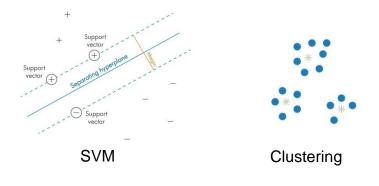


#### AI models in MATLAB

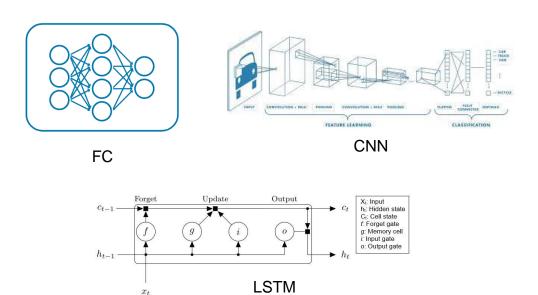
**Machine Learning** 

Deep Learning



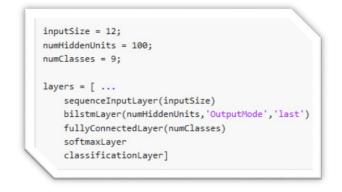


Decision trees

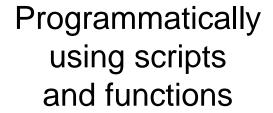


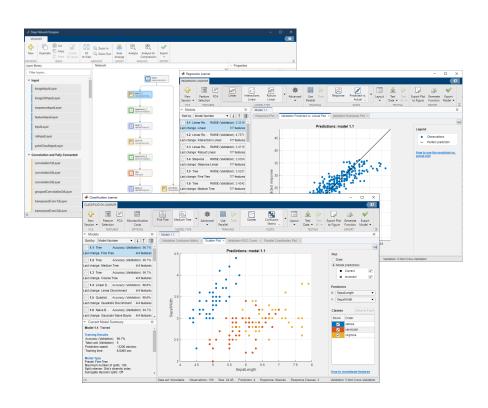


#### 3 ways how to create AI model in MATLAB

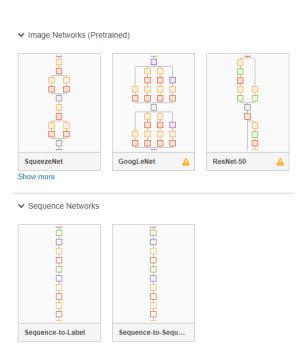


fitcauto / fitrauto





Interactive design using apps

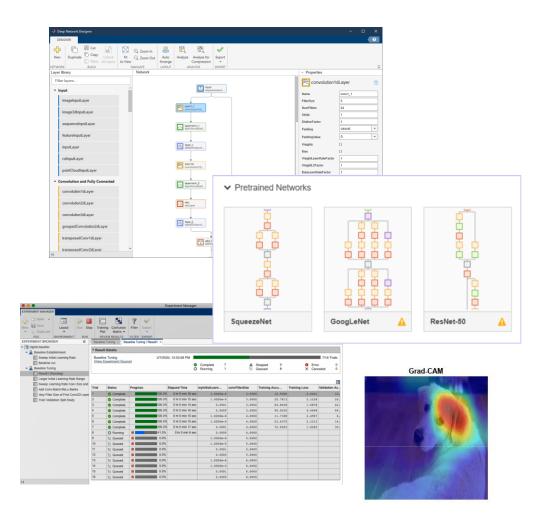


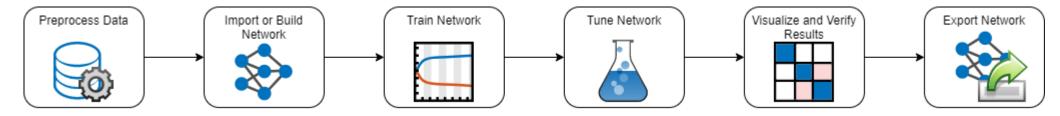
Leverage pre-defined networks and pretrained networks



#### Deep Learning in MATLAB

- Create, train and deploy neural networks
  - variety of applications
  - pre-built networks
- Create networks in the graphical designer
  - design network easier and faster
- Find the optimal network using experiments
- Explain and visualize how networks work
- Interoperability with other environments

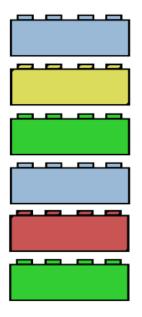




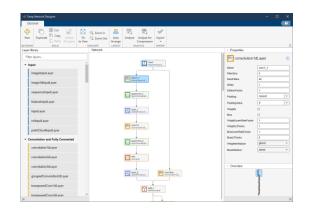


#### Create Deep Neural Networks in MATLAB

~100 layer types



Deep Network Designer



Prepared functions (low code)

Customizations

training using APP\*

```
opts = trainingOptions('solver');
net = trainnet(data,layers,lossfcn,opts);
```

```
scores = minibatchpredict(net,newData);
label = scores2label(scores,classNames);
```

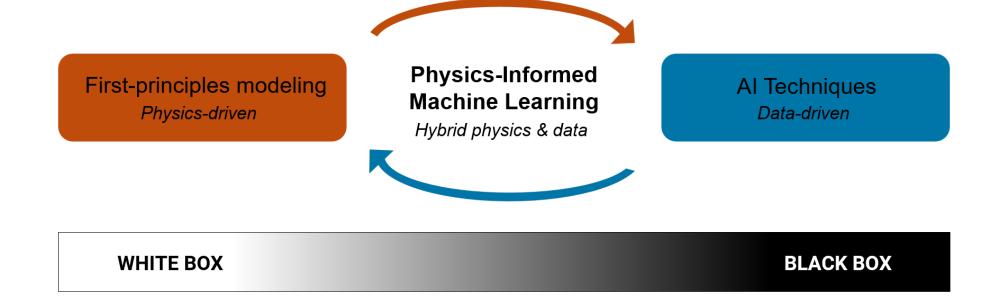
for most deep learning tasks

custom training loops
automatic differentiation
custom loss functions
add physical constraints

PINN networks, GANs, ...

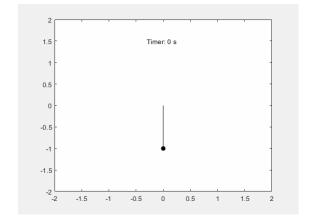


- What is it used for?
  - modeling unknown dynamics
  - discovering equations
  - solving known equations





- A key strategy is to impose constraints based on physics principles to AI model
- How is physics knowledge represented?
  - governing equations
  - conservation laws and symmetries
  - boundary and initial conditions
  - domain-specific knowledge



#### example: simple pendulum

| Туре                          | Given Information                          | Mathematical Formulation  |
|-------------------------------|--|---|
| Governing equations           | Pendulum equation                          | $\ddot{	heta}=\ -\omega_0^2\sin	heta$                                   |
| Conservation Laws             | Conservation of energy                     | $E=\;rac{1}{2}m\ell^2\dot{	heta}^2+mg\ell(1-\cos	heta)$                |
| Boundary / Initial Conditions | Initial angular position, velocity         | $	heta\left(0 ight)=	heta_{0},\dot{	heta}\left(0 ight)=\dot{	heta}_{0}$ |
| Domain knowledge              | Physical limits (e.g. maximum swing angle) | $ 	heta  \leq 	heta_{max}$  |



How is physics knowledge integrated with machine learning?

| Stage                     | Description   |
|---------------------------|---|
| 1. Defining Objective     | Specify what needs to be modeled, including input-output relationships and any known physics.   |
| 2. Curating Training Data | Gather training data through experiments, measurements, or simulations. Preprocess raw data into a format suitable for analysis and modeling.                           |
| 3. Building Model         | Choose a machine learning algorithm or a deep learning architecture that best suits your data and task.   |
| 4. Defining Loss Function | Create a loss function that quantifies the model's performance in meeting its objectives, such as matching observed data or adhering to physical laws, during training. |
| 5. Optimizing Model       | Adjust the model parameters to minimize loss and increase predictive accuracy.  |
| 6. Making Predictions     | Use the trained model to make predictions or simulate system behavior.  |



- Physics can be incorporated at various stages, but often informs:
  - model's structure (stage 3)
  - evaluation (stage 4)
- Soft enforcement:
  - add physics-based constraints in the loss function (stage 4)
  - during training, the model is penalized for violating constraints
  - once trained, its predictions may not strictly satisfy them
  - e.g. PINN's
- Hard enforcement:
  - design the model architecture (stage 3) so that physical constraints are always satisfied
  - e.g. constrained deep learning



# Examples of PIML methods

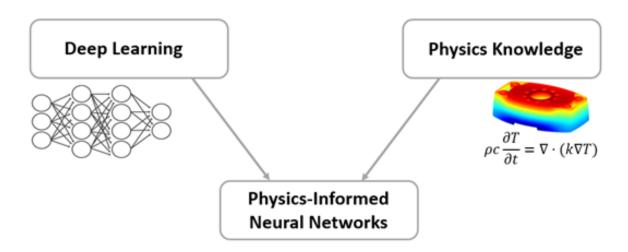
\* weak embedding of physical knowledge, e.g. physics-inspired architecture

| Approach  | Description   |
|---|---|
| Neural Ordinary Differential Equation *             | $\dot{x} = f(x, u)$ , use a neural network to learn $f$ directly from data  |
| Neural State-Space *                                | $\dot{x}=f(x,u),y=g(x,u),$ use neural networks to learn $f$ and $g$ directly from data  |
| Universal Differential Equation                     | combine known physics with machine-learned components   |
| Hamiltonian Neural Networks                         | account for energy conservation   |
| SINDy (Sparse Identification of Nonlinear Dynamics) | reveal the underlying mathematical relationships from data  |
| Physics-Informed Neural Networks                    | combine governing equations (ODEs, PDEs) with data to find solutions that match both observed data and physical laws                      |
| Fourier Neural Operator *                           | learn a mapping from the space of input functions directly to the space of solution functions, enabling fast prediction for new scenarios |
| Graph Neural Networks *                             | operate directly on mesh or graph-based representations   |



#### Physics-Informed Neural Networks (PINNs)

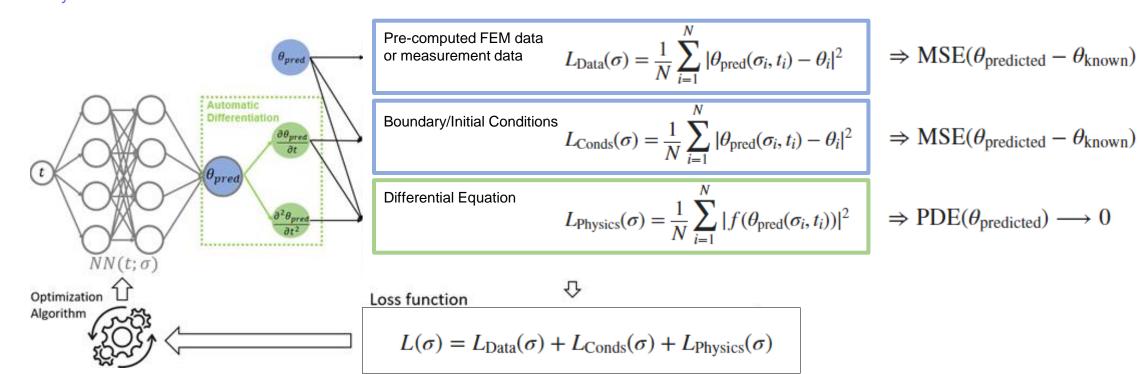
- Neural networks that incorporate physical laws
  - physical laws described by differential equations in their loss functions
- Main purpose
  - guide the learning process toward solutions that are more consistent with the underlying physics
  - use the trained network as the solution of the differential equation





#### Physics-Informed Neural Networks: Loss Function

- Compute loss function L(σ) from three terms
  - $-L_{Data}(\sigma)$ : known input-output data point from FEM solution
  - $-L_{Conds}(\sigma)$ : input-output data points from initial and boundary conditions
  - $-L_{Physics}(\sigma)$ : random input data with physical equation to force the physical constraints



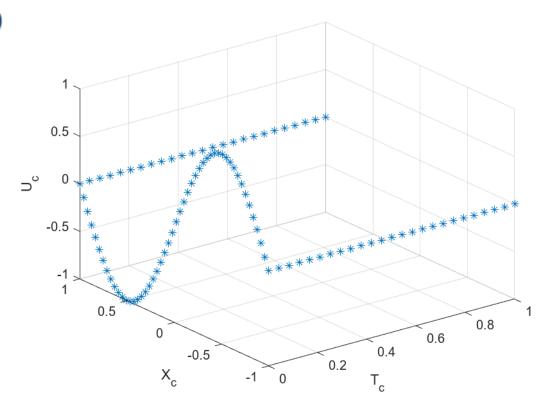


#### **Example: Partial Differential Equation**

• Burger's equation: 
$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \frac{0.01}{\pi} \frac{\partial^2 u}{\partial x^2} = 0$$

• Initial conditions: 
$$u(x, 0) = -\sin(\pi x)$$

- Boundary conditions: u(-1, t) = 0u(1, t) = 0
- Solution space:  $(t, x) \in (0, 1) \times (-1, 1)$

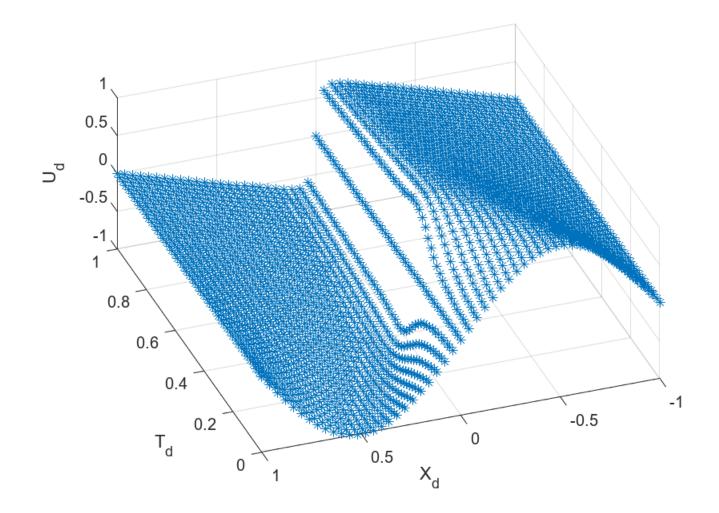


Data points from initial and boundary conditions are used for L<sub>Cond</sub> evaluation



# **Example: FEM Results**

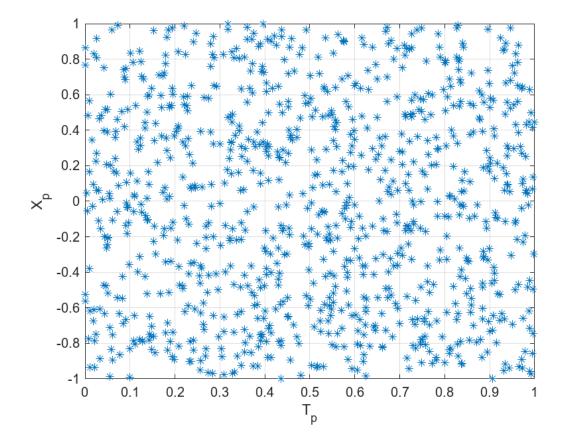
• Data points computed by COMSOL Multiphysics used for L<sub>Data</sub> evaluation





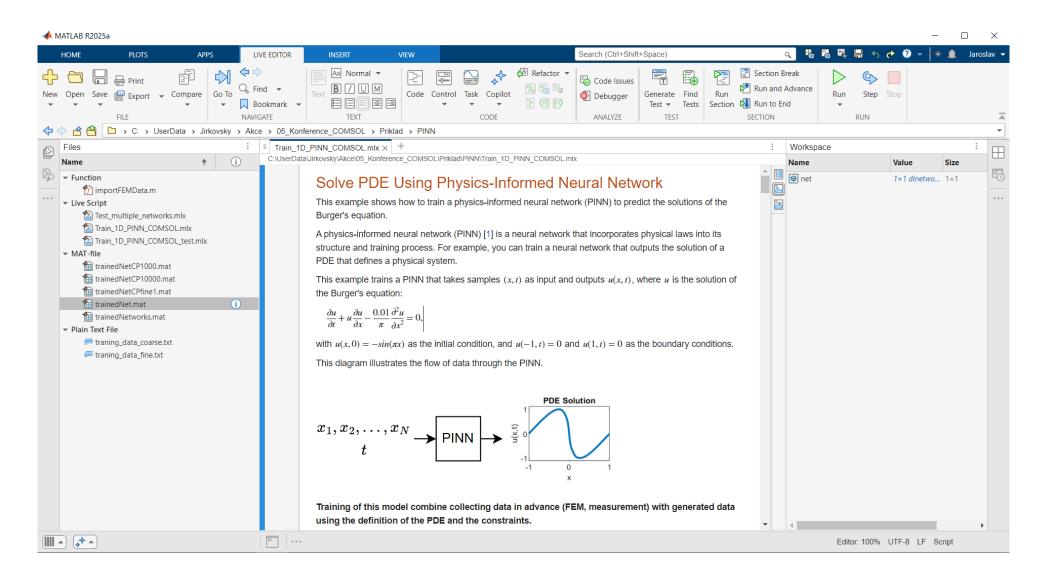
#### Example: Enforce the Physics

- Random data samples used for L<sub>Physiscs</sub> evaluation
- Used to enforce the output of the network to fulfill the Burger's equation





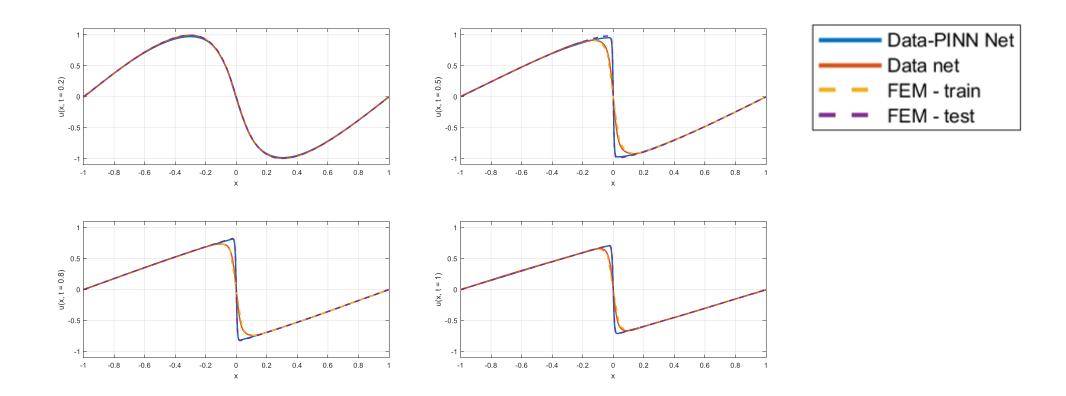
#### Example: Live Script in MATLAB





#### Example: Results

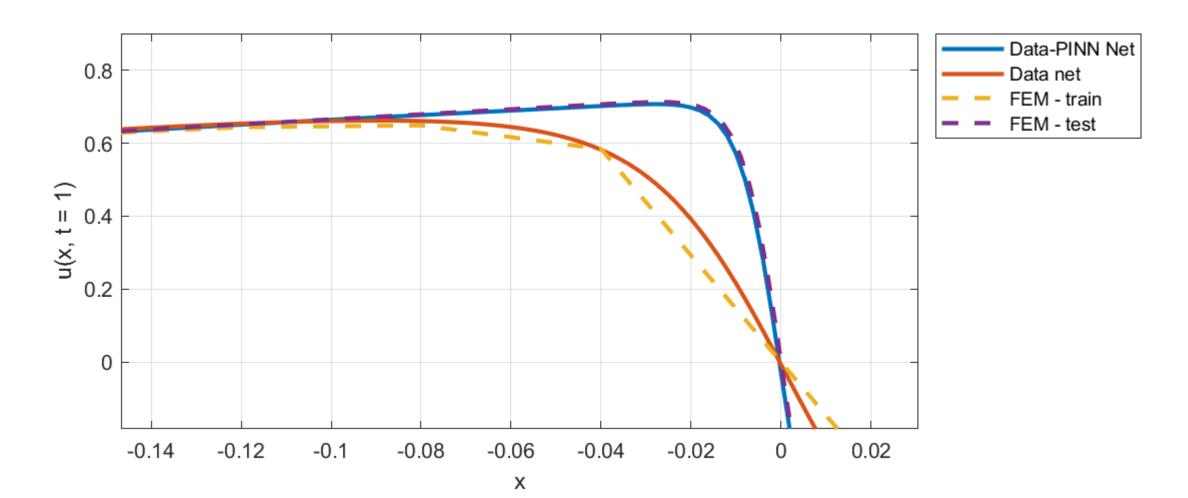
- Solution computed by the trained network at the timestamps 0.2, 0.5, 0.8, 1 sec
- Comparison with the standard (non-PINN) network trained only on the FEM data





### **Example: Results**

Zoom-in the result at t = 1 sec





# Thank you for your attention!