In [3]:

```python
# ============================================================
# Notebook setup: run this before everything
# ============================================================

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(15, 4.5)

from sklearn.neighbors import KernelDensity
from sklearn.model_selection import GridSearchCV
from util import util
import numpy as np
from matplotlib import pyplot as plt
import pandas as pd
import os

# Load data
data_file = os.path.join('..', 'data', 'hpc.csv')
hpc = pd.read_csv(data_file, parse_dates=['timestamp'])

# Identify input columns
inputs = hpc.columns[1:-1]
ninputs = len(inputs)
```

```
The autoreload extension is already loaded. To reload it, use:
  %reload_ext autoreload
```

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 [16]:
```
print(f'#examples: {hpc.shape[0]}, #columns: {hpc.shape[1]}')
hpc.iloc[:3]
```

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

Out[16]:

	timestamp	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	c
0	2018-03-05 22:45:00	0.165639	0.006408	0.012176	0.166835	0.238444	
1	2018-03-05 22:50:00	0.139291	0.007772	0.057400	0.166863	0.238485	
2	2018-03-05 22:55:00	0.141048	0.000097	0.000000	0.166863	0.238444	

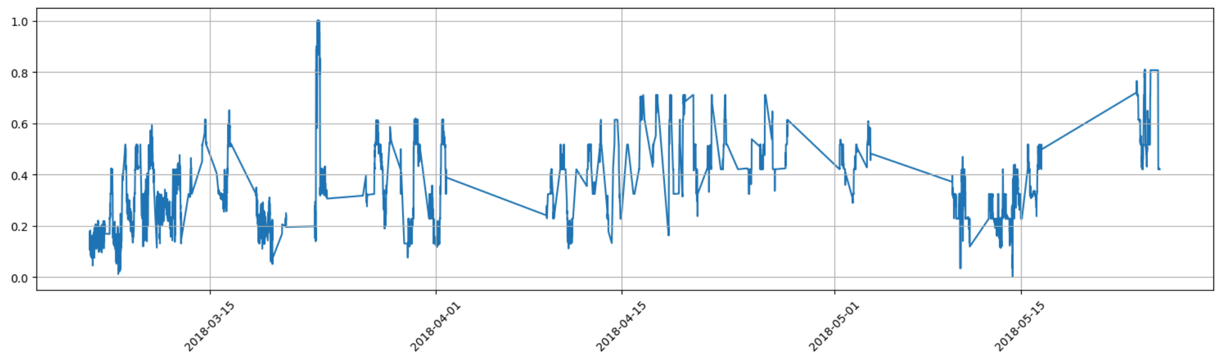
3 rows × 161 columns

- 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 [5]:
```
tmp = pd.Series(index=hpc['timestamp'], data=hpc[inputs[0]].values)
util.plot_series(tmp, figsize=figsize)
```



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

A Look at the Dataset

Approach #2: obtaining *statistics*

In [6]:
```
hpc[inputs].describe()
```

Out[6]:

	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p
count	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.00
mean	0.357036	0.138162	0.060203	0.119616	0.160606	0.18
std	0.166171	0.128474	0.090796	0.098597	0.128127	0.16
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.00
25%	0.227119	0.000073	0.000020	0.000000	0.000000	0.00
50%	0.323729	0.136095	0.000082	0.166835	0.238444	0.23
75%	0.470254	0.261908	0.134976	0.166984	0.238566	0.23
max	1.000000	1.000000	1.000000	1.000000	1.000000	1.00

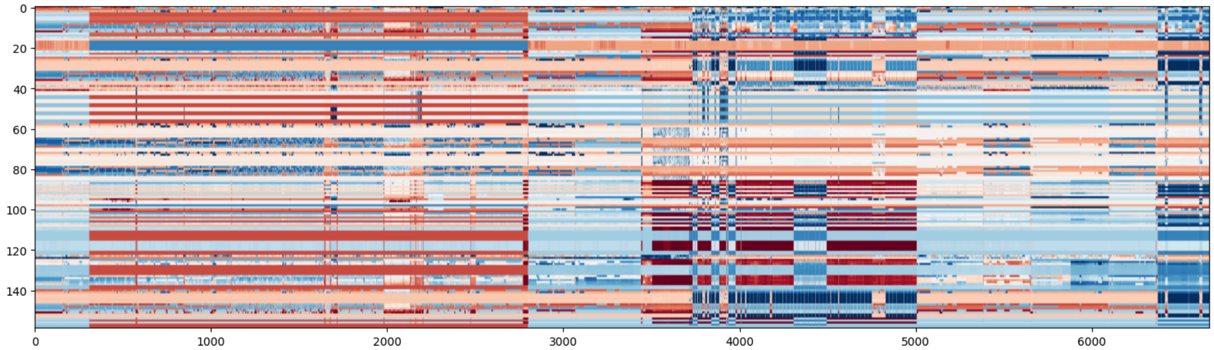
8 rows × 159 columns

- No missing value, *normalized* data

A Look at the Dataset

Approach #3: standardize, then use a *heatmap*

In [7]:
```
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*

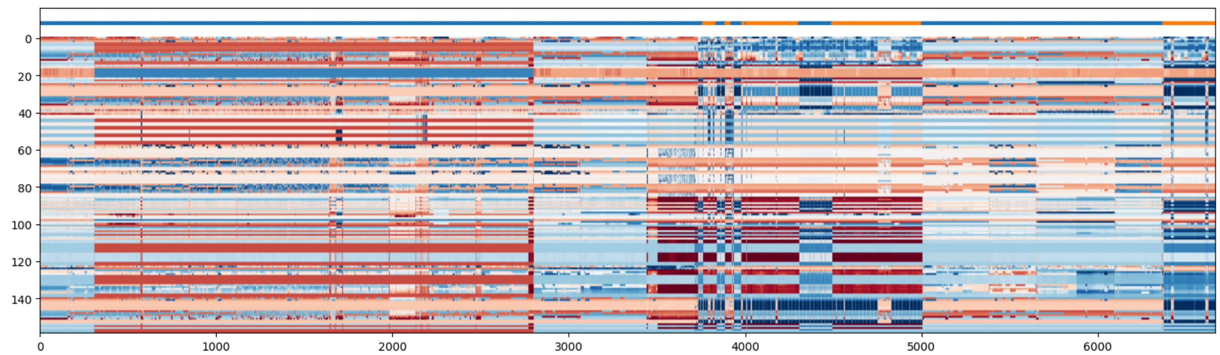
- Since the signals vary so much when the running job changes

Anomalies

We can plot the location of the anomalies:

In [8]:

```
labels = pd.Series(index=hpcsv.index, data=(hpcsv['anomaly'] != 0), dtype=ir
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 [9]:
```
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 [10]:
```
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 [11]:
```
%%time
opt = GridSearchCV(KernelDensity(kernel='gaussian'), {'bandwidth': np.linspa
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)
```

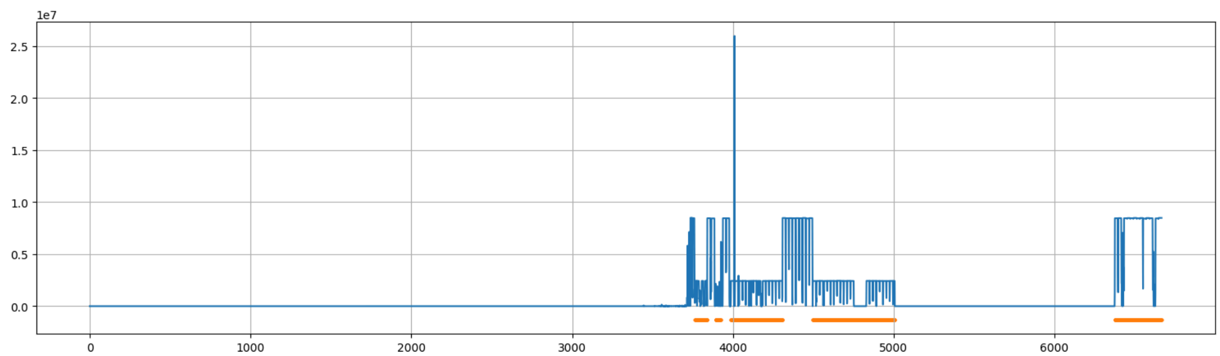
```
Best parameters: {'bandwidth': np.float64(0.5)}
CPU times: user 9.63 s, sys: 34.9 ms, total: 9.67 s
Wall time: 9.67 s
```

> **Both operations are relatively expensive: why?**

KDE Approach

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

In [12]:
```
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 [13]:
```
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 [14]:
```
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_
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:], t
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

The Trouble with KDE

KDE-based approaches work well, but have some *issues*

First, KDE itself runs into trouble with *high-dimensional data*:

- With a larger dimensionality, *prediction times* grows...
- ...And *more data* is needed to obtain reliable results

Second, KDE has trouble with *large training sets*

- The more the samples in the training set
- ...The more the terms to be summed to obtain a density

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*