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SCIENTIFIC MACHINE LEARNING AND TENSORFLOW TUTORIAL

Physics informed neural networks and Inverse Problems

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Numerical PDEs: Analysis, Algorithms, and Data Challenges

ICERM

Brown University

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PHYSICS INFORMED NEURAL NETWORKS

- We previously fit neural networks to functions by regressing against data,
  - We used a loss function that penalized against RSS

    $$\mathcal{J} = ||y - N(x)||_2^2$$

- Neural networks can also be trained using more general loss functions like a PDE residual
  - Solves a PDE

    $$F\left(x, u, Du, D^2u, \ldots\right) = 0 \qquad x \in \Omega$$
    $$G(x, u, Du, D^2u, \ldots) = 0 \qquad x \in \Omega \backslash \partial\Omega$$

  - Residual:

    $$\mathcal{J} = ||F\left(x, u, Du, D^2u, \ldots\right)||^2 + \lambda ||G(x, u, Du, D^2u, \ldots)||^2$$

PHYSICS INFORMED NEURAL NETWORKS[1] (PINNS) AS A PDE COLLOCATION SCHEME

- For the PDE,

$$\begin{aligned} &\partial_t u + \partial_x F(u) = 0 && (x,t) \in interior \\ &\mathcal{B}u = f && (x,t) \in boundary \\ &u = g && t = 0 \end{aligned}$$

Let the solution be defined by a neural network,

$$u = u(x,t;\xi)$$

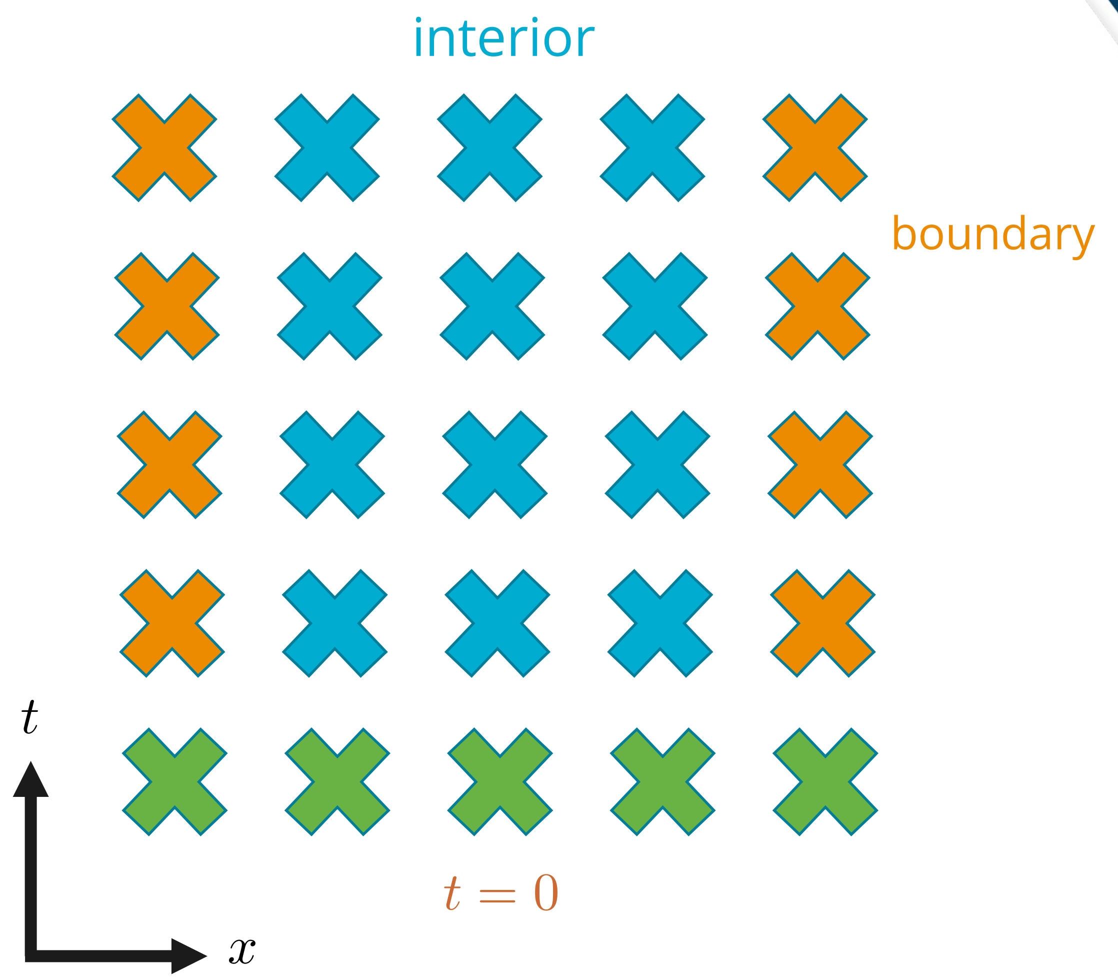
Choose collocation points in space-time

Define a residual,

$$\begin{aligned} R = &||\partial_t u + \partial_x F(u)||^2_{\ell_2 (x,t)_{interior}} \\ &+ \lambda_{BC} ||\mathcal{B}u - f||^2_{\ell_2 (x,t)_{boundary}} \\ &+ \lambda_{IC} ||u - g||^2_{\ell_2 (x,0)} \end{aligned}$$

Minimize

$$\xi = \underset{\hat{\xi}}{\text{argmin}} \ R(\hat{\xi})$$



[1] Raissi et al., *arXiv:1711.10561*

CONTROL VOLUME PINNS[1] (CVPINNS)

- For PDEs of the form,

$$\begin{aligned} &\partial_t u + \partial_x F(u) = 0 && (x,t) \in interior \\ &\mathcal{B}u = f && (x,t) \in boundary \\ &u = g && t = 0 \end{aligned}$$

Let the solution be defined by a neural network,

$$u = u(x, t; \xi)$$

Choose mesh in space-time

Apply divergence theorem to each cell in the mesh

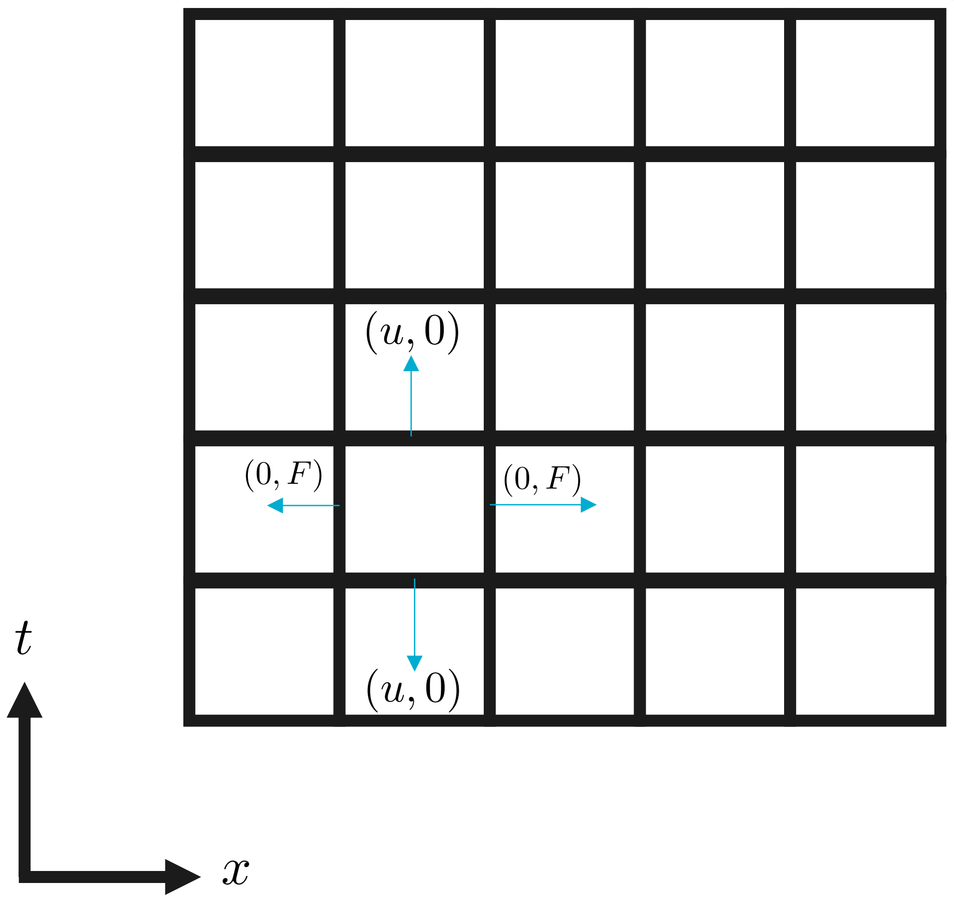
$$R_c = \int_{A_c} \nabla \cdot \begin{pmatrix} u \\ F \end{pmatrix} dA_c = \int_{l_c} \begin{pmatrix} u \\ F \end{pmatrix} \cdot dl_c$$

Approximate integrals with quadrature

Fluxes at boundaries replaced by prescribed values

Minimize residuals

$$\xi = \underset{\hat{\xi}}{\mathrm{argmin}} \sum_c R_c^2$$



[2] R.G. Patel et al., *JCP* (2022)

INVERSE PROBLEMS WITH PINNS

- If we have a data, u_d , and a parameterized PDE, e.g.,

  $F(\partial_t u, \partial_x u, \lambda) = 0$

  $\mathcal{B}u = 0$

- We can find the parameter, λ , using PINNs by adding an extra term to the PINNs loss,

$$\xi, \lambda = \underset{\hat{\xi}, \hat{\lambda}}{\operatorname{argmin}} \; R(\hat{\xi}, \hat{\lambda}) + \alpha ||u - u_d||_{\ell_2}^2$$

- This will simultaneously solve the PDE while adjusting the parameters such that the solution matches the data

CONSTRAINTS FOR PINNS

- Often the parameters we're fitting need to be constrained
  - Well-posedness of the PDE
  - E.g., the conductivity in the heat equation must be positive

    $$\partial_t u = \nabla \cdot \lambda \nabla u$$

  - We can penalize against negative conductivity by adding another term to the loss,

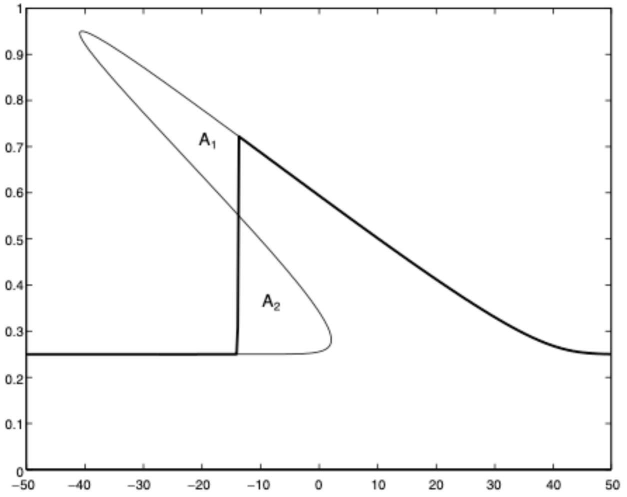
    $$\xi, \lambda = \underset{\hat{\xi}, \hat{\lambda}}{\operatorname{argmin}} \; R(\hat{\xi}, \hat{\lambda}) + \alpha ||u - u_d||_{\ell_2}^2 + \beta || \max(0, -k) ||_{\ell_2}^2$$

  - With a high enough regularization weight, the minima will not have negative conductivity

CVPINNS FOR HYPERBOLIC CONSERVATION LAWS
A CASE STUDY OF PHYSICS INFORMED CONSTRAINED LEARNING

Ingredients needed:

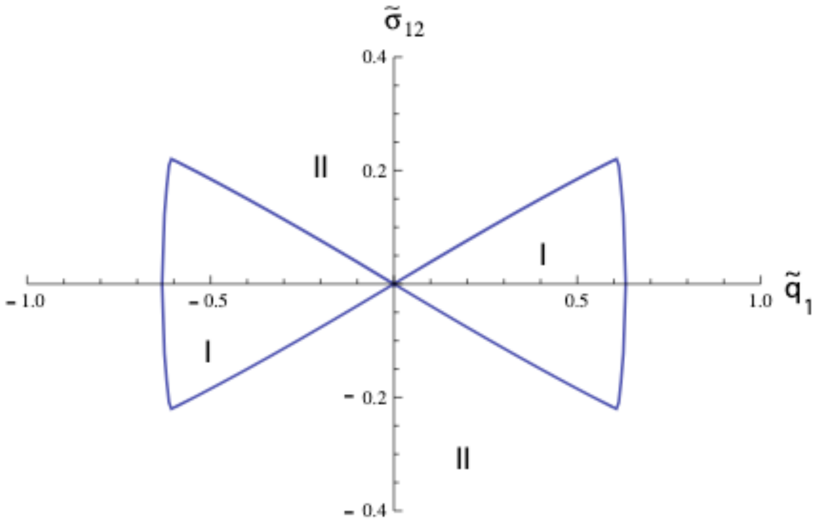
- A numerical method for the PDE,
  $\partial_t \boldsymbol{u} + \boldsymbol{F}(\boldsymbol{u}) = 0$
- A parameterization for $\boldsymbol{F}(\boldsymbol{u})$



Shock solution to the traffic flow equation[1]

Challenges,

- PDE forms discontinuities
- $\boldsymbol{F}(\boldsymbol{u})$ must produce a well-posed IBVP



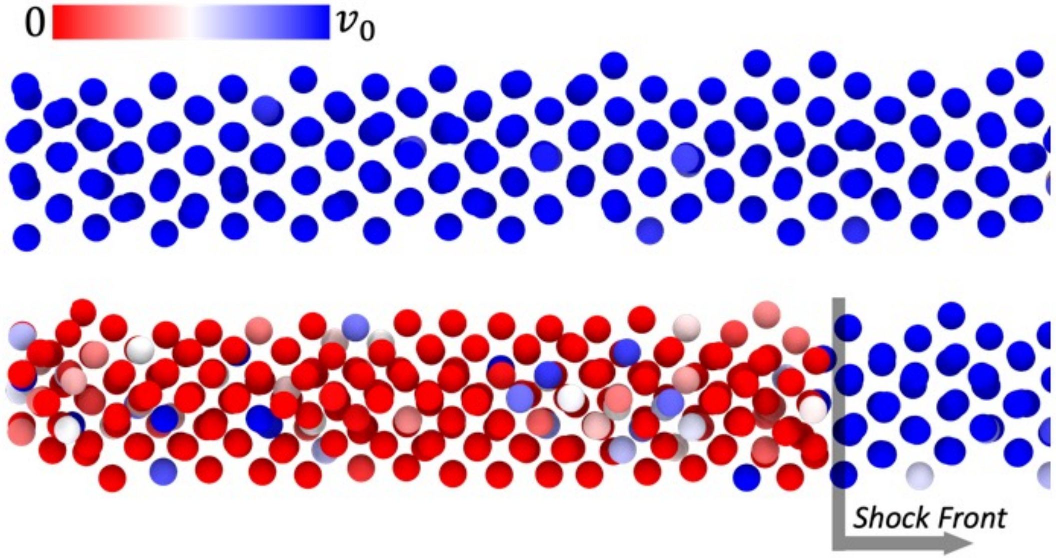
Hyperbolic region for Grad's 13 moment equations[2]

[1] LeVeque, *Finite Volume Methods for Hyperbolic Problems,* 2004

[2] Brini and Ruggeri, *Continuum Mech. Thermodyn.,* 2020

EOS DISCOVERY FOR COPPER UNDER SHOCK

- Perform LAMMPS[1] simulations of the reverse-ballistic impact experiment
  - Various impact velocities and initial temperatures



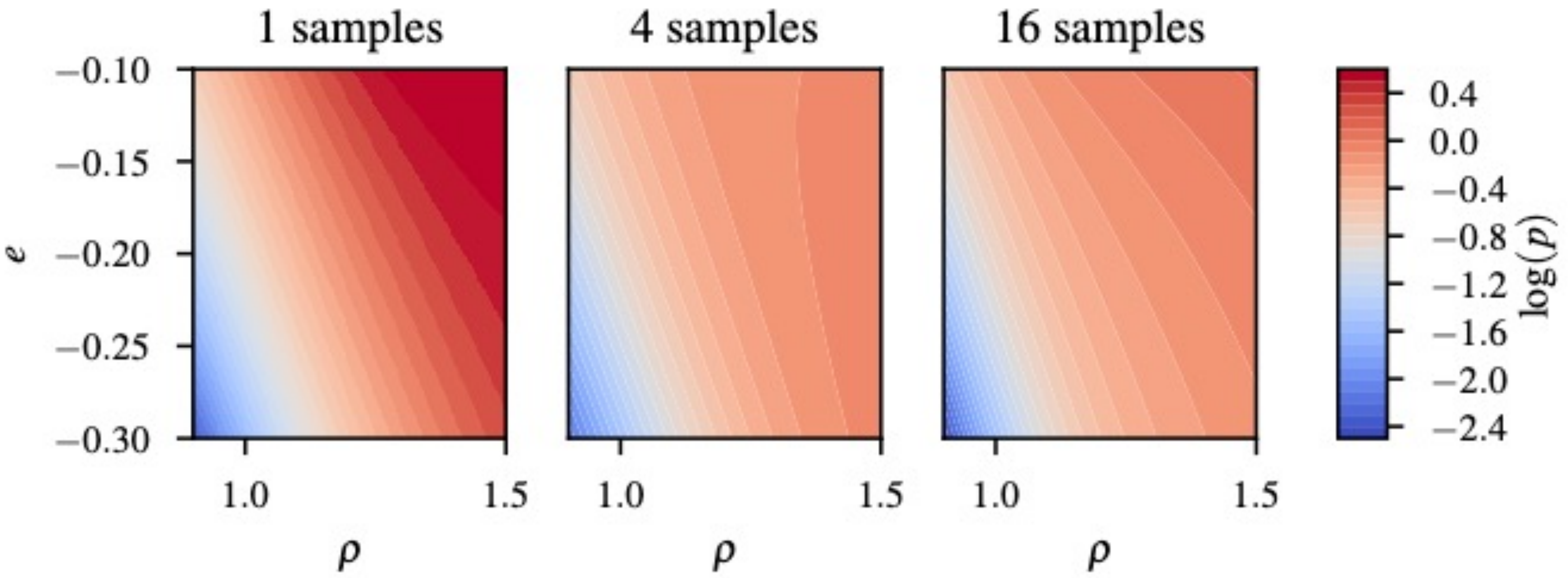
Fit an EOS to the LAMMPS data using CVPINNs

- Regularized neural network parameterization to preserve hyperbolicity in the Euler equations (convex Entropy)

Use fitted EOS to perform FD simulations of a new impact case and compare to LAMMPS

[1]LAMMPS, https://lammps.sandia.gov

EOS FITS FOR SHOCKED COPPER

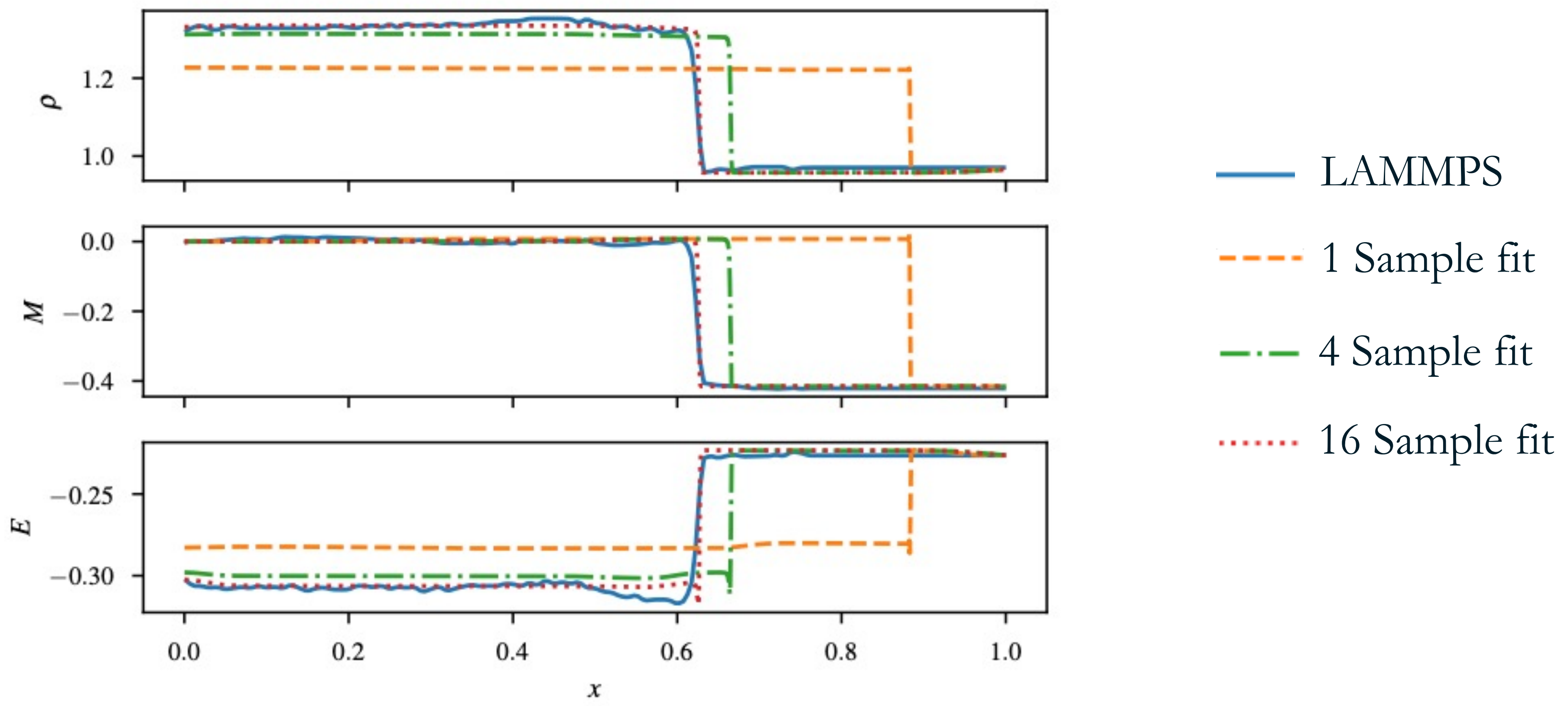


EOS fits using penalty to prevent loss of hyperbolicity

EOS FITS TEST FOR SHOCKED COPPER

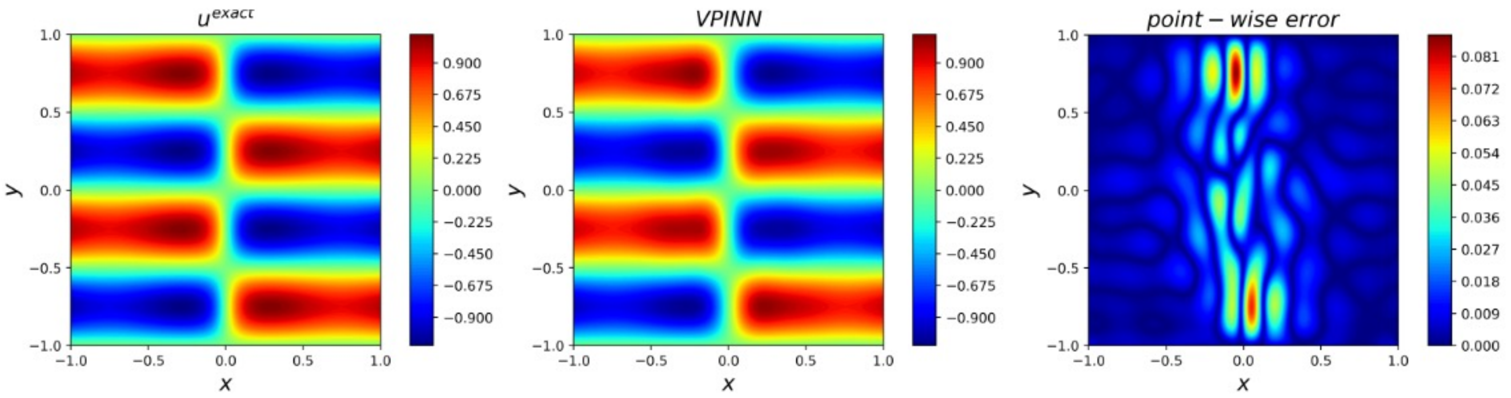
Use fitted EOS's to solve new impact case

- Viscous regularized finite difference (FD) code on a fine mesh

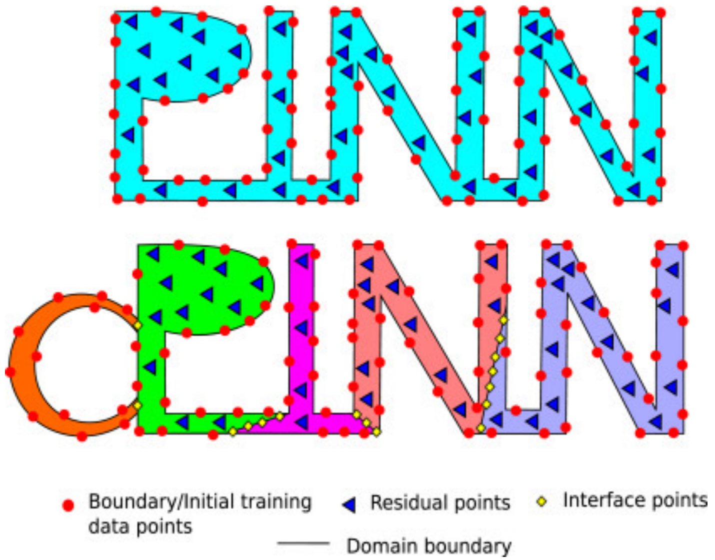


OTHER PINNS VARIANTS

Variational PINNs (E. Kharazmi et al., arXiv:1912.00873 (2019))



Conservative PINNs (A. Jagtap et al., *CMAME* (2020))



EXERCISE

- Exercise 1
  - Develop a PINN for the viscous Burgers equation
  - Solve the forward problem for the viscous Burgers equation
  - Using the provided data, find the viscosity coefficient

- Exercise 2
  - Find the frequency of the forcing term in the Poisson equation