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Optimization-based schemes to solve parabolic PDEs with non-local initial conditions

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INTRODUCTION & AIM

Partial Differential equations (PDEs) with non-local conditions impose *integral constraints* instead of pointwise data — common in heat conduction, thermoelasticity, Ohmic heating, and cell biology (Gierer–Meinhardt model). Non-local operators are fundamentally incompatible with standard automatic differentiation, making classic methods non-trivial to apply.

We present a comparison between two optimization-based numerical methods for PDEs with non-local conditions: a Finite Difference (FD) residual minimization approach and Physics-Informed Neural Networks (PINNs). To ensure a fair evaluation, both methods are tested with equal degrees of freedom and the same optimization algorithms — Adam, AMSGrad, and L-BFGS.

The numerical experiments were carried out in a PDE problem proposed by Sapagovas et al., using nonlocal initial conditions given in articles by Vaquero et al., in a well posed problem.

METHOD

Problem — 1D nonlinear parabolic PDE

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + u^3 = f(x,t) \qquad x \in [0,1], \quad t \in [0,1]$$

Dirichlet boundary conditions (BC)

$$u(0,t) = 0, \qquad u(1,t) = \frac{2}{\pi}\left(1 + \frac{\pi}{8}\right) e^{t/2},$$

Nonlocal initial conditions (IC)

$$u(x,0) = \sum_{j=1}^{m} \alpha_j\, u(x,T_j) + \int_0^T \nu(\tau)\, u(x,\tau)\, d\tau + \varphi(x),$$

Exact solution: $u(x,t) = \frac{2}{\pi}\left(\sin\frac{\pi x}{2} + \frac{\pi x^2}{8}\right) e^{t/2}$

Numerical Methods

FD-based optimization

- Discretize domain on uniform grid; approximate derivatives with 2nd-order central differences
- Approximate integral in non-local IC with the trapezoidal rule
- Create residuals r_{PDE}, r_{BC}, r_{IC}
- Minimize composite loss: $\mathcal{L} = \mathcal{L}_{PDE} + \mathcal{L}_{BC} + \mathcal{L}_{IC}$ using mean squared error (MSE)

PINNs

- Parametrize solution as $u_\theta(x,t)$— fully connected feedforward network with *tanh* activations
- Integral IC via trapezoidal rule at initial collocation points
- Minimize same loss structure: $\mathcal{L} = \mathcal{L}_{PDE} + \mathcal{L}_{BC} + \mathcal{L}_{IC}$ over θ
- Network width chosen so total trainable params ≈ FD grid points

Optimizers

Adam	AMSGrad	L-BFGS
Adaptive learning rates; robust, low cost per iteration; slower convergence	Monotone 2nd-moment accumulation; guaranteed sublinear regret in convex case	Quasi-Newton; R-linear convergence; uses curvature info; memory-efficient

RESULTS

As shown in Figure 1, both methods recover the solution with similar accuracy (~10^{-4}). The FD error (b) concentrates in horizontal bands at intermediate t, while the PINNs error (d) accumulates near $x = 1$, $t = 1$.

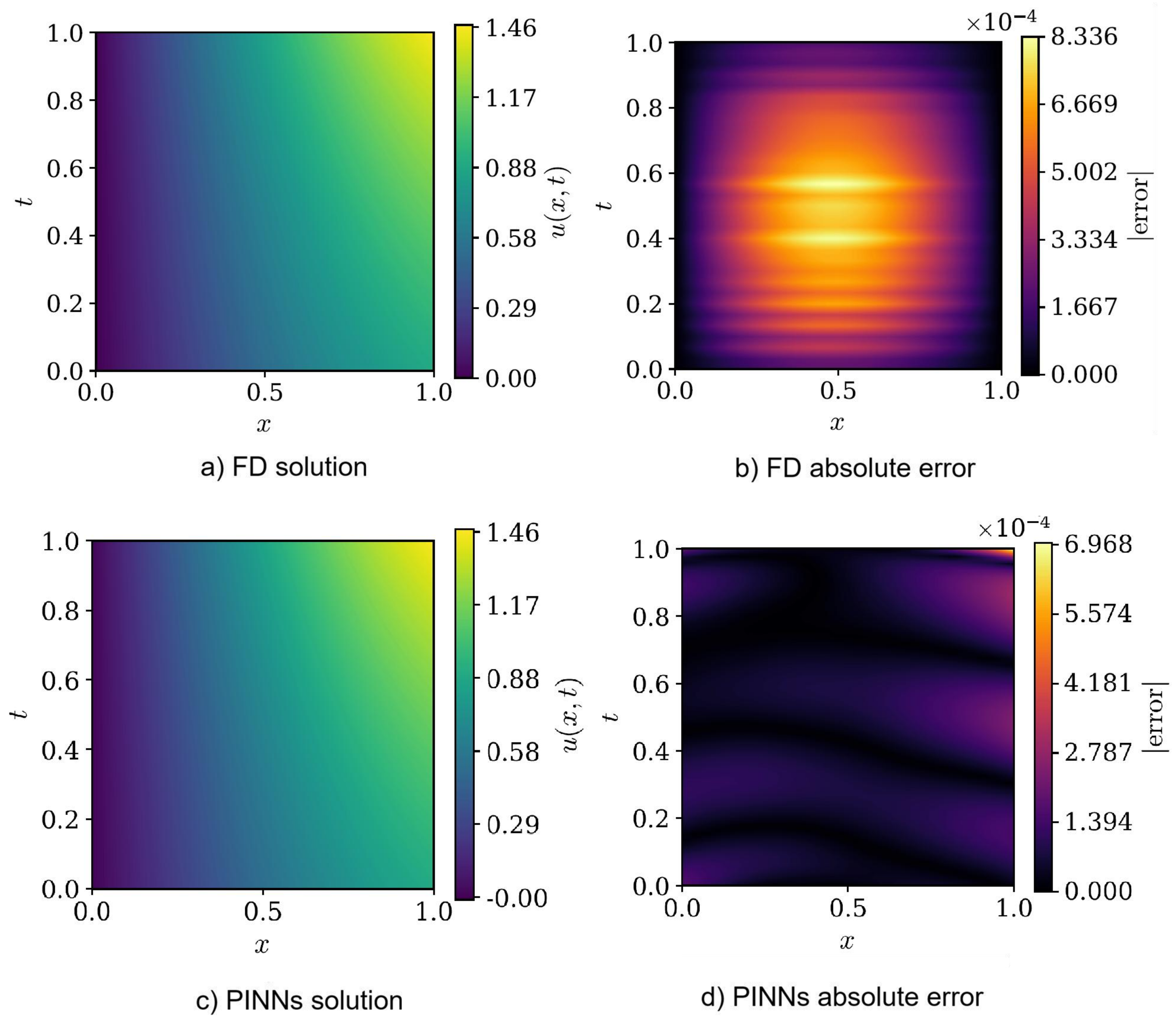

Figure 1: Numerical solution (a, c) and absolute error (b, d) for the FD method (top) and PINNs (bottom) for 30×30 grid, 30 000 iterations.

CONCLUSION

Figure 2: shows that FD methods, particularly with L-BFGS and Adam, reach lower errors in less time across all tested resolutions, while all PINNs variants demand considerably more computation to achieve comparable accuracy.

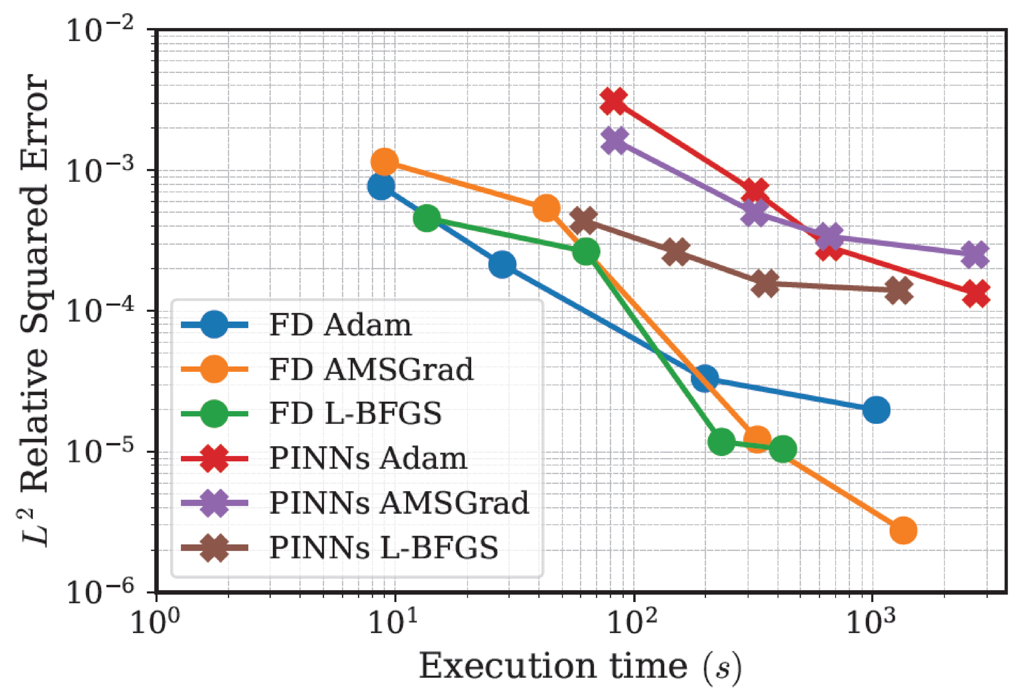

Figure 2: L^2 relative squared error vs. execution time for FD and PINNs methods across four grid resolutions (20×20 to 68×68). FD methods achieve lower errors faster; PINNs require significantly more computation for equivalent accuracy.

- Both methods achieve comparable accuracy (~10^{-4}).
- FD converges faster at small–medium scales but loses accuracy gains beyond 100×100 grids.
- PINNs are mesh-free, though sensitive to initialization.
- L-BFGS outperforms first-order optimizers in both methods but can get stuck in local minima; a hybrid Adam → L-BFGS strategy is recommended.

FUTURE WORK

Future work includes comparing both methods against Fourier Neural Operators (FNOs), extending to higher-dimensional problems, and exploring a broader range of PDE types and non-local operators.

Main References

[1] Martín-Vaquero, J., & Sajavičius, S. (2019). The two-level finite difference schemes for the heat equation with nonlocal initial condition. *Applied Mathematics and Computation*, *342*, 166-177.

[2] Sapagovas, M., Novickij, J., & Pupalaigė, K. (2025). On stability and convergence of difference schemes for one class of parabolic equations with nonlocal condition. *Nonlinear Analysis: Modelling and Control*, *30*(1), 135-155.