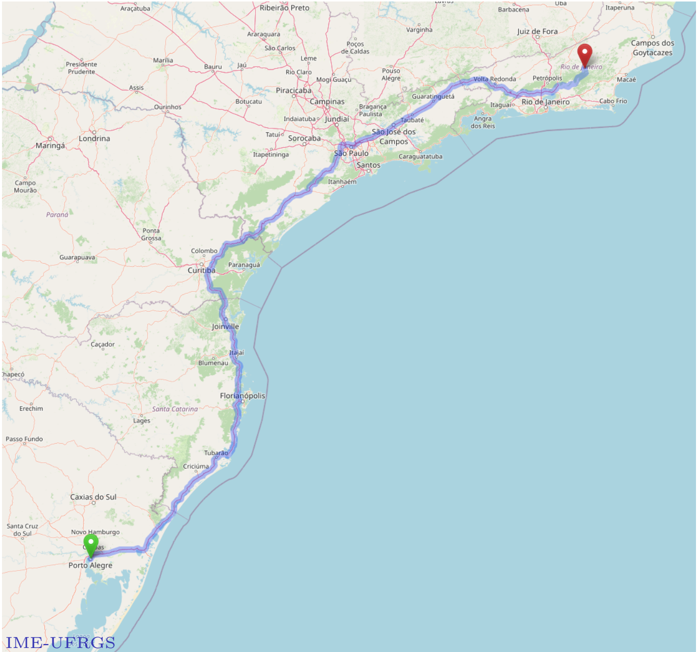
XXVI ENMC
ENCONTRO NACIONAL DE MODELAGEM COMPUTACIONAL
XIV ECTM
ENCONTRO DE CIÊNCIA E TECNOLOGIA DE MATERIAIS
2023

BURGERS' PINNs WITH IMPLICIT EULER TRANSFER LEARNING

Vitória Biesek and Pedro H. A. Konzen

PPGMAp, IME, UFRGS
Porto Alegre, RS

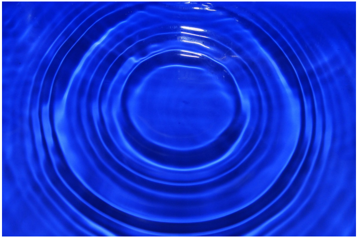
Thank you for having me here!



Contents

Introduction: Burgers' PINNs

$$u_t + uu_x = \nu u_{xx}, \ (t,x) \in (0,t_f] \times (0,1)$$
$$u(0,x) = u_0(x), \ x \in [0,1]$$
$$u(t,0) = u(t,1) = 0, \ t \in [0,t_f]$$



Raissi, M., Perdikaris. 2019a, Journal of Computational Physics **378**, 686-707.

Euler Implicit PINNs

- Euler implicit scheme:
  - Time discretization

$$t^{(k)} = kh_t,\ h_t = t_f/n_t,\ n_t \geq 0$$

  - Time iteration

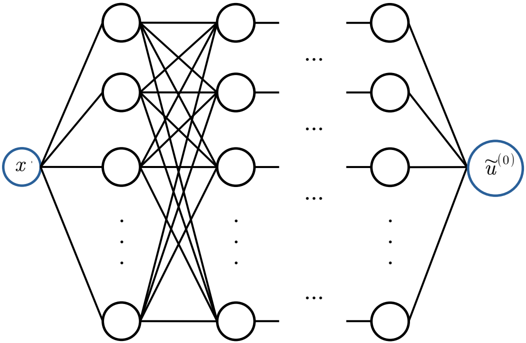
$$\begin{aligned}
&\tilde{u}^{(0)}(x) = u_0(x),\\
&\tilde{u}^{(k)} = \tilde{u}^{(k-1)} + h_t\left(\nu \tilde{u}^{(k)}_{xx} - \tilde{u}^{(k)}\tilde{u}^{(k)}_x\right),\\
&\tilde{u}^{(k)}(0) = \tilde{u}^{(k)}(1) = 0
\end{aligned}$$

- Sequence of multilayer percetrons (MLPs)

$$\begin{aligned}
&\tilde{u}^{(k)} = \mathcal{N}^{(k)}\left(x; \left\{\left(W^{(l)}, \boldsymbol{b}^{(l)}, \boldsymbol{f}^{(l)}\right)\right\}_{l=1}^{n_l}\right),\\
&\boldsymbol{a}^{l} = \boldsymbol{f}\left(W^{(l)}\boldsymbol{a}^{(l-1)} + \boldsymbol{b}^{(l-1)}\right),\\
&a^{(0)} = x,\ \tilde{u}^{(k)} = a^{(n_l)}.
\end{aligned}$$

Initial Condition

- $\tilde{u}^{(0)} = \mathcal{N}^{(0)}(x)$

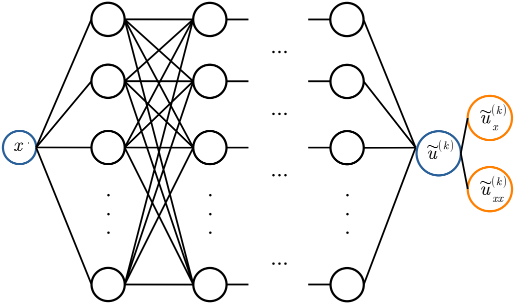


- Loss function (MSE)

$$\mathcal{L}_0 := \frac{1}{n_s} \sum_{s=1}^{n_s} \left| \tilde{u}^{(0)}(x_s) - u_0(x_s) \right|^2$$

Implicit Euler Transfer Learning

- $\mathcal{N}^{(k)} \leftarrow \mathcal{N}^{(k-1)}$
- $\tilde{u}^{(k)} = \mathcal{N}^{(k)}(x)$



- Loss function

$$\mathcal{L} := \frac{1}{n_s - 2} \sum_{s=1}^{n_s-2} \left| \mathcal{R}\left(x; \tilde{u}^{(k)}, \tilde{u}^{(k-1)}\right) \right|^2 + \frac{1}{2}\left(\left| \tilde{u}^{(k)}(0) \right|^2 + \left| \tilde{u}^{(k)}(1) \right|^2 \right)$$

- Residual

$$\mathcal{R}\left(x; \tilde{u}^{(k)}, \tilde{u}^{(k-1)}\right) := \tilde{u}^{(k)} - \tilde{u}^{(k-1)} - h_t \left(\nu \tilde{u}_{xx}^{(k)} - \tilde{u}^{(k)} \tilde{u}_x^{(k)} \right).$$

Problem 1

- Initial condition

$$u_0(x) = 2\nu\pi \frac{\sin(\pi x)}{2 + \cos(\pi x)}$$

- Exact solution ($\nu = 1$)

$$u(t, x) = 2\nu\pi \frac{e^{-\nu\pi^2 t}\sin(\pi x)}{2 + e^{-\nu\pi^2 t}\cos(\pi x)}.$$

- MLP architecture
  - $1 - n_n \times n_l - 1$
  - Hidden activation functions

$$\boldsymbol{a}^{(l)} = \tanh\left(\boldsymbol{z}^{(l)}\right)$$

  - Output activation function

$$a^{(n_l)} = \mathrm{id}(\boldsymbol{z}^{n_l - 1})$$

Problem 1: Initial Condition Training

$n_{\text{epoch}}/\mathcal{L}_0$

$n_l \backslash n_n$	10	20	30	40
		$ns = 10$		
1	5E+4 / 2E−5	5E+4 / 3E−5	5E+4 / 6E−6	4E+4 / 3E−5
2	1E+4 / 6E−7	1E+4 / 7E−7	1E+4 / 7E−7	1E+4 / 5E−7
3	1E+4 / 6E−7	1E+4 / 6E−7	9E+3 / 8E−7	9E+3 / 5E−7
4	1E+4 / 8E−7	1E+4 / 6E−7	2E+4 / 8E−7	1E+4 / 7E−7
		$ns = 100$		
1	5E+4 / 6E−6	5E+4 / 5E−6	5E+4 / 7E−6	5E+4 / 1E−5
2	5E+4 / 9E−7	1E+4 / 9E−7	1E+4 / 9E−7	1E+4 / 9E−7
3	2E+4 / 9E−7	1E+4 / 9E−7	1E+4 / 9E−7	9E+3 / 9E−7
4	2E+4 / 9E−7	1E+4 / 9E−7	1E+4 / 9E−7	1E+4 / 9E−7

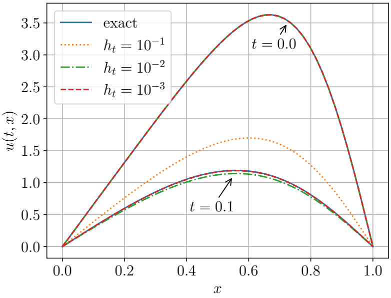
Problem 1: First Time Step

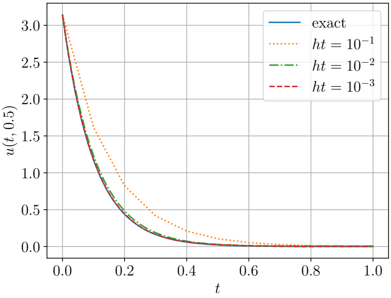
$n_{\text{epoch}}/\mathcal{L}$

$h_t \backslash ns$	10	100	1000
10^{-1}	4E+4 / 2E−1	2E+4 / 2E−1	2E+4 / 2E−1
10^{-2}	2E+4 / 3E−3	2E+4 / 3E−3	2E+4 / 3E−3
10^{-3}	2E+4 / 3E−5	2E+4 / 8E−5	3E+4 / 8E−6

Problem 1: PINN *versus* Exact Solutions

$$h_t = 10^{-3},\ n_s = 100$$



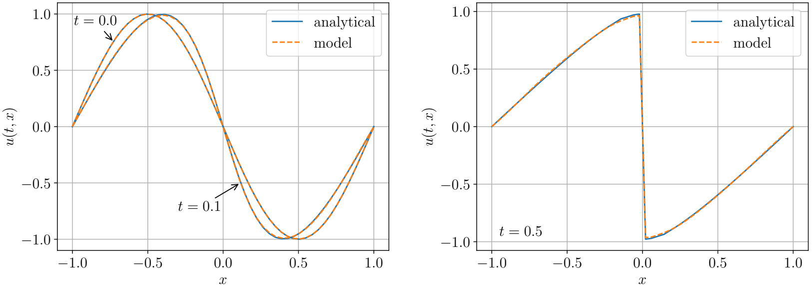


Problem 2

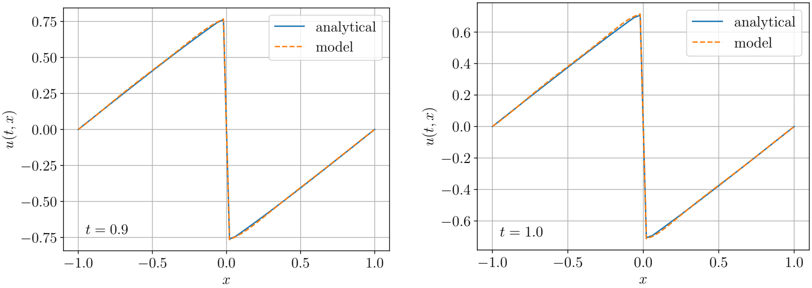
- Initial condition
$$u_0(x) = -\sin(\pi x)$$
- Analytical solution ($\nu = 0.01/\pi$)
$$u(x) = \frac{-\int_{-\infty}^{\infty} \sin(\pi(x-\eta)) f(x-\eta) e^{-\frac{\eta^2}{4\nu t}} \, d\eta}{\int_{-\infty}^{\infty} f(x-\eta) e^{-\frac{\eta^2}{4\nu t}} \, d\eta},$$
where $f(y) = e^{-\cos(\pi y)/(2\pi\nu)}$.
- MLP Architecture
$$1 - 30 \times 3 - 1$$
- Discretization parameters
$$h_t = 10^{-3},\ n_s = 100 \tag{4}$$

Raissi, M., Perdikaris. 2019b, Journal of Computational Physics **378**, 686-707.

Problem 2: First Time Steps



Problem 2: Last Time Steps



Final Considerations

- Simulation of Burgers' equation
  - PINNs - Physical-informed neural networks
  - Implicit Euler transfer learning
- PINNs advantages
  - Simplicity
  - Meshless
  - Generality
- Implicit Euler transfer learning
  - Smaller MLP architecture
  - Potentially enhancing computational resources
- Further developments
  - θ-Scheme
  - Preprocessing
  - Adaptive MLP architecture

Thanks for your attention!

Research group

Site UFRGS

`professor.ufrgs.br/pedro`

Lecture Notes

`notaspedrok.com.br`

Instagram

`@notas.pedrok`

PPGMAp

Instituto de MATEMÁTICA E ESTATÍSTICA UFRGS