Machine Learning for Inverse Problems in Computational Engineering

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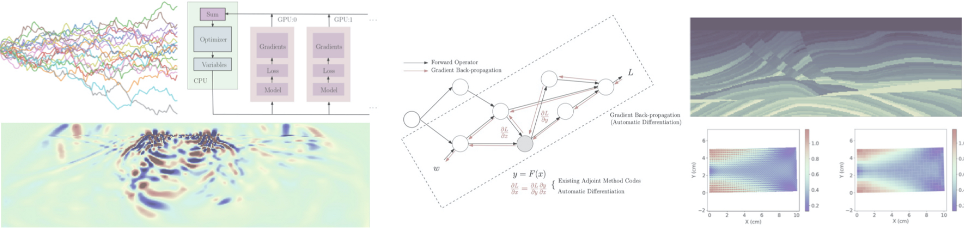
https://github.com/kailaix/ADCME.jl



Outline

Inverse Modeling

Forward Problem

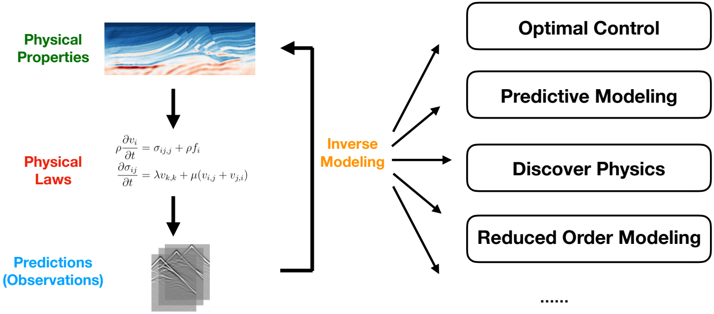
Model Parameters → Physical Laws → Prediction of Observations

Inverse Problem

Observations → Physical Laws → Estimation of Parameters

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.t



Inverse Modeling

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

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

- 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 or differential algebraic equations (DAEs), e.g., $H(u_h', u_h, t; \theta) = 0$. 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?

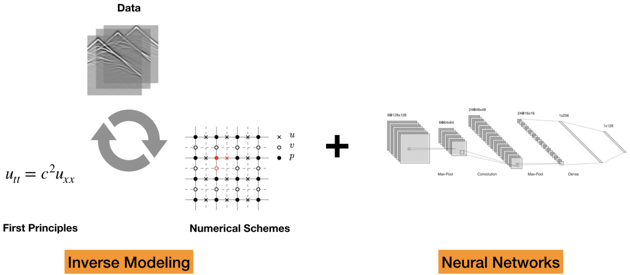
- Koopman operator in dynamical systems.
- Constitutive relations in solid mechanics.
- Turbulent closure relations in fluid mechanics.
- ...

The candidate solution space is infinite dimensional.

Machine Learning for Computational Engineering

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

- 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.

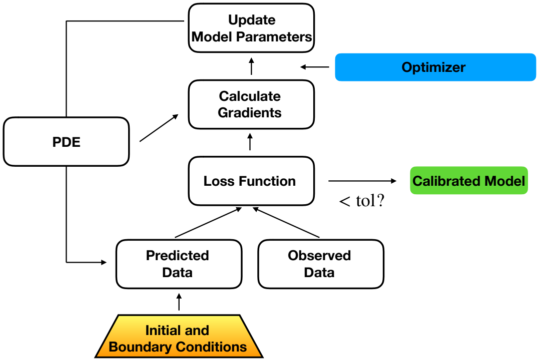


Gradient Based Optimization

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

- We can now apply a gradient-based optimization method to (1).
- 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

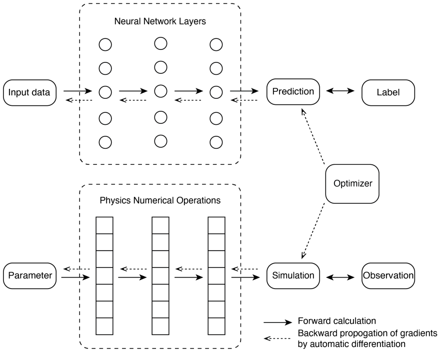
Back-propagation

||

Reverse-mode Automatic Differentiation

||

Discrete Adjoint-State Method



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.

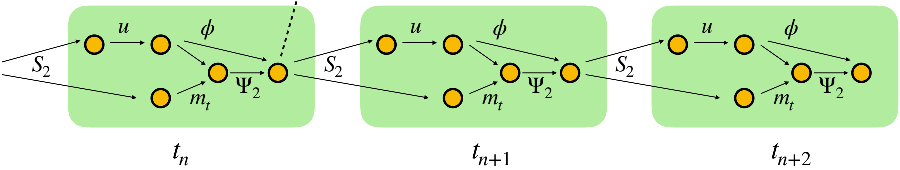
Margossian CC. A review of automatic differentiation and its efficient implementation. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery. 2019 Jul;9(4):e1305.

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

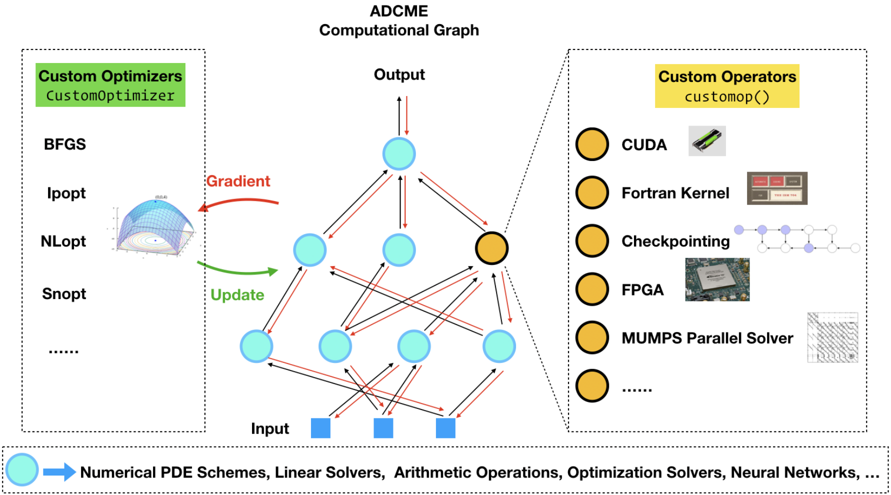
Computational Graph for Numerical Schemes

- 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.

$$\phi(S_2^{n+1} - S_2^n) - \nabla \cdot \left(m_2(S_2^{n+1}) K \nabla \Psi_2^n\right) \Delta t = \left(q_2^n + q_1^n \frac{m_2(S_2^{n+1})}{m_1(S_2^{n+1})}\right) \Delta t$$

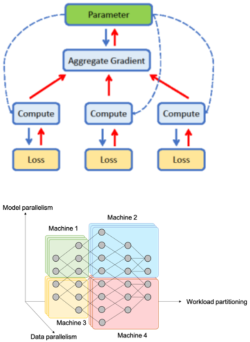


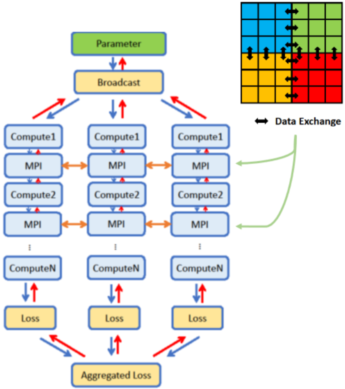
ADCME: Computational-Graph-based Numerical Simulation



Parallel Computing

- Parallel computing is essential for accelerating simulation and satisfying demanding memory requirements.

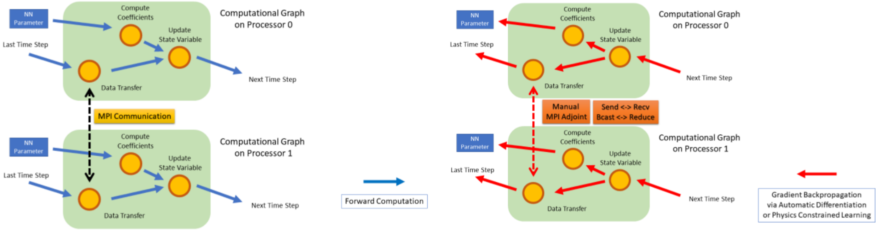




Deep Learning Data/Model Parallelism **Scientific Computing Mixed Parallelism**

Distributed Optimization

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



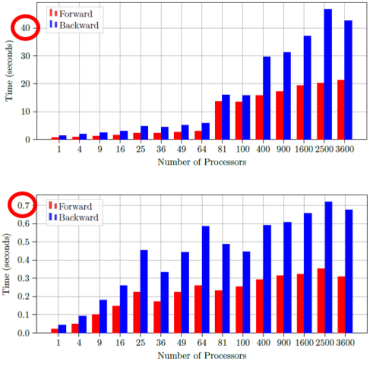
- Key idea: Everything is an operator. Computation and communications are converters of data streams (tensors) through the computational graph.

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

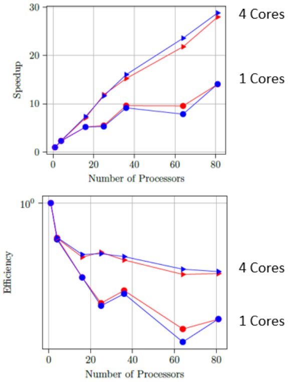
Interoperability with Hypre

$$\nabla \cdot (\textcolor{red}{\mathrm{NN}_\theta(\mathrm{x})} \nabla u(\mathrm{x})) = f(\mathrm{x}) \qquad \mathrm{x} \in \Omega$$
$$u(\mathrm{x}) = 0 \qquad \mathrm{x} \in \partial\Omega$$

The discretization leads to a linear system, which is solved using Hypre.



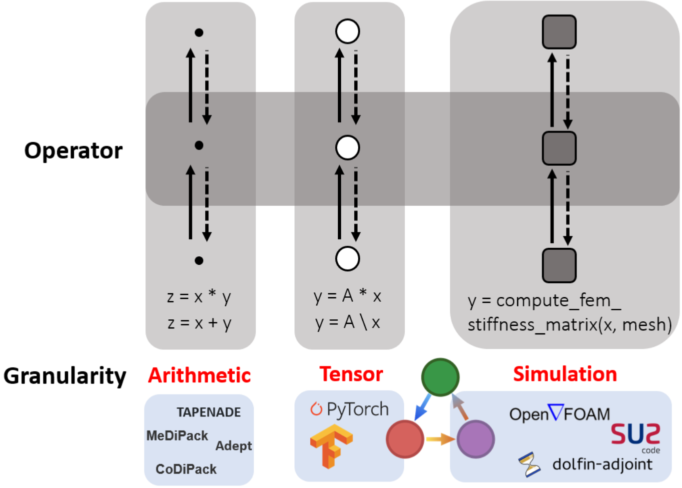
Weak Scalability



Strong Scalability

Granularity of Automatic Differentiation

- Coarser granularity gives researchers more control over gradient back-propagation.



Outline

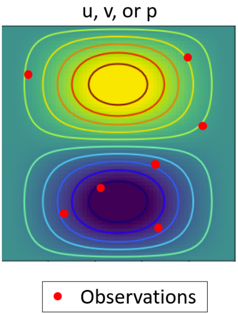
Inverse Modeling of the Stokes Equation

- The governing equation for the Stokes problem

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

- The weak form is given by

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



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
```

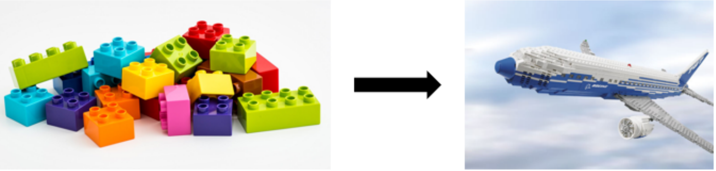
Inverse Modeling of the Stokes Equation

- 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)
```



ADCME/AdFem **Simulation Program**

Outline

Constitutive Modeling

$$
\begin{aligned}
\underbrace{\sigma_{ij,j}}_{\text{stress}} + \rho \underbrace{b_i}_{\text{external force}} &= \rho \underbrace{\ddot{u}_i}_{\text{velocity}} \\
\underbrace{\varepsilon_{ij}}_{\text{strain}} &= \frac{1}{2}(u_{j,i} + u_{i,j})
\end{aligned} \tag{2}
$$

- **Observable**: external/body force b_i, displacements u_i (strains ε_{ij} can be computed from u_i); density ρ is known.
- **Unobservable**: stress σ_{ij}.
- Data-driven Constitutive Relations: modeling the strain-stress relation using a neural network

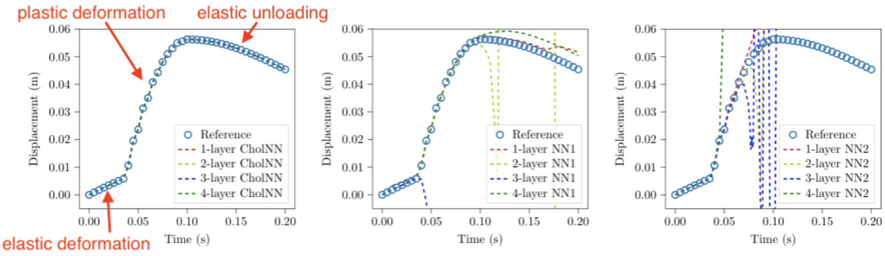
$$
\boxed{\text{stress} = \mathcal{M}_\theta(\text{strain}, \ldots)} \tag{3}
$$

and the neural network is trained by coupling Eq. 2 and Eq. 3.

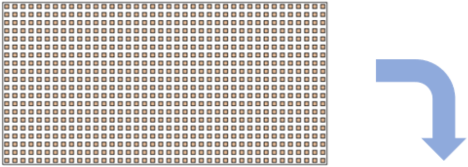
Modeling Elasto-plasticity

- Comparison of different neural network architectures

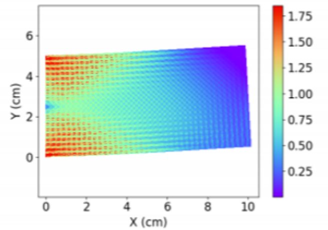
$$\boldsymbol{\sigma}^{n+1} = \mathsf{L}_\theta(\epsilon^{n+1}, \epsilon^n, \boldsymbol{\sigma}^n)\mathsf{L}_\theta(\epsilon^{n+1}, \epsilon^n, \boldsymbol{\sigma}^n)^T(\epsilon^{n+1} - \epsilon^n) + \boldsymbol{\sigma}^n$$
$$\boldsymbol{\sigma}^{n+1} = \mathsf{NN}_\theta(\epsilon^{n+1}, \epsilon^n, \boldsymbol{\sigma}^n)$$
$$\boldsymbol{\sigma}^{n+1} = \mathsf{NN}_\theta(\epsilon^{n+1}, \epsilon^n, \boldsymbol{\sigma}^n) + \boldsymbol{\sigma}^n$$



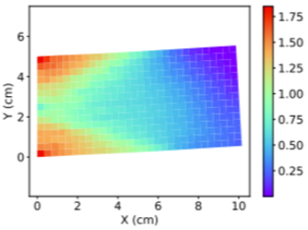
Modeling Elasto-plasticity: Multi-scale



Fiber Reinforced Thin Plate



Reference von Mises stress



SPD-NN

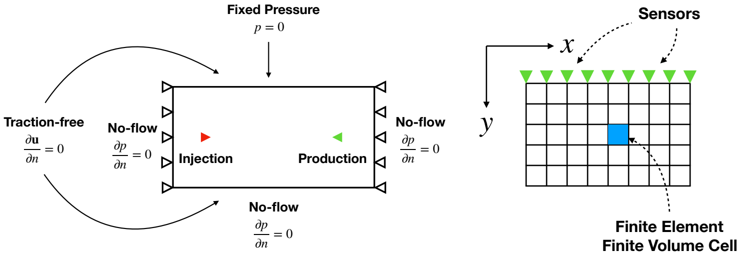
Poroelasticity

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

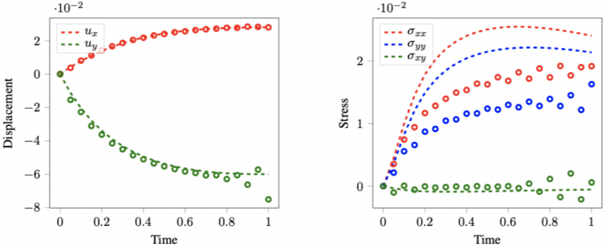
$$
\begin{aligned}
\operatorname{div}\boldsymbol{\sigma}(\mathrm{u}) - b\nabla p &= 0\\
\frac{1}{M}\frac{\partial p}{\partial t} + b\frac{\partial \epsilon_v(\mathrm{u})}{\partial t} - \nabla\cdot\left(\frac{k}{B_f\mu}\nabla p\right) &= f(x,t)\\
\boldsymbol{\sigma} &= \boldsymbol{\sigma}(\epsilon, \dot{\epsilon})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

- Approximate the constitutive relation by a neural network

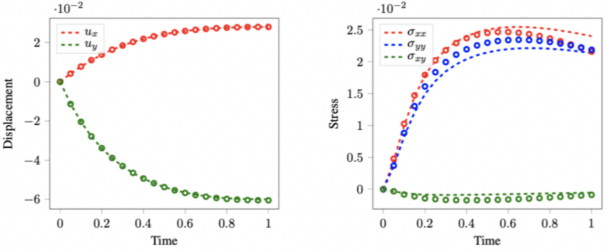
$$
\boldsymbol{\sigma}^{n+1} = \mathcal{NN}_{\boldsymbol{\theta}}(\boldsymbol{\sigma}^n, \boldsymbol{\epsilon}^n) + H\boldsymbol{\epsilon}^{n+1}
$$



Poroelasticity



(a) Space Varying Linear Elasticity

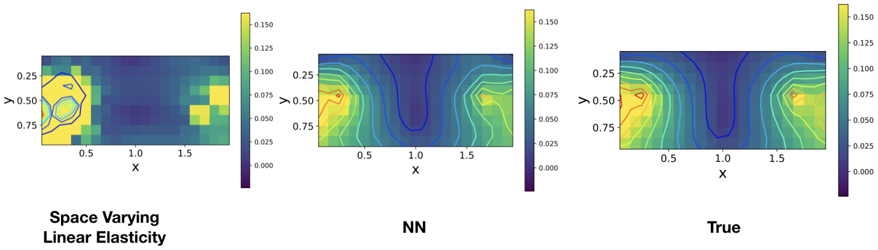


(b) NN-based Viscoelasticity

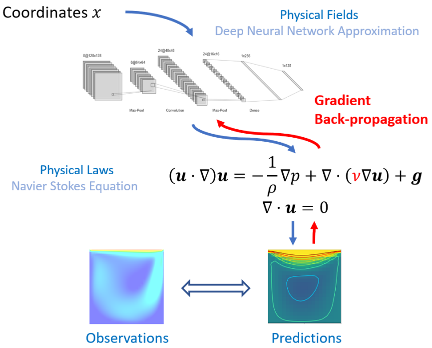
Poroelasticity

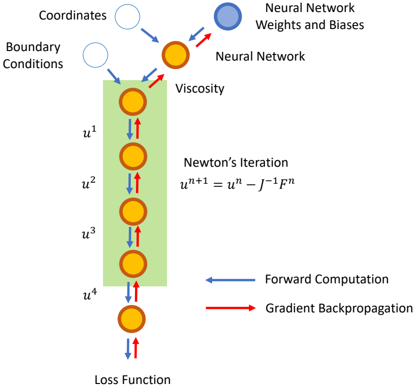
- Comparison with space varying linear elasticity approximation

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

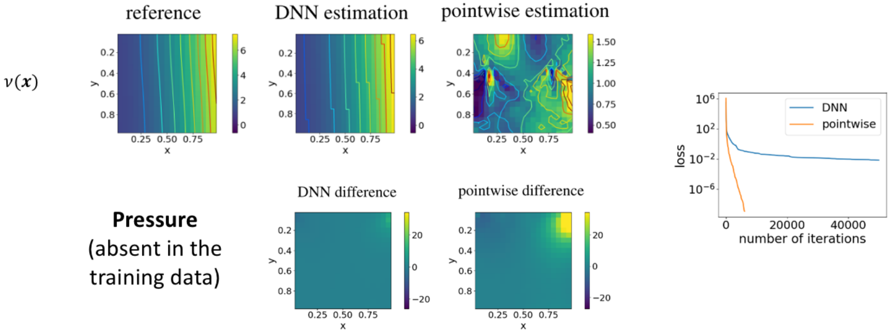


Navier-Stokes Equation



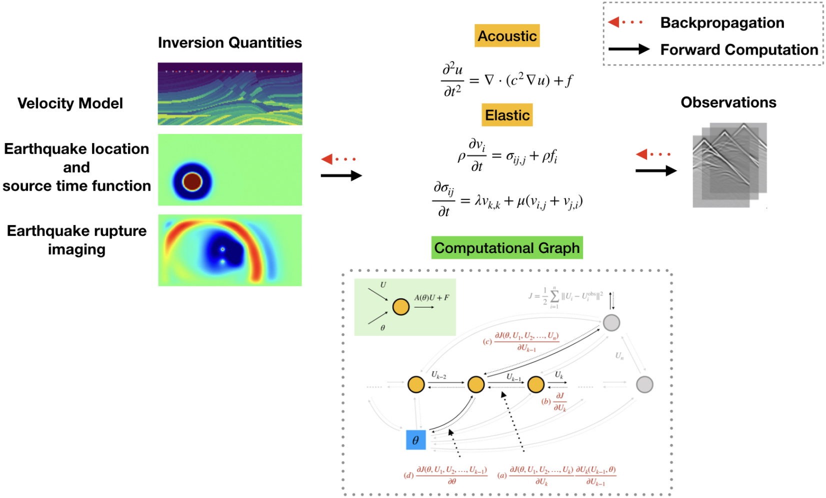


- Data: (u, v)
- Unknown: $\nu(\mathrm{x})$ (represented by a deep neural network)
- Prediction: p (absent in the training data)
- The DNN provides regularization, which generalizes the estimation better!



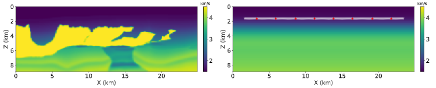
ADSeismic.jl: A General Approach to Seismic Inversion

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

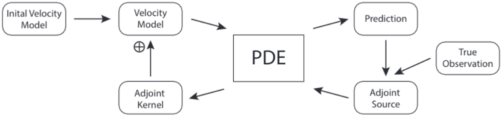


- Estimate velocity models from seismic observations.

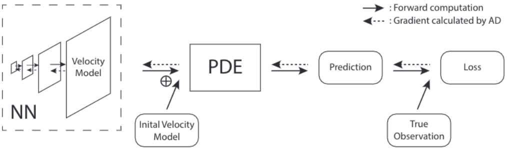
$$\frac{\partial^2 u}{\partial t^2} = \nabla\cdot(m^2\nabla u)+f$$



(a) Traditional FWI:

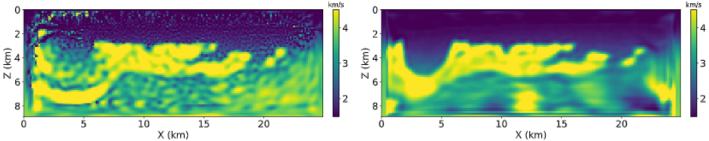


(b) NNFWI:

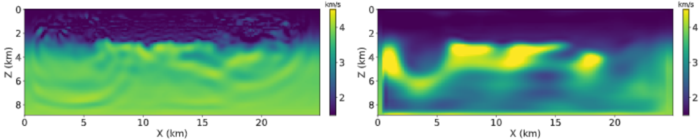


NNFWI: Neural-network-based Full-Waveform Inversion

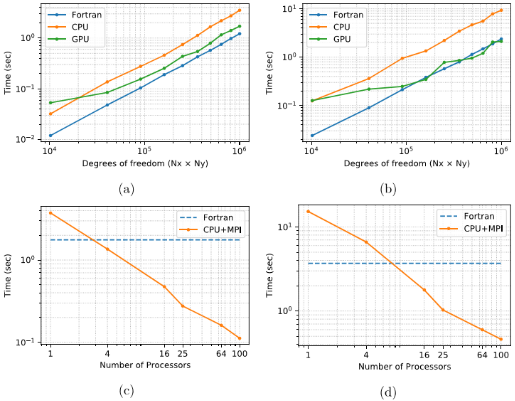
- Inversion results with a noise level $\sigma = \sigma_0$



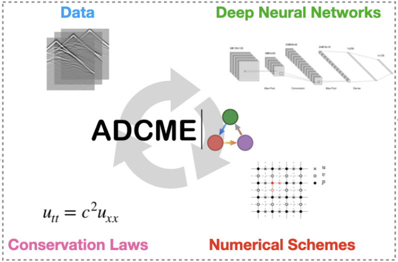
- Inversion results for the same loss function value:



- 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



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