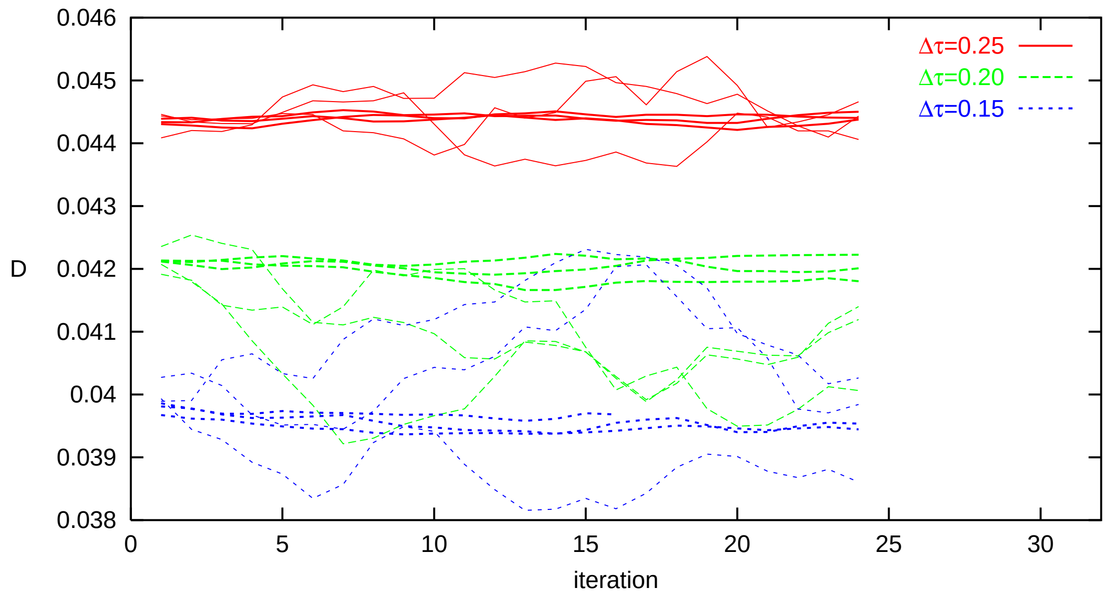

Figure 3.65: Convergence and fluctuations of double occupancy D for $T = 0.055$ and $U = 4.65$, very close to the critical end point ($T^* = 0.055$, $U^* = 4.665$) for $\Delta\tau = 0.0$. Thin lines correspond to runs with 10^5 sweeps per iteration, thick lines to runs with $4 \cdot 10^6$ sweeps.

$U = 4.65$, i.e., very close to our estimate of the critical end point (for $\Delta\tau = 0.0$). Figure 3.65 shows results for the discretizations $\Delta\tau = 0.25$, $\Delta\tau = 0.20$, and $\Delta\tau = 0.15$, with three statistically independent runs using 10^5 sweeps ("low" accuracy) and three runs using $4 \cdot 10^6$ sweeps per iteration ("high" accuracy) each. Evidently, the amplitude of fluctuations indeed increases for decreasing $\Delta\tau$ at $T = 0.055$ and $U = 4.65$. The fluctuations are strongly reduced by a 40-fold increase in the number of sweeps, i.e., by a reduction of the statistical error of the solution of each impurity model to about 1/6. Note that the long "time" scale (i.e., the large number of iterations) associated with the fluctuations of the runs with low accuracy generically leads to an underestimation of error bars for averages obtained from a single run. One way of detecting such extremely long autocorrelation time is the comparison of several independent runs as seen in Fig. 3.65 for $\Delta\tau = 0.15$. For a finite number of runs, however, the deviations of all iteration runs may have the same sign as seen for $\Delta\tau = 0.20$ in the same figure. Thus, accurate and controlled estimates can only be obtained from runs with high accuracy, i.e., a large number of sweeps.

Corresponding data for the slightly higher temperature $T = 1/15$ is shown in Fig. 3.66. For each of the combinations of a representative sets of values of the interaction ($U = 4.4$, $U = 4.55$, $U = 4.65$, and $U = 4.8$) and of the discretization (here limited to $\Delta\tau = 0.25$, $\Delta\tau = 0.2$, and $\Delta\tau = 0.15$ by the computational resources), we used our best previous estimate of the converged solution for initializing 3 runs with high accuracy and 3 runs with low accuracy. While some initial trend is visible even in some high accuracy runs, the rapid convergence of each run and the agreement