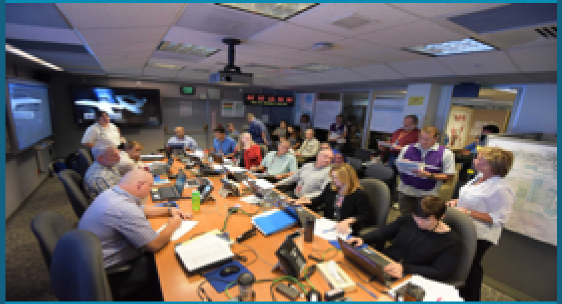
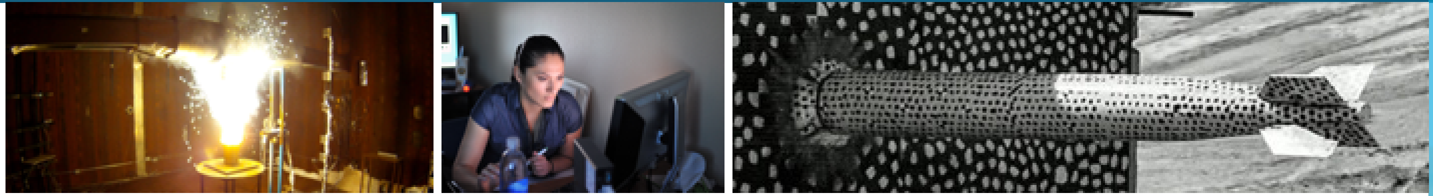
SAND2021-2236C

Thermodynamically consistent physics-informed neural networks for hyperbolic systems





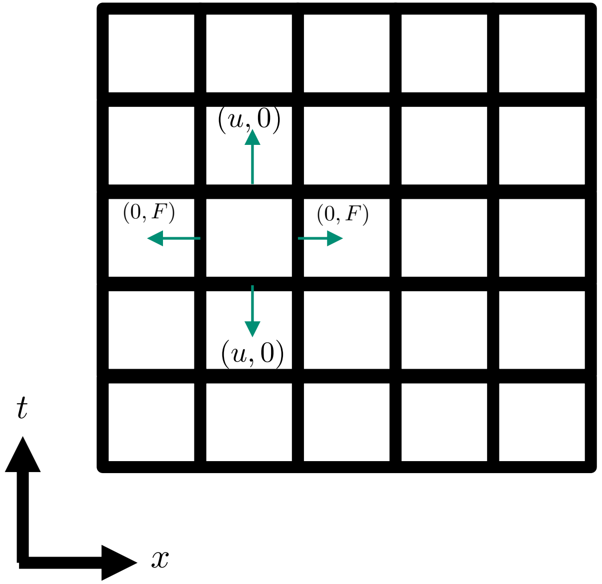
Indu Manickam
Mission Algorithms Research and Solutions

SIAM Conference on Computational Science and Engineering
Learning Operators from Data
March 2021

Control Volume Physics Informed Neural Networks (cvPINNs)

- Deep learning method for solving hyperbolic PDEs.
- Assimilates traditional finite volume methodology.
- Introduce regularizations that bias solutions towards the zero-viscosity limit.
- Ensures a thermodynamically consistent treatment of forward and inverse problems.
- Extract data-driven equations of state for shock hydrodynamic problems.

$$L = \underbrace{\sum_c R_c^2}_{\text{conservation law residual}} + \underbrace{\lambda_E \sum_c \max(0, R_c^E)^2}_{\text{entropy regularization}} + \underbrace{\lambda_T \sum_n \max(0, \mathrm{TV}(u^{n+t}) - \mathrm{TV}(u^n))^2}_{\text{total variation diminishing property}}$$



Hyperbolic conservation laws

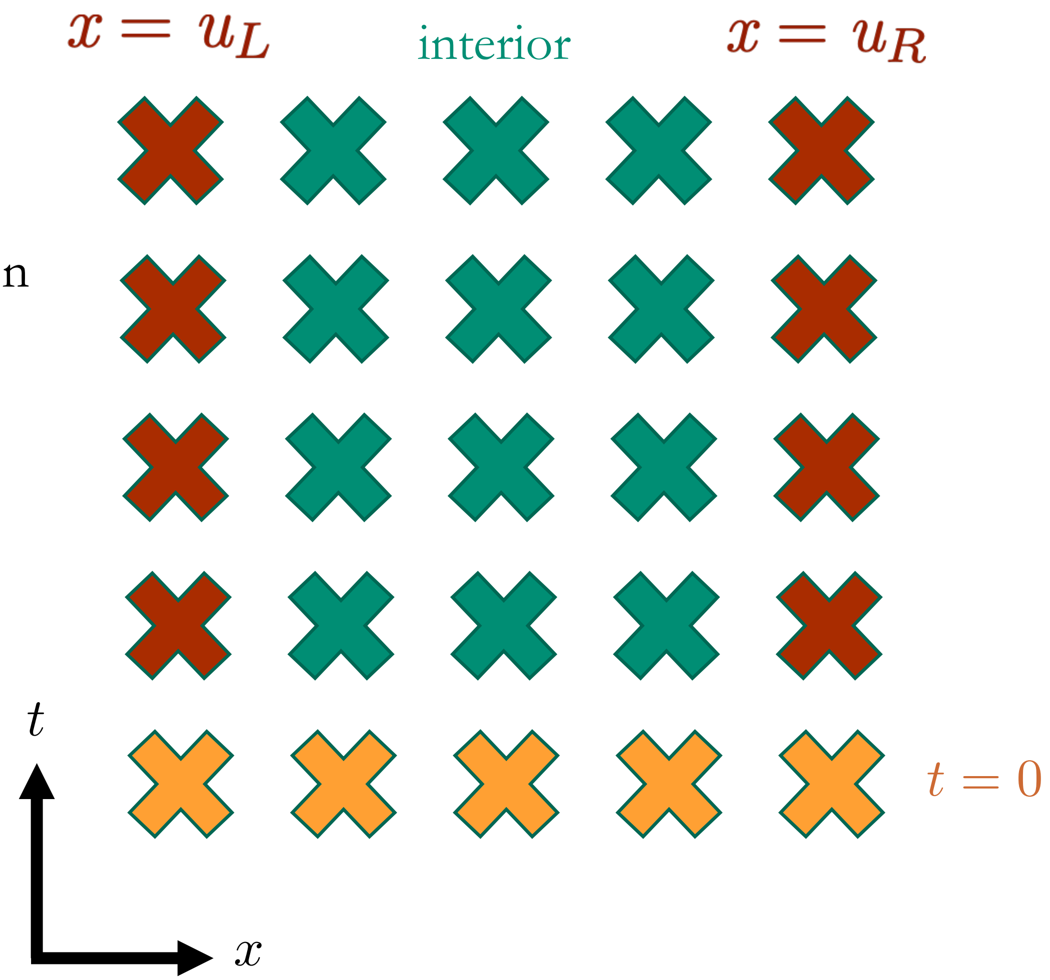
Hyperbolic PDE for a conserved variable $u(x, t)$

$\partial_t u + \partial_x F(u) = 0$ $(x, t) \in interior$ Conservation Law

$\mathcal{B}u = f$ $(x, t) \in boundary$ Boundary condition

$u = g$ $t = 0$ Initial condition

Solve for $u(x, t)$



Euler Equations

Conserved Variables

$\rho =$ density

$v =$ velocity

$p =$ pressure

Conservation Laws

$$\partial_t \rho + \partial_x \rho v = 0$$

$$\partial_t \rho v + \partial_x (\rho v^2 + p) = 0$$

$$\partial_t E + \partial_x v(E + p) = 0$$

$$E = \rho e + \frac{1}{2}\rho v^2$$

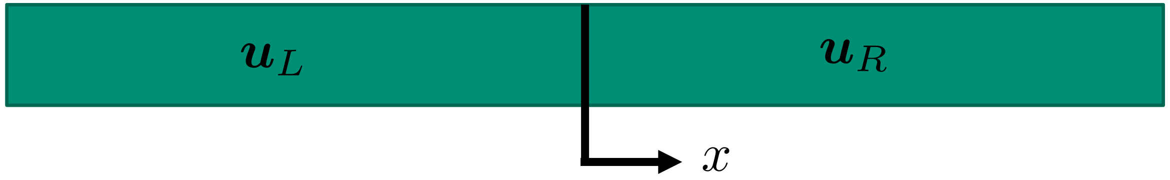
Equation of State (EOS)

$$s = \log(e^{1/(\gamma-1)}/\rho)$$

$$p = -\rho^2(\partial_\rho s)(\partial_e s)^{-1}$$

We will consider solutions to Riemann problems,

$$\begin{aligned} \boldsymbol{u}(x,0) &= \boldsymbol{u}_L \quad \text{if } x < 0 \\ \boldsymbol{u}(x,0) &= \boldsymbol{u}_R \quad \text{if } x \geq 0 \end{aligned}$$



Outline

1. cvPINNs as a numerical method for hyperbolic PDEs **(Forward problem)**

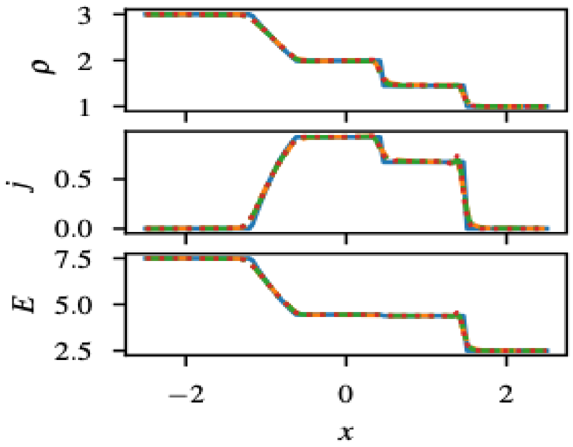
$$\partial_t \rho + \partial_x \rho v = 0$$

$$\partial_t \rho v + \partial_x (\rho v^2 + p) = 0$$

$$\partial_t E + \partial_x v(E + p) = 0$$

$$s = \log(e^{1/(\gamma-1)}/\rho)$$

$$p = -\rho^2 (\partial_\rho s)(\partial_e s)^{-1}$$



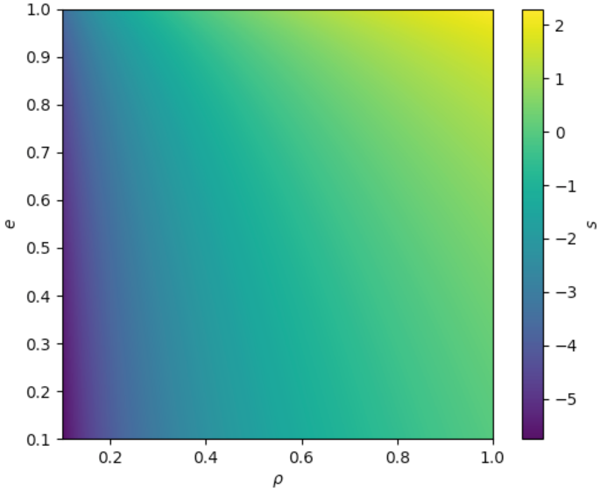
2. Equation of state discovery with cvPINNs **(Inverse problem)**

$$\partial_t \rho + \partial_x \rho v = 0$$

$$\partial_t \rho v + \partial_x (\rho v^2 + p) = 0$$

$$\partial_t E + \partial_x v(E + p) = 0$$

$$s = s(\rho, e)$$



Physics informed neural networks[1] (PINNs) as a PDE collocation scheme

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

Let the solution be defined by a neural network,

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

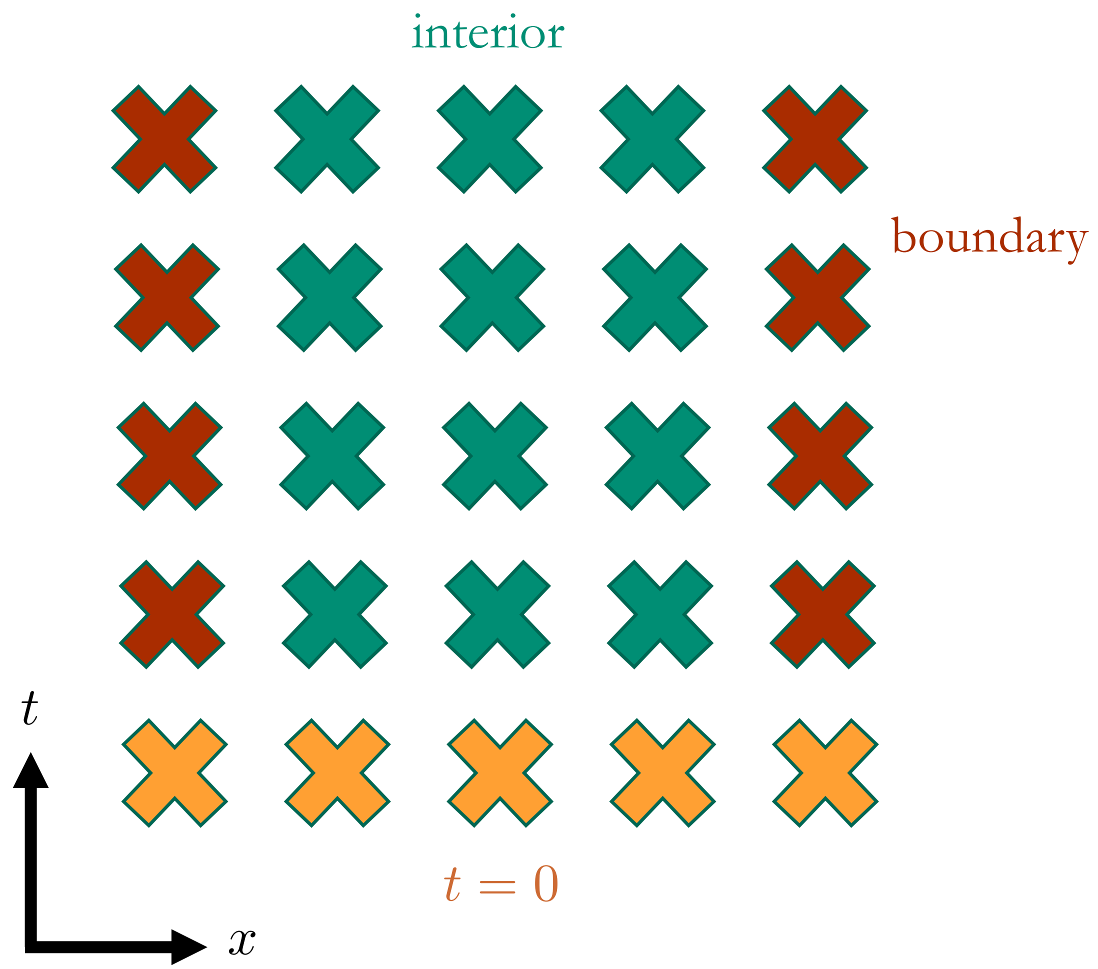
Choose collocation points in space-time

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

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



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

Control volume PINNs (cvPINNs)

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

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

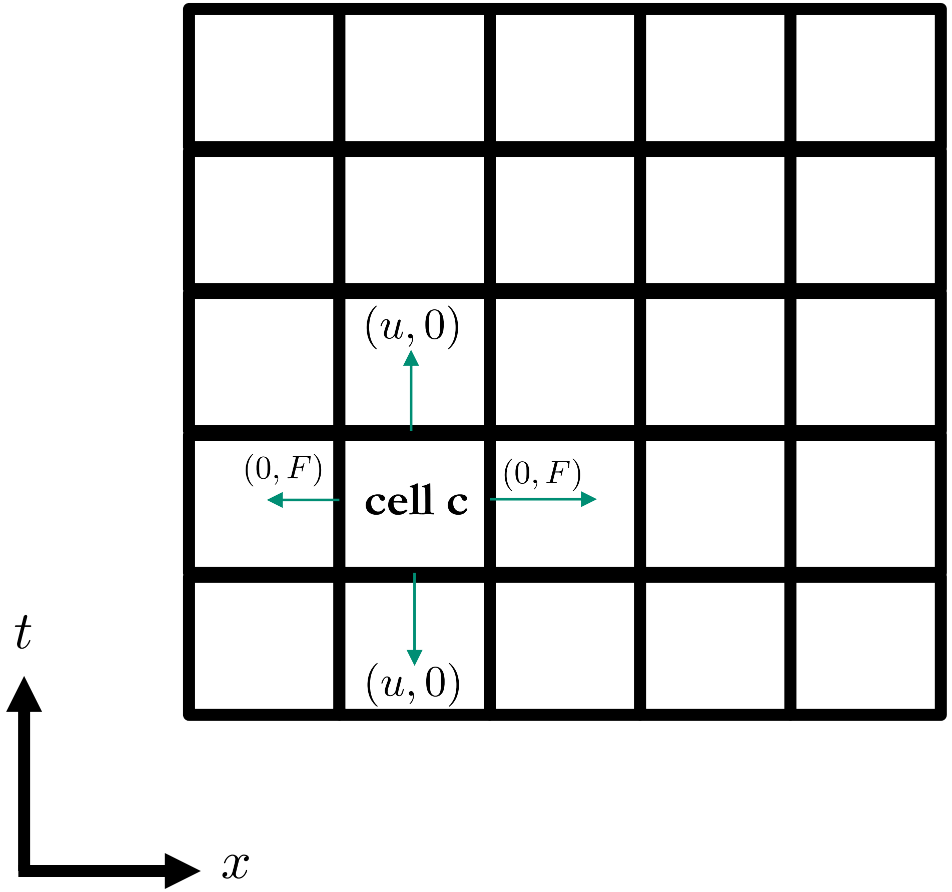
$$R_c = \int_{A_c} \nabla \cdot \begin{pmatrix} u \\ F \end{pmatrix} dA_c = \int_{l_c} \begin{pmatrix} u \\ F \end{pmatrix} \cdot dl_c$$

Approximate integrals with quadrature

Fluxes at boundaries replaced by prescribed values

Minimize residuals

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



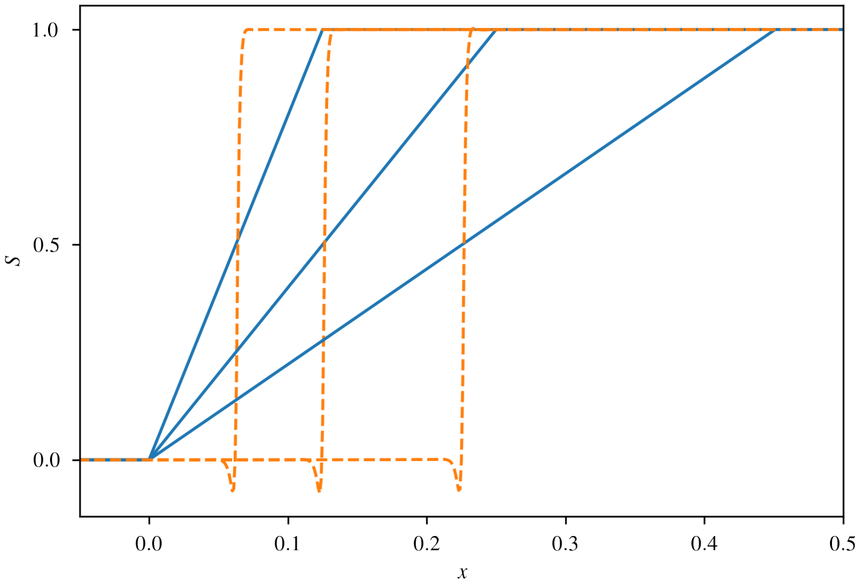
Potential issues with cvPINNs

Converging to unphysical solution

Solutions to the integral form aren't unique.

We want the physically meaningful entropy solution,

$$\lim_{\nu \to 0} \partial_t u + \partial_x F(u) = \nu \partial_x^2 u$$



▬ Entropy solution to Burgers equation

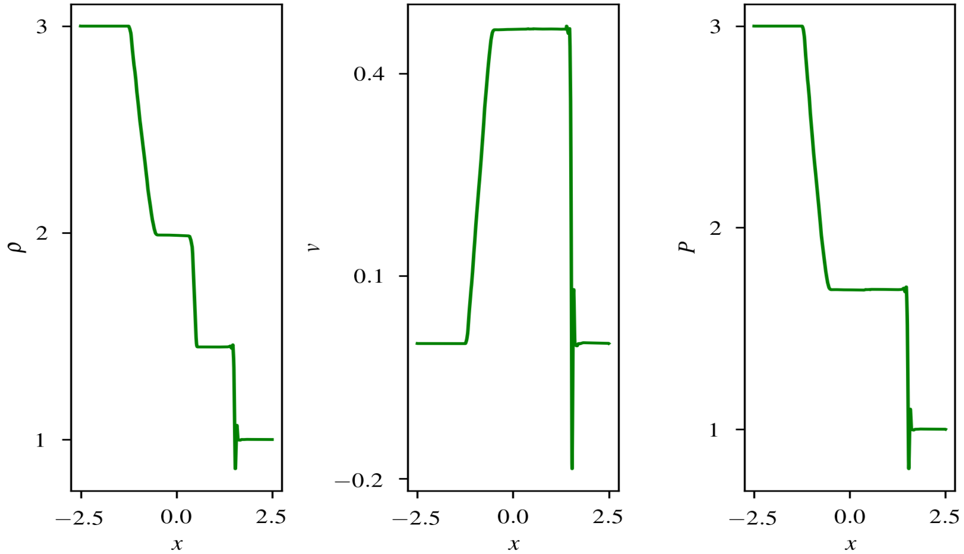
▪▪▪ Unphysical solution from unregularized cvPINNs

Oscillatory behavior near shock

May occur due to:

- Estimating discontinuous solutions using an L_2 framework
- Suboptimal training/approximation of the deep neural network

Euler equation



Entropy regularization – Bias Towards Entropy Solution

Given entropy pair,(q, η), the entropy solution obeys:

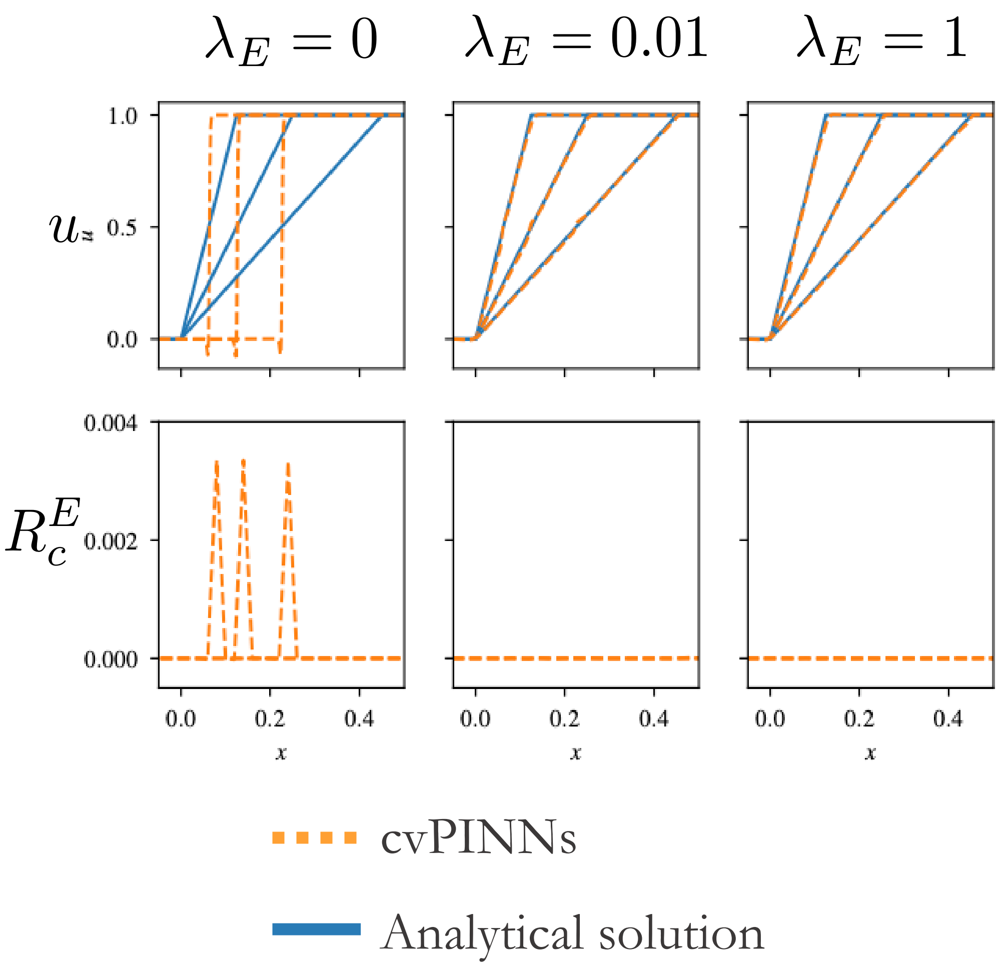
$$\partial_t q(u) + \partial_x \eta(u) \leq 0$$

Add the entropy penalty, R_c^E , for each cell c to the loss:

$$R_c^E = \int_{\partial_c} \partial_t q(u) + \partial_x \eta(u) \cdot dA$$

$$L = \sum_c R_c^2 + \lambda_E \underline{\sum_c max(0, R_c^E)^2}$$

Burgers equation with neural network initialized to unphysical solution.



TVD regularization- Prevent Oscillations Near Shocks

TVD schemes in standard discretizations prevent oscillations

For $u(x,t)$ at grid values $u_i^n = u(x_i, t_n)$

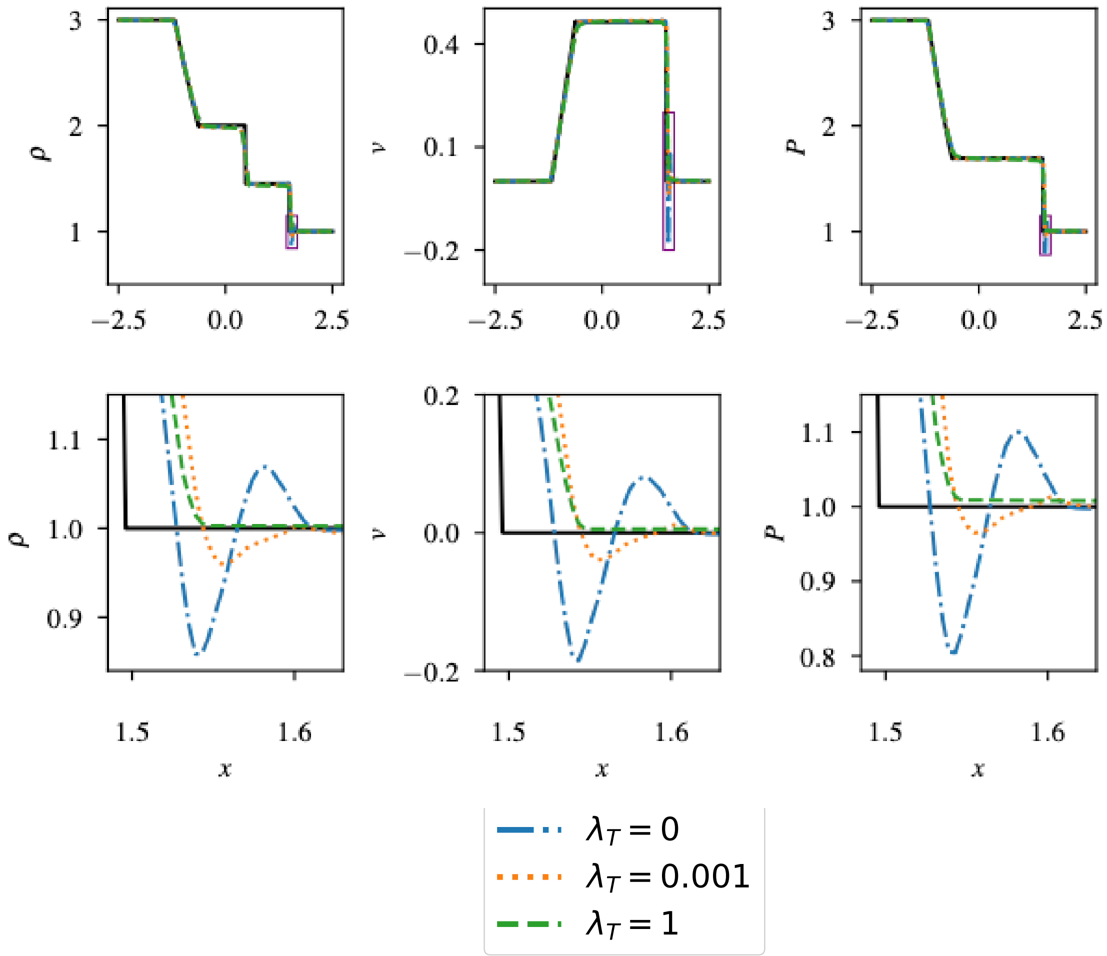
$$TV(u^n) = \sum_i |u_{i+1}^n - u_i^n|$$

$$TV(u^{n+1}) - TV(u^n) \leq 0$$

Define a regular grid on top of the mesh and add another term to the loss:

$$L = \sum_c R_c^2 + \lambda_E \sum_c \max(0, R_c^E)^2$$
$$+ \lambda_T \sum_n \max(0, \mathrm{TV}(u^{n+t}) - \mathrm{TV}(u^n))^2$$

Euler equations with gamma law gas



Outline

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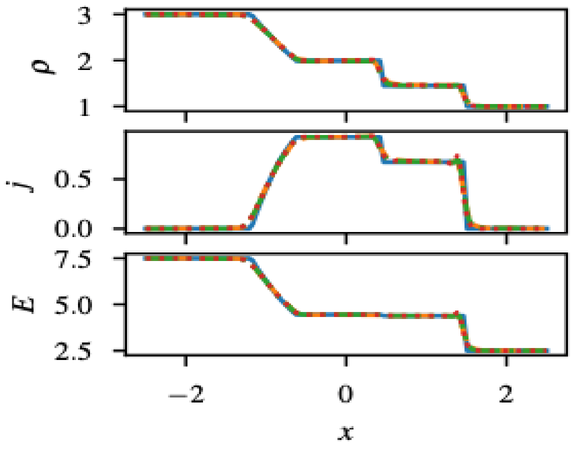
$$s = \log(e^{1/(\gamma-1)}/\rho)$$

$$p = -\rho^2 (\partial_\rho s)(\partial_e s)^{-1}$$



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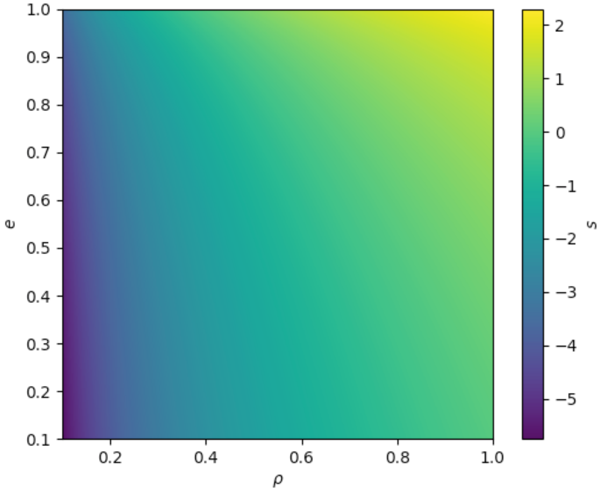
$$s = s(\rho, e)$$



Inverse problems with hyperbolic conservation laws: Equation of state discovery

Objective: learn both $u(x, t)$ and the equation of state, $s(\rho, e; \xi_{EOS})$

Given a set of scattered point observations, $u_{\textbf{data}}$

Simultaneously minimize the PDE residual and the data residual

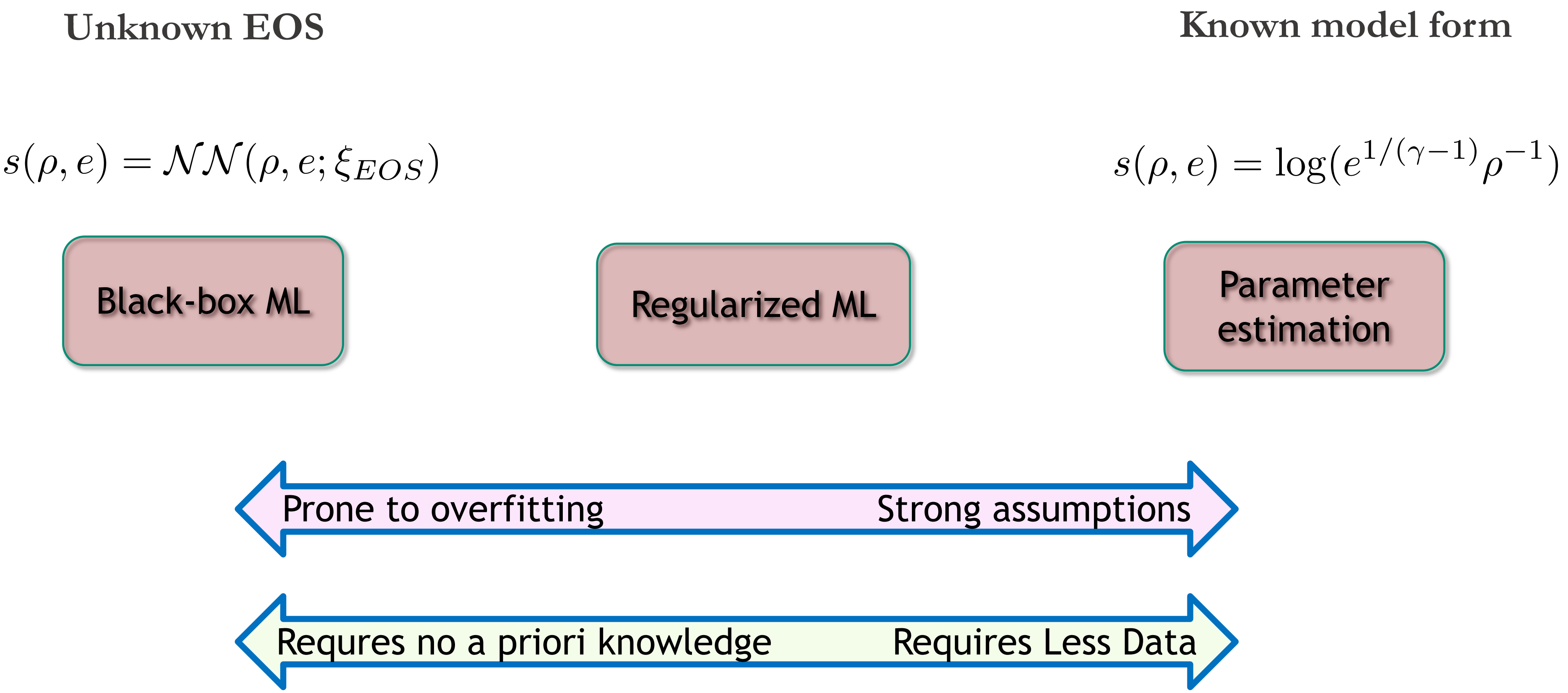
$$\partial_t \rho + \partial_x \rho u = 0$$
$$\partial_t \rho u + \partial_x (\rho u^2 + p) = 0$$
$$\partial_t E + \partial_x u(E + p) = 0$$

$$\underline{s(\rho, e; \xi_{EOS})}$$

$$\longrightarrow$$

$$L = \sum_c R_c^2 + \lambda_E \sum_c \max(0, R_c^E)$$
$$+ \lambda_T \sum_n \max(0, TV(u^{n+1}) - TV(u^n))$$
$$+ \lambda_D \underline{||u - u_{data}||_{\ell_2(x,t)_{data}}}$$

EOS Parameterizations



Unknown EOS

Known model form

$$s(\rho, e) = \mathcal{N}\mathcal{N}(\rho, e; \xi_{EOS})$$

$$s(\rho, e) = \log(e^{1/(\gamma-1)}\rho^{-1})$$

Black-box ML

Regularized ML

Parameter estimation

Prone to overfitting

Strong assumptions

Requres no a priori knowledge

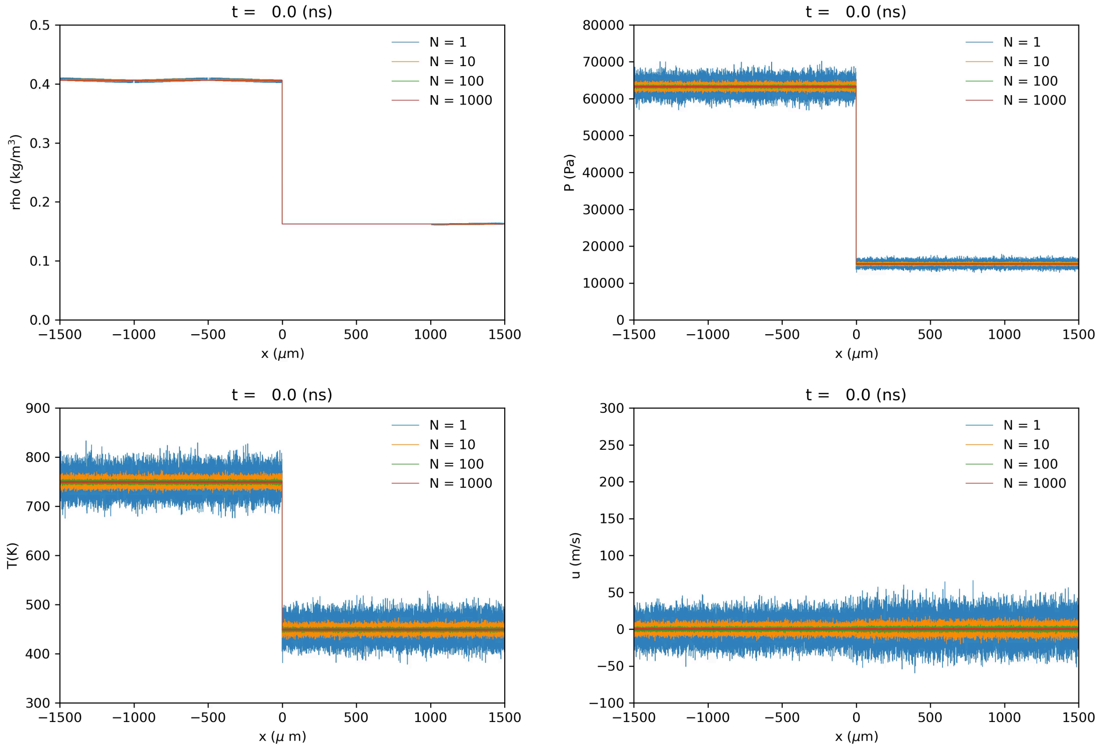
Requires Less Data

Verification with DSMC data

DSMC simulations of Sod shock problems performed in Sparta[1]

- Argon gas
- Varying density, pressure initial conditions
- Constructed to match Riemann problem with gamma gas law.

$$s(\rho, e) = \log(e^{1/(\gamma-1)}\rho^{-1})$$



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[1] Sparta, https://sparta.sandia.gov/

Parameterized gamma law gas vs Black-box ML

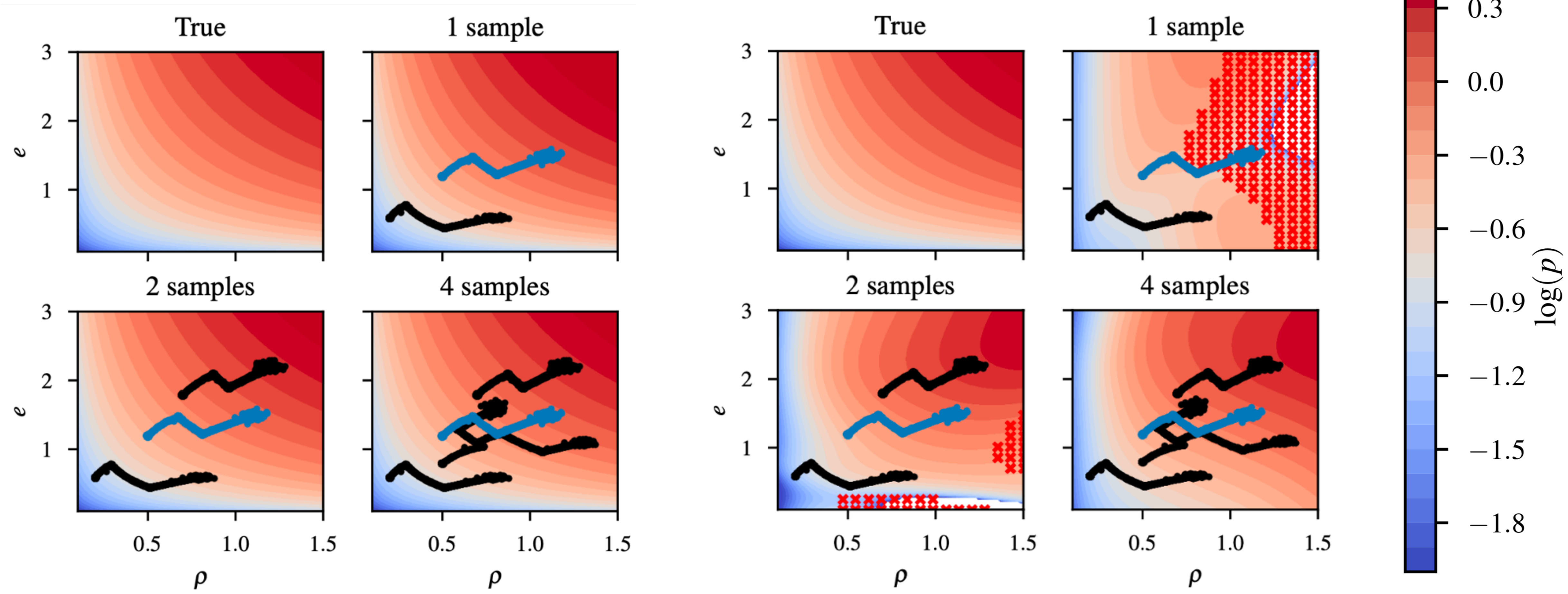
● Training data

✖ Elliptic regions

● Test data

Parameter estimation

Black-box ML



Thermodynamic regularization

For a physical reasonable EOS[1],

$$\partial_e s > 0 \qquad \partial_e^2 s \leq 0 \qquad \partial_\rho(\rho^2 \partial_\rho s) < 0$$

Guarantee hyperbolicity of Euler equations

- Necessary for well-posedness of IBVP

Add another term to the loss,

$$L = \sum_c R_c^2 + \lambda_E \sum_c \max(0, R_c^E)$$

$$+ \lambda_T \sum_n \max(0, TV(u^{n+1}) - TV(u^n))$$

$$+ \lambda_D ||u - u_{data}||_{\ell_2(x,t)_{data}}$$

$$+ \lambda_R \sum_{(\rho,e)_{regularize}} \left[\max\left(0, -\partial_e s\right) + \max\left(0, \partial_e^2 s\right) + \max\left(0, \partial_\rho(\rho^2 \partial_\rho s)\right)\right]$$

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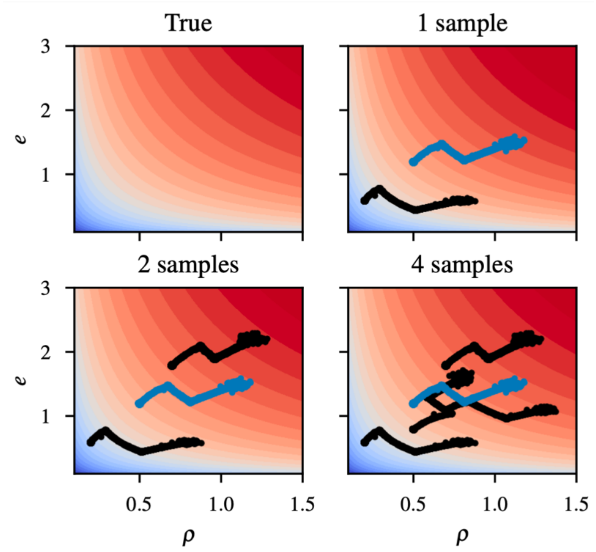
[1] Menikoff and Plohr, *Rev. Modern Phys*, 1989

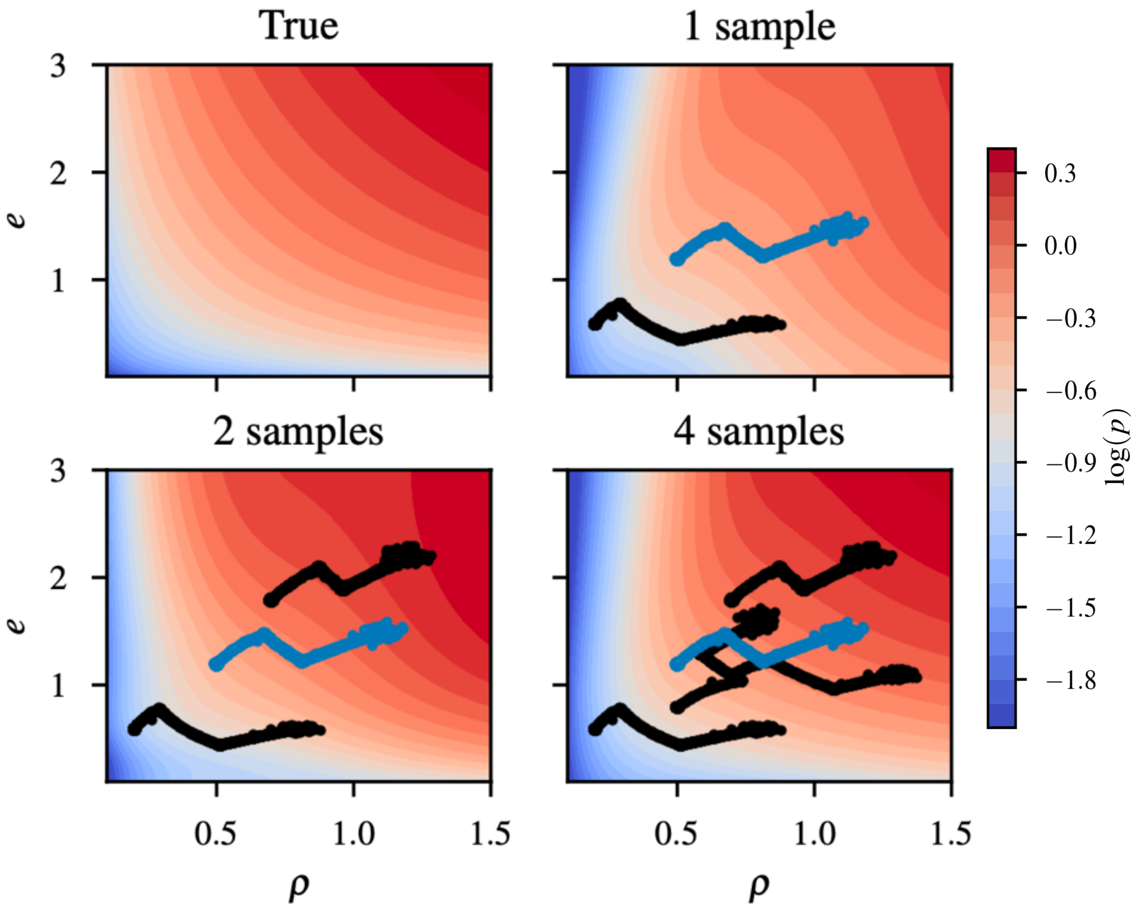
Neural network with thermodynamic regularization

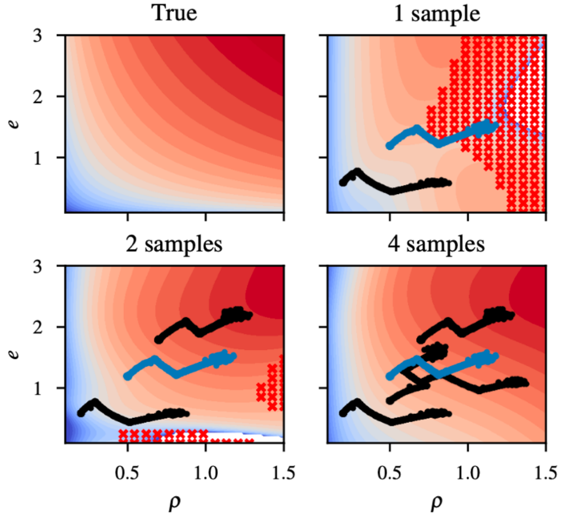
- ● Training data
- ✖ Elliptic regions
- ● Test data



Parameter estimation

Regularized ML

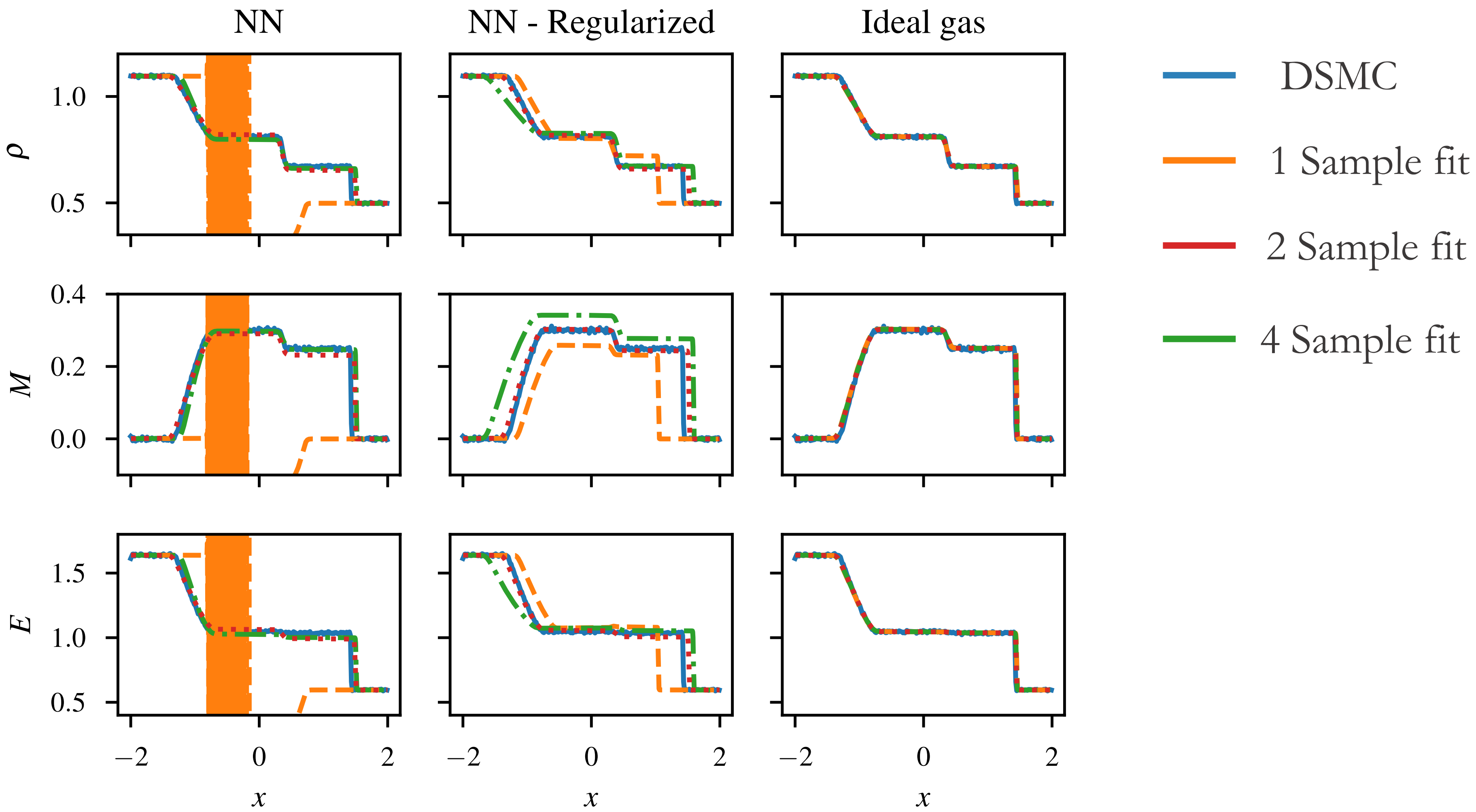




Black-box ML

Comparison of EOS Parameterizations

Prone to overfitting Strong assumptions

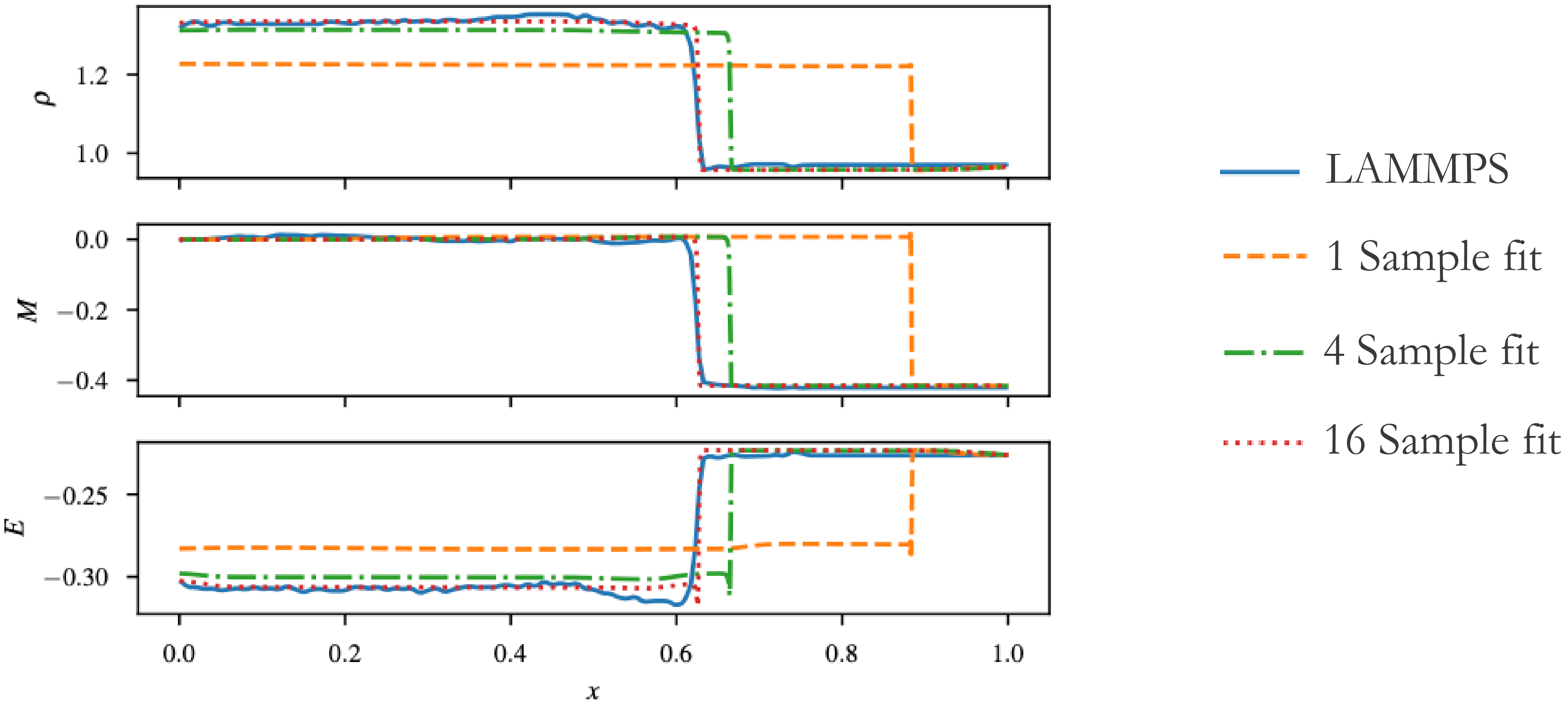


Requres no a priori knowledge Requires Less Data

EOS fits test for shocked copper

Perform LAMMPS[1] simulations of a copper bar in a reverse-ballistic impact experiment

Unknown EOS



Conclusion

Preprint:

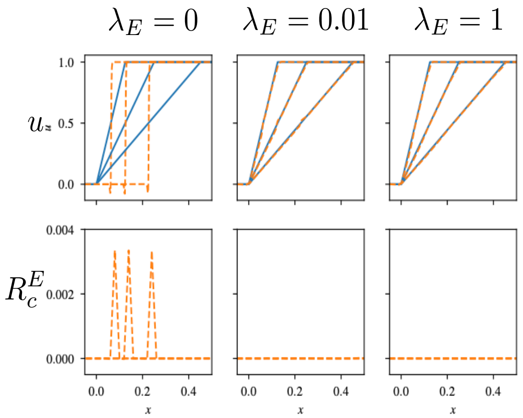
- Patel et al. *arXiv:2012.05343*

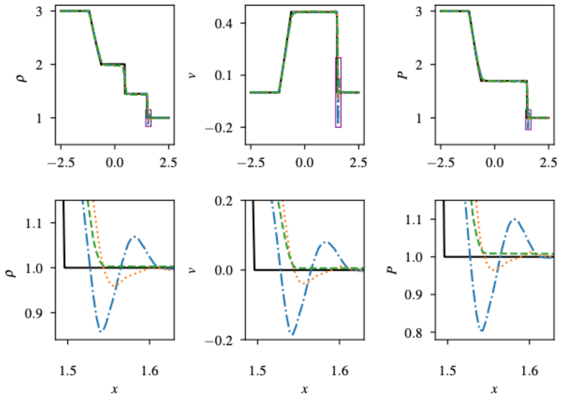
Code:

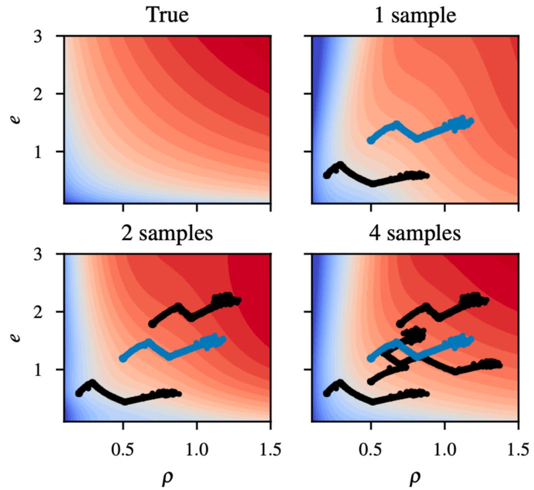
- https://github.com/rgp62/cvpinns

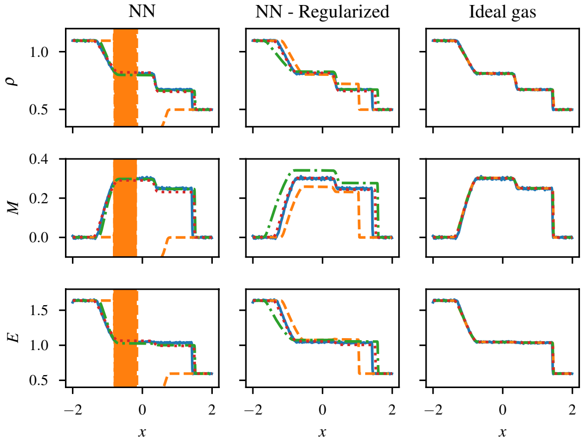
1. cvPINNs as a numerical method for hyperbolic PDEs
   - Less regularization needed
   - Reduces solution regularity requirements
   - Bias solution towards entropy solution and total variation diminishing property

2. Equation of state discovery with cvPINNs
   - Extract data-driven EOS
   - Impose thermodynamic bias
   - EOS parameterizations
     - Parameterized model
     - Neural network
     - Regularized neural network



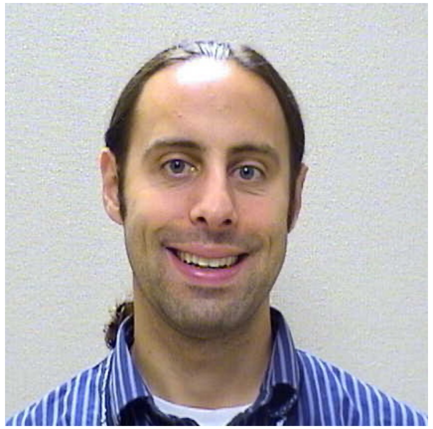






Acknowledgements

Ravi Patel



Eric Cyr

Nat Trask

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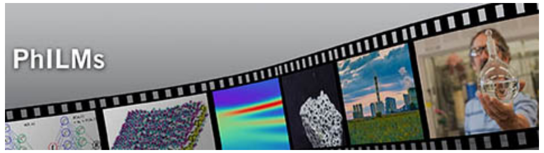
Ignacio Tomas

Mitch Wood

MK Lee



www.pnnl.gov/computing/philms

cvPINNs is less sensitive to hyperparameters than PINNs

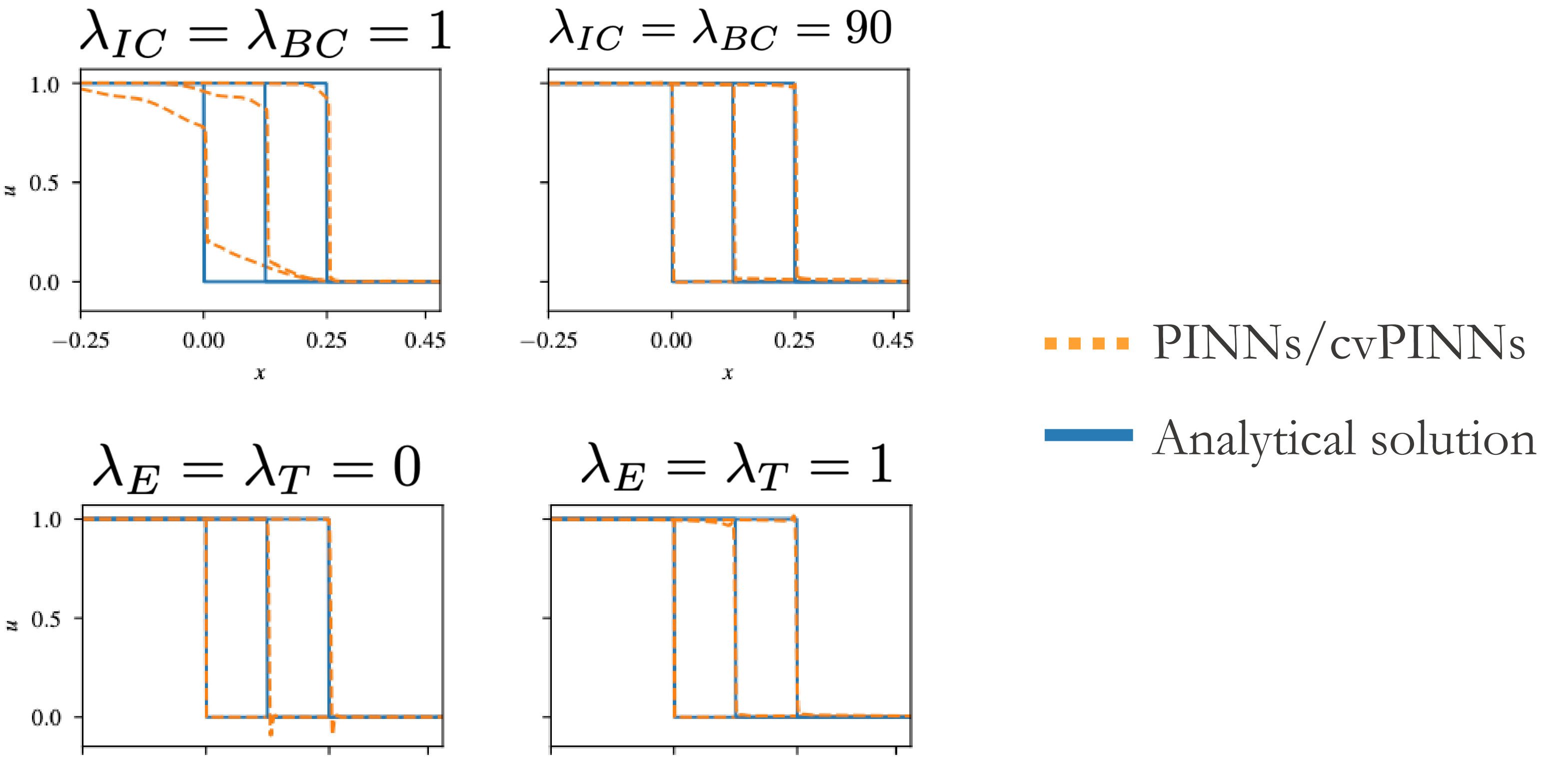
PINNs has been used successfully for hyperbolic PDEs[1]

- We observed reduced sensitivity to hyperparameters in cvPINNs
  - BC and IC penalties in PINNs
  - Entropy+TVD penalties in cvPINNs

For Burgers equation,

PINNs solution

cvPINNs solution



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[1] Mao et al. *CMAME*, 2020

PINNs can fail to find the entropy solution without artificial viscosity

Buckley-Leverett: PDE with nonconvex flux produces solutions with mixed type waves,

$$\partial_t u + \partial_x \left(\frac{u^2}{u^2 + \frac{1}{M}(1-u)^2} \right) = 0$$

Without AV

With AV

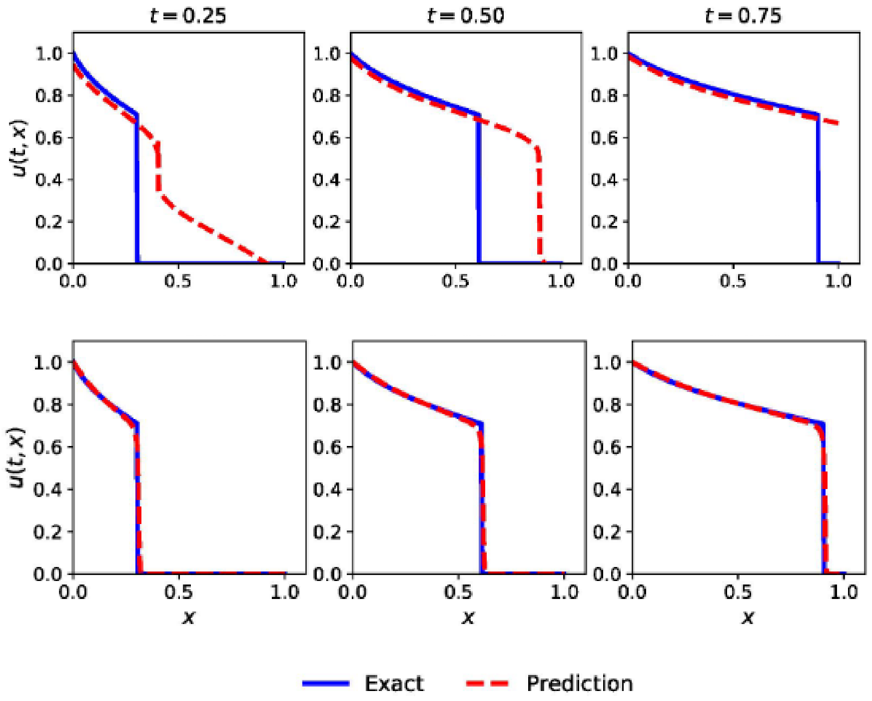

Figure reproduced from [1]

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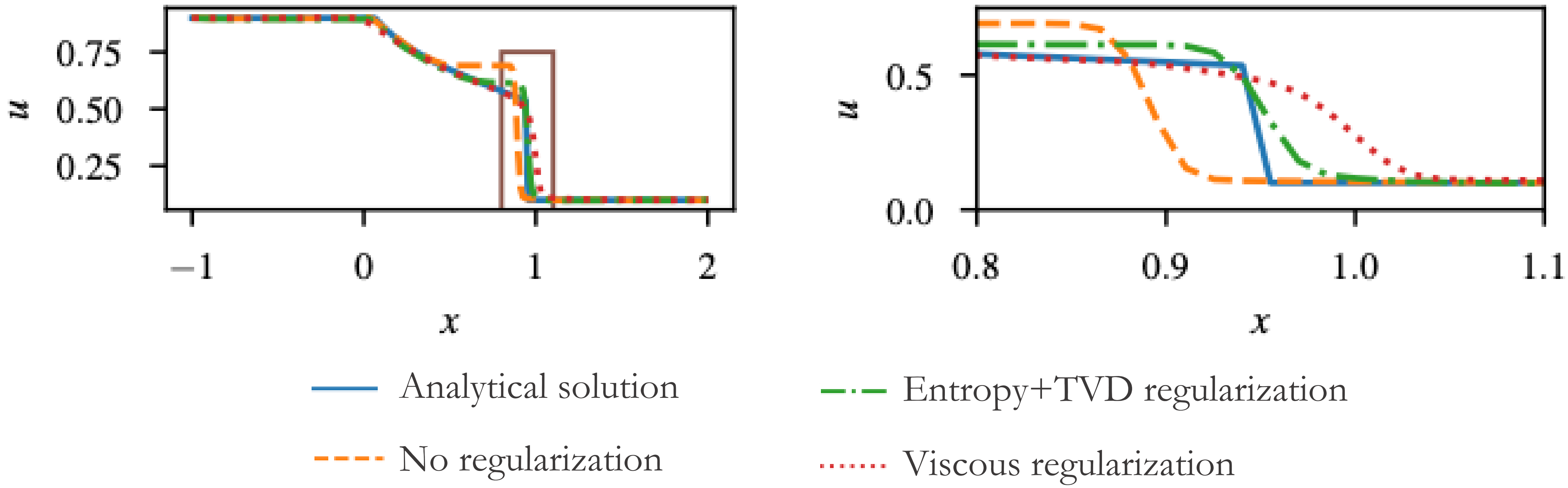
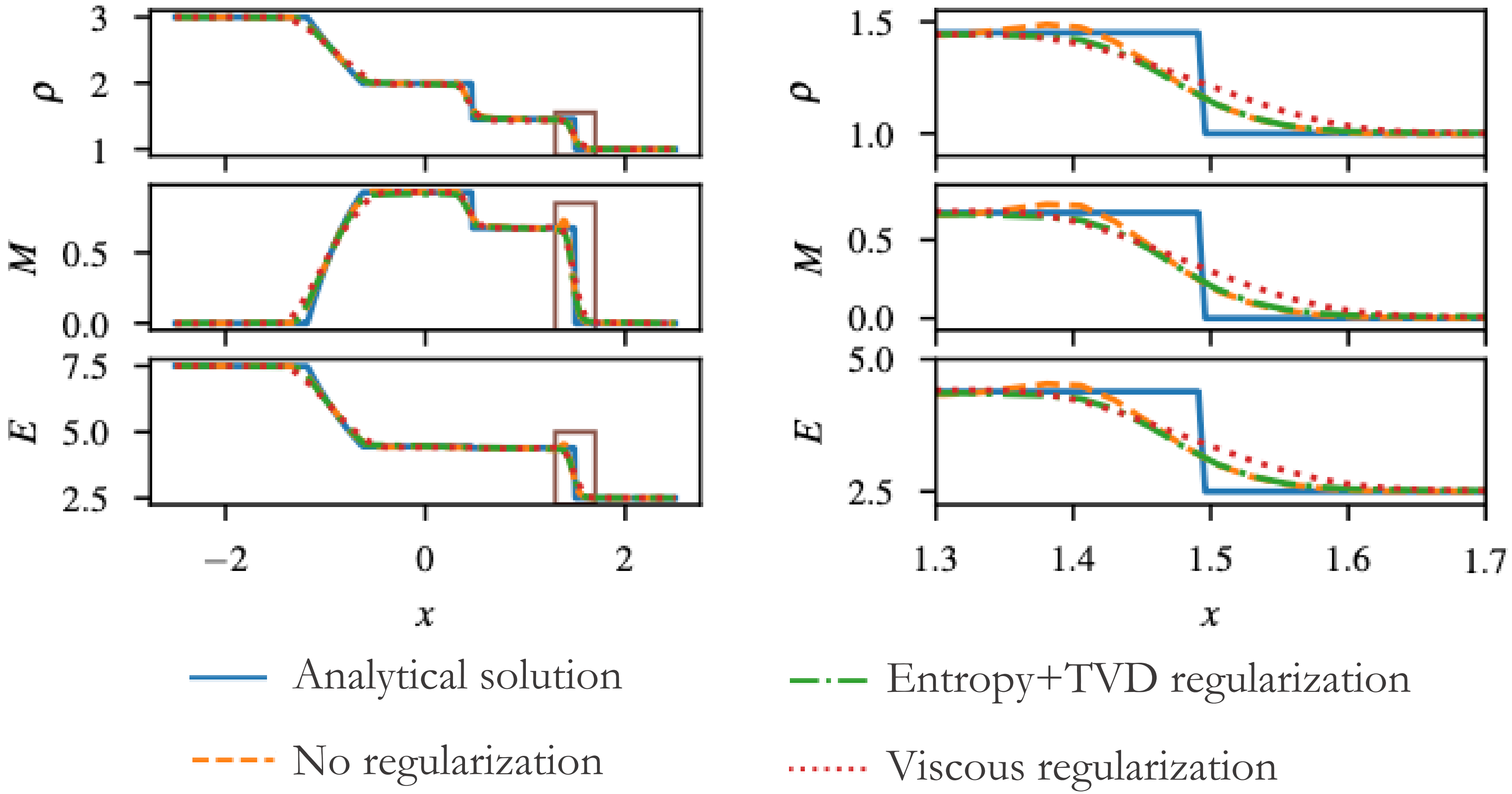
[1] Fuks and Tchelepi, *JMLMC*, 2020

cvPINNs forward solution: Buckley-Leverett equation

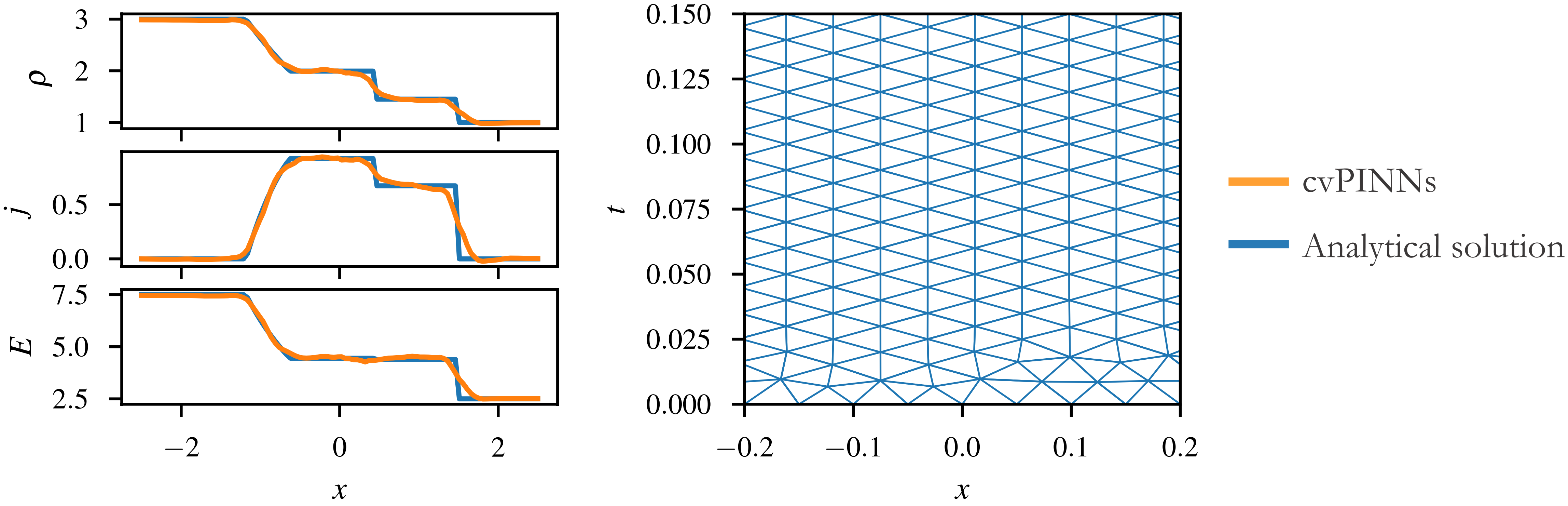


cvPINNs forward solution: Euler equations



cvPINNs on unstructured meshes

For Euler equations with gamma law gas on triangular mesh[1],



Solution

Mesh

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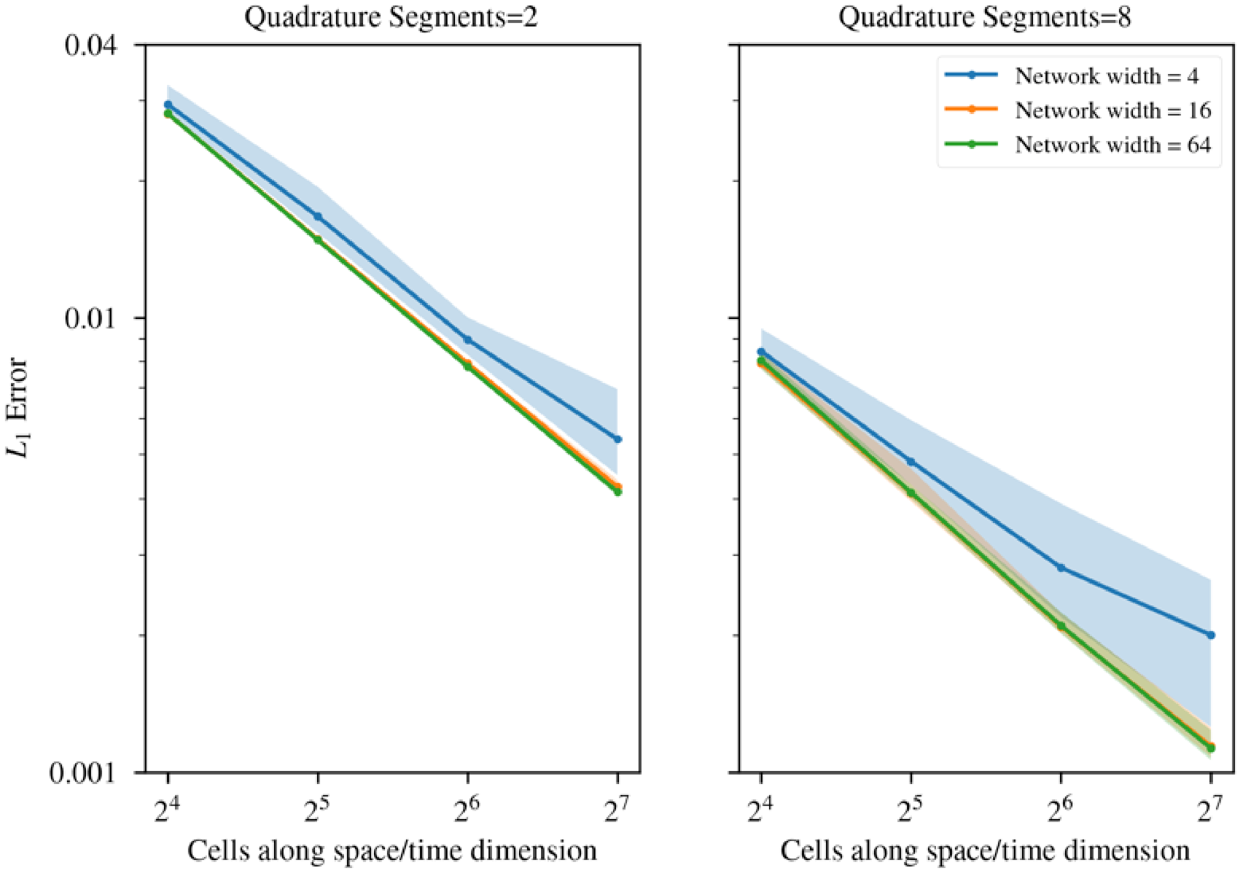
[1] pygmsh, https://pypi.org/project/pygmsh/

cvPINNs: L1 error for Burgers rarefaction

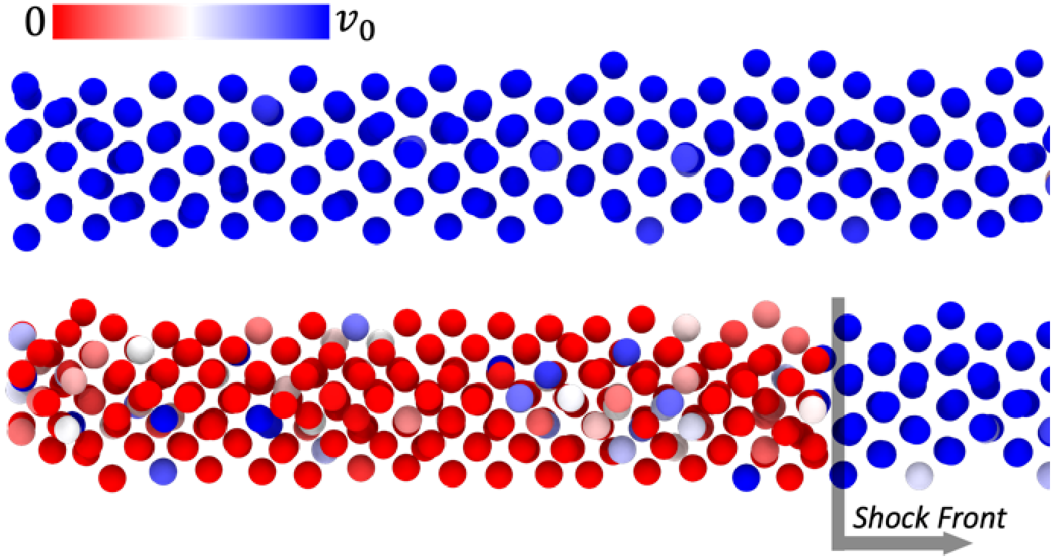
Mean and standard deviation computed over 10 runs



EOS discovery application: shock hydrodynamics of copper

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

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

EOS fits test for shocked copper

Use fitted EOS's to solve new impact case