A program is CPU bound if it would go faster if the CPU were faster, i.e. it spends the majority of its time simply using the CPU (doing calculations). A program that computes new digits of π will typically be CPU-bound, it's just crunching numbers.

A program is I/O bound if it would go faster if the I/O subsystem was faster. Which exact I/O system is meant can vary; I typically associate it with disk, but of course networking or communication in general is common too. A program that looks through a huge file for some data might become I/O bound, since the bottleneck is then the reading of the data from disk (actually, this example is perhaps kind of old-fashioned these days with hundreds of MB/s coming in from SSDs).