A Comparative Study of Galerkin and Mixed Galerkin Methods in Optimal Control Problems with Applications to Semiconductor Modeling

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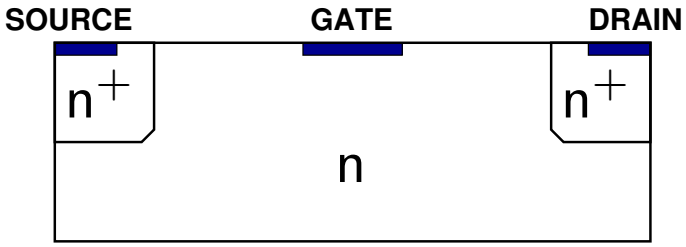
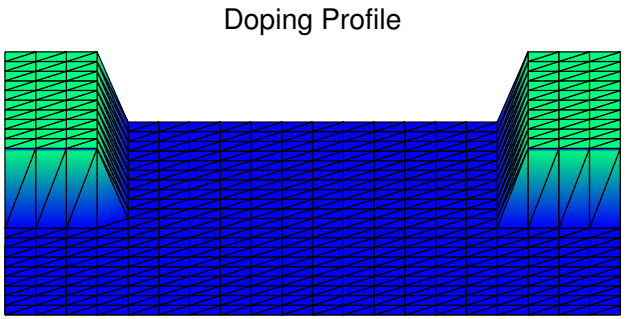
Outline

- Introduction: Motivation and Problem Statement
- Survey of Discretization Techniques
- The Discrete Problem: Galerkin vs. Mixed Galerkin
- Numerical Results
- Conclusion

Motivation

- **How does the choice of the finite element discretization affect the solution of PDE–constrained optimization problems arising in the control and design of semiconductor devices?**
- collaboration with the *Charon* project (Sandia National Labs): modeling of electrical semiconductor devices at high fidelities; in addition to simulation, Charon enables the solution of related parameter estimation, optimal design, and inverse problems





Example Problems:

- increase the current flow over a contact by tweaking the doping profile
- determine the doping profile based on a profile measurement and the corresponding (experimental) current data

Problem Statement

$$\text{minimize} \quad \mathcal{J} = \frac{1}{2}\|J(x)\cdot\nu - \widehat{J}(x)\cdot\nu\|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2}\|(u(x)-\widehat{u}(x)\|^2_{0,\Omega}$$

subject to

$$\left.\begin{aligned} J_n(x) &= \mu_n(\nabla n(x) + n(x)\nabla y(x)) \\ J_p(x) &= \mu_p(\nabla p(x) - p(x)\nabla y(x)) \\ \nabla\cdot J_n(x) &= 0 \\ \nabla\cdot J_p(x) &= 0 \\ -\nabla\cdot(k(x)\nabla y(x)) &= n(x) - p(x) - u(x), \end{aligned}\right\} \text{DRIFT–DIFFUSION}$$

where y is the electrostatic potential, n and p are electron and hole densities, u is the doping profile, μ_n and μ_p are electron and hole mobilities, k is the permittivity, and the total current density is given by

$$J(x) = J_n(x) + J_p(x).$$

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Survey

Discretization of the Drift–Diffusion Equations

- primal Galerkin FE schemes with streamline or flux upwinding (SUPG – Hughes, Brooks; FUPG – Carey, Sharma)
- mixed and hybrid FE methods with exponential fitting (Brezzi, Marini, Pietra; Holst, Jüngel, Pietra)
- exponentially fitted triangular and tetrahedral FE methods (Wang, Miller, Angermann)

- finite volume / covolume methods, e.g. the *box method* with Scharfetter–Gummel upwinding (McCartin, Bank et al., Mock)

Survey

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Optimization

- while the discretization of the D–D equations is fairly well studied, there are virtually no studies on the impact of the discretization on the solution of the PDE–constrained optimization problem
- one example: study of the SUPG method in discretize-then-optimize vs. optimize-then-discretize (Collis and Heinkenschloss)

- numerical study of Galerkin versus mixed Galerkin discretizations

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Simplified Model Problem

$$\text{minimize} \quad \mathcal{J} = \frac{1}{2}\|J(x)\cdot\nu - \widehat{J}(x)\cdot\nu\|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2}\|(u(x) - \widehat{u}(x)\|^2_{0,\Omega}$$

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Simplified Model Problem

minimize $\mathcal{J} = \frac{1}{2}\|\nabla y(x)\cdot\nu - \nabla\widehat{y}(x)\cdot\nu\|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2}\|(u(x)-\widehat{u}(x)\|^2_{0,\Omega}$

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\end{aligned}
$$

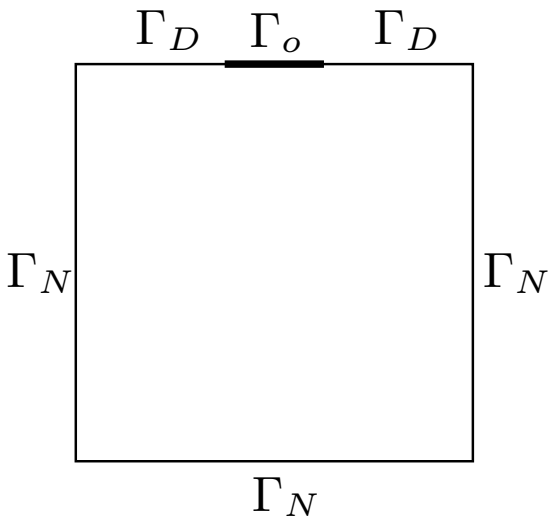
$$J \to \nabla y$$

Simplified Model Problem

minimize $\mathcal{J} = \frac{1}{2}\|\nabla y(x)\cdot\nu - \nabla\widehat{y}(x)\cdot\nu\|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2}\|(u(x)-\widehat{u}(x)\|^2_{0,\Omega}$

subject to

$$
\begin{aligned}
-\nabla\cdot(k(x)\nabla y(x)) &= f(x)+u(x) && \text{in } \Omega\\
y(x) &= y_D(x) && \text{on } \Gamma_D\\
(k(x)\nabla y(x))\cdot\nu &= g(x) && \text{on } \Gamma_N
\end{aligned}
$$



Galerkin Discretization

- state and control spaces

$$Y = \left\{ y \in H^1(\Omega) \ : \ y = y_D \text{ on } \Gamma_D \right\}, \quad U = L^2(\Omega)$$

- test function space

$$V = \left\{ v \in H^1(\Omega) \ : \ v = 0 \text{ on } \Gamma_D \right\}$$

- (bi)linear forms

$$a(y,v) = \int_\Omega k \nabla y \cdot \nabla v \, dx, \qquad b(u,v) = -\int_\Omega uv \, dx,$$
$$\langle f, v \rangle = \int_\Omega f v \, dx, \qquad \langle g, v \rangle_{\Gamma_N} = \int_{\Gamma_N} g v \, dx$$

- **Weak form**: Find $y \in Y, u \in U$, which solve, *for all* $v \in V$

minimize $\frac{1}{2} \| \nabla y(x) \cdot \nu - \nabla \widehat{y}(x) \cdot \nu \|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2} \| (u(x) - \widehat{u}(x) \|^2_{0,\Omega}$

subject to

$$a(y,v) + b(u,v) = \langle f, v \rangle + \langle g, v \rangle_{\Gamma_N}.$$

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subject to

$$a(y,v) + b(u,v) = \langle f, v \rangle + \langle g, v \rangle_{\Gamma_N}.$$

Galerkin Discretization

Flux Term: $\|\nabla y(x)\cdot\nu - \nabla\widehat{y}(x)\cdot\nu\|^2_{-1/2,\Gamma_o}$

- **Standard approach.** Restrict the states to a finite element subspace Y_h, compute terms $\nabla y_h \cdot \nu$ directly, and use a weighted L^2 norm to approximate the norm on $H^{-1/2}(\Gamma_o)$:

$$\|\nabla y\cdot\nu - \nabla\widehat{y}\cdot\nu\|^2_{-1/2,\Gamma_o} \approx h\|\nabla y_h\cdot\nu - \nabla\widehat{y}_h\cdot\nu\|^2_{0,\Gamma_o}$$

- **Better choice: Variational Flux Approximation (VFA).** Replace flux $\nabla y_h \cdot \nu$ by a more accurate, C^0 approximation λ_h, obtained by solving the equation

$$\int_{\Gamma_0} \lambda_h v_h \, dl = k^{-1}\left(a(y_h, v_h) + b(u_h, v_h) - (f, v_h) - \int_{\Gamma\setminus\Gamma_o} k\nabla y_h\cdot\nu v_h \, dl\right)$$

then approximate the flux term as follows:

$$\|\nabla y\cdot\nu - \nabla\widehat{y}\cdot\nu\|^2_{-1/2,\Gamma_o} \approx h\|\lambda_h - \widehat{\lambda}_h\|^2_{0,\Gamma_o}$$

Galerkin Discretization

Variational Flux Approximation

$$\int_{\Gamma_0} \lambda_h v_h \, dl = k^{-1} \left(a(y_h, v_h) + b(u_h, v_h) - (f, v_h) - \int_{\Gamma \setminus \Gamma_o} k \nabla y_h \cdot \nu v_h \, dl \right)$$

- PDEs: Wheeler, Babuška, Brezzi, Hughes, etc.
  When used to postprocess a given finite element solution (y_h, u_h), the right hand side above involves only known quantities.
- Optimal control (to date): Berggren, et al. (Thanks!)
  VFA is used in an already defined optimality system to improve the accuracy of the solution.
- Our case, NEW use of VFA:
  VFA *changes* the optimization problem, because the discretization

  $$\|\nabla y \cdot \nu - \nabla \widehat{y} \cdot \nu\|^2_{-1/2,\Gamma_o} \approx h \|\lambda_h - \widehat{\lambda}_h\|^2_{0,\Gamma_o},$$

  where λ_h is given above, is a function of *both* the unknown states y_h and the unknown controls u_h!

Mixed Galerkin Discretization

- consider the Poisson equation as a first–order system:
  Given $u \in L^2(\Omega)$, $f \in L^2(\Omega)$, $g \in L^2(\Gamma_N)$, and $y_d \in H^1(\Omega) \cap C(\overline{\Omega})$, seek $y \in L^2(\Omega)$ and $p \in \left[L^2(\Omega)\right]^2$, with $\nabla \cdot p \in L^2(\Omega)$, satisfying

$$
\begin{aligned}
\nabla \cdot p + u &= -f && \text{in } \Omega \\
k^{-1}\, p - \nabla y &= 0 && \text{in } \Omega \\
y &= y_D && \text{on } \Gamma_D \\
(k \nabla y) \cdot \nu &= g && \text{on } \Gamma_N.
\end{aligned}
$$

- for the weak form, we introduce the spaces

$$
\begin{aligned}
H(\text{div}, \Omega) &= \left\{ q \in \left[L^2(\Omega)\right]^2 : \nabla \cdot q \in L^2(\Omega) \right\}, \\
H_{0,N}(\text{div}, \Omega) &= \left\{ q \in H(\text{div}, \Omega) : q \cdot \nu = 0 \text{ on } \Gamma_N \right\}, \\
H_{g,N}(\text{div}, \Omega) &= \left\{ q \in H(\text{div}, \Omega) : (k\, q) \cdot \nu = g \text{ on } \Gamma_N \right\}.
\end{aligned}
$$

Mixed Galerkin Discretization

- state spaces $Y = L^2(\Omega)$ and $P = H_{g,N}(\text{div}, \Omega)$
- control space $U = L^2(\Omega)$
- test function spaces $V = L^2(\Omega)$ and $Q = H_{0,N}(\text{div}, \Omega)$
- (bi)linear forms

$$a(p,q) = \int_\Omega \frac{1}{k}\, p \cdot q \, dx, \qquad b(q,y) = \int_\Omega (\nabla \cdot q) y \, dx, \qquad c(u,v) = \int_\Omega uv \, dx,$$

$$\langle f, v \rangle = \int_\Omega f v \, dx, \qquad \langle y_d, q \cdot \nu \rangle_{\Gamma_D} = \int_{\Gamma_D} y_D \, q \cdot \nu \, dx$$

- **Weak form**: Find $(y,p) \in Y \times P$, and $u \in U$, which solve, *for all* $q \in Q$ *and all* $v \in V$, the problem

$$\text{minimize} \quad \frac{1}{2} \| k^{-2} (p \cdot \nu - \widehat{p} \cdot \nu) \|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2} \| u - \widehat{u} \|^2_{0,\Omega}$$

subject to

$$a(p,q) + b(q,y) = \langle y_d, q \cdot \nu \rangle_{\Gamma_D}$$
$$b(p,v) + c(u,v) = -\langle f, v \rangle .$$

Mixed Galerkin Discretization

Flux Term: $\|k^{-2}(p \cdot \nu - \widehat{p} \cdot \nu)\|^2_{-1/2,\Gamma_o}$

- **Direct approximation.** The flux is approximated directly by p_h:

$$\|k^{-2}(p \cdot \nu - \widehat{p} \cdot \nu)\|^2_{-1/2,\Gamma_o} \approx h\|k^{-2}(p_h \cdot \nu - \widehat{p}_h \cdot \nu)\|^2_{0,\Gamma_o} \cdot$$

- A more natural, "compatible" flux approximation!

Preliminary Comparison

$$\text{minimize} \quad \frac{1}{2}\|J(x)\cdot\nu - \widehat{J}(x)\cdot\nu\|^2_{-1/2,\Gamma_o} + \frac{\alpha}{2}\|(u(x)-\widehat{u}(x)\|^2_{0,\Omega}$$

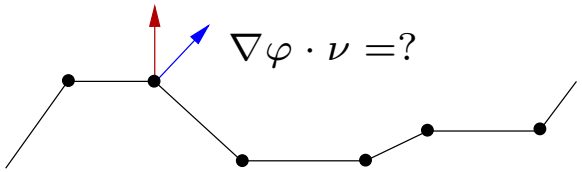
subject to

$$\begin{aligned} -\nabla\cdot(k(x)\nabla y(x)) &= f(x)+u(x) && \text{in } \Omega \\ y(x) &= y_D(x) && \text{on } \Gamma_D \\ (k(x)\nabla y(x))\cdot\nu &= g(x) && \text{on } \Gamma_N \end{aligned}$$

GALERKIN

$\int_{\Gamma_o} \nabla\varphi_i\cdot\nu\ \nabla\varphi_j\cdot\nu\ dx$

$\varphi_{i,j}$ nodal basis functions **VFA**



⊖ STD: innacurate flux computations
⊖ VFA: cumbersome implementation!

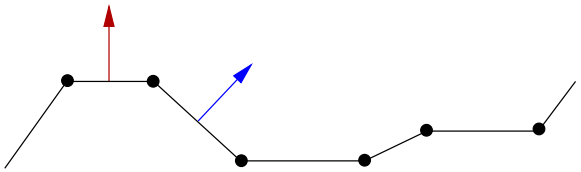
$$a(y,v)+b(u,v) = \langle f,v\rangle + \langle g,v\rangle_{\Gamma_N}$$

⊕ less expensive solution of the PDE

MIXED GALERKIN

$\int_{\Gamma_o} k^{-2}\ \psi_i\cdot\nu\ \psi_j\cdot\nu\ dx$

$\psi_{i,j}$ "face" basis functions



⊕ more natural choice for flux objectives

$$a(p,q)+b(q,y) = \langle y_d, q\cdot\nu\rangle_{\Gamma_D}$$

$$b(p,v)+c(u,v) = -\langle f,v\rangle$$

⊖ more expensive solution of the PDE

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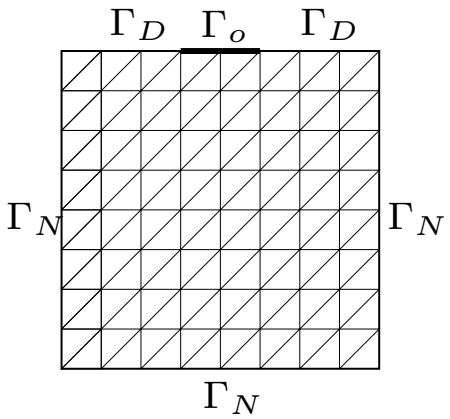
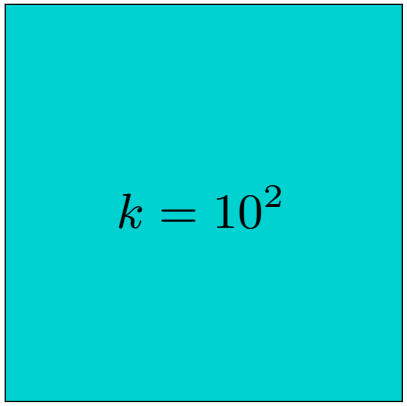
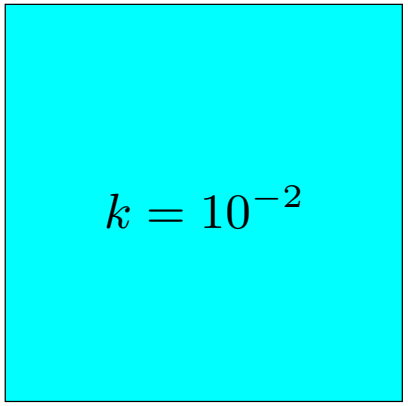
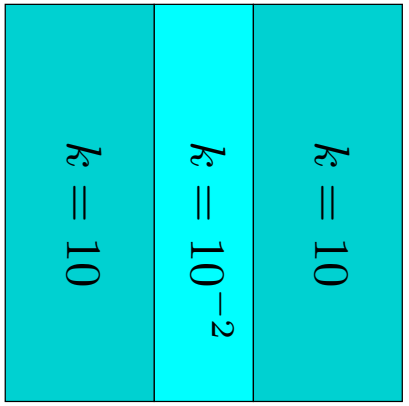
Experimental Setup



- Galerkin: first–order nodal elements ($\mathcal{P}^1$)
- Mixed: lowest–order Raviart–Thomas elements (RT_0)
- $32 \times 32 \times 2$ triangular mesh
- forcing term $f(x) = 0$, $y_D = 0$ on Γ_D
- target doping $\widehat{u} = 1$, reg. param. $\alpha = 6.25 \cdot 10^{-4}$
- $g = 0$ on left, right Γ_N; $g(x) = -k(x)$ on bottom Γ_N
- **parameter study**: (a) diffusivity profile k
  (b) target flux $\nabla \widehat{y} \cdot \nu$







Experimental Setup ... cont'd

Example 1. The desired flux is $\nabla\widehat{y}\cdot\nu = 1$ and $k(x) = 10^2$ in Ω.

Example 2. The desired flux is $\nabla\widehat{y}\cdot\nu = 1$ and $k(x) = 10^{-2}$ in Ω.

Example 3. The desired flux is $\nabla\widehat{y}\cdot\nu = 1$ and

$$k(x) = \begin{cases} 10 & \text{in } [-1,-0.25]\times[-1,1] \\ 10^{-2} & \text{in } [-0.25,0.25]\times[-1,1] \\ 10 & \text{in } [0.25,1]\times[-1,1], \end{cases}$$

Example 4. The desired flux is $\nabla\widehat{y}\cdot\nu = 100$ and $k(x)$ is as in Ex. 3.

Objective Functional

	Example 1: $k(x) = 10^2$			Example 2: $k(x) = 10^{-2}$		
	GM	Mixed	GM-VFA	GM	Mixed	GM-VFA
$\mathcal{J}_F$	1.99e-06	1.88e-06	1.95e-04	6.42e-09	2.51e-09	2.70e-09
$\mathcal{J}_u$	1.10e-08	1.10e-08	3.81e-07	1.12e-03	1.08e-03	1.11e-03
$\mathcal{J}$	2.00e-06	1.89e-06	1.95e-04	1.12e-03	1.08e-03	1.11e-03
	Example 3: $k(x)$ discontinuous			Example 4: $k(x)$ disocntinuous		
	GM	Mixed	GM-VFA	GM	Mixed	GM-VFA
$\mathcal{J}_F$	6.07e-05	8.10e-10	2.83e-07	1.06e+01	2.56e-07	6.29e-07
$\mathcal{J}_u$	7.17e-05	4.62e-05	4.50e-03	3.63e+00	4.57e-03	7.19e-03
$\mathcal{J}$	1.32e-04	4.62e-05	4.50e-03	1.42e+01	4.57e-03	7.19e-03

Table: $\mathcal{J}_F$, $\mathcal{J}_u$ and $\mathcal{J}$ denote the values of the flux term, the control term and their sum (the total value of the objective functional).

Example 3

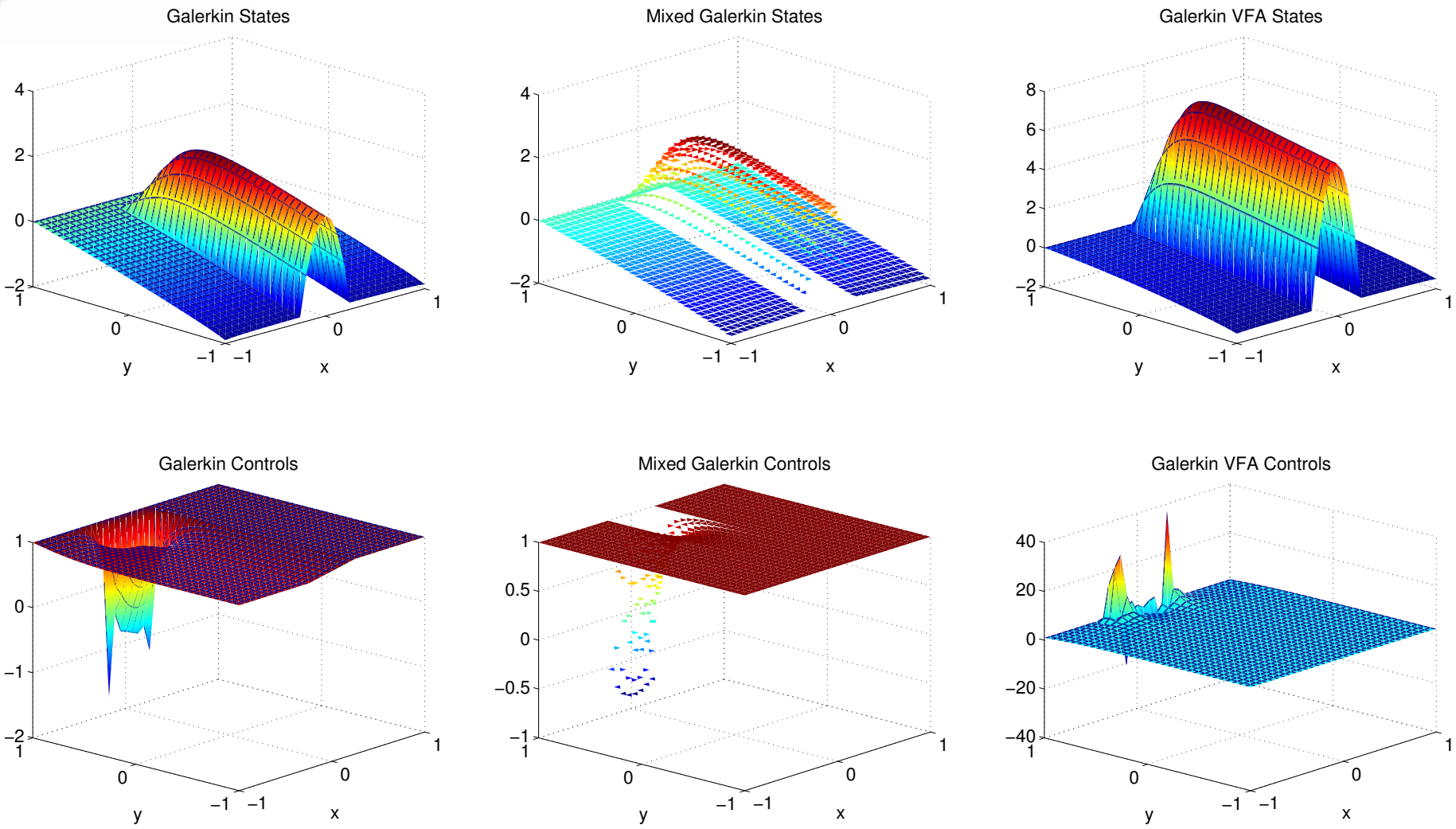


Figure: Galerkin, mixed Galerkin, and Galerkin VFA optimal states (top row) and optimal controls (bottom row) for Example 3.

Example 4

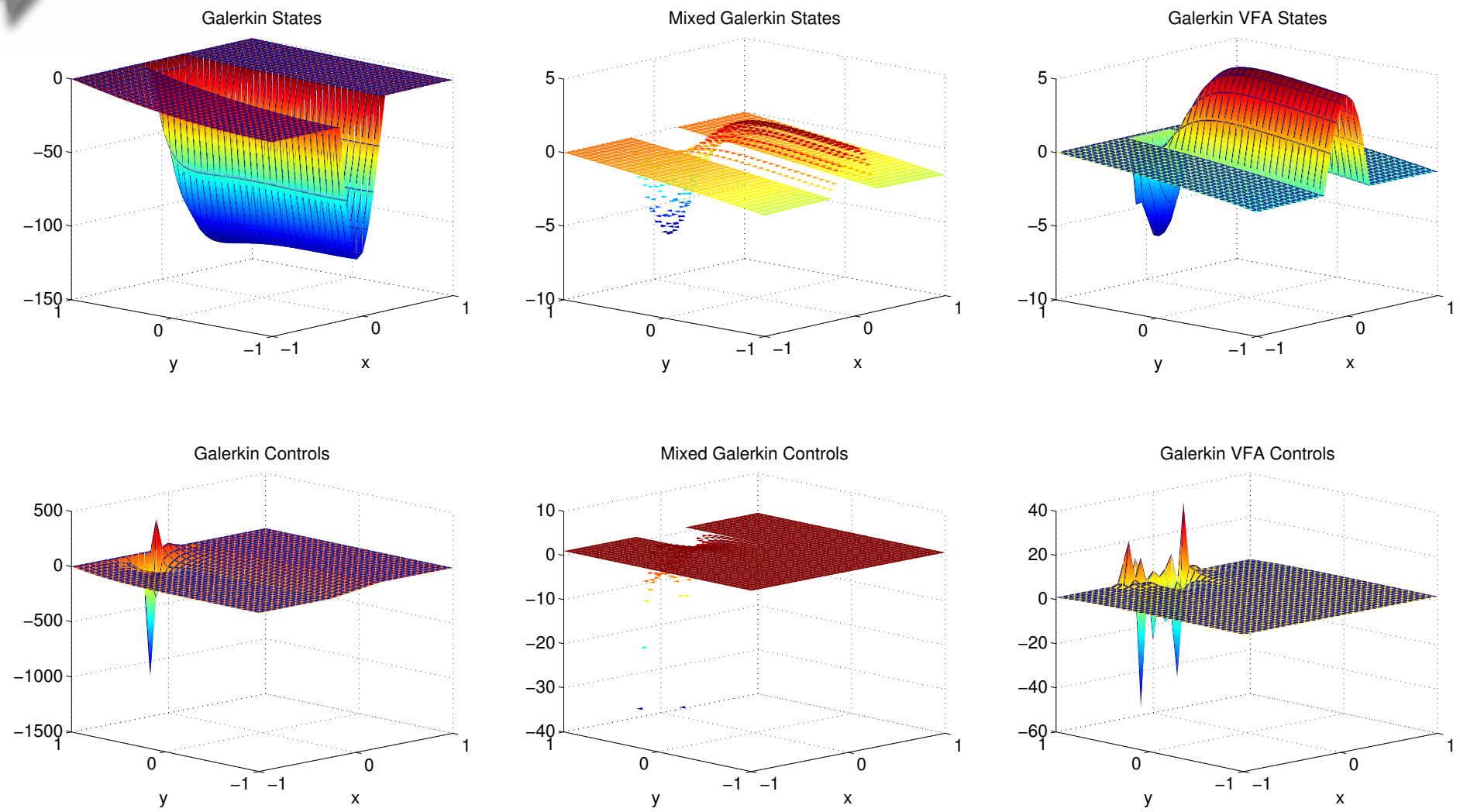


Figure: Galerkin, mixed Galerkin, and Galerkin VFA optimal states (top row) and optimal controls (bottom row) for Example 4.

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Summary & Conclusion

- performed study of Galerkin and mixed Galerkin discretizations used for the numerical solution of PDE–constrained optimization problems with applications to semiconductor design
- *unique problem feature*: objective functionals involve flux terms, which have fundamentally different discrete representations depending on the type of FE discretization
- for problems with heterogeneous material properties the mixed Galerkin method offers the most robust performance and the most accurate results
- the worst performer is the standard Galerkin method (not recommended!), which may yield state and control approximations that are many orders of magnitude less accurate than those computed by the mixed method
- if, for whatever reason, the use of the mixed method is not feasible, then the Galerkin discretization of the state equations should be combined with the VFA approach in order to improve robustness and accuracy