ADCME MPI: Distributed Machine Learning for Computational Engineering

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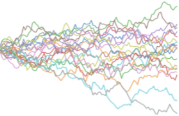
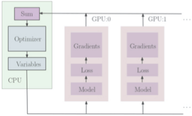
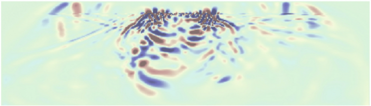
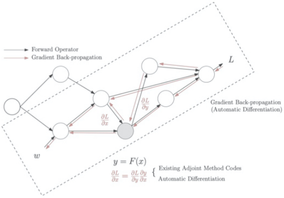
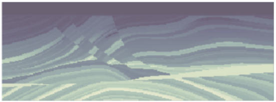
https://github.com/kailaix/ADCME.jl

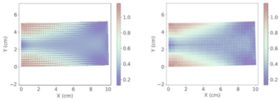








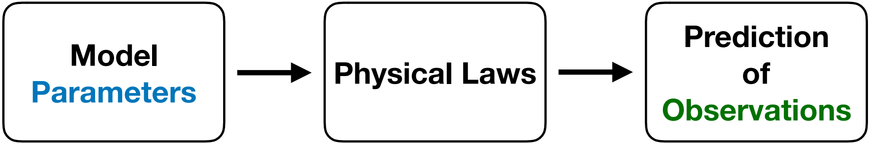




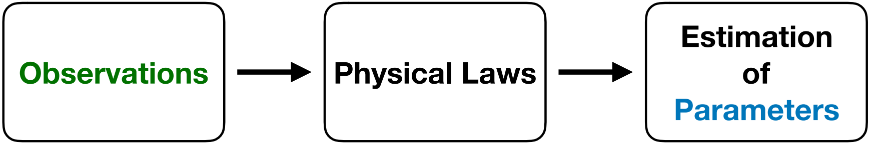
Outline

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

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

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.
- ...

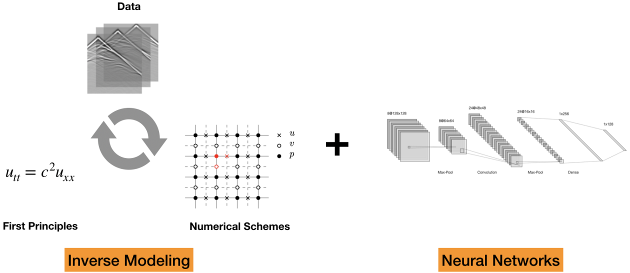
The candidate solution space is infinite dimensional.

Machine Learning for Computational Engineering

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

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

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

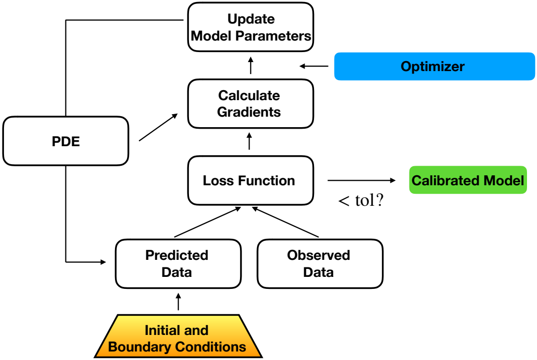


Gradient Based Optimization

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

- We can now apply a gradient-based optimization method if we can calculate a 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

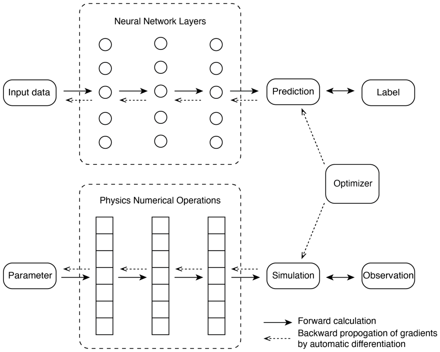
Back-propagation

||

Reverse-mode Automatic Differentiation

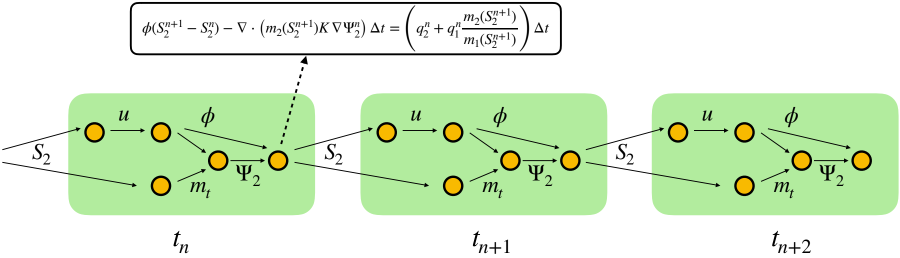
||

Discrete Adjoint-State Method

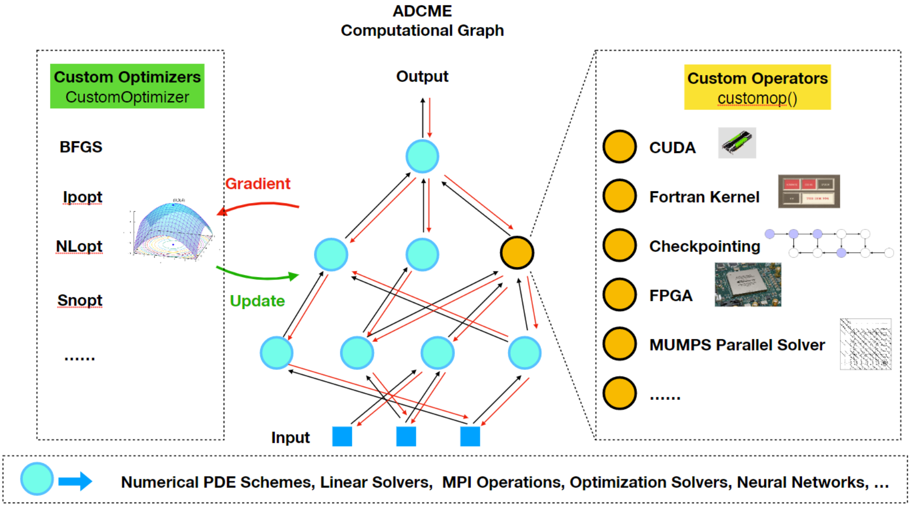


Computational Graph for Numerical Schemes

- 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

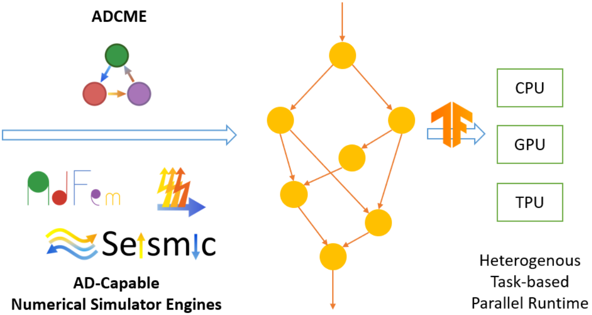


How ADCME works

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

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

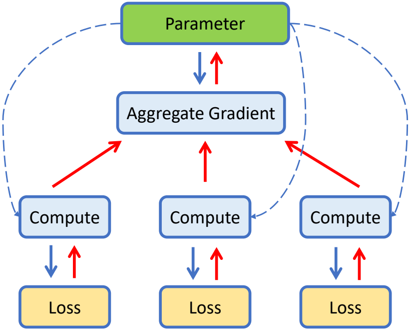
```
mmesh = Mesh(50, 50, 1/50, degree=2)

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
```

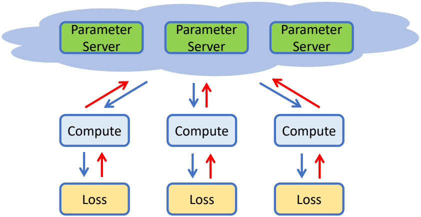


Outline

Common Distributed Computing Patterns in DL

$$L(\theta) = \sum_{i=1}^{N} (NN(x_i; \theta) - y_i)^2$$





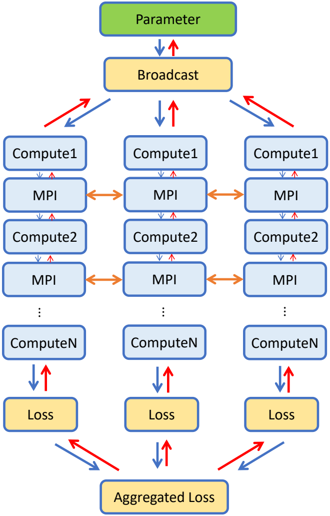
Distributed Computing in ML for Computational Engineering

Consider a time-dependent PDE, where the state variable

$$u_k = [u_k^{(1)} \; u_k^{(2)} \; \cdots u_k^{(P)}]$$

is stored on P machines. Each time step requires a distributed numerical solver.

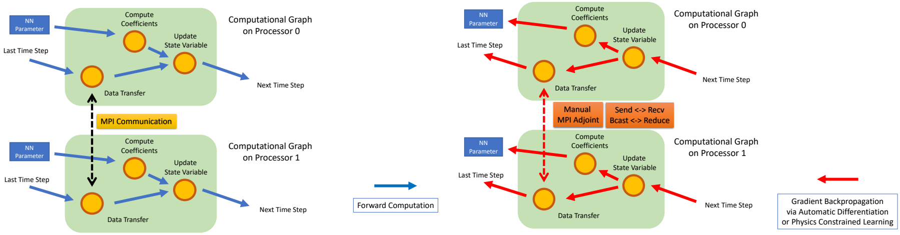
$$\begin{aligned} \min_{\theta} \; & L(u_n) \\ \text{s.t. } & A(\theta)u_2 = h(u_1;\theta) + g \\ & A(\theta)u_3 = h(u_2;\theta) + g \\ & \vdots \\ & A(\theta)u_n = h(u_{n-1};\theta) + g \end{aligned}$$



ADCME-MPI

ADCME-MPI abstracts distributed computing as a node in the computational graph. The ADCME-MPI model is **transparent**.

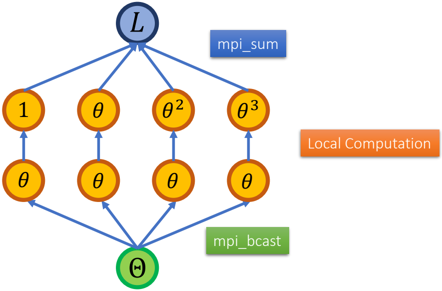
- ADCME takes responsibility for MPI communication and gradient back-propagation across clusters;
- users can adapt their single processor codes to a distributed computing environment with little efforts.



Example

Consider a simple function:

$$L(\theta) = 1 + \theta + \theta^2 + \theta^3$$




```julia
using ADCME
mpi_init() # initialize MPI
theta0 = placeholder(1.0)
theta = mpi_bcast(theta0)
l = theta^mpi_rank()
L = mpi_sum(l)
g = gradients(L, theta0)
# initialize a Session
sess = Session(); init(sess)
L_value = run(sess, L)
g_value = run(sess, g)
mpi_finalize() # finalize MPI
```

Distributed Optimization

In the ADCME-MPI, we can convert a serial optimizer to a distributed optimizer by inserting some communication codes:

flag

Master

```
for k = 1, 2, 3, ...
    flag = COMPUTE_OBJ
    mpi_sync!(flag)
    f = compute_objective_function(x)
    ...
    flag = COMPUTE_GRAD
    mpi_sync!(flag)
    dx = compute_gradient(x)
    ...
    x = x – alpha * dx
flag = OPTIMIZATION_STOP
mpi_sync!(flag)
```

Worker

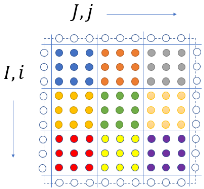
```
while true
    mpi_sync!(flag)
    if (flag==COMPUTE_OBJ)
        compute_objective_function(x)
    elseif (flag==COMPUTE_GRAD)
        compute_gradient(x)
    else
        break
    end
end
```

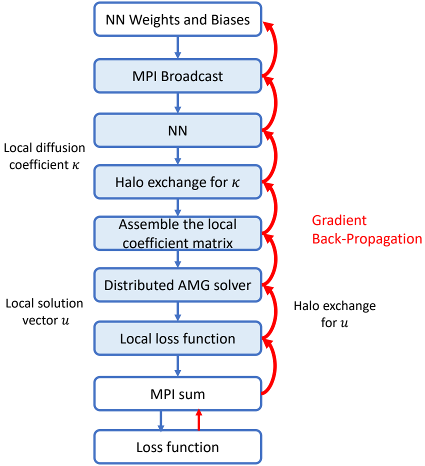
Benchmarks

$$\min_{\theta} J(\theta) := \sum_{i \in \mathcal{I}} (u(\mathrm{x}_i) - u_i)^2$$

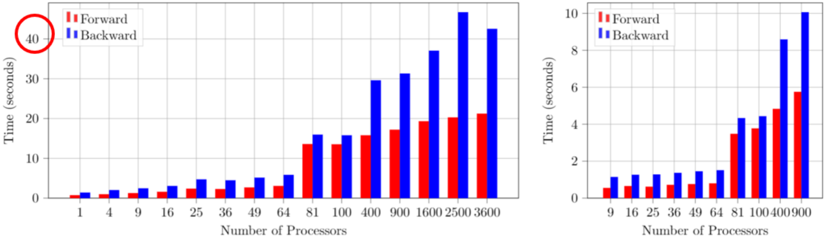
$$\text{s.t. } \nabla \cdot ({\color{red}NN_\theta(\mathrm{x})} \nabla u(\mathrm{x})) = f(\mathrm{x}), \ \mathrm{x} \in \Omega$$

$$u(\mathrm{x}) = 0, \ \mathrm{x} \in \partial\Omega$$

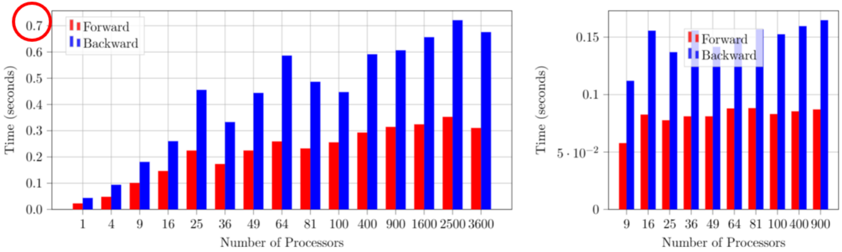




Total Time



ADCME Overhead = Total Time – Hyper Time



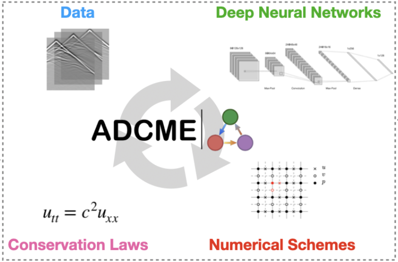
1 Core per MPI processor **4 Core per MPI processor**

Reference

For more technical details, benchmarks, or use cases:

- AAAI Conference Paper: *ADCME MPI: Distributed Machine Learning for Computational Engineering*
- Full paper: *Distributed Machine Learning for Computational Engineering using MPI*
  `https://arxiv.org/pdf/2011.01349.pdf`
- Software documentation:
  `https://kailaix.github.io/ADCME.jl/dev/`

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

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