We use advanced numerical methods to model fluid-structure coupling with transport phenomena (fluid flow and mass transfer) involved in biomedical systems, such as controlled drug delivery and transport of deformable microcapsules into microfluidic chips. The simulations require high grid resolution to predict and to capture the details of each particle deformation and the released drug spatial distribution. The computer code solver that is based on the lattice-Boltzmann method, which is a state-of-the-art computational fluid dynamics method, is parallelized using both the MPI (Message Passing Interface) and the CAF (Co-Array Fortran 2008). We present the performance of the code on different machines when using either MPI or CAF. We show original results and data obtained with our computer codes. The drug release rate as a function of the flow around a capsule, and the clog and no-clog states of multiple capsules when squeezed into a microfluidic constriction. The HPC has allowed us to speed up the simulation run time, and therefore, to explore a wide range of the key control parameters. These studies are used to guide experimental studies with the hope to be used in the near future as a computer-aided design tool in pharmaceutics and biomedical industry.