{ik} A_{ik}$

    A_{ik}: k-th eigenvector, λ_{ik}: k-th eigenvalue (k=1,...,N)

  - ◇ Calculation of empirical eigenfunctions: $\phi_{ik} = \sum_{j=1}^{N} a_{ik}^j x_i^j$

    α_{ik}^j: j-th element of A_{ik}

COMPUTATION OF EMPIRICAL EIGENFUNCTIONS

- Non-dimensionalized process dynamic model:

$$\frac{1}{t_f}\frac{\partial x}{\partial \tau} = \frac{1}{l^2}\frac{\partial}{\partial \zeta}(k(\zeta)\frac{\partial x}{\partial \zeta}) + \beta_T(\zeta)(e^{-\dfrac{\gamma}{1+x}} - e^{-\gamma}) + \beta_U(b(\zeta)u(\tau) - x)$$

$$x(0,\tau) = 0, \quad x(1,\tau) = 0, \quad x(\zeta,0) = x_0(\zeta)$$

- Construction of ensemble in space:

Set 1

◇ 2 different initial conditions.

◇ 6 t-profiles × 1 design variable.

◇ 296 snapshots.

Set 2

◇ 2 different initial conditions.

◇ 6 t-profiles × 3 design variables.

◇ 1554 snapshots.

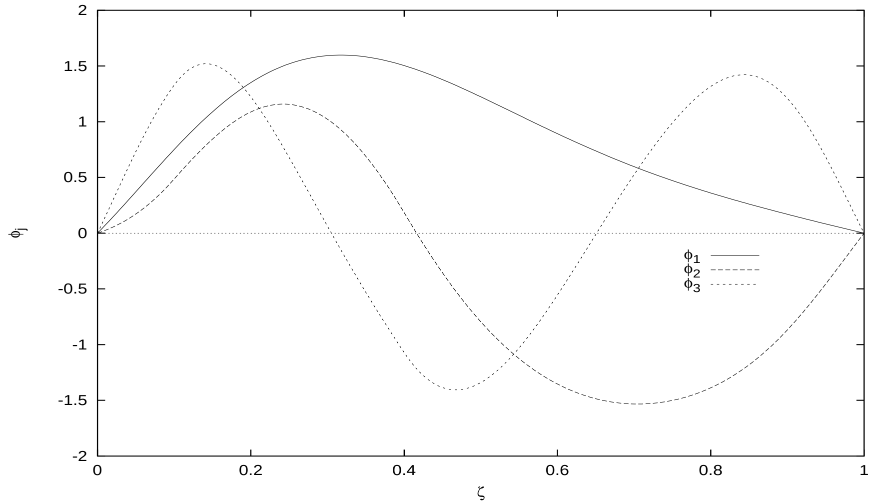
- Karhunen-Loève expansion:

◇ Eight empirical eigenfunctions.

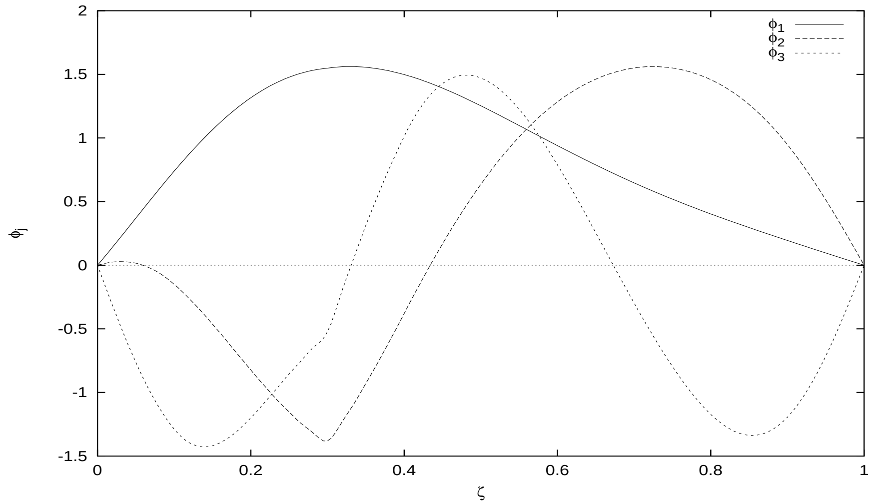
◇ Nine empirical eigenfunctions.

EMPIRICAL EIGENFUNCTIONS

First three empirical eigenfunctions (one actuator).



First three empirical eigenfunctions (three actuators).



REDUCED OPTIMIZATION PROBLEM

- Nondimensionalized spatial domain $\zeta = \dfrac{z}{l}$

- Applying Galerkin's method with N basis functions.

$$\min\left(\int_0^{t_f}\int_0^1 w_s(\sum_{i=1}^{N} a_i(t)\phi_i(\zeta))^2 + w_u u^2(t)d\zeta dt\right)$$

$$s.t.$$

$$\frac{da_i}{dt} = \sum_{j=1}^{N}\alpha_j\int_0^1 \frac{1}{l}\frac{d}{d\zeta}\frac{k(\zeta)}{l}\frac{d\phi_j(\zeta)}{d\zeta}\phi_i(\zeta)d\zeta - \beta_U a_i + \beta_U\int_0^1 \bar{u}\phi_i(\zeta)$$

$$+\int_0^1 \beta_T\left(exp(-\gamma(\sum_{j=1}^{N}\alpha_j\phi_j(\zeta)+1)^{-1}) - exp(-\gamma)\right)d\zeta,\ i = 1, ..., N$$

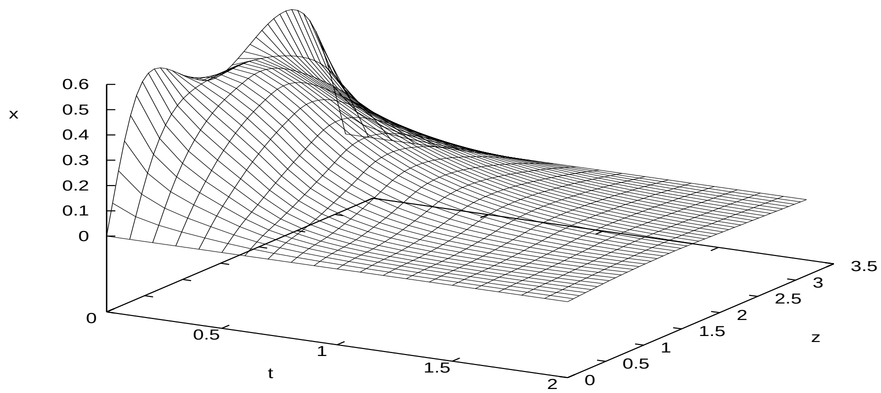
$$\|u(t)\| \leq 0.6, \qquad \forall t \in [0, t_f]$$

- Temporal discretization using finite differences.

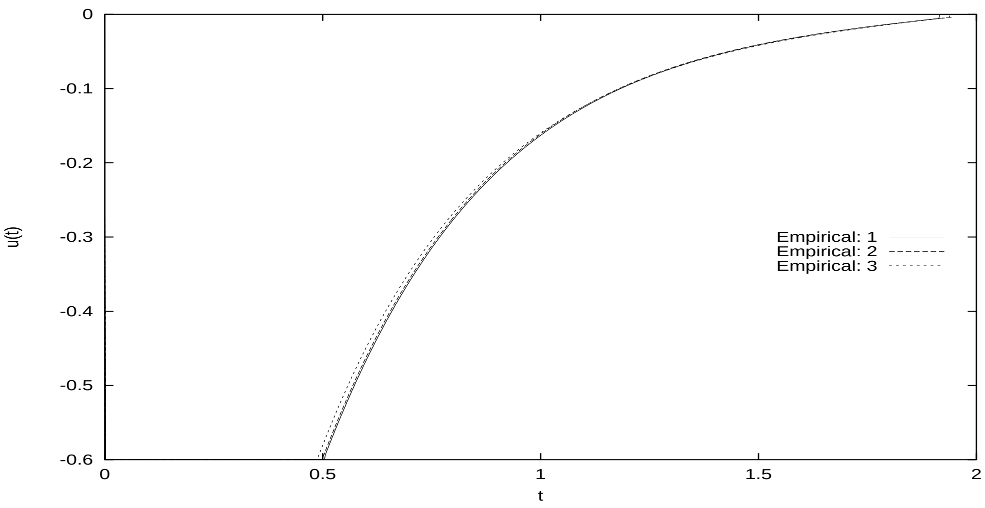
OPTIMIZATION RESULTS

Nominal conditions, Set 1, actuator $b_1(z)$

Spatiotemporal profile of solution ($N = 3$).



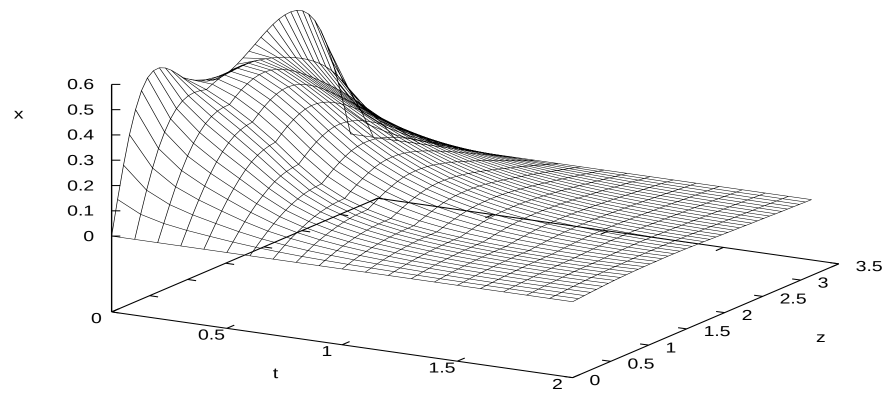
Independent variable profile.



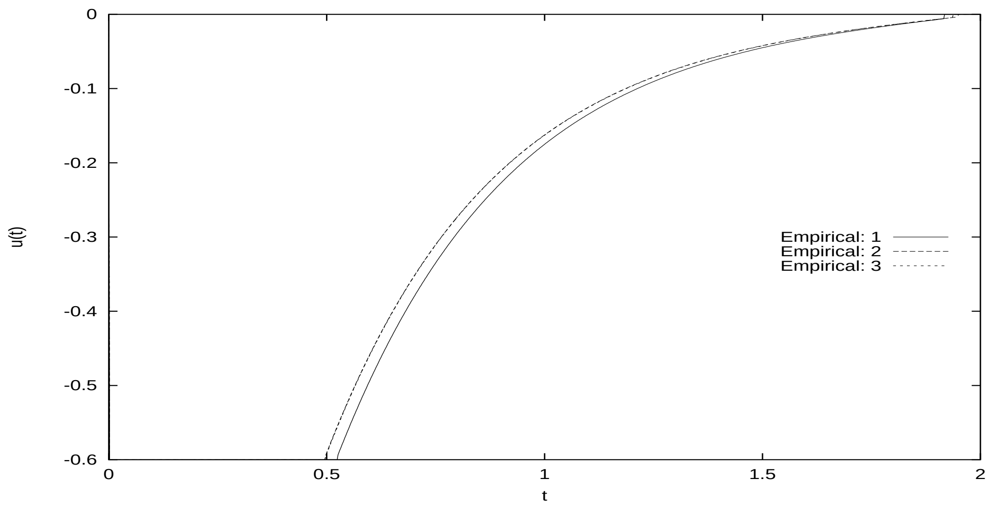
OPTIMIZATION RESULTS

Nominal conditions, Set 2, actuator $b_1(z)$

Spatiotemporal profile of solution ($N = 3$).



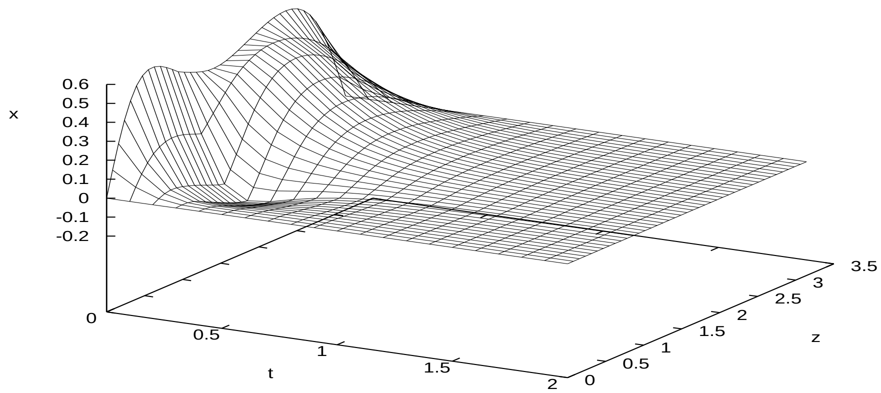
Design variable profile.



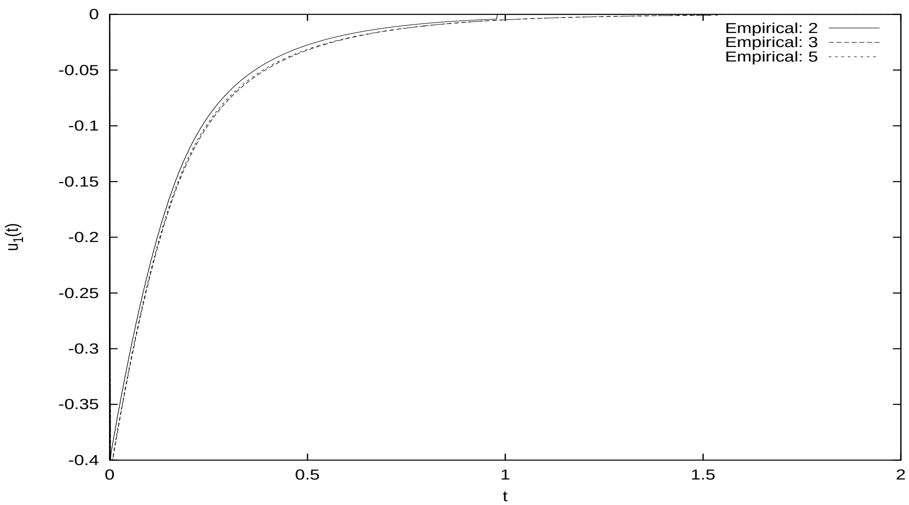
OPTIMIZATION RESULTS

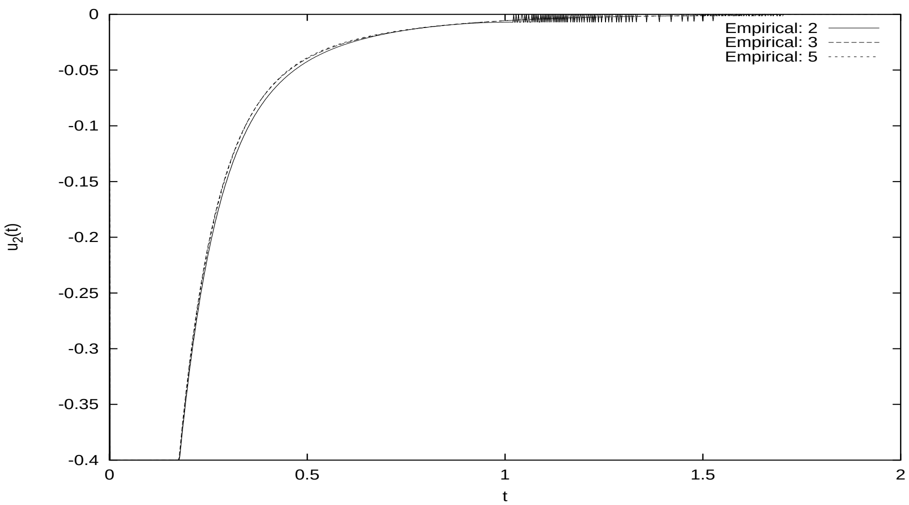
Nominal, Set 2, actuators $b_1(\zeta)$ (distributed), $b_2(\zeta)$ (point)

Spatiotemporal profile of solution ($N = 3$).



Design variable profile.

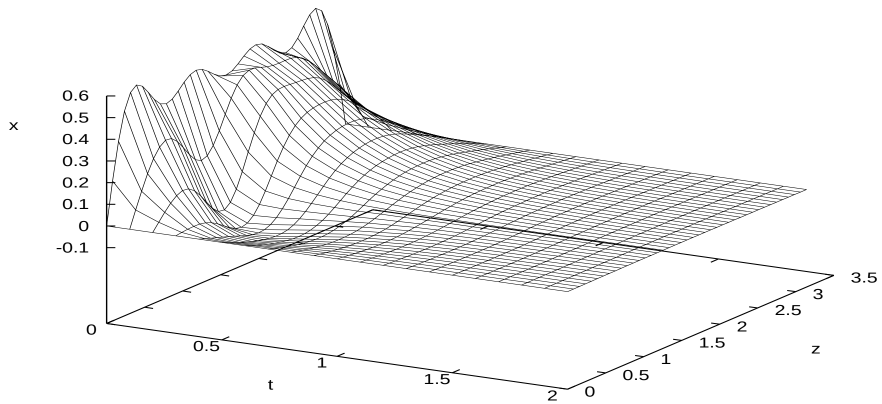




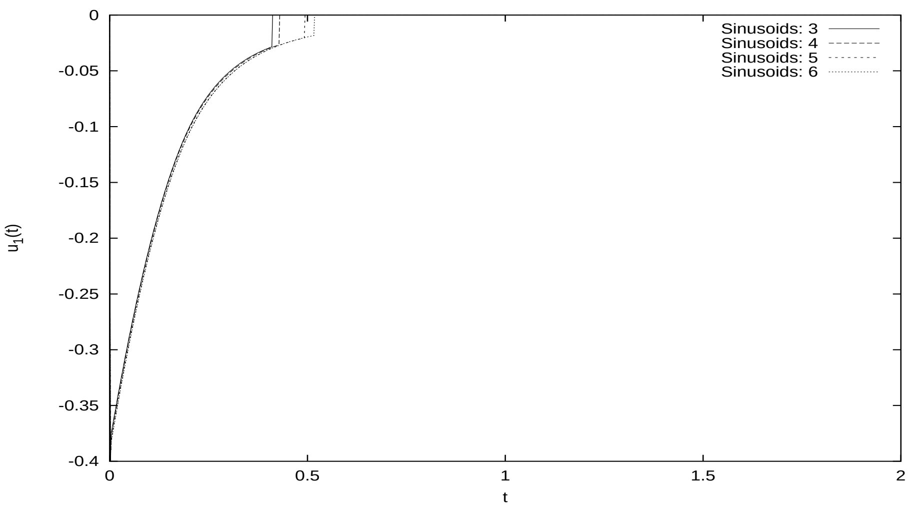
OPTIMIZATION RESULTS

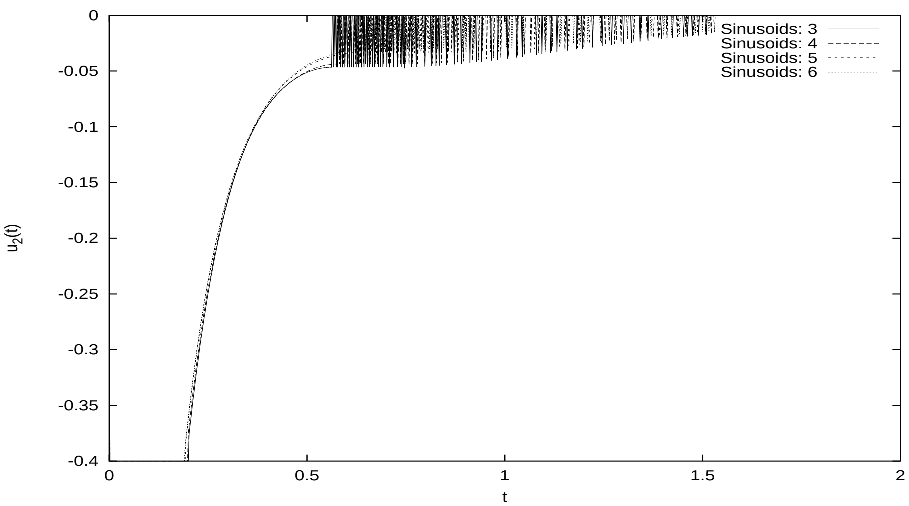
Nominal, sinusoid basis, actuators $b_1(\zeta)$ (distributed), $b_2(\zeta)$ (point)

Spatiotemporal profile of solution ($N = 8$).



Design variable profiles.





- Stiffness problems preclude further order increase.

TWO-TIME-SCALE BEHAVIOR OF MODAL EQUATIONS

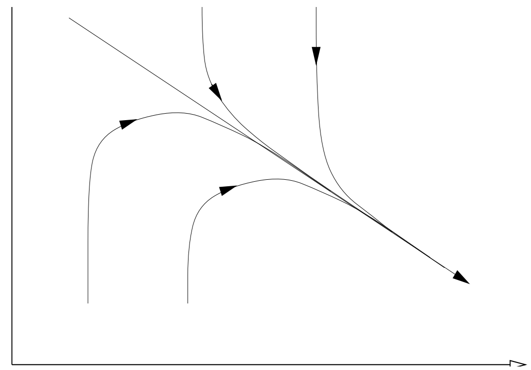
- Finite-dimensional dynamic nonlinear program.

$$min \int_0^{t_f} G(a_N, d)dt$$

$$\dot{a}_N = \tilde{f}(a_N, d)$$

$$\tilde{g}(a_N, d) \leq 0$$

- Pictorial representation of fast and slow motions of modal equations.



TWO-TIME-SCALE BEHAVIOR OF MODAL EQUATIONS

- a_N modes can be decomposed into coupled fast (a_f) and slow (a_s) modes.

$$min \int_0^{t_f} G(a_s, a_f, d)dt$$

$$\dot{a}_s = \tilde{f}_s(a_s, a_f, d)$$

$$\dot{a}_f = \tilde{f}_f(a_s, a_f, d)$$

$$\tilde{g}(a_s, a_f, d) \leq 0$$

- $\dot{a}_f = 0$ - reduced-order dynamic nonlinear program.

$$min \int_0^{t_f} G(a_s, a_f, d)dt$$

$$\dot{a}_s = \tilde{f}_s(a_s, a_f, d)$$

$$0 = \tilde{f}_f(a_s, a_f, d)$$

$$\tilde{g}(a_s, a_f, d) \leq 0$$

- Justification within the framework of approximate inertial manifolds.

FAST AND SLOW DYNAMIC NONLINEAR PROGRAMS

- Dynamic nonlinear program at fast time-scale.

$$min \int_0^{\tau_f} G(a_s(0), a_f(t), d)dt$$

$$\dot{a}_f = \tilde{f}_f(a_s(0), a_f(t), d)$$

$$\tilde{g}(a_s(0), a_f(t), d) \leq 0$$

- Dynamic nonlinear program at slow time-scale.

$$min \int_0^{t_f} G(a_s, a_f, d)dt$$

$$\dot{a}_s = \tilde{f}_s(a_s, a_f, d)$$

$$0 = \tilde{f}_f(a_s, a_f, d)$$

$$\tilde{g}(a_s, a_f, d) \leq 0$$

KURAMOTO-SIVASHINSKY EQUATION

- Mathematical description:

$$\frac{\partial U}{\partial t} = -\nu \frac{\partial^4 U}{\partial z^4} - \frac{\partial^2 U}{\partial z^2} - U \frac{\partial U}{\partial z} + \sum_{i=1}^{l} b_i(z) u_i(t)$$

- Initial conditions:

$$\text{Case 1:} \quad U(z,0) = U_{0,1} = \sum_{j=1}^{4} sin(j\ z)$$

$$\text{Case 2:} \quad U(z,0) = U_{0,2} = 0.5 \sum_{j=1}^{3} sin(j\ z) + 1.5 \sum_{j=4}^{6} sin(j\ z)$$

- Boundary conditions:

$$\frac{\partial^j U}{\partial z^j}(-\pi, t) = \frac{\partial^j U}{\partial z^j}(+\pi, t), \quad j = 0, \ldots, 3$$

◇ For $\nu = 0.12$, $U(z,t) = 0$ is unstable.

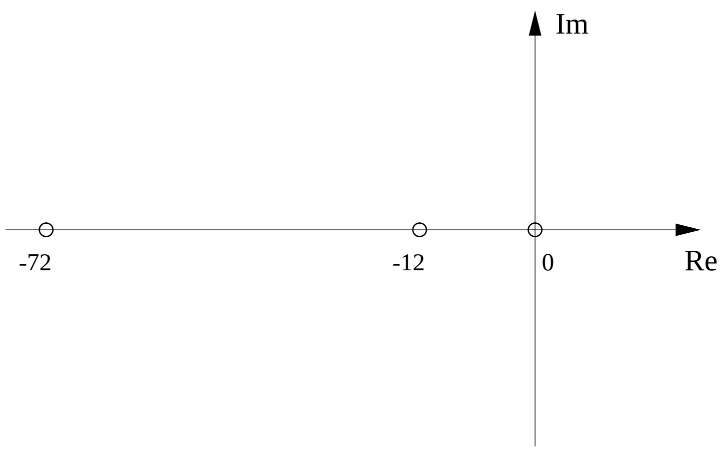
EIGENSPECTRUM / OPEN-LOOP DYNAMICS

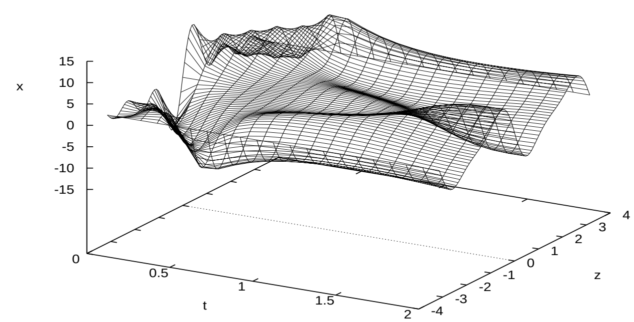
- Eigenvalue problem:

$$\mathcal{A}\phi_j \;=\; -\nu\frac{\partial^4\phi_j}{\partial z^4} - \frac{\partial^2\phi_j}{\partial z^2} \;=\; \lambda_j\phi_j$$

$$\frac{\partial^j\phi_j}{\partial z^j}(-\pi,t) = \frac{\partial^j\phi_j}{\partial z^j}(+\pi,t)\,, \quad j = 0,\ldots,3$$

- $\begin{array}{rl} \text{Eigenvalues:} & \lambda_j = -\nu j^4 + j^2 \\ \text{Eigenfunctions:} & \phi_j(z) = sin(j\ z) \end{array}$ $, \; j = 1,\ldots,\infty$:





$(\nu = 1)$ $(\nu = 0.12)$

Open-loop spatio-temporal profile of $U(z,t)$.

REDUCED OPTIMIZATION PROBLEM

- Applying Galerkin's method with N analytical eigenfunctions using an N'-dimensional AIM.

$$min\left(\int_0^{t_f}\int_0^{\pi} w_s(\sum_{i=1}^{6} a_i(t)\phi_i(z))^2 + w_u u^2(t)dzdt\right)$$

$$s.t.$$

$$\frac{da_i}{dt} = \lambda_i a_i + \sum_{j=1}^{N+N'}\sum_{k=1}^{N+N'} \alpha_j\alpha_k \int_{-\pi}^{\pi}\phi_j(z)\frac{d\phi_k(z)}{dz}\phi_i(z)dz + \sum_{j=1}^{l} u_j(t)\int_{-\pi}^{\pi} b_j(z)\phi_i(z)\,dz,$$

$$i = 1, ..., N$$

$$0 = \lambda_i a_i + \sum_{j=1}^{N+N'}\sum_{k=1}^{N+N'} \alpha_j\alpha_k \int_{-\pi}^{\pi}\phi_j(z)\frac{d\phi_k(z)}{dz}\phi_i(z)dz + \sum_{j=1}^{l} u_j(t)\int_{-\pi}^{\pi} b_j(z)\phi_i(z)\,dz,$$

$$i = N+1, ..., N'$$

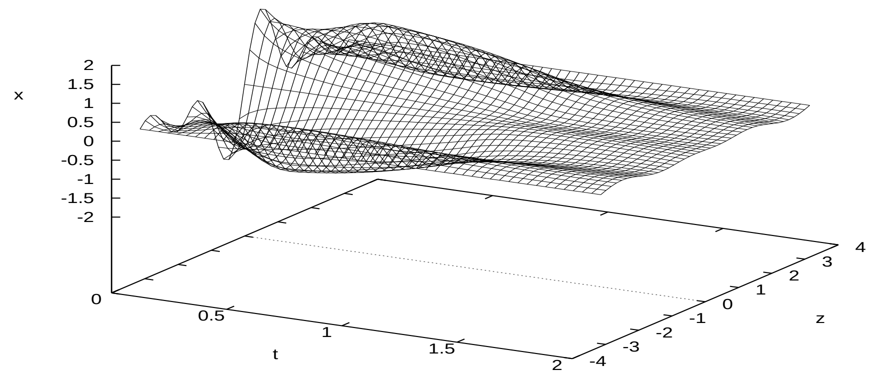
$$b_1(z) = \delta(z-0.5\pi),\;\; b_2(z) = \delta(z+0.5\pi),\quad \|u(t)\| \leq 3.0,\qquad \forall t \in [0, t_f]$$

- Temporal discretization using finite differences.

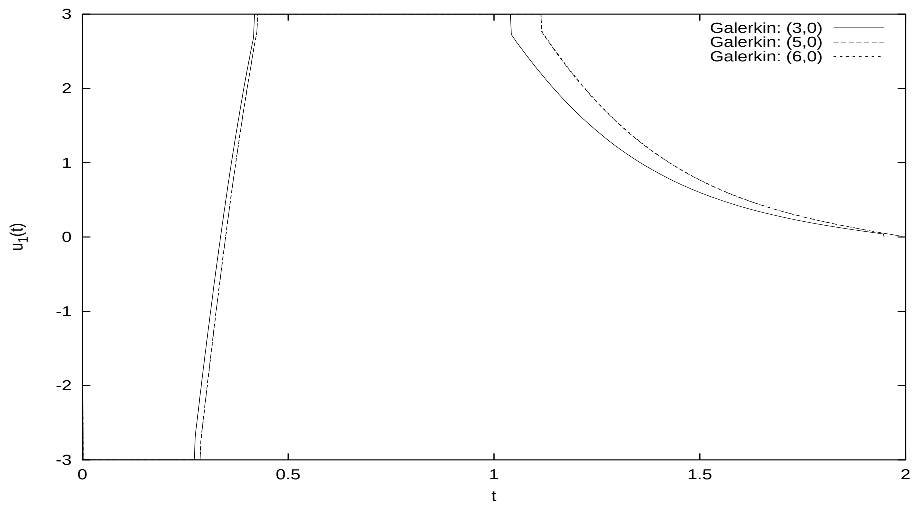
OPTIMIZATION RESULTS

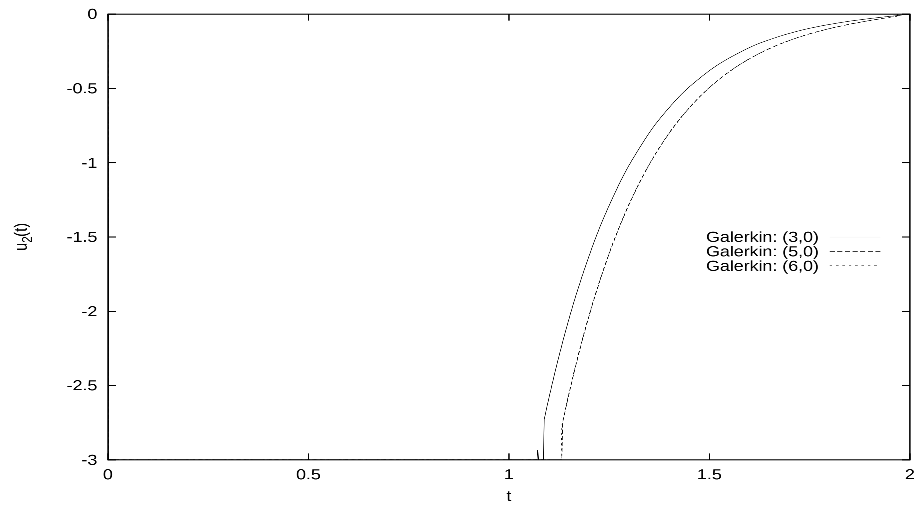
Nominal, $U_{0,1}$, linear Galerkin (N'=0)

Spatiotemporal profile of solution ($N = 6$).



Design variable profile.

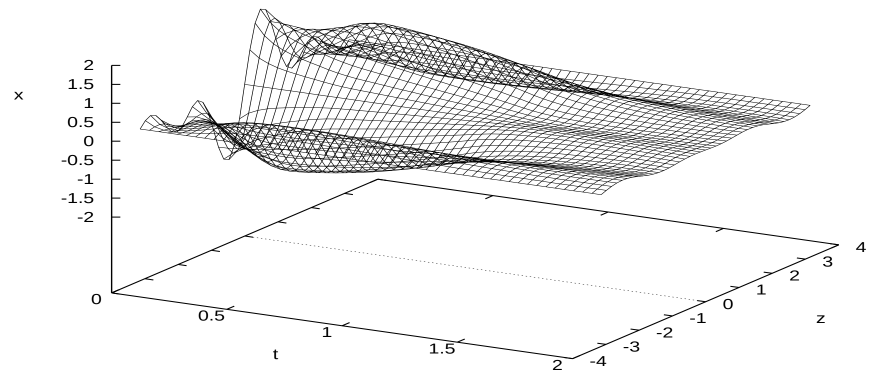




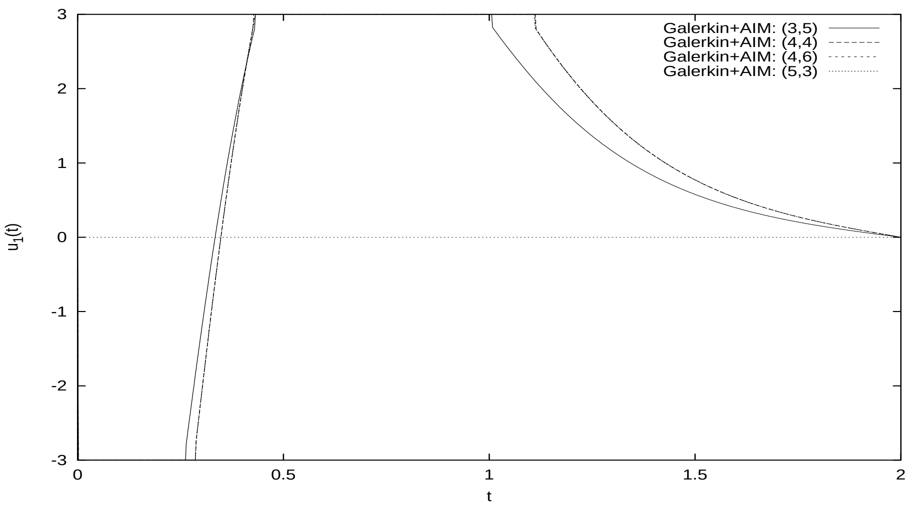
OPTIMIZATION RESULTS

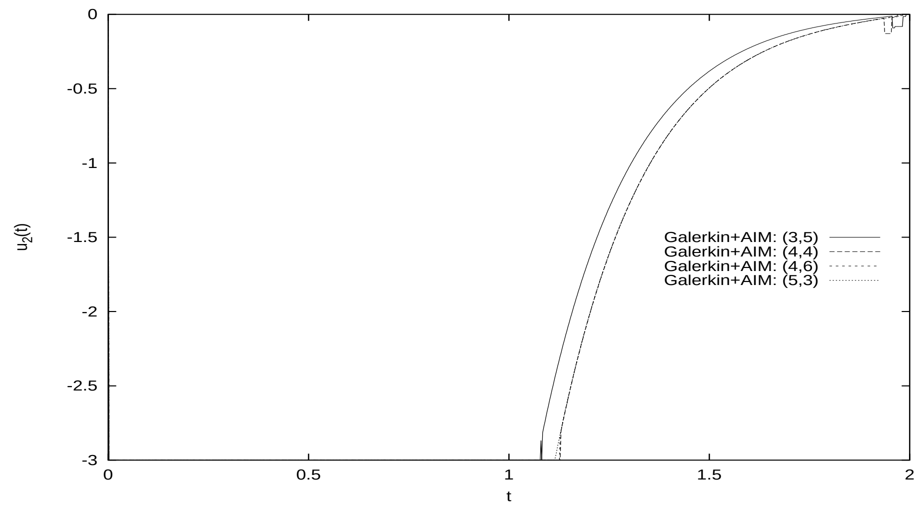
Nominal, $U_{0,1}$, combination Galerkin AIM

Spatiotemporal profile of solution ($N = 5, N' = 3$).



Independent variable profile.

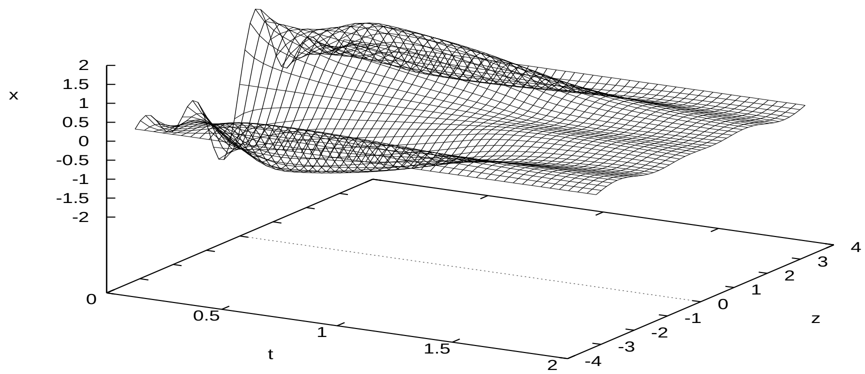




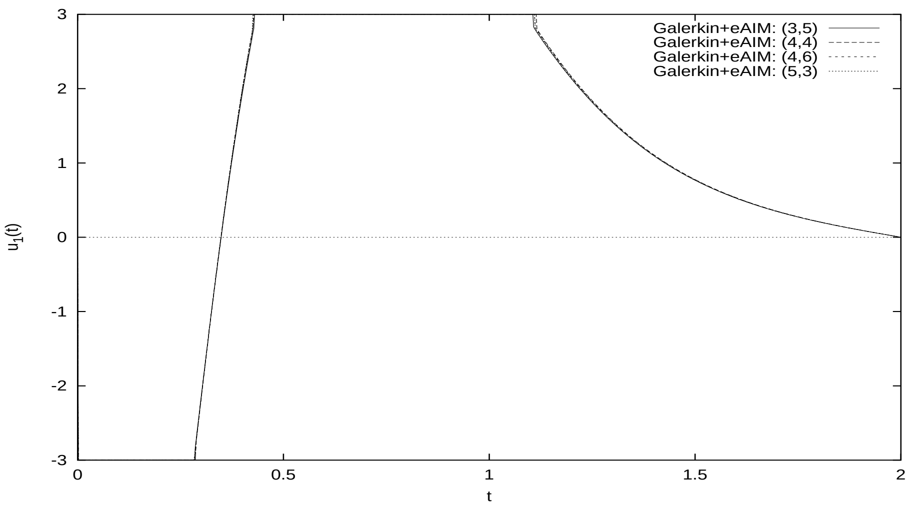
OPTIMIZATION RESULTS

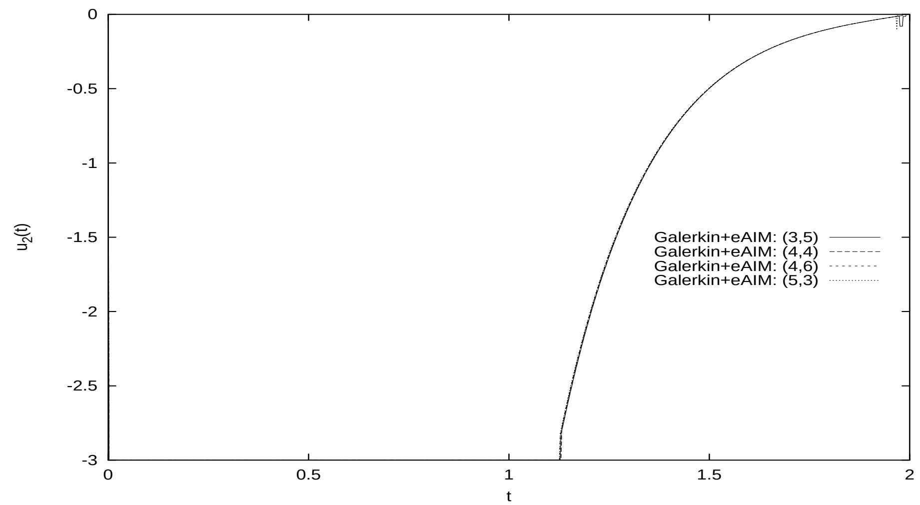
Nominal, $U_{0,1}$, combination Galerkin eAIM

Spatiotemporal profile of solution ($N = 5, N' = 3$).



Design variable profile.

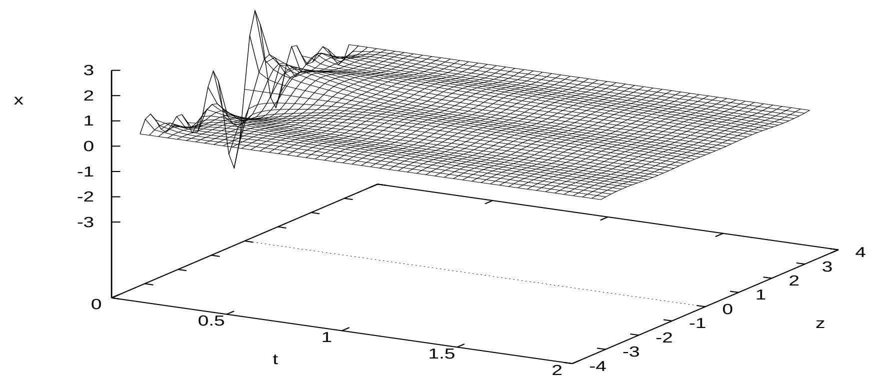




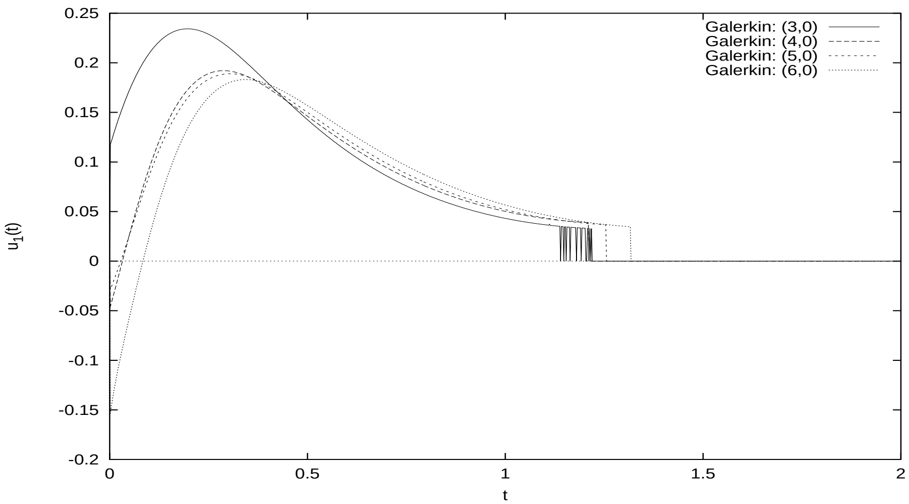
OPTIMIZATION RESULTS

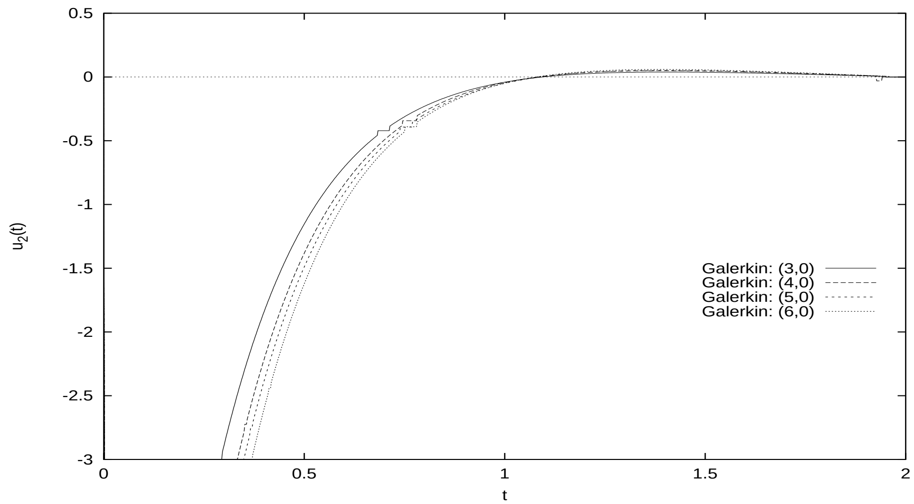
Nominal, $U_{0,2}$, linear Galerkin (N'=0)

Spatiotemporal profile of solution ($N = 6$).



Design variable profile.

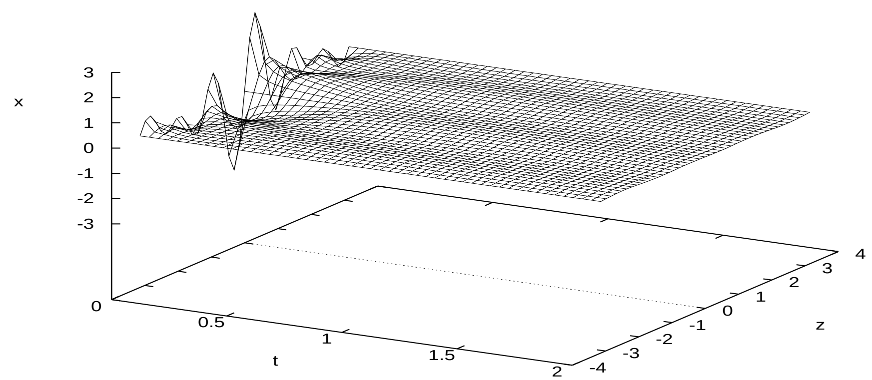




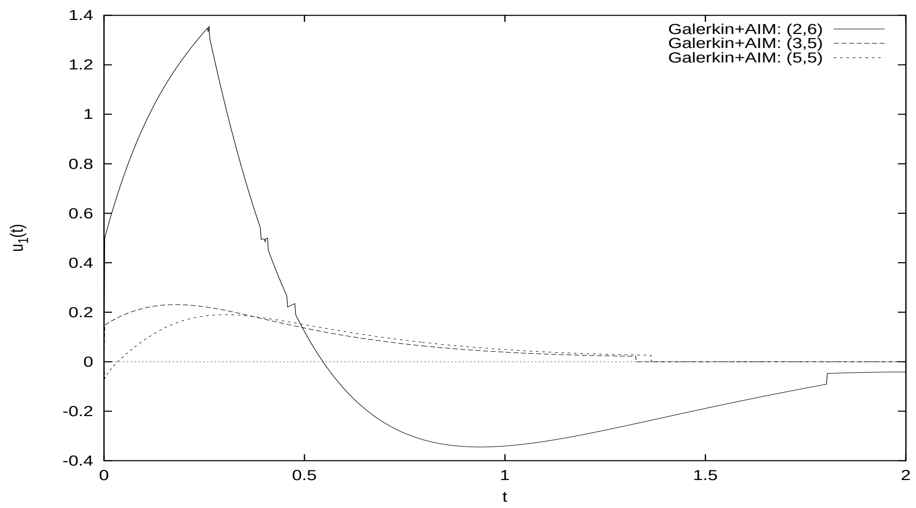
OPTIMIZATION RESULTS

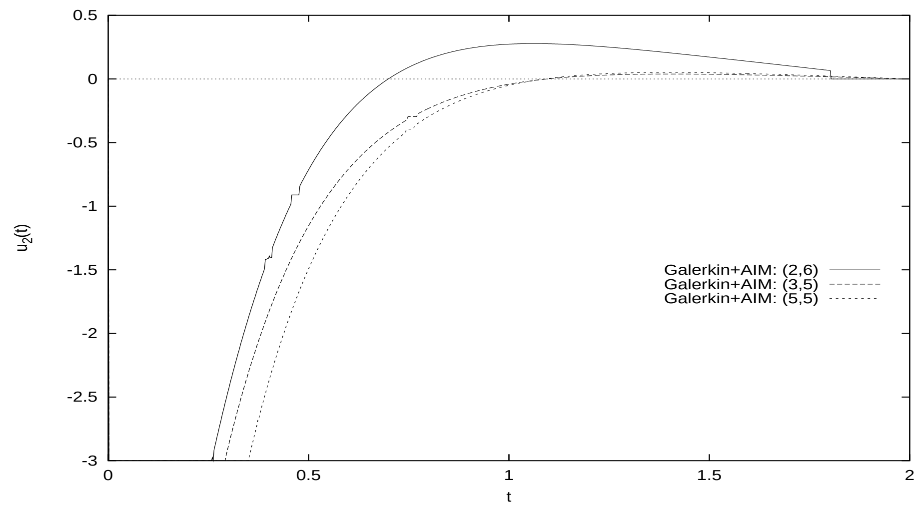
Nominal, $U_{0,2}$, combination Galerkin AIM

Spatiotemporal profile of solution ($N = 5, N' = 5$).



Design variable profile.

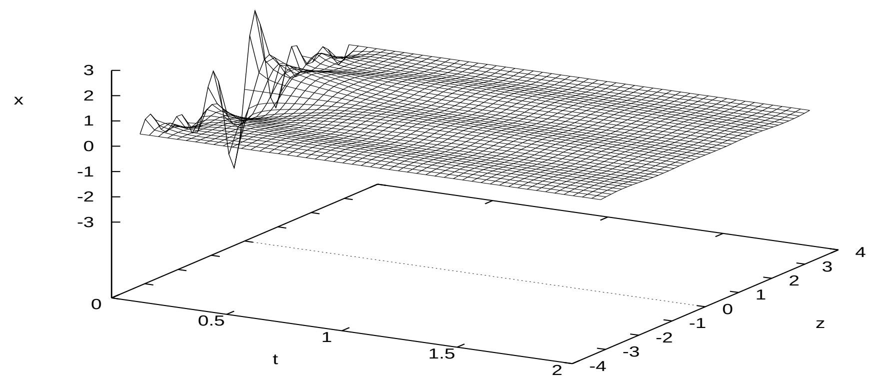




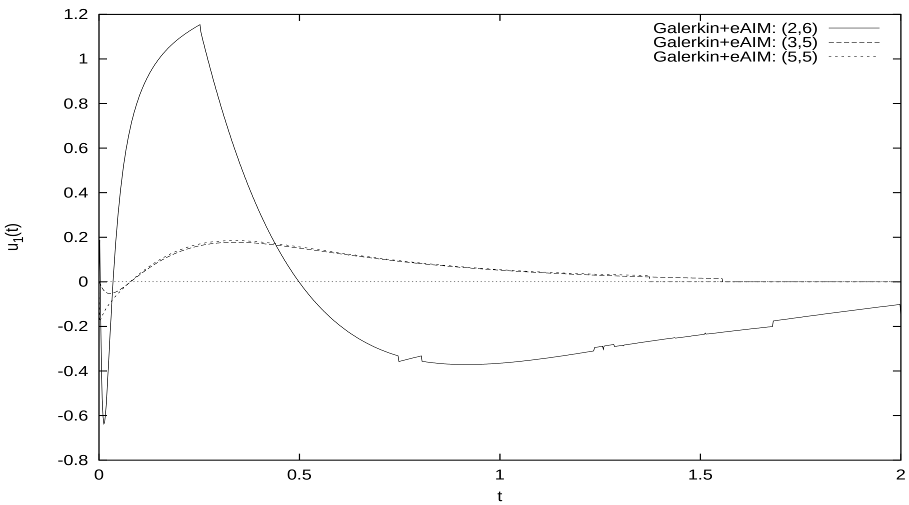
OPTIMIZATION RESULTS

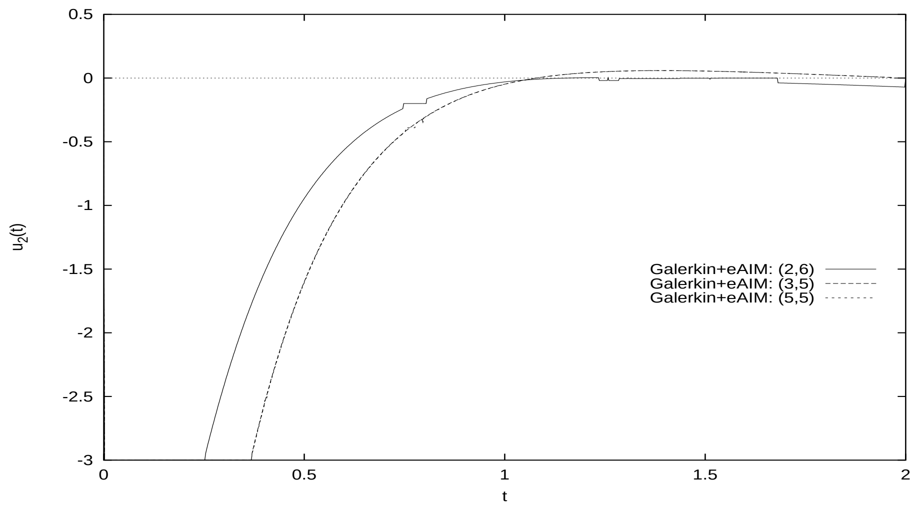
Nominal, $U_{0,2}$, combination Galerkin eAIM

Spatiotemporal profile of solution ($N = 5, N' = 5$).



Design variable profile.





CONCLUSIONS

- Computationally-efficient methods for the solution of dynamic optimization problems arising in systems modeled by highly dissipative PDEs.
  - ◇ Analytical eigenfunctions / off-the-shelf sets of basis functions.
  - ◇ Empirical eigenfunctions derived via Karhunen-Loève expansion.
  - ◇ Approximate inertial manifolds.
- Applications:
  - ◇ Diffusion-reaction processes.
  - ◇ Kuramoto-Sivashinsky equation.

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