Experiments Report

December 3, 2016

Abstract

This report will include the discussion for the experiments. The experiments section will have data plotting and an initial analysis (model and discussion) based on the developed understanding. A Q & A subsection will follow after the discussion. I will add questions there that still need answering. It would be nice if others contributed with questions!

CPPTraj RMSD

The data reported are CPPTraj comparing experiments between Vanilla (MPI) execution and the task parallel execution of CPPTraj via RADICAL-Pilot. The experiments setup is the following:

- RMSD over 160000 frames as a single trajectory and as an ensemble of 2 trajectories that contain 80000 frames each. (105GB filesize)
- RMSD over 320000 frames as a single trajectory and as an ensemble of 4 trajectories that contain 80000 frames each. (209GB filesize)
- RMSD over 640000 frames as a single trajectory and as an ensemble of 8 trajectories that contain 80000 frames each. (418GB filesize)

The configuration was from a core per 80000 trajectories up to a node per 80000 frames. All experiments were done on Stampede.

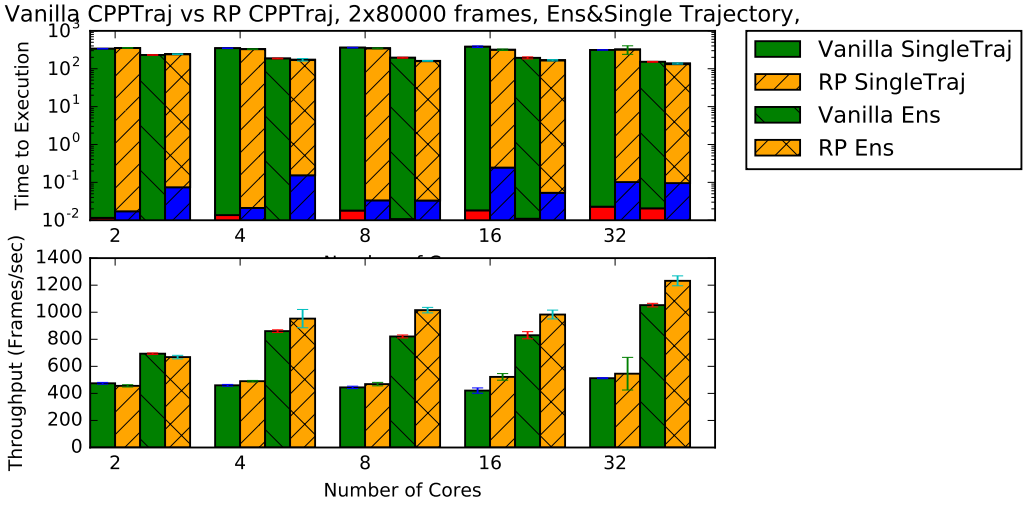


Figure 1: Time to Execution and Throughput comparison between different ways of executing the same CPPTraj analysis. There are in total 160K frames organized as a single trajectory file for the Single trajectory case and as an ensemble of 2 trajectories for the ensemble case

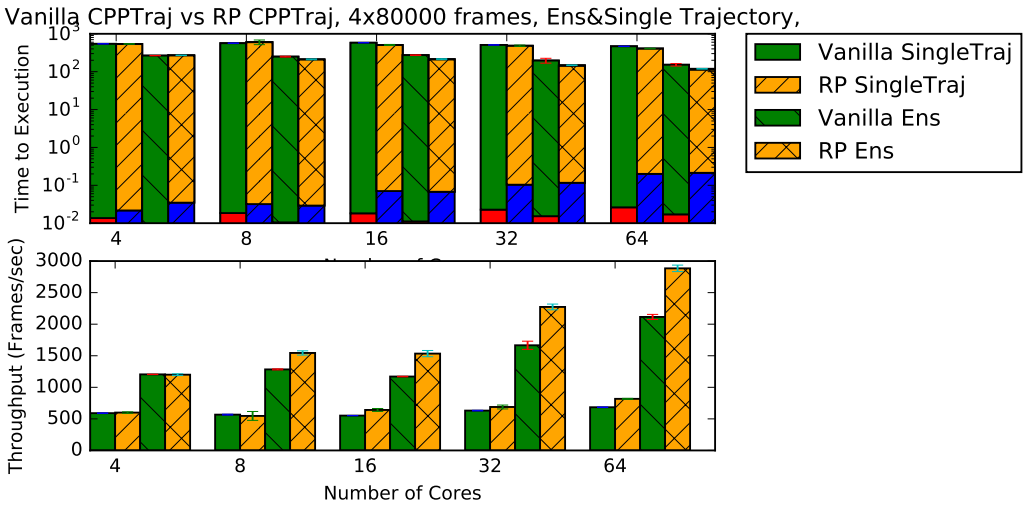


Figure 2: Time to Execution and Throughput comparison between different ways of executing the same CPPTraj analysis. There are in total 320K frames organized as a single trajectory file for the Single trajectory case and as an ensemble of 4 trajectories for the ensemble case.

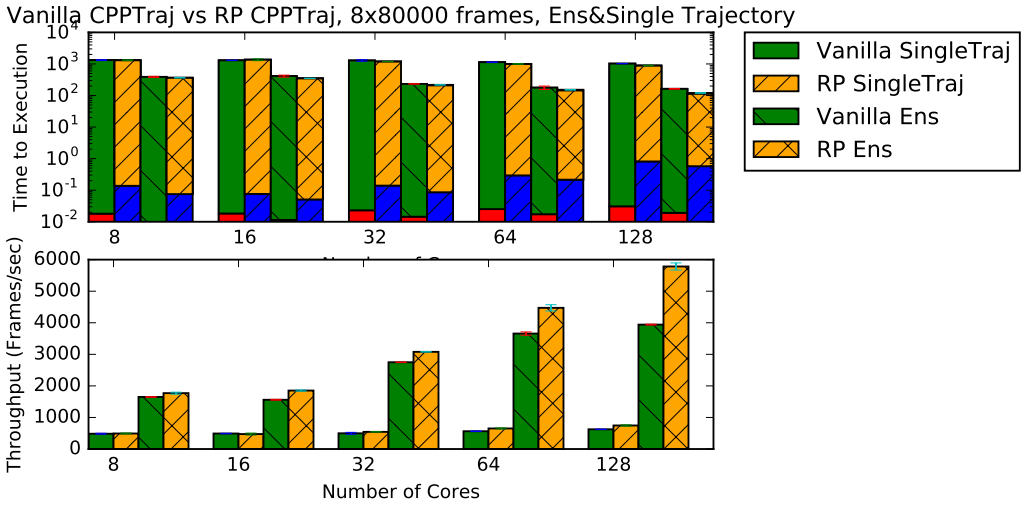


Figure 3: Time to Execution and Throughput comparison between different ways of executing the same CPPTraj analysis. There are in total 640K frames organized as a single trajectory file for the Single trajectory case and as an ensemble of 8 trajectories for the ensemble case.

The top subplot show the Execution time for Vanilla and RADICAL-Pilot. The bottom subplot shows the Average Throughput. In all figures the order of the bars is from right to left:

1 Single Trajectory Vanilla,

2 RP-CPPTraj single trajectory,

3 CPPTraj Vanilla Ensemble and

4 RP-CPPTraj Ensemble

One important note to make, is that as the core count increases, the MPI implementation does not scale

in ensemble case as the task level parallel for the 320K, Figure 2, and 640K frames, Figure 3. The main difference between those two is that the CPPTraj execution via RADICAL-Pilot introduces a small delay between the launching of each CPPTraj process. I believe that this delay reduces the strain CPPTraj's MPI implementation puts to the filesystem and the data are read faster. In the next set of experiments with RMSD, I want to find the filesize, or better the system size, where the MPI implementation cannot scale anymore and the task level parallel can.

The reason behind the above statement is the fact that throughput remains relatively stable. Throughput, here measured as frames per second, is the amount of computed data per time unit. We can say it is the computation velocity. Throughput is a function of input rate and the number of computing blocks. By computating blocks, I mean a self contained element that takes an input, does some sort of processing on the input and gives an output. In this case,it can either be a MPI process or a task.

Assuming that the input rate, throughin, is infinite and it can feed continuously and steadily any number of computing blocks, the throughput will increase linearly as we increase the number of computing blocks. Say that such a block can process N inputs per time unit. Adding a second computing block $2N$ inputs per time unit can now be processed. Thus, with K computing blocks the throughput is KN inputs per time unit. It is now established how throughput changes when the computation blocks vary and the input rate is large enough to accomodate any number of them.

Assume now that the input rate is finite to a maximum of M inputs per time unit. In case $M < N$, throughput is dectated by the input rate. In case $M \geq N$, throughput will increase linearly as long as the number of computing blocks is less or equal to $\lfloor \frac{M}{N} \rfloor$. When the number of computing blocks, becomes larger than the previous number, throuput flats to a rate equal to the rate in which the input is produced.

The question that needs to be answered now is what is the rate that CPPTraj reads in data. The experiments will read the file and do nothing else.

Hausdorff Distance

The data reported here are comparing the Hausdorff Distance calculation via a RADICAL-Pilot and a Spark implementation. Both use the same implementation for the main function and both use parallel read. The experiments were executed over 192 trajectories of CA atoms on Comet. Figure 4 show the mean time to execution for all three cases of trajectory size for the CA atoms.

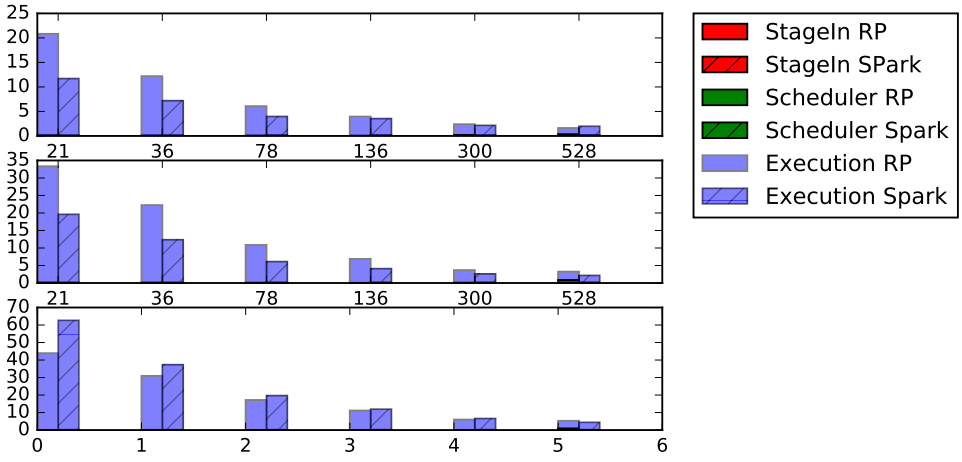


Figure 4: Time to Execution Hausdorff Distance. From top to bottom Short trajectory, Medium Trajectory, Long Trajectory

Figures 5,6 and 7 show in more detail how the execution between the two frameworks differ. Two main differences is that RADICAL-Pilot spends more time to stage in and stage out data to and from a task, where Spark is more expensive in scheduling tasks.

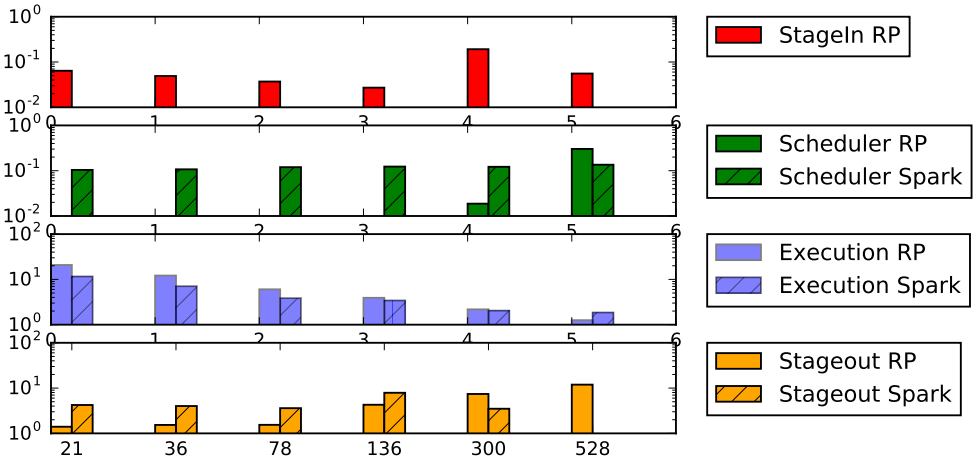


Figure 5: Execution break down between RADICAL-Pilot and Spark execution. The Y axis represents the time spent in each part and the X axis the number of core. This is short trajectory size

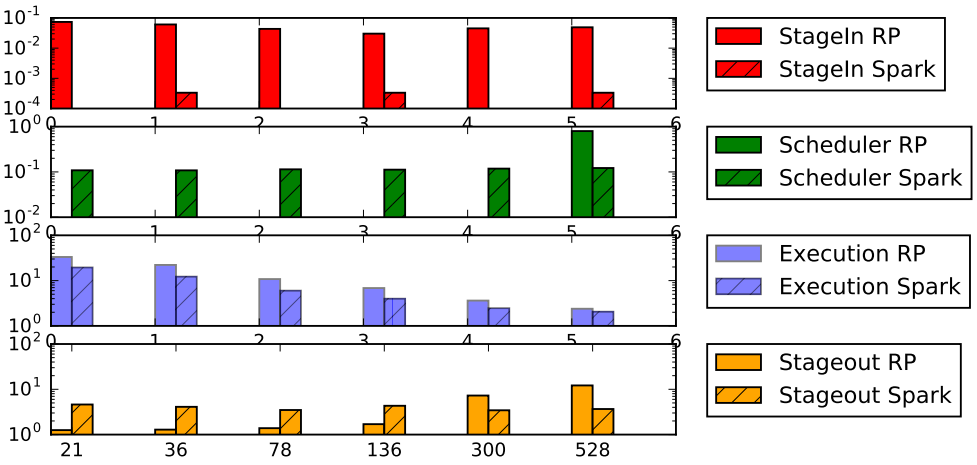


Figure 6: Execution break down between RADICAL-Pilot and Spark execution. The Y axis represents the time spent in each part and the X axis the number of core. This is medium trajectory size

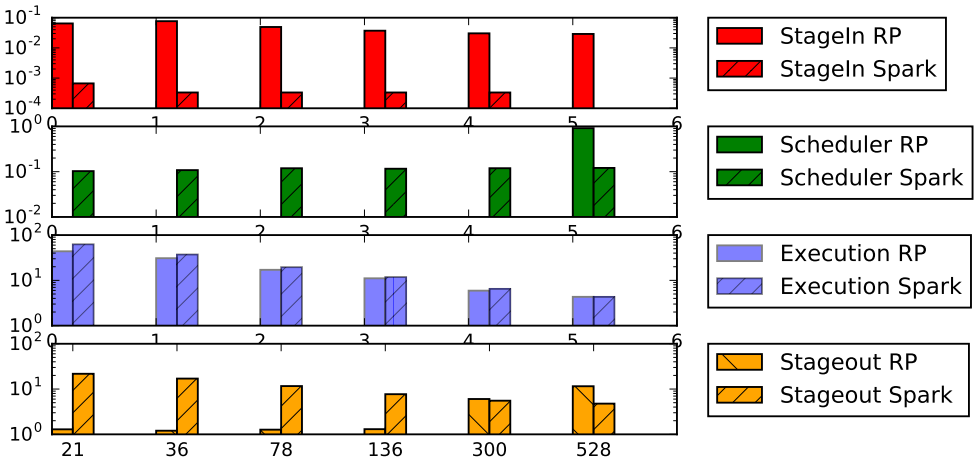
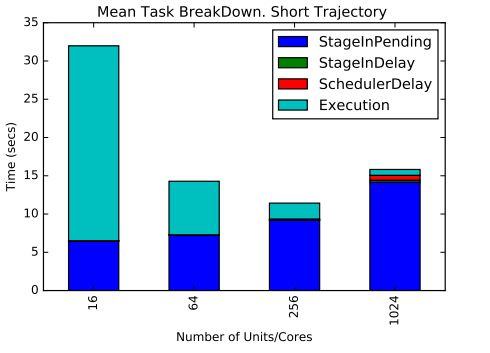


Figure 7: Execution break down between RADICAL-Pilot and Spark execution. The Y axis represents the time spent in each part and the X axis the number of core. This is Long trajectory size

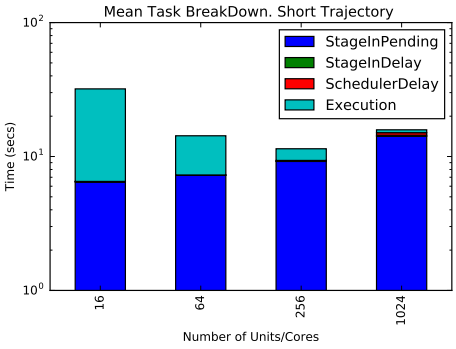
Extra experiments were executed with the following configuration on Comet:

- Number of trajectories is 128
- Number of atoms 214 and frames 102. Trajectory sizes are Short, Medium and Long. This is equivalent to 214 atoms per frame, 428 and 856 respectively.
- The whole matrix was calculated
- Core count: 16, 64, 256 and 1024
- Execution was done with RADICAL-Pilot and Pilot-Spark.

The following figures show that comparison.



Average Task execution time for four core counts. 128 trajectories were compared. Each trajectory has 102 frames of 214 atoms. The execution partitioned the calculation of the distance matrix into the calculation of a number of submatrices (16,64,256,1024).Resource: Comet,Date:12/1/2016



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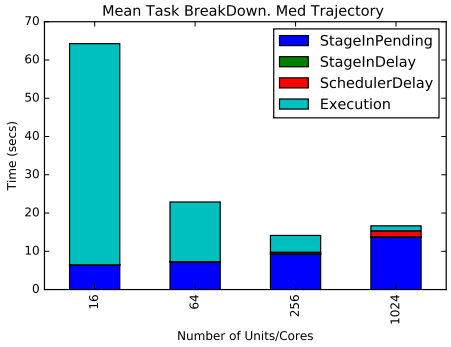
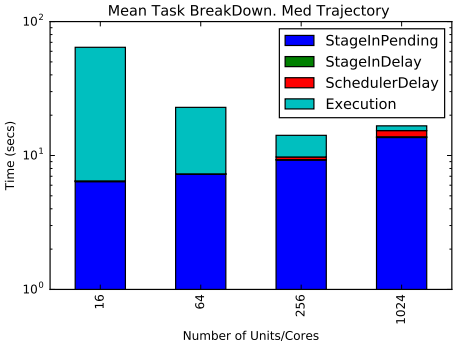


Average Task execution time for four core counts. 128 trajectories were compared. Each trajectory has 102 frames of 428 atoms. The execution partitioned the calculation of the distance matrix into the calculation of a number of submatrices (16,64,256,1024).Resource: Comet,Date:12/1/2016



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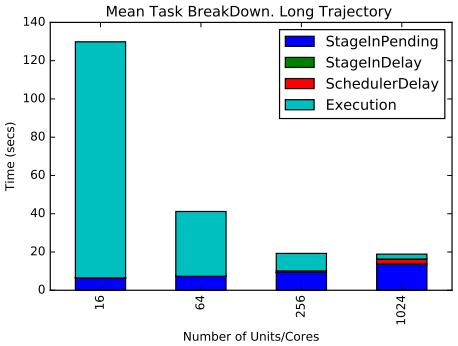
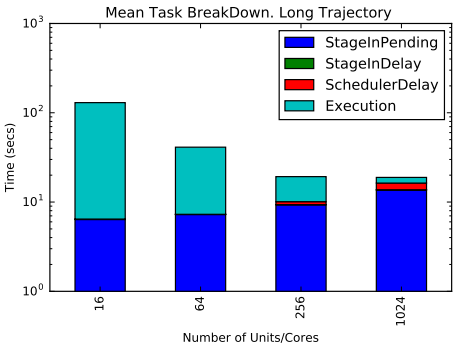


Average Task execution time for four core counts. 128 trajectories were compared. Each trajectory has 102 frames of 856 atoms. The execution partitioned the calculation of the distance matrix into the calculation of a number of submatrices (16,64,256,1024).Resource: Comet,Date:12/1/2016



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Useful Definitions [Updated*]

- N_{Tr}: Number of Trajectories per task
- N_A: Number of atoms in a frame.
- N_F: Number of frames per trajectory. All trajectory files have the same number of frames, 102.
- N_T: Number of tasks
- α: the coefficient of Staging In
- β: the coefficient of the Scheduling delay
- γ: the coefficient of the Execution
- δ: the coefficient of the Staging Out

Analysis

The execution model can be easily broken to different parts. First part of the model is data StageIn. In case of RADICAL-Pilot StageIn is rather easy to undeerstand. In case of Spark, I consider as StageIn the part of the code that is written before partitioning the data. Second part is the time need to schedule a task. Third is the actual execution of the task, which can be broken further more to read, exec and write. Finally, the last part of the model is the time necessary to stage out the data. In case of RADICAL-Pilot it is easy to

understand. In Spark, I consider as the time needed from the time that all tasks have returned their data until the end of the script.

***giannis: Why is the need for every parameter?

Essentially, the model will look like:

$$T = \alpha(N_I) + \beta N_T + \gamma Y + \delta\Big(N_O S_O + \frac{k(k+1)}{2}\Big)$$

Y is the tme of the execution of the task.

Task Execution Analysis

That is dependent to the number of trajectories being processed and the number of points in each trajectory. Let T_N be the number of trajectories per task and T_S the size of each trajectory, i.e. the number of points.Thus, the above execution time can be

$$Y = O((N_T r N_F N_A)^2)$$

Let dH be the time to calculate the Hausdorff distance between two trajectories. The following algorithm describes it in pseudocode. The description will help the following analysis:

```
1: procedure HausdorffDistance(T1, T2)                ▷ T1 and T2 are a set of 3D points
2:     for ∀t1 in T1 do
3:         for ∀t2 in T2 do
4:             Append in D1 calculated d(t1, t2)
5:         end for
6:         Dt1 append max(D1)
7:     end for
8:     N1 = min(Dt1)
9:     for ∀t2 in T2 do
10:        for ∀t1 in T1 do
11:            Append in D2 calculated d(t2, t1)
12:        end for
13:        Dt2 append max(D2)
14:    end for
15:    N2 = min(Dt2)
16:    return max(N1,N2)
17: end procedure
```

Thus, the complexity of dH is

$$dH = \mathcal{O}({T_S}^2) + T_S\mathcal{O}(T_S) + \mathcal{O}({T_S}^2) + T_S\mathcal{O}(T_S)$$

RP Fitting

Before solving any system, I will add some assumptions that will try to simplify the model as well as better understand how the scheduler and data stage in overheads affect the execution.

- RADICAL-Pilot's staging output does not affect the execution pattern of the tasks. All tasks are executed in parallel and there is no data movement from the executing resource to the client. Also, there is no continuation in the execution since only one pass is done over the data.

- Any delay between the moment a Compute Unit goes to the Executing state and starts execute as well as the delay from the moment it returns until it moves to the next stage, are assumed as part of the execution time of the task.
- Parameter γ is set to 1 in this case, because the timing parameters for the execution are captured inside Y.

***giannis: What is x^2 value? What is the goodness of the values? What is the error in all these?

[Update] The execution time of the tasks depend on the number of trajectory files that it gets, the number frames per trajectory and the number of atoms. The number of atoms affects the exeution time linearly, the number of frames and the number of trajectories affect in a squared fashion.

Thus $T_{Ex}(N_{Tr}, N_A, N_F) = e_1 N_{Tr}^2 N_F^2 N_A + e_2$

After appling the least square method the values found for e_1 and e_2 are:

$$e_1 = 1.33271794e-08 \quad e_2 = 8.09404416e-02$$

The χ^2 test was applied to the following points:

Trajectories	Frames	Atoms	Observed Time	Predicted Time
32	102	214	25.46786774	30.46545617
16	102	214	7.00346226	7.67706937
8	102	214	2.0758777	1.97997267
4	102	214	0.76485454	0.5556985
32	102	418	57.81401424	60.84997191
16	102	418	15.59695303	15.27319831
8	102	418	4.39942563	3.87900491
4	102	418	1.3047394	1.03045656
32	102	856	123.41059877	121.61900337
16	102	856	33.88301111	30.46545617
8	102	856	9.16800458	7.67706937
4	102	856	2.56352096	1.97997267

The tested null hypothesis is the observed values belong to the predicted distribution

The χ^2 is calculated with the following formula:

$$\chi^2 = \sum_{1}^{12} \frac{(O_i - P_i)^2}{P_i}$$

The χ^2 value is 2.13474849056. This value is smaller than the $\chi_0^2.05$ for 11 degress of freedom, thus we cannot reject the null hypothesis for the 0.05 significance level.

The Last Unit arrival time is considered as the time the last CU entered the State AgentStagingInput where input staging start to be executed.

The Least Squares Fit was done over the points obtained for 16, 64, 256 and 1024 CUs. The line that was obtained is the following

$$T_A(N_T) = 0.01313076 N_T + 7.66860076$$

Spark Fitting

The Spark execution model requires one extra term. That term is shows the time that is needed to for Spark to launch its executors. An executor is the process responsibe to execute the tasks. An assumption that is made is the fact that stagein in the Spark execution does not significantly change the execution time since it creates an RDD with the paths where the file are. So, the model will be

$$T = \beta\frac{k(k+1)}{2} + Y + \delta\Big(N_O S_O + \frac{k(k+1)}{2}\Big) + \epsilon W$$

where W is the number of worker nodes.

***giannis: TODO: Solve the system