Chapter 1

Quick start guide

The ClusteringSuite is the software package that includes the cluster analysis tool developed at the Barcelona Supercomputing Center Tools Team. It is composed by a set of binaries and libraries implemented in C and C++. The main tool included in this package is BurstClustering, which performs the cluster analysis of Paraver traces (see section ??).

As a short summary, the cluster analysis tool finds groups in the different computations (CPU bursts, i.e. regions between call to the parallel runtime) a parallel application performs. To characterize these bursts we can use any information gathered in the input trace. In almost all cases we use the information provided by the Performance Hardware Counters.

In this first chapter of this manual we detail the contents of the package as well as we guide how to run the first cluster analysis, following the example distributed with the ClusteringSuite package.

1.1 ClusteringSuite package

The package is distributed in compressed tar format (e.g., clusteringsuite.tar.gz). To unpack it, execute from the desired target directory the following command line:

```
> tar xvfz clusteringsuite.tar.gz
```

The unpacking process will create different directories on the current directory (see table 1.1). We suggest adding the `<clusteringsuite_dir>/bin` directory to your PATH environment variable, so as to easily access to the tools included in the package.

```
<table>
<thead>
<tr>
<th>Directory</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>bin</td>
<td>Contains the binary files of the ClusteringSuite package.</td>
</tr>
<tr>
<td>include</td>
<td>Contains the different library headers to extend the package.</td>
</tr>
<tr>
<td>lib</td>
<td>Contains the different libraries files to extend the package.</td>
</tr>
<tr>
<td>share/doc</td>
<td>Contains the ClusteringSuite manuals (pdf version).</td>
</tr>
<tr>
<td>share/example</td>
<td>Contains an example to illustrate the package operation.</td>
</tr>
</tbody>
</table>
```

Table 1.1: Package contents description
1.2 Running the cluster analysis example

As listed in Table 1.1, in the ClusteringSuite package we include an example to illustrate the basic operation of BurstClustering, the main analysis tool included in the package. If you move into the directory share/example you will find the files 6 listed in Table 1.2.

The XML configuration files provided use Completed Instructions hardware counter, PAPI_TOT_INS in PAPI terminology, and Instructions Per Cycle (IPC), derived using PAPI_TOT_INS / PAPI_TOT_CYC counters, as clustering parameters. It sets a duration filter of 1000µs and a Completed Instructions filter of $3 \times 10^8$. It configures the extrapolation of all the counters present in the input trace and defines a single output plot combining the two clustering metrics, depicting the raw values.

The input trace provided is a two iteration chop from an execution with 16 tasks of SU3_AHiggs, a lattice quantum chromodynamics code, part of the PRACE benchmark suite.

1.2.1 Executing BurstClustering tool

You can execute the cluster analysis with the provided XMLs without modification running the following command:

```bash
> BurstClustering -d cluster.xml -i su3.lat256_2it.16tasks.prv -o su3.lat256_2it.16tasks.clustered.prv
```

As a result of this execution, the 'BurstClustering' tool will detect 14 clusters in the input data.

1.2.2 BurstClustering outputs

The BurstClustering tool will generate the following outputs:

- `su3.lat256_2it.16tasks.clustered.[prv|pcf|row]`: a Paraver trace with clusters information. You can load this trace in Paraver, and use the clustering configuration files to analyse the clusters behaviour with the time context. In the default distribution of Paraver, these configuration files are installed in the directory `$PARAVER_HOME/cfgs/clustering`.

---

Table 1.2: Contents of share/example directory

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>README</td>
<td>Text file with the same instructions of this section.</td>
</tr>
<tr>
<td>cluster_explained.xml</td>
<td>Clustering configuration XML file with brief descriptions about the different fields.</td>
</tr>
<tr>
<td>cluster.xml</td>
<td>Same clustering configuration XML file as the previous one, without the descriptions.</td>
</tr>
<tr>
<td>su3.lat256_2it.16tasks.[prv</td>
<td>pcf</td>
</tr>
</tbody>
</table>

---

1. http://www.prace-ri.eu/ueabs#QCD - Kernel B
• **su3.lat256_2it.16tasks.clustered.clusters_info.csv**: a CSV file with clusters statistics, including the aggregated duration of each cluster, the average duration of the bursts of each cluster, and the average values of the cluster parameters and the extrapolation parameters. You can import this file to a regular spreadsheet application to analyse the clusters behaviour as a group.

• **su3.lat256_2it.16tasks.clustered.IPC.PAPI_TOT_INS.gnuplot**: a GNUPlot script to observe the resulting clusters in a 2D scatter plot. To visualize it, execute:

```
> gnuplot su3.lat256_2it.16tasks.clustered.IPC.PAPI_TOT_INS.gnuplot
```

• **su3.lat256_2it.16tasks.clustered.DATA.csv**: a CSV file with the characterization of each burst read from the input trace, including its clustering and extrapolation parameters value, as well as the timestamps and cluster id assigned. This file is used by the GNUPlot script, but you can also load it in a spreadsheet or any other software to analyse the different CPU burst instances that took part in the cluster analysis process.

### 1.3 About Extrae and Paraver

**Extrae** and **Paraver** are two of the core tools of the BSC Performance Analysis Tools ecosystem.

**Extrae** is a dynamic instrumentation package to trace programs compiled and run with the shared memory model (like OpenMP and pthreads), the message passing (MPI) programming model or both programming models (different MPI processes using OpenMP or pthreads within each MPI process). It generates trace files that can be latter visualized with **Paraver**.

**Paraver** is a flexible parallel program visualization and analysis tool based on an easy-to-use GUI. **Paraver** was developed responding to the need of having a qualitative global perception of the application behavior by visual inspection and then to be able to focus on the detailed quantitative analysis of the problems. **Paraver** provides a large amount of information useful to decide the points on which to invest the programming effort to optimize an application.

#### 1.3.1 Where the Extrae and Paraver can be found?

The **Extrae** and **Paraver** distributions can be found at URL:

```
http://www.bsc.es/performance-tools/downloads
```

This tools are open-source (LGPL v2), so you can download both the source code and precompiled packages for different architectures and operating systems.

If you have any doubts about how to download these tools, you can send an e-mail to BSC Tools support at tools@bsc.es.
Chapter 2

The BurstClustering tool

In the previous chapter we have seen how to unpack the contents of the ClusteringSuite package, and also how to execute our first cluster analysis using the BurstClustering tool. In this chapter, we deeply describe the operation of this tool, both the inputs it requires and the outputs it generates. For this reason, some descriptions of the previous chapter can be repeated in the current one.

2.1 BurstClustering operation

The BurstClustering tool receives two inputs, the ParaVer trace where the information will be extracted and a XML configuration file, where the user indicates the clustering parameters, extrapolation parameters, etc. With this two inputs, the tool first extracts the data from the ParaVer trace, as defined in the XML file, then applies the cluster algorithm and finally creates the different outputs.

In brief, the cluster analysis process its composed by 6 steps. First four steps are required to generate the XML configuration file, while the last two are the execution of the BurstClustering tool itself and the observation and analysis of the results.

1. Select the clustering/extrapolation parameters.
2. Define the filters and normalization applied to the input data
3. Select the cluster algorithm and its parameters
4. Define the output plots
5. Execute the cluster analysis
6. Analyse the tool outputs

The actual definition of the different records in the XML file are described in the following chapter, while this one include the guidelines to detect the information it will contain.

1. Select the clustering parameters

The first decision to take when performing a cluster analysis is which of the data present in the input trace will be used to describe each CPU burst, in the ClusteringSuite terminology, we call them simply the parameters.
Using the Paraver vocabulary, a CPU burst is expressed in a trace as a State Record of value 1 (Running State). The parameters available to characterize a CPU burst are those events that appear at the end time of the given Running State. As a Paraver event is a pair event/value, in the XML file we use the event type to indicate events we whose values will be stored in the different bursts. We can also use Running State duration (difference between end time and begin time) as a CPU burst parameter.

In the XML we will express those parameters that will be used by the cluster algorithm, the clustering parameters, and those that will be used in the extrapolation process, the extrapolation parameters. The parameters can be defined as single event reads (single events) or combinations of pair of events (mixed events). In case we use the CPU burst duration, it will always be used as a clustering parameter.

It could be obvious, but to define the different parameters it is essential to know first which ones we want to use and which are the event type codification present in the trace. To do that we need to go through to the Paraver Configutarion File (.pcf file generated by Extrae) and check which events appear in the trace and their event type encoding. Almost in all analyses we use the Performance Hardware Counters events, being Completed Instructions and IPC the usual metrics combinations used by the cluster algorithm.

2. Define the filters and normalizations

Once knowing which are the clustering parameters, we have to decide the possible filters we want to apply. The filters prevent the cluster algorithm of analysing CPU bursts that can bias the result or do not add any valuable information. We found two different filters: a duration filter to discard those burst whose duration is shorter than a given value, and a range filter that can be defined to each parameter and eliminates those bursts than are out of the boundaries.

To tune the duration filter we use the stats tools provided by the CEPBA-Tools package. Using the -bursts_histo parameter this tool computes a plot as the one presented in Figure 2.1 for a given Paraver trace. This plot is an histogram where the $x$ axis is the duration of the CPU bursts and quantifies both the aggregated time of the CPU bursts, the green bars, and the number of bursts, the red line. Observing this plot we can select the duration that eliminates de maximum number of bursts (red line at left of the select duration), while maintaining a high value of aggregated time (green bars at right of the selected point). For example, in the Figure 2.1 a reasonable duration filter will be 10 milliseconds.

With respect to the normalizations, we provide the possibility of applying first a logarithmic normalization, useful when the parameter range is wide and can bias the results of the cluster analysis. The logarithmic normalization can be applied to each parameter independently. The second normalization is a pure range normalization to set the parameter values in range $[0, 1]$, following the formula range ($\forall a_i \in A, a_i \leftarrow (a_i - \min(A))/(\max(A) - \min(A))$). When using the range normalization, it will be applied to each parameter used, so as to guarantee that all of them have the same weight in the analysis. If we to add more weight one of the parameters used in the cluster analysis, we can apply a multiplicative factor.

To clarify how the different normalizations and filters work, this is the order as they are applied: when a CPU burst is read, its duration is checked and then the different parameters that have range filters defined; to those bursts that pass the filters its performed the logarithmic normalization of each parameter that requires it and afterwards the range normalization. Finally, the scaling factor is applied.
3. Select the output plots

We can combine the parameters defined previously to generate GNUplot scripts of 2D and 3D scatter-plots. The plots can print both the normalized data or the raw data (before normalizations). The user can tune the ranges to print and also the axis-labels of the plots. In addition, users can let the library to produce all 2D plots obtained combining all metrics defined.

Once having the parameters, filters and plots, we can run the application ClusteringDataExtractor to extract the data and produce the plots described before running the cluster algorithm. The resulting plots will show all the data available, distinguishing between the duration filtered bursts, the range filtered bursts and the ones that will take part in the cluster analyses. These plots are an useful aid to fine tune the parameter filters and normalizations.

4. Select the cluster algorithm

Even though the Aggregative Cluster Refinement and DBSCAN are the two basic algorithms offered by the ClusteringSuite package, there is a few more clustering algorithms offered to the user. Table 2.1 contains the list of these algorithms and their parameters. It is interesting to note that the Aggregative Cluster Refinement is the only algorithm that does not require any parameter and it not have to be expressed in the XML configuration file.

For further information about the different algorithms included in the package, we point to the following papers: [1] for DBSCAN algorithm, [2] for GMEANS and [3] for CAPEK, PAM and XCLARA.

In case of DBSCAN we provide the application DBSCANParametersApproximation to help the parameter selection, according to the technique described in [1].
<table>
<thead>
<tr>
<th>Cluster Algorithm Name</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>DBSCAN</td>
<td>epsilon, min_points</td>
</tr>
<tr>
<td>GMEANS</td>
<td>critical_value, max_clusters</td>
</tr>
<tr>
<td>CAPEK(^1)</td>
<td>k</td>
</tr>
<tr>
<td>MUSTER_PAM(^1)</td>
<td>max_clusters</td>
</tr>
<tr>
<td>MUSTER_XCLARA(^1)</td>
<td>max_clusters</td>
</tr>
</tbody>
</table>

\(^1\) libClustering includes a common interface to this algorithms offered by the MUSTER library [http://tgamblin.github.com/muster/main.html](http://tgamblin.github.com/muster/main.html)

Table 2.1: Cluster algorithms included in the libClustering and their parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Required parameters</strong></td>
<td></td>
</tr>
<tr>
<td>-d &lt;clustering_definition.xml&gt;</td>
<td>Clustering definition XML to be used</td>
</tr>
<tr>
<td>-i &lt;input_trace.prv&gt;</td>
<td>Input (Paraver) trace to be used</td>
</tr>
<tr>
<td>-o &lt;output_trace.prv&gt;</td>
<td>Output (Paraver) trace with cluster information added</td>
</tr>
<tr>
<td><strong>Optional parameters</strong></td>
<td></td>
</tr>
<tr>
<td>-h</td>
<td>Show help message and exit</td>
</tr>
<tr>
<td>-s</td>
<td>Performs a silent execution, without informative messages</td>
</tr>
<tr>
<td>-m &lt;number_of_samples&gt;</td>
<td>Performs a cluster analysis using the number of burst indicated and classifying the rest</td>
</tr>
<tr>
<td>-a[f]</td>
<td>Generates an output file with the aligned sequences (in FASTA format when using <code>-af</code>)</td>
</tr>
<tr>
<td>-ra[p]</td>
<td>Executes the Aggregative Cluster Refinement instead of the cluster algorithm indicated in the XML. When using <code>-rap</code> generates plots and outputs from intermediate steps</td>
</tr>
<tr>
<td>-t</td>
<td>Print accurate timings (in (\mu)seconds) of different algorithm parts</td>
</tr>
<tr>
<td>-e EvtType1, EvtType2,...</td>
<td>Changes the Paraver trace processing, to capture information by the events defined instead of CPU bursts</td>
</tr>
</tbody>
</table>

Table 2.2: BurstClustering tool parameters
5. Execute the cluster analysis

Once defined the different elements necessary to perform the analysis, we need to execute the BurstClustering tool. The different parameters of this tool and a short description of them are listed in Table 2.2. Basically, to perform a regular analysis using the cluster algorithm defined in the XML file we need to execute the command:

```
> BurstClustering -d <clustering_definition.xml> -i <input_trace> -o <output_trace>
```

The tool will process the information provided in the configuration file, extract the data from the input trace, execute the cluster algorithm and then generate the required output plots, extrapolation files and the output trace. These files will be explained in the further step.

In case we want to execute the Aggregative Cluster Refinement algorithm, the command varies slightly:

```
> BurstClustering -d <clustering_definition.xml> -ra -i <input_trace> -o <output_trace>
```

By adding the `-ra` parameter, the tool discards the algorithm indicated in the clustering definition XML file and then applies this different algorithm. In case we use the parameter `-rap`, the tool will produce, apart from the regular outputs, the traces and plots of intermediate steps of the Aggregative Cluster Refinement algorithm.

6. BurstClustering tool outputs

The BurstClustering offers three main outputs: scatter-plots of the different metrics, a cluster statistics file (including the extrapolation) and a reconstructed Paraver trace. In addition, it also generates the refinement tree, when using the Aggregative Cluster Refinement. Optionally, it can produce the a file with the sequence alignment and a file containing the Cluster Sequence Score values. Here we will describe briefly all of them.

The scatter-plots are simply GNUplot scripts that can be load using this plotting tool. As seen in previous steps, they can be 2 or 3 dimensional combinations of different metrics used to characterize the CPU bursts. In any case, the points in the scatter plots are coloured to distinguish the different clusters found. These plots are useful to observe, qualitatively, variations in the clusters with respect to the metrics used. In Figure 2.2 we show 4 different plots combining 8 different hardware counters. First plot, 2.2a, show the metrics used by the cluster algorithm. In the rest of combinations we can observe that the clusters represent clear isolated clouds, with a minor exception of the plot comparing Main Memory Accesses vs. L2 Data Cache Accesses, 2.2c, where Cluster 4 (in red) appear in two different clouds.

The plot scripts are named using the output trace prefix plus a trailing string expressing the combination of metrics used. They have the extension `.gnuplot`. All of them use a file ended in `.DATA.csv` that contain on each line the different parameters described in the XML file plus the cluster identifier assigned for each CPU burst analysed.

The clustering statistics file is a CSV file that contains the number of individuals, the aggregated duration and the average duration per CPU burst, and the average values of extrapolation parameters defined in XML, for each cluster found. This file is really useful to analysed quantitatively the behaviour of the different clusters found. The clusters statistics file is named using the prefix of the input trace, but ending in `.clusters_info.csv`. 

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Figure 2.2: Output plots produced by BurstClustering tool combining different metrics
Next output that is always produced is the **output trace**. Basically, this is exactly the same input trace where all the CPU burst have been surrounded using a certain events to identify them. Thanks to these events, we can take advantage of the vast analysis power of Paraver and Dimemas to perform further analyses and correlate the clusters with all the information present on the trace. For example, we can observe the time-line distribution of the different computation regions detected. An example of Paraver time-line and its corresponding duration profile can be seen in Figure 2.3.

We provide a set of Paraver configuration files with pre-defined views and histograms related to cluster events.

In case we executed the Aggregative Cluster Refinement algorithm, the tool will also produce a **refinement tree** file. This file has the same prefix as the output trace and the extension `TREE.dot`. It is a text file that describes the refinement tree using the DOT language. To visualize it we require the GraphViz\(^1\) software package. We also recommend using of the interactive tool `xdot\(^2\)` to navigate through the refinement tree output. An example of a refinement tree can be seen in Figure 2.4.

Finally, using the parameter `-a`, the tool will produce a CSV file containing the sequences obtained after applying the Cluster Sequence Score. This file, named as the output trace with the extension `.seq`, contains the sequence of the cluster identifiers (numbers) and gaps (marked as hyphens) introduced by the alignment algorithm for each task and thread present on the input trace. If use the parameter `-af`, the file will be generated in the FASTA format, transforming the first 21 clusters in an amino-acid identifier. The FASTA file can be load in any alignment software, such as ClustalX\(^3\) for its visualization. In Figure 2.5 we can see a ClustalX window with a set of aligned sequences.

If we use any of these last two parameters, the tool will also produce a file with the extension `SCORES.csv`, that contains the numerical results of the Cluster Sequence Score.

When using the Aggregative Cluster Refinement with the parameter `-rap` the tool will produce the plots, traces, refinement trees, sequence files and score files for each refinement step. The intermediate statistics files will not be generated and these intermediate trace files will only contain cluster events, to check the intermediate cluster distribution, but not to correlate them with other information. The intermediate files will have an inter-fix `STEPX` in their file name, to distinguish at which step (iteration) of refinement were produced.

Finally, it is interesting to note that we guarantee the colour coherence in all those outputs generated by the BurstClustering that use colour information to distinguish the cluster identifiers. In case of ClustalX we provide a modified version of software package with the required amino-acid colouring.

\(^{1}\)http://www.graphviz.org/
\(^{2}\)http://code.google.com/p/jrfonseca/wiki/XDot
\(^{3}\)http://www.clustal.org/
Figure 2.3: A ParaVer time-line and profile showing information related to a cluster analysis
Figure 2.4: Example of a refinement tree produced by BurstClustering tool
Figure 2.5: ClustalX sequence alignment window
Chapter 3

Creating the clustering definition XML

In this chapter we deeply describe the structure of the clustering definition XML.

3.1 Clustering definition XML description

In brief, the clustering definition XML file contains the description of four elements of the clustering process: the parameters associated to each CPU burst in the trace used by cluster analysis and the extrapolation process; the filtering ranges and normalizations applied to this data; the cluster algorithm to be used; and finally, the description of the different output plots, generated as GNUplot scripts. We can see how these different parts are distributed in the XML file in Figure 3.1.

Following the current description of the file it could be easily generated using a regular text editor or a XML editor.

3.2 Parameter selection

There are two ways to define how the parameters are read from a Paraver trace. First, the values of individual events situated at the end of the Running State, using single_event nodes. Second, combining the values of two different events with a basic mathematical operation, using mixed_events nodes.

A single_event node, see Figure 3.2a, contains first two attributes: apply_log that indicates if a logarithmic normalization will be applied to its values; the name parameter is the label the will be used in the different output file. The inner node event_type is mandatory, to define the event type that appears in the Paraver trace. Optional nodes range_min and range_max are used to filter the CPU burst outside these boundaries. Finally, optional node factor is a multiplicative value so as to weight the parameter value.

A mixed_events node, see Figure 3.2b, is pretty similar to the previous one, but includes two mandatory internal nodes event_type_a and event_type_b, to define the two types of events involved, and the attribute operation to define the mathematical operation applied to the values read. Possible operations are +, -, *, and /. The operation is applied to the values of the two events defined, before the logarithmic normalization.

To define the CPU bursts parameters that will be used by the cluster algorithm, they have to be placed below the clustering_parameters node, see Figure 3.1. To define those that will be used to characterize the resulting clusters (as averages in the clusters_info.csv file), we have to place them below the extrapolation_parameters node.
Figure 3.1: Clustering definition XML file structure
If we want to use the duration of the CPU bursts as a parameter, we need to set to yes the attribute use_duration present in the root node (clustering_definition).

Filtering and normalization

The filtering and normalization is expressed at two points of the XML file. We have seen that the parameter definition nodes include both a range filtering and also a logarithmic normalization. The filtering information included in the extrapolation parameters is not taken into account.

The second point is the root node. In this node we find different attributes, see Figure 3.1 regarding filters and normalizations. First one is apply_log, that indicates if logarithmic normalization will be applied to the burst duration, if used. Next one is normalize_data, that indicates if a final range normalization will be applied to the values of all parameters (independently). Next we find the duration_filter, expressed in µs, to discard those burst with less duration than the indicated. Finally, the threshold_filter is a percentage to discard all the clusters found whose aggregated duration represents less percentage of the total clusters duration than the indicated.

Output plots

Once defined the parameters used to characterize the CPU bursts, below the output_plots node we can define the output plots combining the different metrics.

If we set the attribute all_plots of this main node to yes, the libTraceClustering library will generate all possible 2D plots combining the parameters defined (clustering parameters and extrapolation parameters). If we want to manually define the combinations we can use the plot_definition structure, see Figure 3.3.

What we find first in the plot_definition node is the attribute raw_metrics. In case we applied normalization to the clustering parameters setting this attribute to “yes” indicates that the resulting plot will use the raw values of the parameters. Then we find three kind of nodes [x|y|z]_metric. Each of these nodes has a mandatory attribute title that will be used as the plot label for the corresponding axis. They have two optional attributes max and min to define the axis range. Finally, the content of each of these nodes must be the name attribute of any of the parameters defined previously (clustering parameter of extrapolation parameter). In case we want
to use the duration, as it is defined differently from regular parameters, it has to be referenced simply using the text `Duration`.

We can combine up to three metrics to create a 3 dimensional scatter-plot, where the individuals will be distinguished in series according to the cluster identifier assigned. The same is applicable when using just two metrics (`x` and `y`). If we just define a single metric (`x metric`), the resulting plot will be a 2 dimensional plot using the cluster identifier as `y axis`. 

Figure 3.3: `plot definition` node of the clustering definition XML.
Bibliography

