



A supercomputer consists of millions of identical 'processors' that work in parallel to perform thousands of trillions of calculations each second.

A supercomputer can perform a large number of calculations very fast compared to ordinary computers such as your desk or lap-top computer. This makes them very important for mathematically modeling complex systems such as the movement of millions of particles through space, the folding of complicated proteins, or the sequencing of DNA.

Let's have a look at one simple application to see how this works!

Imagine that you are following the movement of three stars through space, and that their distance from our sun in light years is given by the following three equations, where T is the elapsed time in millions of years:

$$d_1 = 3T + 2$$

$$d_2 = 4T - 2$$

$$d_3 = 8T + 3$$

Problem 1 - Using a calculator, A) evaluate by hand the values for d_1 , d_2 and d_3 for the three time steps $T = 1, 2$ and 3 . B) How long did it take you, in seconds, to perform the calculations? C) How many key strokes were involved? D) How many mathematical operations were involved?

Problem 2 - Suppose you wanted to follow the movement of 300 stars in a star cluster for three time steps. A) How many equations would be involved? B) How many keystrokes would you have to execute? C) How many mathematical operations would you have to perform? D) How long would the calculation take for three time steps? E) If N is the number of particles in your simulation, what is the general formula that gives the computation time in seconds for N particles?

Problem 3 - Suppose that you wrote a computer program to perform the calculations on a high-end laptop computer using a programming language such as FORTRAN, or C. With a 'clock speed' of 1 billion operations per second, how long would the computer take to evaluate the three particle positions after three time steps?

Problem 4 - A supercomputer not only performs an individual mathematical operation very fast, (3 million billion 'floating point operations per second' which is called 3 petaFLOPS) but it can perform many operations simultaneously by using parallel processing. In the example above, for each time step, suppose the computer might be built to use three 'processors', (one for each particle), to evaluate all three values for d in one step! How long would it take a 3 petaFLOP supercomputer to calculate three time steps for 10 million particles?

Problem 1 - Using a calculator, A) evaluate by hand the values for d_1 , d_2 and d_3 for the three time steps $T= 1, 2$ and 3 . B) How long did it take you, in seconds, to perform the calculations? C) How many key strokes were involved? D) How many mathematical operations were involved?

Answer: A) $d_1 = 5, 8$ and 11 . $d_2 = 2, 6$ and 10 ; $d_3 = 11, 19, 27$.

B) It takes about 5 seconds per evaluation, or **45 seconds for all three particles for 3 time intervals**, not including the time to write down the answer.

C) For one value: $3 \times 1 + 1 =$ each entry is a key stroke. There are 3 timesteps \times 3 particles \times 6 keystrokes = **54 keystrokes** total.

D) There are only 2 operations per evaluation 'x' and '+' or '-' so a total of **18 operations**.

Problem 2 - Suppose you wanted to follow the movement of 300 stars in a star cluster for three timesteps. A) How many equations would be involved? B) How many keystrokes would you have to execute? C) How many mathematical operation would you have to perform? D) How long would the calculation take for three time steps? E) If N is the number of particles in your simulation, what is the general formula that gives the computation time in seconds for N particles? E) How long, in hours ,will it take to calculate the position of 300 particles for three timesteps?

Answer: A) There would be **300 equations** for ; $d_1, d_2, d_3, \dots d_{300}$.

B) 6 keystrokes \times 3 timesteps \times 300 equations = **5400 keystrokes**

C) 2 operations \times 3 timesteps \times 300 equations = **1800 operations**

D) From your answer to Problem 1A it takes about 5 seconds to calculate one time step for one particle, so $T = 3$ timesteps \times 5 seconds \times N or **$T = 15 N$ seconds**.

E) $T = 15 \times 300 = 4500$ seconds or **1.25 hours**.

Problem 3 - Suppose that you wrote a computer program to perform the calculations on a high-end laptop computer using a programming language such as FORTRAN, or C. With a 'clock speed' of 1 billion operations per second, how long would the computer take to evaluate 10 million particle positions after three time steps?

Answer: $T = 3$ timesteps \times (2 operations/timestep) \times (1 second/1 billion operations) \times 10 million particles

= **0.06 seconds**.

Problem 4 - A supercomputer not only performs an individual mathematical operation very fast, (3 million billion 'floating point operations per second' which is called 3 petaFLOPS) but it can perform many operations simultaneously by using parallel processing. In the example above, for each time step, suppose the computer might be built to use three 'processors', (one for each particle), to evaluate all three values for d in one step! How long would it take a 3 petaFLOP supercomputer to calculate three time steps for 10 million particles?

Answer: The supercomputer would use 10 million 'parallel processors' so that

$T = 3$ timesteps \times (2 operations/timestep) \times (1 second/ 3×10^{12} operations)

= **2×10^{-12} seconds**.