# 基于机器学习的材料设计方法及参数反演研究

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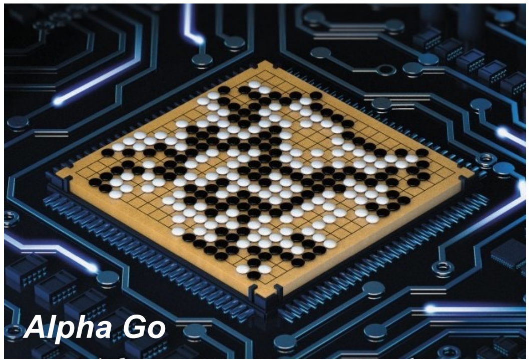
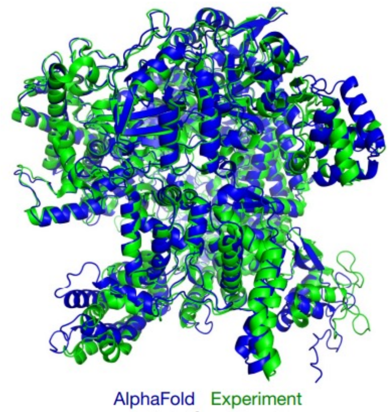
# 报告提纲

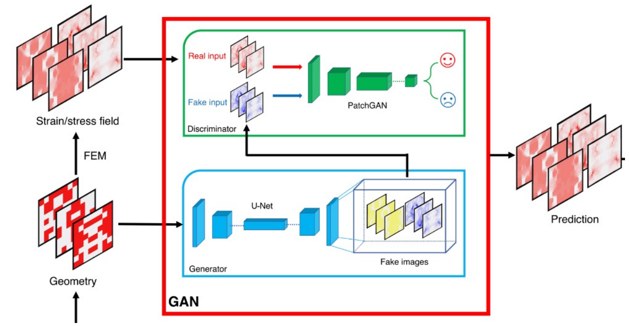
# 研究背景



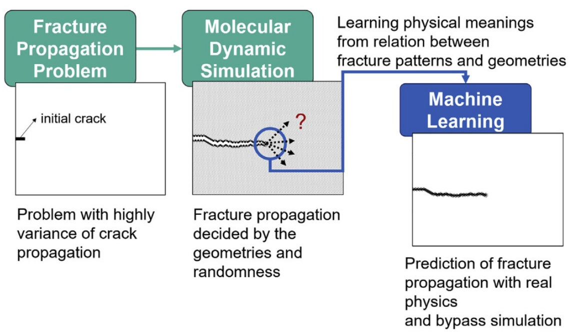

*Nature, 2016*



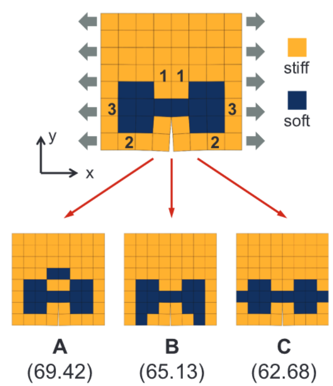

*Nature, 2021*



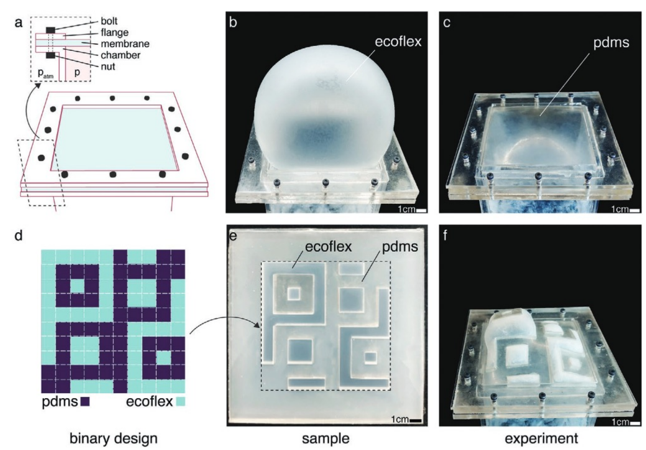

*Sci. Adv., 2021*




*Matter, 2020*

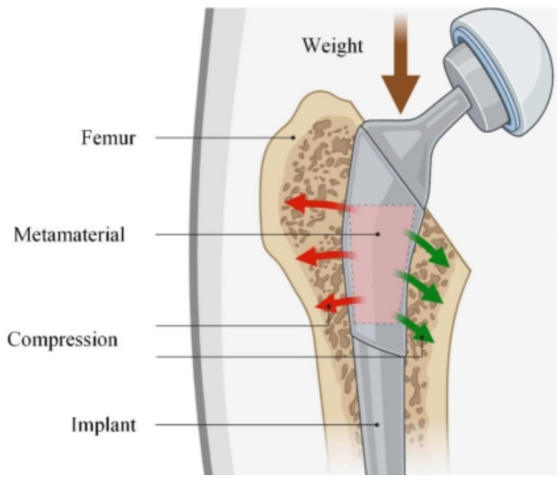



*Adv. Sci., 2020*



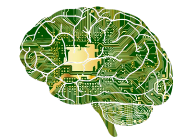

*Adv. Funct. Mater. 2022*

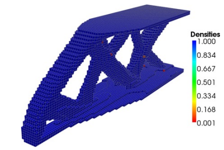
# 研究背景




优化算法

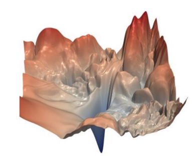
梯度下降法

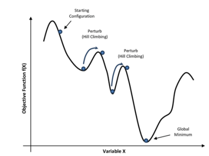




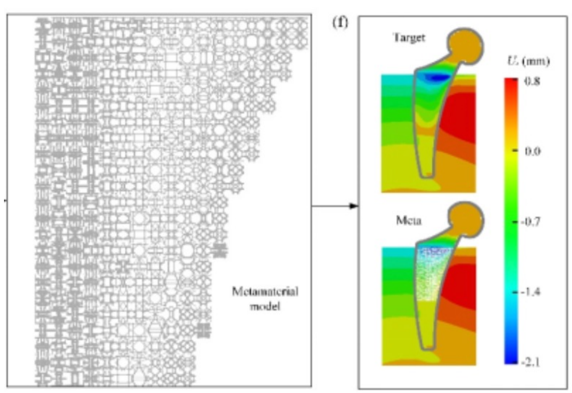
机器学习，拓扑优化

无梯度方法





遗传算法，模拟退火




*Int. J. Mech. Sci., 2022*

| EA time cost (24 × 4 voxels) | | | |
|---|---|---|---|
| Design | ML-EA | FE-EA | RMS errors |
| One-period: | 11 m | 1053 h | 0.82 and 1.11 mm |
| Two-period: | 11 m | 1053 h | 0.70 and 0.89 mm |
| Three-period: | 54 m | 5263 h | 1.37 and 1.34 mm |
| Half-butterfly: | 22 m | 2105 h | 0.96 and 1.02 mm |

*Adv. Funct. Mater. 2021*

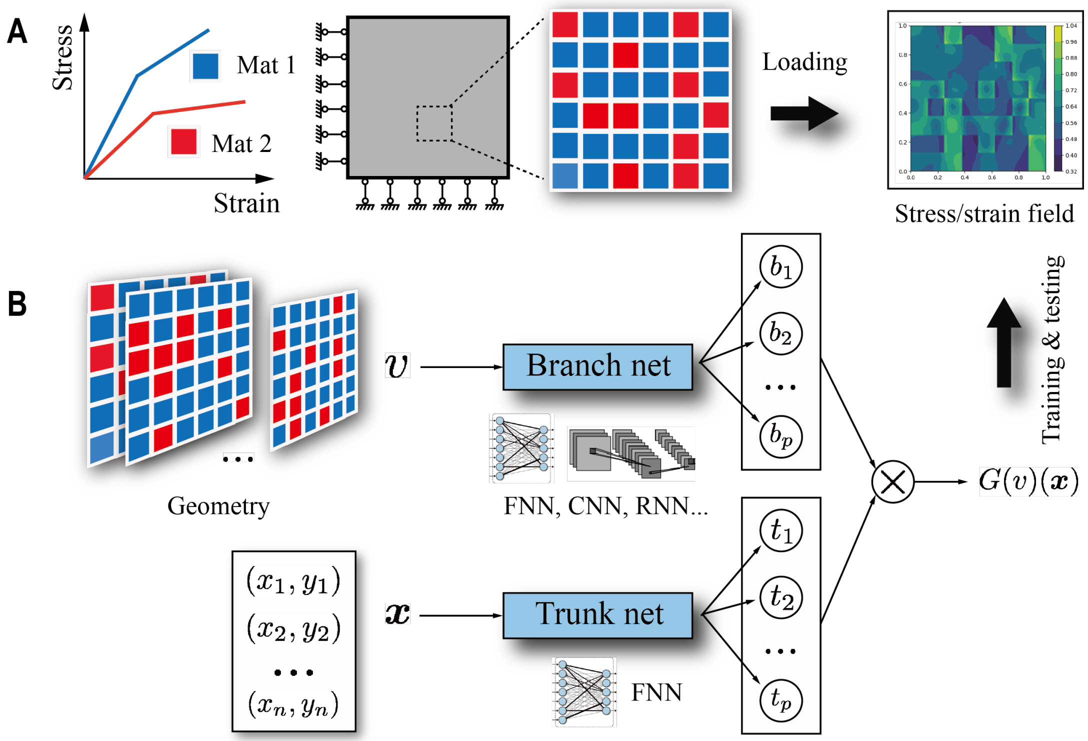
**挑战：适应复杂几何外形、减少训练数据**

# 报告提纲

# 网络架构



网络将材料分布和位置坐标结合



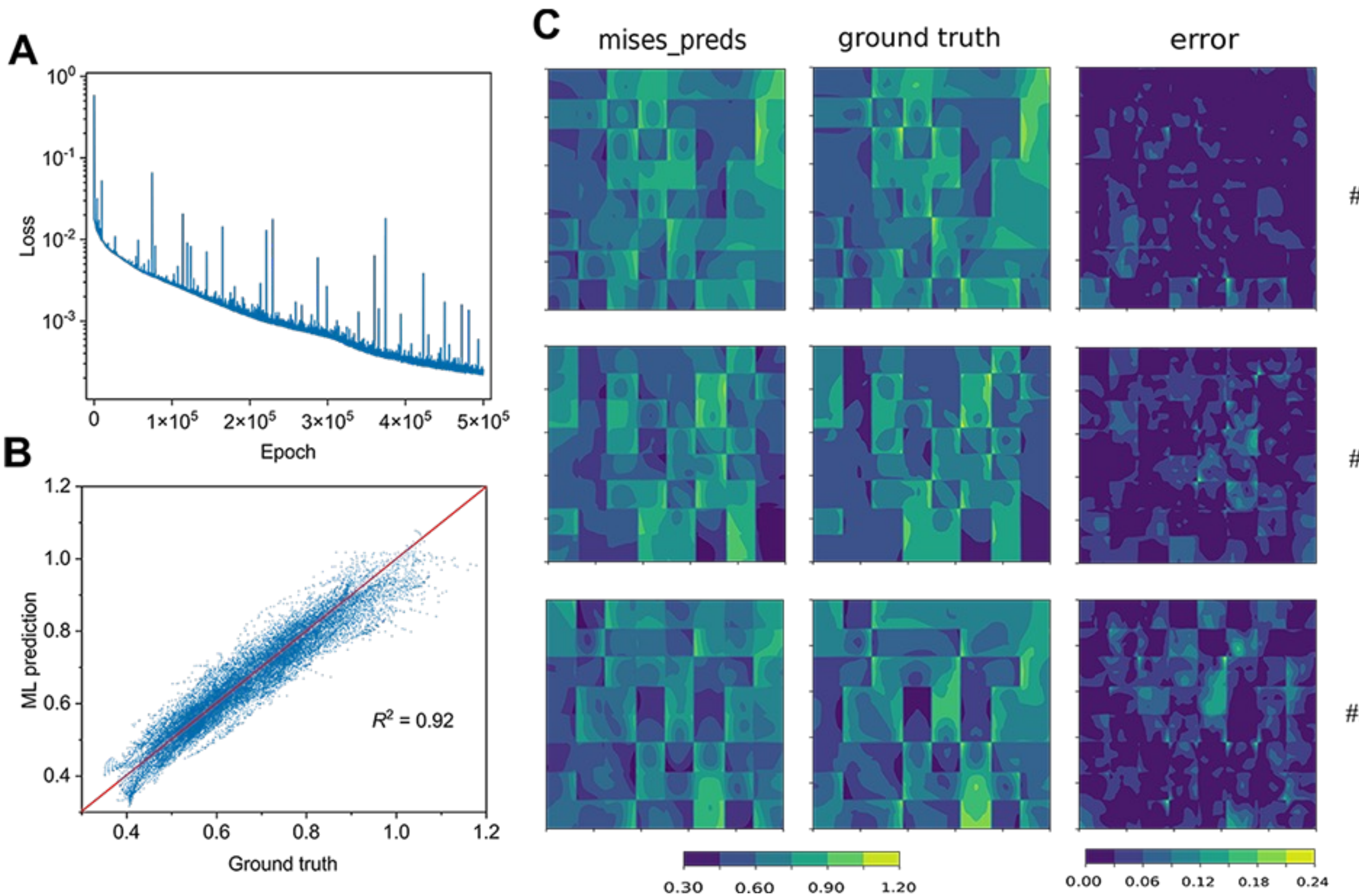

考虑 8×8 的分布组合，共有$2^{64} \approx 1.84\times10^{19}$种分布方式

采用有限元建立2000个数据样本，其中80%用于训练，20%测试，两则无交集

$$G(v)(\boldsymbol{x}) \approx \sum_{k=1}^{p} b_k t_k + b_0 \qquad l_2 = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{m}\left(G(v^i)(\boldsymbol{x}_j) - G_{\theta}(v^i)(\boldsymbol{x}_j)\right)^2$$

# 力学响应预测

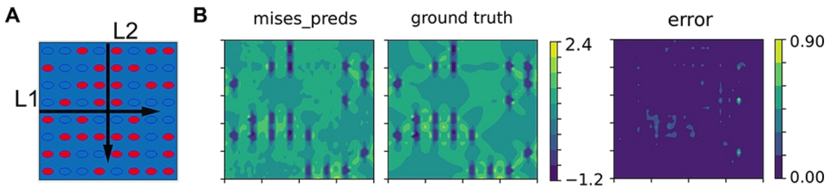
从测试数据集中随机抽取3个样本验证

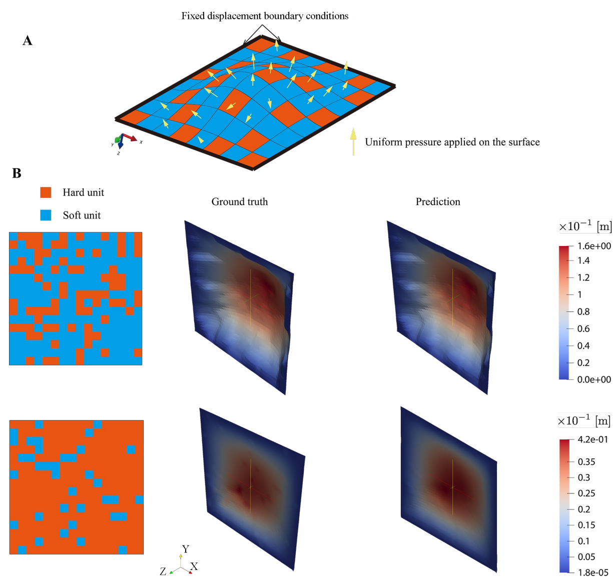


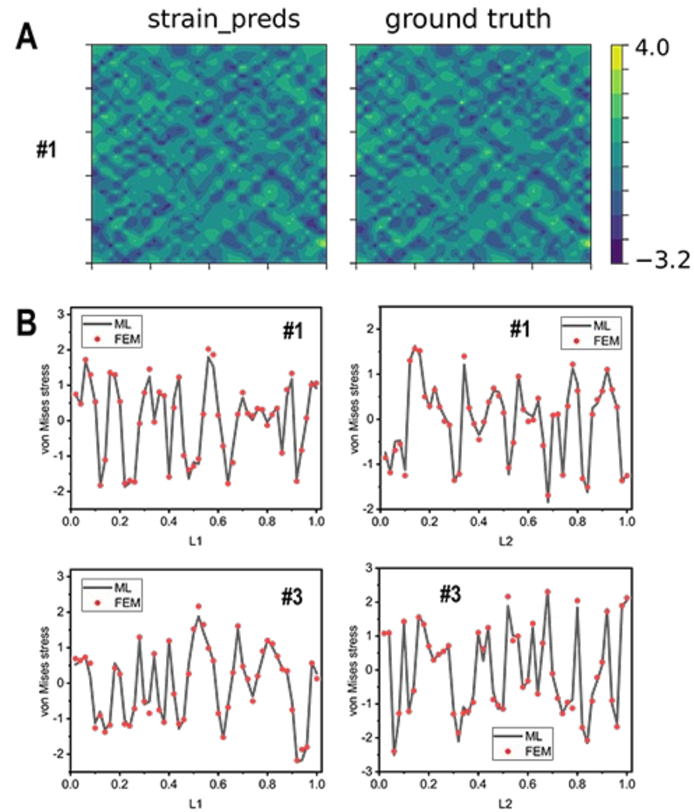
# 力学响应预测

NANJING TECH UNIVERSITY

测试了模型能准确预测大变形、非规则几何结构及三维薄壳的力学响应

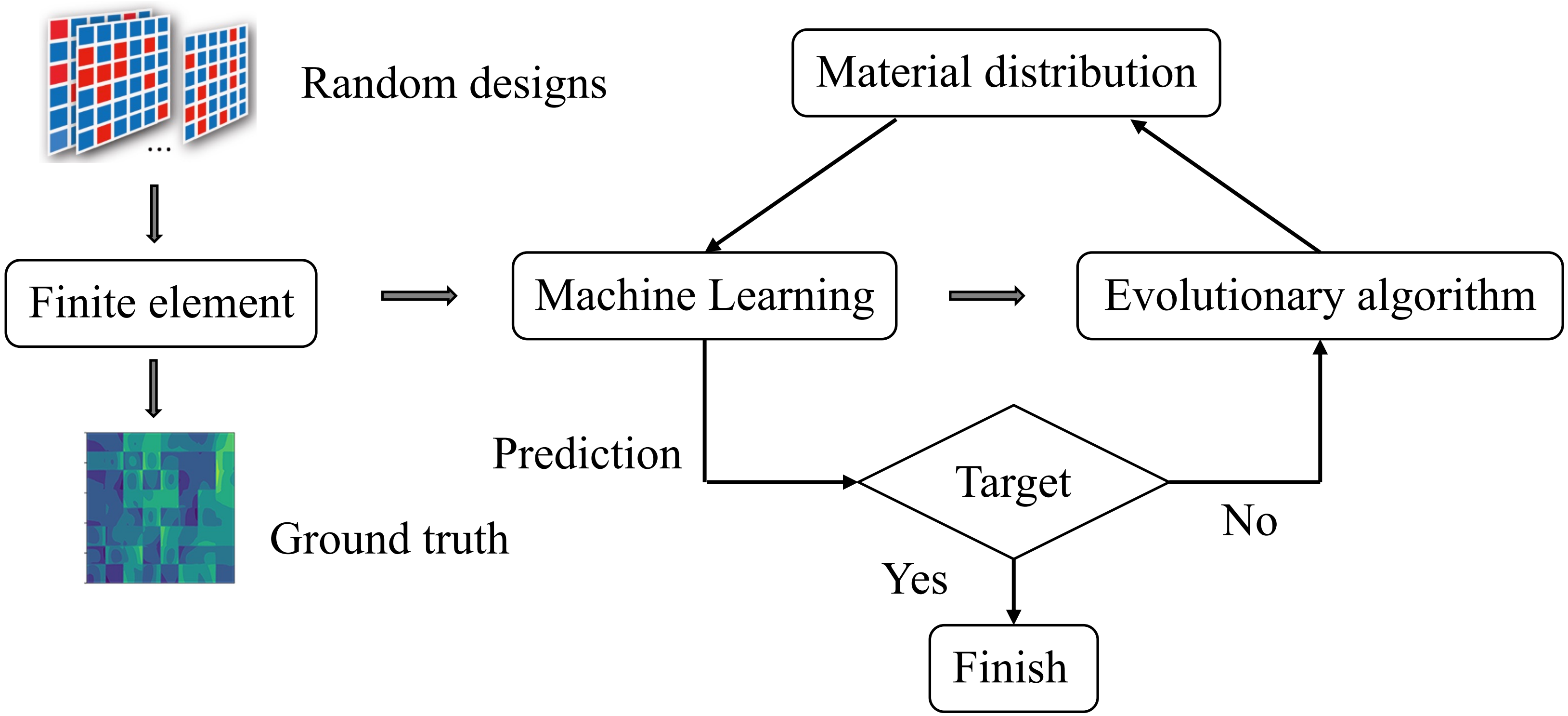


# 材料设计优化算法






- 遗传算法每次迭代需要对大量样本进行评估，若采用有限元计算量惊人；
- 训练好的 ML 网络能够在 5-6 秒实现上万次力学响应计算。

# 材料分布优化

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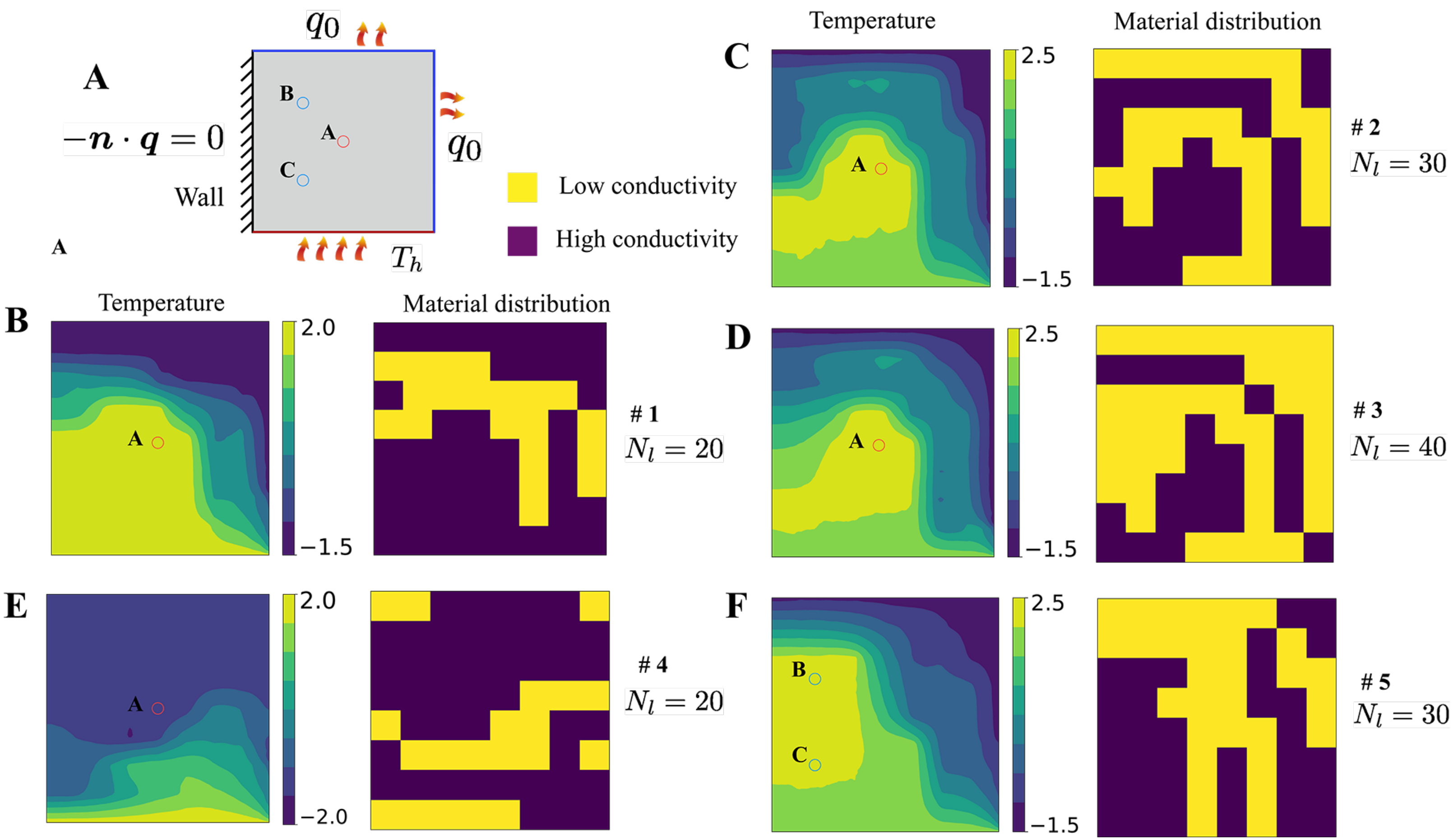
目标：使得特定位置温度最大/最小

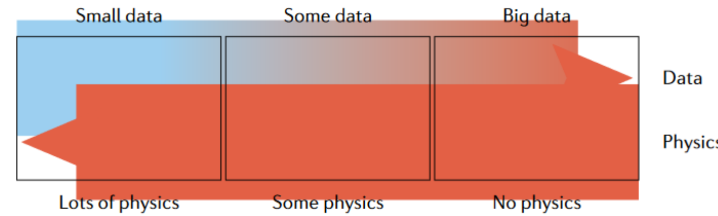


# 报告提纲

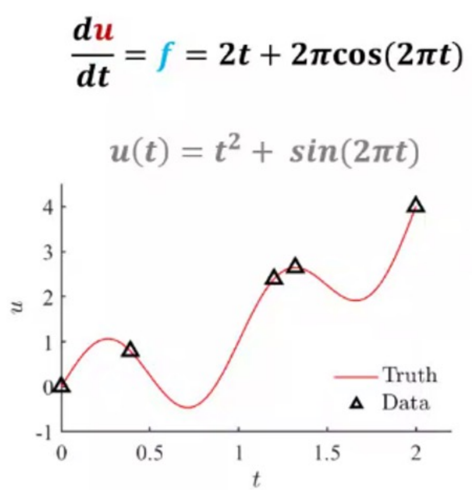
南京工业大学 NANJING TECH UNIVERSITY

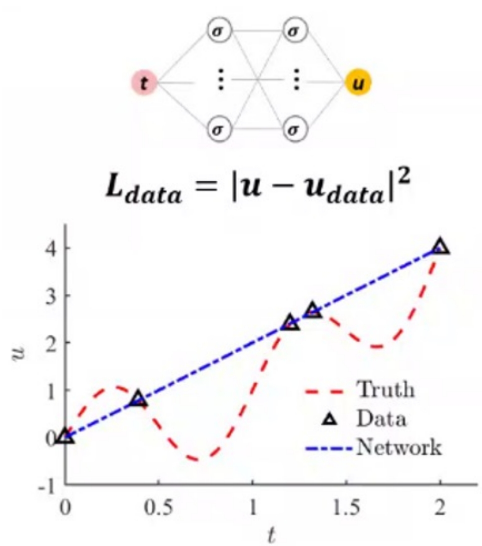
# 物理内嵌网络（PINNs）

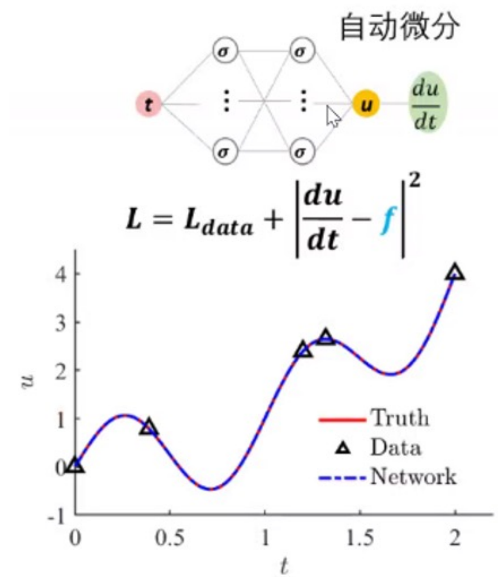
- Physics-informed neural networks (PINNs) – (Raissi, et al., JCP, 2019)
- 用于求解偏微分方程的正问题和**反问题**
- 用神经网络表示 PDE 的解 $\boldsymbol{u} = NN(\boldsymbol{x})$




*Nature Reviews Physics, 2021*



# 物理内嵌网络（PINNs）



- 用神经网络表示PDEs的解 $\boldsymbol{u} = NN(\boldsymbol{x})$
- 基于域分解和Gauss–Legendre积分
- 给出PDEs不同类型等效积分形式以构造Loss
- 引入参数网络，反演未知材料参数

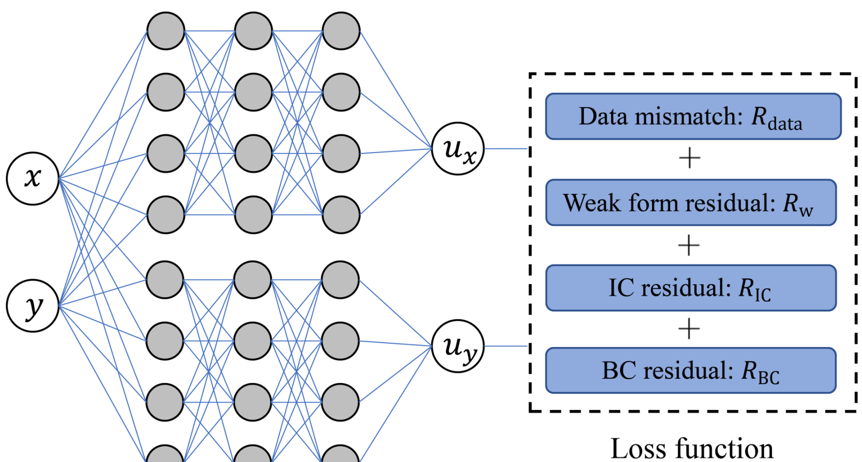
$$\sigma_{ij,j} + f_i = 0 \quad \text{B.C.} \begin{cases} u_i = \bar{u}_i \\ \sigma_{ij} = \bar{\sigma}_{ij} \end{cases}$$

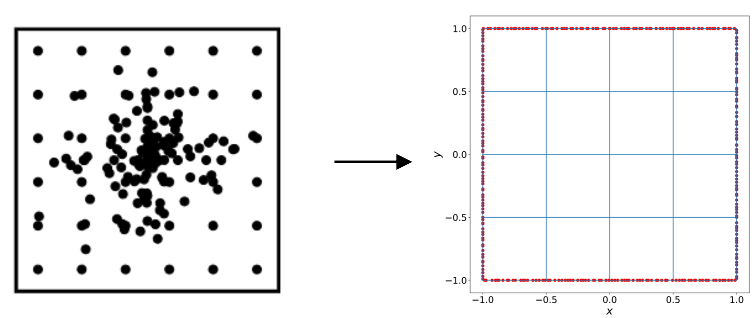
弹性力学Loss函数

$$R_{\mathrm{w}} = -\sum_{e}^{N_e}\sum_{k}^{N_k}\sum_{i}^{N_{\mathrm{dim}}}\sum_{j}^{N_{\mathrm{dim}}}\int_{\Omega}(w_{k,j}^{e}\sigma_{ij}^{e} + w_k^e f_i^e)\mathrm{dV}$$

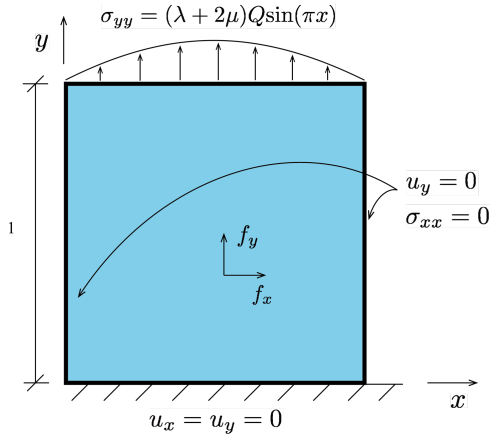
$$R_{\mathrm{BC}} = \frac{1}{N_{\mathrm{BC}}}\sum_{i}^{N_{\mathrm{BC}}}[u_j^{\mathrm{NN}}(\boldsymbol{x_i}) - \bar{u}_j]$$

$$\mathcal{L} = \lambda_{\mathrm{w}}R_{\mathrm{w}} + \lambda_{\mathrm{BC}}R_{\mathrm{BC}}$$



# 物理内嵌网络（PINNs）



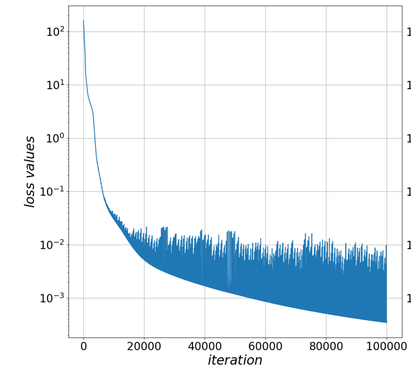

$\lambda = 1$, $\mu = 0.5$, and $Q = 4$.

$$f_x = \lambda \left[4\pi^2 \cos(2\pi x)\sin(\pi y) - \pi \cos(\pi x) Q y^3\right] + \mu \left[9\pi^2 \cos(2\pi x)\sin(\pi y) - \pi \cos(\pi x) Q y^3\right]$$

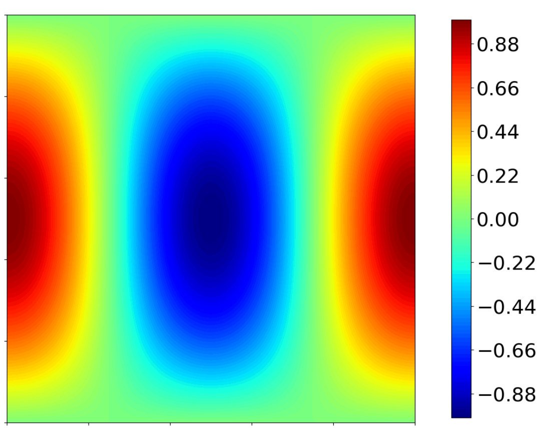
$$f_y = \lambda \left[-3\sin(\pi x) Q y^2 + 2\pi^2 \sin(2\pi x)\cos(\pi y)\right] + \mu \left[-6\sin(\pi x) Q y^2 + 2\pi^2 \sin(2\pi x)\cos(\pi y) + \pi^2 \sin(\pi x) Q y^4/4\right]$$

解析解：

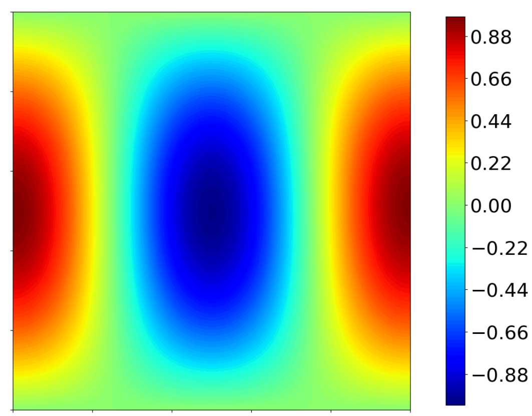
$$u_x(x, y) = \cos(2\pi x)\sin(\pi y),$$
$$u_y(x, y) = \sin(\pi x) Q y^4/4.$$



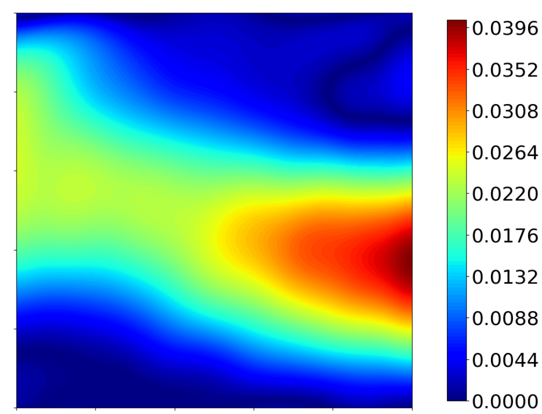

$u_x$ exact




$u_x$ predicted

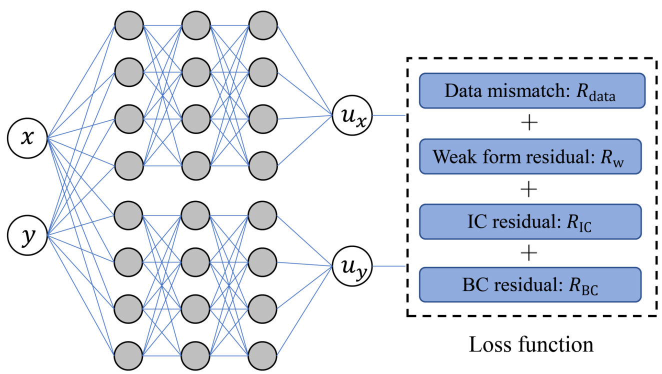


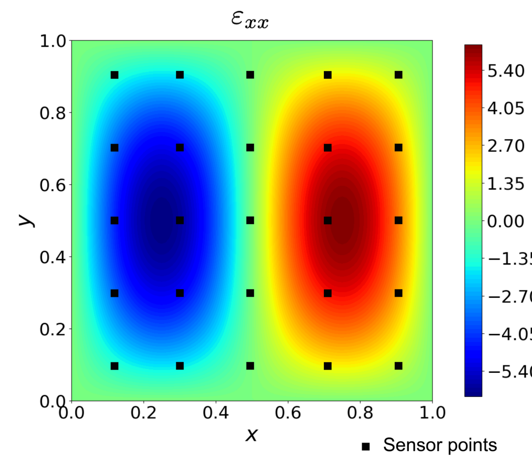

Point-wise error

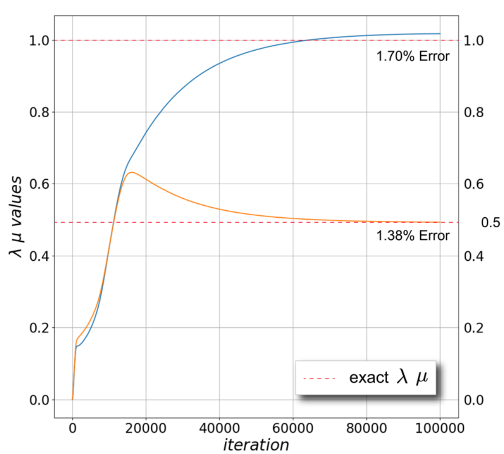


# 材料参数反演

## 已知部分测量数据，如何得到材料参数的数值




- 利用25个位置的 x 方向应变数据
- 两个 Lamé 参数误差约 1%
- 材料参数收敛速度快于全局Loss

# 总结与展望

- ML模型在学习少量数据的基础上，能够预测大量未看过的结果；嵌入位置坐标信息可应用于不规则结构；
- 网络中嵌入物理方程可进行无监督学习获得PDEs的解，理论上能够实现大部分有限元法所能处理的问题；
- 结合一定量的测量数据，ML能够推算出材料参数；

# 谢谢！