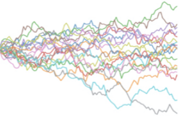
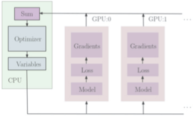
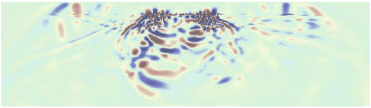
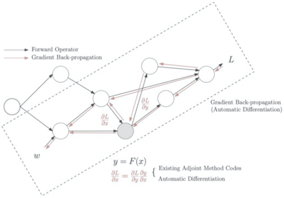
Machine Learning for Inverse Problems in Computational Engineering

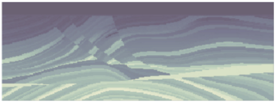
Kailai Xu, and Eric Darve
https://github.com/kailaix/ADCME.jl

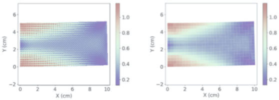








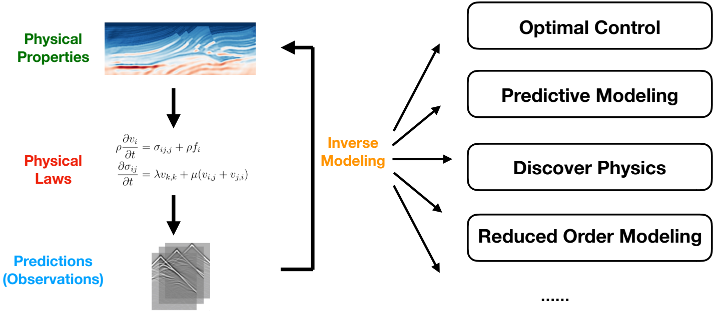




Outline

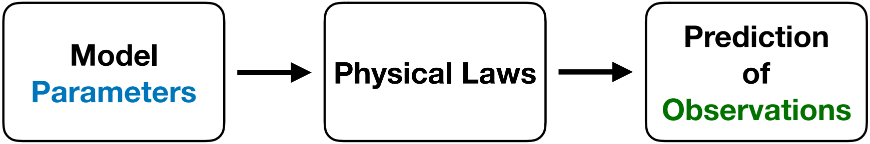
Inverse Modeling

- **Inverse modeling** identifies a certain set of parameters or functions with which the outputs of the forward analysis matches the desired result or measurement.
- Many real life engineering problems can be formulated as inverse modeling problems: shape optimization for improving the performance of structures, optimal control of fluid dynamic systems, etc.

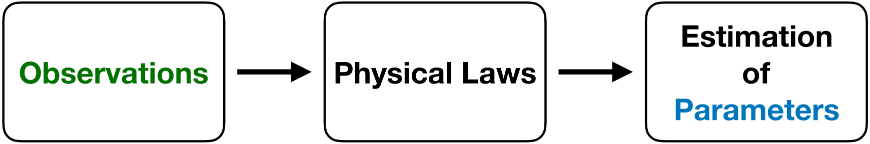


Inverse Modeling

Forward Problem



Inverse Problem



Inverse Modeling

We can formulate inverse modeling as a PDE-constrained optimization problem

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

- The loss function L_h measures the discrepancy between the prediction u_h and the observation u_{obs}, e.g., $L_h(u_h) = \|u_h - u_{\mathrm{obs}}\|_2^2$.
- θ is the model parameter to be calibrated.
- The physics constraints $F_h(\theta, u_h) = 0$ are described by a system of partial differential equations. Solving for u_h may require solving linear systems or applying an iterative algorithm such as the Newton-Raphson method.

Function Inverse Problem

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

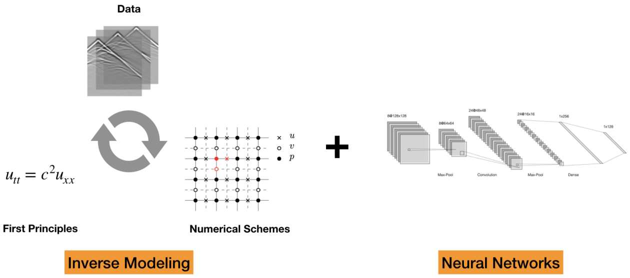
What if the unknown is a function instead of a set of parameters?

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

The candidate solution space is infinite dimensional.

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

- Deep neural networks exhibit capability of approximating high dimensional and complicated functions.
- **Machine Learning for Computational Engineering**: 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.

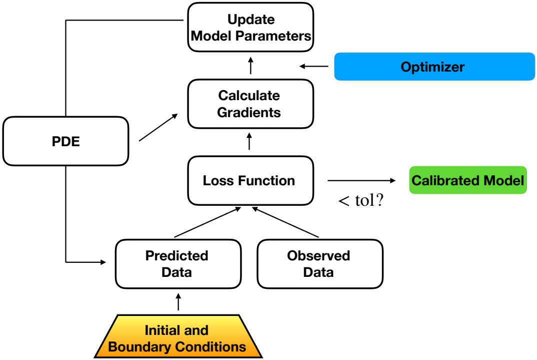


Gradient Based Optimization

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

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

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



Outline

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

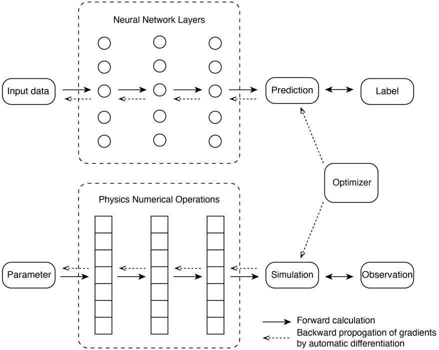
Back-propagation

||

Reverse-mode Automatic Differentiation

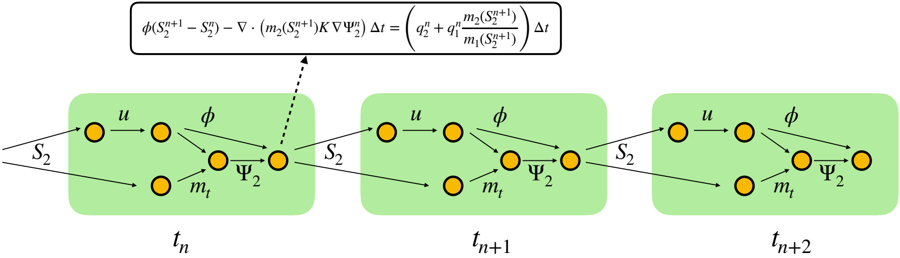
||

Discrete Adjoint-State Method

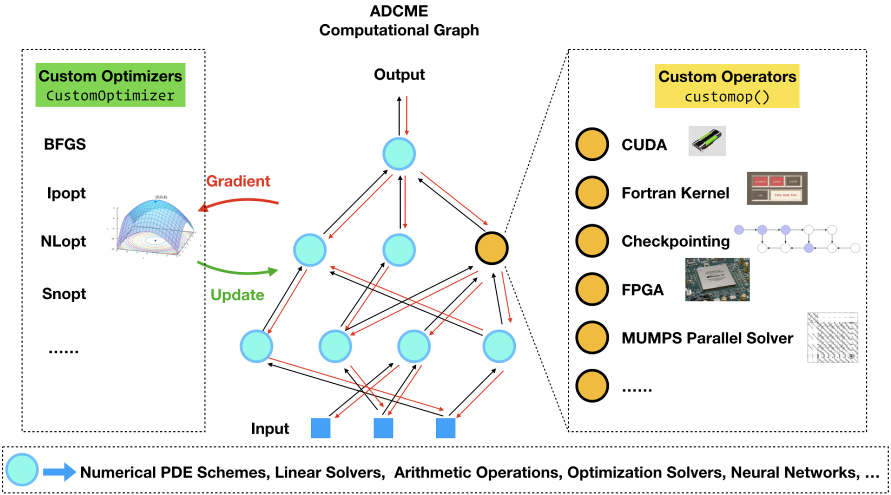


Computational Graph for Numerical Schemes

- 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.

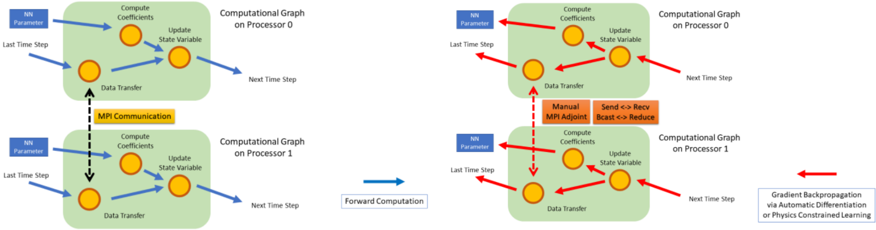


ADCME: Computational-Graph-based Numerical Simulation



Distributed Optimization

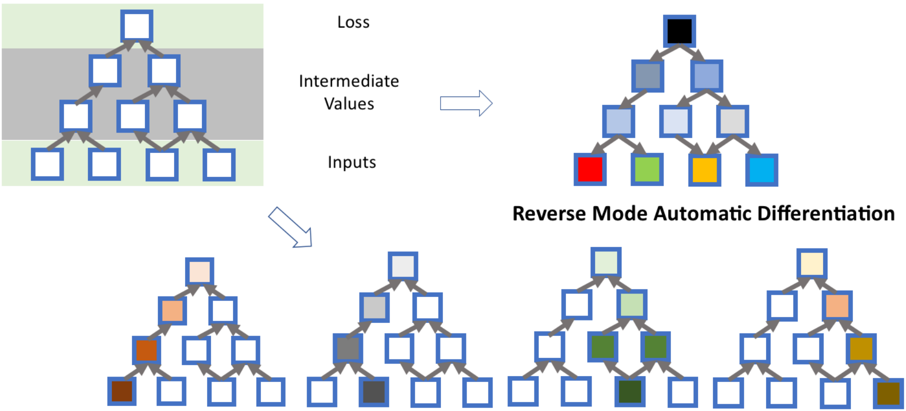
- ADCME also supports MPI-based distributed computing. The parallel model is designed specially for scientific computing.



- Key idea: Everything is an operator. Computation and communications are converters of data streams (tensors) through the computational graph.

`mpi_bcast`, `mpi_sum`, `mpi_send`, `mpi_recv`, `mpi_halo_exchange`, ...

Automatic Differentiation: Forward-mode and Reverse-mode



Forward Mode Automatic Differentiation

What is the Appropriate Model for Inverse Problems?

- In general, for a function $f : \mathbb{R}^n \to \mathbb{R}^m$

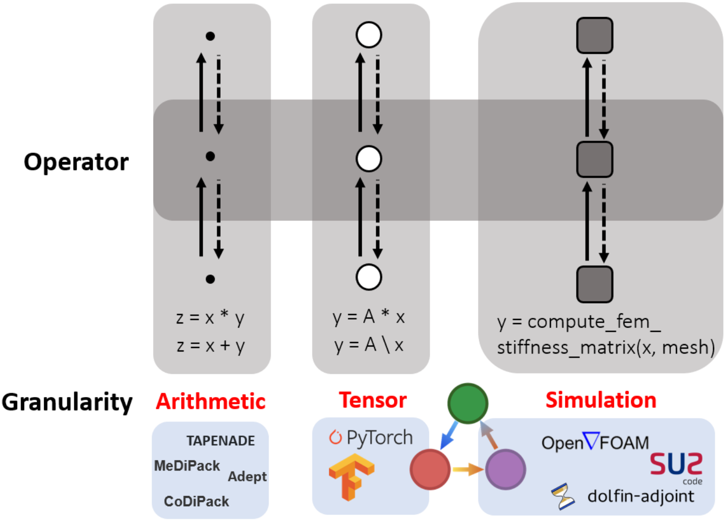
Mode	Suitable for ...	Complexity[1]	Application
Forward	$m \gg n$	$\leq 2.5\,\mathrm{OPS}(f(x))$	UQ
Reverse	$m \ll n$	$\leq 4\,\mathrm{OPS}(f(x))$	Inverse Modeling

- There are also many other interesting topics
  - Mixed mode AD: many-to-many mappings.
  - Computing sparse Jacobian matrices using AD by exploiting sparse structures.

Margossian CC. A review of automatic differentiation and its efficient implementation. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery. 2019 Jul;9(4):e1305.

[1] OPS is a metric for complexity in terms of fused-multiply adds.

Granularity of Automatic Differentiation



Outline

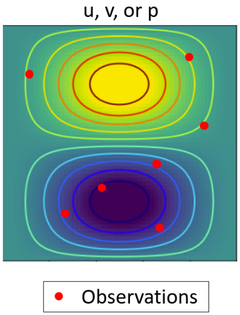
Inverse Modeling of the Stokes Equation

- The governing equation for the Stokes problem

$$\begin{aligned} -\nu\Delta\mathbf{u} + \nabla p &= \mathbf{f} && \text{in } \Omega \\ \nabla\cdot\mathbf{u} &= 0 && \text{in } \Omega \\ \mathbf{u} &= \mathbf{0} && \text{on } \partial\Omega \end{aligned}$$

- The weak form is given by

$$\begin{aligned} (\nu\nabla u, \nabla v) - (p, \nabla\cdot v) &= (f, v) \\ (\nabla\cdot u, q) &= 0 \end{aligned}$$



Inverse Modeling of the Stokes Equation

```
nu = Variable(0.5)
K = nu*constant(compute_fem_laplace_matrix(m, n, h))
B = constant(compute_interaction_matrix(m, n, h))
Z = [K -B'
-B spdiag(zeros(size(B,1)))]

# Impose boundary conditions
bd = bcnode("all", m, n, h)
bd = [bd; bd .+ (m+1)*(n+1); ((1:m) .+ 2(m+1)*(n+1))]
Z, _ = fem_impose_Dirichlet_boundary_condition1(Z, bd, m, n, h)

# Calculate the source term
F1 = eval_f_on_gauss_pts(f1func, m, n, h)
F2 = eval_f_on_gauss_pts(f2func, m, n, h)
F = compute_fem_source_term(F1, F2, m, n, h)
rhs = [F;zeros(m*n)]
rhs[bd] .= 0.0

sol = Z\rhs
```

Inverse Modeling of the Stokes Equation

- The distinguished feature compared to traditional forward simulation programs: the model output is differentiable with respect to model parameters!

```
loss = sum((sol[idx] - observation[idx])^2)
g = gradients(loss, nu)
```

- Optimization with a one-liner:

```
BFGS!(sess, loss)
```

PoreFlow/ADCME

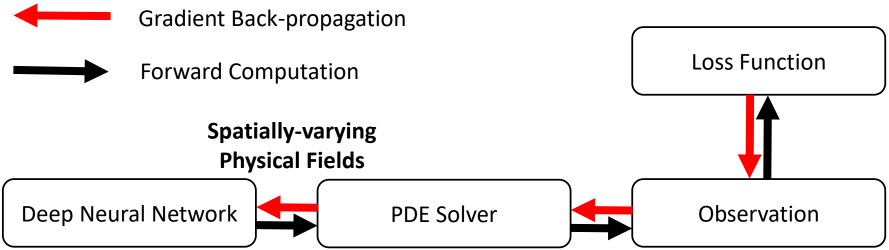
Simulation Program

Outline

Learning spatially-varying physical parameters using deep neural networks

- It is easy to adopt ADCME for modeling spatially-varying physical parameters using deep neural networks with a PDE solver.

$$\boxed{\text{DNN} + \text{PDE} + \text{Data} = \text{Physics Constrained Data-driven Modeling}}$$



Linear Elasticity

DNN + Linear Elasticity + Displacement Data

$$\boxed{\begin{aligned} &\sigma_{ij,j} + b_i = 0,\ x \in \Omega \\ &\varepsilon_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j}),\ x \in \Omega \\ &\sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + \mu(\varepsilon_{ij} + \varepsilon_{ji}),\ x \in \Omega \\ &\sigma_{ij} n_j = t_j,\ x \in \Gamma_N; \quad u_i = (u_0)_i,\ x \in \Gamma_D \\ &\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad \mu = \frac{E\nu}{1-\nu^2} \end{aligned}}$$

Stokes' Problem

DNN + Stokes' Problem + Pressure Data

$$\boxed{\begin{aligned} -\nabla \cdot (\nu \nabla u) + \nabla p &= f \quad \text{in } \Omega \\ \nabla \cdot u &= 0 \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned}}$$

Hyperelasticity

DNN + Hyperelasticity + Displacement Data

$$
\boxed{
\begin{aligned}
\min_u \psi &= \frac{\mu}{2}(I_c - 2) - \frac{\mu}{2}\log(J) + \frac{\lambda}{8}\log(J)^2\\
F &= I + \nabla u,\ \ C = F^T F,\ \ J = \det(C),\ \ I_c = \mathrm{trace}(C)\\
\lambda &= \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}
\end{aligned}
}
$$

Burgers' Equation

DNN + Burgers' Equation + Velocity Data

$$\boxed{\begin{aligned}\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} &= \nabla\cdot(\nu\nabla u)\\ \frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} &= \nabla\cdot(\nu\nabla v)\\ (x,y)\in\Omega,\ t&\in(0,T)\end{aligned}}$$

- Steady-state Navier-Stokes equation

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

- Inverse problem are ubiquitous in fluid dynamics:

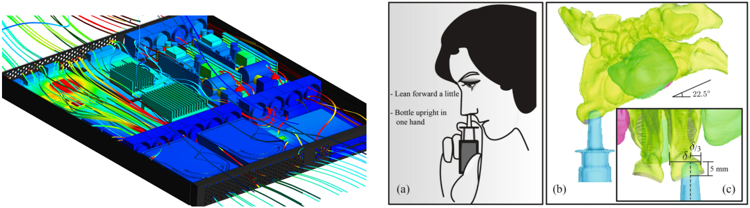
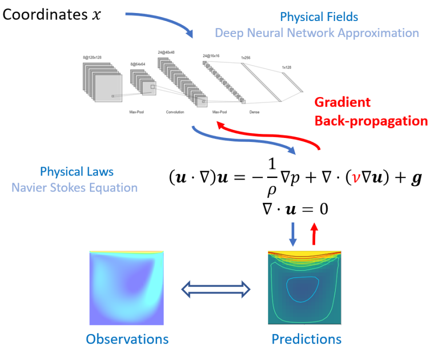
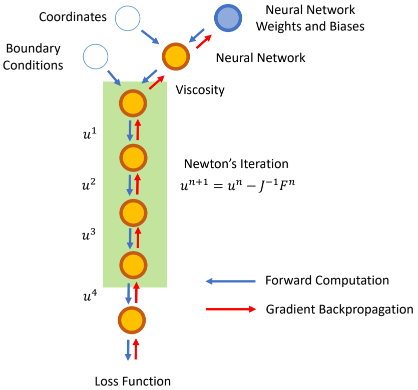


Figure: Left: electronic cooling; right: nasal drug delivery.

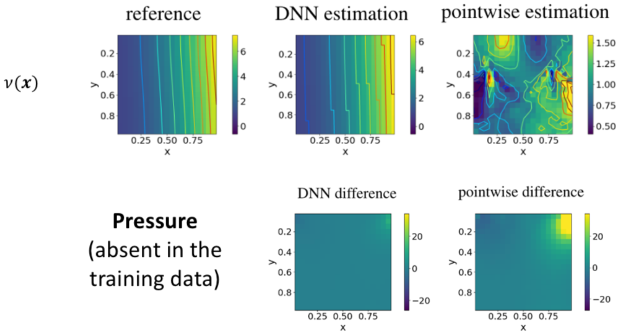
Navier-Stokes Equation

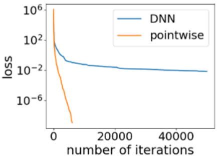




Navier-Stokes Equation

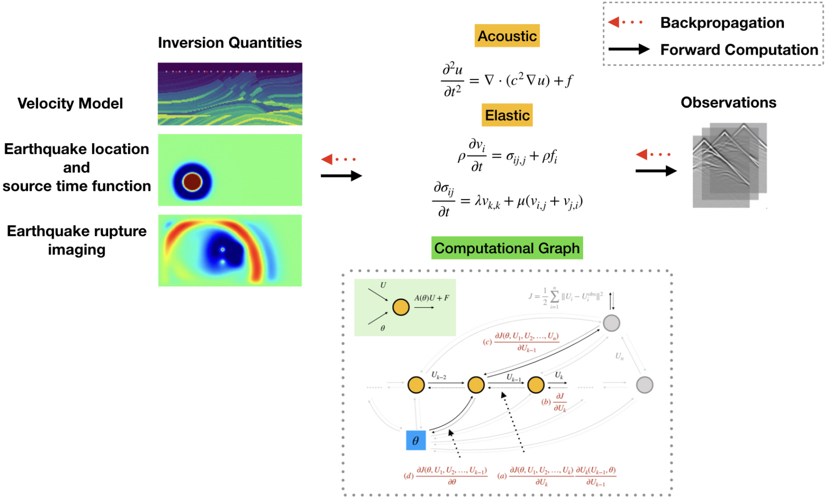
- Data: (u, v)
- Unknown: $\nu(\mathbf{x})$ (represented by a deep neural network)
- Prediction: p (absent in the training data)
- The DNN provides regularization, which generalizes the estimation better!





ADSeismic.jl: A General Approach to Seismic Inversion

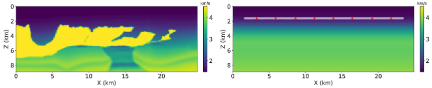
- Many seismic inversion problems can be solved within a unified framework.

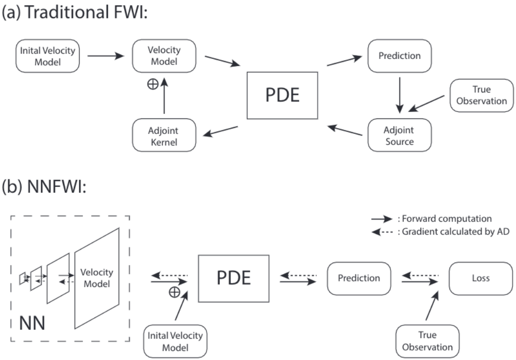


NNFWI: Neural-network-based Full-Waveform Inversion

- Estimate velocity models from seismic observations.

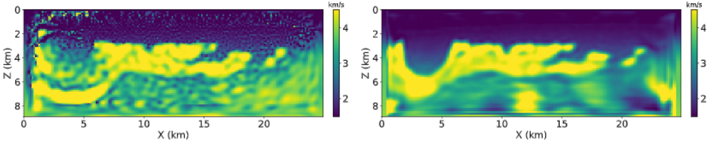
$$\frac{\partial^2 u}{\partial t^2} = \nabla\cdot(m^2 \nabla u) + f$$



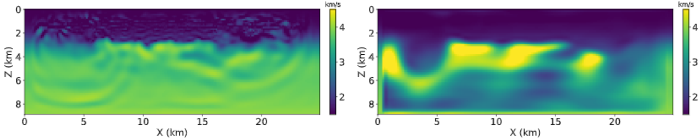


NNFWI: Neural-network-based Full-Waveform Inversion

- Inversion results with a noise level $\sigma = \sigma_0$



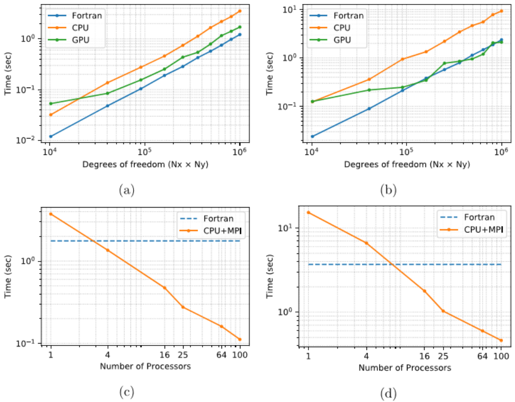
- Inversion results for the same loss function value:



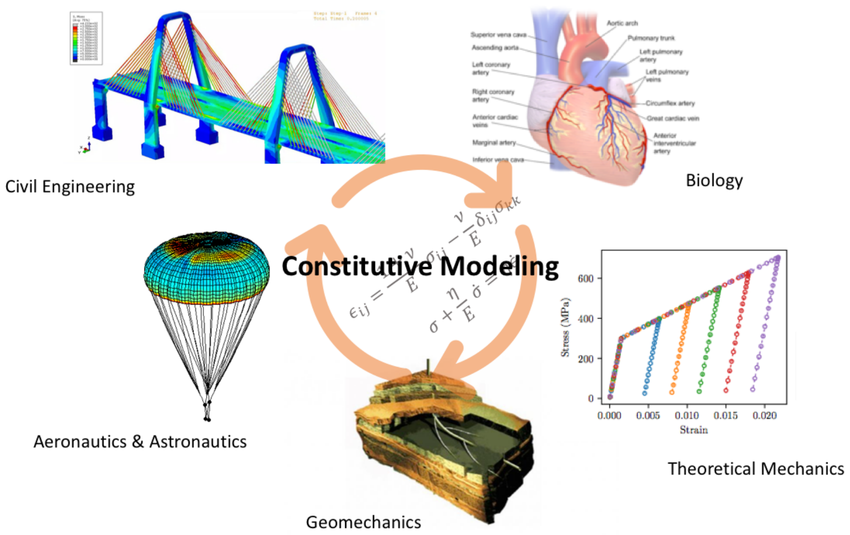
ADSeismic.jl: Performance Benchmark

- Performance is a key focus of ADCME.
- ADCME enables us to utilize heterogeneous (CPUs, GPUs, and TPUs) and distributed (CPU clusters) computing environments.

  Fortran: open-source Fortran90 programs SEISMIC_CPML



Constitutive Modeling



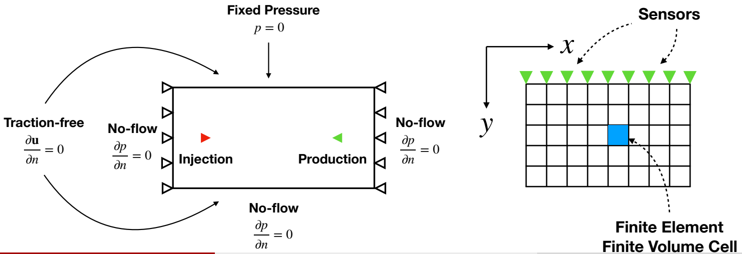
Poroelasticity

- Multi-physics Interaction of Coupled Geomechanics and Multi-Phase Flow Equations

$$\mathrm{div}\boldsymbol{\sigma}(\mathbf{u}) - b\nabla p = 0$$
$$\frac{1}{M}\frac{\partial p}{\partial t} + b\frac{\partial \epsilon_v(\mathbf{u})}{\partial t} - \nabla\cdot\left(\frac{k}{B_f\mu}\nabla p\right) = f(x,t)$$
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{\epsilon}, \dot{\boldsymbol{\epsilon}})$$

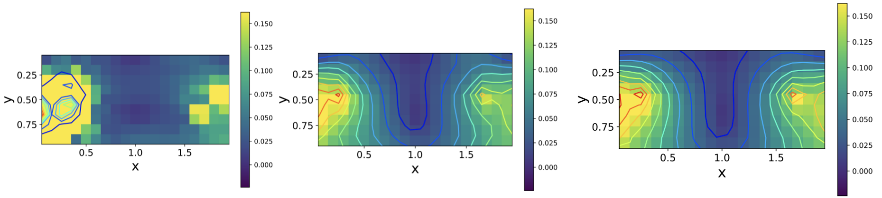
- Approximate the constitutive relation by a neural network

$$\boldsymbol{\sigma}^{n+1} = H(\boldsymbol{\epsilon}^{n+1} - \boldsymbol{\epsilon}^n) + \mathcal{NN}_{\boldsymbol{\theta}}(\boldsymbol{\sigma}^n, \boldsymbol{\epsilon}^n)$$



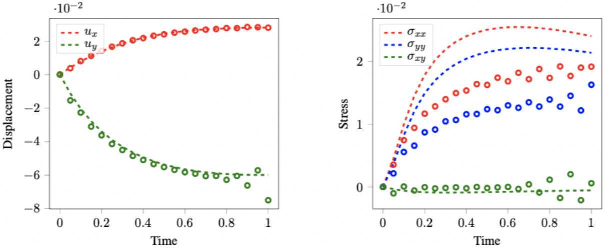
- Comparison with space varying linear elasticity approximation

$$\boldsymbol{\sigma} = H(x, y)\epsilon$$

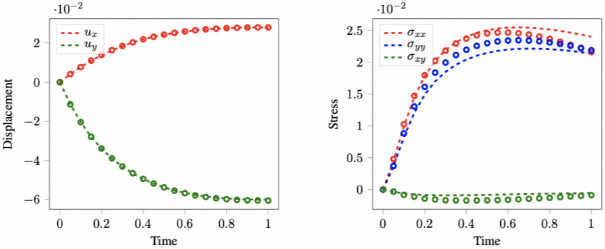


Space Varying Linear Elasticity | **NN** | **True**

Poroelasticity



(a) Space Varying Linear Elasticity



(b) NN-based Viscoelasticity

A Paradigm for Inverse Modeling

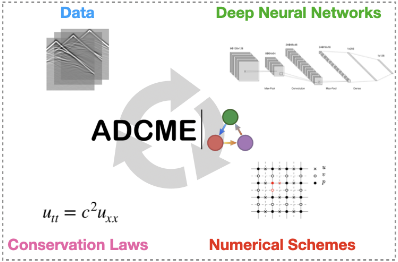
- Most inverse modeling problems can be classified into 4 categories. To be more concrete, consider the PDE for describing physics

$$\nabla \cdot (\theta \nabla u(x)) = 0 \quad \mathcal{BC}(u(x)) = 0 \tag{2}$$

We observe some quantities depending on the solution u and want to estimate θ.

Expression	Description	ADCME Solution	Note
$\nabla \cdot (c\nabla u(x)) = 0$	Parameter Inverse Problem	Discrete Adjoint State Method	c is the minimizer of the error functional
$\nabla \cdot (f(x)\nabla u(x)) = 0$	Function Inverse Problem	Neural Network Functional Approximator	$f(x) \approx \mathcal{NN}_w(x)$
$\nabla \cdot (f(u)\nabla u(x)) = 0$	Relation Inverse Problem	Residual Learning Physics Constrained Learning (PCL)	$f(u) \approx \mathcal{NN}_w(u)$
$\nabla \cdot (\varpi\nabla u(x)) = 0$	Stochastic Inverse Problem	Physical Generative Neural Networks (PhysGNN)	$\varpi = \mathcal{NN}_w(v_{\text{latent}})$

A General Approach to Inverse Modeling



AdFem.jl
Finite Element Library for Inverse Modeling
https://github.com/kailaix/AdFem.jl

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

Reference

- Methodology and Implementation:
  - Physics Constrained Learning for Data-driven Inverse Modeling from Sparse Observations (Core techniques!)
  - A General Approach to Seismic Inversion with Automatic Differentiation
  - Time-lapse Full-waveform Inversion for Subsurface Flow Problems with Intrusive Automatic Differentiation
- Consistutive Modeling:
  - Learning Constitutive Relations from Indirect Observations Using Deep Neural Networks
  - Learning Constitutive Relations using Symmetric Positive Definite Neural Networks
  - Inverse Modeling of Viscoelasticity Materials using Physics Constrained Learning
- Learning Spatially-varying Fields:
  - Solving Inverse Problems in Steady State Navier-Stokes Equations using Deep Neural Networks