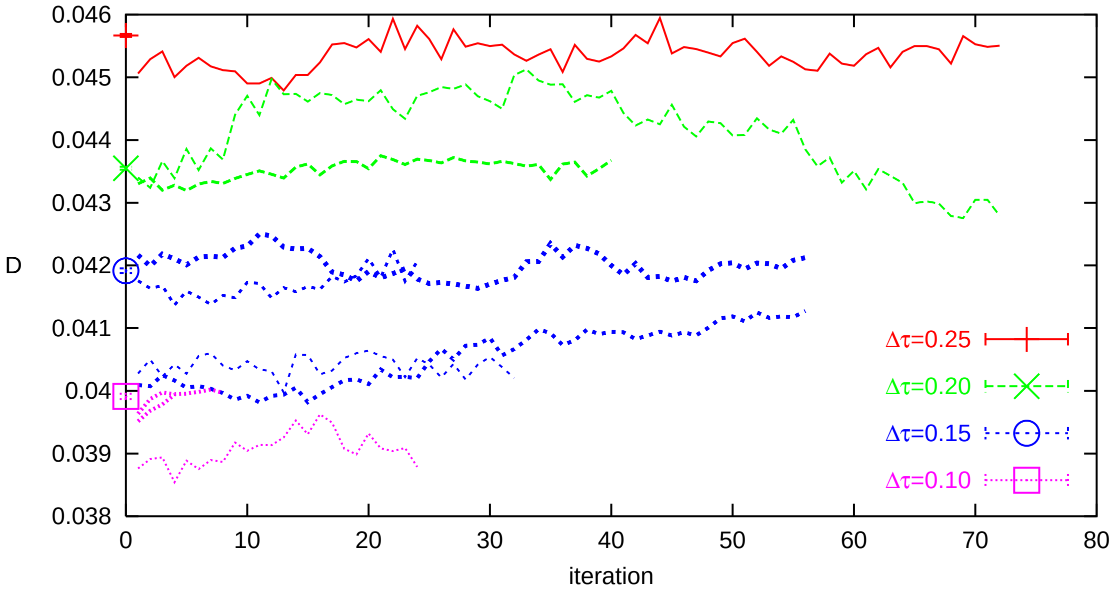

Figure 3.64: Convergence of double occupancy D for $T = 0.067$ and $U = 4.55$. The number of sweeps is about 10^5 for thin lines and about 10^6 for thick lines. Symbols at the left axis indicate our best estimate of D for each value of $\Delta\tau$.

versus iteration number for several independent iteration runs. Line types (solid, long-dashed, short-dashed, and dotted) denote the time discretization $\Delta\tau$ while the width of the lines give a rough indication of the numerical accuracy, i.e., the number of sweeps used in each convergence run which is larger for thicker lines. Apparently, the overall convergence is not good since not all solutions for the same value of $\Delta\tau$ tend to a common fixed point. Instead, long-scale fluctuations appear, e.g., for the run with lower accuracy for $\Delta\tau = 0.2$ (thin long-dashed line). This is exactly what we expect from Landau theory: as soon as the gradient of the free energy is smaller than statistical fluctuations, the iterated solutions follow an asymptotically free random walk (predominantly in the soft-mode direction). Two strategies for overcoming the associated problems are also apparent from Fig. 3.64: On the one hand, it is important to increase the numerical precision near critical regions in order to reduce fluctuations. On the other hand, trends can be much better recognized when comparing several independent self-consistency runs. By comparing the evolution (as a function of iteration number) of different runs with more metallic or insulating initial conditions, one can establish boundaries for the fixed point or accelerate convergence by preparing initial states near the assumed fixed point.[56] We used such strategies extensively throughout the numerical parts of this thesis. For example, the upward trend of initial solutions for $\Delta\tau = 0.15$ (two lower short-dashed lines in Fig. 3.64) prompted us to initialize runs with $D \approx 0.042$; those are seen to be stable.

In order to further illustrate these considerations and to demonstrate increased fluctuations near the critical point, we perform sets of iteration runs for $T = 0.055$,

[56] The possibilities for initialization are obviously more limited very close to a stability edge.