Preliminary Research Project Report: Mountain–Pass Algorithms for High–Index Critical Points of the Allen–Cahn PDE on Triangularisable Domains

Siddharth Berera Supervisor: Prof. Marco Guaraco

2 July 2025

1 Context and motivation

The Allen–Cahn PDE

$$\varepsilon\Delta u - \frac{1}{\varepsilon}\big(u - u^3\big) = 0 \qquad (\ u|_{\partial\Omega} = 0\ )$$

is a variational PDE and so has a Dirichlet Energy,

$$E_\varepsilon(u) = \int_\Omega \Big(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{(1-u^2)^2}{4\varepsilon}\Big)\,dx.$$

The extremes of this energy correspond to solutions of the PDE. We look to find extrema of this energy of different Morse Indices, where the Morse Index of a point in the function space is the number of orthogonal directions in which the functional on the function space is decreasing at that point. The goal of our project is to efficiently and robustly approximate these solutions of different Morse indices using the Mountain Pass algorithm. We approximate our function space of possible solutions to the PDE by restricting to only the value of functions on a finite triangular mesh, which we dynamically adjust as our algorithm evolves the approximating solution. The Mountain Pass Algorithm is based on the Mountain Pass Lemma, which guarantees the existence of a saddle point of a functional given that the functional has two minima. The algorithm which is based on the proof of this lemma takes a 1-parameter family of curves in the domain, connecting the minima and deforms the path at some sliced points via gradient descent, the max value of the functional on this deformed 1-parameter family is now our approximation of the saddle point. Later theory developed, allows one to begin our approximating algorithm with a k-parameter family of curves in a way to guarantee finding a saddle point where the index of the saddle+nullity of the hessian at that point is k, provided we control this nullity as outlined in Choi–McKenna (1992) we can get a saddle of the index we require, provided it exists.

2 Objectives

O1. Theoretical grounding – obtain an intuitive working definition of p-widths and their relationship with the Allen–Cahn PDE - try summarise the introductions of the four core papers.

O2. Closed-form element formulas – derive by hand exact Dirichlet + potential energy on a simplex, gradient on a simplex and Hessian on a simplex (program symbolically).

O3. Finite-element objects – build `Mesh`, `FunctionSet` and `SweepOut_k` classes for triangularisable planar domains in PyTorch; verify gradient flow on a torus mesh converges to $u \equiv 0$.

O4. Mountain-pass engine (index 1) – implement whole-path descent with arc-length re-parametrisation and add-max routine; demonstrate convergence on the torus mesh.

O5. Index control – study how to control index and find index 5 solution

O6. Parameter & geometry study – vary ε and domain shape; observe Γ-convergence of interfaces to minimal curves.

O7. Compute Morse-index – assemble the discrete Hessian, run `eigsh`, and automate index counting for every computed saddle.

O8. Documentation & dissemination – maintain living LaTeX report; produce final report and research-fair poster; release reproducible, documented code.

3 Literature snapshot

- **Origin of p-widths:** Gromov, "Dimension, nonlinear spectra and width" (arXiv: math/0702066).
- **p-widths of polygons:** Chodosh–Cholsaipant, *The p-widths of a polygon* (arXiv: 2505.03047).
- **Allen–Cahn min-max:** Guaraco (2018) and Gaspar–Guaraco (2018) — introduce phase-transition min-max and show $\omega_p \le \beta_p$.
- **Phase-transition spectrum:** Gaspar–Guaraco, "The phase transition spectrum of a closed manifold" (arXiv: 2004.05120).
- **Equality of spectra:** Dey, *A comparison of the Almgren–Pitts and the Allen–Cahn min-max theory* (2024) — proves $\beta_p = \omega_p$.

- **Mountain-pass theory:** Ambrosetti–Rabinowitz (1973); Struwe, *Variational Methods* (Ch. 2).
- **Index bounds and Allen–Cahn saddles:** Hiesmayr (2018); Gaspar (2020).
- **Numerical mountain-pass:** Choi–McKenna (1992); Li–Nirenberg (2005).
- **FEM background:** Braess, *Finite Elements*; Dziuk–Elliott (2013).
- **Index computation:** Davies, *Spectral Theory*; SLEPc manuals.

4 Methods (overview)

1. **Basis.** P^1 nodal functions $\{\varphi_i\}$ on a conforming triangular mesh; Dirichlet condition by zeroing boundary DOFs.
2. **Energy on one triangle.**

$$E_\varepsilon(\Delta) = \frac{\varepsilon^2}{4} \sum_{\text{edges}} \cot\alpha\,(u_j - u_k)^2 + \frac{|\Delta|}{60\varepsilon} P_4(u_j, u_k, u_\ell).$$

3. **Gradient & Hessian.** Assemble sparse matrices M (mass) and K (stiffness); $H = \varepsilon^2 K + M - 3\,\mathrm{diag}(u^2)M$.
4. **Mountain–pass loop.** 20 slices; each interior slice updated by projected gradient descent, followed by arc–length reparametrisation.
5. **Index check.** `eigsh`(H, k=10, sigma=0) counts negative eigenvalues.

5 Work plan

wb 1 Jul	Read intros of width papers; fix domain list; draft Section 1; derive symbolic triangle energy.
wb 8 Jul	Write 1-page Mt-pass proof note; state infin-dim MpL; validate energy formulas in SymPy. Create poster.
wb 15 Jul	Implement Mesh, FunctionSet, SweepOut_k in PyTorch; gradient flow test on torus mesh.
wb 22 Jul	Code energy & auto-grad in PyTorch; finite-difference validation; draft Section 3.
wb 29 Jul	Add-max + Mp-loop (index 1) on torus; energy plot; Hessian / eigsh check.
wb 5 Aug	$k = 3$ symmetry mask on hexagon; compute index 3 saddle; start ε-sweep scripts.
wb 12 Aug	ε-dependence study; Möbius band run; collect figures for poster.
wb 19 Aug	Code clean-up; final report PDF; poster draft; Git release v1.0.

6 Expected outcomes

1. Robust FEM mountain–pass implementation on triangulable domains.

2. Catalogue of index $1, 3, 5$ saddles on representative geometries.
3. Visual evidence of Γ–convergence of interfaces to unstable minimal curves.
4. Reproducible code repository and poster for the summer research fair.