Learning Adaptive Step Sizes in Iterative PDE Solvers: Harmonic Map Heat Flow

Tatjana Schreiber, University of Freiburg

November 22, 2025

Workshop: The Mathematics of Scientific Machine Learning and Digital Twins

Overview

Goal: Replace expensive line search with a learned adaptive step size that preserves stability and minimizes energy faster.

- Step-size selection is a key hyperparameter in iterative PDE solvers
- "Safe" steps guarantee stability but can be *very* slow
- We learn an *adaptive* step size τ_k for the harmonic map heat flow
  $\Rightarrow$ Nonlinear Problem with non convex constraint
- Classical methods $\Rightarrow$ ground truth & features

Model Problem

Harmonic maps

Variational problem

Find $u : \Omega \to \mathbb{S}^2$ **such that**

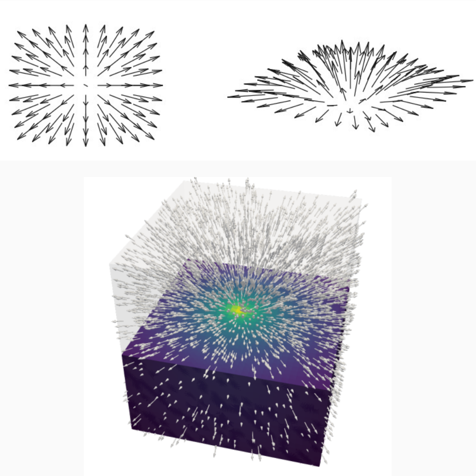
$$E(u) = \frac{1}{2}\|\nabla u\|_{L^2}^2 \quad \text{is minimized,}$$

subject to

$$|u(x)| = 1 \quad \text{for } x \in \Omega, \qquad u = g \quad \text{on } \partial\Omega.$$

Applications

Physical models: Micromagnetics, Liquid crystals, Robotic, . . .
Geometry and data: Minimal surfaces, . . .



Examples of a harmonic map into $\mathbb{S}^2$.

Discrete Harmonic Map Heat Flow

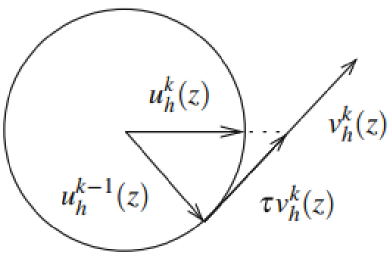
Iterative Algorithm

1. Compute tangent gradient v_h^k:

$$(\nabla v_h^k, \nabla w_h) = -(\nabla u_h^{k-1}, \nabla w_h) \quad \forall w_h \perp u_h^{k-1}.$$

2. Update & Project:

$$u_h^k(z) = \frac{u_h^{k-1}(z) + \tau\, v_h^k(z)}{|u_h^{k-1}(z) + \tau\, v_h^k(z)|}.$$



Reference: F. Alouges, "A new algorithm for computing liquid crystal stable configurations: the harmonic mapping case," SIAM J. Numer. Anal. 34(5), 1708–1726 (1997).

Harmonic map with singularity

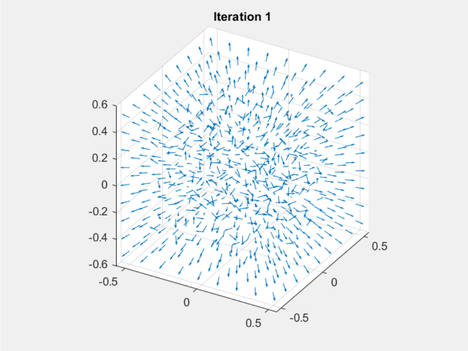
- Domain $\Omega = (-\frac{1}{2}, \frac{1}{2})^2 \subset \mathbb{R}^2$
- Boundary data

$$g(x) = \frac{x}{|x|}, \qquad x \in \partial\Omega,$$

has topological degree 1.

Consequence (Hopf)

H^1-flow must converge to solution with singularity near the origin.



Why adaptive step sizes?

- Iterative schemes must balance **stability** vs. **speed**
- For harmonic map heat flow: if $\tau \leq 2$, the energy decreases in every step

Example: fixed problem, varying step size

τ	0.5	0.75	1.0	1.25	1.5	1.75	2.0
Iterations	411	251	186	149	124	107	797

Classical Step-Size Strategies

Barzilai–Borwein (BB) step sizes

Define $s_{k-1} = u_h^k - u_h^{k-1}$ and $y_{k-1} = v_h^k - v_h^{k-1}$.

Two BB choices for the time step τ_k:

$$\alpha_k^{(1)} = \frac{\langle s_{k-1}, s_{k-1} \rangle}{\langle s_{k-1}, y_{k-1} \rangle}, \qquad \alpha_k^{(2)} = \frac{\langle s_{k-1}, y_{k-1} \rangle}{\langle y_{k-1}, y_{k-1} \rangle}.$$

- Encodes local curvature (approximation of inverse Hessian)
- Very effective in practice
- No guaranteed energy decrease in each step

Golden-Section search

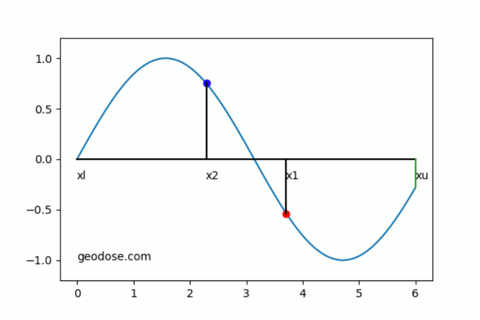
For fixed u and descent direction v, define

$$\Phi(\tau) := E\left(\frac{u+\tau v}{|u+\tau v|}\right).$$

Golden-Section search efficiently finds

$$\arg\min_{\tau\in[a,b]} \Phi(\tau)$$

under a mild near-unimodality assumption.



- Robust and derivative-free $\Rightarrow$ high-quality "oracle" step sizes τ_{gold}
- Main drawback: several energy evaluations per iteration

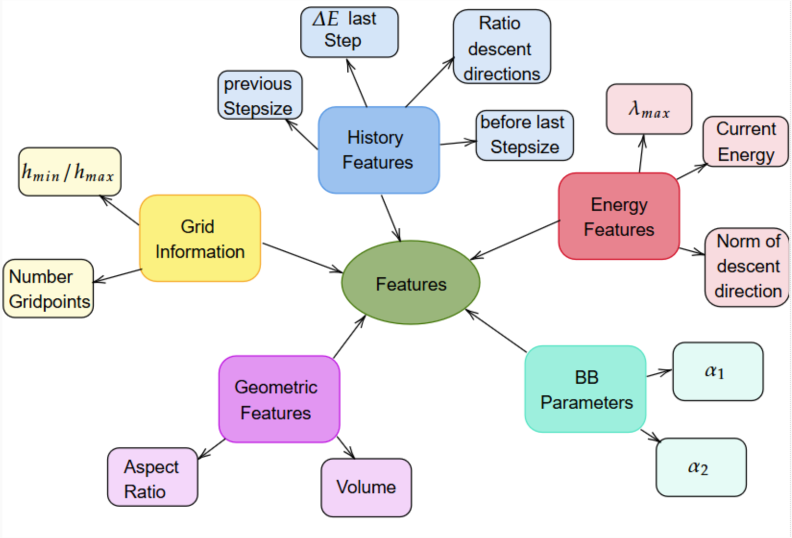
Learning the Step Size

Supervised learning of τ_k

Goal: learn a map $f_\theta : S_k \mapsto \hat{\tau}_k$ from a state representation S_k

- Training data: $(S_k, \tau_k^{\text{gold}})$ pairs from Golden-Section line searches
- State vector: encodes information about the current iterative and history
- Goal: Choose τ by a single forward pass
- Safeguard: If the energy increases, repeat the step with τ_{safe}

State representation



Energy regret bound

Define

$$\Phi(\tau) := E\left(\frac{u+\tau v}{|u+\tau v|}\right).$$

Regret bound

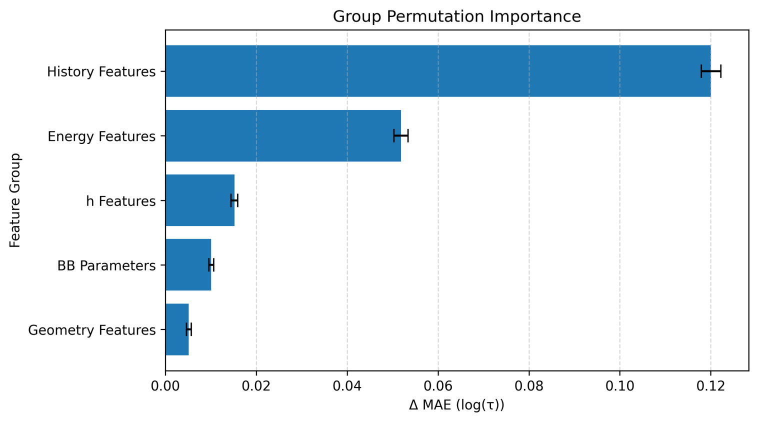
If $\Phi''(\tau) \leq M_v$ on $[0, \tau_{\text{safe}}]$, then

$$0 \leq R := \Phi(\tau_\theta) - \Phi(\tau_{\text{gold}}) \;\leq\; \tfrac{M_v}{2}\,(\tau_\theta - \tau_{\text{gold}})^2.$$

- In expectation, $\mathbb{E}[R] \leq \frac{M}{2}\,\mathrm{MSE}$
- Over K steps: energy gap is quadratically controlled by the prediction error

Results

What does the network learn?



Results

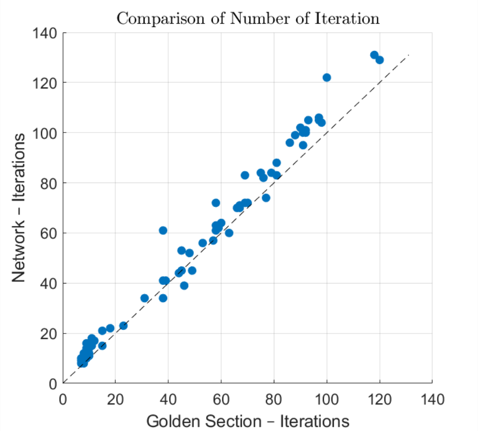


Figure 1: Direct comparison of iterations

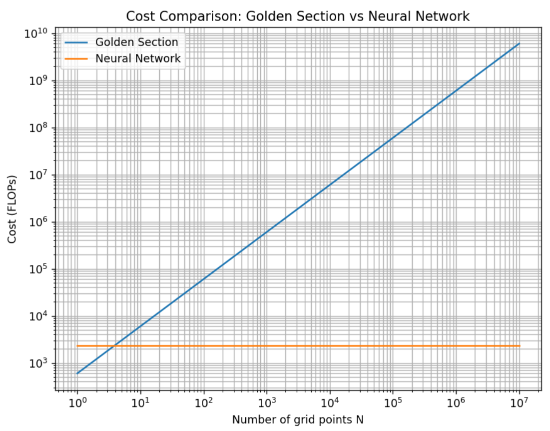


Figure 2: Cost of step–size selection (log–log scale)

Summary

- **Numerical analysis meets Scientific Machine Learning:**
  Learning a step-size rule as a surrogate for classical line search
- **Stable by design:**
  Projection and safeguarding ensure monotone energy decrease
- **Theoretical insight:**
  A regret bound links step-size prediction error to energy gap
- **Practical impact:**
  Replaces a costly line search by a constant-time forward pass, reducing the per-step cost by **3–4 orders of magnitude** for typical 3D meshes

Thank you for your attention!