Machine Learning for Computational Engineering

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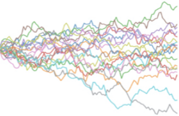
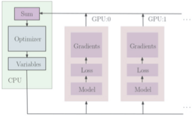
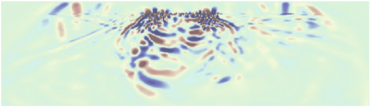
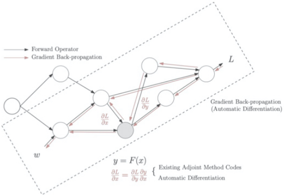
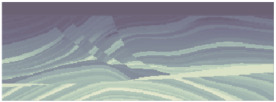
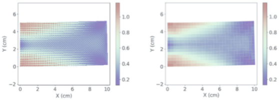












Outline

Inverse Modeling

Forward Problem

Model Parameters → Physical Laws → Prediction of Observations

Inverse Problem

Observations → Physical Laws → Estimation of Parameters

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., $L_h(u_h) = \|u_h - u_{\text{obs}}\|_2^2$.
- 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.,

$$F_h(\theta, u_h) = \mathsf{A}(\theta)u_h - f_h = 0$$

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.
- ...

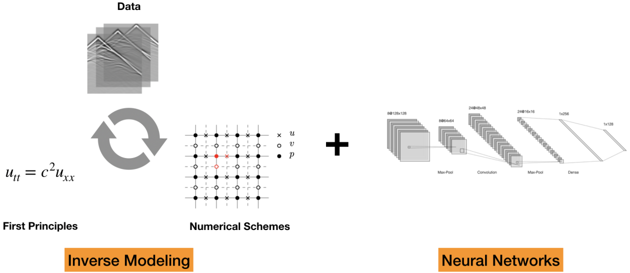
The candidate solution space is infinite dimensional.

Machine Learning for Computational Engineering

$$\min_{\theta} L_h(u_h) \quad \text{s.t.} \quad \boxed{F_h(\mathrm{N}_\theta, u_h) = 0} \leftarrow \text{Solved numerically}$$

1. Use a deep neural network to approximate the (high dimensional) unknown function;
2. Solve u_h from the physical constraint using a numerical PDE solver;
3. Apply an unconstrained optimizer to the reduced problem

$$\min_{\theta} L_h(u_h(\theta))$$

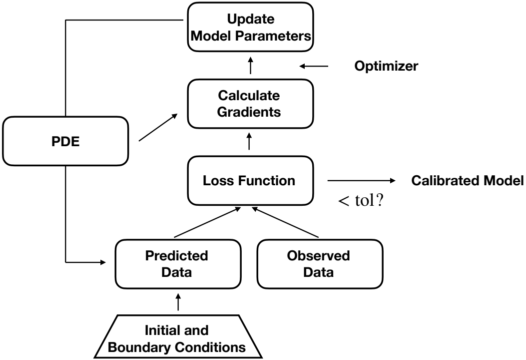


Gradient Based Optimization

$$\min_\theta L_h(u_h(\theta))$$

- Steepest descent method:

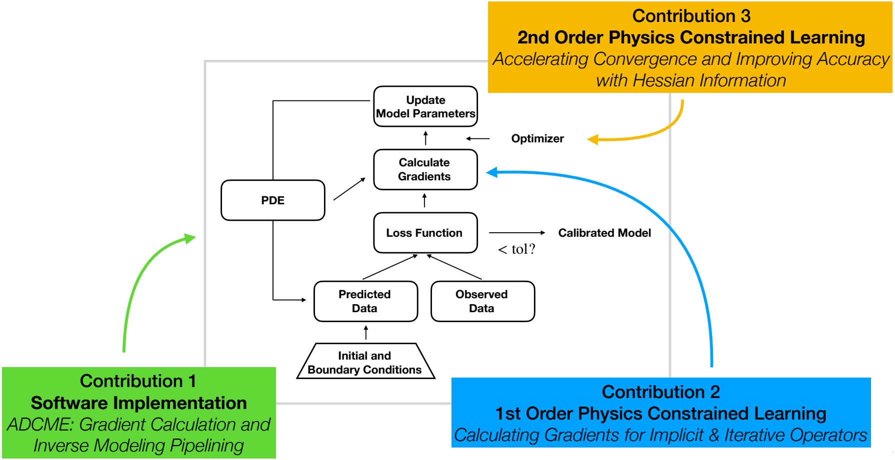
$$\theta_{k+1} \leftarrow \theta_k - \alpha_k \nabla_\theta L_h(u_h(\theta_k))$$

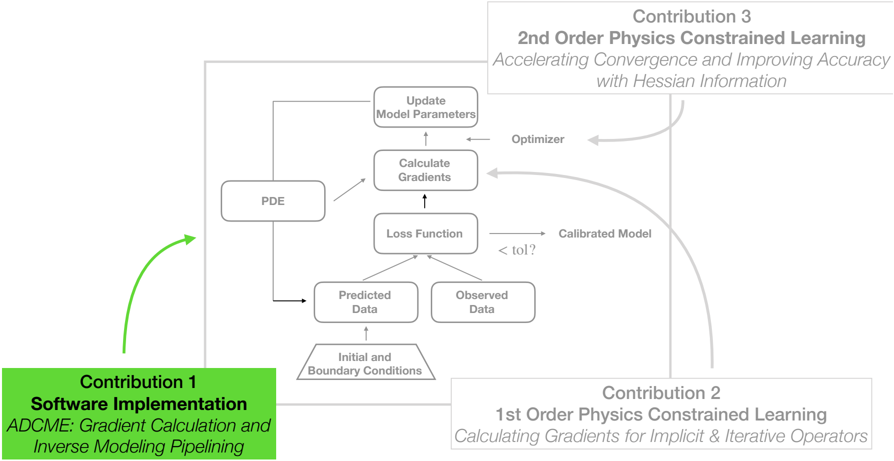


Contributions

Goal

Develop algorithms and tools for solving inverse problems by combining DNNs and numerical PDE solvers.

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2nd Order Physics Constrained Learning
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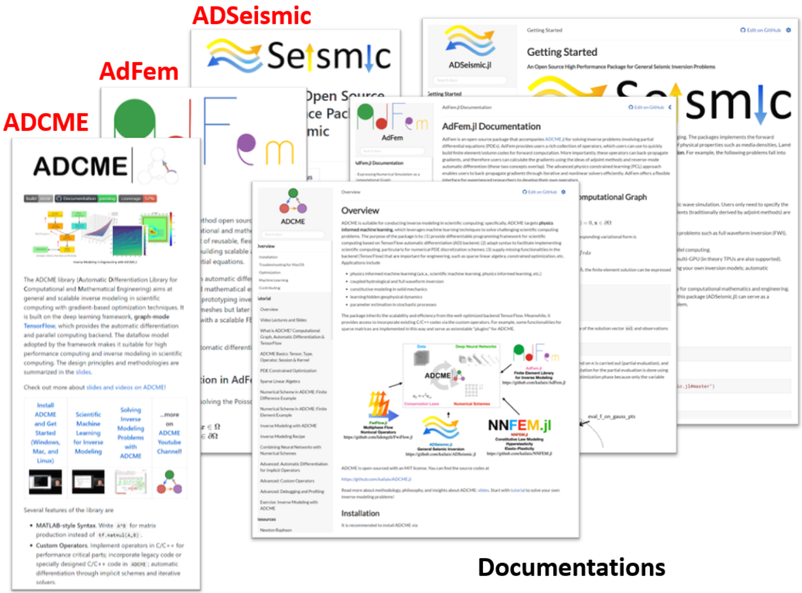
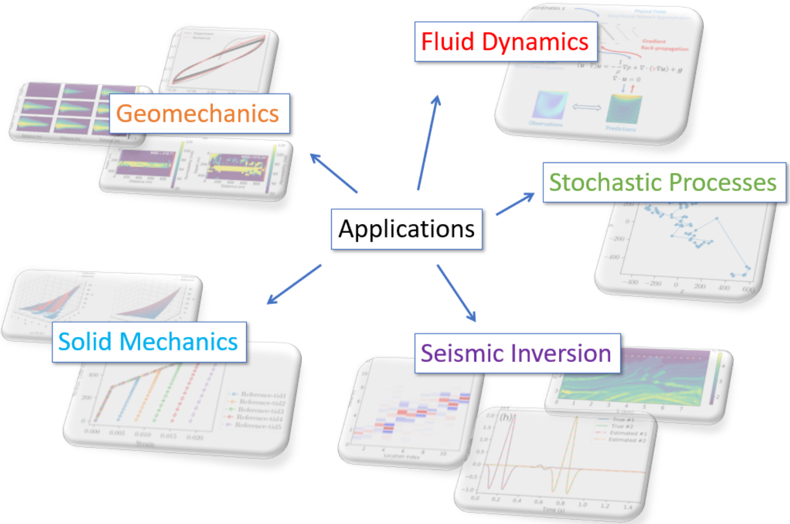
Ecosystem for Inverse Modeling



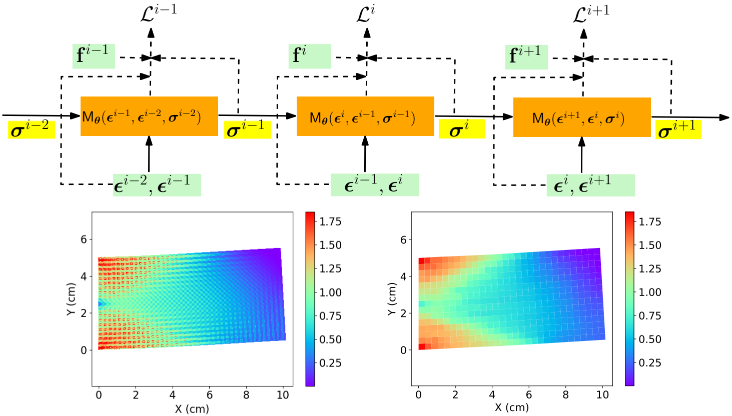
Applications



See the publication list at: https://github.com/kailaix/ADCME.jl

Applications: Solid Mechanics

- Modeling constitutive relations with deep neural networks

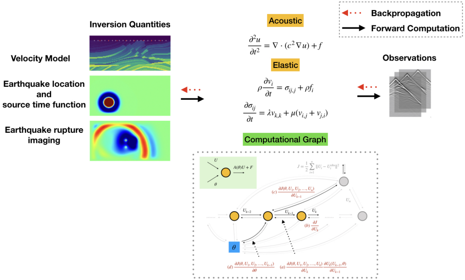


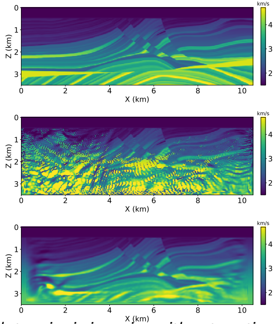
Kailai Xu*, Daniel Z. Huang*, and Eric Darve. *Learning constitutive relations using symmetric positive definite neural networks*. Journal of Computational Physics 428 (2021): 110072.

Daniel Z. Huang*, Kailai Xu*, Charbel Farhat, and Eric Darve. *Learning constitutive relations from indirect observations using deep neural networks*. Journal of Computational Physics 416 (2020): 109491.

Applications: Seismic Inversion

- **ADSeismic**: AD + Seismic Inversion
- **NNFWI**: DNN + FWI

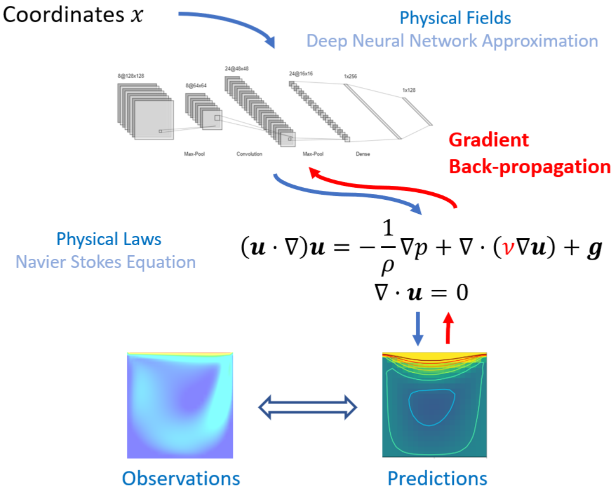




Weiqiang Zhu*, Kailai Xu*, Eric Darve, and Gregory C. Beroza. *A general approach to seismic inversion with automatic differentiation*. Computers & Geosciences (2021): 104751.

Weiqiang Zhu*, Kailai Xu*, Eric Darve, Biondo Biondi, and Gregory C. Beroza. *Integrating Deep Neural Networks with Full-waveform Inversion: Reparametrization, Regularization, and Uncertainty Quantification*. Submitted.

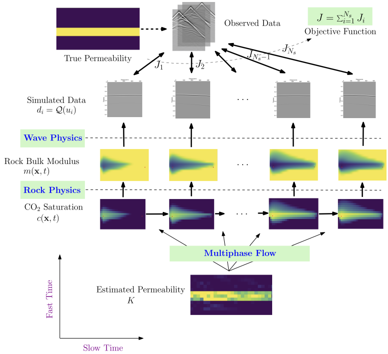
Applications: Fluid Dynamics

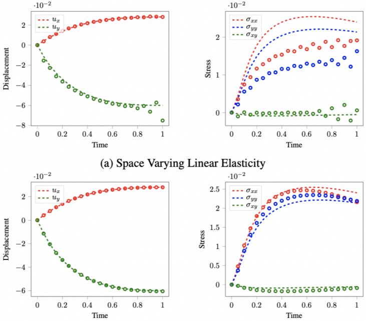


Tiffany Fan, Kailai Xu, Jay Pathak, and Eric Darve. *Solving Inverse Problems in Steady State Navier-Stokes Equations using Deep Neural Networks*. PGAI-AAAI (2020)

Applications: Geo-mechanics

- Learning intrinsic fluid properties from indirect seismic data using automatic differentiation
- Modeling viscoelasticity using deep neural networks





(a) Space Varying Linear Elasticity

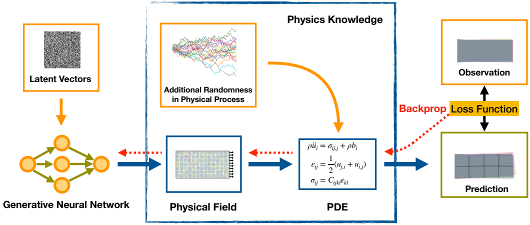
(b) NN-based Viscoelasticity

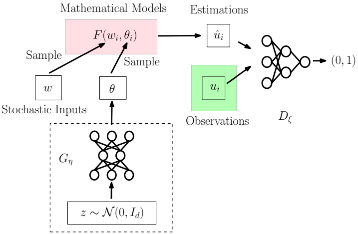
Dongzhuo Li*, Kailai Xu*, Jerry M. Harris, and Eric Darve. *Coupled Time-Lapse Full-Waveform Inversion for Subsurface Flow Problems Using Intrusive Automatic Differentiation*. Water Resources Research 56, no. 8 (2020): e2019WR027032.

Kailai Xu, Alexandre M. Tartakovsky, Jeff Burghardt, and Eric Darve. *Learning Viscoelasticity Models from Indirect Data using Deep Neural Networks*. Submitted.

Applications: Stochastic Processes

- Approximating unknown distributions with deep neural networks in a stochastic process/differential equation.
  - **Adversarial Inverse Modeling (AIM)**: adversarial training
  - **Physics Generative Neural Networks (PhysGNN)**: optimal transport





Kailai Xu and Eric Darve. *Solving Inverse Problems in Stochastic Models using Deep NeuralNetworks and Adversarial Training*. Submitted.

Kailai Xu, Weiqiang Zhu, and Eric Darve. *Learning Generative Neural Networks with Physics Knowledge*. Submitted.

Automatic Differentiation

Bridging the technical gap between deep learning and inverse modeling:

Mathematical Fact

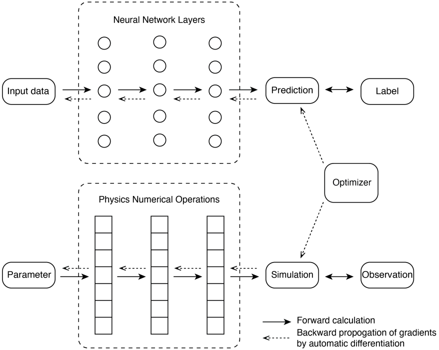
Back-propagation

||

Reverse-mode Automatic Differentiation

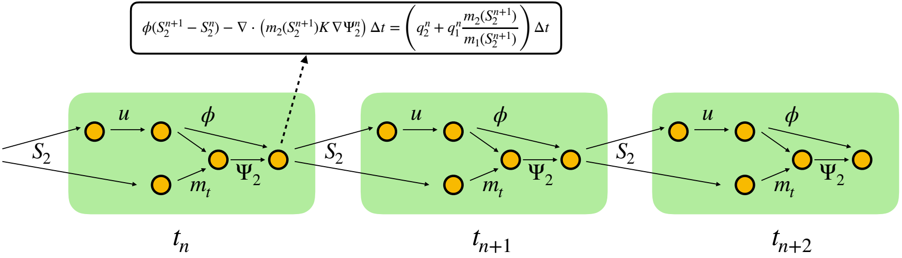
||

Discrete Adjoint-State Method

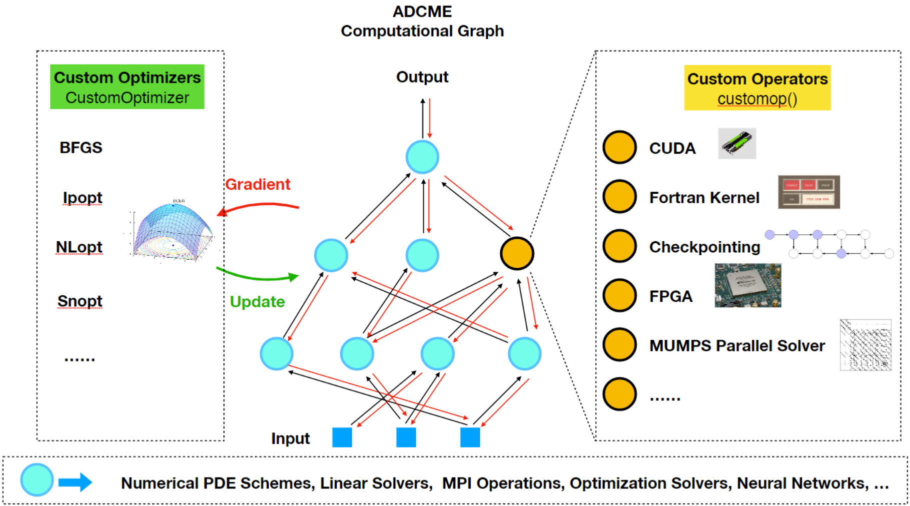


Computational Graph for Numerical Schemes

- 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

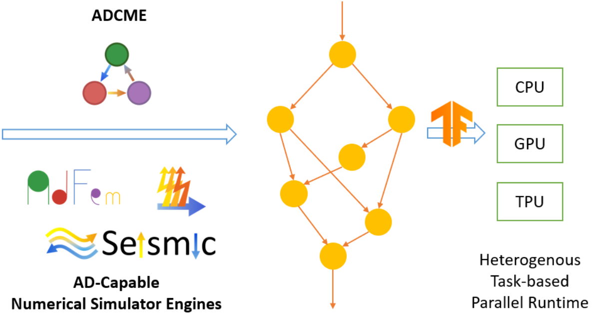


How ADCME works

- ADCME translates your numerical simulation codes to computational graph and then the computations are delegated to a heterogeneous task-based parallel computing environment through TensorFlow runtime.

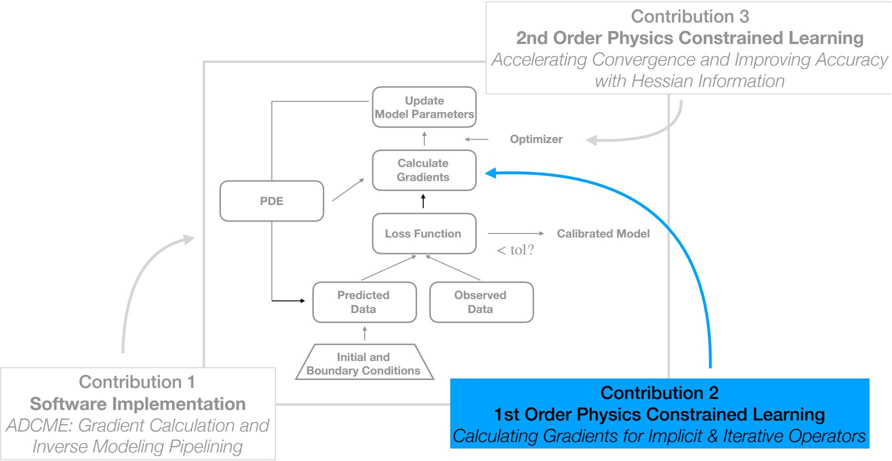
$$
\begin{aligned}
\operatorname{div} \sigma(u) &= f(x) && x \in \Omega \\
\sigma(u) &= C\varepsilon(u) && \\
u(x) &= u_0(x) && x \in \Gamma_u \\
\sigma(x)n(x) &= t(x) && x \in \Gamma_n
\end{aligned}
$$

```
mmesh = Mesh(50, 50, 1/50, degree=2)

left = bcnode((x,y)->x<1e-5, mmesh)
right = bcedge((x1,y1,x2,y2)->(x1>0.049-1e-5) && (x2>0.049-1e-5), mmesh)

t1 = eval_f_on_boundary_edge((x,y)->1.0e-4, right, mmesh)
t2 = eval_f_on_boundary_edge((x,y)->0.0, right, mmesh)
rhs = compute_fem_traction_term(t1, t2, right, mmesh)

nu = 0.3
x = gauss_nodes(mmesh)
E = abs(fc(x, [20, 20, 20, 1])|>squeeze)
# E = constant(eval_f_on_gauss_pts(f, mmesh))

D = compute_plane_stress_matrix(E, nu*ones(get_ngauss(mmesh)))
K = compute_fem_stiffness_matrix(D, mmesh)

bdval = [eval_f_on_boundary_node((x,y)->0.0, left, mmesh);
         eval_f_on_boundary_node((x,y)->0.0, left, mmesh)]
DOF = [left;left .+ mmesh.ndof]
K, rhs = impose_Dirichlet_boundary_conditions(K, rhs, DOF, bdval)
u = K\rhs
```



Summary

- Mathematically equivalent techniques for calculating gradients:
  - gradient back-propagation (DNN)
  - discrete adjoint-state methods (PDE)
  - reverse-mode automatic differentiation
- Computational graphs bridge the gap between gradient calculations in numerical PDE solvers and DNNs.
- ADCME extends the capability of TensorFlow to PDE solvers, providing users a single piece of software for numerical simulations, deep learning, and optimization.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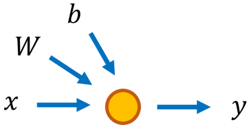
Calculating Gradients for Implicit & Iterative Operators

Motivation

- Most AD frameworks only deal with explicit operators, i.e., the functions that has analytical derivatives, or composition of these functions.
- Many scientific computing algorithms are iterative or implicit in nature.

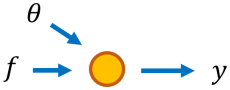
Linear/Nonlinear	Explicit/Implicit	Expression
Linear	Explicit	$y = Ax$
Nonlinear	Explicit	$y = F(x)$
Linear	**Implicit**	$Ay = x$
Nonlinear	**Implicit**	$F(x, y) = 0$

DNN: Explicit



$$y = \sigma(Wx + b)$$

Numerical Schemes: Implicit, Iterative



$$A(y, \theta)y = f$$

Example

- Consider a function $f : x \to y$, which is implicitly defined by

$$F(x, y) = x^3 - (y^3 + y) = 0$$

If not using the cubic formula for finding the roots, the forward computation consists of iterative algorithms, such as the Newton's method and bisection method

$y^0 \leftarrow 0$
$k \leftarrow 0$
while $|F(x, y^k)| > \epsilon$ **do**
  $\delta^k \leftarrow F(x, y^k)/F'_y(x, y^k)$
  $y^{k+1} \leftarrow y^k - \delta^k$
  $k \leftarrow k + 1$
end while
Return y^k

$l \leftarrow -M$, $r \leftarrow M$, $m \leftarrow 0$
while $|F(x, m)| > \epsilon$ **do**
  $c \leftarrow \frac{a+b}{2}$
  if $F(x, m) > 0$ **then**
    $a \leftarrow m$
  else
    $b \leftarrow m$
  end if
end while
Return c

Example

- An efficient way to do automatic differentiation is to apply the implicit function theorem. For our example, $F(x, y) = x^3 - (y^3 + y) = 0$; treat y as a function of x and take the derivative on both sides

$$3x^2 - 3y(x)^2 y'(x) - y'(x) = 0 \Rightarrow y'(x) = \frac{3x^2}{3y^2 + 1}$$

The above gradient is exact.

Can we apply the same idea to inverse modeling?

Physics Constrained Learning (PCL)

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

- Assume that we solve for $u_h = G_h(\theta)$ with $F_h(\theta, u_h) = 0$, and then

$$\tilde{L}_h(\theta) = L_h(G_h(\theta))$$

- Applying the implicit function theorem

$$\frac{\partial F_h(\theta, u_h)}{\partial \theta} + \frac{\partial F_h(\theta, u_h)}{\partial u_h} \frac{\partial G_h(\theta)}{\partial \theta} = 0 \Rightarrow \frac{\partial G_h(\theta)}{\partial \theta} = -\Big(\frac{\partial F_h(\theta, u_h)}{\partial u_h} \Big)^{-1} \frac{\partial F_h(\theta, u_h)}{\partial \theta}$$

- Finally we have

$$\boxed{\frac{\partial \tilde{L}_h(\theta)}{\partial \theta} = \frac{\partial L_h(u_h)}{\partial u_h} \frac{\partial G_h(\theta)}{\partial \theta} = -\frac{\partial L_h(u_h)}{\partial u_h} \left(\frac{\partial F_h(\theta, u_h)}{\partial u_h}\Big|_{u_h = G_h(\theta)} \right)^{-1} \frac{\partial F_h(\theta, u_h)}{\partial \theta}\Big|_{u_h = G_h(\theta)}}$$

Penalty Methods

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

- Penalty Method: parametrize f with f_θ (DNNs, linear finite element basis, radial basis functions, etc.) and incorporate the physical constraint as a penalty term (regularization, prior, ...) in the loss function.

$$\min_{\theta,\, u_h} L_h(u_h) + \lambda \|F_h(f_\theta, u_h)\|_2^2$$

  + Easy to implement (no need for differentiating numerical solvers)
  − May not satisfy physical constraint $F_h(f_\theta, u_h) = 0$ accurately;
  − High dimensional optimization problem; both θ and u_h are variables.

Physics Constrained Learning for Stiff Problems

- PCL is superior for stiff problems.
- Consider a model problem

$$\min_\theta \|u-u_0\|_2^2 \qquad \text{s.t. } Au=\theta y$$

$$\text{PCL}: \qquad \min_\theta \tilde L_h(\theta) = \|\theta A^{-1}y-u_0\|_2^2 = (\theta-1)^2\|u_0\|_2^2$$

$$\text{Penalty Method}: \qquad \min_{\theta,u_h} \tilde L_h(\theta,u_h) = \|u_h-u_0\|_2^2+\lambda\|Au_h-\theta y\|_2^2$$

Theorem

The condition number of A_λ *is*

$$\liminf_{\lambda\to\infty}\kappa(\mathrm{A}_\lambda)=\kappa(A)^2, \qquad \mathrm{A}_\lambda=\begin{bmatrix} I & 0\\ \sqrt{\lambda}A & -\sqrt{\lambda}y\end{bmatrix}, \qquad \mathrm{y}=\begin{bmatrix}u_0\\0\end{bmatrix}$$

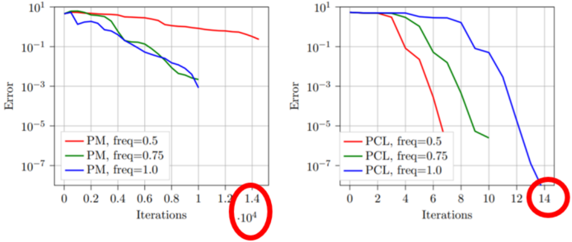
and therefore, the condition number of the unconstrained optimization problem from the penalty method is equal to the square of the condition number of the PCL asymptotically.

Physics Constrained Learning for Stiff Problems

Parameter Inverse Problem

$$\Delta u + k^2 g(x) u = 0$$
$$g(x) = 5x^2 + 2y^2$$

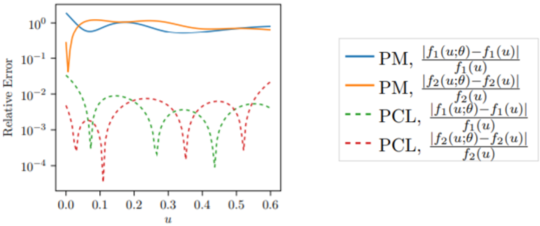
$$g_\theta(x) = \theta_1 x^2 + \theta_2 y^2 + \theta_3 xy + \theta_4 x + \theta_5 y + \theta_6$$



Approximate Unknown Functions using DNNs

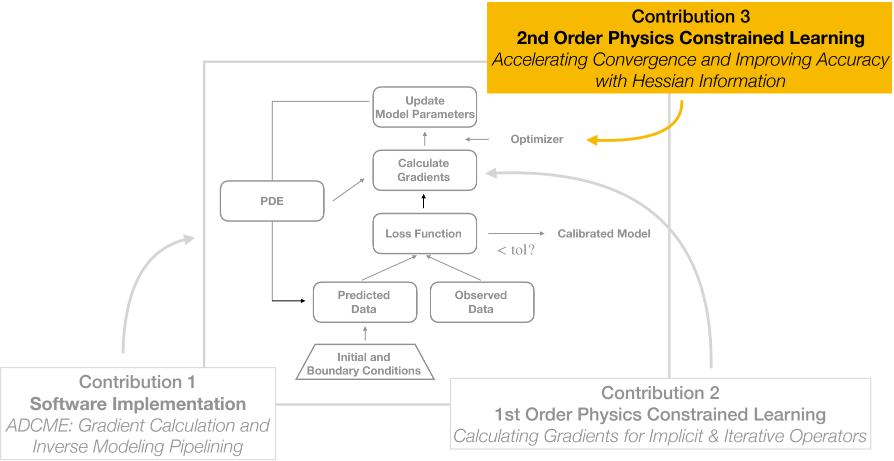
$$-\nabla \cdot (\boldsymbol{f}(u) \nabla u) = h(\boldsymbol{x})$$

$$\boldsymbol{f}(u) = \begin{bmatrix} NN(u;\theta_1) & 0 \\ 0 & NN(u;\theta_2) \end{bmatrix}$$



Summary

- Implicit and iterative operators are ubiquitous in numerical PDE solvers. These operators are insufficiently treated in deep learning software and frameworks.
- PCL helps you calculate gradients of implicit/iterative operators efficiently.
- PCL leads to faster convergence and better accuracy compared to penalty methods for stiff problems.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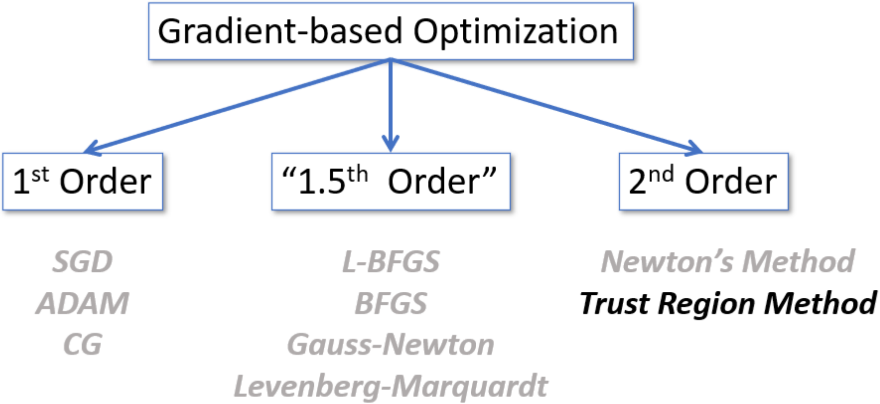
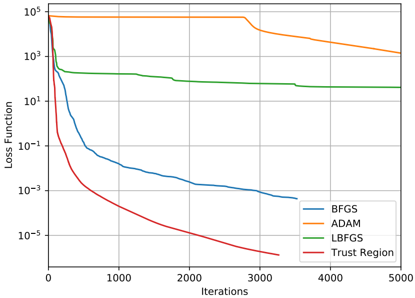

Gradient-based Optimization
1st Order
"1.5th Order"
2nd Order
SGD
ADAM
CG
L-BFGS
BFGS
Gauss-Newton
Levenberg-Marquardt
Newton's Method
Trust Region Method

Overview



Goal

Accelerate convergence and improve accuracy with Hessian information

Challenge

Calculate Hessians for coupled systems of PDEs and DNNs

Trust Region vs. Line Search

Trust Region

- Approximate $f(x_k + p)$ by a model quadratic function

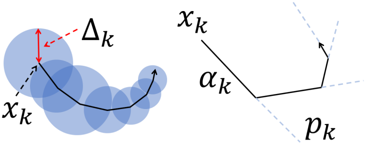
$$m_k(p) = f_k + g_k^T p + \frac{1}{2} p^T B_k p$$

$$f_k = f(x_k), g_k = \nabla f(x_k), B_k = \nabla^2 f(x_k)$$

- Solve the optimization problem within a trust region $\|p\| \leq \Delta_k$

$$p_k = \arg\min_p \; m_k(p) \quad \text{s.t. } \|p\| \leq \Delta_k$$

- If decrease in $f(x_k + p_k)$ is sufficient, then update the state $x_{k+1} = x_k + p_k$; otherwise, $x_{k+1} = x_k$ and improve Δ_k.



Trust Region   Line Search

Line Search

- Determine a descent direction p_k
- Determine a step size α_k that sufficiently reduces $f(x_k + \alpha_k p_k)$
- Update the state $x_{k+1} = x_k + \alpha_k p_k$

Second Order Physics Constrained Learning

- Consider a composite function with a vector input x and scalar output

$$v = f(G(x)) \tag{1}$$

- Define

$$f_{,k}(y) = \frac{\partial f(y)}{\partial y_k}, \quad f_{,kl}(y) = \frac{\partial^2 f(y)}{\partial y_k \partial y_l}$$
$$G_{k,l}(x) = \frac{\partial G_k(x)}{\partial x_l}, \quad G_{k,lr}(x) = \frac{\partial^2 G_k(x)}{\partial x_l \partial x_r}$$

- Differentiate Equation (1) with respect to x_i

$$\frac{\partial v}{\partial x_i} = f_{,k} G_{k,i} \tag{2}$$

- Differentiate Equation (2) with respect to x_j

$$\boxed{\frac{\partial^2 v}{\partial x_i \partial x_j} = f_{,kr} G_{k,i} G_{r,j} + f_{,k} G_{k,ij}}$$

Second Order Physics Constrained Learning

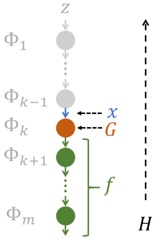
In the vector form,

$$\boxed{\nabla^2 v = (\nabla G)^T \nabla^2 f (\nabla G) + \nabla^2(\bar{G}^T G) \qquad \bar{G} = \nabla f}$$

- Consider a function composed of a sequence of computations

$$v = \Phi_m(\Phi_{m-1}(\cdots(\Phi_1(z))))$$

Initialize $H \leftarrow 0$
for $k = m-1, m-2, \ldots, 1$ **do**
    Define $f := \Phi_m(\Phi_{m-1}(\cdots(\Phi_{k+1}(\cdot))))$, $G := \Phi_k$
    Calculate the gradient (Jacobian) $J \leftarrow \nabla G$
    Extract $\bar{G}$ from the saved gradient back-propagation data
    Calculate $Z = \nabla^2(\bar{G}^T G)$
    Update $H \leftarrow J^T H J + Z$
end for



Numerical Benchmark

- We consider the heat equation in $\Omega = [0,1]^2$

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \nabla \cdot (\kappa(x,y)\nabla u)) + f(x,y) && x \in \Omega \\
u(x,y,0) &= x(1-x)y^2(1-y)^2 && (x,y) \in \Omega \\
u(x,y,t) &= 0 && (x,y) \in \partial\Omega
\end{aligned}
$$

- The diffusivity coefficient κ and exact solution u are given by

$$
\begin{aligned}
\kappa(x,y) &= 2x^2 - 1.05x^4 + x^6 + xy + y^2 \\
u(x,y,t) &= x(1-x)y^2(1-y)^2 e^{-t}
\end{aligned}
$$

- We learn a DNN approximation to κ using full-field observations of u

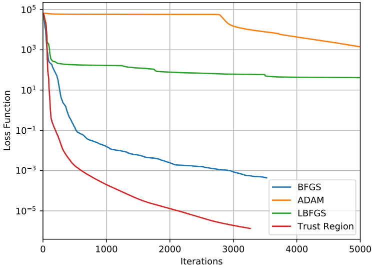
$$
\kappa(x,y) \approx \mathrm{N}_\theta(x,y)
$$

Convergence

- The optimization problem is given by

$$\min_{\theta} \; L(\theta) = \sum_n \sum_{i,j} \left(\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} - F_{i,j}(u^{n+1}; \theta) - f_{i,j}^{n+1} \right)^2$$

$F_{i,j}(u^{n+1}; \theta)$: the 4-point finite difference approximation to the Laplacian $\nabla \cdot (\mathrm{N}_\theta \nabla u)$.



Effect of PDEs

$$N_\theta \rightarrow \text{(PDE Solver)} \rightarrow \text{Loss Function}$$

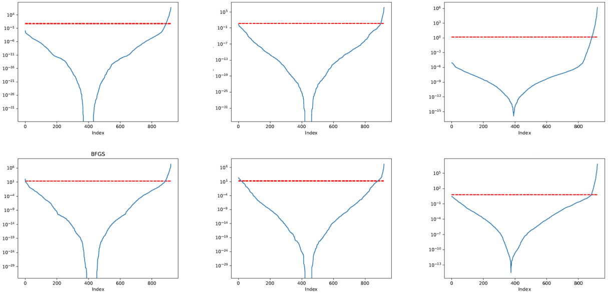
- Consider the loss function excluding the effects of PDEs

$$l(\theta) = \sum_{i,j} (N_\theta(x_{i,j}, y_{i,j}) - \kappa(x_{i,j}, y_{i,j}))^2$$

- Eigenvalue magnitudes of $\nabla^2 L(\theta)$ and $\nabla^2 l(\theta)$

$\nabla^2 L(\theta)$
DNN-PDE

$\nabla^2 l(\theta)$
DNN Only



BFGS LBFGS Trust Region

Effect of PDEs

- Most of the eigenvalue directions at the local landscape of loss functions are “flat” $\Rightarrow$ “effective degrees of freedom (DOFs)”.
- Physical constraints (PDEs) further reduce effective DOFs:

	BFGS	LBFGS	Trust Region
DNN-PDE	**31**	**22**	**35**
DNN Only	34	41	38

Effect of Widths and Depths

- The ratio of zero eigenvalues **increases** as
  - the number of hidden layers increase for a fixed number (20) of neurons per layer (unit: %)

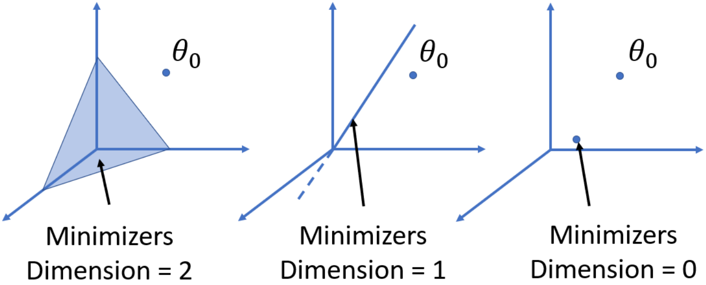
# Hidden Layers	LBFGS	BFGS	Trust Region
1	76.54	72.84	77.78
2	98.2	94.41	93.21
3	98.7	98.15	96.09

  - the number of neurons per layer increases for a fixed number (3) of hidden layers (unit: %)

# Neurons per Layer	LBFGS	BFGS	Trust Region
5	93.83	85.19	69.14
10	97.7	83.52	89.66
20	96.2	97.39	96.42

Effect of Widths and Depths: Conjecture

- Implications for overparametrization: **the minimizer lies on a relatively higher dimensional manifold of the parameter space**.
- Conjecture: overparameterization makes the optimization easier due to a larger chance of hitting the minimizer manifold.



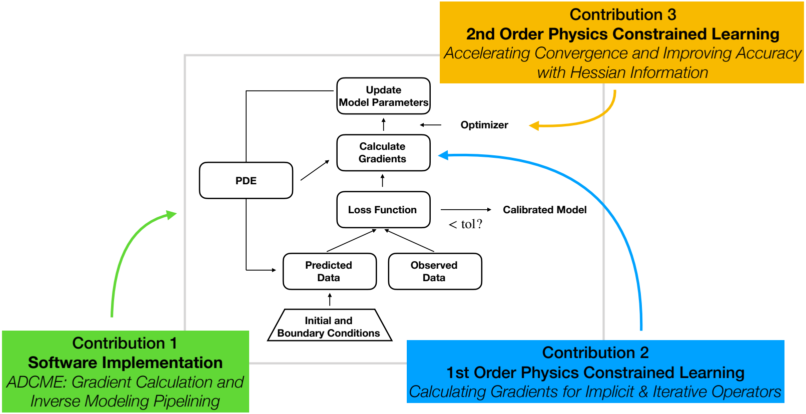
Summary

- Trust region methods converge significantly faster compared to first order/quasi second order methods by leveraging Hessian information.
- Second order physics constrained learning helps you calculate Hessian matrices efficiently.
- The local minimum of DNNs have small effective degrees of freedom compared to DNN sizes.

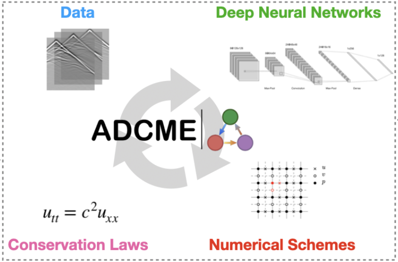
Conclusion

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

✓ *Develop algorithms and tools for solving inverse problems by combining DNNs and numerical PDE solvers.*



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

Supporting Materials

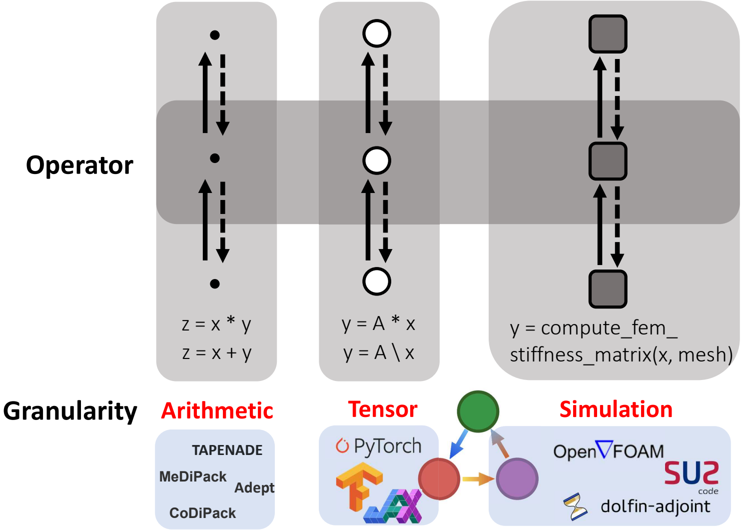
Limitations and Future Work

- Computational cost
  - A PDE needs to be solved per inner iteration in the optimization process
  - Calculating Hessians are very expensive: exploit the Hessian structure to accelerate computations
- Convergence and accuracy of DNNs
- Ill-posed inverse problems
  - Regularization
  - Bayesian approach
- Robustness to noise
- Theoretical investigations

Major AD Frameworks

	TensorFlow 1.x	PyTorch	JAX
Computational graph	static and explicit	dynamic and explicit	dynamic and implicit
Programming	declarative	imperative	imperative
Focus	graph optimization, AD	AD	AD
Computing	CPU/GPU/TPU	CPU/GPU, TPU(-)	CPU/GPU/TPU
Highlights	• graph optimizations and manipulations • optimized tensor libraries	intuitive APIs	• just-in-time compilation from Python functions to XLA-optimized kernels • arbitrary composition of pure functions • high order derivatives

AD Frameworks



Static Graph versus Dynamic Graph

	Static Graph	Dynamic Graph
Pros	• graph optimizations, rewriting, and simplifications; • easy to reason about and analyze	• intuitive: run to define.
Cons	• compiled-language-like: define to run.	• difficult to reason about and optimize; • encourage trial and error instead of computations itself.