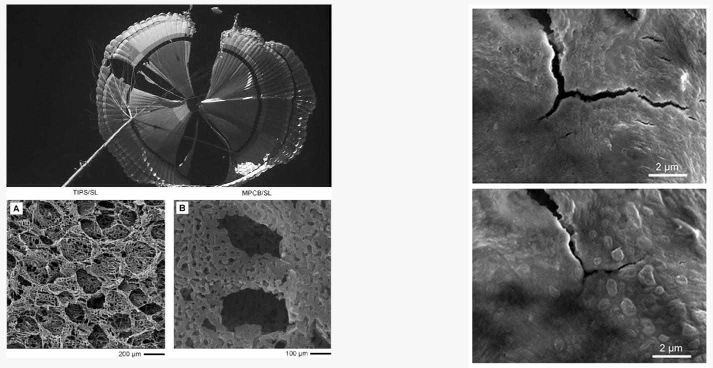
Learning Constitutive Relations using Symmetric Positive Definite Neural Networks

Background



How to model complex constitutive behaviors from observations?

Failure of parachute test; multiscale porous scaffolds; fracture in batteries. Source: NBC News; Luigi Ambrosio; Technologyreview

- It is challenging to model complex material constitutive behavior with conventional mathematical modeling approaches.
- Deep neural networks emerge as an empirically successful function approximator for complex and high dimensional functions.
- To leverage the physics to the largest extent, we **couple neural-network-based constitutive relations and partial differential equations**.
- Training the neural network requires back-propagating through both the numerical partial differential equation solvers and deep neural networks.
- Most important of all, **what conditions should deep neural networks satisfy to stabilize numerical solvers?**

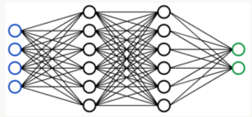
Software

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

SPD-NN

- Conventional neural-network-based constitutive relations

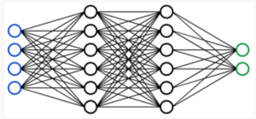
Strain ϵ^n
Strain ϵ^{n+1}
Stress σ^n



Stress σ^{n+1}

- Symmetric positive definite neural networks (SPD-NN)

Strain ϵ^n
Strain ϵ^{n+1}
Stress σ^n



Cholesky Factor L

Incremental form: $\boxed{\Delta\sigma = LL^T\Delta\epsilon}$

Residual Learning

PDE + NN + Data

$$\begin{aligned} \rho\ddot{u} &= \mathrm{div}\,\sigma + \rho b && \text{in } \Omega \\ u &= \bar{u} && \text{on } \Gamma_u \\ \sigma n &= \bar{t} && \text{on } \Gamma_t \end{aligned}$$

$$\Delta\sigma = LL^T\Delta\epsilon$$

Strain-Stress Pairs or Displacement Data

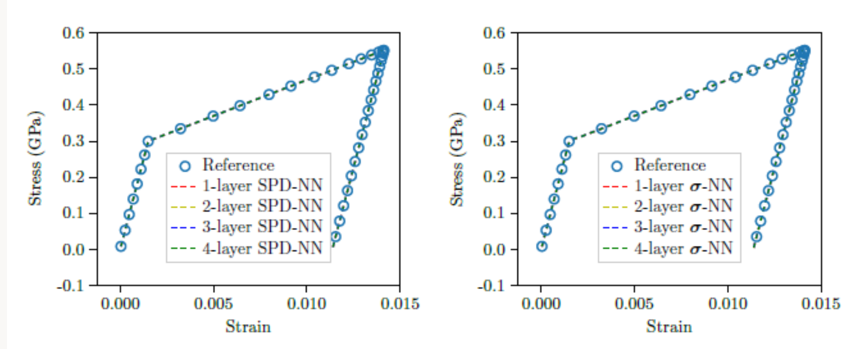
Finite Element Residual

$$\arg\min_\theta \mathcal{L}(\theta) := \sum_{j=1}^{N}\sum_{i=2}^{n-1}\left(M\ddot{u}_j^i + P(u_j^i, \sigma_j^i(\theta)) - f_j^i\right)^2$$

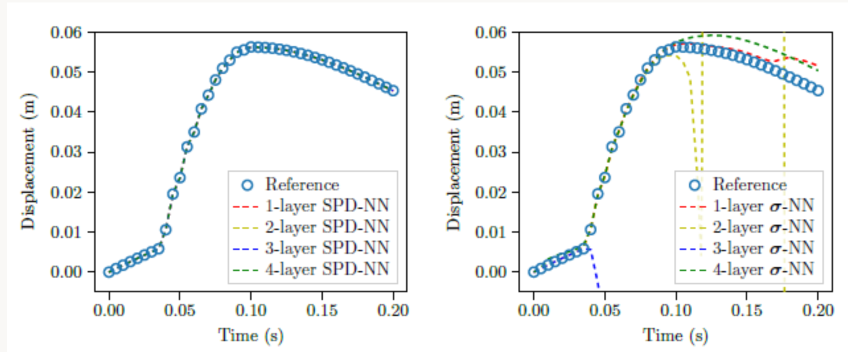
- The time integrator of the PDE resembles a recurrent neural network.
- Automatic differentiation through both PDE solvers and neural networks.

Result

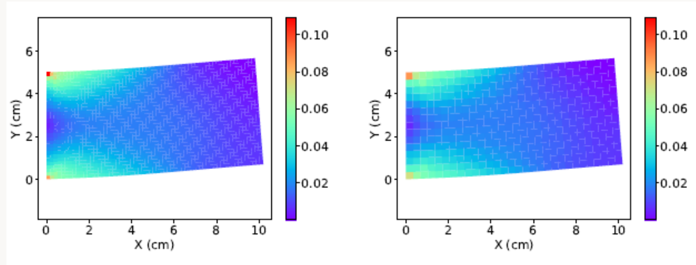
- Elasto-plasticity
  - Both SPD-NNs and conventional NNs predict strain-stress curves accurately.



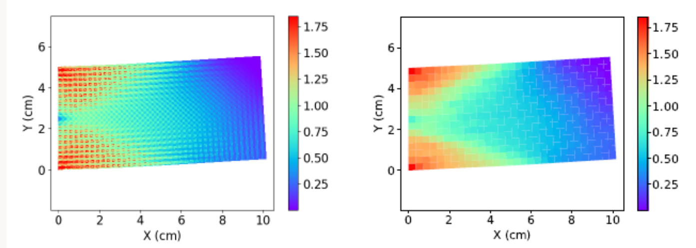
  - But when they are coupled with a numerical solver, only SPD-NNs are stable.



- Hyperelasticity



- Multi-scale



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