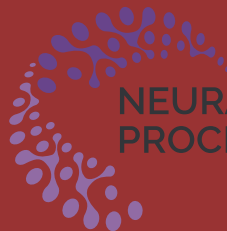


# Physics-Constrained Flow Matching:

Sampling Generative Models with Hard Constraints



LEARNING MATTER



NEURAL INFORMATION  
PROCESSING SYSTEMS

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# Problem Setup

$$\begin{aligned}\partial_t u(x, t) + \nabla \cdot \mathcal{F}_\phi(u(x, t)) &= 0, \\ u(x, 0) &= \alpha_0(x), \\ \mathcal{B}u(x, t) &= 0,\end{aligned}$$

$$\begin{aligned}\forall x \in \Omega, t \in [0, T], \\ \forall x \in \Omega, \\ \forall x \in \partial\Omega, t \in [0, T],\end{aligned}$$

**Pre-trained PDE  
Generative Model**

$$\mathcal{H}u(x, t) = 0$$

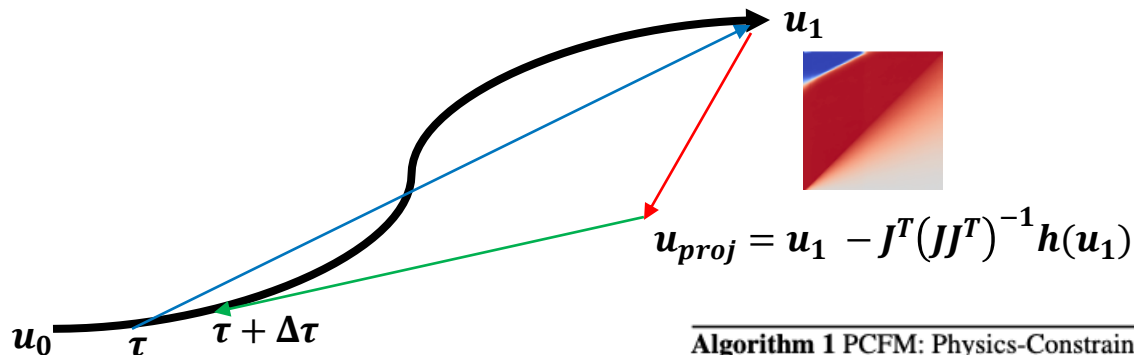
**Constraint information  
at Inference**

**Goal: Generate hard constrained PDE solutions  
by inference-only guidance**

# Landscape of Constrained Guidance

Software	Zero-shot	Continuous Guidance	Hard Constraint	Complex Constraints
Conditional FFM	✗	✓	✓	✗
DiffusionPDE	✓	✗	✗	✓
D-Flow	✓	✓	✗	✓
ECI	✓	✓	✓	✗
PCFM (Ours)	✓	✓	✓	✓

# PCFM: Physics-Constrained Flow Matching



Zero-shot constraint enforcement!

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## Algorithm 1 PCFM: Physics-Constrained Flow Matching

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**Require:** Flow model  $v_\theta(u, \tau)$ , constraint residual  $h(u)$ , initial state  $u_0$ , steps  $N$ , penalty  $\lambda$

**Ensure:** Final state  $u_1$  such that  $h(u_1) = 0$

- 1:  $\Delta\tau \leftarrow 1/N, \quad u \leftarrow u_0$
  - 2: **for**  $k = 0, \dots, N - 1$  **do**
  - 3:    $\tau \leftarrow k \cdot \Delta\tau, \quad \tau' \leftarrow \tau + \Delta\tau$
  - 4:    $u_1 \leftarrow \text{ODESolve}(u, v_\theta, \tau, 1, \theta)$
  - 5:    $J \leftarrow \nabla h(u_1)^\top$
  - 6:    $u_{proj} \leftarrow u_1 - J^\top (JJ^\top)^{-1} h(u_1)$
  - 7:    $\hat{u}_{\tau'} \leftarrow \text{ODESolve}(u_{proj}, -(u_{proj} - u_0), 1, \tau')$
  - 8:    $u_{\tau'} \leftarrow \arg \min_u \|u - \hat{u}_{\tau'}\|^2 + \lambda \|h(u + (1 - \tau')v_\theta(u_{\tau'}, \tau'))\|^2$
  - 9: **if**  $\|h(u)\| > \epsilon$  **then**
  - 10:    $u \leftarrow \arg \min_u \|u - u_1\|^2 \quad \text{s.t.} \quad h(u) = 0$
  - 11: **return**  $u$
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# What Constraints?

Table 2: Summary of constraint types commonly encountered in PDE-based physical systems, categorized by their mathematical form and scope.

Constraint Type	Representative Form	Linearity
Dirichlet IC / BC	$\mathcal{H}u = Au - b = 0$	Linear
Global mass conservation (periodic BCs)	$\mathcal{H}u = \int_{\Omega} u(x, t) dx - C = 0$	Linear
Nonlinear conservation law	$\mathcal{H}u = \frac{d}{dt} \int_{\Omega} \rho(u(x, t)) dx = 0$	Nonlinear
Neumann or flux boundary condition	$\mathcal{H}u = \partial_n u(x, t) - g(x, t) = 0$	Potentially nonlinear
Coupled or implicit constraints	Nonlinear spatial/temporal relationships	Nonlinear

# PCFM: Physics-Constrained Flow Matching

“Easy” to  
learn PDEs  
(Linear constraints)

“Harder” to  
learn PDEs  
(Nonlinear constraints)

Dataset	Metric	PCFM	ECI	DiffusionPDE	D-Flow	FFM
Heat Equation	MMSE / $10^{-2}$	<b>0.241</b>	0.697	4.49	1.97	4.56
	SMSE / $10^{-2}$	<b>0.937</b>	0.973	3.93	1.14	3.51
	CE (IC) / $10^{-2}$	<b>0</b>	<b>0</b>	599	102	579
	CE (CL) / $10^{-2}$	<b>0</b>	<b>0</b>	2.06	64.8	2.11
	FPD	<b>1.22</b>	1.34	1.70	2.70	1.77
Navier-Stokes	MMSE / $10^{-2}$	<b>4.59</b>	5.23	17.4	–	16.5
	SMSE / $10^{-2}$	<b>4.17</b>	7.28	9.48	–	7.90
	CE (IC) / $10^{-2}$	<b>0</b>	<b>0</b>	288	–	328
	CE (CL) / $10^{-2}$	<b>0</b>	<b>0</b>	21.4	–	18.6
	FPD	<b>1.00</b>	1.04	3.70	–	2.81
Reaction-Diffusion IC	MMSE / $10^{-2}$	<b>0.026</b>	0.324	3.16	0.318	2.92
	SMSE / $10^{-2}$	0.583	<b>0.060</b>	2.54	6.86	2.54
	CE (IC) / $10^{-2}$	<b>0</b>	<b>0</b>	451	215	445
	CE (CL) / $10^{-2}$	<b>0</b>	6.00	3.82	29.7	3.87
	FPD <sup>†</sup>	<b>15.7</b>	136	44.1	28.3	24.9
Burgers BC	MMSE / $10^{-2}$	0.335	0.359	5.42	<b>0.224</b>	4.86
	SMSE / $10^{-2}$	0.123	<b>0.089</b>	1.30	0.948	1.38
	CE (BC) / $10^{-2}$	<b>0</b>	20.3	426	95.7	409
	CE (CL) / $10^{-2}$	<b>0</b>	15.7	6.20	15.0	6.91
	FPD	<b>0.292</b>	0.307	25.9	1.44	24.7
Burgers IC	MMSE / $10^{-2}$	<b>0.052</b>	10.0	14.3	9.97	13.7
	SMSE / $10^{-2}$	<b>0.272</b>	6.65	8.06	7.91	7.90
	CE (IC) / $10^{-2}$	<b>0</b>	<b>0</b>	471	397	462
	CE (CL) / $10^{-2}$	<b>0</b>	205	6.22	8.66	6.91
	FPD	<b>0.101</b>	1.31	35.8	22.1	33.5

<sup>†</sup> Pretrained Poseidon requires spatially square inputs; we bilinearly interpolated solution grids to  $128 \times 128$ , which may introduce artifacts in FPD evaluation. D-Flow results are omitted due to numerical instabilities.

# Captures shocks in Hyperbolic PDEs

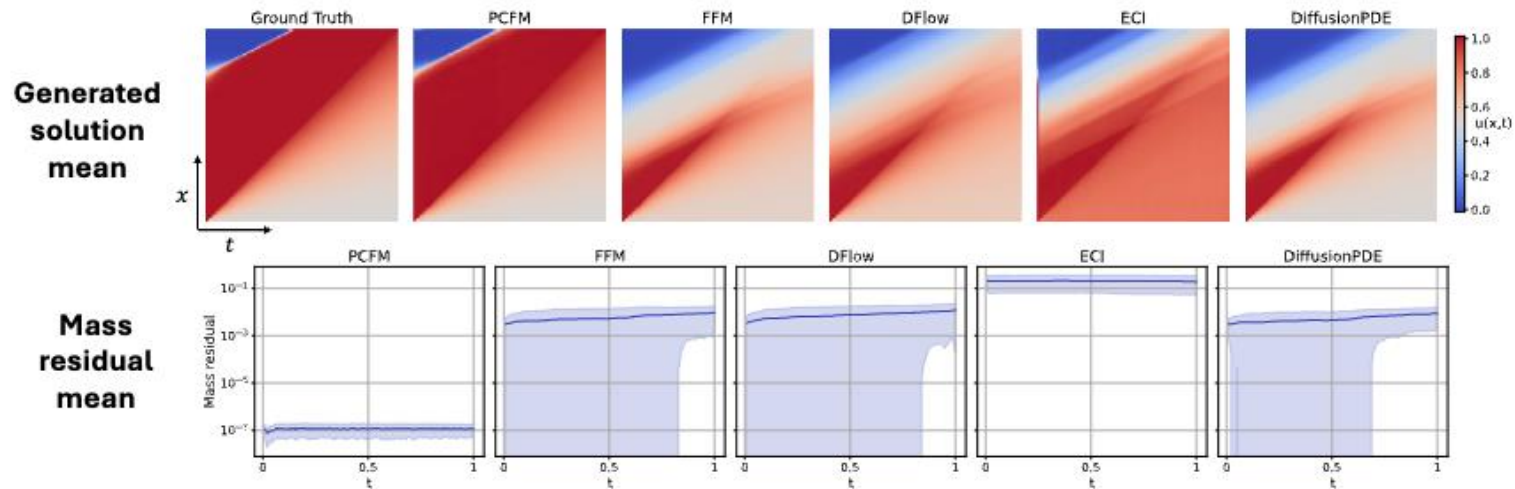
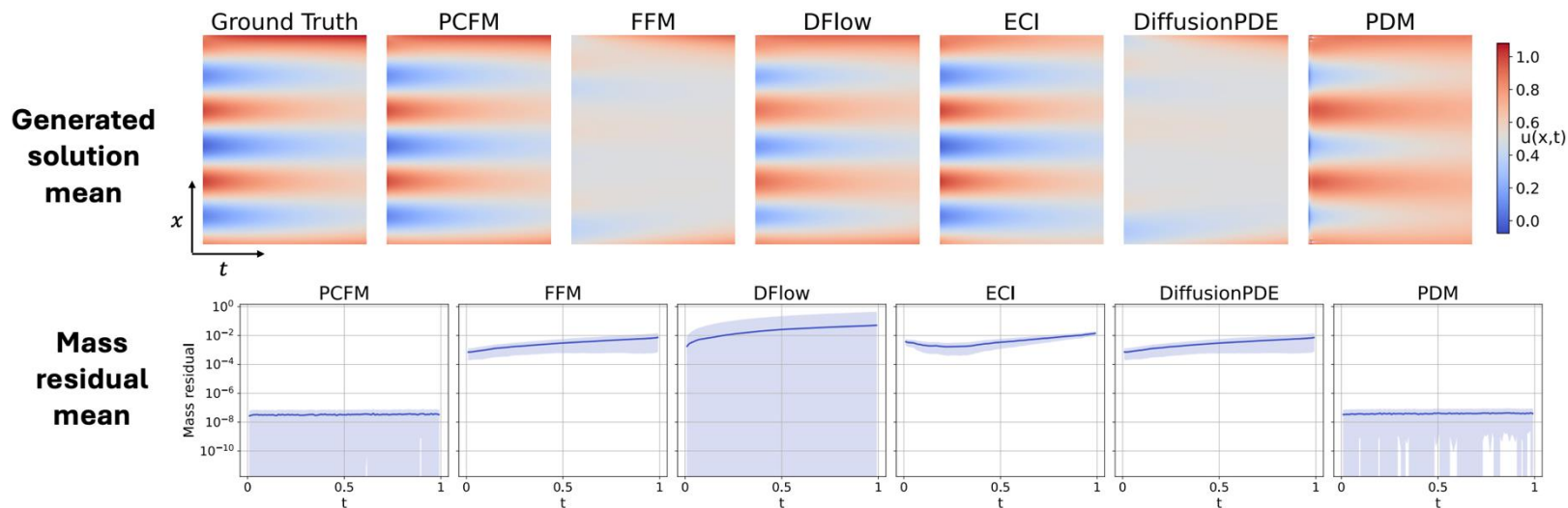


Figure 3: Comparison of mean generated solutions and mass conservation errors for the Burger's problem with IC fixed. By enforcing nonlinear conservation constraints via PCFM, our method captures the Burgers' shock phenomenon, ensures global mass conservation in the generated solution, while improving solution quality. Shaded bands show  $\pm 1$  std. of mass residuals across samples.

# Comparison with other methods



**PCFM improves reaction-diffusion solutions by exactly enforcing mass conservation, ensuring superior quality and zero residuals.**



# More Constraints = More Performance?

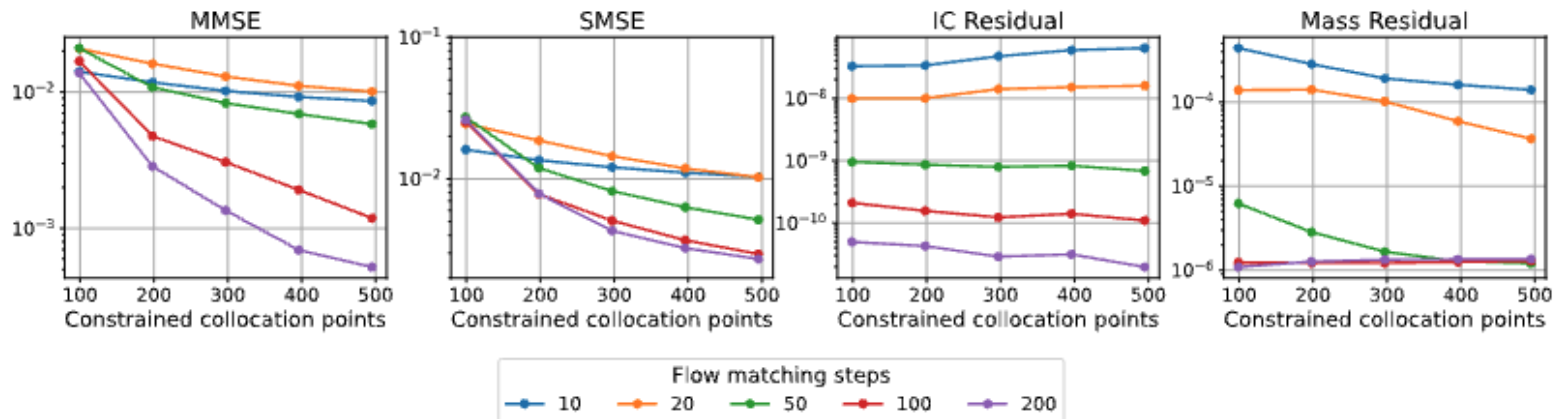


Figure 4: Increasing the number of constraints (constraint collocation points) can improve solution fidelity while maintaining strong satisfaction of other constraints (IC and global mass conservation), demonstrating the ability of PCFM to handle chaining of multiple constraints.

**Akin to what is seen in PINNs where additional constraints may hinder the performance**

# Thank you!

Checkout our paper: <https://arxiv.org/abs/2506.04171>

Python: <https://github.com/cfpengfei/PCFM>

Julia: <https://github.com/utkarsh530/PCFM.jl>