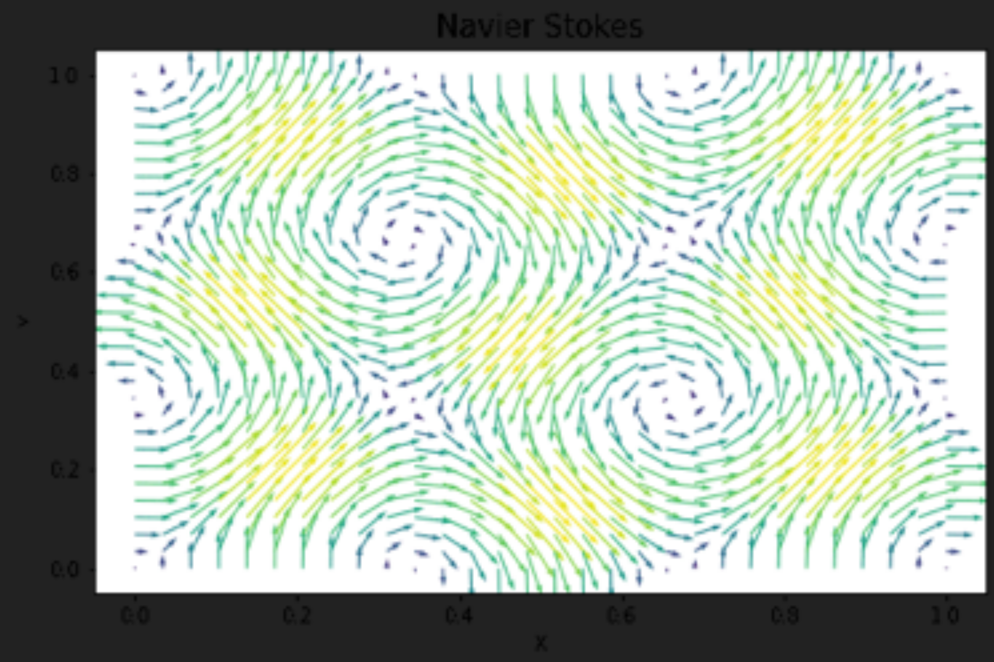


ARXIV: 2103.08662

dNNsolve

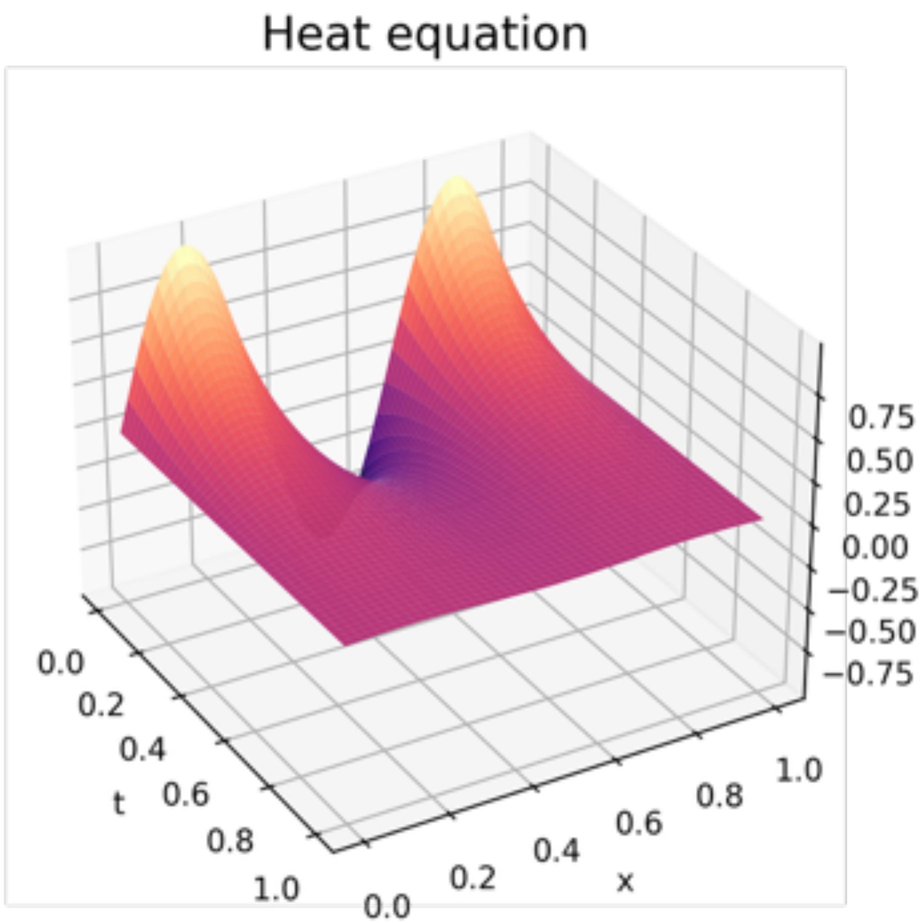
an efficient NN-based PDE solver

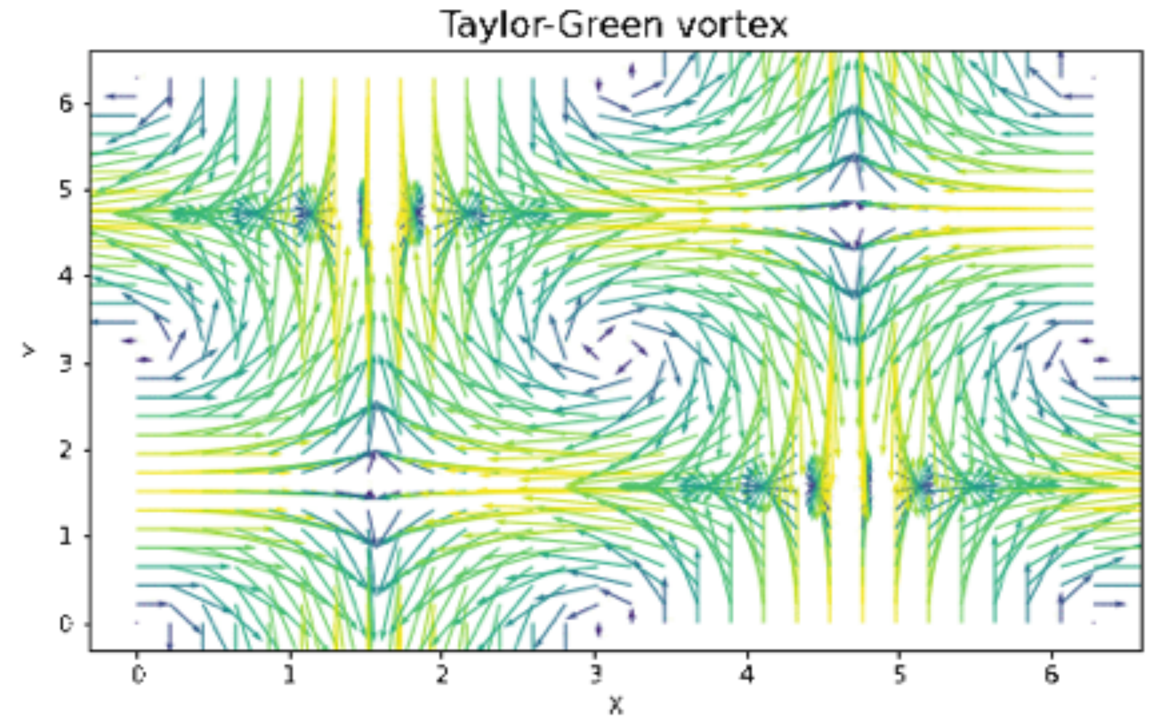
V. Guidetti

F.Muia

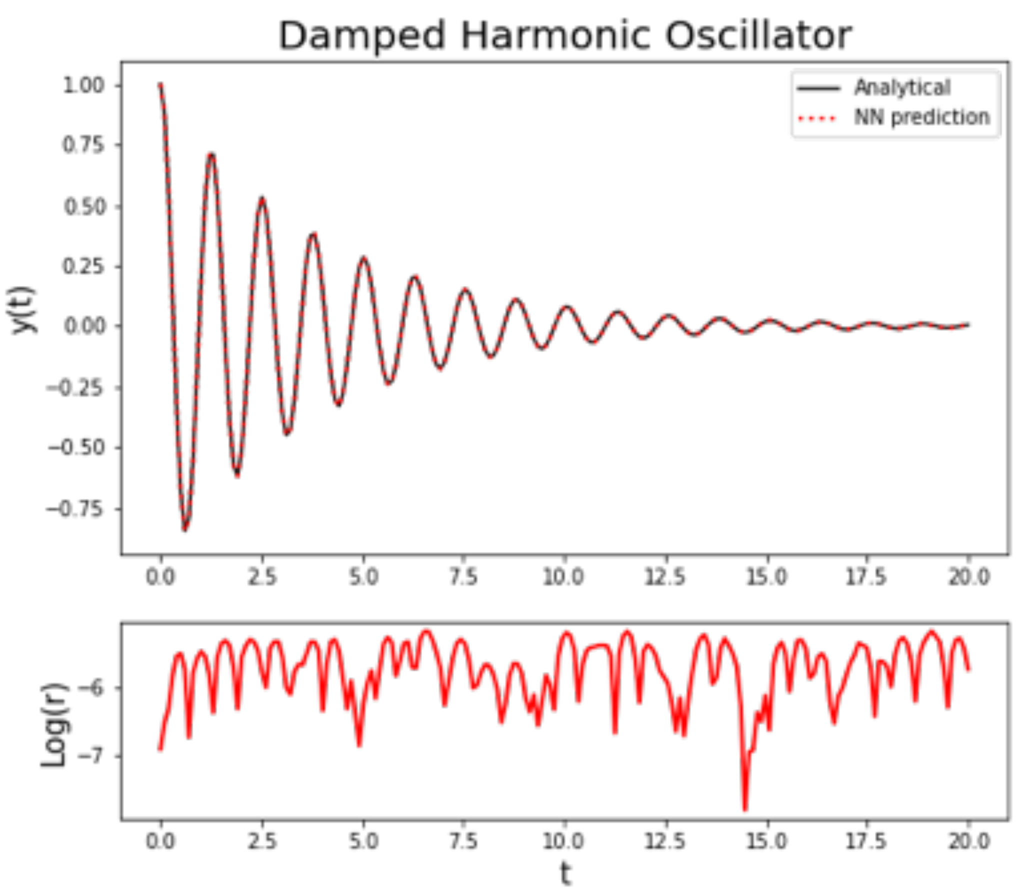
Y. Welling

A. Westphal





PDES ARE UBIQUITOUS IN NATURE



NN OPTIMISATION PROBLEM

(Lagaris, Likas, Fotiadis, 1998) and **`PINNs'** (Raissi, Perdikaris, Karniadakis, 2017) + more

- Neural network approximates solution u(x) of PDE
- Loss function: physical laws + additional constraints

$$\mathcal{L}(\hat{u}(\vec{x}), \alpha_\bullet) \equiv \frac{\alpha_\Omega}{n_\Omega} \sum_i \underline{[\mathcal{G}[\hat{u}](\vec{x}_i)]^2} + \frac{\alpha_0}{n_0} \sum_j \underline{[\mathcal{B}_0[\hat{u}](\vec{x}_j)]^2} + \frac{\alpha_{\partial\Omega}}{n_{\partial\Omega}} \sum_k \underline{[\mathcal{B}_{\partial\Omega}[\hat{u}](\vec{x}_k)]^2} + \ldots$$

PDE i.c. b.c.

UNSUPERVISED

Beautifully simple idea!

ADVANTAGES OVER STANDARD SOLVERS

- Solve multiple types of PDEs with same simple method
  - initial value problem
  - boundary value problem
  - delay equation
  - additional constraints
  - inverse problem
  - …

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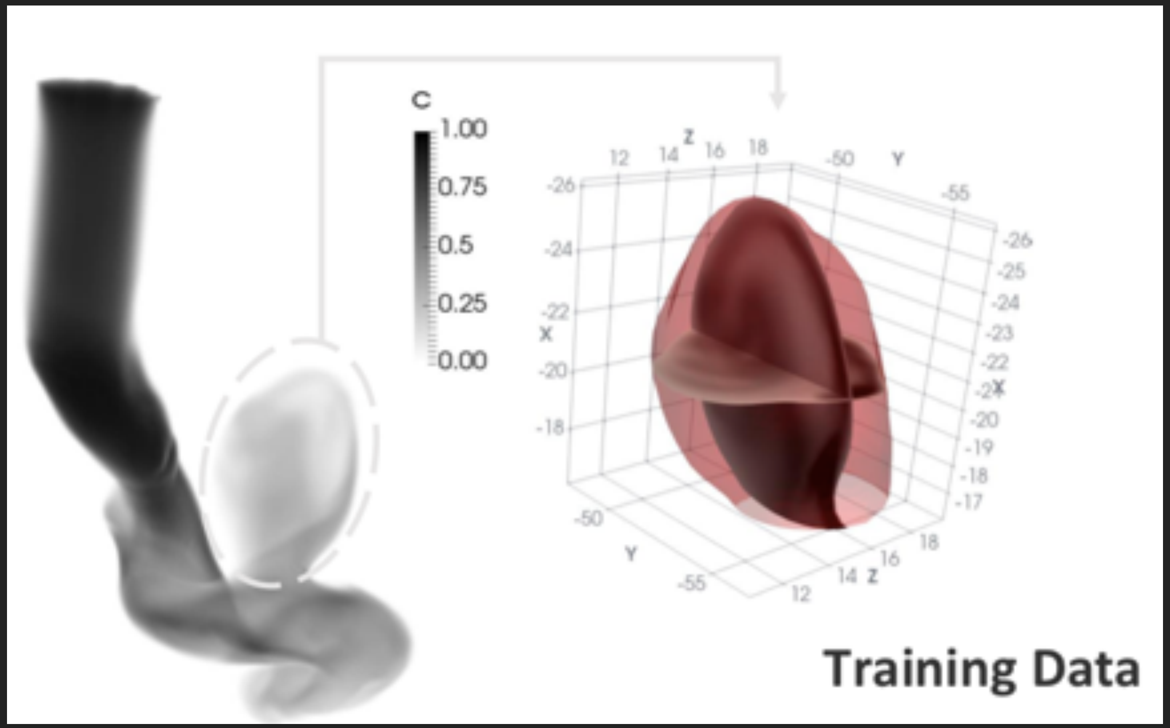
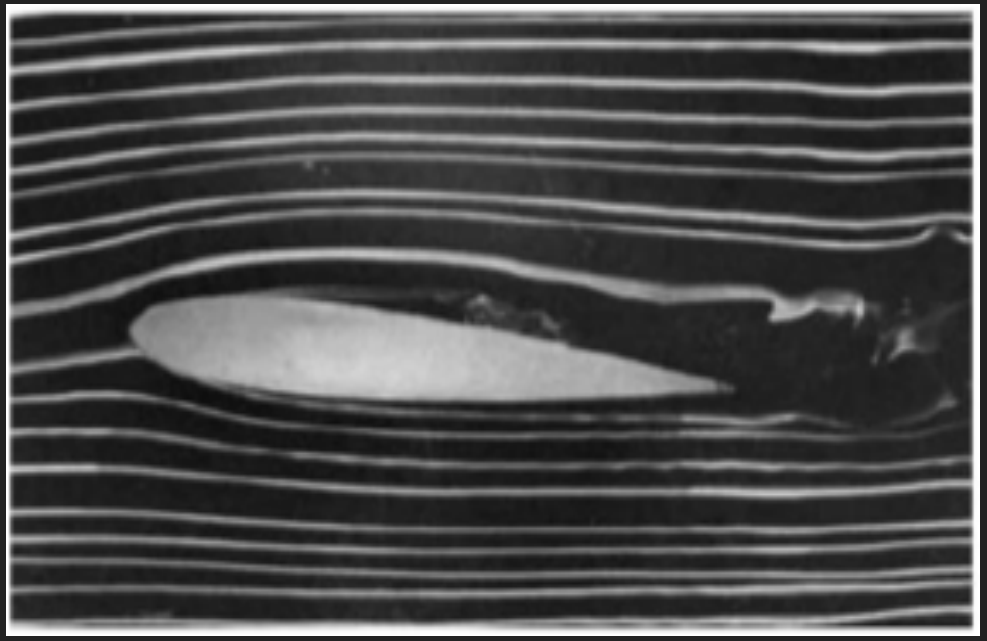
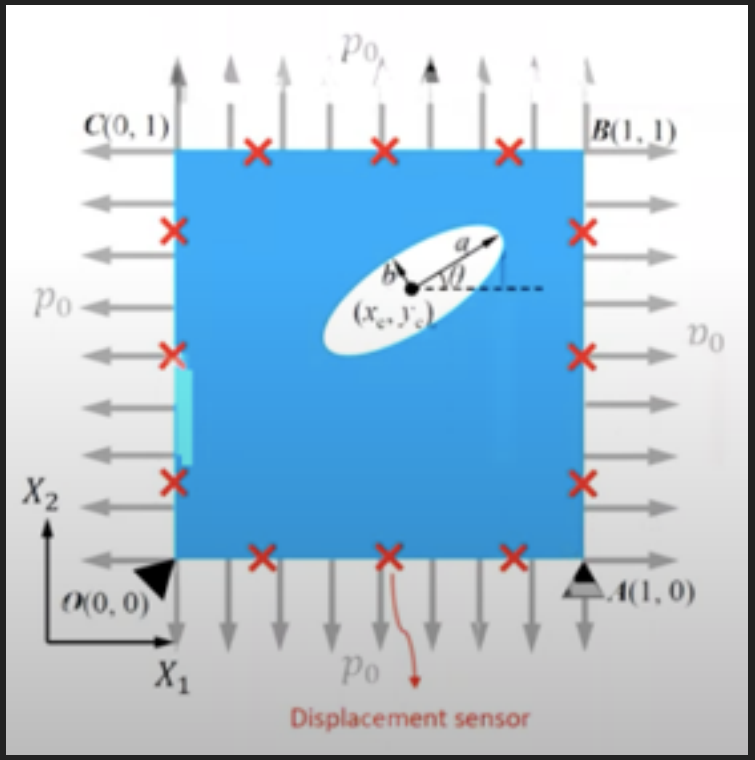
- PINNs already improve on memory complexity (≥3D) and time complexity (≥5D) as compared to FDM (Avrutskiy,2020)
- Cosmologist's dream: have competitive NN-based cosmo codes
  This calls for time efficiency improvements in 3+1D

Hidden Fluid Mechanics (Raissi, Yazdani, Karniadakis, Science 2020)





Identify location hole



PROMISING PINNS

(see talk by Karniadakis MLTP 2020)

https://www.youtube.com/watch?v=FQ0vsqU-K00

MAIN DRAWBACK OF PINNS

- Fine tuning of hyper parameters NN for each problem at hand

  Also remarked in (DeepXDE; Lu, Meng, Zao, Karniadakis, 2020). See also (PyDEns; Koryagin, Khudorozkov, & Tsimfer, 2019) + (NeuroDiffEq; Chen, Sondak, Pavlos Protopapas, Mattheakis, Liu, Agarwal, Di Giovanni, 2019)

  E.g. we failed to solve for the harmonic oscillator

$$\ddot{u}(t) + \omega^2 u(t) = 0; \;\; u(t_0) = 1; \;\; \dot{u}(t_0) = 0 \quad \longrightarrow \quad u(t) = \cos(\omega t)$$

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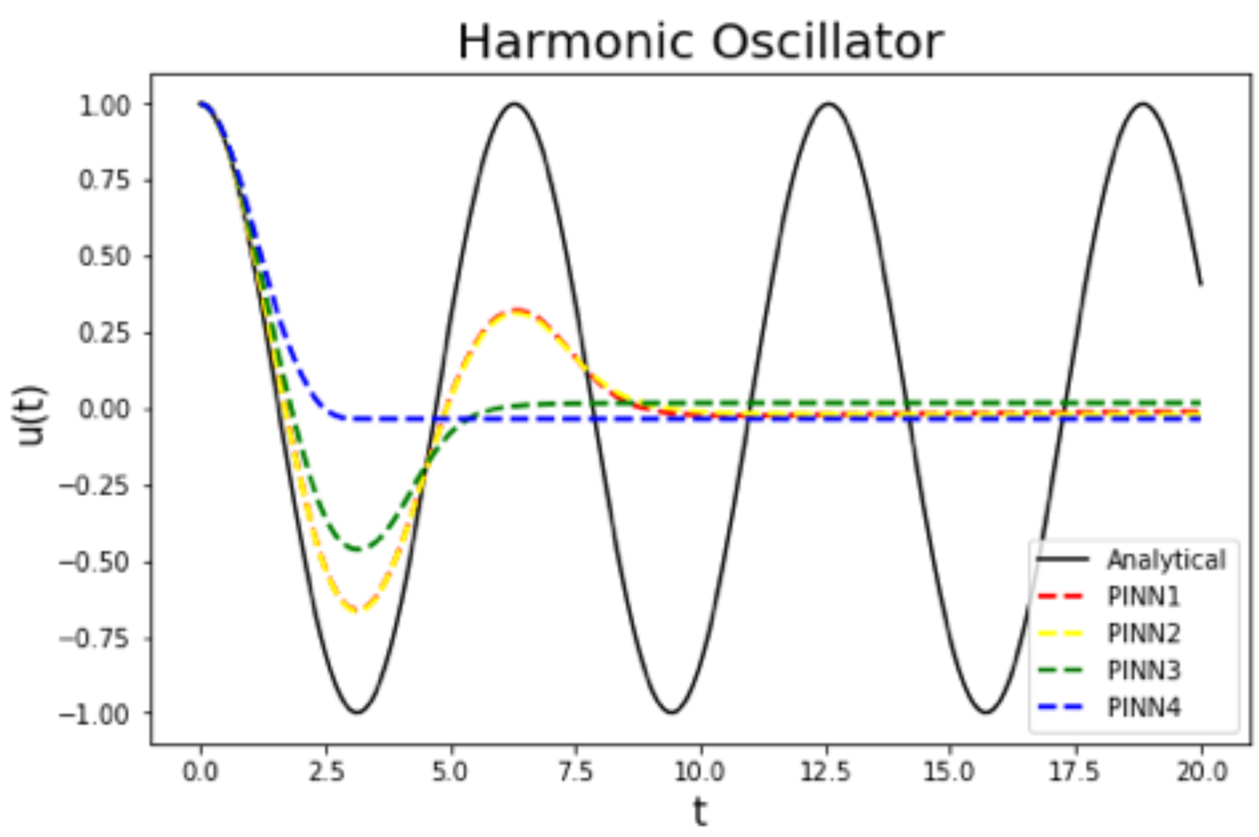
  - *3000* collocation points
  - *PINNi* ≡ *i* layers × *20* nodes of sigmoids
  - *2000* epochs of ADAM



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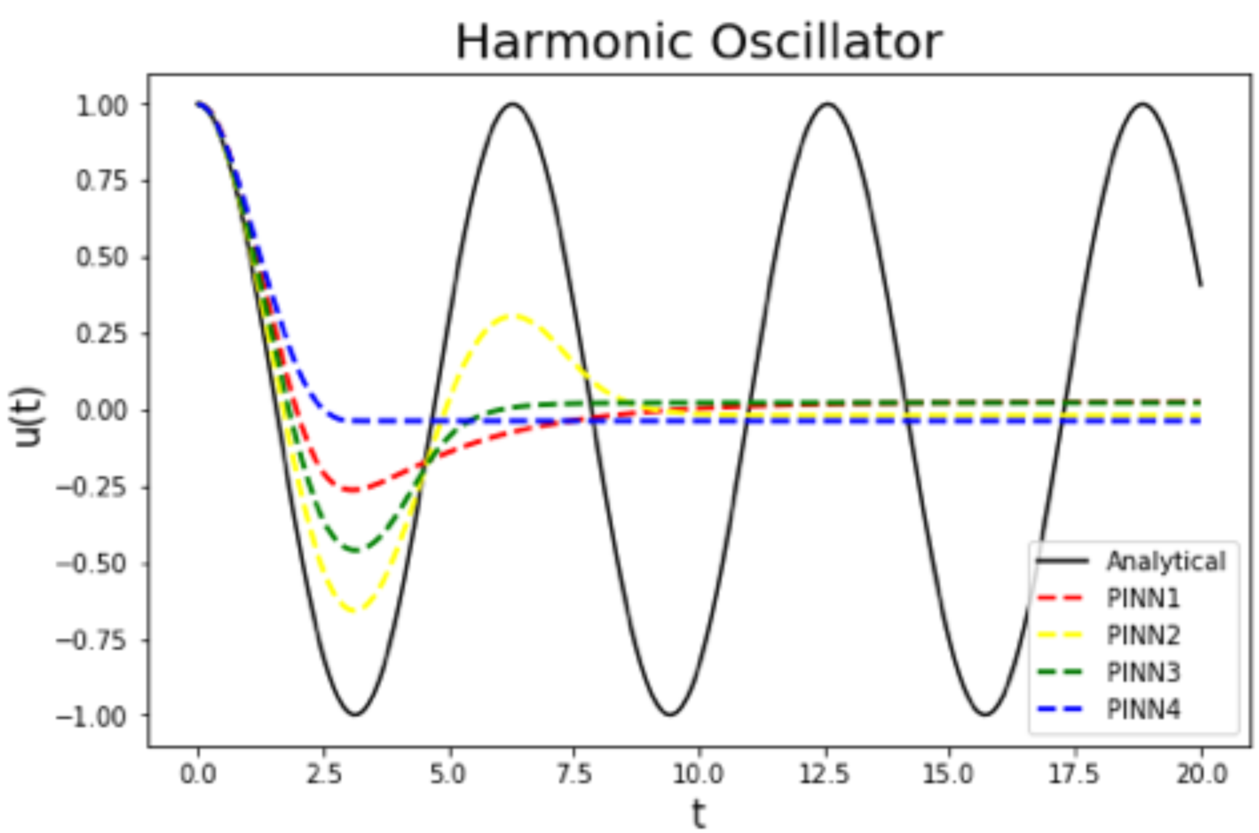
E.g. we failed to solve for the harmonic oscillator

- *3000* collocation points
- *PINNi* ≡ *i* layers × *20* nodes of sigmoids
- *20.000* epochs of ADAM



Wait.. what's going on?

BACK TO THE BASICS: UNIVERSAL APPROXIMATION THEOREM

- PINNs are motivated by UAT (Cybenko 1989)

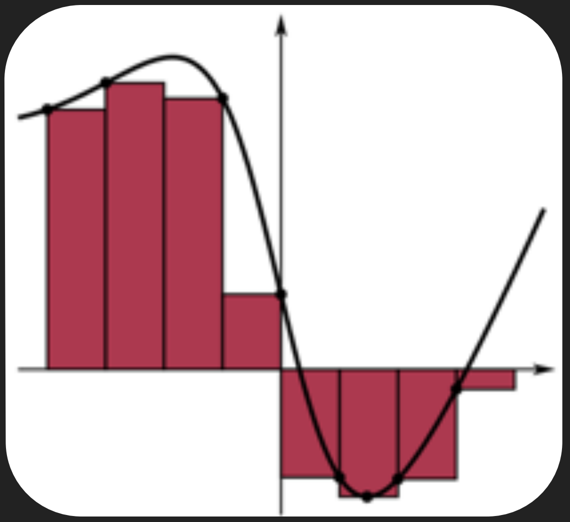
Theorem 1. *Let σ be any continuous discriminatory function. Then finite sums of the form*

$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma(y_j^T x + \theta_j) \tag{2}$$

are dense in $C(I_n)$. In other words, given any $f \in C(I_n)$ and $\varepsilon > 0$, there is a sum, $G(x)$, of the above form, for which

$$|G(x) - f(x)| < \varepsilon \quad \text{for all} \quad x \in I_n.$$

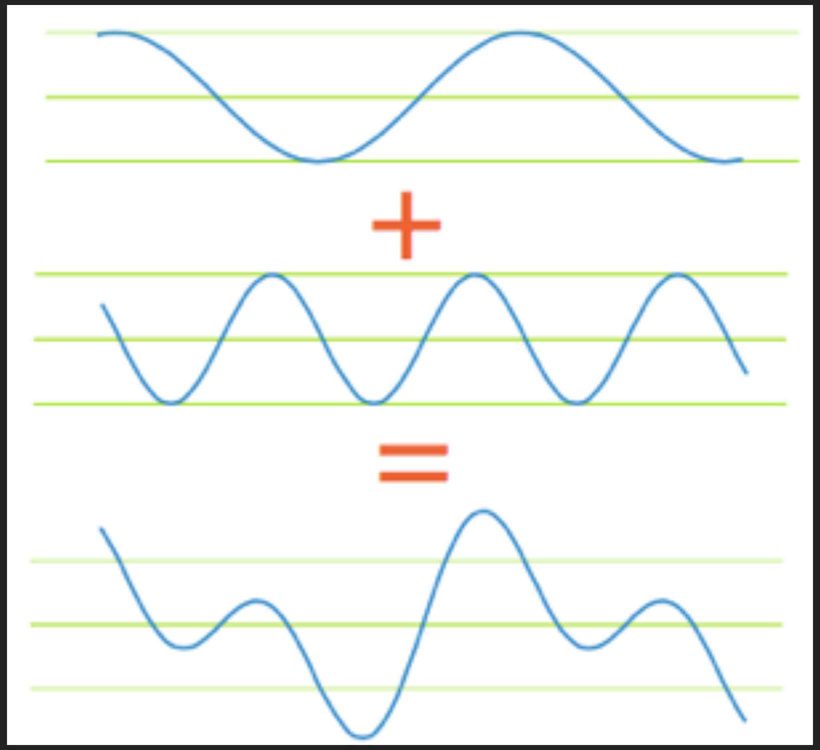
- Proof: based on binning a function



(Riemann Sum - Wikipedia)

BACK TO THE BASICS: UNIVERSAL APPROXIMATION THEOREM

- For many PDEs there exist more efficient basis functions! Fourier series, polynomials, …



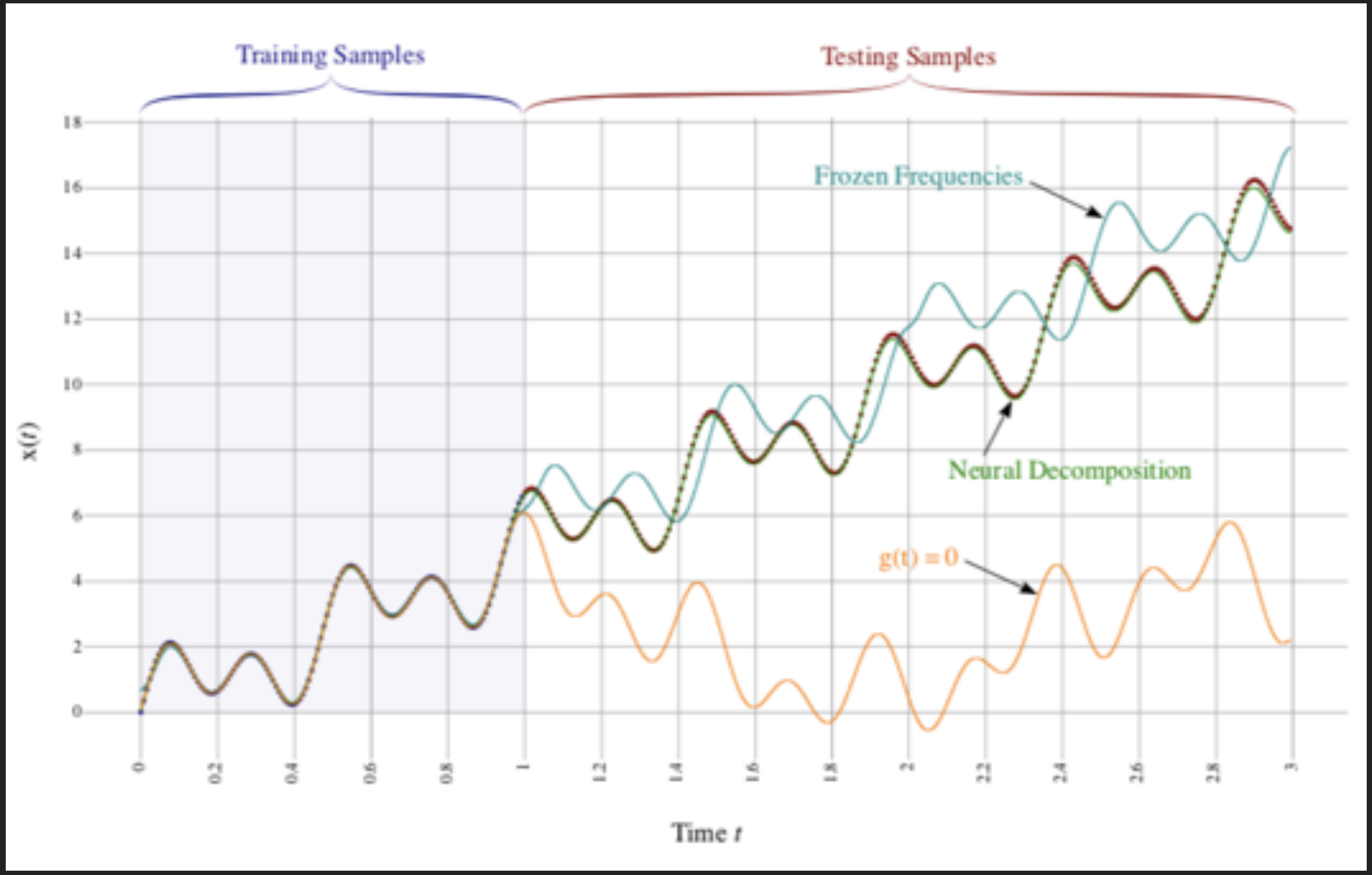
mathisfun.com

- Plus: how a NN actually learns: https://cs.stanford.edu/people/karpathy/convnetjs/demo/regression.html

BACK TO THE BASICS: UNIVERSAL APPROXIMATION THEOREM

- We propose to use Fourier series AND a secular expansion

Just like e.g. time-series extrapolation



(Godfrey, Gashler, 2017)

DNNSOLVE TWO-STREAM FOURIER+SECULAR BASIS

1D

$$\hat{u}(x) = \sum_{k=1}^{N} \underbrace{d_k \sin(f_k x + \phi_k)}_{\text{Fourier}} + \underbrace{d_{N+k}\sigma(w_k x + b_k)}_{\text{Secular}} + \underbrace{d_{2N+k} \sin(f_k x + \phi_k)\sigma(w_k x + b_k)}_{\text{Non-linear combi}} + a$$

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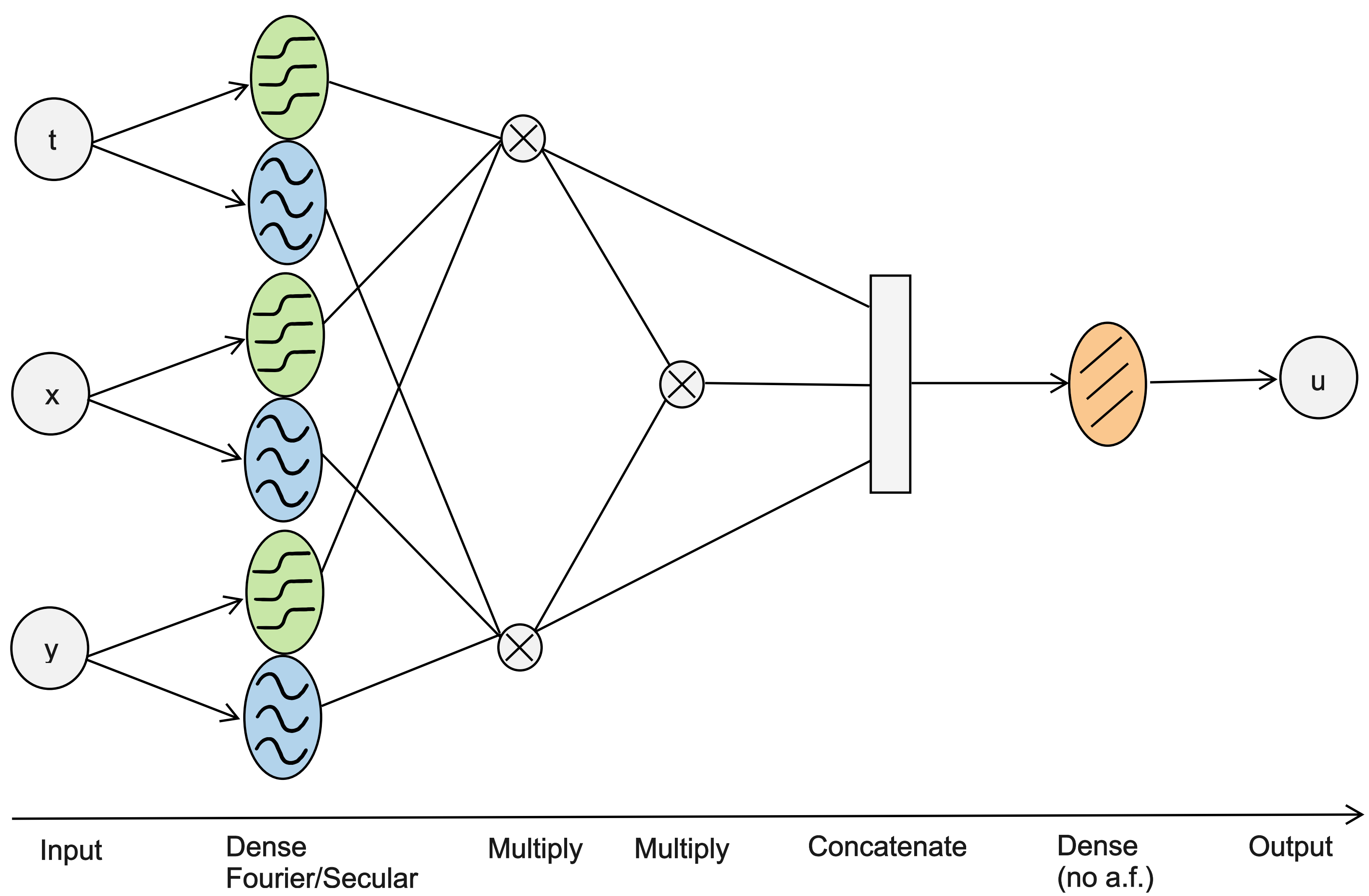
3D



OUR LOSS FUNCTION

- We use sum of RMSE (empirically: faster convergence & better accuracy)

$$\mathcal{L}(\hat{u}(\vec{x}),\alpha_\bullet) \equiv \alpha_\Omega \sqrt{\frac{1}{n_\Omega}\sum_i \left[\mathcal{G}[\hat{u}](\vec{x}_i)\right]^2} + \alpha_0 \sqrt{\frac{1}{n_0}\sum_j \left[\mathcal{B}_0[\hat{u}](\vec{x}_j)\right]^2} + \alpha_{\partial\Omega} \sqrt{\frac{1}{n_{\partial\Omega}}\sum_k \left[\mathcal{B}_{\partial\Omega}[\hat{u}](\vec{x}_k)\right]^2}$$

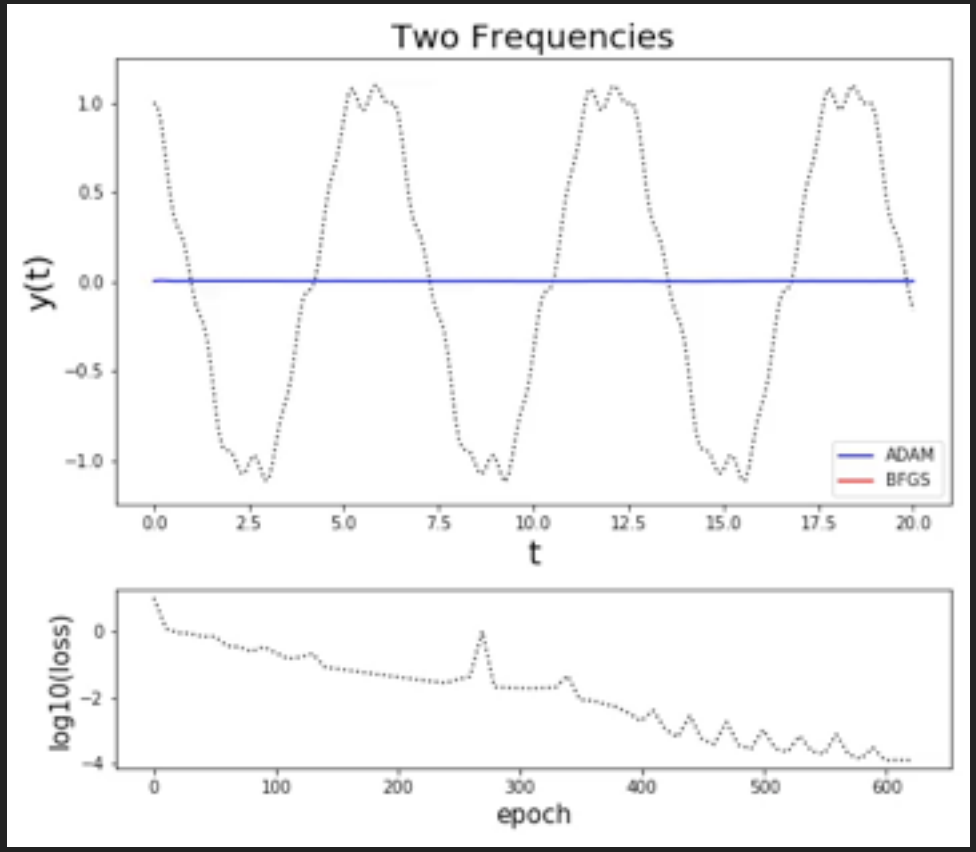
PDE   i.c.   b.c.

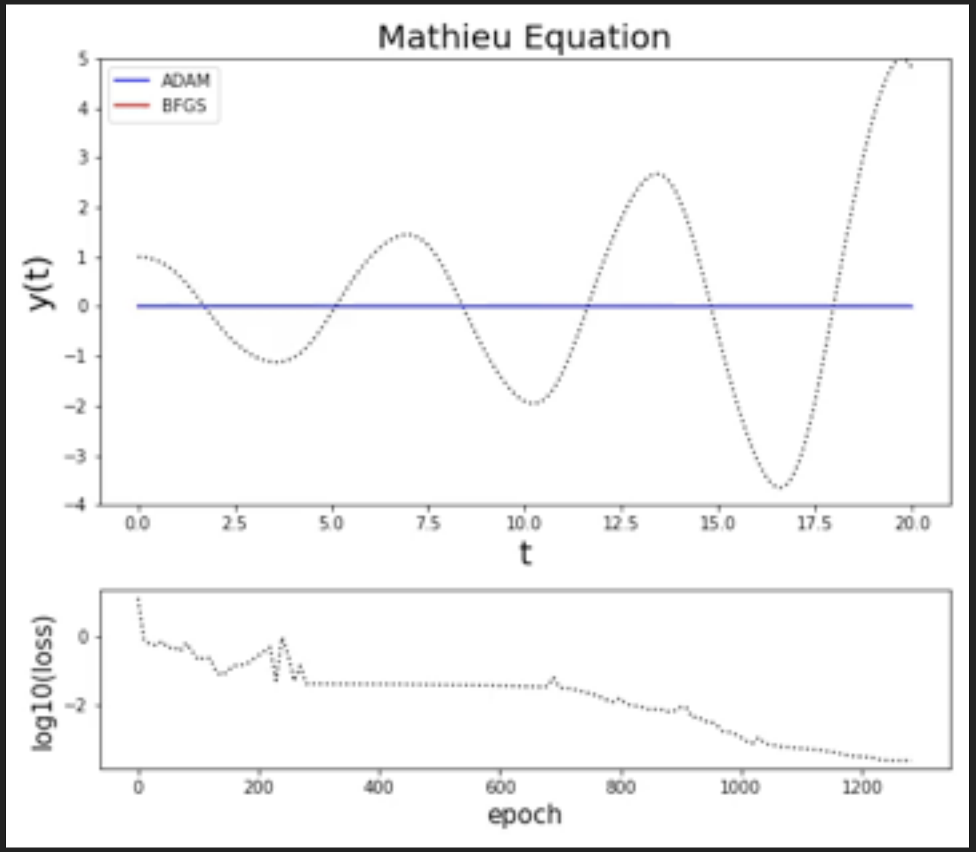
- Loss weights α are necessary to escape local minima
- Only tuning we will encounter is the intrinsically required mild tuning of these weights in 3D!

RESULTS 1D

Data and loss weights: 2000+1 points, $\alpha_0 = \alpha_\Omega = \alpha_{\delta\Omega} = 1$
Neural network size: 35 nodes per branch (10 for oscillon)
Training: 150 epochs of Adam (mini-batches of size 256) + BFGS until convergence

- Evolution solution during training





high and low freq are learned simultaneously

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- Accuracies of the tested ODEs

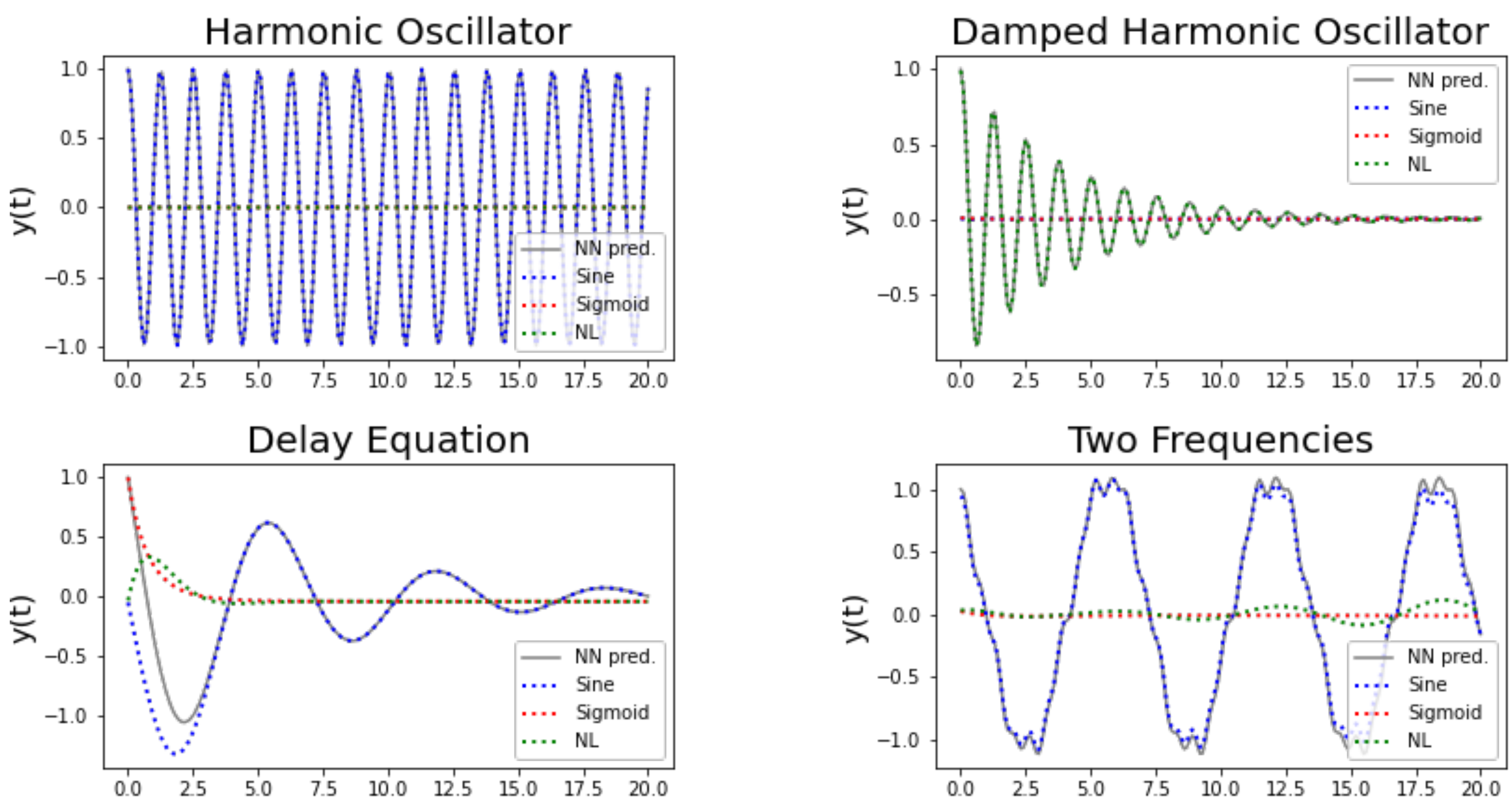
ODE	Epochs	$\log_{10}(r)$
Mathieu equation	1283	-3.6 (*)
Decaying exponential	393	-4.1
Harmonic oscillator	728	-5.8
Damped harmonic oscillator	765	-5.1
Linear equation	513	-3.1
Delay equation	414	-2.5 (*)
Stiff equation	642	-4.3
Gaussian	380	-3.7
Two frequencies equation	622	-4.2
Oscillon profile equation	748	-5.2

$$r \equiv \sqrt{\frac{1}{n_{\mathrm{tot}}} \sum_i |\hat{u}(\vec{x}_i) - u(\vec{x}_i)|^2}$$

all results are obtained with one random initialisation, hence don't correspond to our best results

RESULTS 1D

- Contributions of the sine, secular and non-linear branches



To do: reduce noise from superfluous neurons

RESULTS 2D

Data and loss weights: 1000+200+200 points, $\alpha_0 = 10$, $\alpha_\Omega = \alpha_{\delta\Omega} = 1$
Neural network size: 10 nodes per branch
Training: 210 epochs of Adam (mini-batches of size 256) + BFGS until convergence

- Accuracies of the tested PDEs

PDE	Epochs	r
Wave equation (1)	528	-5.3
Wave equation (2)	538	-6.3
Traveling wave	496	-6.1
Heat equation (1)	911	-4.6
Heat equation (2)	3764	-3.9
Heat equation (3)	762	-4.5
Poisson equation (1)	533	-6.4
Poisson equation (2)	1437	-4.8
Advective diffusion equation	942	-5.2
Burgers' equation	3744	-3.9 (*)
Parabolic equation	1158	-5.4
Poisson equation (3, disk)	4574	-5.6 (*)

$$r \equiv \sqrt{\frac{1}{n_{\rm tot}}\sum_i |\hat{u}(\vec{x}_i) - u(\vec{x}_i)|^2}$$

RESULTS 3D

Data and loss weights: 1000+1200+500 points, α: see table
Neural network size: 10 nodes per branch (20 for Lamb-Oseen)
Training: 210 epochs of Adam (mini-batches of size 256) + BFGS until convergence

- Accuracies of the tested PDEs

PDE	Epochs	$(\alpha_\Omega, \alpha_0, \alpha_{\partial\Omega})$	r
Wave equation (1)	706	(1,10,1)	-5.8
Wave equation (2)	524	(1,10,1)	-5.8
Traveling wave	715	(1,1,1)	-4.5
Heat equation (1)	750	(1,10,10)	-4.5
Heat equation (2)	1484	(1,10,10)	-4.8
Poisson equation (1)	1546	(1,1,1)	-3.7
Poisson equation (2)	3277	(1,1,1)	-2.8
Poisson equation (3)	1640	(1,1,1)	-3.0
Taylor-Green vortex	1165	(1,10,1)	-4.2
Lamb-Oseen vortex	7389	(1,1,1)	-2.4
Vorticity equation	11232	(1,1,1)	(*)

$$r \equiv \sqrt{\frac{1}{n_{\text{tot}}} \sum_i |\hat{u}(\vec{x}_i) - u(\vec{x}_i)|^2}$$

choice α required max 4 trials ↑ to do: automatised weight selection

DNNSOLVE IMPROVES ON ONE-STREAM PINNS

- No hyper parameter tuning: every *d*-dimensional PDE is solved with the *same* architecture and initialisation and reaches precision 10^{-3}-10^{-6} (Only mild tuning for loss weights in 3D)

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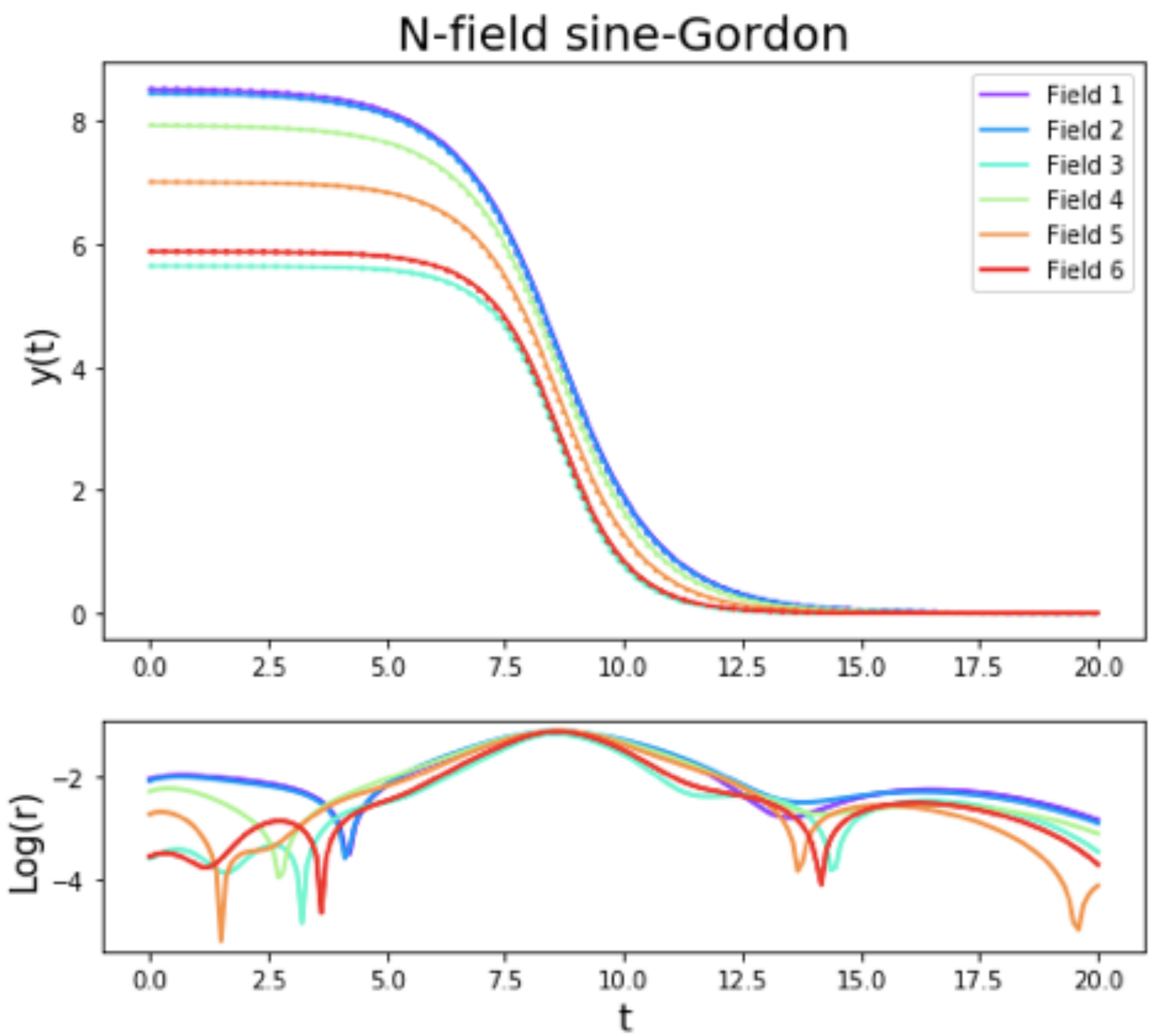
- No hyper parameter tuning: every *d*-dimensional PDE is solved with the *same* architecture and initialisation and reaches precision 10^{-3}-10^{-6} (Only mild tuning for loss weights in 3D)

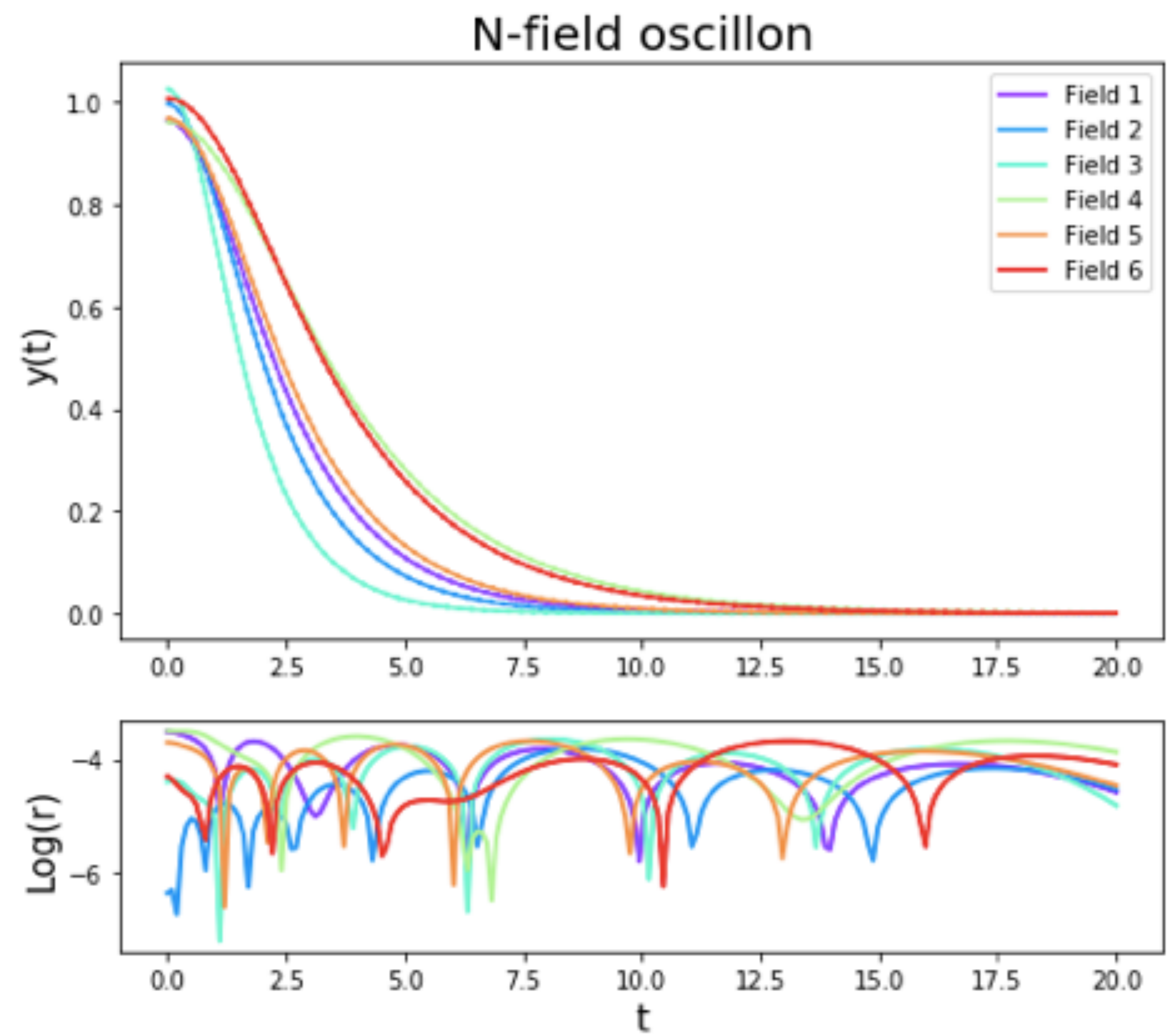
- We use $d \cdot \mathcal{O}(100\text{-}200)$ trainable parameters and $\mathcal{O}(1000)$ epochs of Adam (or $\mathcal{O}(100)$ with mini-batches)

  Compare e.g. to *1000-8000* trainable parameters and *15000-80000* epochs for 1,2 D examples presented in (DeepXDE; Lu, Meng, Zao, Karniadakis, 2020)

KINKS & OSCILLONS

Data and loss weights: 300+1 points, $a_0 = a_\Omega = a_{\delta\Omega} = 1$
Neural network size: 10 nodes per branch
Training: 500 epochs of Adam + BFGS until convergence



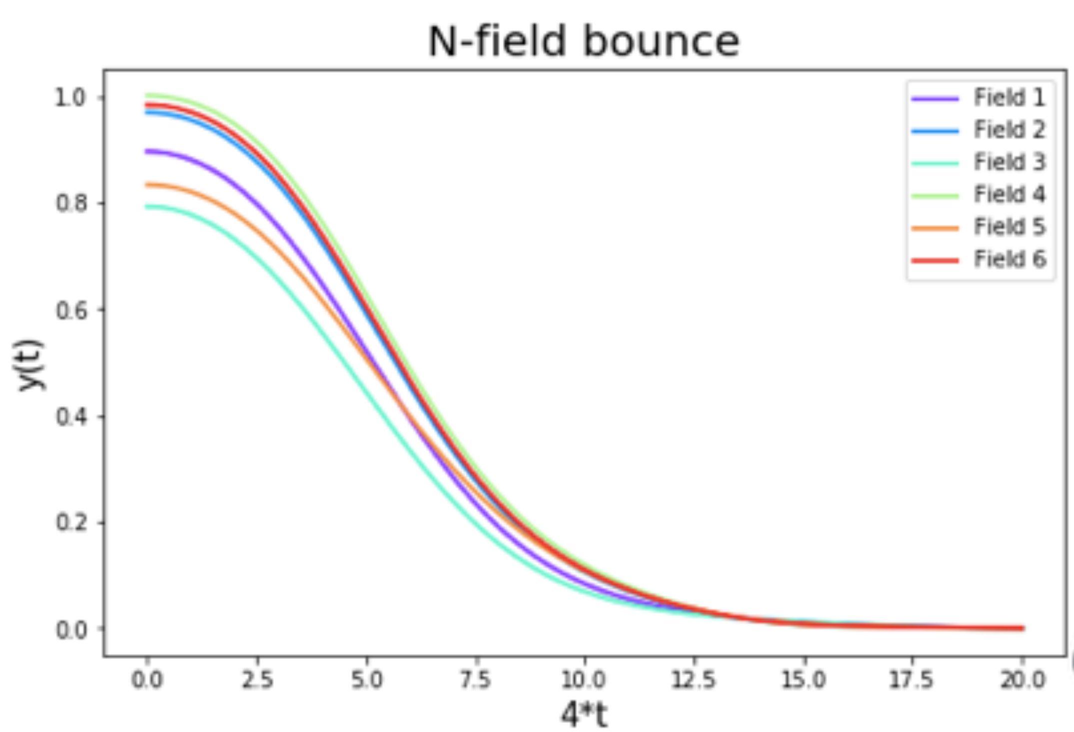


position kink is arbitrary
accuracy is not accurate ;-)

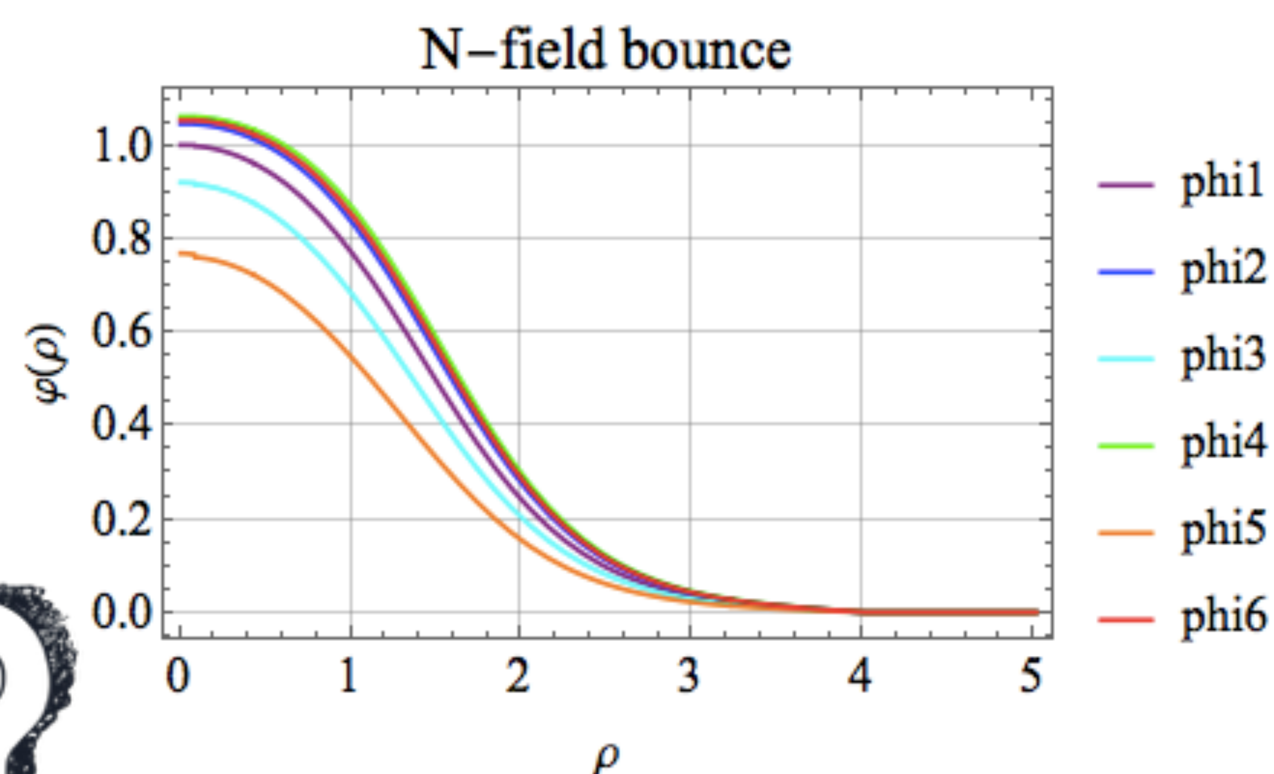
BOUNCES?

- N-field benchmark example (BubbleProfiler; Athron et al, 2019) (SimpleBounce; Sato, 2020) (FindBounce; Guada, 2020) (OptiBounce; Bardsley, 2021) see also (Piscopo, Spannowsky, Waite, 2019)

$$\ddot{\phi}_i^{\,B} + \frac{D-1}{\rho}\dot{\phi}_i^{\,B} = \frac{\partial V}{\partial \phi_i^B} \qquad V_{n_\phi} = \left(\left[\sum_{i=1}^{n_\phi} c_i(\phi_i - 1)^2\right] - \delta\right)\left(\sum_{i=1}^{n_\phi} \phi_i^2\right)$$



dNNsolve



FindBounce

CONCLUSIONS

- dNNsolve: a two-stream Fourier + secular architecture
- dNNsolve improves on PINNs:
  (1) it can solve a wide range of PDEs without (or mild in 3D) hyper parameter tuning and good precision 10^{-3}-10^{-6}
  (2) it requires much fewer NN parameters and converges much faster during training
- We gained new insights how to further improve dNNsolve
  - automatised a weight tuning
  - reduce noise from superfluous neurons
- Code becomes available soon
- We are open for new ideas/collaborations

Thank you!

FUNDING ACKNOWLEGDMENT

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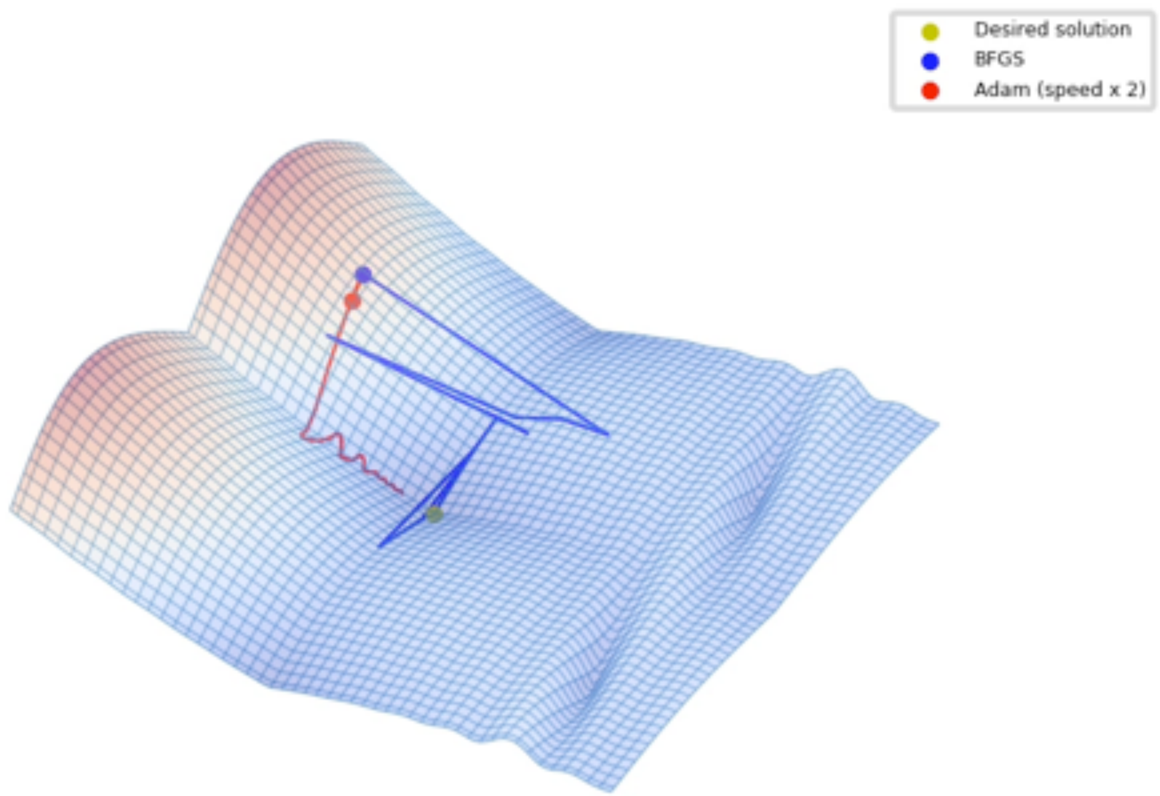
ADAM VS BFGS



1D ODES

Mathieu equation:

$$\begin{cases} u''(t) + (a - 2\,q\,\cos(2t))u(t) = 0 & a = 1, q = 0.2 \\ u(0) = 1 \\ u'(0) = 0 \end{cases}$$

Damped harmonic oscillator:

$$\begin{cases} u''(t) + \beta\,u'(t) + \omega^2\,u(t) = 0 \\ u(0) = 1 \\ u'(0) = 0 \end{cases}$$

with analytical solution

$$u(t) = e^{-\beta\,t/2}\left(\cos(f\,t) + \frac{\beta}{2f}\sin(f\,t)\right), \quad f \equiv \sqrt{\omega^2 - \beta^2/4}$$

1D ODES

Two frequencies:

$$\begin{cases} u''(t) + u(t) + A_1 \cos(\omega_1 t) + A_2 \sin(\omega_2 t), & A_1 = 2, A_2 = 6, \omega_1 = 5, \omega_2 = 10 \\ u(0) = 1 \\ u'(0) = 0 \end{cases}$$

with analytical solution

$$u(t) = \frac{1}{132}(121\cos(t) + 11\cos(5t) - 80\sin(t) + 8\sin(10t)$$

Oscillon Profile equation:

$$\begin{cases} u''(t) + \frac{d-1}{r}u'(t) + m^2 u(t) - 2u^3(t) = 0, & d = 1 \\ u' + mu = 0 \quad \text{when} \quad t \to \infty \\ u'(0) = 0 \end{cases}$$

with analytical solution

$$u(t) = \frac{m}{\cosh(m\,t)}$$

1D ODES

Decaying exponential:

$$\begin{cases} u'(t) + \beta\, u(t) = 0 & \beta = 0.52 \\ u(0) = 1 \end{cases}$$

with analytical solution

$$u(t) = e^{-\beta t}$$

Harmonic oscillator:

$$\begin{cases} u''(t) + \omega^2 u(t) = 0 & \omega = 5 \\ u(0) = 1 \\ u'(0) = 0 \end{cases}$$

with analytical solution

$$u(t) = \cos(\omega\, t)$$

1D ODES

Linear function:

$$\begin{cases} u'(t) - 1 = 0 \\ u(0) = 1 \end{cases}$$

with analytical solution

$$u(t) = 1 + t$$

Delay equation:

$$\begin{cases} u'(t) - \beta u(t) + u(t-d) = 0, u(t|t<0) = t-1, \qquad d = 1 \\ u(0) = 1 \end{cases}$$

1D ODES

Stiff equation::

$$\begin{cases} u'(t) + 21\,u(t) - e^{-t} = 0 \\ u(0) = 1 \end{cases}$$

with analytical solution

$$u(t) = \frac{1}{20}\left(e^{-t} + 19e^{-21t}\right)$$

Gaussian:

$$\begin{cases} u'(t) + 2\,b\,t\,u(t) = 0 \qquad b = 0.1 \\ u(0) = 1 \end{cases}$$

with analytical solution

$$u(t) = e^{-bt^2}$$

2D PDES

Advenction diffusion equation:

$$\begin{cases} \partial_t u - \frac{1}{4}\partial^2_{xx} = 0 \\ u(0,x) = \frac{1}{4}\sin(\pi x) \\ u(t,0) = u(t,1) = 0 \end{cases}$$

with analytical solution

$$u(t,x) = \frac{1}{4}e^{-\frac{1}{4}\pi^2 t}\sin(\pi x)$$

Burger's equation:

$$\begin{cases} \partial_t u + u\partial_x u - \frac{1}{4}\partial^2_{xx} = 0 \\ u(0,x) = x(1-x) \\ u(t,0) = u(t,1) = 0 \end{cases}$$

Parabolic equation on unit disk:

$$\begin{cases} \partial^2_{tt} u + \partial^2_{xx} u - 4 = 0 \\ u|_{\partial\Omega} = 1 \end{cases}$$

with analytical solution

$$u(t,x) = \frac{1}{4}e^{-\frac{1}{4}\pi^2 t}\sin(\pi x)$$

2D PDES

Heat equation 1:

$$\begin{cases} \partial_t u - 0.05\, \partial^2_{xx} u = 0 \\ u(0,x) = \sin(3\pi x) \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x) = \sin(3\pi x) e^{-0.05(3\pi)^2 t}$$

Heat equation 2:

$$\begin{cases} \partial_t u - 0.01\, \partial^2_{xx} u = 0 \\ u(0,x) = 2\sin(9\pi x) + 0.3\sin(4\pi x) \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x) = 2\sin(9\pi x) e^{-0.01(9\pi)^2 t} - 0.3\sin(4\pi x) e^{-0.01(4\pi)^2 t}$$

Heat equation 3:

$$\begin{cases} \partial_t u - 0.05\, \partial^2_{xx} u = 0 \\ u(0,x) = \sin(3\pi x) \\ \partial_x u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x) = \cos(3\pi x) e^{-0.05(3\pi)^2 t}$$

2D PDES

Poisson equation 1:

$$\begin{cases} \partial_{tt}^2 u + \partial_{xx}^2 u + 2\pi^2 \sin(\pi t)\sin(\pi x) = 0 \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x) = \sin(\pi x)\sin(\pi t)$$

Poisson equation 2:

$$\begin{cases} \partial_{tt}^2 u + \partial_{xx}^2 u + 10(t-1)\cos(5x) + 25(t-1)(x-1)\sin(5x) = 0 \\ u(0,x) = (1-x)\sin(5x) \\ u(1,x) = u(t,0) = u(t,1) = 0 \end{cases}$$

with analytical solution

$$u(t,x) = (1-t)(1-x)\sin(5x)$$

Poisson equation on unit disk:

$$\begin{cases} \partial_{tt}^2 u + \partial_{xx}^2 u - e^{-(t^2+10x^2)} = 0 \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

2D PDES

Wave equation:

$$\begin{cases} \partial_{tt}^2 u - \partial_{xx}^2 u = 0 \\ u(0,x) = \sin(3\pi x) \\ \partial_t u(0,x) = 0 \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x) = \cos(3\pi t)\sin(3\pi x)$$

Wave equation:

$$\begin{cases} \partial_{tt}^2 u - \partial_{xx}^2 u = 0 \\ u(0,x) = \sin(3\pi x) \\ \partial_t u(0,x) = 0 \\ \partial_x u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x) = \cos(3\pi t)\cos(3\pi x)$$

Traveling Wave equation:

$$\begin{cases} \partial_t u - \partial_x u = 0 \\ u(0,x) = \sin(2\pi x) \\ u\,|_{\partial\Omega} = \sin(2\pi t) \end{cases}$$

with analytical solution

$$u(t,x) = \cos\left(2\pi(t+x)\right)$$

3D PDES

Taylor-Green vortex:

$$\begin{cases} \partial_t u + u\partial_x u + v\partial_y u + \frac{1}{2}e^{-4t}\sin 2x - (\partial_{xx}u + \partial_{yy})u = 0 \\ \partial_t v + u\partial_x v + v\partial_y v + \frac{1}{2}e^{-4t}\sin 2y - (\partial_{xx}v + \partial_{yy}v) = 0 \\ \partial_x u + \partial_y v = 0 \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$\begin{cases} u(t,x,y) = \cos(x)\sin(y)e^{-2t} \\ v(t,x,y) = \sin(x)\cos(y)e^{-2t} \end{cases}$$

Vorticity equation:

$$\begin{cases} \omega = \partial_x v - \partial_y u \\ \partial_t \omega + u\partial_x \omega + v\partial_y \omega - 5 \cdot 10^{-3}(\partial_{xx}\omega + \partial_{yy})\omega - 0.75\left[\sin\left(2\pi(x+y)\right) + \cos\left(2\pi(x+y)\right)\right] = 0 \\ \partial_x u + \partial_y v = 0 \end{cases}$$

where

$$\begin{cases} w(0,x,y) = \pi\left[\cos(3\pi x) - \cos(3\pi y)\right] \\ u(t,0,y) = u(t,1,y) \\ u(t,x,0) = u(t,x,1) \\ u(t,0,y) = u(t,1,y) \\ v(t,x,0) = u(t,x,1) \end{cases}$$

3D PDES

Lamb-Oseen vortex:

$$\begin{cases} \omega = \partial_x v - \partial_y u \\ \partial_t \omega + u\partial_x \omega + v\partial_y \omega - 5 \cdot 10^{-3}(\partial_{xx}\omega + \partial_{yy})\omega = 0 \\ \partial_x u + \partial_y v = 0 \end{cases}$$

where

$$\begin{cases} w(0,x,y) = \frac{1}{4\pi t} \exp\left[-\frac{x^2+y^2}{4t}\right] \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$\begin{cases} u(t,x,y) = -\frac{y}{2\pi(x^2+y^2)}\left(1 - \exp\left[-\frac{x^2+y^2}{4t}\right]\right) \\ v(t,x,y) = \frac{x}{2\pi(x^2+y^2)}\left(1 - \exp\left[-\frac{x^2+y^2}{4t}\right]\right) \end{cases}$$

3D PDES

Heat equation 1:

$$\begin{cases} \partial_t u - (\partial^2_{xx} + \partial^2_{yy})u = 0 \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$u(t, x, y) = e^{x+y+2t}$$

Heat equation 2:

$$\begin{cases} \partial_t u - (\partial^2_{xx} + \partial^2_{yy})u = 0 \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$u(t, x, y) = (1 - y)e^{x+t}$$

3D PDES

Poisson equation 1:

$$\begin{cases} \partial_{tt}^2 u + \partial_{xx}^2 u + \partial_{yy}^2 u + 3\pi^2 \sin(\pi t)\sin(\pi x)\sin(\pi y) = 0 \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x,y) = \sin(\pi t)\sin(\pi x)\sin(\pi y)$$

Poisson equation 2:

$$\begin{cases} \partial_{tt}^2 u + \partial_{xx}^2 u + \partial_{yy}^2 u - 6 = 0 \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$u(t,x,y) = u(t,x,y) = t^2 + x^2 + y^2$$

Poisson equation 3:

$$\begin{cases} \partial_{tt}^2 u + \partial_{xx}^2 u + \partial_{yy}^2 u - 6 = 0 \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$u(t,x,y) = t^2 + x^2 - y^2$$

3D PDES

Wave equation:

$$\begin{cases} \partial_{tt}^2 u - (\partial_{xx}^2 u + \partial_{yy}^2 u) = 0 \\ u(0,x,y) = \sin(\pi x)\sin(\pi y) \\ \partial_t u(0,x,y) = 0 \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x,y) = \cos(\sqrt{2}\pi t)\sin(\pi x)\sin(\pi y)$$

Wave equation:

$$\begin{cases} \partial_{tt}^2 u - (\partial_{xx}^2 u + \partial_{yy}^2 u) = 0 \\ u(0,x,y) = \sin(3\pi x)\sin(4\pi y) \\ \partial_t u(0,x,y) = 0 \\ u\,|_{\partial\Omega} = 0 \end{cases}$$

with analytical solution

$$u(t,x,y) = \cos(5\pi t)\sin(3\pi x)\sin(4\pi y)$$

Traveling wave equation:

$$\begin{cases} \partial_t u - \frac{1}{5}(\partial_x u + \partial_y u) = 0 \\ u(0,x,y) = \sin(3\pi x + 2\pi y) \\ \text{Dirichlet BC} \end{cases}$$

with analytical solution

$$u(t,x,y) = \sin(3\pi x + 2\pi y + \pi t)$$