Recurrent Localization Networks applied to the Lippman-Schwinger Equation

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BACKGROUND:

- Designing new materials requires linkages between process, structure, and property
- Estimating and understanding these linkages involves testing and simulation
- Simulating physics over high-dimensional structures is expensive
- Machine learning models are faster than traditional simulations, but less accurate and interpretable
- Physics-informed learning is a rapidly-growing field

METHODS

1. Convert governing equation to equivalent Lippman-Schwinger (L-S) form
2. Approximate L-S operator with an ML model and solve iteratively
3. Train end-to-end on synthetic data
4. Result: learned L-S iteration!

RESULTS

- $\approx$1000X speedup over FEA baseline
- More accurate and efficient than standard deep learning models
- Iterative model was more powerful than a single feed-forward network with identical structure and number of parameters

CONCLUSIONS & FUTURE WORK

- Baking physics into a learning method creates more efficient and accurate models
- Recurrent, fully-convolutional networks are excellent for modeling physical systems
- Gradient-based formulation allows for property optimization through ML model

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Embedding physics into machine learning creates better models.

These models can accelerate the development of new materials.

$$\boldsymbol{\sigma} = C\boldsymbol{\varepsilon}, \quad \nabla \cdot \boldsymbol{\sigma} = 0.$$

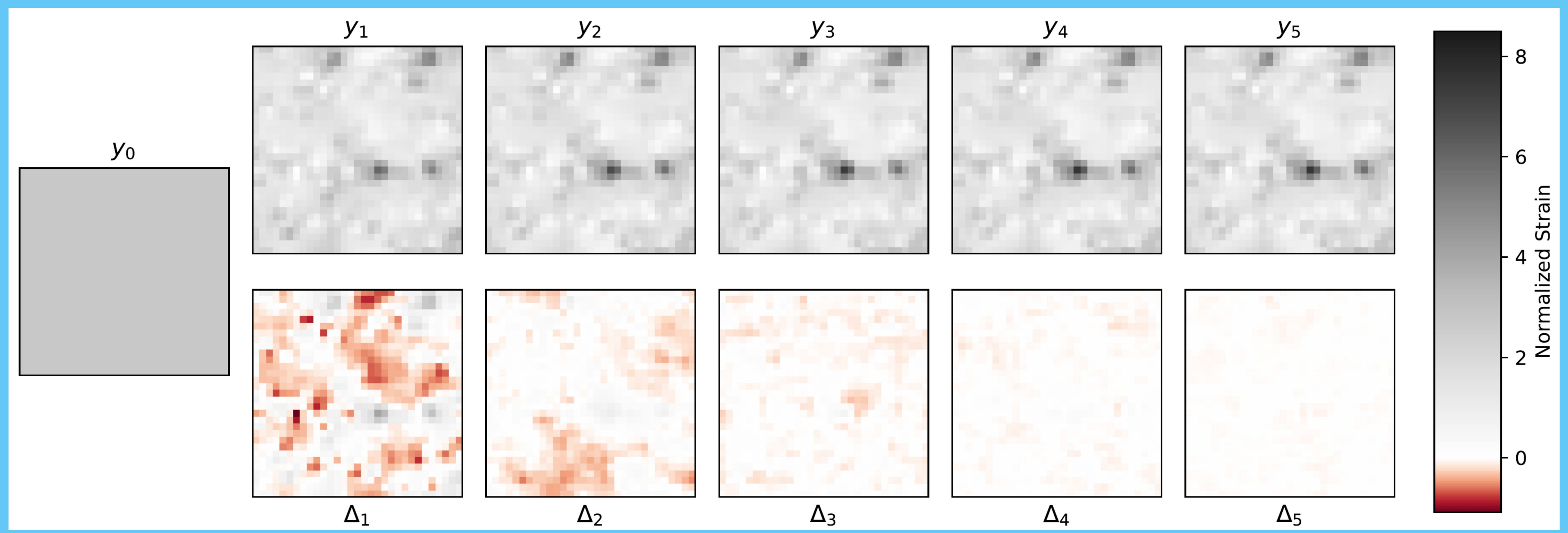
Original Physics

$$y(x) = y^R + \underbrace{\int_X G(x,s)B(y(s))ds}_{F(y)}$$

Lippmann-Schwinger Form

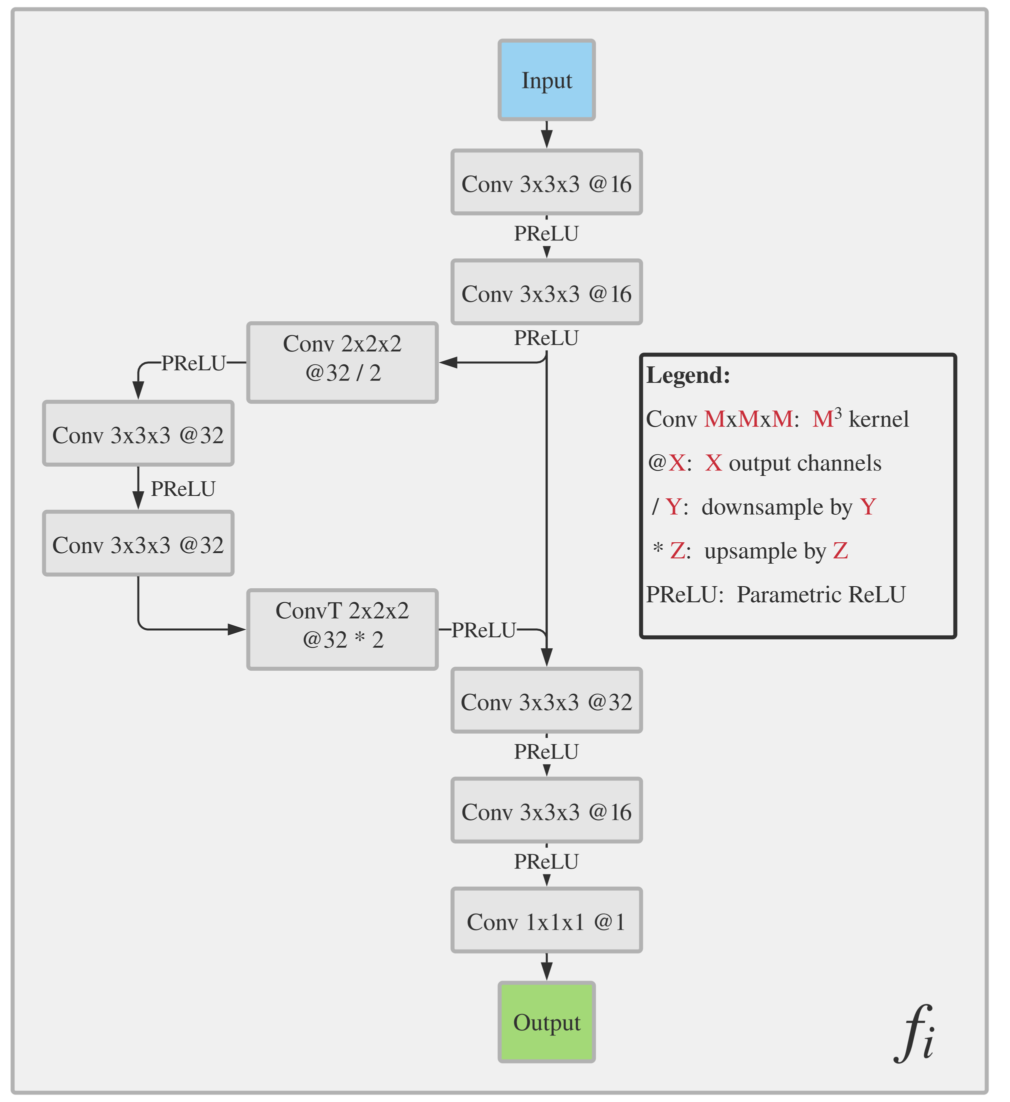
$$\begin{aligned}&\textbf{def } \hat{F}_\theta(y_0; m):\\ &\quad \textbf{for } i = 1, \dots, N:\\ &\qquad y_i = y^R + f_{\theta_i}(y_{i-1}, m)\\ &\quad \textbf{return } y_N\end{aligned}$$

Learned L-S iteration

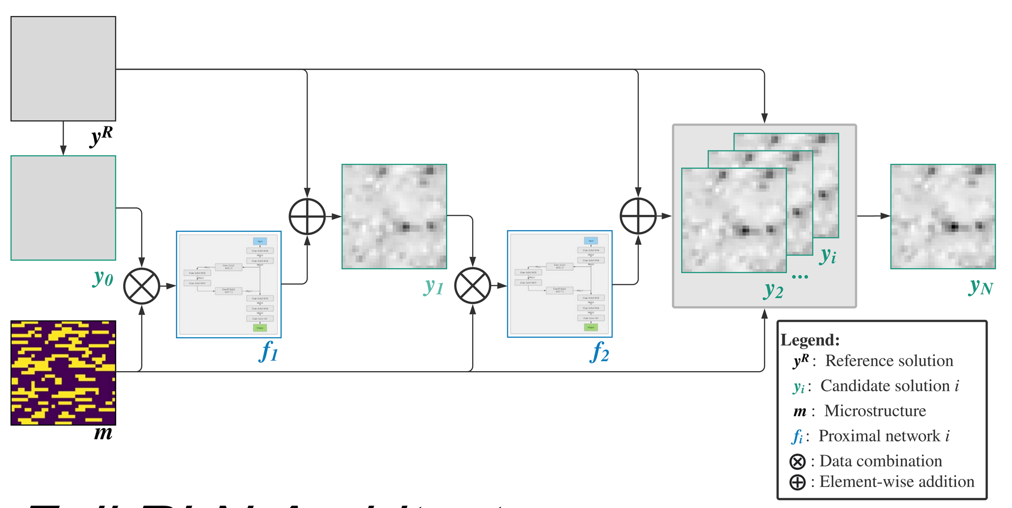


Fast, approximate physics solver

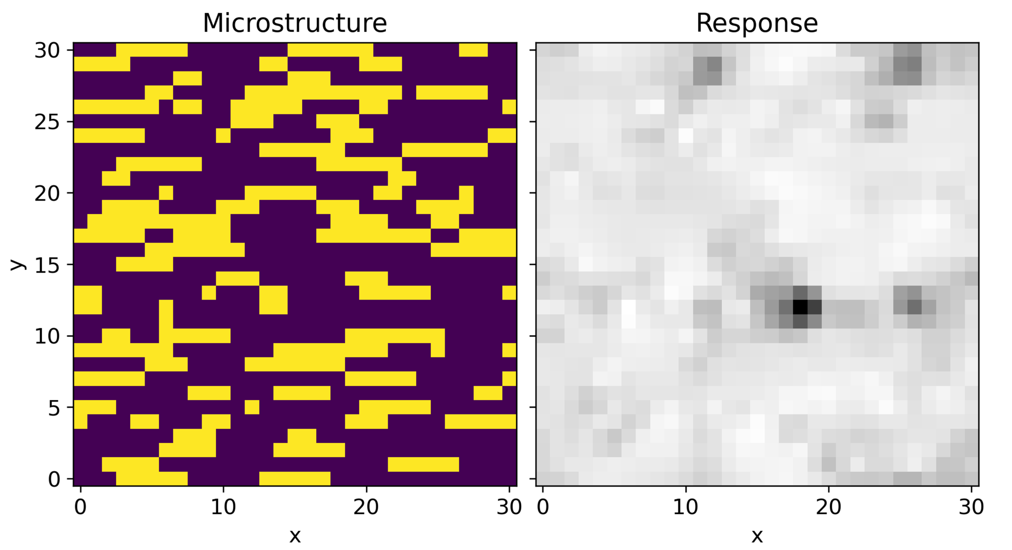
Scan me to download the full paper!



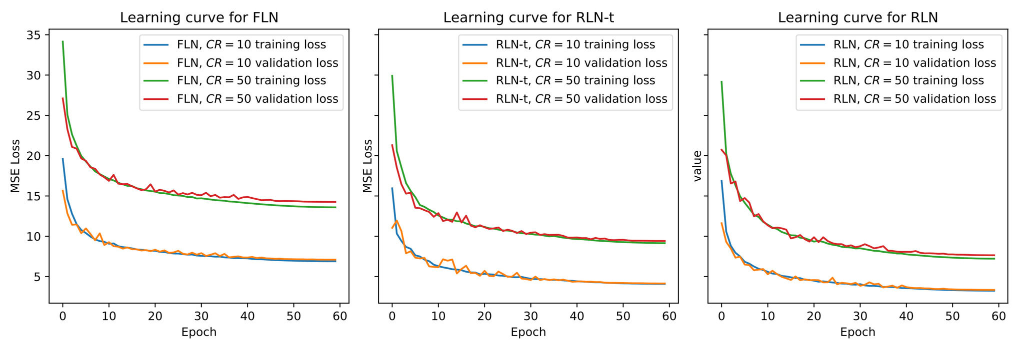
Proximal Network Architecture



Full RLN Architecture



Example input/output pair



Learning curves for each configuration

Model	MASE (mean $\pm$ std. dev.)
Contrast-10	
Comparison DL model [11]	3.07%±1.22%
FLN	4.98%±1.49%
RLN-t	1.81%±0.58%
RLN	1.21%±0.37%
Contrast-50	
Comparison DL model	5.71%±2.46%
FLN	9.23%±3.29%
RLN-t	4.26%±1.65%
RLN	2.92%±1.17%

Results for each configuration

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