

1 Square-to-Circle Reference Case

The square-to-circle case is included in the HeavyMetal validation suite as a reference-history test for large-scale mass transport by surface diffusion. In contrast to the Mullins and ATG cases, this problem is not compared with a closed-form analytical time-history solution. Instead, it provides a simple geometric reference case in which the expected long-time behavior is clear: an initial square should evolve toward a circular shape.

The physical formulation is the same as that used in the Mullins validation case. The chemical potential is written in terms of the normal stress as

$$\mu = \mu_0 - \Omega \sigma_{nn}, \quad (1.1)$$

where the normal stress is generated by the applied surface energy. Gradients in this chemical potential drive surface diffusion along the boundary. For an isotropic surface energy and fixed area, the circle is the minimum-energy shape, so the square-to-circle evolution provides a direct test of whether the surface transport formulation can move material over large distances toward the expected equilibrium morphology.

Figure 1.1 shows the predicted evolution. The initial square rapidly loses its sharp corners, then progressively approaches a nearly circular shape as material is redistributed along the free surface. This case was the first test of the ability of HeavyMetal to simulate large-scale mass transport by stress-driven surface diffusion, beyond the small-amplitude or idealized perturbations used in the analytical Mullins and ATG benchmarks.

In the automated validation workflow, the square-to-circle problem is treated as a reference-history case. The current solution is compared against trusted reference output in order to detect unintended changes as the code evolves. The case therefore serves two purposes: it verifies reproducibility of an established HeavyMetal calculation, and it demonstrates that the same surface-energy and surface-diffusion formulation used in the analytical benchmarks can also produce large-scale morphological evolution toward the correct geometric end state.

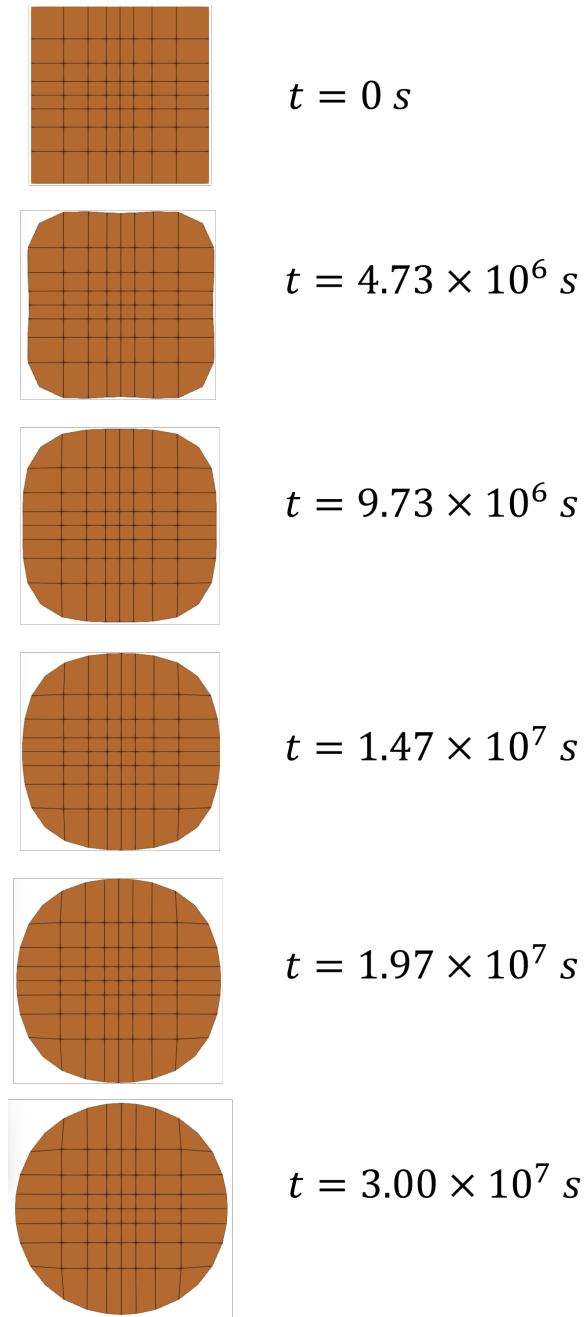


Figure 1.1: Predicted evolution of an initially square region toward a circular shape under the action of surface energy and stress-driven surface diffusion. The calculation demonstrates large-scale redistribution of material toward the expected minimum-energy morphology.