Anomaly Detection in HPC Centers

High Performance Computing

High Performance Computing

HPC refers to HW/SW infrastructures for particularly intensive workloads

High Performance Computing

HPC is (somewhat) distinct from cloud computing

- Cloud computing is mostly about running (and scaling) services
- ...HPC is all about performance

Typical applications: simulation, massive data analysis, training large ML models

HPC systems follow a batch computation paradigm

- Users send jobs to the systems (i.e. configuration for running a program)
- Jobs end in one of several queues
- A job scheduler draws from the queue
- ...And dispatches jobs to computational nodes for execution

High Performance Computing

HPC systems can be large and complex

E.g. Leonardo, 7-th on the top 500 list on June 2024

7	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy	1,824,768	241.20	306.31	7,494

- The system has 1,824,768 cores overall!

Configuring (and maintaining the configuration) of these systems

- ...Is of paramount importance, as it has an impact on the performance
- ...Is challenging, due to their scale and the presence of node heterogeneity

Hence the interest in detecting anomalous conditions

The Dataset

As an example, we will consider the DAVIDE system

Small scale, energy-aware architecture:

- Top of the line components (at the time), liquid cooled
- An advanced monitoring and control infrastructure (ExaMon)
- ...Developed together with UniBo

The system went out of production in January 2020

The monitoring system enables anomaly detection

- Data is collected from a number of samples with high-frequency
- Long term storage only for averages over 5 minute intervals
- Anomalies correspond to unwanted configurations of the frequency governor
- ...Which can throttle performance to save power or prevent overheating

A Look at the Dataset

Our dataset refers to the non-idle periods of a single node

In [3]:
```
print(f'#examples: {hpc.shape[0]}, #columns: {hpc.shape[1]}')
hpc.iloc[:3]
```

```
#examples: 6667, #columns: 161
```

Out[3]:

	timestamp	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p0_12	cmbw_p0_13	cmbw_p0_14	cmbw_p0_
0	2018-03-05 22:45:00	0.165639	0.006408	0.012176	0.166835	0.238444	0.230092	0.145691	0.227682	0.000094
1	2018-03-05 22:50:00	0.139291	0.007772	0.057400	0.166863	0.238485	0.230092	0.145691	0.227682	0.176855
2	2018-03-05 22:55:00	0.141048	0.000097	0.000000	0.166863	0.238444	0.230092	0.145691	0.227682	0.252403

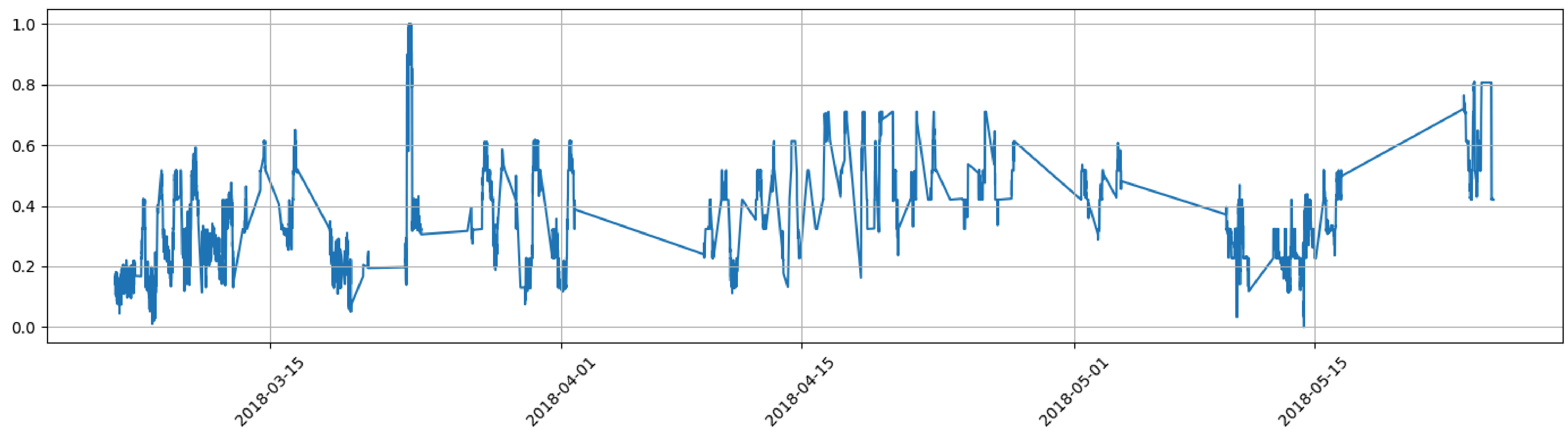
3 rows × 161 columns

- This still a time series, but a multivariate one

A Look at the Dataset

How to display multivariate series? Approach #1: showing individual columns

In [4]:
```
tmp = pd.Series(index=hpc['timestamp'], data=hpc[inputs[0]].values)
util.plot_series(tmp, figsize=figsize)
```



A Look at the Dataset

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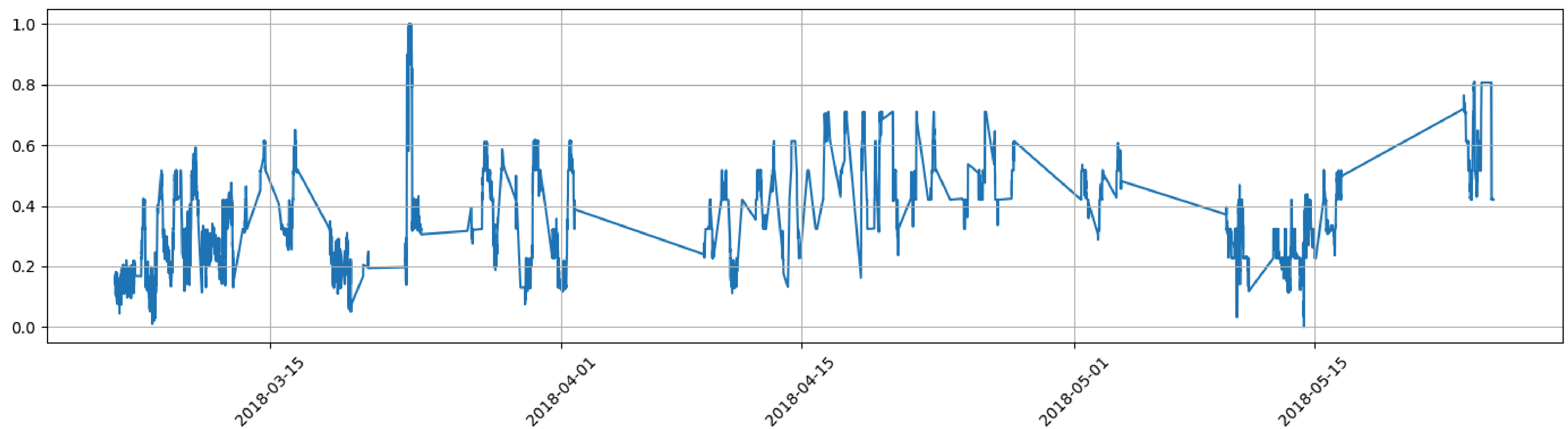


- The series contains significant gaps (i.e. the idle periods)

A Look at the Dataset

Approach #2: obtaining statistics

In [5]:
```
hpc[inputs].describe()
```

Out[5]:

	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p0_12	cmbw_p0_13	cmbw_p0_14	cmbw_p0_
count	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.00000
mean	0.357036	0.138162	0.060203	0.119616	0.160606	0.184970	0.118305	0.151434	0.143033
std	0.166171	0.128474	0.090796	0.098597	0.128127	0.163190	0.104490	0.120793	0.125052
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	0.227119	0.000073	0.000020	0.000000	0.000000	0.000000	0.000000	0.000000	0.000117
50%	0.323729	0.136095	0.000082	0.166835	0.238444	0.230092	0.145691	0.227682	0.174933
75%	0.470254	0.261908	0.134976	0.166984	0.238566	0.230406	0.145908	0.227779	0.251910
max	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000

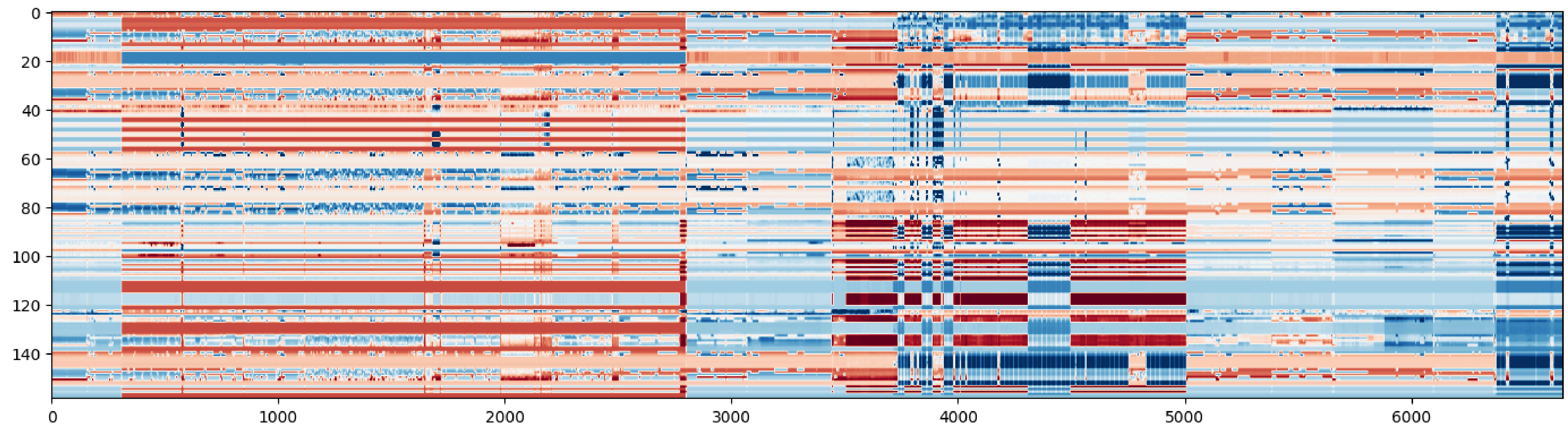
8 rows × 159 columns

- No missing value, normalized data

A Look at the Dataset

Approach #3: standardize, then use a heatmap

In [6]:
```
hpcsv = hpc.copy()
hpcsv[inputs] = (hpcsv[inputs] - hpcsv[inputs].mean()) / hpcsv[inputs].std()
util.plot_dataframe(hpcsv[inputs], figsize=figsize)
```



- White = mean, red = below mean, blue = above mean

Anomalies

There are three possible configurations of the frequency governor:

- Mode 0 or "normal": frequency proportional to the workload
- Mode 1 or "power saving": frequency always at the minimum value
- Mode 2 or "performance": frequency always at the maximum value

On this dataset, this information is known

...And it will serve as our ground truth

- We will focus on discriminating normal from non-normal behavior
- I.e. we will treat both "power saving" and "performance" cases as anomalous

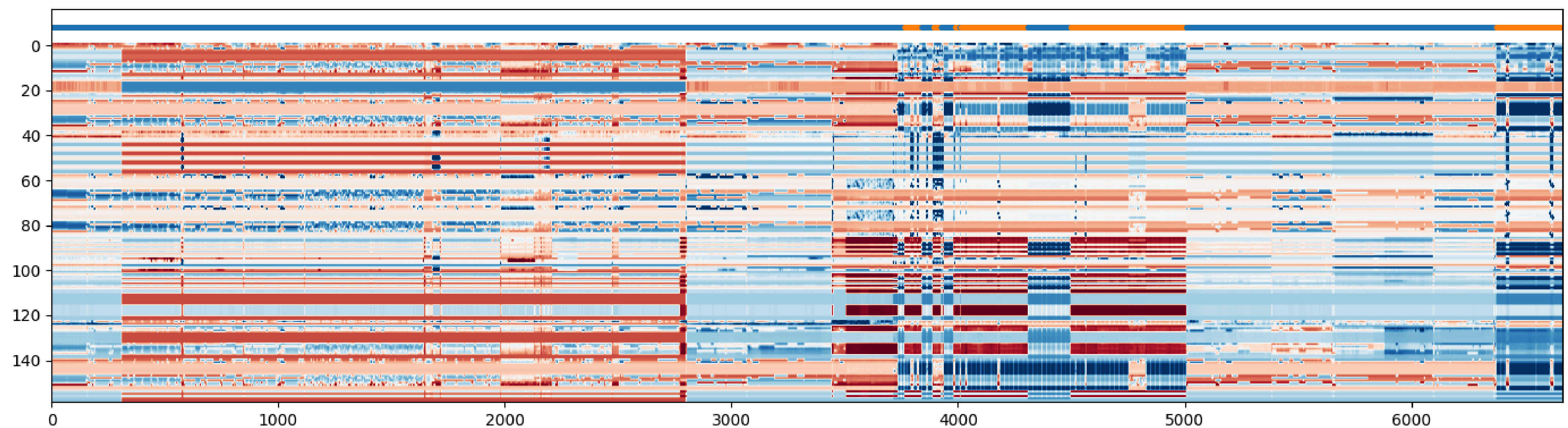
Detecting them will be challenging

- Since the signals vary so much when the running job changes

Anomalies

We can plot the location of the anomalies:

In [7]:
```
labels = pd.Series(index=hpcsv.index, data=(hpcsv['anomaly'] != 0), dtype=int)
util.plot_dataframe(hpcsv[inputs], labels, figsize=figsize)
```



- On the top, blue = normal, orange = anomaly

A KDE Approach

KDE Approach

Let's try first a density estimation approach (once again using KDE)

First, we standardize the data again, based on training information alone

```
In [8]: tr_end, val_end = 3000, 4500

        hpcs = hpc.copy()
        tmp = hpcs.iloc[:tr_end]
        hpcs[inputs] = (hpcs[inputs] - tmp[inputs].mean()) / tmp[inputs].std()
```

- This is needed so that we do not accidentally exploit test set information
- The training set separator was chosen so as not to include anomalies

Then we can separate training, validation, and test data:

```
In [9]: trdata = hpcs.iloc[:tr_end]
        valdata = hpcs.iloc[tr_end:val_end]
        tsdata = hpcs.iloc[val_end:]
```

A KDE Approach

Then we calibrate the bandwidth and generate the alarm signal

In [10]:
```
%%time
opt = GridSearchCV(KernelDensity(kernel='gaussian'), {'bandwidth': np.linspace(0.1, 1, 10)},
opt.fit(trdata[inputs])
print(f'Best parameters: {opt.best_params_}')

ldens = opt.score_samples(hpcs[inputs])
signal_kde = pd.Series(index=hpcs.index, data=-ldens)
```

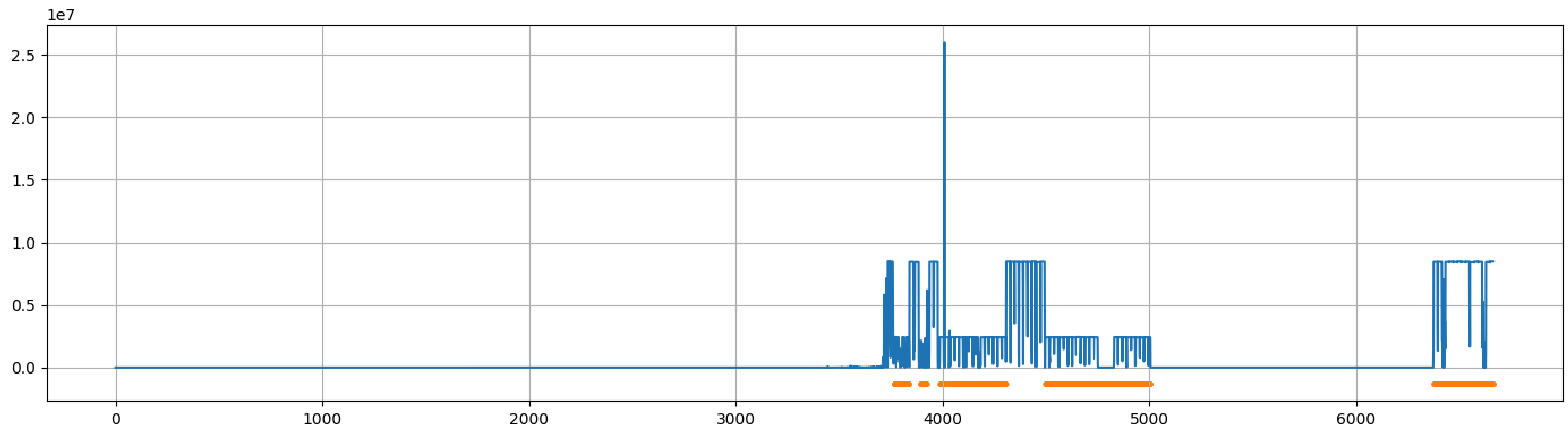
```
Best parameters: {'bandwidth': 0.5}
CPU times: user 9.27 s, sys: 114 ms, total: 9.38 s
Wall time: 9.38 s
```

Both operations are relatively expensive: why?

KDE Approach

There is a good match with the anomalies, but also some spurious peaks

In [11]:
```
util.plot_signal(signal_kde, labels, figsize=figsize)
```



- This is mostly due to the large variations due to job changes

KDE Approach

We then need to define the threshold, but for that we need a cost model

Our main goal is to detect anomalies, not anticipating them

- Misconfigurations in HPC are usually not critical
- ...And cause little issue, unless they stay unchecked for very long

We will use a simple cost model:

- c_{alarm} for false positive (erroneous detections)
- c_{missed} for false negatives (undetected anomalies)
- Detections are fine as long as they are within $tolerance$ units from the anomaly

In [12]:
```
c_alarm, c_missed, tolerance = 1, 5, 12
cmodel =  util.HPCMetrics(c_alarm, c_missed, tolerance)
```

The implementation details can be found in the `util` utility module

KDE Approach

We can now optimize the threshold over the validation set

```
In [13]: th_range = np.linspace(1e4, 2e5, 200)
         th_kde, val_cost_kde = util.opt_threshold(signal_kde[tr_end:val_end],
                                                   valdata['anomaly'],
                                                   th_range, cmodel)
         print(f'Best threshold: {th_kde:.3f}')
         tr_cost_kde = cmodel.cost(signal_kde[:tr_end], hpcs['anomaly'][:tr_end], th_kde)
         print(f'Cost on the training set: {tr_cost_kde}')
         print(f'Cost on the validation set: {val_cost_kde}')
         ts_cost_kde = cmodel.cost(signal_kde[val_end:], hpcs['anomaly'][val_end:], th_kde)
         print(f'Cost on the test set: {ts_cost_kde}')
```

```
Best threshold: 148442.211
Cost on the training set: 0
Cost on the validation set: 263
Cost on the test set: 265
```

- The `opt_threshold` function runs the usual line search process
- In this case the training and validation set are completely separated

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KDE-based approaches work well, but have some issues

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- ...And more data is needed to obtain reliable results

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- The more the samples in the training set
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Third, KDE gives you nothing more than an anomaly signal

- Determining the cause of the anomaly is up to a domain expert
- This is ok in low-dimensional spaces, but harder on high-dimensional ones