Physics-Aware Recurrent Convolutions (PARC)

Stephen Baek

Recap of PINN and Neural Operator from a Differential Geometry Point of View

- Physics-informed loss (Raissi et al.)

$$\partial_t u - \mathcal{N}(u) = 0$$

Recap of PINN and Neural Operator from a Differential Geometry Point of View

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$$\partial_t u - \alpha \nabla^2 u = 0$$

Heat equation

Recap of PINN and Neural Operator from a Differential Geometry Point of View

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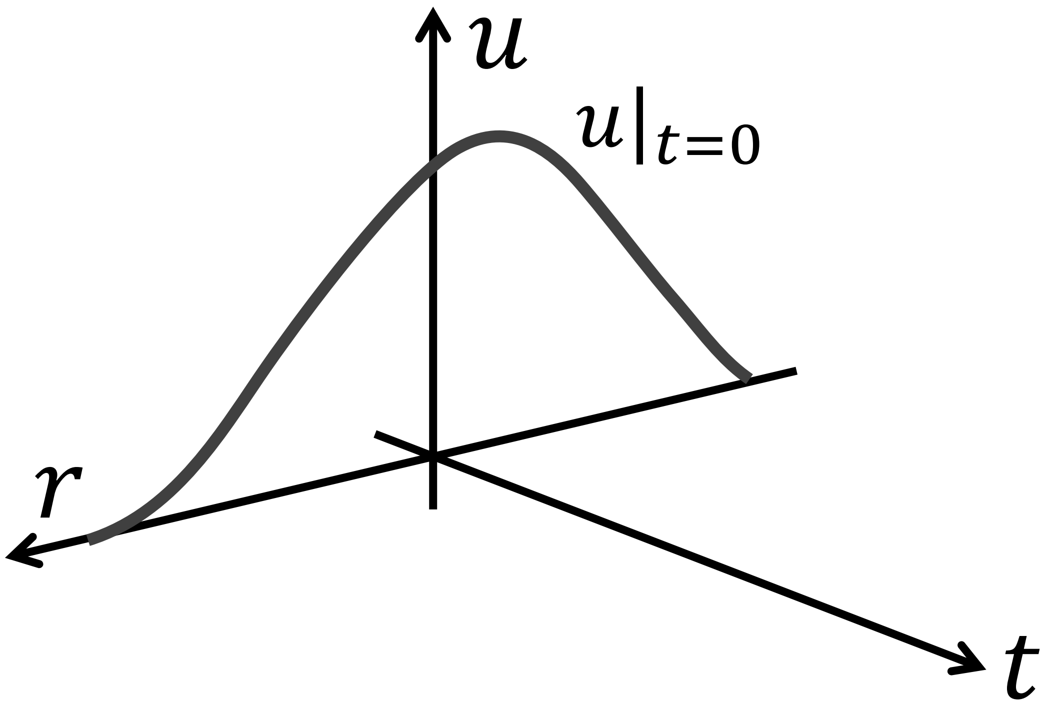

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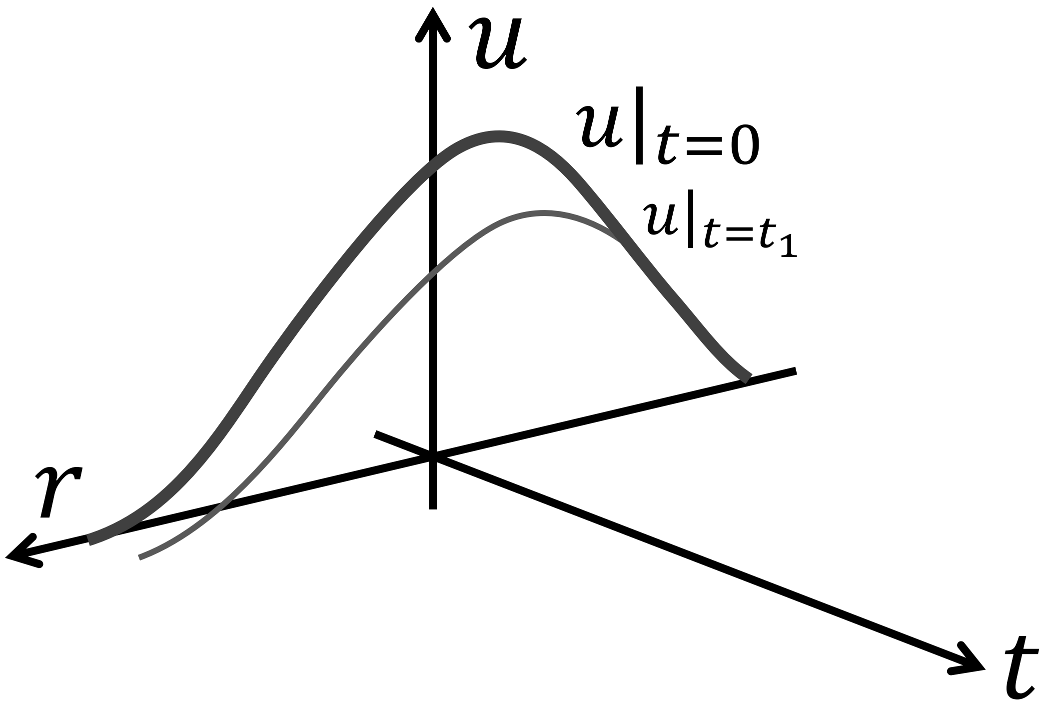

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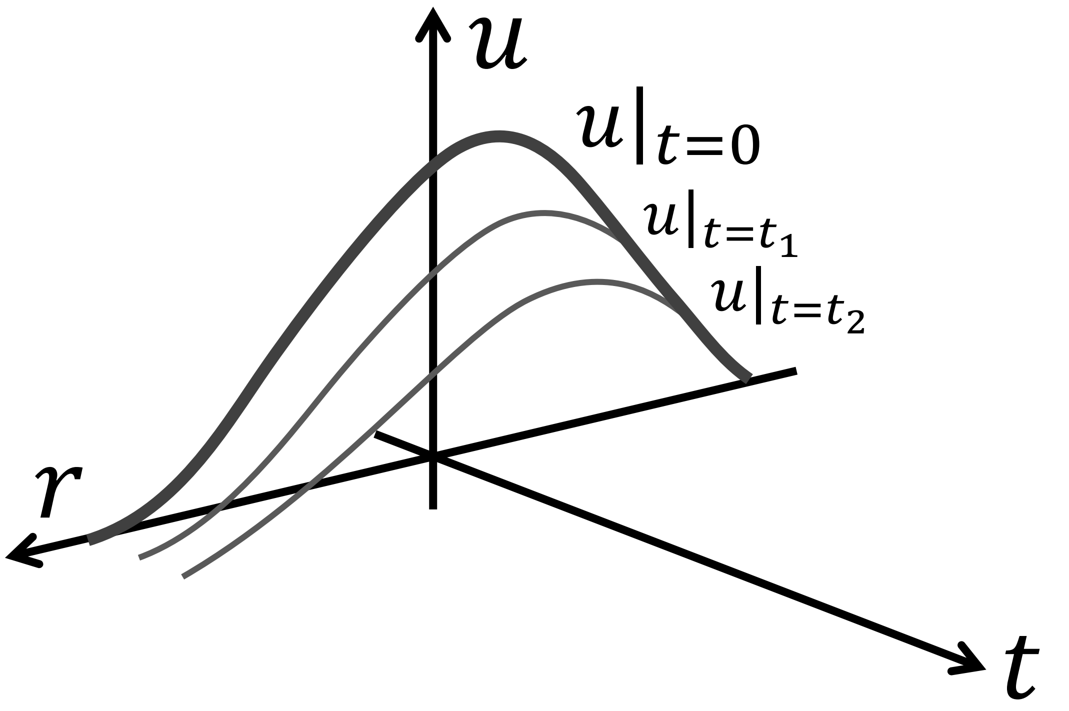

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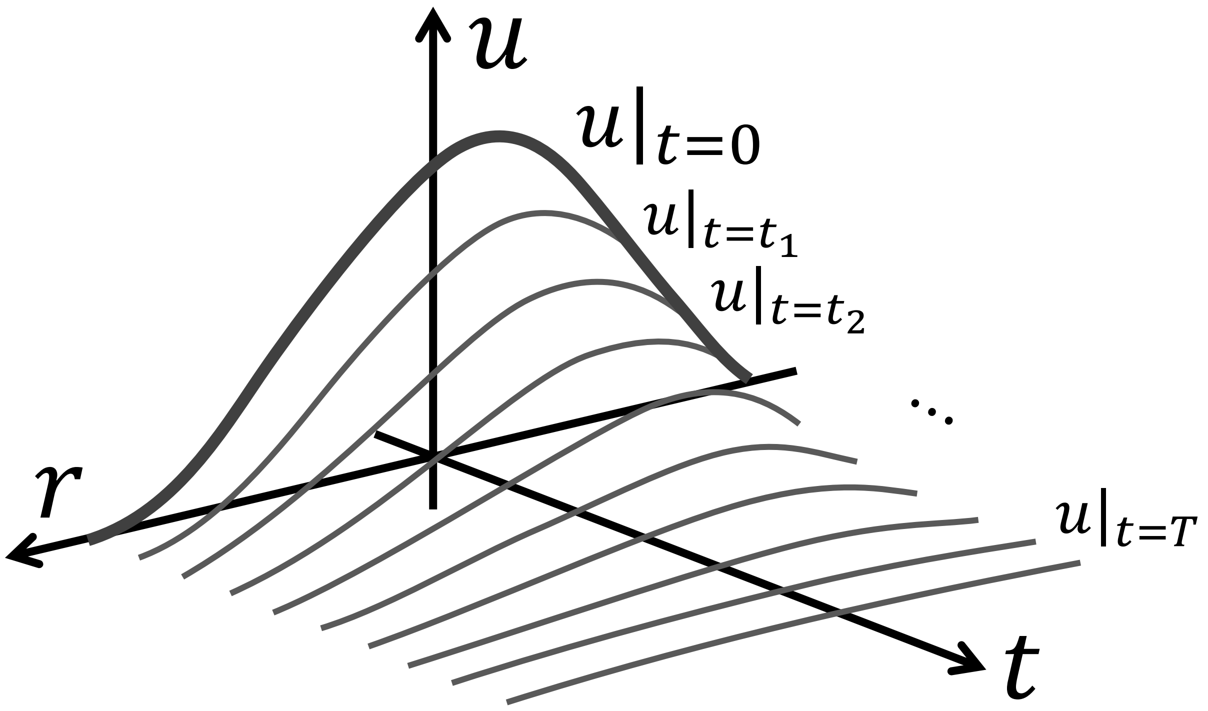

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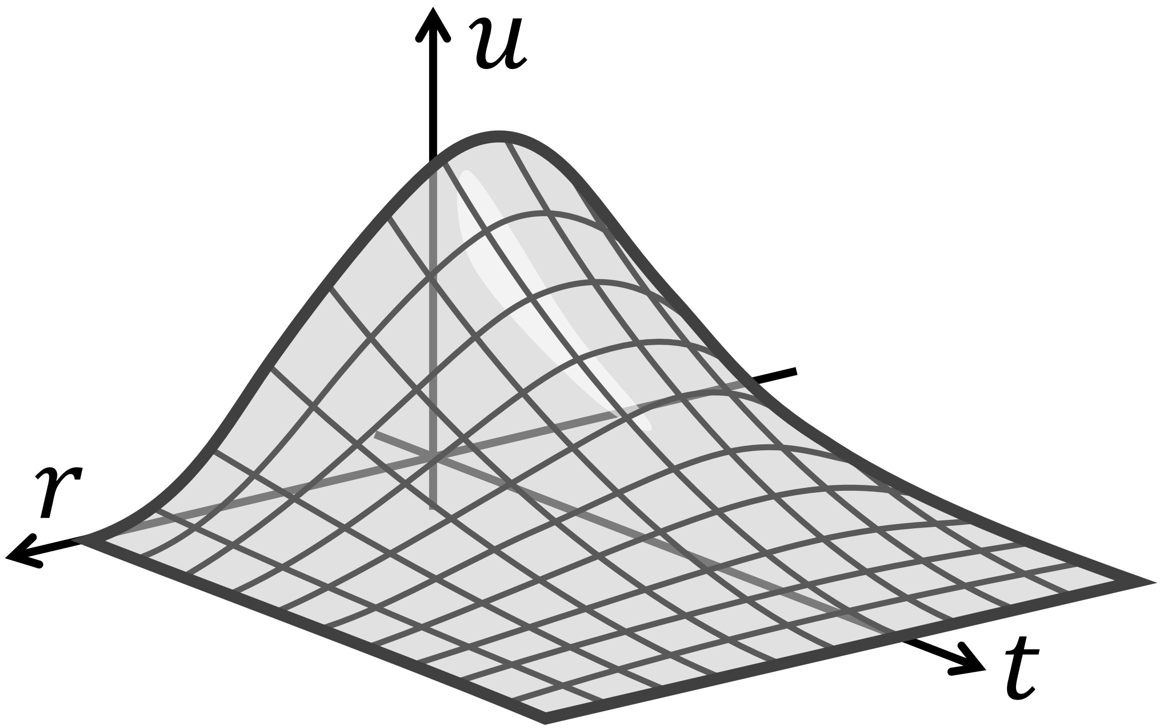

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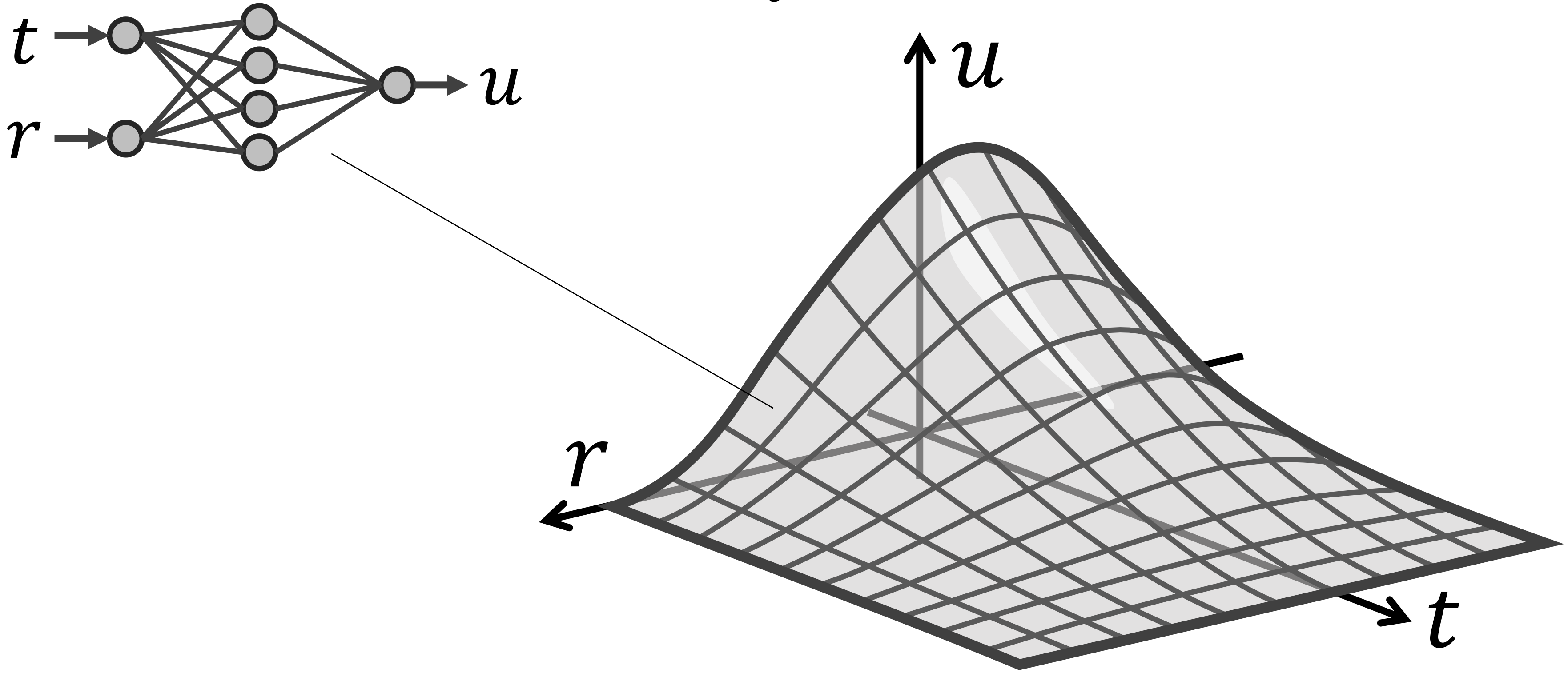

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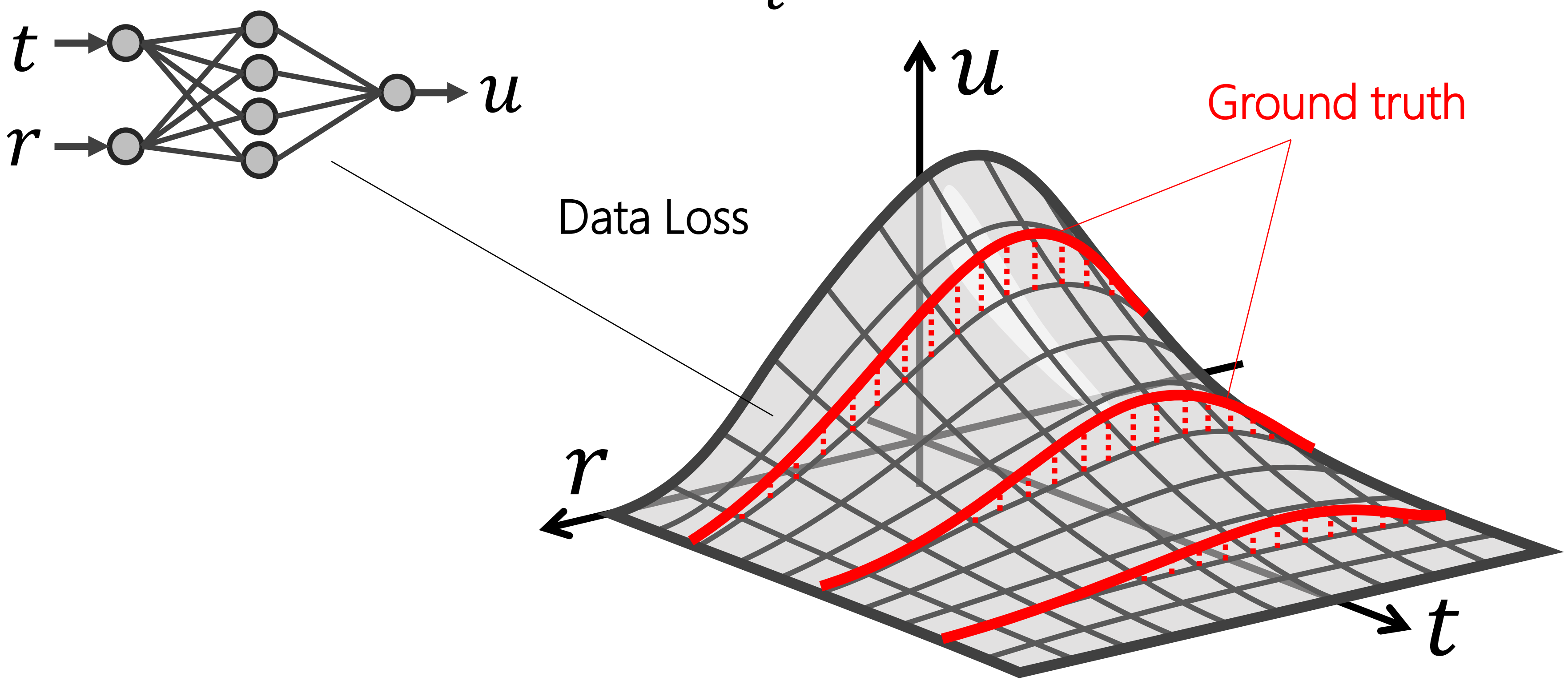

Recap of PINN and Neural Operator from a Differential Geometry Point of View

- Physics-informed loss (Raissi et al.)

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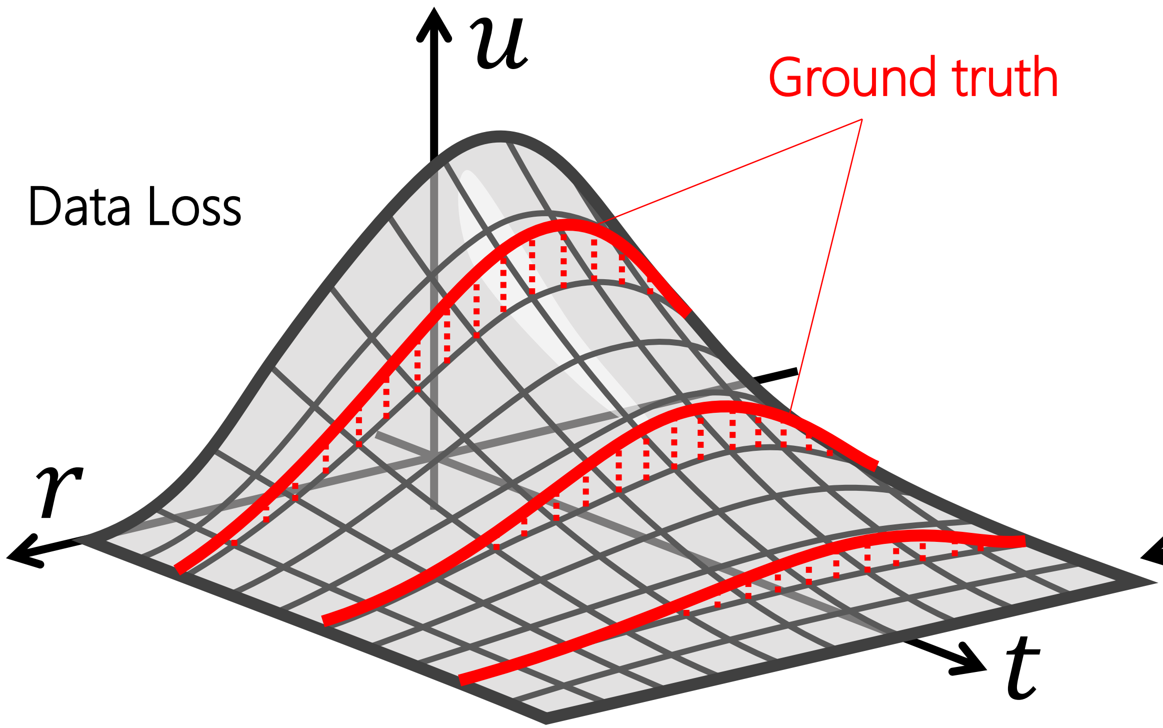
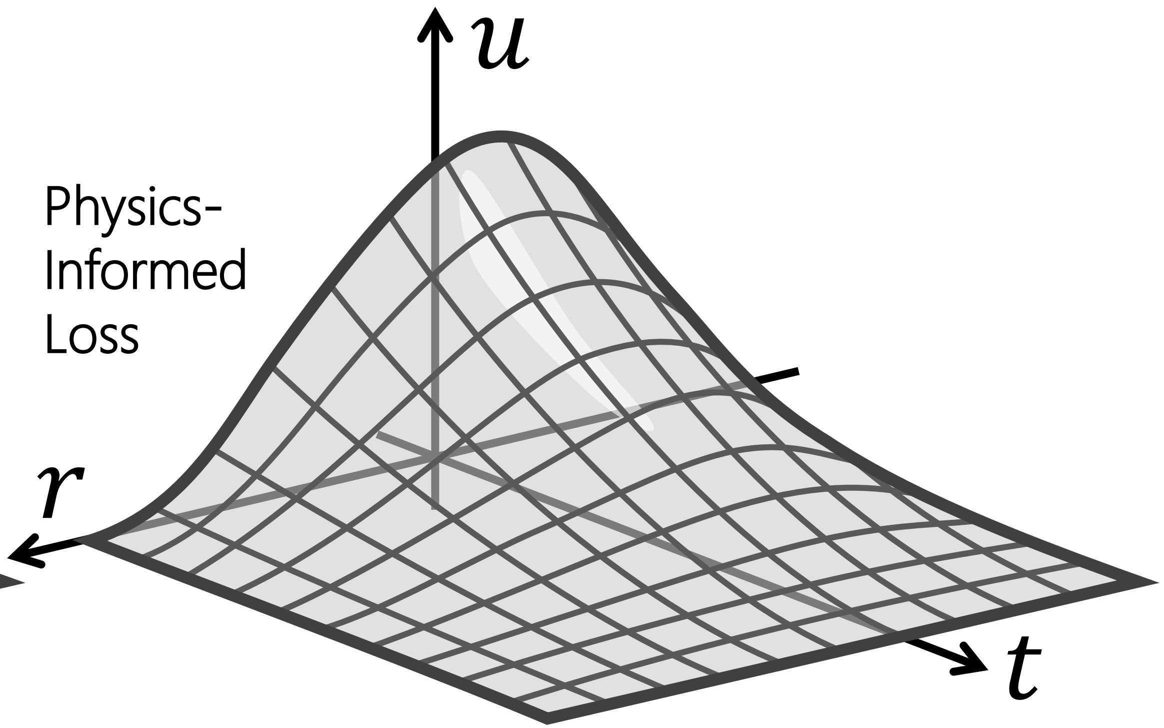
Data Loss



Physics-Informed Loss



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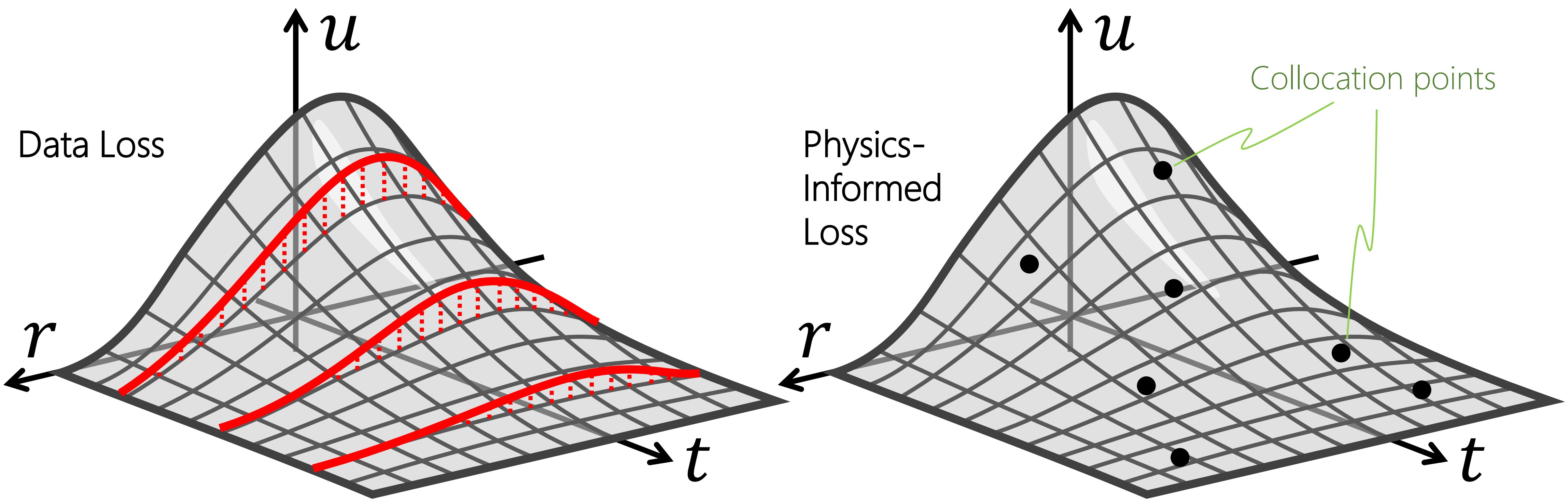

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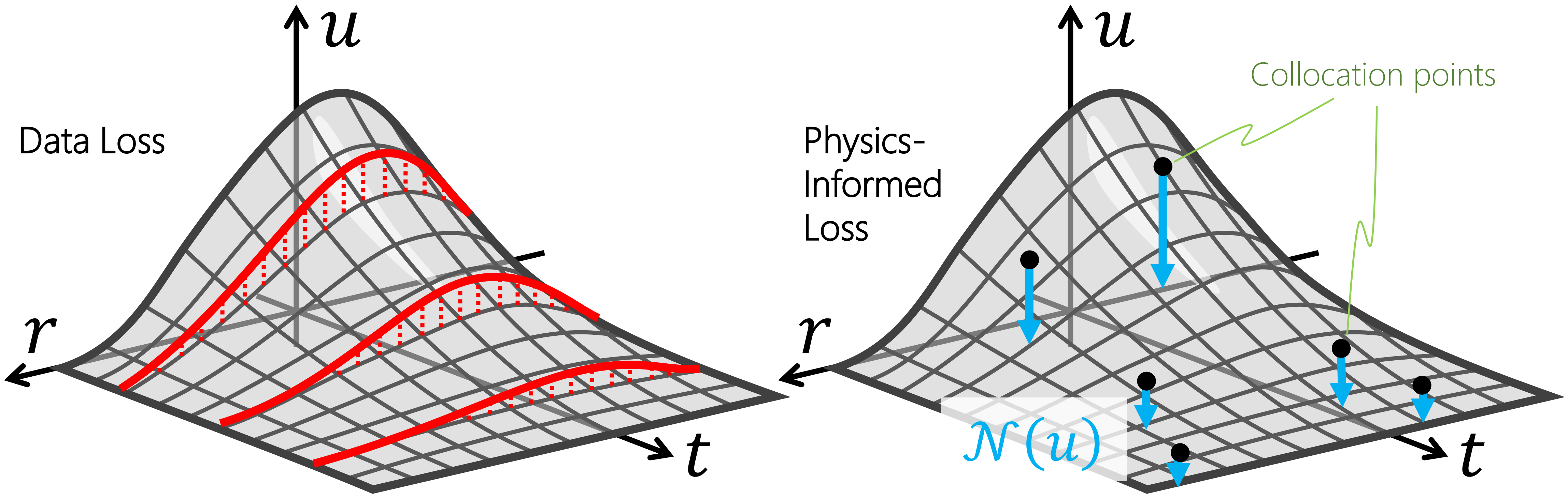

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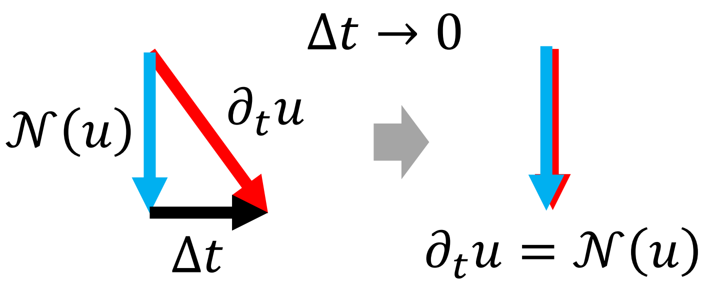

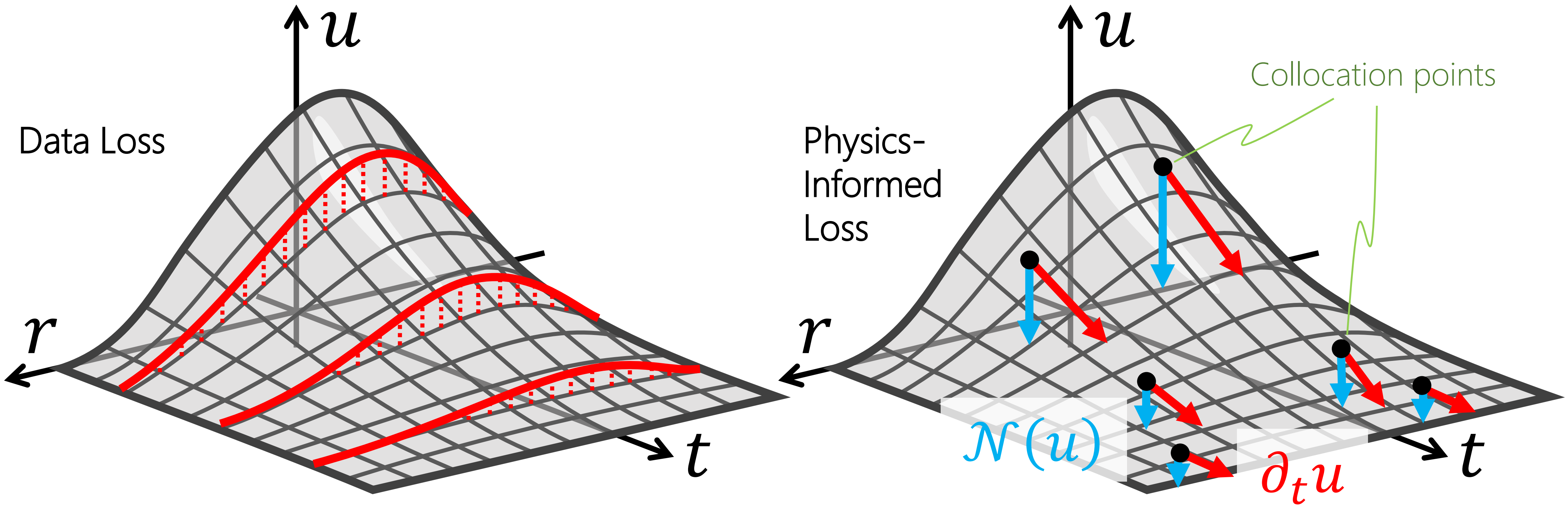

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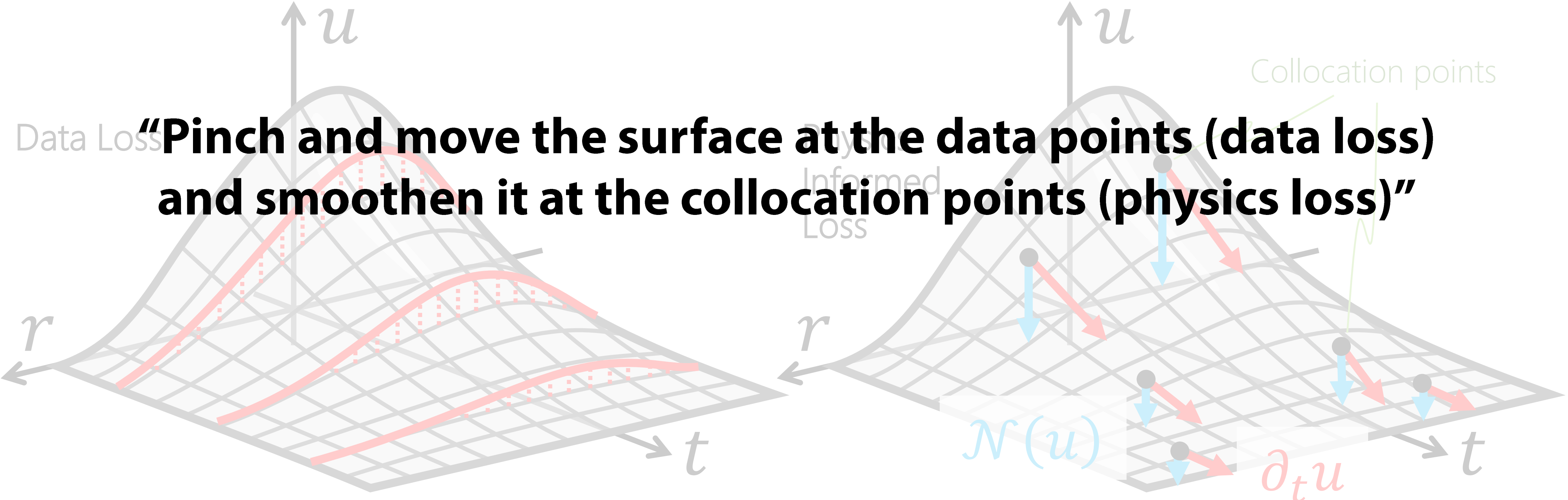
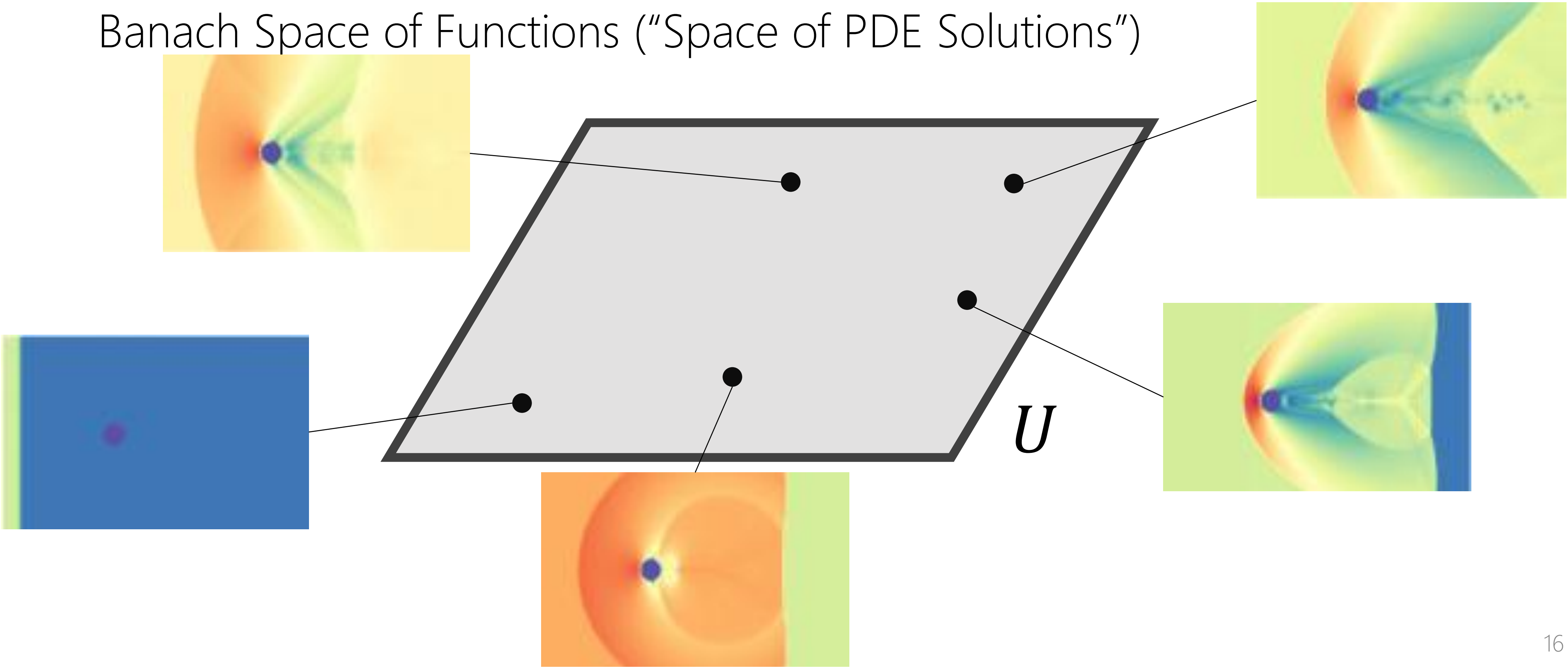


"Pinch and move the surface at the data points (data loss) and smoothen it at the collocation points (physics loss)"

Recap of PINN and Neural Operator from a Differential Geometry Point of View

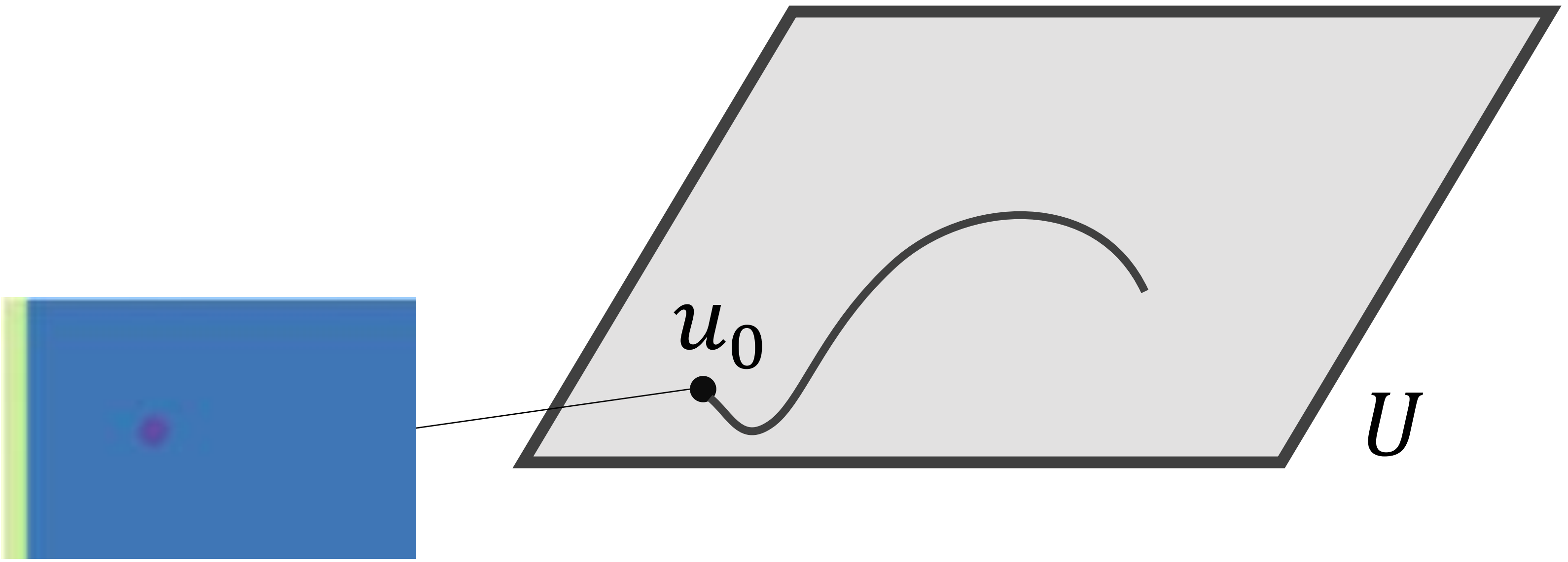
- Neural Operators (Kovachki, Li, et al.)



Recap of PINN and Neural Operator from a Differential Geometry Point of View

- Neural Operators (Kovachki, Li, et al.)

Banach Space of Functions ("Space of PDE Solutions")



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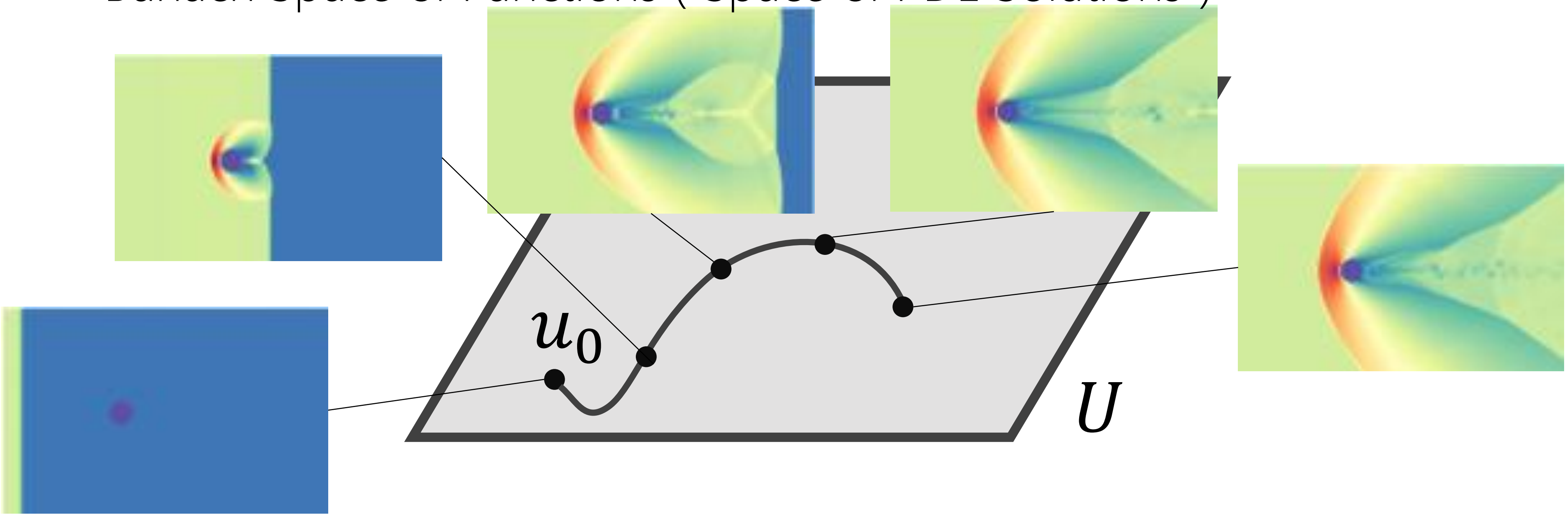

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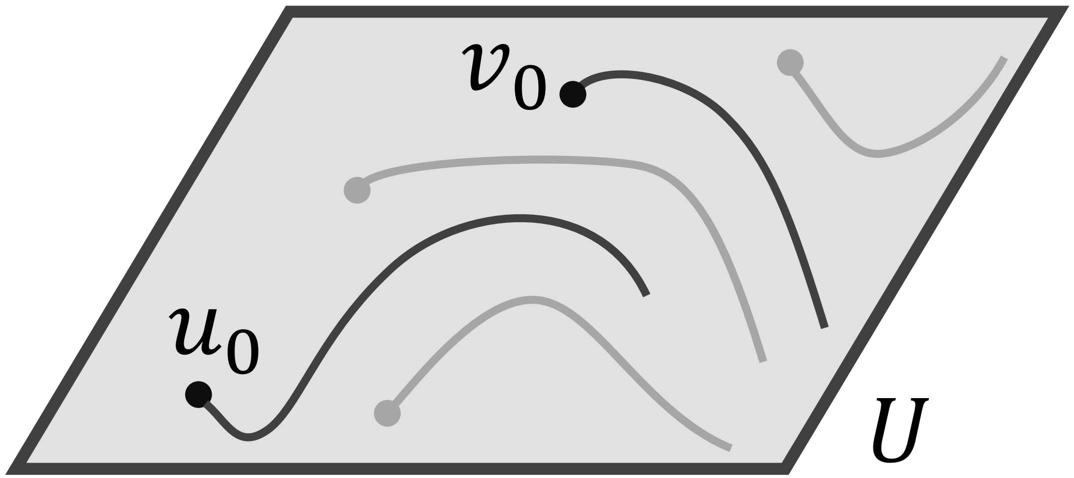
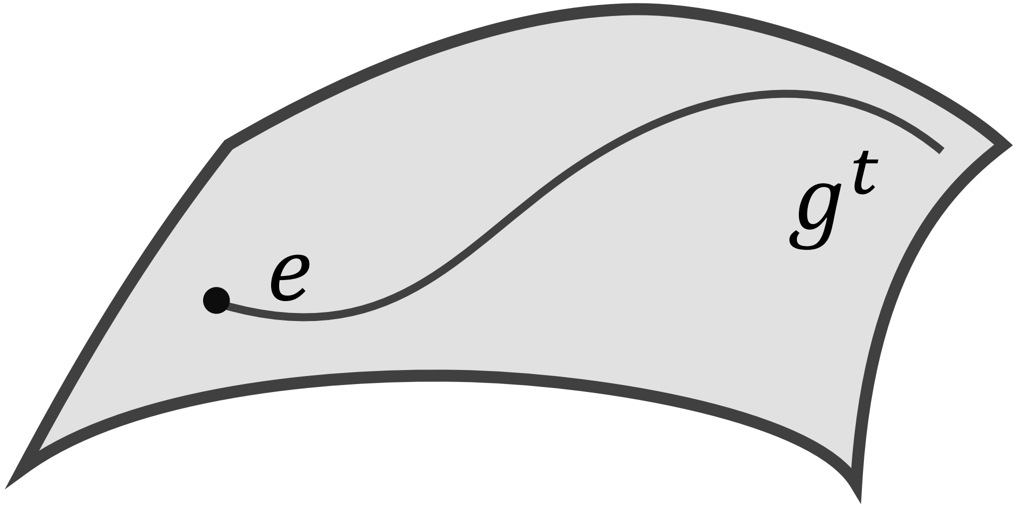


Recap of PINN and Neural Operator from a Differential Geometry Point of View

- Neural Operators (Kovachki, Li, et al.)

Space of Operators

$G = \mathrm{Aut}(U)$



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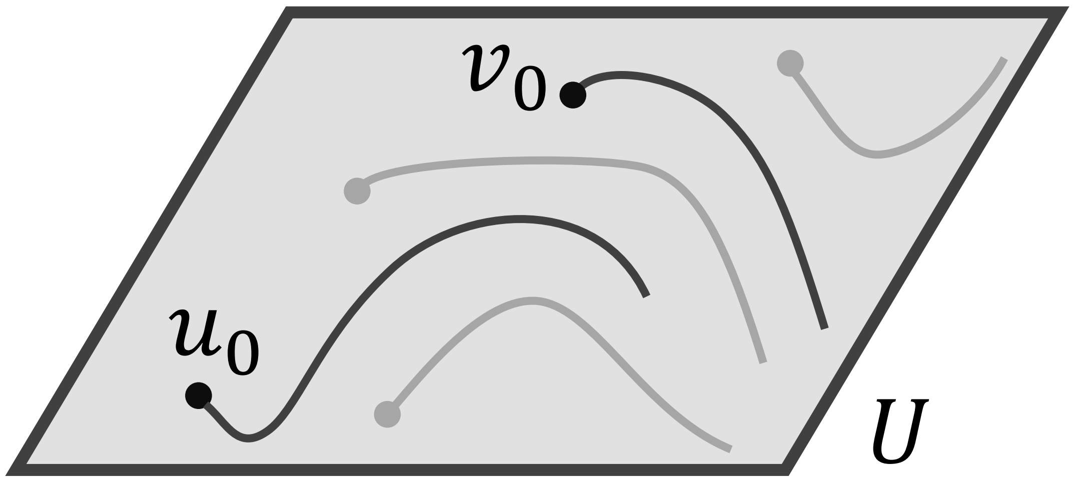

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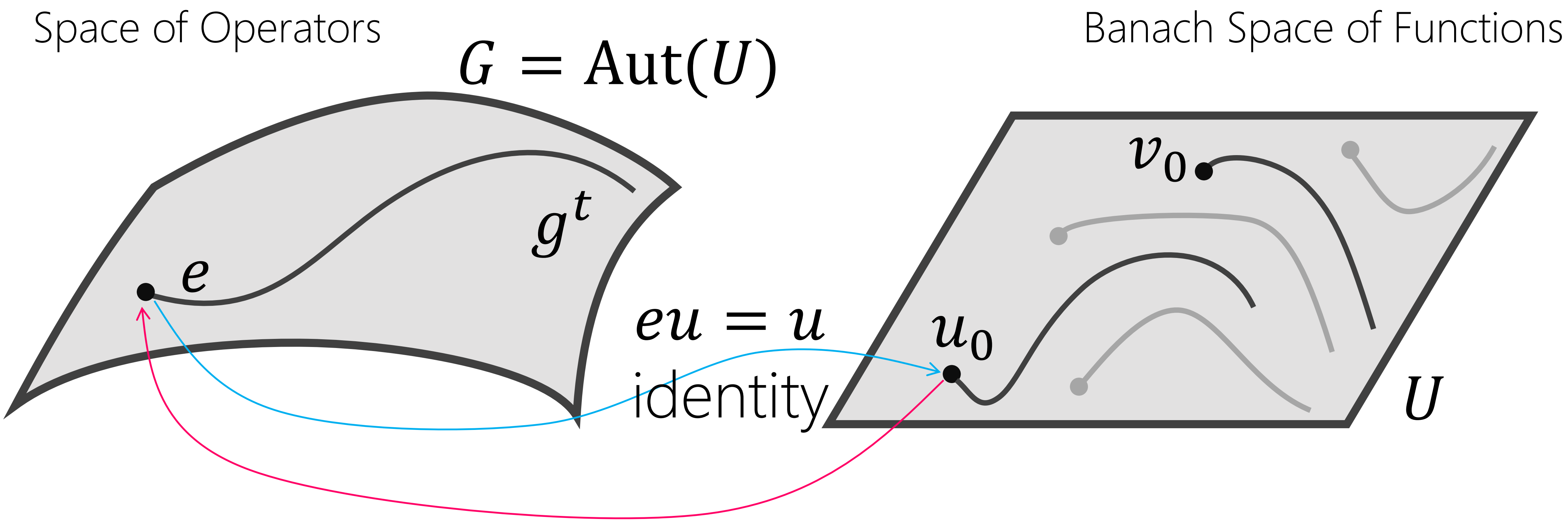

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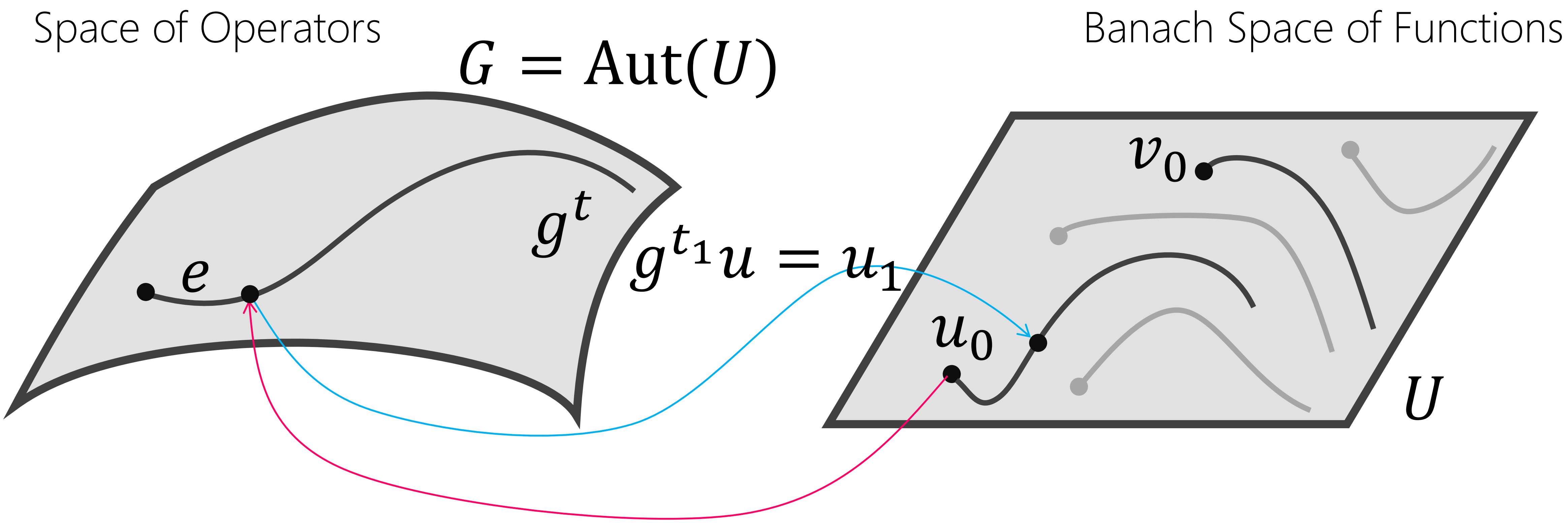

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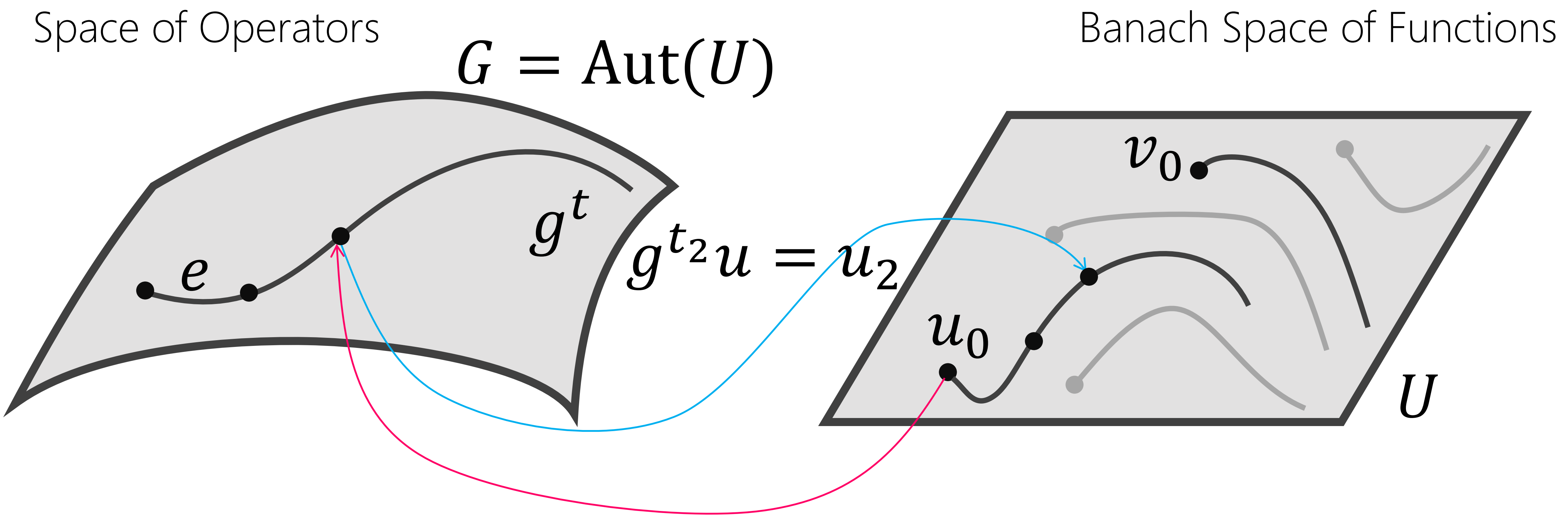

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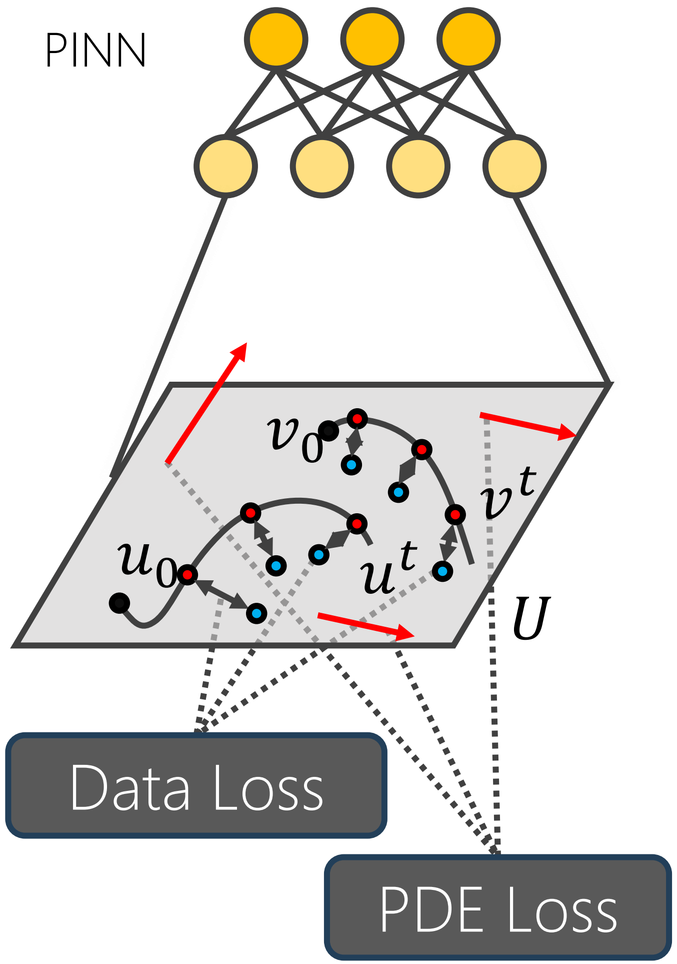
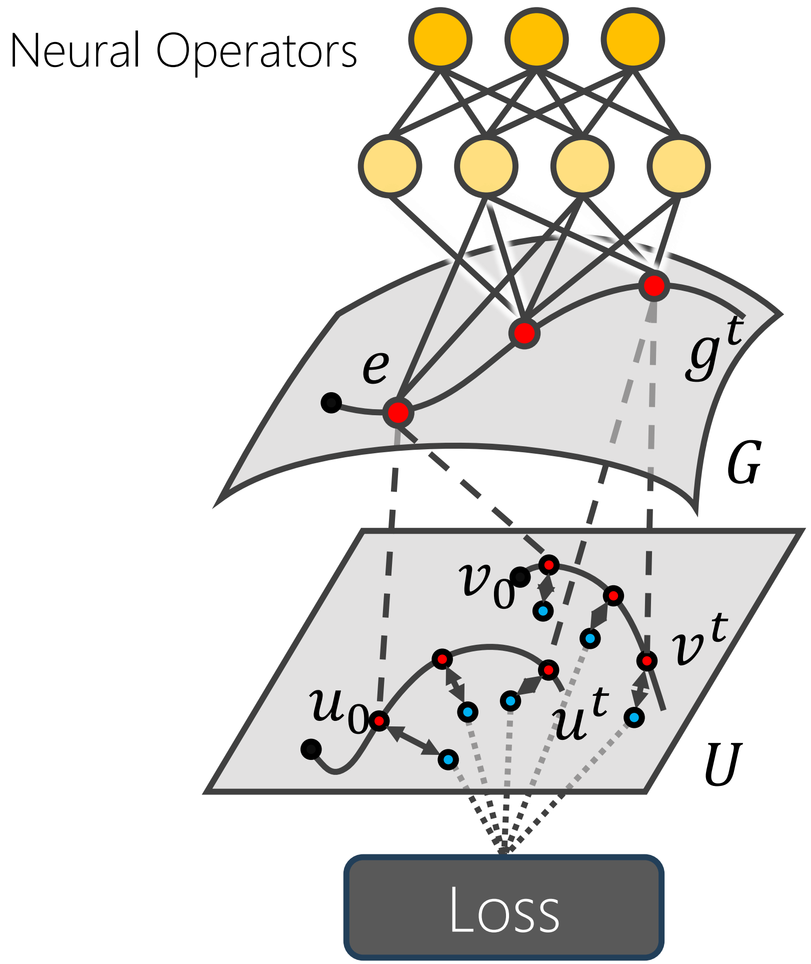




Re-thinking the Physics Learning

- PINN: Learning the solution function
  - Approximate the solution function using neural networks
  - Search space: Entire space of functions $\mathcal{U}$

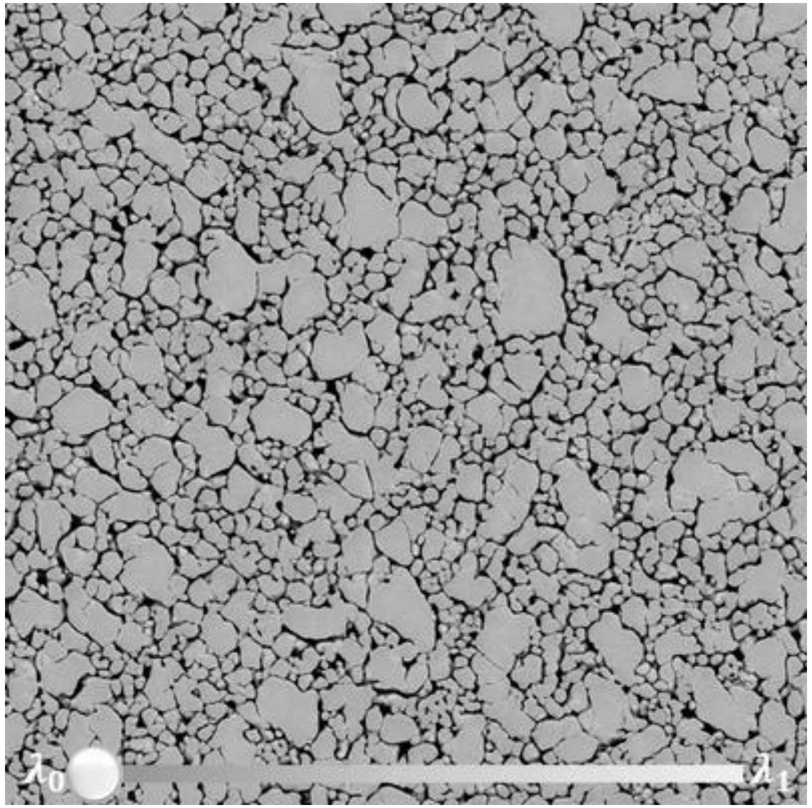
  - If IC/BC/other physical conditions change, the model needs to be retrained.
  - When the solution function u is nonlinear, the model is harder to fit with small data

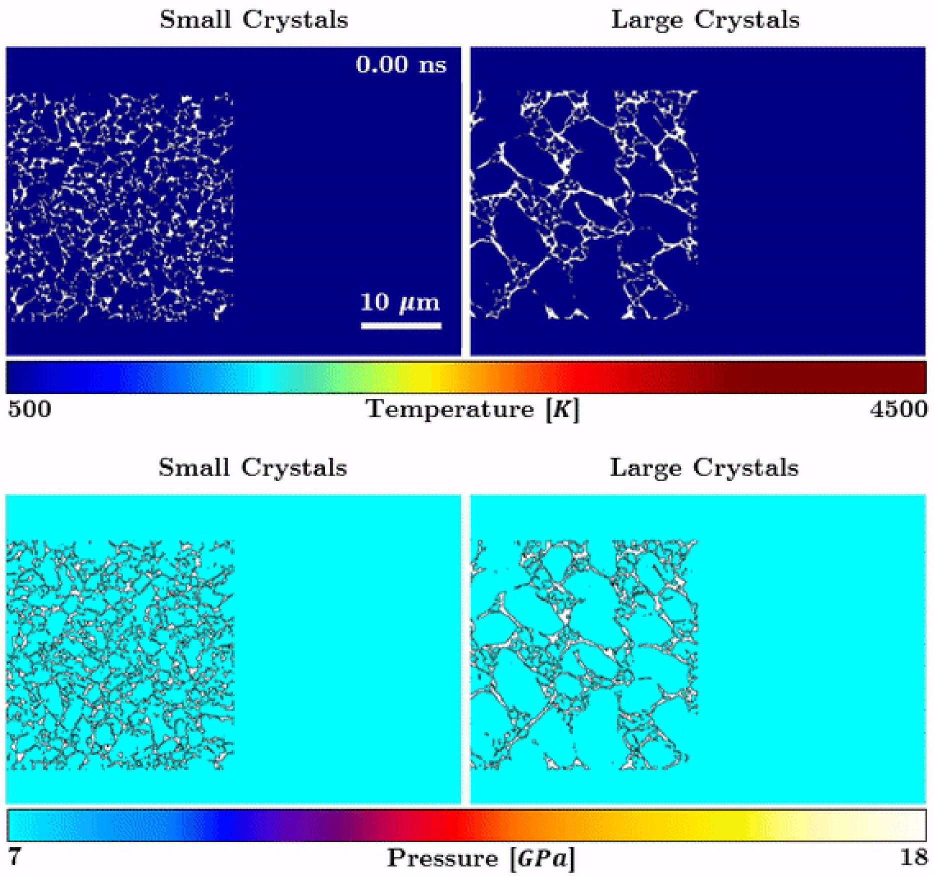
- Neural Operators: Learning the operator
  - Approximate the solution operator using neural networks
  - Search space: Space of operators $\mathcal{G}$

  - Model is still valid for different IC/BC/physical parameters
  - Relatively easier to learn nonlinear dynamics

Physics-Aware Recurrent CNNs (PARC)

- Initial & boundary value problems





Chun et al. (2020) https://www.nature.com/articles/s41598-020-70149-0

Visual Intelligence Laboratory

A generic nonlinear differential operator

Morphology

$$\frac{\partial X}{\partial t} = \mathcal{D}(X, \mu)$$

Quantities of interest

(in our case, temperature & pressure)

Visual Intelligence Laboratory

Deep neural network

model parameters

$$\frac{\partial X}{\partial t} = f(X, \mu \mid \theta) + \varepsilon$$

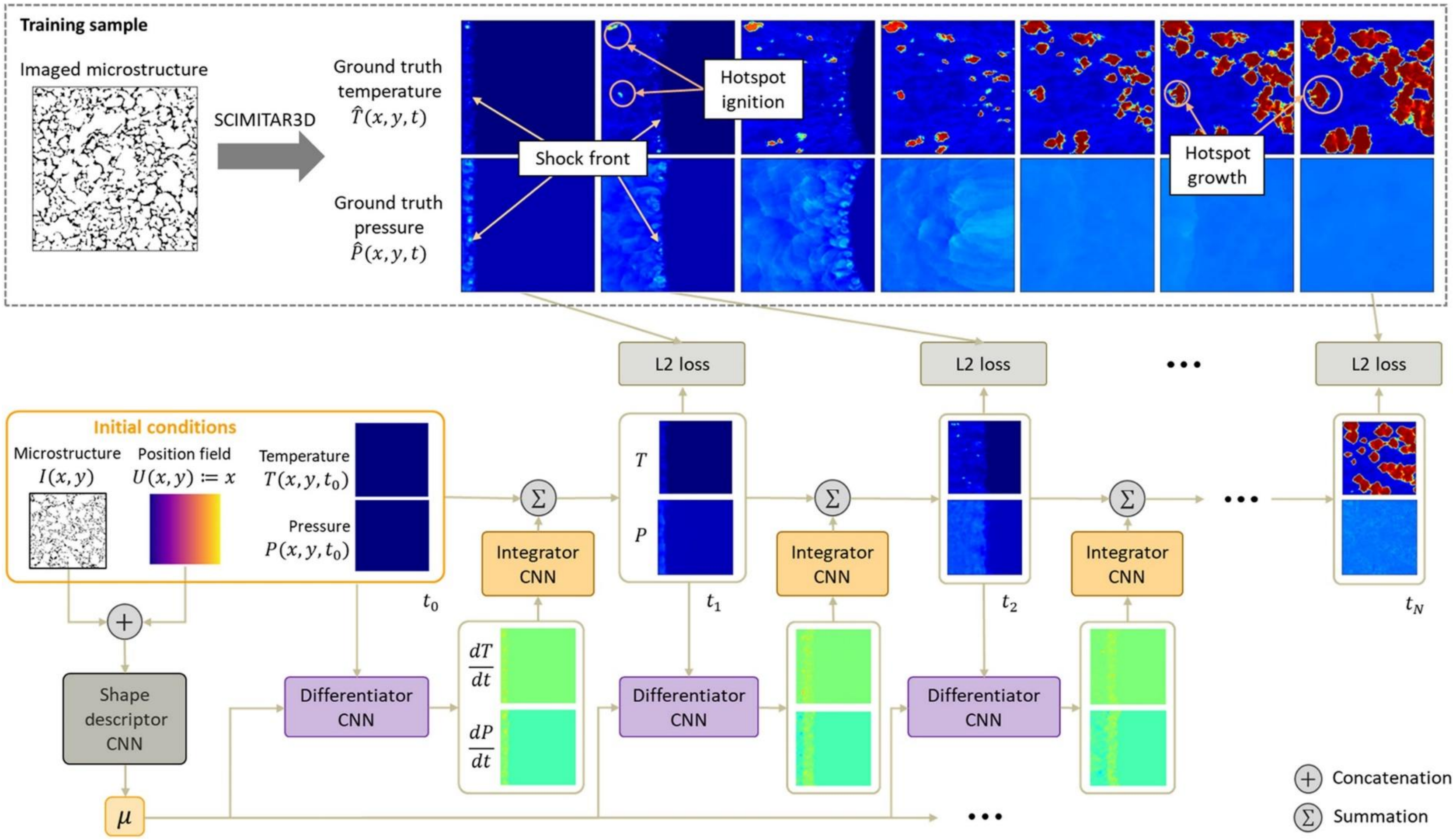
stochastic noise + prediction error

Visual Intelligence Laboratory

$$\frac{\partial X}{\partial t} = f(X, \mu \mid \theta) + \varepsilon$$

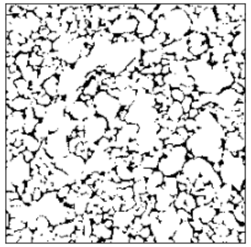
$$X(t + \Delta t) = X(t) + \int_0^{\Delta t} f(X, \mu \mid \theta) dt$$

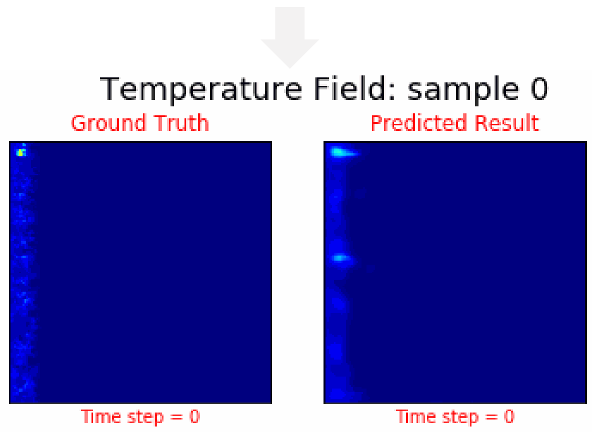
Physics-Aware Recurrent CNNs (PARC)



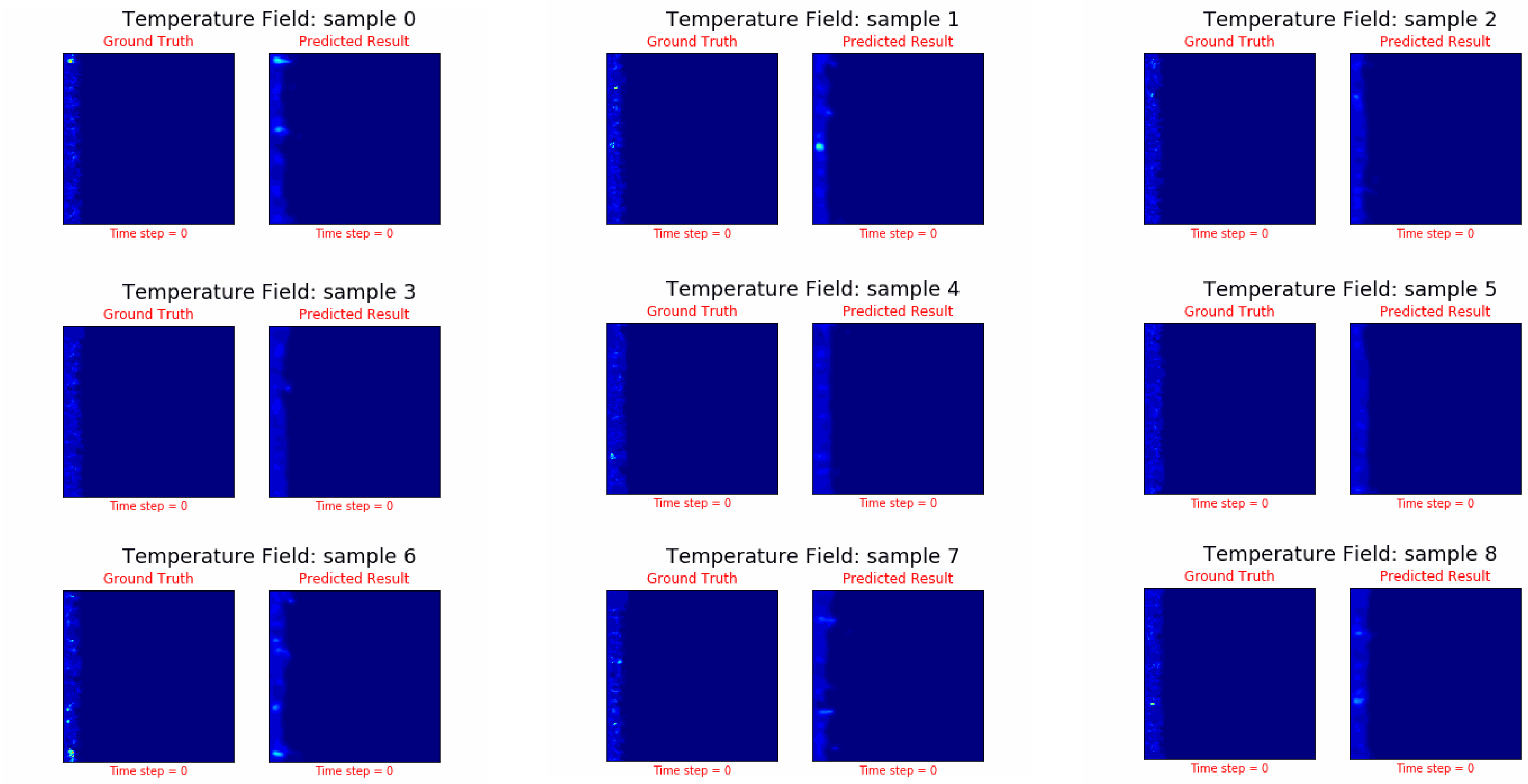
$$\frac{\partial X}{\partial t} = f(X, \mu \mid \theta) + \varepsilon$$

$$X(t + \Delta t) = X(t) + \int_0^{\Delta t} f(X, \mu \mid \theta) dt$$





Nguyen et al. (2023a). https://www.science.org/doi/10.1126/sciadv.add6868



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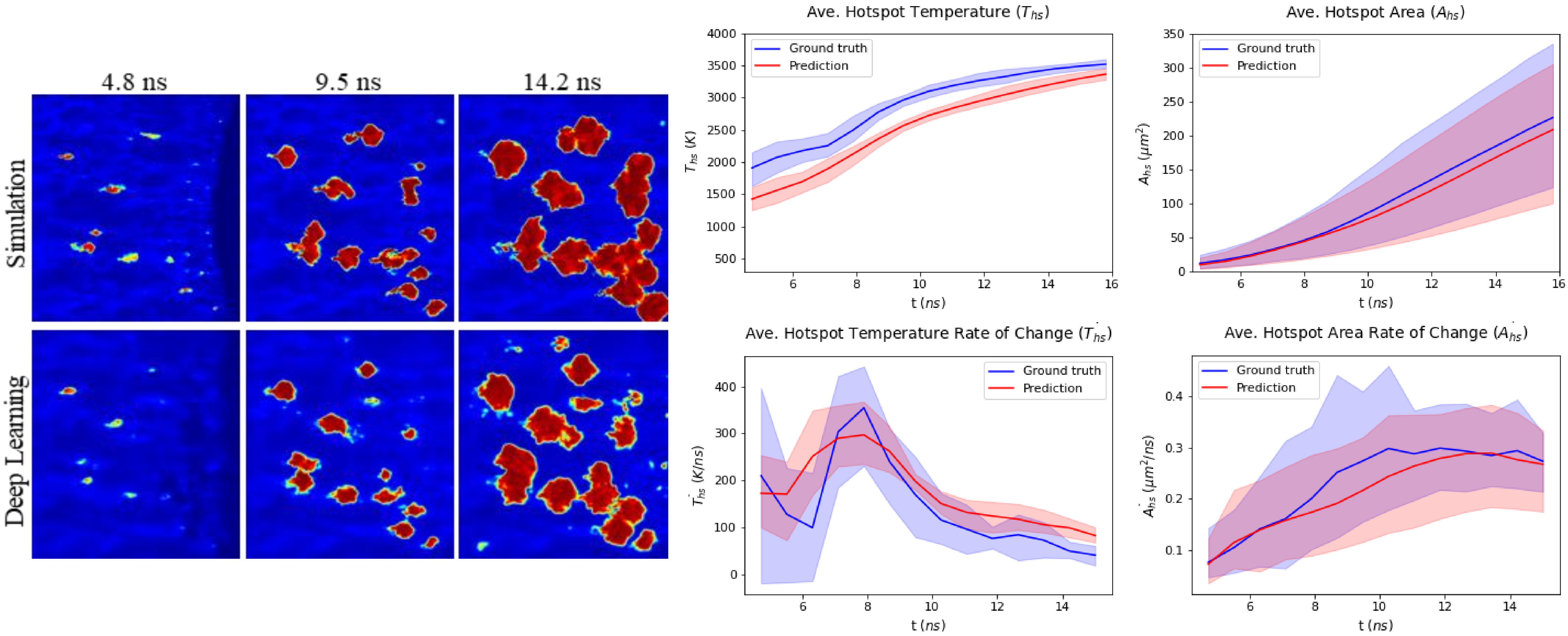
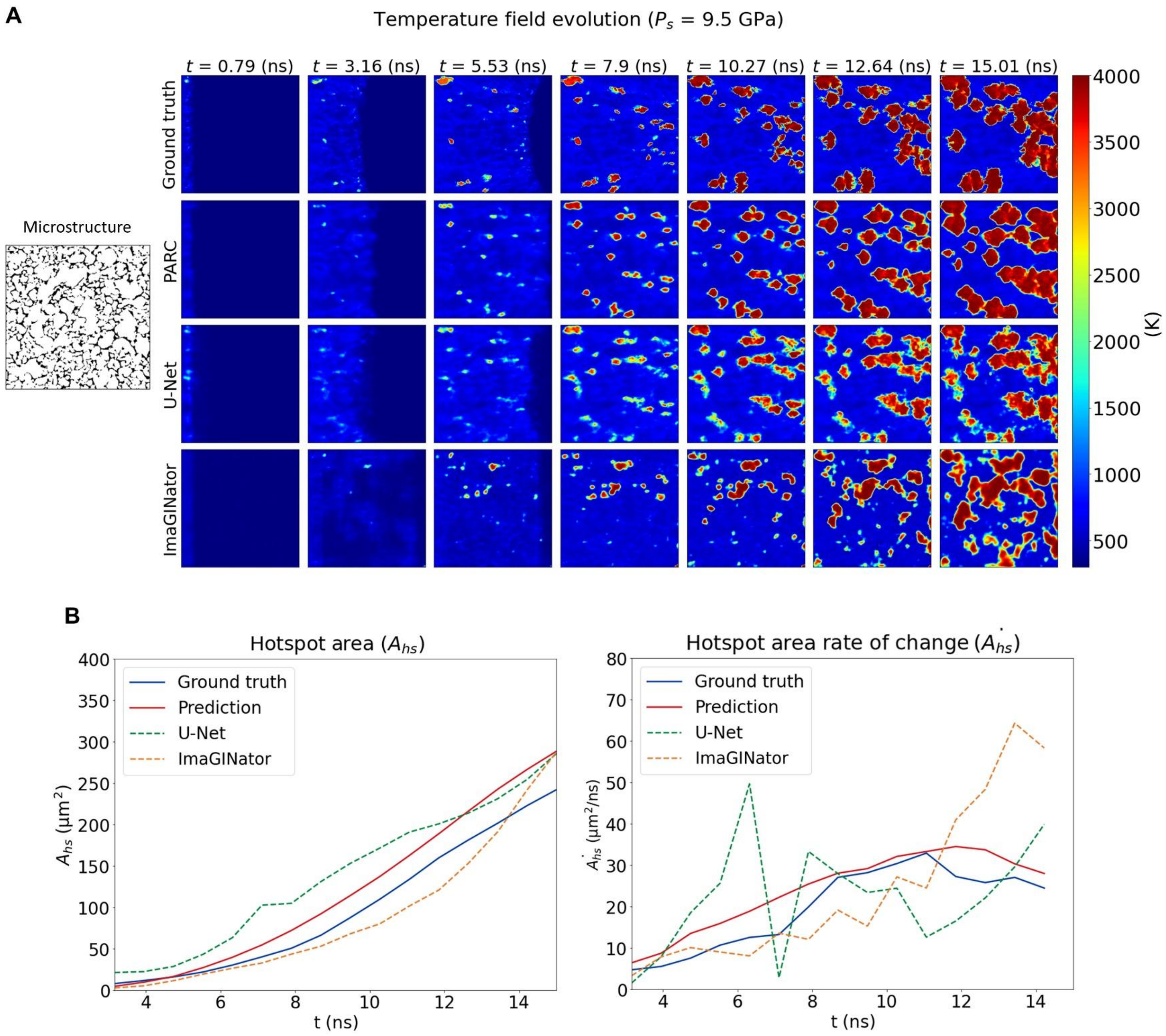


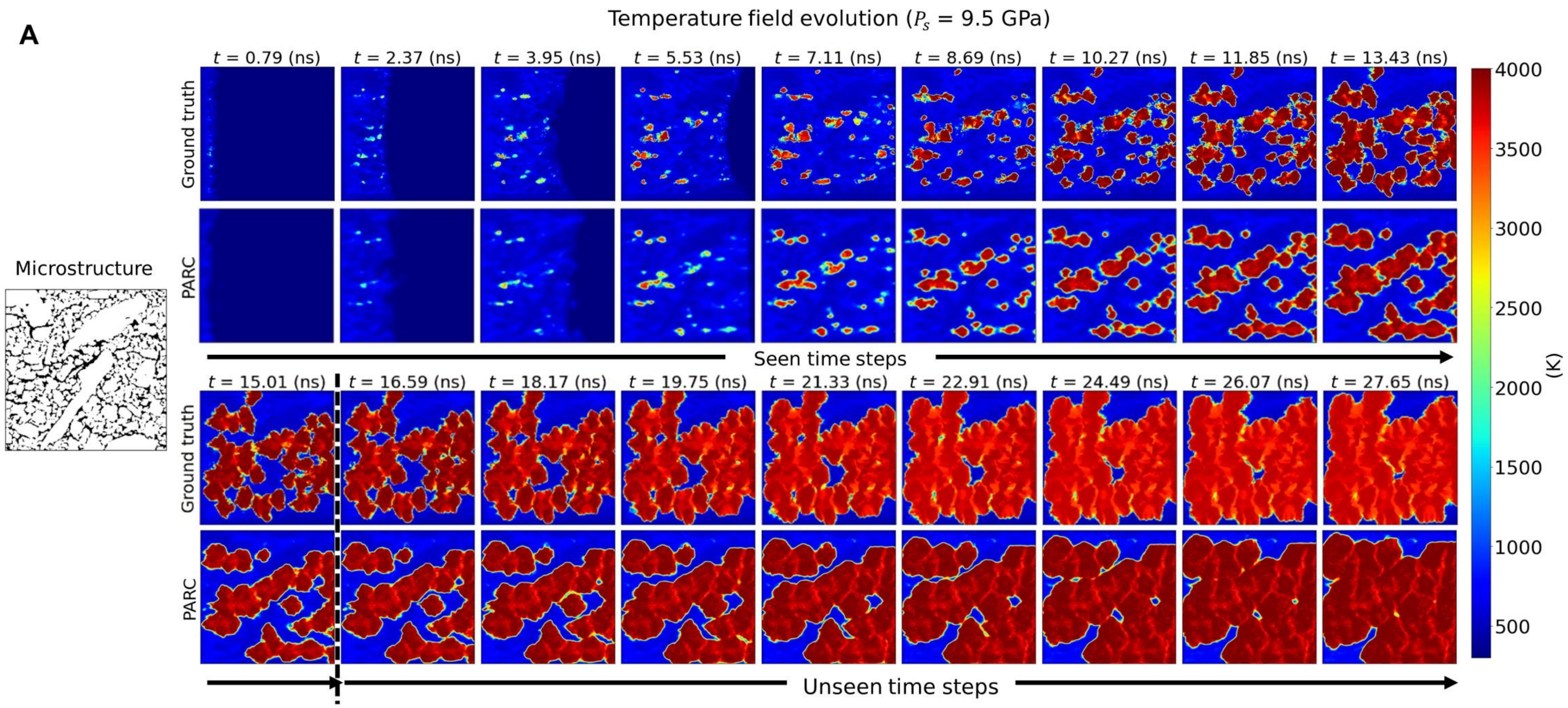
https://www.science.org/doi/10.1126/sciadv.add6868

Physics-Aware
vs
Physics-Naïve



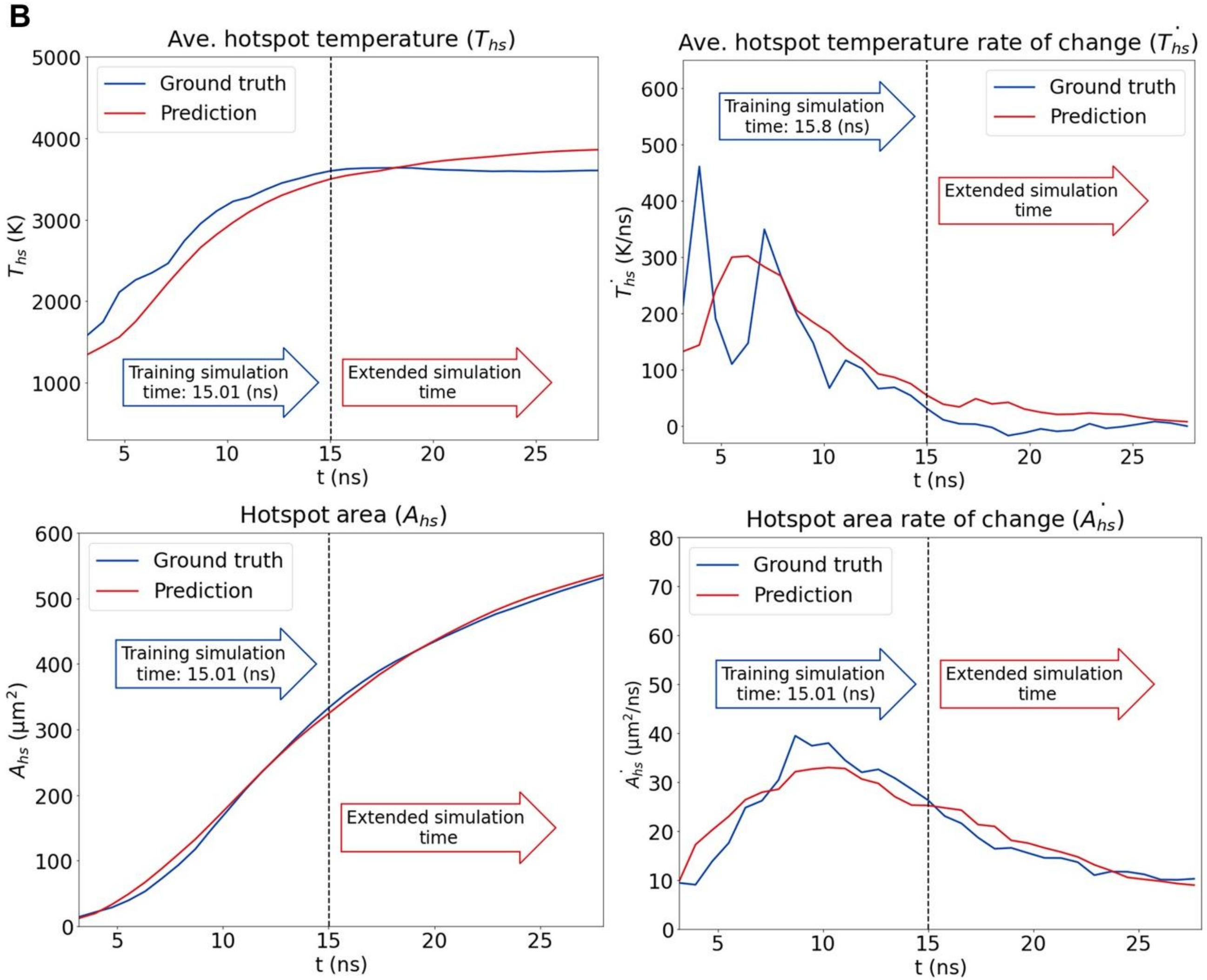
https://www.science.org/doi/10.1126/sciadv.add6868

Physics-Awareness



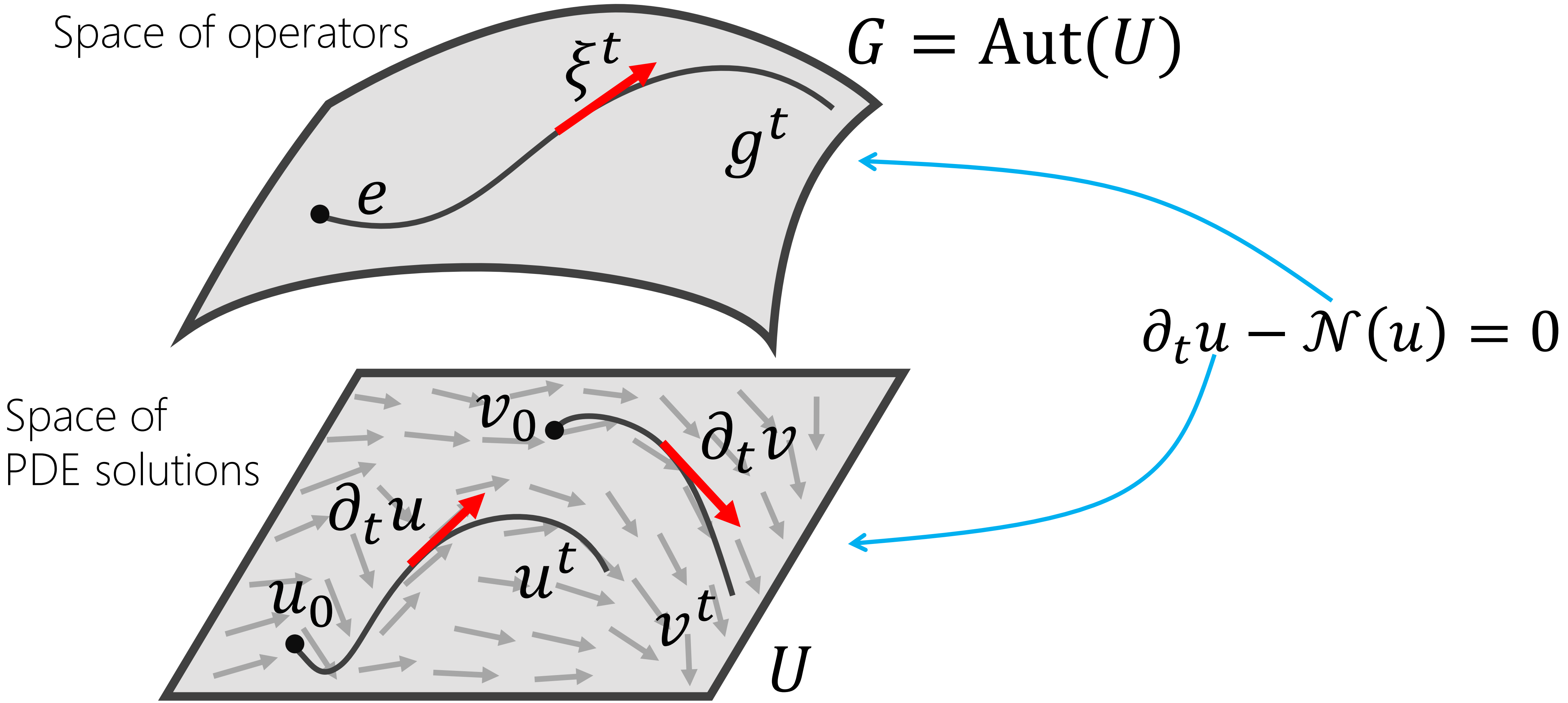
https://www.science.org/doi/10.1126/sciadv.add6868

Physics-Awareness

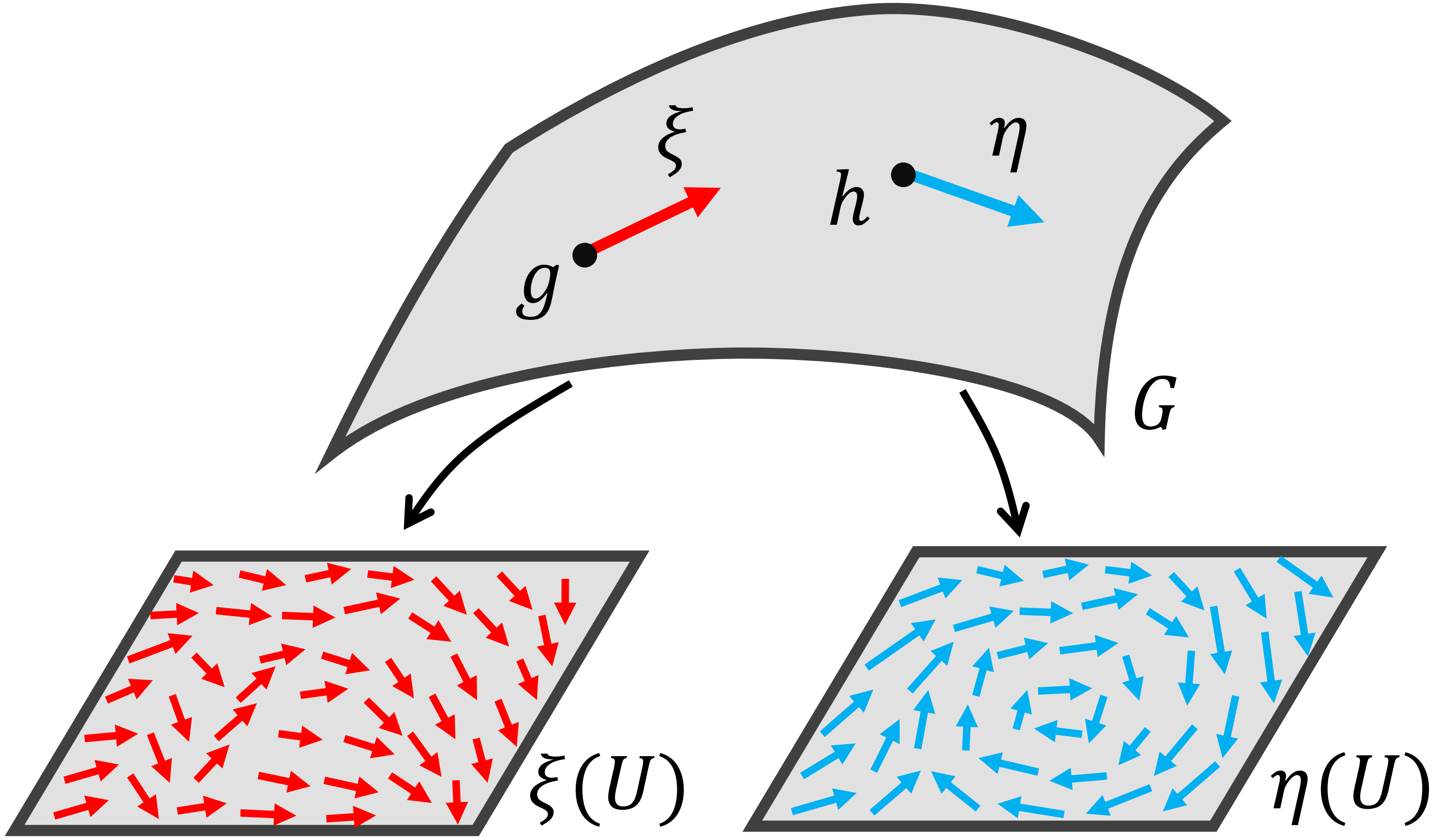


https://www.science.org/doi/10.1126/sciadv.add6868

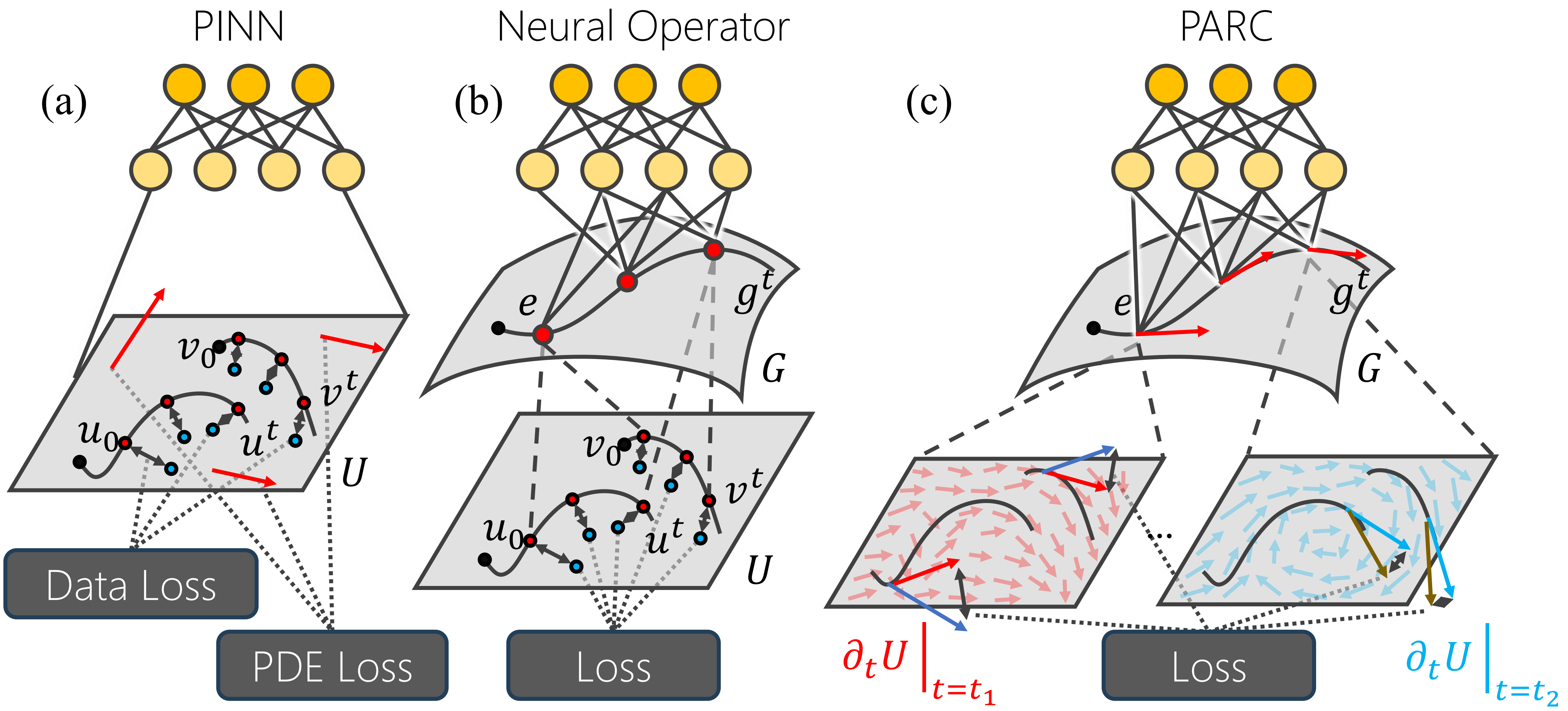
Differential Geometry Perspective



Differential Geometry Perspective

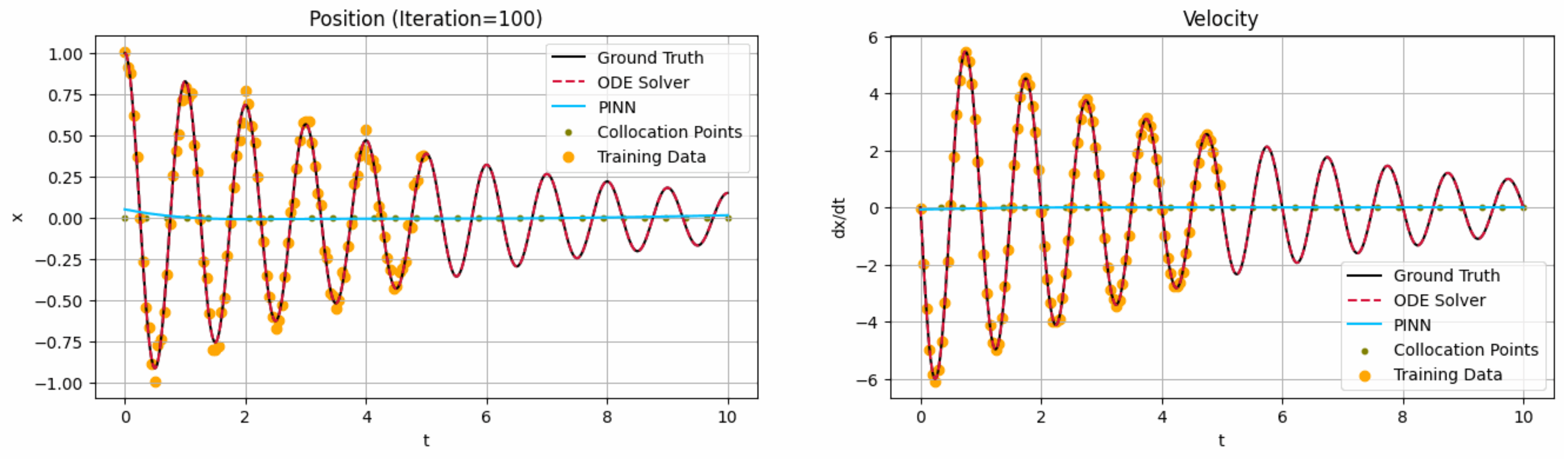


Different Ways to Inform Physics

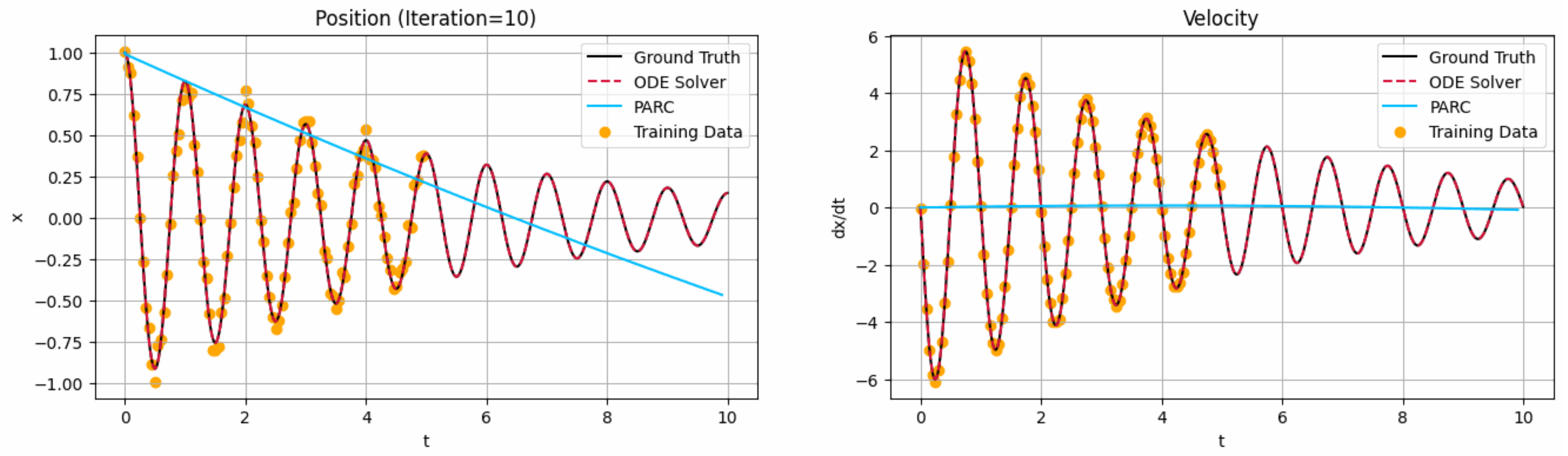


Learning on the Banach Space
Vs. Learning on the Operator Manifold

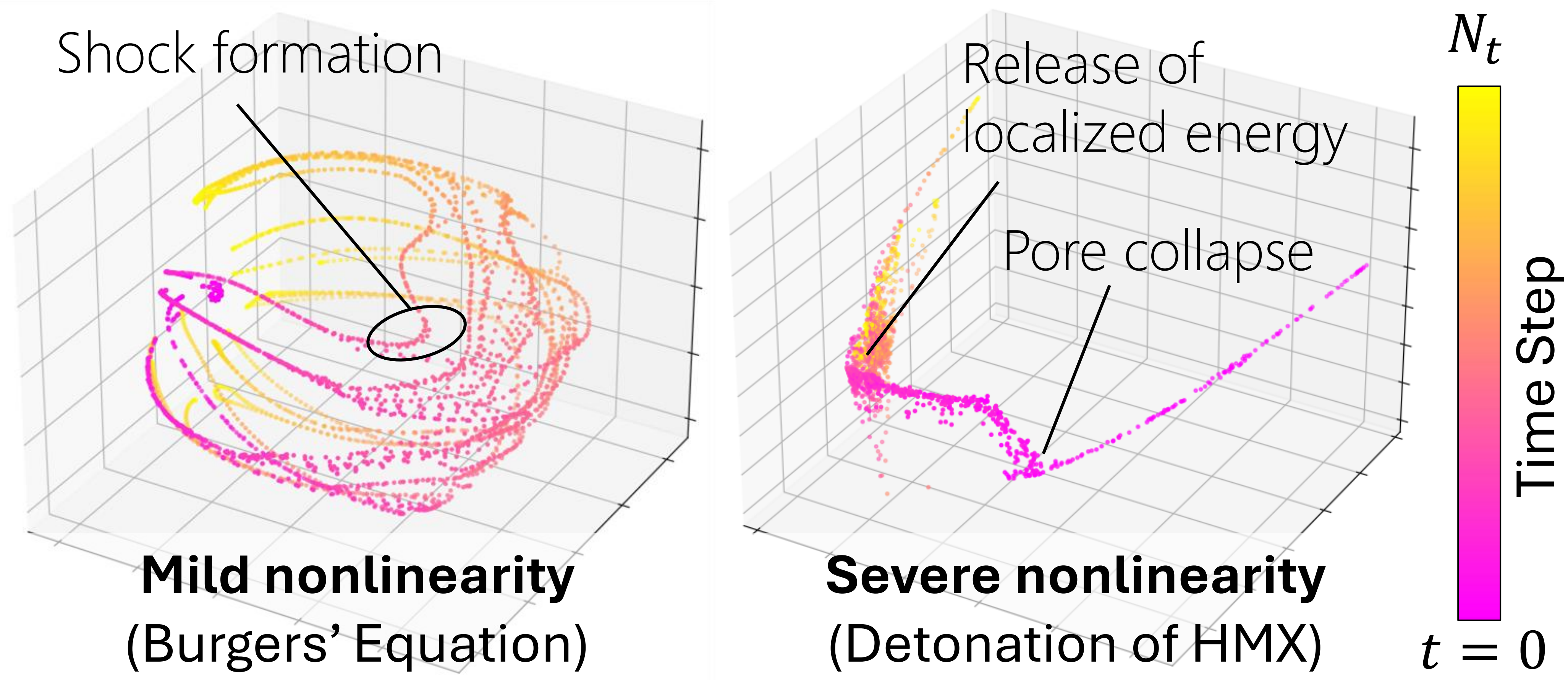
Physics-Informed Neural Network
(3 hidden layers – 256, 256, 256)



Physics-Aware Recurrent Conv.
(2 hidden layers – 16, 32)



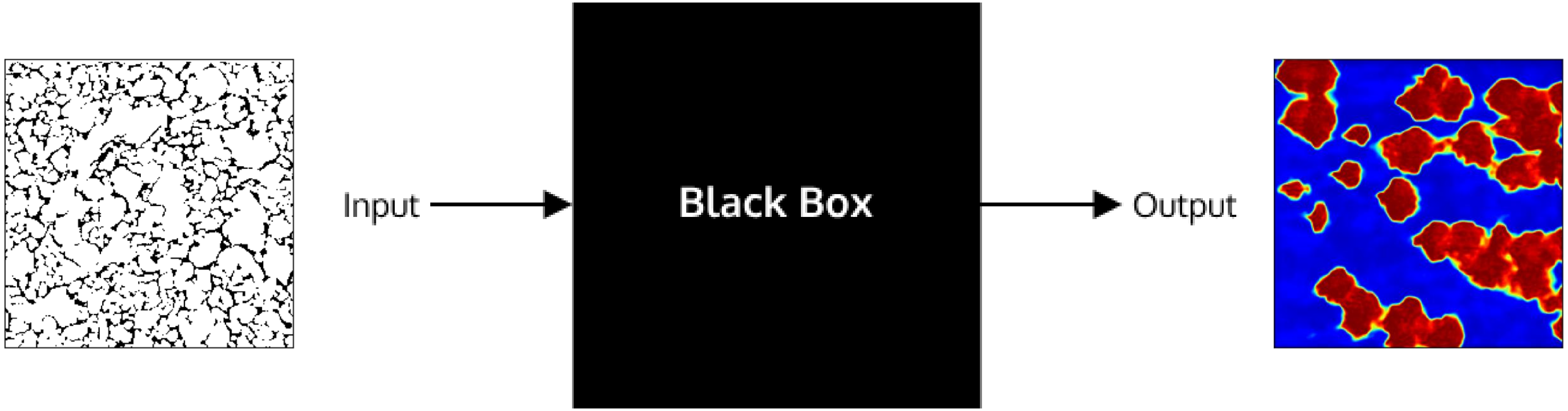
Geometry of Extreme Dynamics



Mild nonlinearity
(Burgers' Equation)

Severe nonlinearity
(Detonation of HMX)

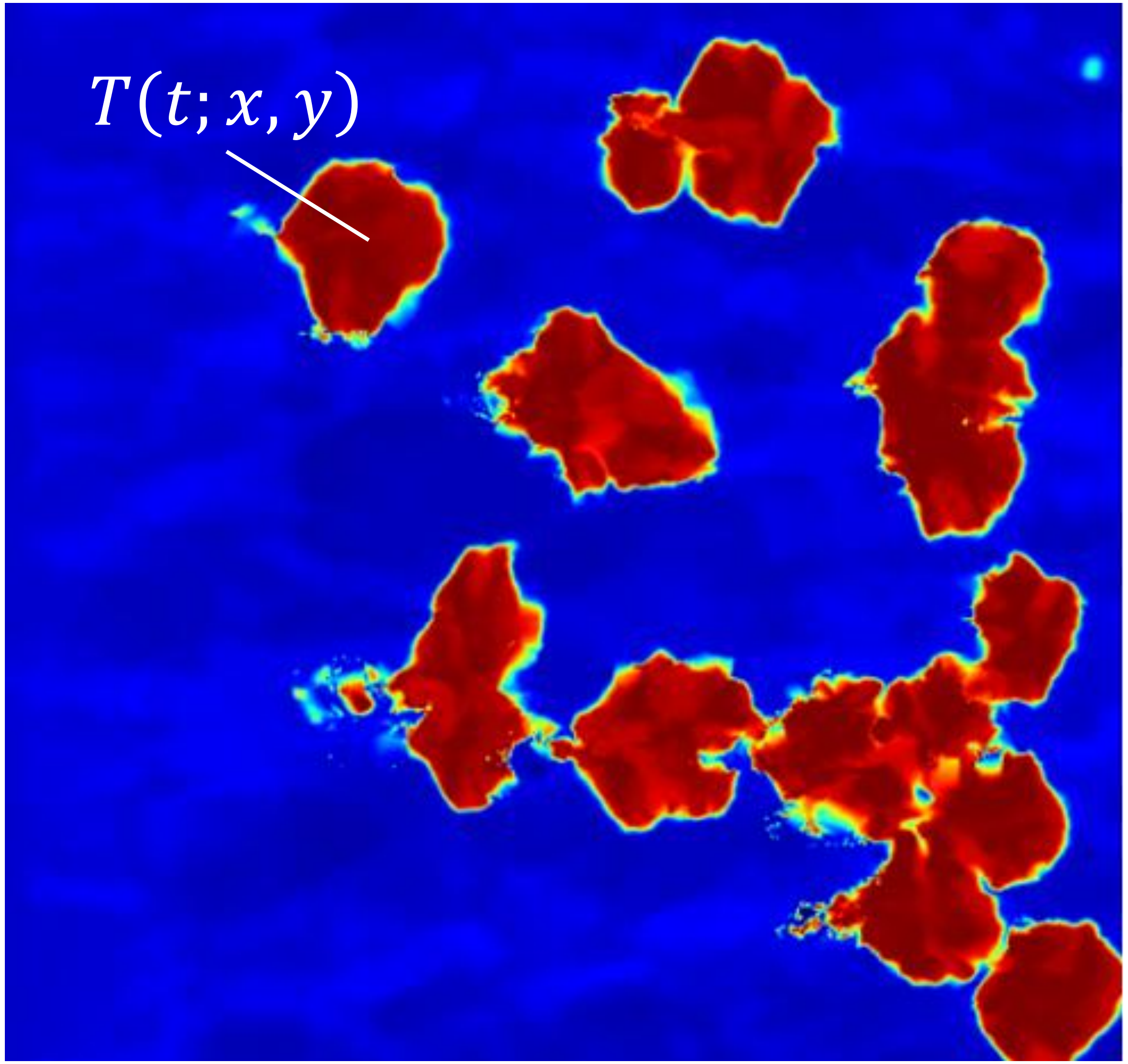
What does PARC see in microstructure images?

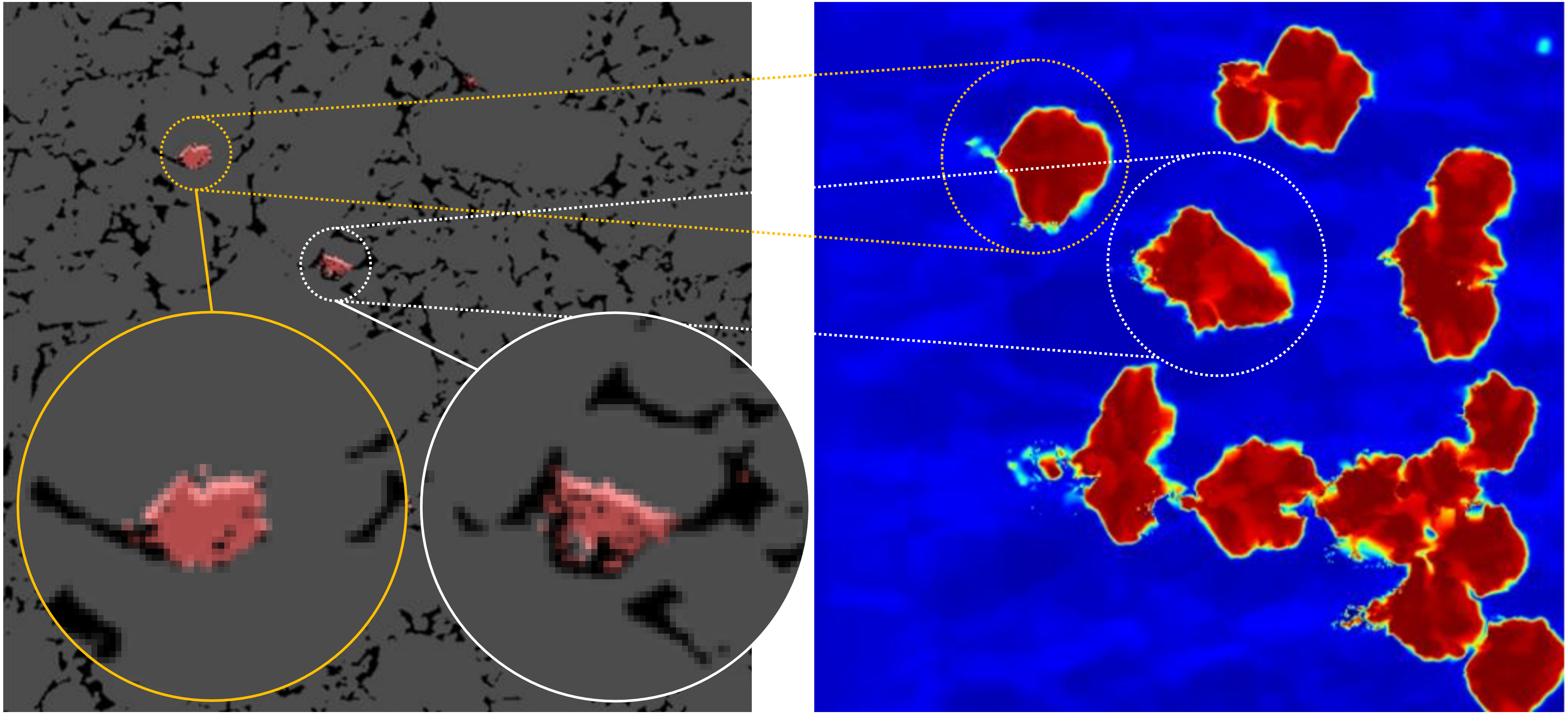


Saliency Map

Which element in the microstructure had the biggest influence on the hotspot formation?

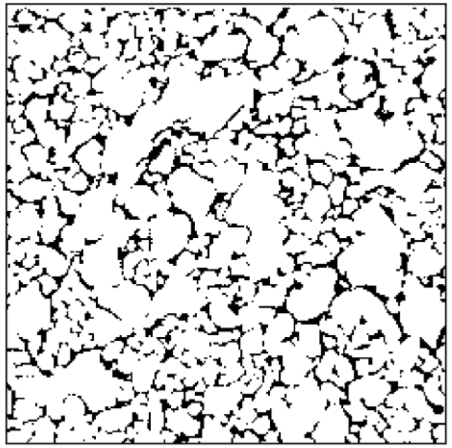
$$\frac{\partial T}{\partial \mu(x, y)}$$



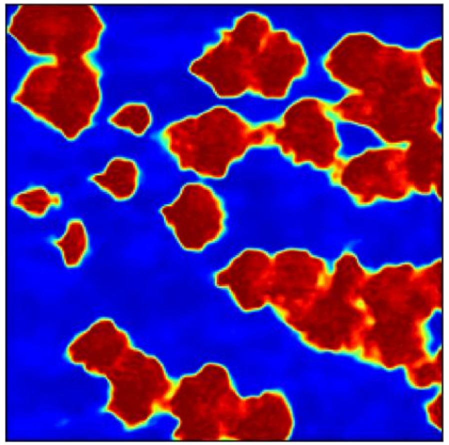


Saliency Map

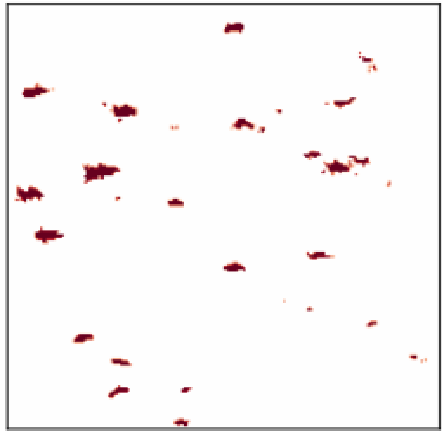
Microstructure $\mu(x, y)$



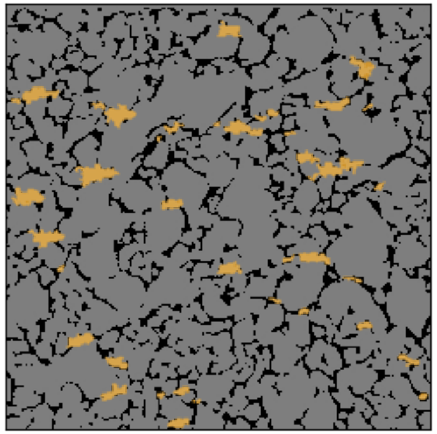
Temperature field $\boldsymbol{T}(\boldsymbol{x}, \boldsymbol{y})$

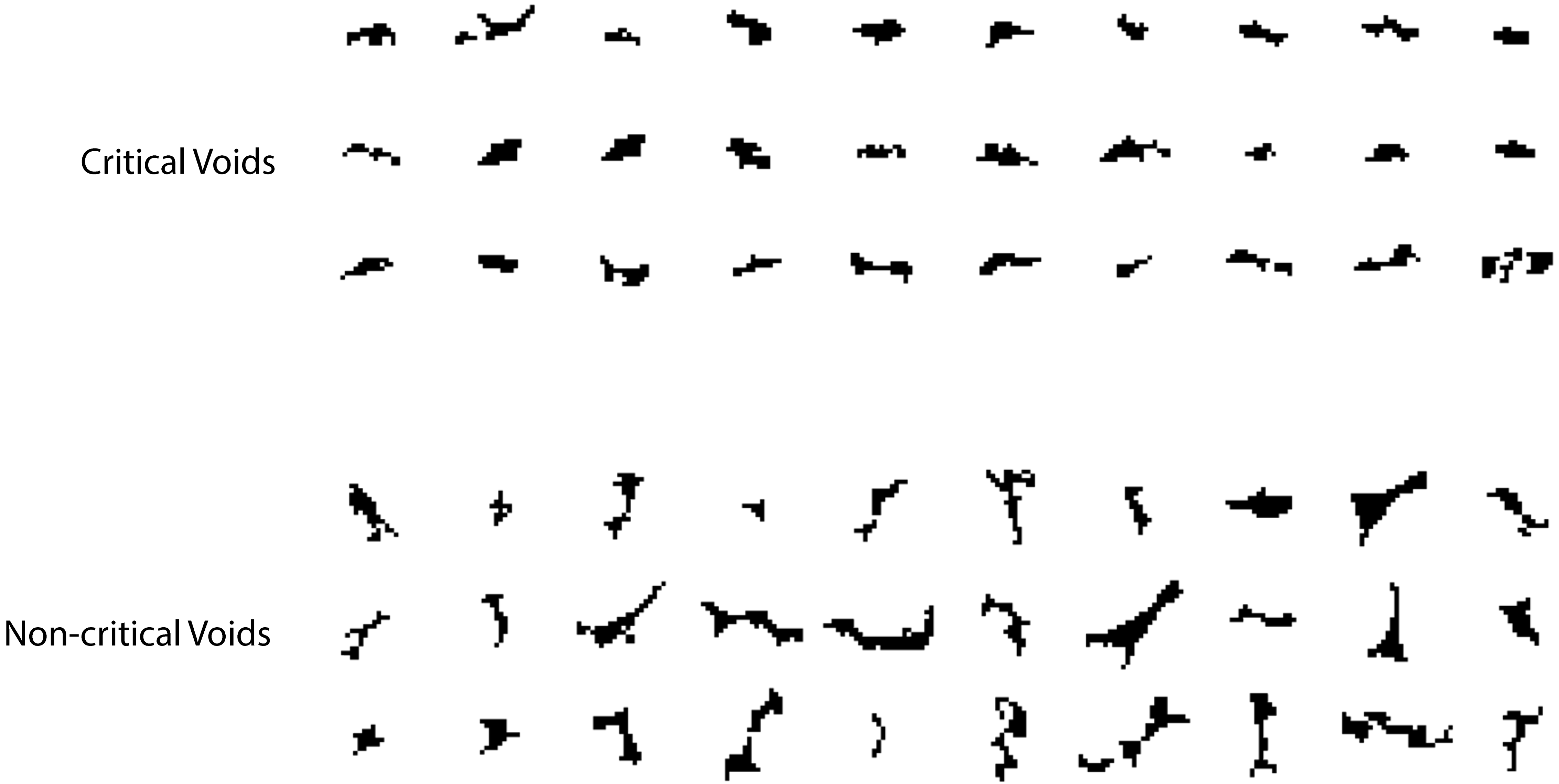


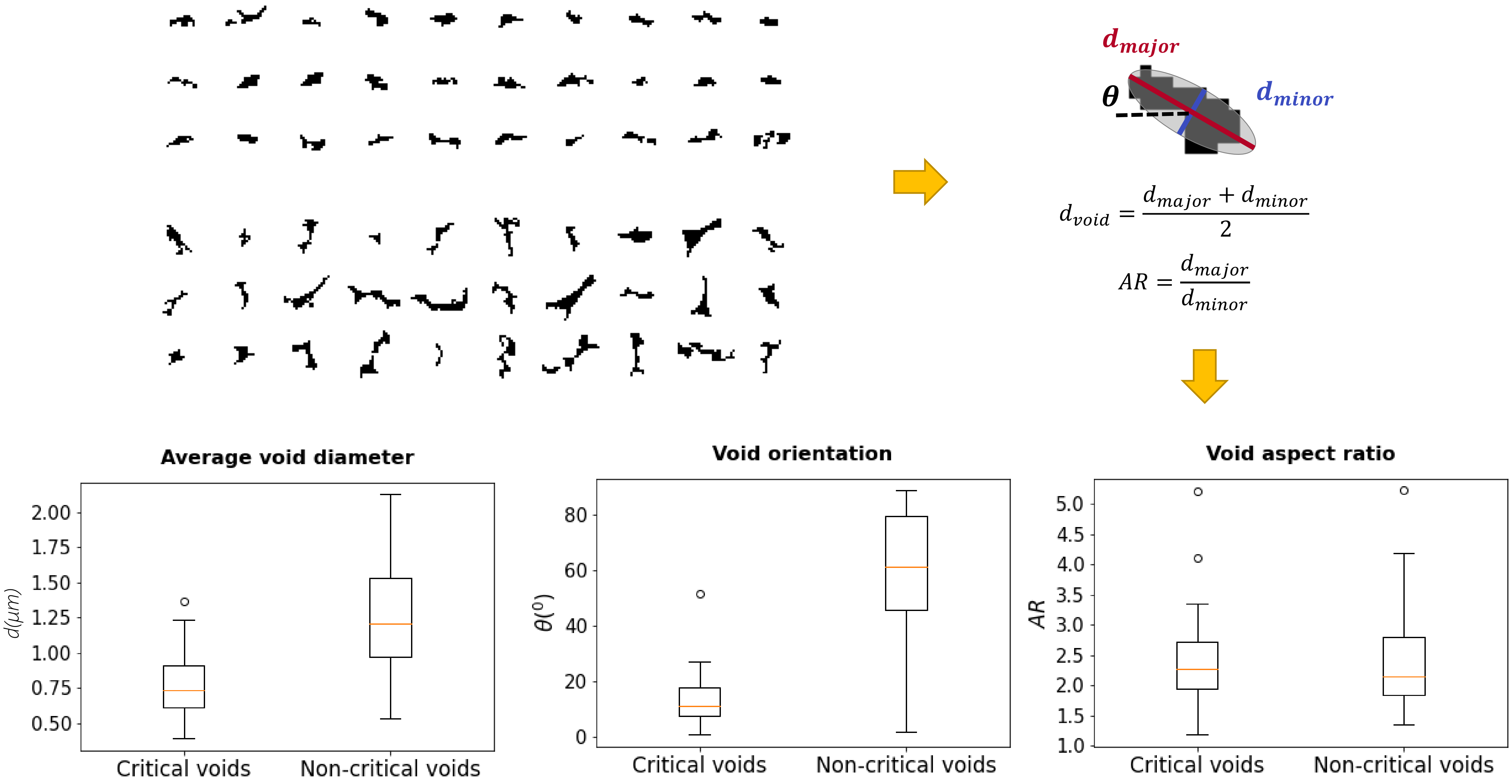
Saliency map $G(x, y)$



Saliency map superimposed on microstructure



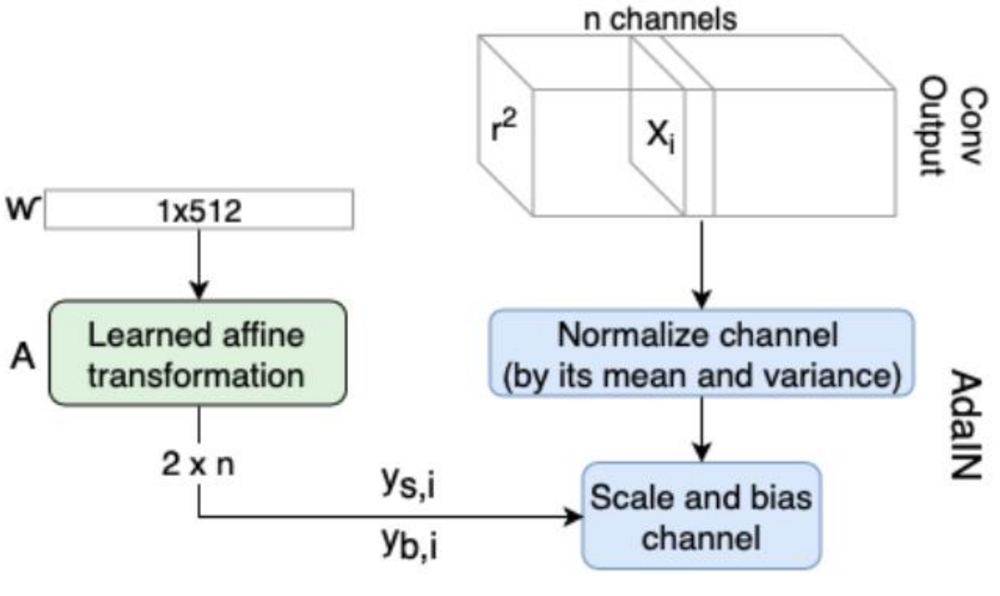

Critical Voids
Non-critical Voids



d_{major}
θ
d_{minor}
$d_{void} = \frac{d_{major} + d_{minor}}{2}$
$AR = \frac{d_{major}}{d_{minor}}$
Average void diameter
$d(\mu m)$
2.00
1.75
1.50
1.25
1.00
0.75
0.50
Critical voids
Non-critical voids
Void orientation
$\theta(^{o})$
80
60
40
20
0
Critical voids
Non-critical voids
Void aspect ratio
AR
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
Critical voids
Non-critical voids

PARCel – Extending PARC to other operating conditions

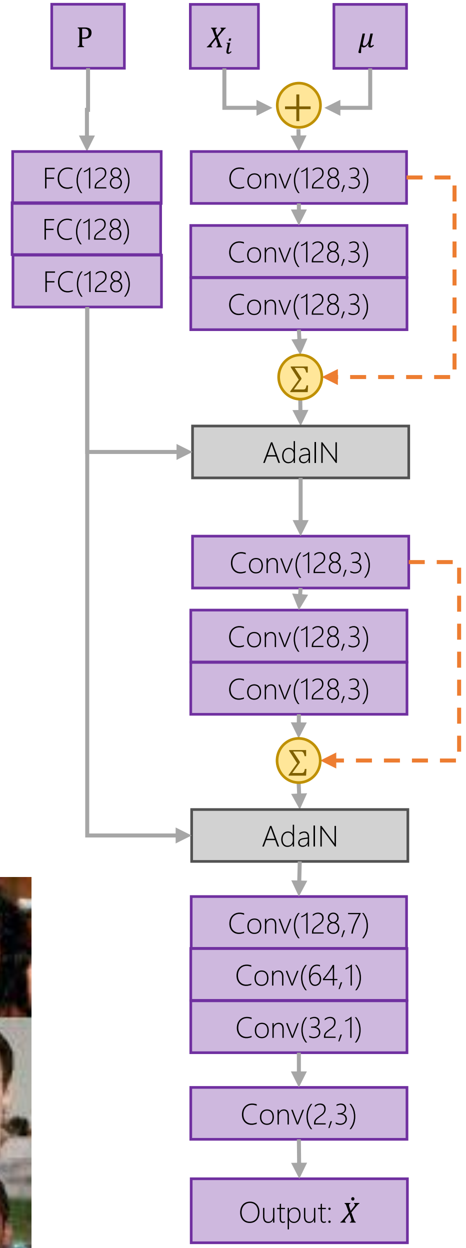
- "Style-vector" in StyleGAN



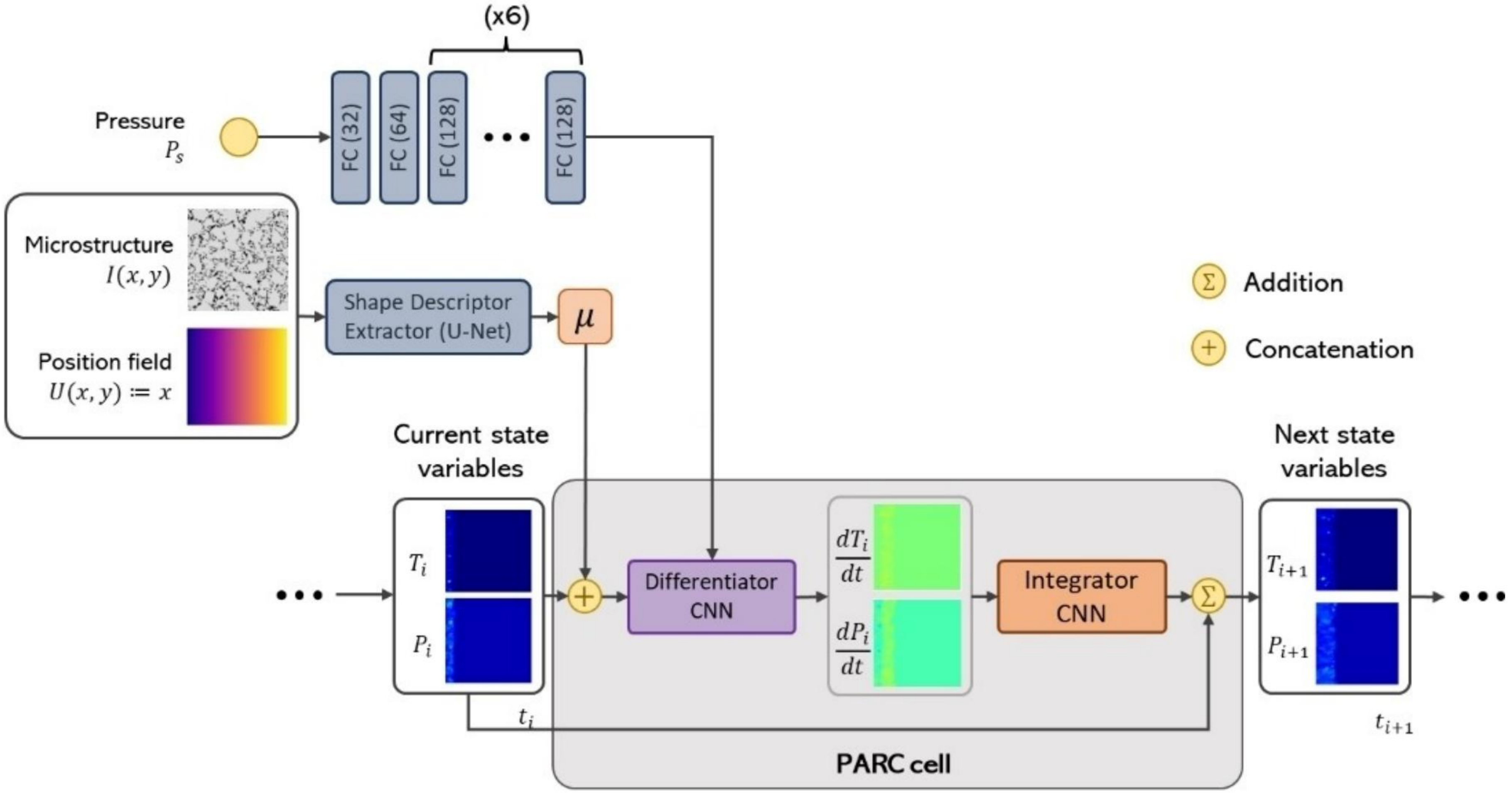
$$\mathrm{AdaIN}(\mathbf{x}_i, \mathbf{y}) = \mathbf{y}_{s,i}\frac{\mathbf{x}_i - \mu(\mathbf{x}_i)}{\sigma(\mathbf{x}_i)} + \mathbf{y}_{b,i},$$

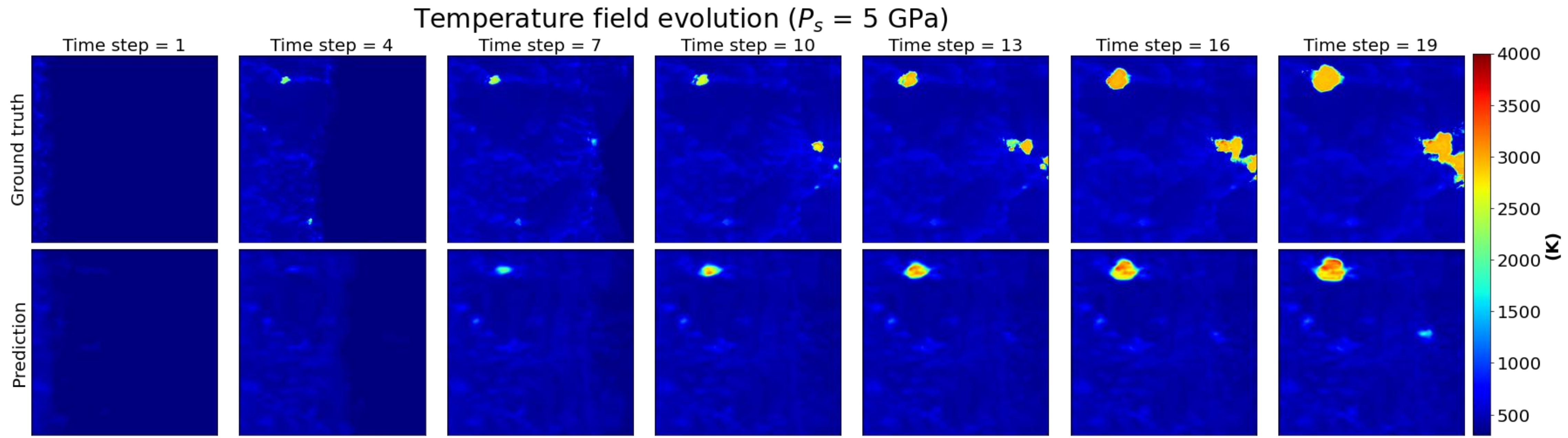
Karras, Laine, & Aila. "A Style-Based Generator Architecture for Generative Adversarial Networks," CVPR 2019

Introducing "Bias" to represent the effects of different shock loadings.

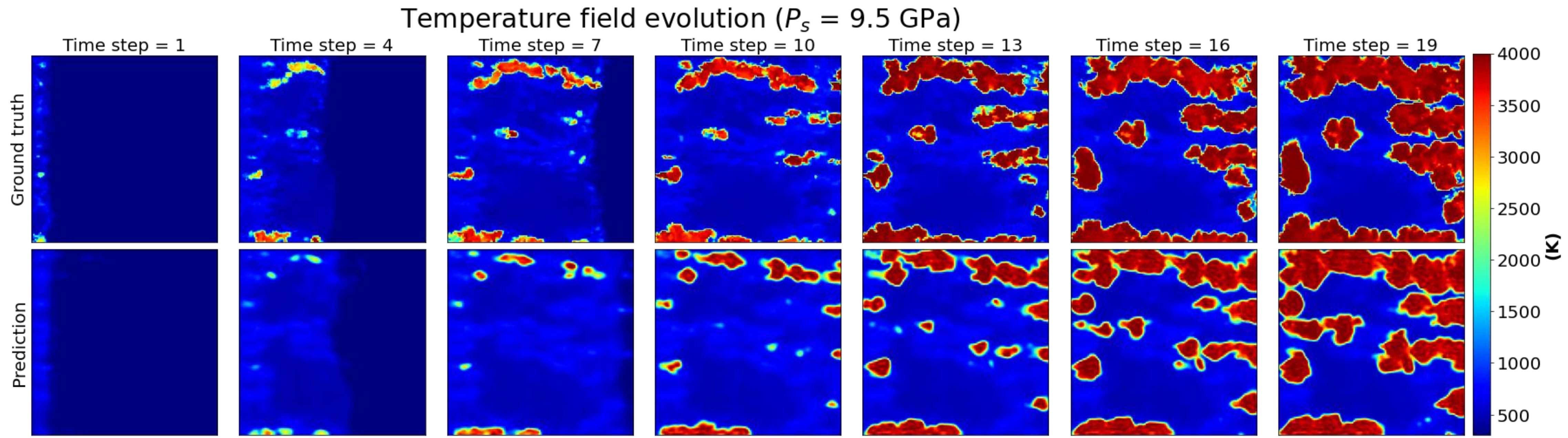


PARCel – Extending PARC to other operating conditions

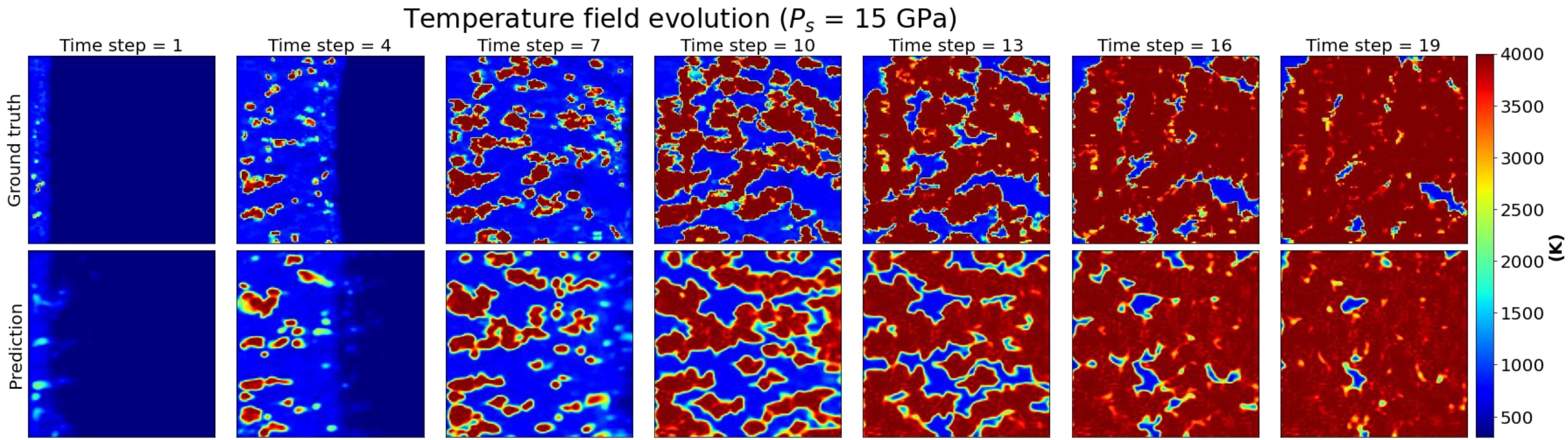




Nguyen et al. (2023). https://doi.org/10.1002/prep.202200268

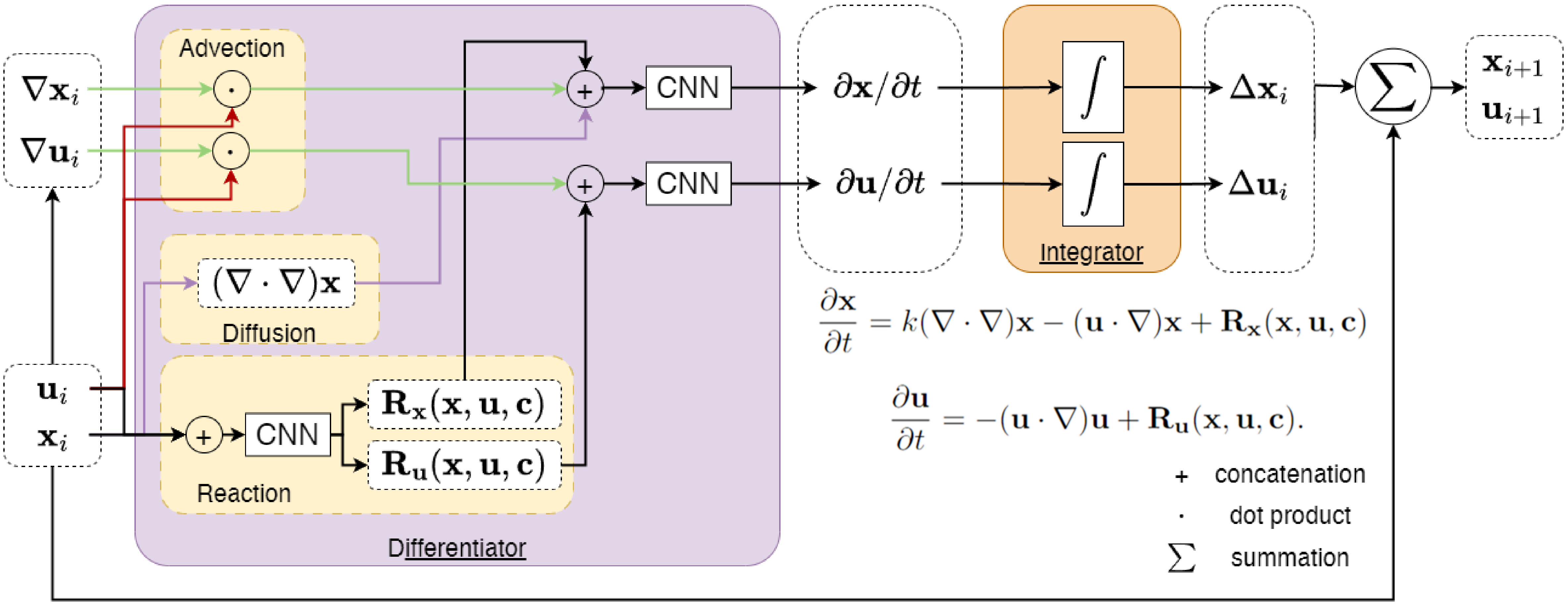


Nguyen et al. (2023). https://doi.org/10.1002/prep.202200268



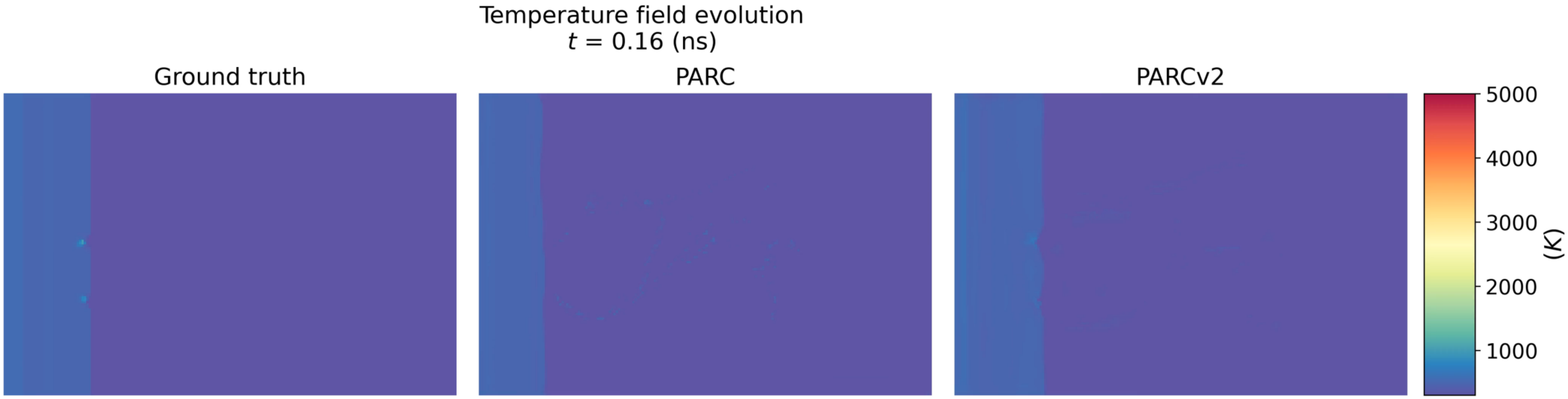
Nguyen et al. (2023). https://doi.org/10.1002/prep.202200268

Physics-Aware Recurrent CNNs (PARCv2)



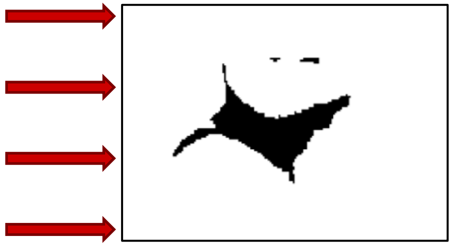
Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

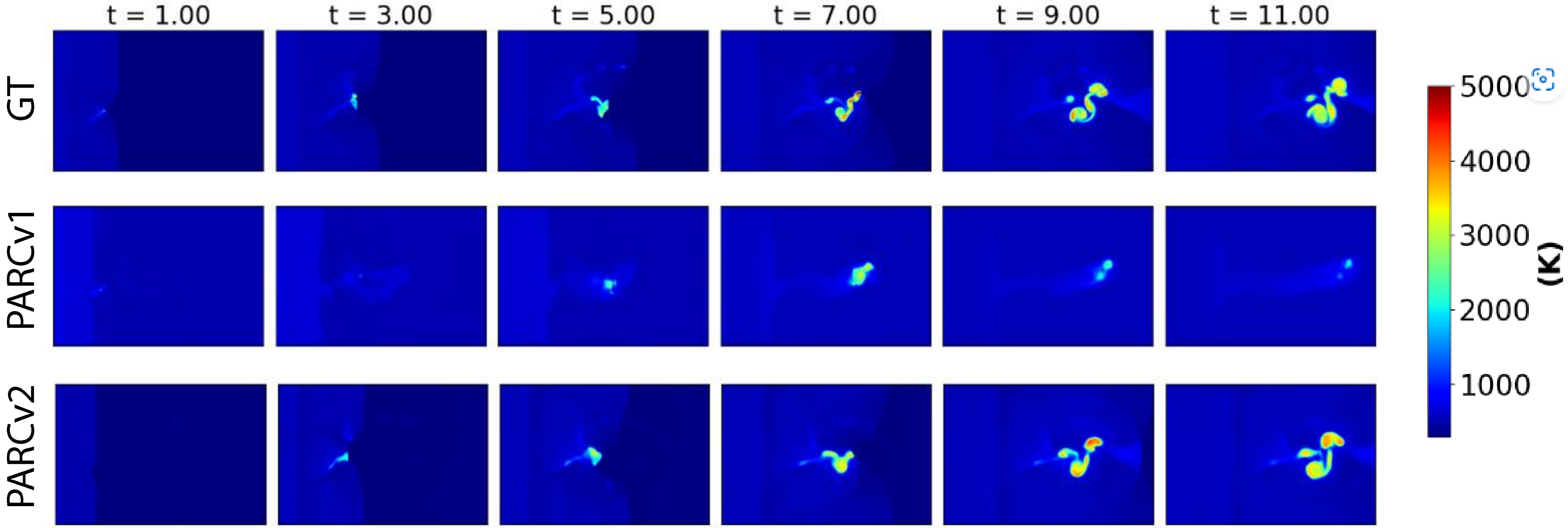
Pore Collapse Simulation



Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

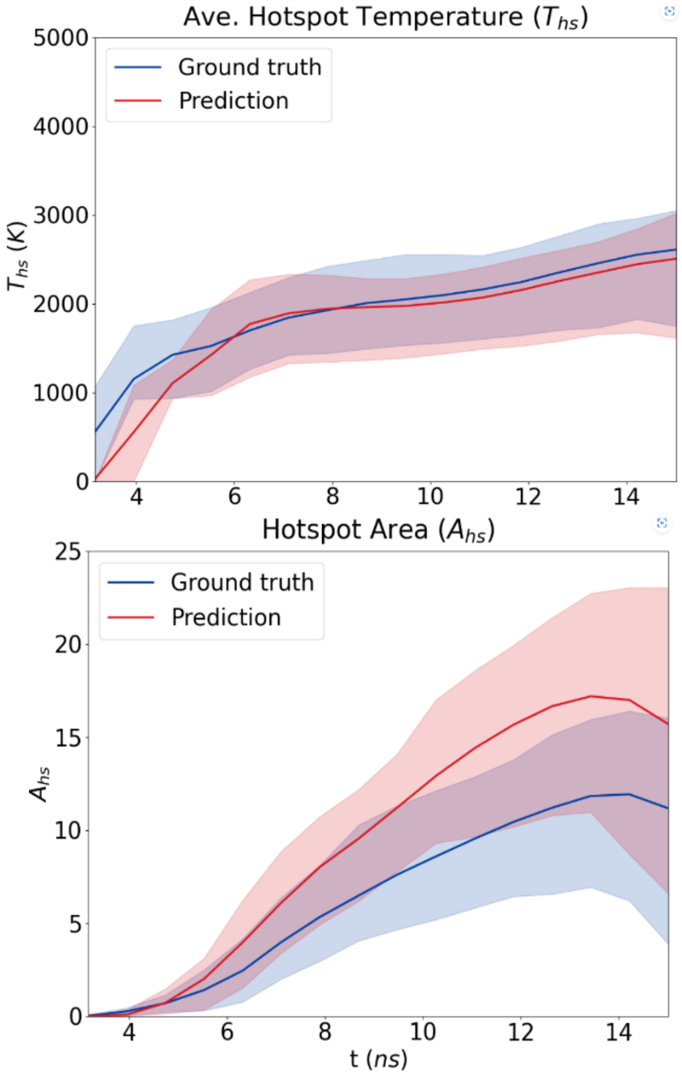
Pore Collapse Simulation

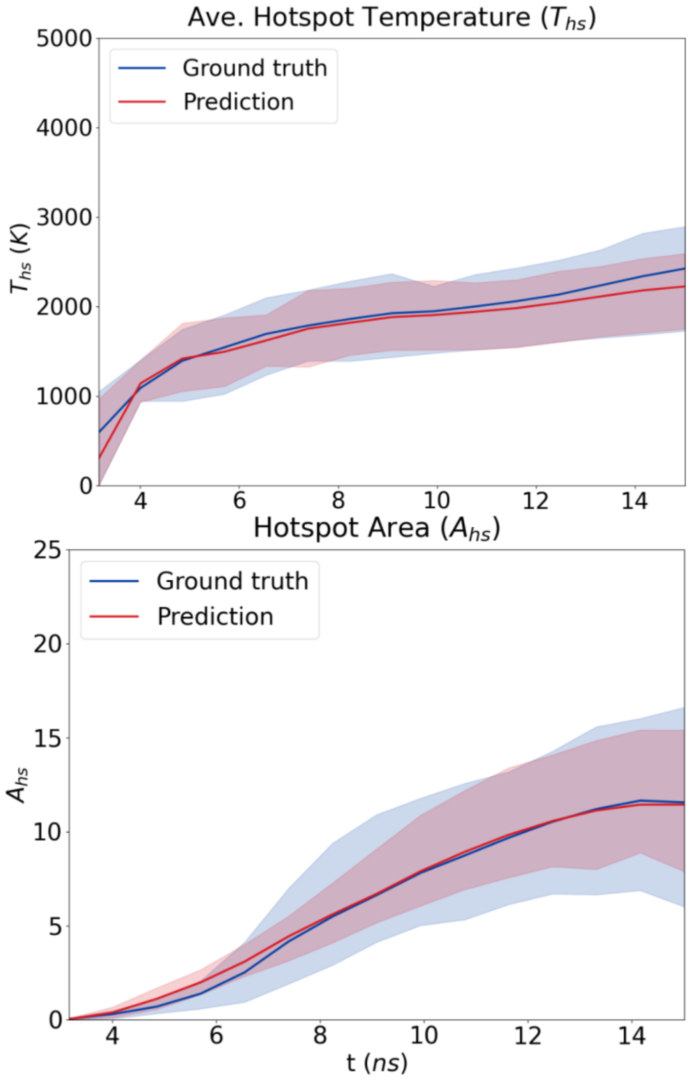




Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

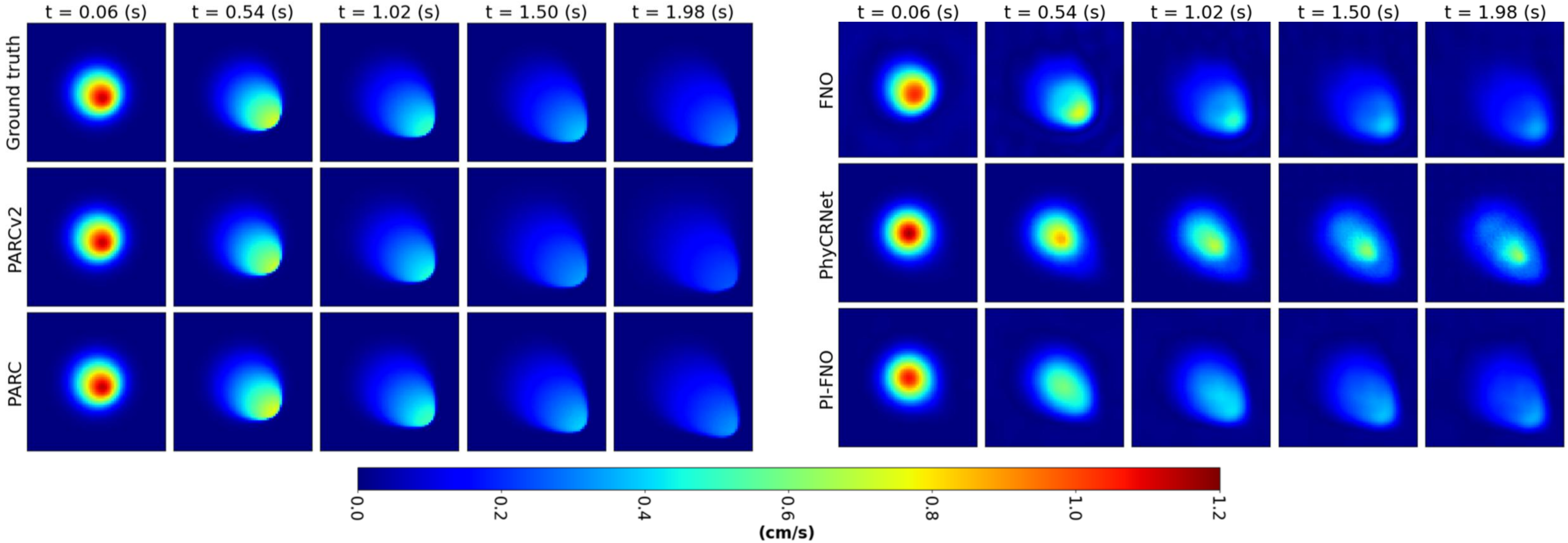
PARCv1 vs. PARCv2





Burgers' Equation

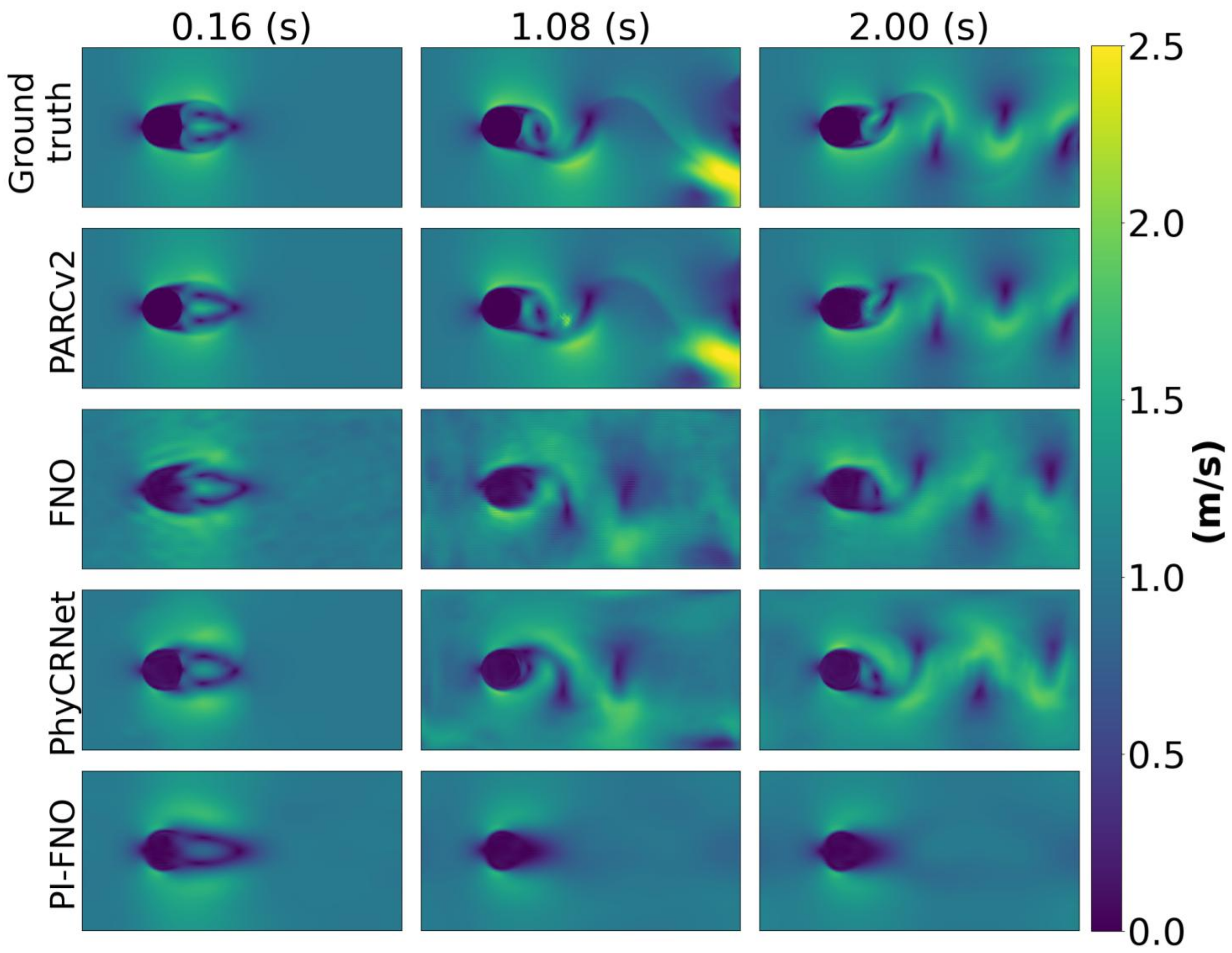
Model	$RMSE_u$ (cm/s)	$\|\|\mathbf{f_u}\|\|$ (cm/s^2)
DNS		0.1241
PARC (numerical int.)	0.0074	0.1262
PARC (data-driven int.)	0.0236	0.1176
FNO	0.0289	0.1537
PhyCRNet	0.0588	0.0560
PIFNO	0.0338	0.1058
PARCv2 (This Study)	0.0129	0.1292



Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

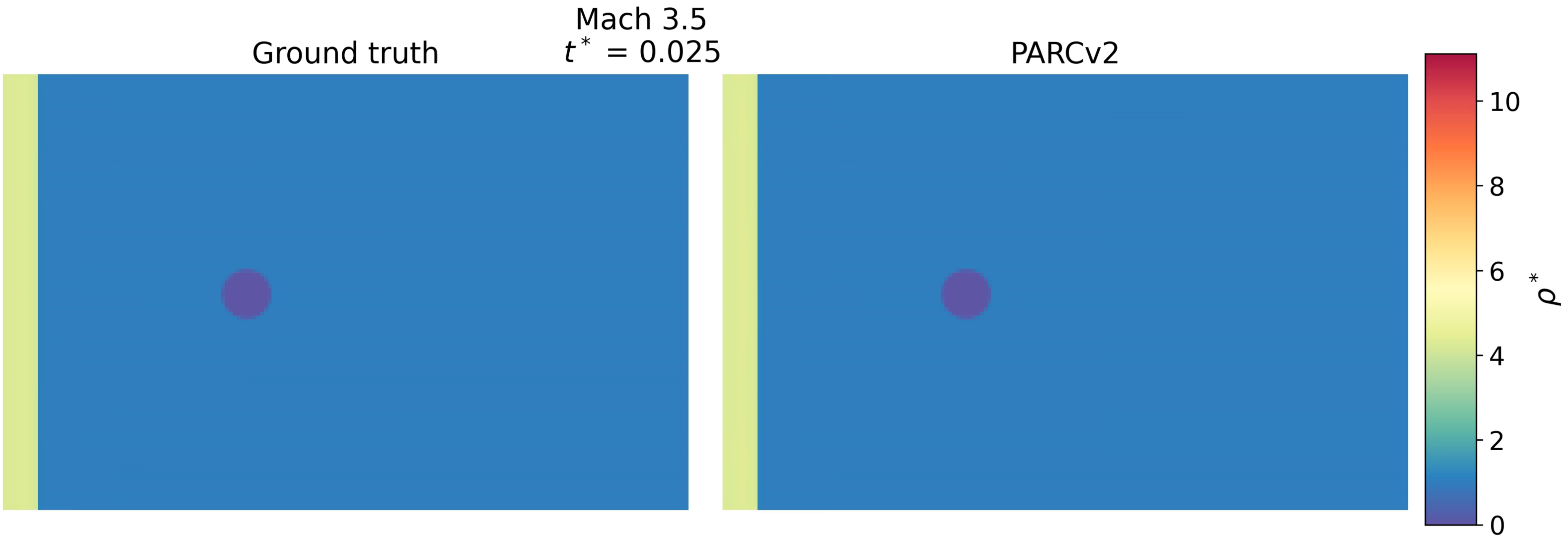
Navier-Stokes Equations

Model	RMSE (cm/s^2)	$\|\|f_{\mathbf{u}}\|\|$ (m/s^2)	ε_{div} $(1/s)$
DNS (Ground truth)	-	2.2339	0.0198
FNO	0.2411	3.2804	1.0471
PhyCRNet	0.2324	2.6994	0.0597
PI-FNO	0.2230	1.4488	0.0307
PARCv2	0.1556	3.0402	0.3655



Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

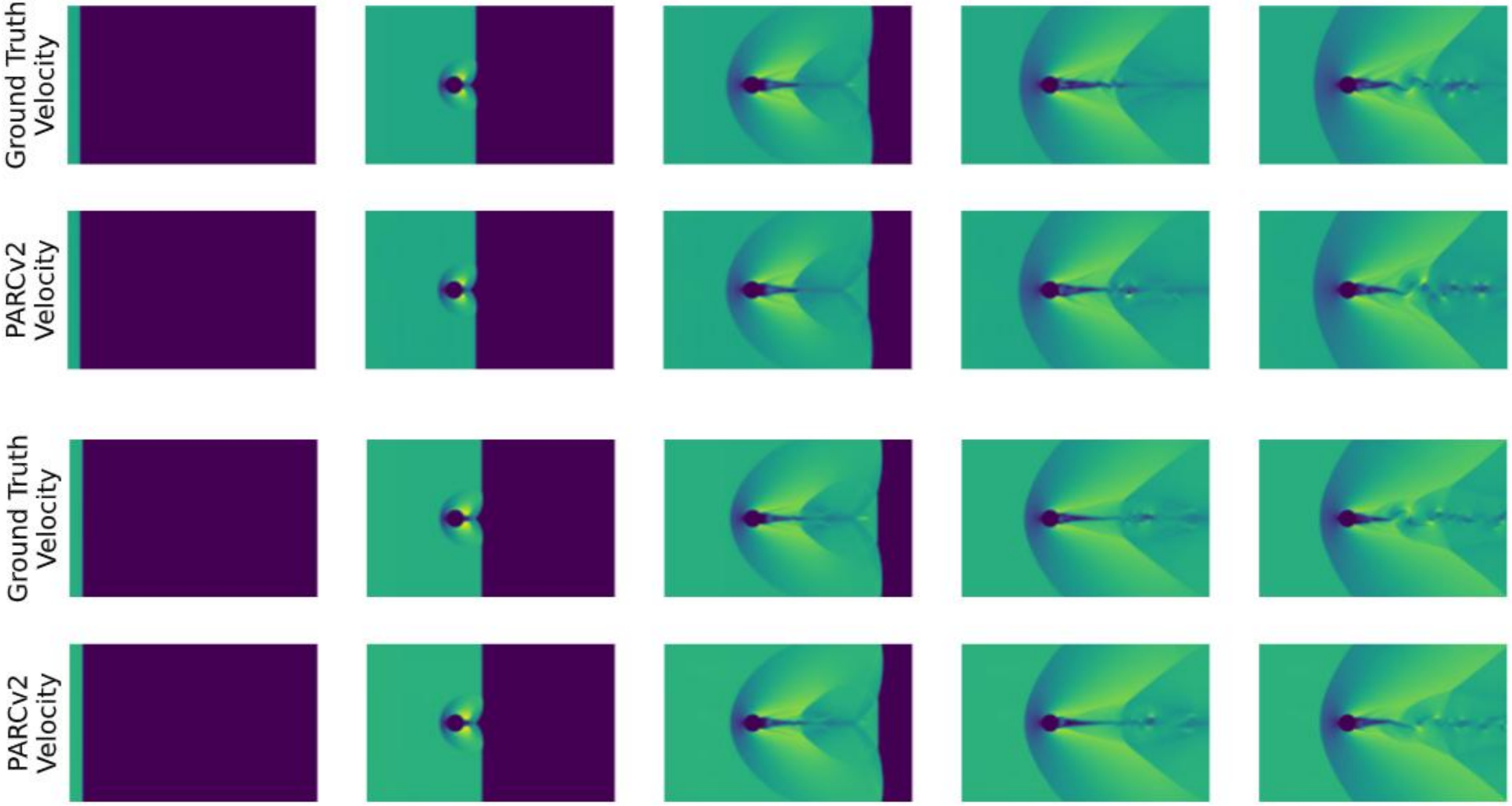
Compressible, Supersonic Flow



Compressible, Supersonic Flow

Mach 3

Mach 4



Summary

- PARC features its "differentiator-integrator architecture" mimicking how PDEs are solved in physics-based solvers
- Comparable accuracy & fidelity to DNS, but multiple orders of magnitude faster (hours on an HPC versus less than a second on a laptop)
- Tends to capture sharp gradients & fast transients better, compared to other physics-informed models.