ADCME
Machine Learning for Computational Engineering

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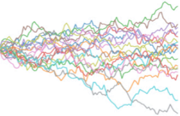
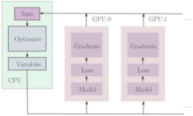
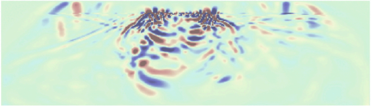
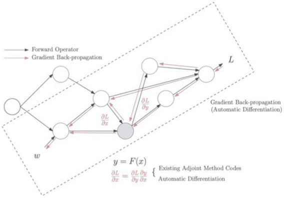
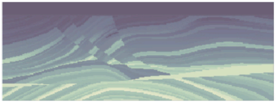
https://github.com/kailaix/ADCME.jl

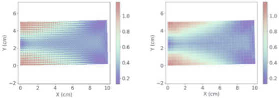






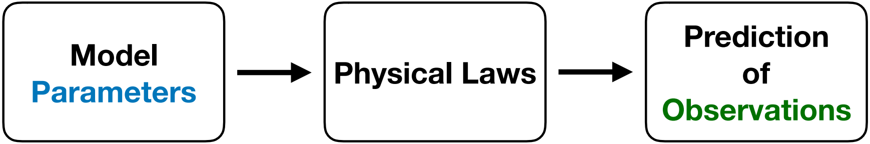




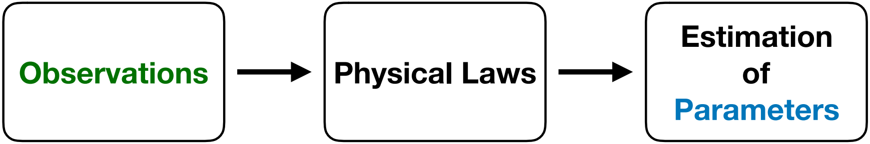


Inverse Modeling

Forward Problem



Inverse Problem



Function Inverse Problem

$$\min_{f} L_h(u_h) \quad \text{s.t. } F_h(f, u_h) = 0$$

What if the unknown is a function instead of a set of parameters?

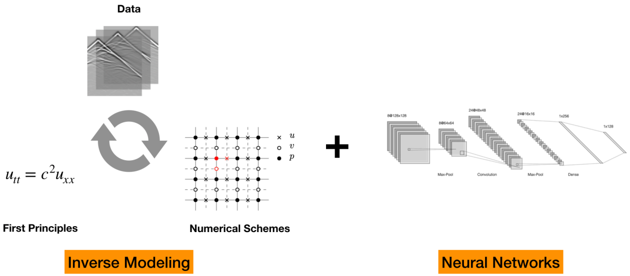
- Koopman operator in dynamical systems.
- Constitutive relations in solid mechanics.
- Turbulent closure relations in fluid mechanics.
- ...

The candidate solution space is infinite dimensional.

Physics Based Machine Learning

$$\min_{\theta} L_h(u_h) \quad \text{s.t. } F_h(NN_\theta, u_h) = 0$$

- Deep neural networks exhibit capability of approximating high dimensional and complicated functions.
- **Physics based machine learning**: the unknown function is approximated by a deep neural network, and the physical constraints are enforced by numerical schemes.
- Satisfy the physics to the largest extent.

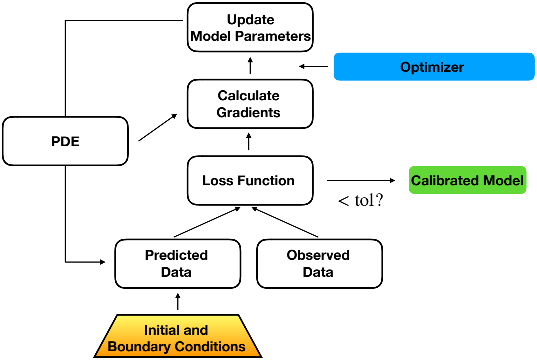


Gradient Based Optimization

$$\min_{\theta} L_h(u_h) \quad \text{s.t. } F_h(\theta, u_h) = 0 \tag{1}$$

- We can now apply a gradient-based optimization method to (1).
- The key is to calculate the gradient descent direction g^k

$$\theta^{k+1} \leftarrow \theta^k - \alpha g^k$$



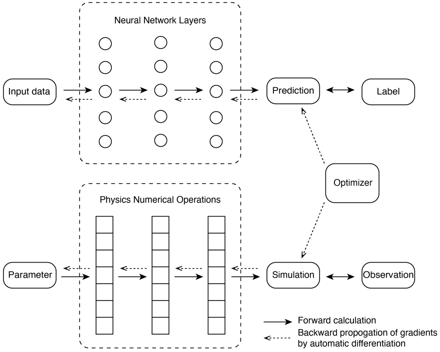
Automatic Differentiation

The fact that bridges the technical gap between machine learning and inverse modeling:

- Deep learning (and many other machine learning techniques) and numerical schemes share the same computational model: composition of individual operators.

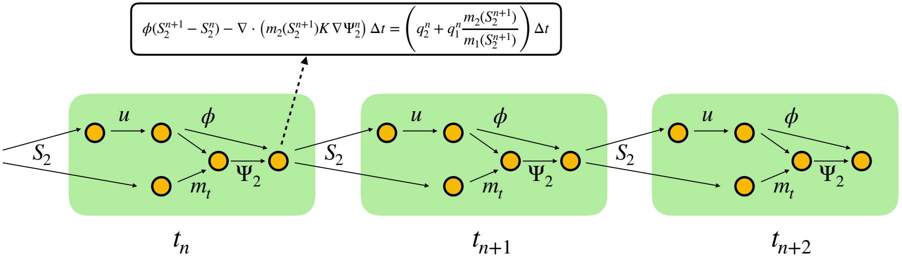
Mathematical Fact

Back-propagation
||
Reverse-mode
Automatic Differentiation
||
Discrete
Adjoint-State Method

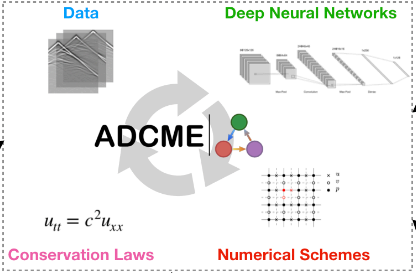


Computational Graph for Numerical Schemes

- To leverage automatic differentiation for inverse modeling, we need to express the numerical schemes in the "AD language": computational graph.
- No matter how complicated a numerical scheme is, it can be decomposed into a collection of operators that are interlinked via state variable dependencies.



A General Approach to Inverse Modeling



PoreFlow.jl
Geomechanics
Viscoelasticity
Multiphase Flow
Multiphysics
* coming soon

FwiFlow.jl
Multiphase Flow
Nonlocal Operators
https://github.com/lidongzh/FwiFlow.jl

ADSeismic.jl
General Seismic Inversion
https://github.com/kailaix/ADSeismic.jl

NNFEM.jl
Constitutive Law Modeling
Hyperelasticity
Elasto-Plasticity
https://github.com/kailaix/NNFEM.jl

FEM/FVM on Structured Grids

- Steady-state Navier-Stokes equation

$$
\begin{aligned}
(\mathbf{u}\cdot\nabla)\mathbf{u} &= -\frac{1}{\rho}\nabla p + \nabla\cdot(\nu(\mathbf{x})\nabla\mathbf{u}) + \mathbf{g}\\
\nabla\cdot\mathbf{u} &= 0
\end{aligned}
$$

- Inverse problem are ubiquitous in fluid dynamics:

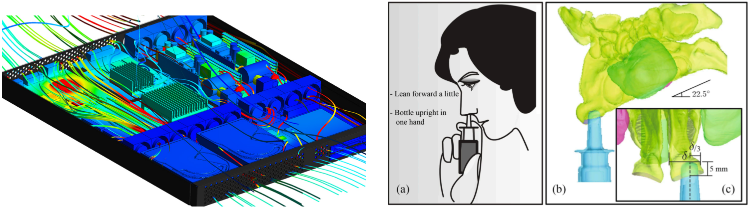
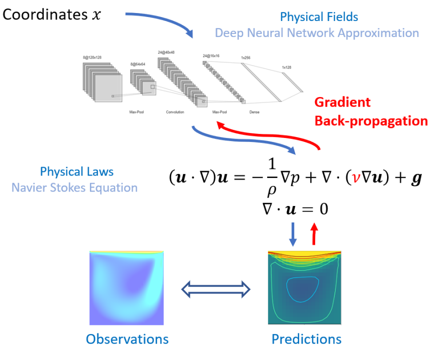
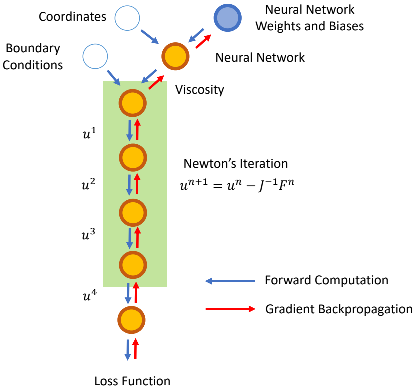


Figure: Left: electronic cooling; right: nasal drug delivery.

FEM/FVM on Structure Grids





FEM/FVM on Structure Grids

- Data: (u, v)
- Unknown: $\nu(\mathbf{x})$ (represented by a deep neural network)
- Prediction: p (absent in the training data)
- The DNN provides regularization, which generalizes the estimation better!