PDE-Constrained Optimization in Dynamic Systems

Theory and Environmental Applications

Dr. Maryam Iqbal

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Academy of Computer Science and Software Engineering
University of Johannesburg
South Africa

Presentation Outline

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Introduction

Motivation

Environmental systems are becoming increasingly complex due to

- Climate change
- Air and water pollution
- Energy demand
- Sustainable resource management

To make optimal decisions we combine

$$\boxed{\text{Mathematical Modeling} + \text{Optimization} + \text{Numerical Computing}}$$

which naturally leads to

$$\boxed{\textbf{PDE-Constrained Optimization}}$$

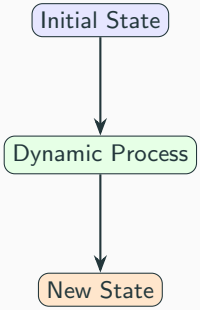
Dynamic Systems

Dynamic Systems

A dynamic system changes continuously with time.

Examples

- Heat transfer
- River pollution
- Groundwater flow
- Climate systems
- Population dynamics



General model

$$\frac{\partial y}{\partial t} = F(y, u)$$

Partial Differential Equations

Partial Differential Equations (PDEs)

Definition

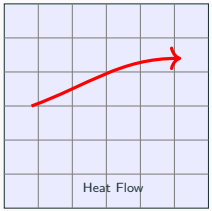
A Partial Differential Equation (PDE) describes the evolution of a physical quantity with respect to space and time.

General form

$$F(x, t, y, \nabla y, \nabla^2 y) = 0$$

Examples

- Heat Equation
- Diffusion Equation
- Wave Equation
- Navier–Stokes Equation



PDE-Constrained Optimization

PDE-Constrained Optimization

Definition

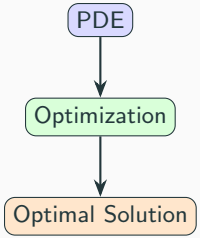
PDE-constrained optimization seeks the best control while satisfying a governing PDE.

General problem

$$\min_u J(y, u)$$

subject to

$$E(y, u) = 0$$



Applications

- Pollution Control
- Heat Transfer
- Water Management
- Climate Modeling

Mathematical Formulation

The optimization problem is

$$\min_{u} J(y, u)$$

subject to

$$\frac{\partial y}{\partial t} - \nabla \cdot (k \nabla y) = f + u$$

Objective function

$$J(y, u) = \frac{1}{2}\|y - y_d\|^2 + \frac{\alpha}{2}\|u\|^2$$

where

- y : State
- u : Control
- y_d : Desired State

Optimization Workflow



Pipeline

Model → Simulation → Optimization → Decision Making

Environmental Applications

Case Study: River Pollution Control

Objective

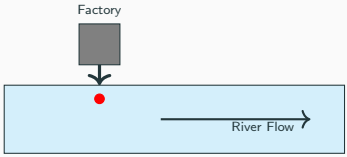
Minimize pollutant concentration while reducing treatment cost.

The transport of pollutants is governed by the Advection–Diffusion Equation

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = D\nabla^2 c + S(x,t)$$

where

- c : Pollutant concentration
- $\mathbf{v}$: Flow velocity
- D : Diffusion coefficient
- S : Pollution source

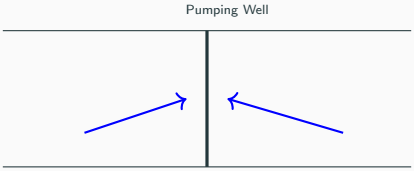


Groundwater Optimization

Groundwater systems are modeled using PDEs to simulate water flow and contaminant transport.

Optimization objectives

- Minimize contaminant spread
- Optimal pumping strategy
- Protect drinking water
- Reduce remediation cost



Artificial Intelligence

Physics-Informed Neural Networks (PINNs)

PINNs integrate deep learning with governing PDEs.

Advantages

- No mesh generation
- Fast approximation
- Data + Physics together
- Suitable for inverse problems
- Reduced computational cost



Climate and Energy Applications

PDE-constrained optimization contributes significantly to sustainable development.

Applications include

- Climate prediction
- Carbon emission reduction
- Wind energy
- Solar energy
- Smart grids
- Heat management
- Ocean circulation
- Weather forecasting

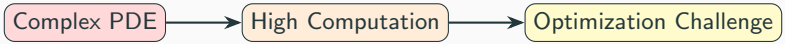
$$\boxed{\text{Optimization} + \text{AI} + \text{PDEs} = \text{Sustainable Future}}$$

Challenges

Current Challenges

Despite significant progress, several challenges remain.

- Large-scale optimization
- High computational cost
- Nonlinear PDE models
- Uncertainty in data
- High-dimensional systems
- Real-time optimization
- Complex boundary conditions
- Multi-objective optimization



Future Research

Future Research Directions

Future developments are expected in

- Physics-Informed Machine Learning
- Artificial Intelligence
- Digital Twins
- Real-Time Optimal Control
- Quantum Computing
- Smart Environmental Monitoring
- Sustainable Development

$$\boxed{\text{AI} + \text{Big Data} + \text{PDE Optimization} = \text{Next Generation Decision Making}}$$

Conclusion

Conclusion

1. PDEs model dynamic environmental systems.
2. Optimization identifies the best control strategy.
3. Numerical algorithms solve large-scale problems efficiently.
4. AI and PINNs are transforming PDE optimization.
5. These techniques support sustainable environmental management.

Better Models $\Rightarrow$ Better Decisions $\Rightarrow$ Better Environment

References

References i

Hinze M., Pinnau R., Ulbrich M., Ulbrich S.
Optimization with PDE Constraints.
Springer, 2009.

Tröltzsch F.
Optimal Control of Partial Differential Equations.
AMS, 2010.

Biegler L. T.
Nonlinear Programming.
SIAM, 2010.

References ii

Quarteroni A.

Numerical Models for Differential Problems.

Springer, 2017.

Raissi M., Perdikaris P., Karniadakis G.

Physics-Informed Neural Networks.

Journal of Computational Physics, 2019.

Chen X. et al.

AI-Driven PDE-Constrained Optimization for Environmental Systems.

Applied Mathematics and Computation, 2024.

Wang Y. et al.

Physics-Informed Machine Learning for Scientific Computing.

Journal of Scientific Computing, 2025.

Thank You

Questions?

Dr. Maryam Iqbal

University of Johannesburg