Comparison of Classical Numerical PDE Methods and Deep Learning-Based PDE Solvers

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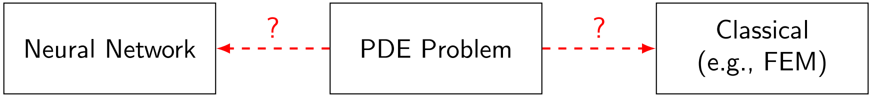
Which Solver Should We Use?



Observation

From what we have seen so far, it's still unclear when to use classical numerical methods or neural networks to solve a given PDE problem.

- Classical methods are reliable and well-understood — but expensive in high dimensions
- Neural networks can generalize — but may lack guarantees or interpretability
- Choosing between them is still an open research question

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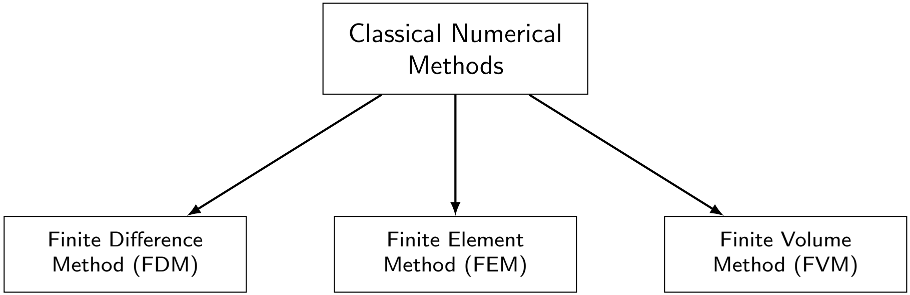
Classical Numerical Methods


Classical Numerical Methods
Finite Difference Method (FDM)
Finite Element Method (FEM)
Finite Volume Method (FVM)

Advantages of Classical Methods

Accuracy & Convergence Theory

- Well-established mathematical theories ensure convergence and stability
- Rigorous error estimates for FDM and FEM

Flexibility & Generality

- Handle arbitrary PDEs with proper formulation
- FEM particularly powerful for complex geometries and adaptive meshing

Interpretability & Reliability

- Solutions based on first-principles physics
- No need for large datasets

Computational Inefficiency

High-dimensional PDEs suffer from the curse of dimensionality:

- Boltzmann equation: $d = 7$
- Radiative Transfer: $d \geq 5$
- Black-Scholes: $d >> 1$
- Schrödinger: $d >> 1$

Fine grids required:

- Both spatial and temporal resolution
- High computational costs

Complexity of Implementation:

- Assembly of system matrices requires careful integration over elements.
- Boundary condition enforcement can be subtle and error-prone.
- Handling curved boundaries, adaptive refinement, and mesh conformity adds significant code complexity.

Many-Query Problems

Applications requiring multiple PDE solves:

- Design optimization
- Uncertainty quantification
- Inverse problems (EIT, Seismic Waves)

Example: Flow past airfoils

- Various Mach numbers
- Different angles of attack
- Lift & drag evaluation

Additional Challenges

Multiscale & Multiphysics

- Turbulence modeling
- Geophysics applications
- Material science
- Multiple spatial & temporal scales
- Mesh resolution constraints

Grid Generation Dependency

- Careful meshing required
- Complex for irregular geometries
- Poor meshing leads to numerical errors and instability

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Why Use Deep Learning for PDEs?

Deep learning-based PDE solvers address computational challenges of classical methods:

- Mesh-free approaches
- High-dimensional capability
- Fast inference
- Data-driven solutions

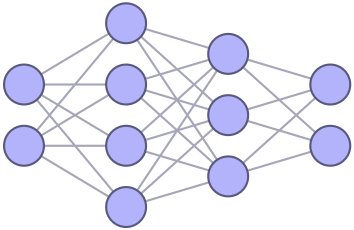


Figure: Deep Neural Network Architecture

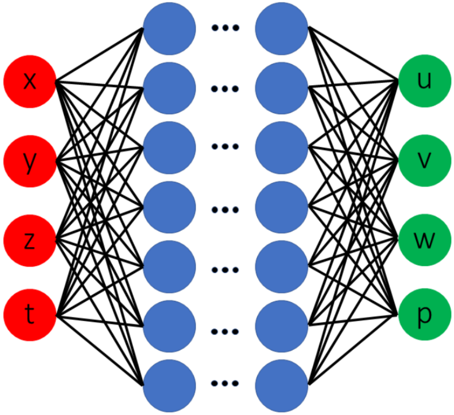
Mesh-Free Methods

Traditional methods:

- Require mesh generation
- Grid-dependent solutions
- Complex for irregular geometries

Deep learning methods:

- Physics-Informed Neural Networks (PINNs)
- Deep Ritz method (DeepRitz)
- No mesh generation required



Mesh-free approaches

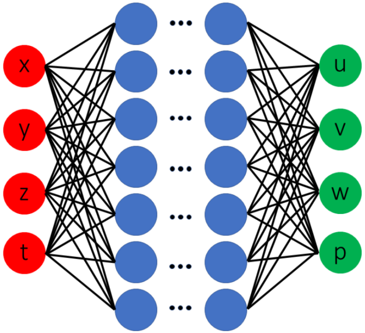
High-Dimensional PDE Handling

Classical methods:

- Struggle with curse of dimensionality
- Exponential growth in computational cost
- Limited to low-dimensional problems

Neural networks:

- Approximate high-dimensional operators efficiently
- Scale better with dimension
- Universal approximation properties



Scaling with dimension

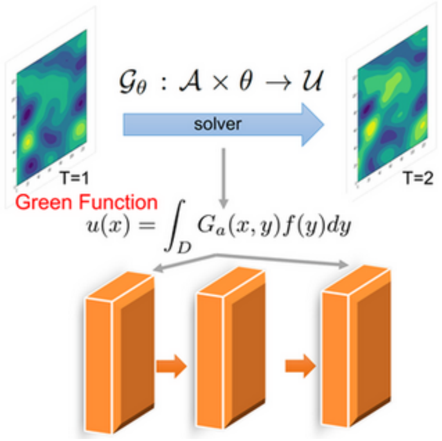
Computational Efficiency

Training Phase:

- One-time computational cost
- Learn PDE solution patterns
- Neural operator learning (FNO)

Inference Phase:

- Instantaneous solutions
- Ideal for many-query problems
- Optimization, inverse problems, UQ



$\mathcal{G}_\theta : \mathcal{A} \times \theta \to \mathcal{U}$
solver
T=1
T=2
Green Function
$u(x) = \int_D G_a(x,y) f(y) dy$

Neural Operator

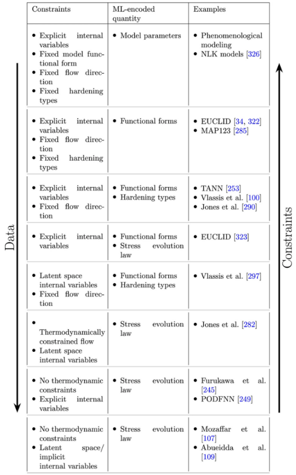
Data-Driven PDE Solving

Real-world challenges:

- Unknown or incomplete physics
- Turbulence modeling
- Climate modeling
- Complex material behavior

Deep learning advantages:

- Learn from experimental data
- Observational data integration
- Solutions where first-principles fail


Data
Constraints

Constraints	ML-encoded quantity	Examples
• Explicit internal variables • Fixed model functional form • Fixed flow direction • Fixed hardening types	• Model parameters	• Phenomenological modeling • NLK models [326]
• Explicit internal variables • Fixed flow direction • Fixed hardening types	• Functional forms	• EUCLID [34, 322] • MAP123 [285]
• Explicit internal variables • Fixed flow direction	• Functional forms • Hardening types	• TANN [253] • Vlassis et al. [100] • Jones et al. [290]
• Explicit internal variables	• Functional forms • Stress evolution law	• EUCLID [323]
• Latent space internal variables • Fixed flow direction	• Functional forms • Hardening types	• Vlassis et al. [297]
• Thermodynamically constrained flow • Latent space internal variables	• Stress evolution law	• Jones et al. [282]
• No thermodynamic constraints • Explicit internal variables	• Stress evolution law	• Furukawa et al. [245] • PODFNN [249]
• No thermodynamic constraints • Latent space/ implicit internal variables	• Stress evolution law	• Mozaffar et al. [107] • Abueidda et al. [109]

Data-driven modeling of constitutive laws

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Classical vs. Deep Learning Methods

Feature	Classical Methods	Deep Learning
Accuracy	High for well-resolved grids	Approximate, improves with training
Interpretability	High, first-principles physics	Lower, but improving
Computational Cost	Expensive for high-dim & many-query	Fast inference after training
High-Dimensional PDEs	Struggles beyond 3D	Efficient for high-dim
Inverse & UQ Problems	Many PDE solves, costly	Fast trained solutions
Data Dependency	No data needed	Can learn from data

When to Use Each Method?

Use Classical Methods when:

- High accuracy required
- Well-understood physics
- Low-dimensional problems
- Single or few PDE solves
- Interpretability crucial

Use Deep Learning when:

- High-dimensional PDEs
- Many-query problems
- Unknown/incomplete physics
- Real-time applications
- Large datasets available

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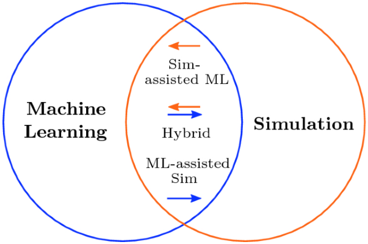
Hybrid Approaches

Combining the best of both worlds:

- Physics-informed deep learning
- Neural-enhanced classical solvers
- Multi-fidelity approaches
- Adaptive mesh refinement with ML

Emerging trends:

- Scientific machine learning
- Differentiable programming
- Neural operators



Hybrid classical-ML approach

Mini Game: Classical vs Neural Network?

Can you guess the right solver for each case?

1. **Parametric FEM is too slow**
   A company simulates heat transfer in engine blocks for different materials. Each FEM run takes 2 hours. They want quick temperature field predictions during design.
2. **No PDE, just data**
   A hospital collects data from patients with a rare lung disease. They have stress-strain curves but no clear mechanical model of the tissue.
3. **Safety-critical simulation**
   An aerospace firm needs accurate stress predictions on a turbine blade. These simulations inform certification and safety margins.

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Discussion:

- (1) $\rightarrow$ **Neural Network Surrogate** trained on offline FEM runs
- (2) $\rightarrow$ **Neural Network Model** fit to the data, no physics known
- (3) $\rightarrow$ **Classical FEM Solver** for reliability and interpretability

Conclusion

- Classical methods remain gold standard for accuracy and interpretability
- Deep learning excels in high-dimensional and many-query scenarios
- Method choice depends on specific problem requirements
- Future lies in hybrid approaches combining both strengths
- Scientific machine learning is rapidly evolving field

Thank you for your attention!