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An approach to data mining inside PostgreSQL based on parallel implementation of UDFs

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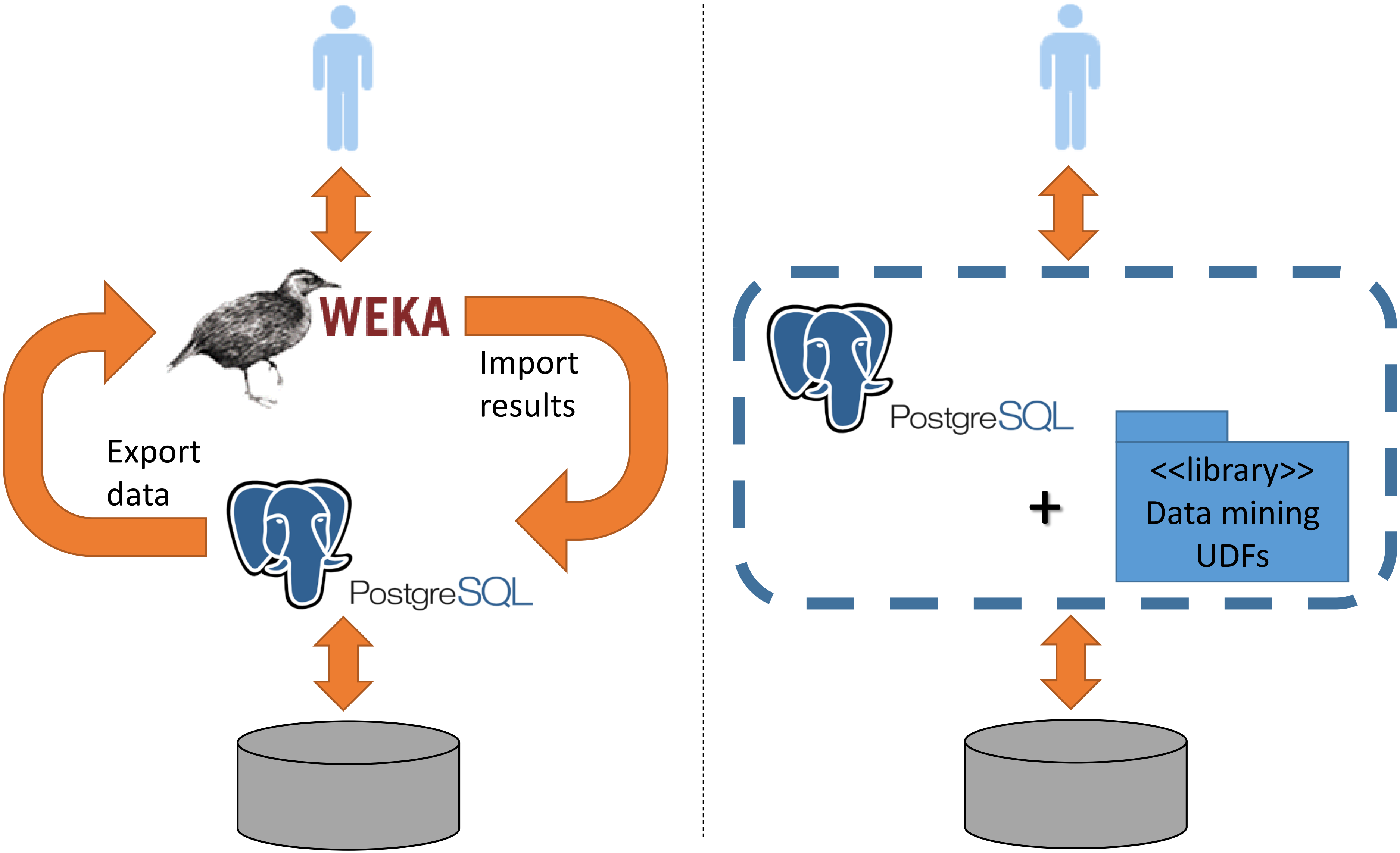
Data mining outside *vs.* inside DBMS



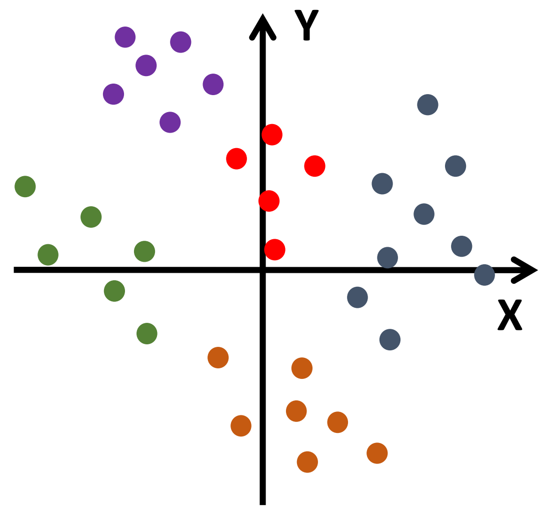
Data mining inside DBMS

Points

X	Y	Z	I	J	K	…
…						
…						

dim=2 k=5

```
procedure Clustering (
  inpTable text,  -- Input table name
  dim int,        -- # of columns
  k int,          -- # of clusters
  Eps real        -- Accuracy
) return text
begin
…
end
```




```
sql> exec Clustering('Points', 2, 5, 0.001);
```

X	Y	CLUSTER
…	…	
…	…	
…	…	
…	…	
…	…	

Data mining inside PostgreSQL

```
#include <libpq-fe.h> // API of PostgreSQL
#include "pgmining.h" // API of pgMining library

void main (void)
{
   char *inpTable = "Points“;// Table with data to be mined
   int dim = 3;                // Number of columns
   int k = 5;                  // Number of clusters
   float Eps = 0.001;          // Accuracy
   char *outTable = "Clusters"; // Table to save mining results

   // Connect to server
   char *conninfo = "user=postgres port=5432 host=localhost";
   PGconn *conn = PQconnectdb (conninfo);

   // Call mining UDF
   pgClustering (conn, inpTable, dim, k, Eps, outTable);

   PQexec (conn, strcat ("SELECT * FROM ", outTable));// Show results
   PQfinish (conn); // Cleanup
}
```

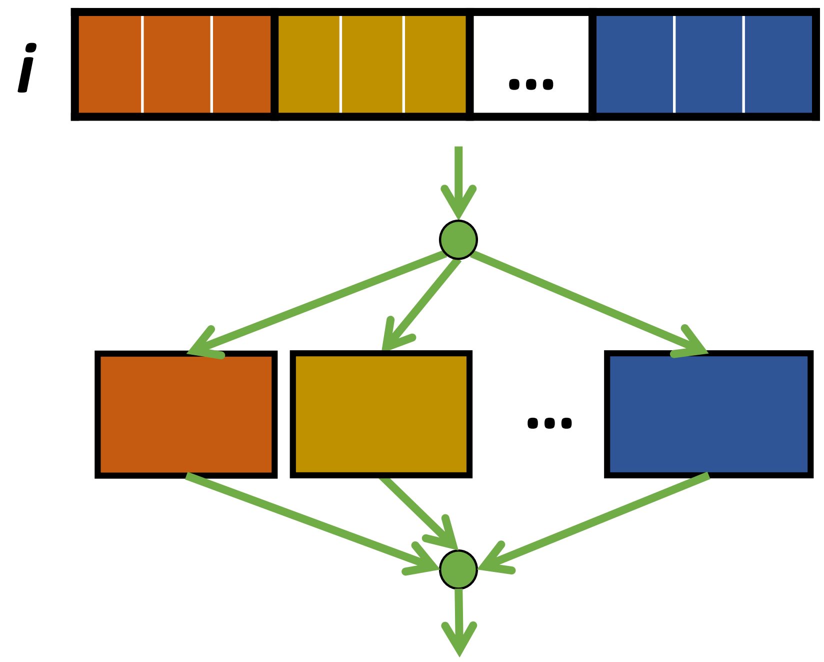
What mining UDF encapsulates

- Parallel implementation by OpenMP

```
#pragma omp parallel for
for (i=0; i<n; i++) {
  ...
  ...
}
```

fork

join



What mining UDF encapsulates

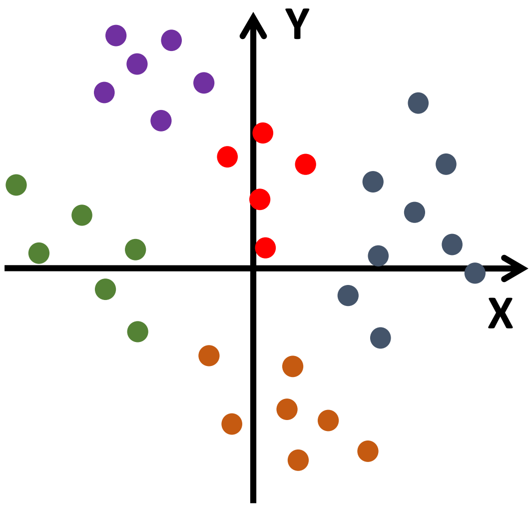
- … for Intel MIC (Many Integrated Core) platforms

Device / Feature	Intel Xeon X5680	**Intel Xeon Phi, Knights Corner** SE10X	**Intel Xeon Phi, Knights Landing** 7250
# of physical cores	6	**61**	**68**
Hyper threading factor	2	**4**	**4**
# of logical cores	12	**244**	**272**
Frequency, GHz	3.33	**1.1**	**1.4**
Vector processing unit	No	**512 bit**	**512 bit**
Bootable	Yes	**No**	**Yes**
Peak performance, TFLOPS	0.371	**1.076**	**3.046**

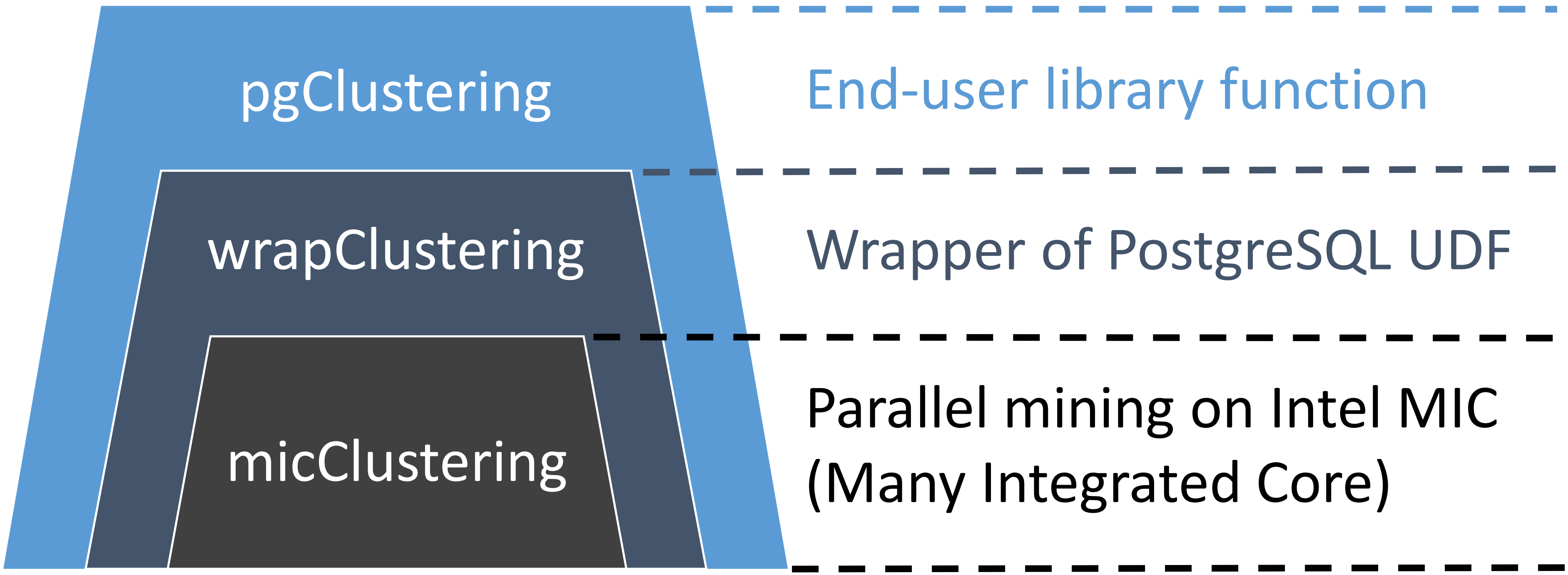

What mining UDF encapsulates

- Using cache of pre-computed mining structures
  - E.g. distance matrix to perform clustering

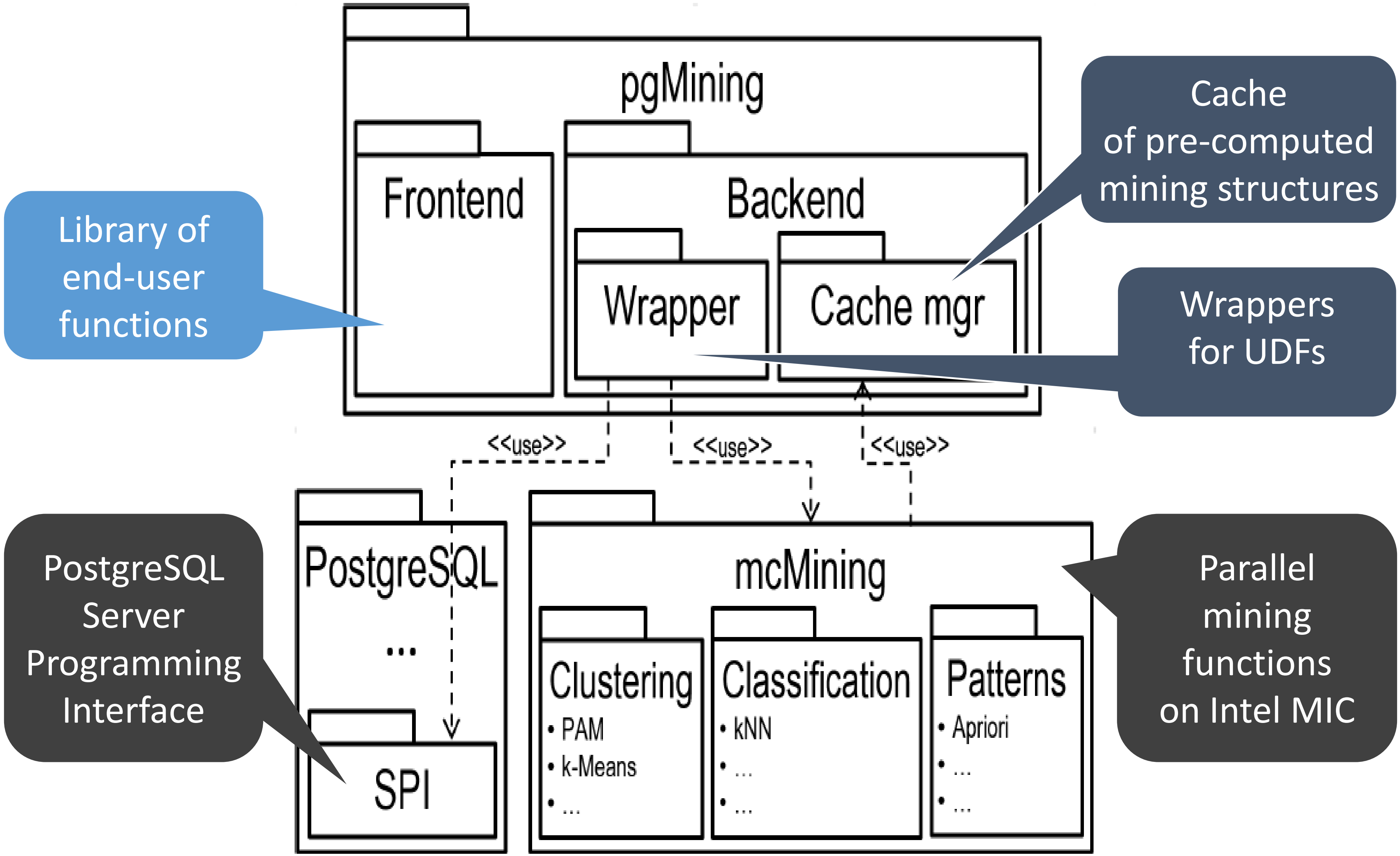
	0	1	...	*n*-1
0	0	dist(a_0, a_1)	...	dist(a_0, a_{n-1})
1		0	dist(a_1, a_j)	dist(a_1, a_{n-1})
...			0	dist(a_j, a_{n-1})
***n*-1**				0



How mining UDF is designed



Module structure



End-user library function

```
int pgClustering (
   PGconn * conn,     // ID of PostgreSQL connection
   char * inpTable,   // Name of input table
   int dim,           // Number of coordinates in data point
   int k,             // Number of clusters
   float Eps,         // Accuracy
   char * outTable)   // Name of output table
{
   // Register UDF
   PQexec (conn, "CREATE OR REPLACE FUNCTION
   wrapClustering (text, integer, integer, real) RETURNS text AS
       ' pgmining ', 'wrapClustering' LANGUAGE C STRICT;");
   // Create resulting table
   PQexec (conn, "CREATE %s TABLE IF NOT EXISTS (data text)",
              outTable);
   // Execute UDF
   return PQexec (conn, "INSERT INTO %s
       SELECT wrapClustering (%s, %d, %d, %f);",
              outTable, inpTable, dim, k, Eps);
}
```

Wrapper of PostgreSQL UDF


```
Datum wrapClustering(PG_FUNCTION_ARGS)
{
    // Extract input parameters of clustering
    // from the PostgreSQL parameters
        char * inpTable = text_to_cstring (PG_GETARG_TEXT_P (0));
        int dimension = PG_GETARG_INT32 (1);
        int k = PG_GETARG_INT32 (2);
        float Eps = PG_GETARG_FLOAT4 (3);
        int N;

    // Check if we have pre-calculated mining structures
    // in our cache, else calculate (in parallel) and load it
        void * distMatr = cache_getObject (strcat (inpTable, "_distMatrix" ));
        if (distMatr == NULL) {
                // Check if input table is in our cache
                void * inpData = cacheGet (inpTable);
                if (inpData == NULL) {
                        // Allocate memory and load input table to cache
                        inpData = (float4 *) palloc (dimension * sizeof (float4));
                        wrapTabRead (inpData , inpTable, dim, &N);
                        cachePut (inpTable, inpData, sizeof (inpData));
                }
                distMatr = micCalcDistMatr (inpData, dim, N);
                cache_putObject (strcat (inpTable, "_distMatrix"), distMatr, sizeof (distMatr));
        }

    // Cluster data (in parallel) using mining structures
    // and save results in output table
        micClusteringRes * outData = micClusteringResCreate ();
        micClustering (N, k, Eps , outData , distMatr);
        PG_RETURN_TEXT (data2String(outData));
}
```

Wrapper of PostgreSQL UDF

```
Datum wrapClustering(PG_FUNCTION_ARGS)
{
   // Extract input parameters of clustering
   // from the PostgreSQL parameters
   char * inpTable = text_to_cstring (PG_GETARG_TEXT_P (0));
   int dim = PG_GETARG_INT32 (1);
   int k = PG_GETARG_INT32 (2);
   float Eps = PG_GETARG_FLOAT4 (3);
   int N;

   // Check if we can use pre-calculated mining structures
   void * distMatr = cacheGet(strcat (inpTable , "_distMatr" ));
   if (distMatr == NULL) {
      // Check if input table is in our cache
      void * inpData = cacheGet (inpTable);
      if (inpData == NULL) {
         // Allocate memory and load input table to cache
         inpData = (float4 *) palloc (dim * sizeof (float4));
         wrapTabRead (inpData, inpTable, dim, &N);
         cachePut(inpTable, inpData, sizeof (inpData));
      }
      distMatr = micCalcDistMatr (inpData, dim, N);
      cachePut (strcat (inpTable, "_distMatr"), distMatr, sizeof (distMatr));
   }
   micClustering_res * outData = micClustering_resCreate ();
   micClustering (N, k, Eps, outData , distMatr); // Perform clustering
   PG_RETURN_TEXT (data2String(outData)); // Write results to the output table
}
```

Wrapper of PostgreSQL UDF

```
Datum wrapClustering(PG_FUNCTION_ARGS)
{
    char * inpTable = text_to_cstring (PG_GETARG_TEXT_P (0));
    int dim = PG_GETARG_INT32 (1);
    int k = PG_GETARG_INT32 (2);
    float Eps = PG_GETARG_FLOAT4 (3);
    int N;
    // Check if we can use pre-calculated distance matrix
    void * distMatr = cacheGet (strcat (inpTable, "_distMatr"));
    if (distMatr == NULL) {
       // Check if input table is in our cache and load if not
       void * inpData = cacheGet (inpTable);
       if (inpData == NULL) {
           inpData = (float4 *) palloc (dim * sizeof (float4));
           wrapTabRead (inpData, inpTable, dim, &N);
           cachePut (inpTable, inpData, sizeof (inpData));
        }
       // Calculate distance matrix in parallel and load it to cache
       distMatr = micCalcDistMatr (inpData, dim, N);
       cachePut (strcat (inpTable, "_distMatr"), distMatr,
                 sizeof (distMatr));
    }
    micClusteringRes * outData = micClusteringResCreate ();
    micClustering (N, k, Eps , outData , distMatr); // Perform clustering
    PG_RETURN_TEXT (data2String(outData)); // Write results to the output table
}
```

Wrapper of PostgreSQL UDF

```
Datum wrapClustering(PG_FUNCTION_ARGS)
{
    // Extract input parameters
    char * inpTable = text_to_cstring (PG_GETARG_TEXT_P (0));
    int dim = PG_GETARG_INT32 (1);
    int k = PG_GETARG_INT32 (2);
    float Eps = PG_GETARG_FLOAT4 (3);
    int N;
    // Check if we can use pre-calculated distance matrix
    void * distMatr = cacheGet (strcat (inpTable, "_distMatr"));
    if (distMatr == NULL) {
       // Check if input table is in our cache and load if not
       void * inpData = cacheGet (inpTable);
       if (inpData == NULL) {
            inpData = (float4 *) palloc (dim * sizeof (float4));
            wrapTabRead (inpData, inpTable, dim, &N);
            cachePut (inpTable, inpData, sizeof (inpData));
        }
       // Calculate distance matrix in parallel and load it to cache
       distMatr = micCalcDistMatr (inpData, dim, N);
       cachePut (strcat (inpTable, "_distMatr"), distMatr,
                    sizeof (distMatr));
    }

    // Cluster data (in parallel) using mining structures
    micClusteringRes * outData = micClusteringResCreate ();
    micClustering (N, k, Eps, outData, distMatr);
    // Save results in output table
    PG_RETURN_TEXT (data2String(outData));
}
```

Methods of Cache manager

- `void * cacheGet(char * objName)`

  // Searches for a specified object in the cache.

  // Updates internal statistics of the mined object
  // (number of calls, timestamp of recent call, etc.).

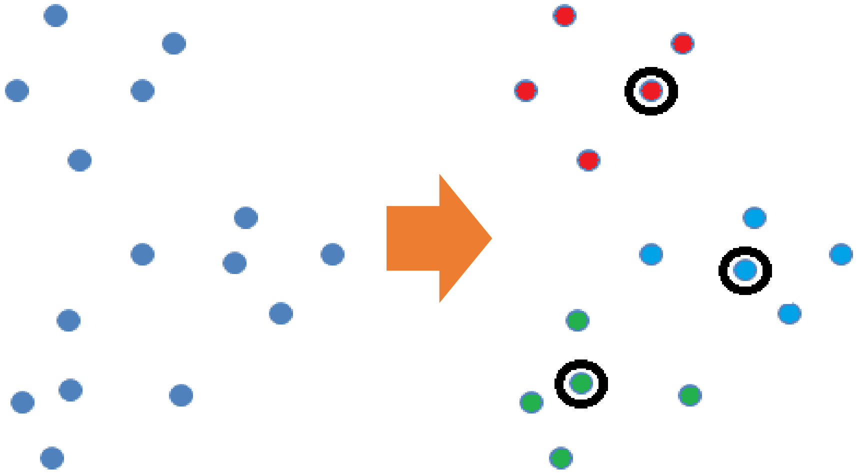
- `int cachePut(char * objName)`

  // Loads a specified object into the cache.

  // Pops out a victim object if it is not enough space in the cache
  // (according to a cache management policy,
  // e.g. Least Recently Used, Least Frequently Used, etc.).

PAM: Partition Around Medoids

- Goal
  - Organize *n* objects of data set in *k* clusters
- Key idea
  - Cluster centers are chosen as objects of data set (*medoids*)
- Method
  - BUILD phase
    - Initially choose cluster centers
  - SWAP phase
    - Iteratively move objects across clusters to improve value of an objective function



Parallel PAM: basic optimizations

```
void calcDistMatr (const float* rowData, const float* colData,
        float* distances, const int n, const int pointWidth){
  const int vecLen = 32;
  #pragma omp parallel
  {
    float point[pointWidth] __attribute__((aligned(64)));
    float result[vecLen]    __attribute__((aligned(64)));
    #pragma omp for
    for(int i=0; i<n; ++i){
      point[:]=rowData[i*pointWidth:pointWidth];
      for(int ii = 0; ii < n; ii += vecLen){
        result[:]=0;
        for(int j=0; j < pointWidth; ++j){
          const float* restrict point2 = colData+ii*pointWidth;
          result[:]+=(point[j]-point2[j*vecLen:vecLen])*
                     (point[j]-point2[j*vecLen:vecLen]);
        }
        distances[i*n+ii:vecLen] = sqrtf(result[:]);
      }
    }
  }
}
```

OpenMP
Rewriting loops
Loop tiling
Data alignment

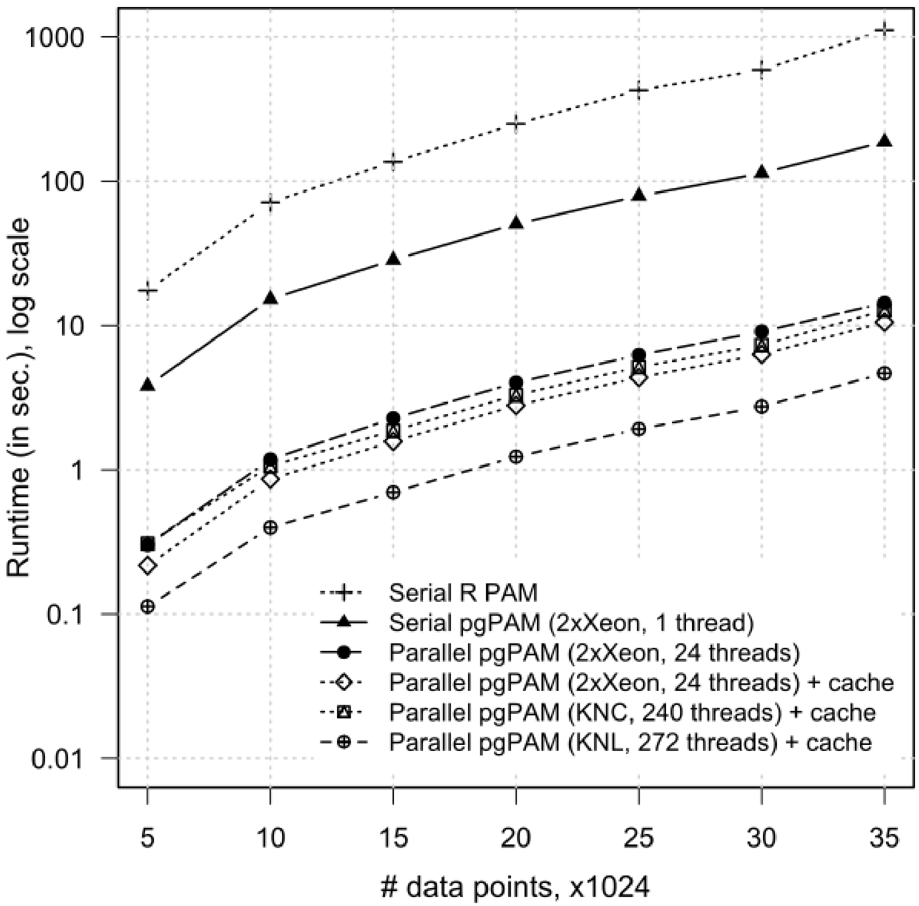
Experimental evaluation

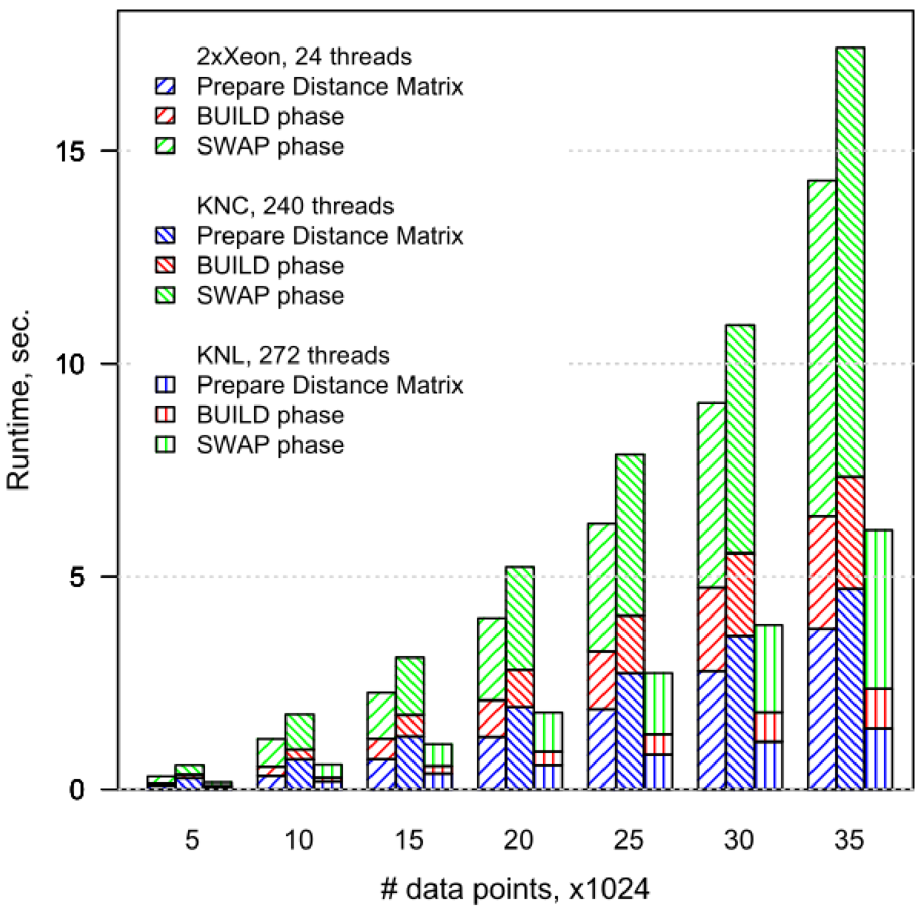
- Clustering algorithm: PAM (Partition Around Medoids)
  - Represents cluster centers as points of input data set (*medoids*)
  - *CALCULATION* of distance matrix
  - *BUILD phase*: initial clustering by the successive selection of medoids
  - *SWAP phase*: improving clustering according to an objective function
- Datasets

Name	dim	# of clusters	# of points, $\times 2^{10}$	Semantic
Census	67	10	35	Population surveys by the US Census Bureau
MixSim	5	10	35	Generator of synthetic datasets for evaluation of clustering algorithms
Power	3	10	35	Individual household electricity consumption
FCS Human	423	10	18	Aggregated human gene information

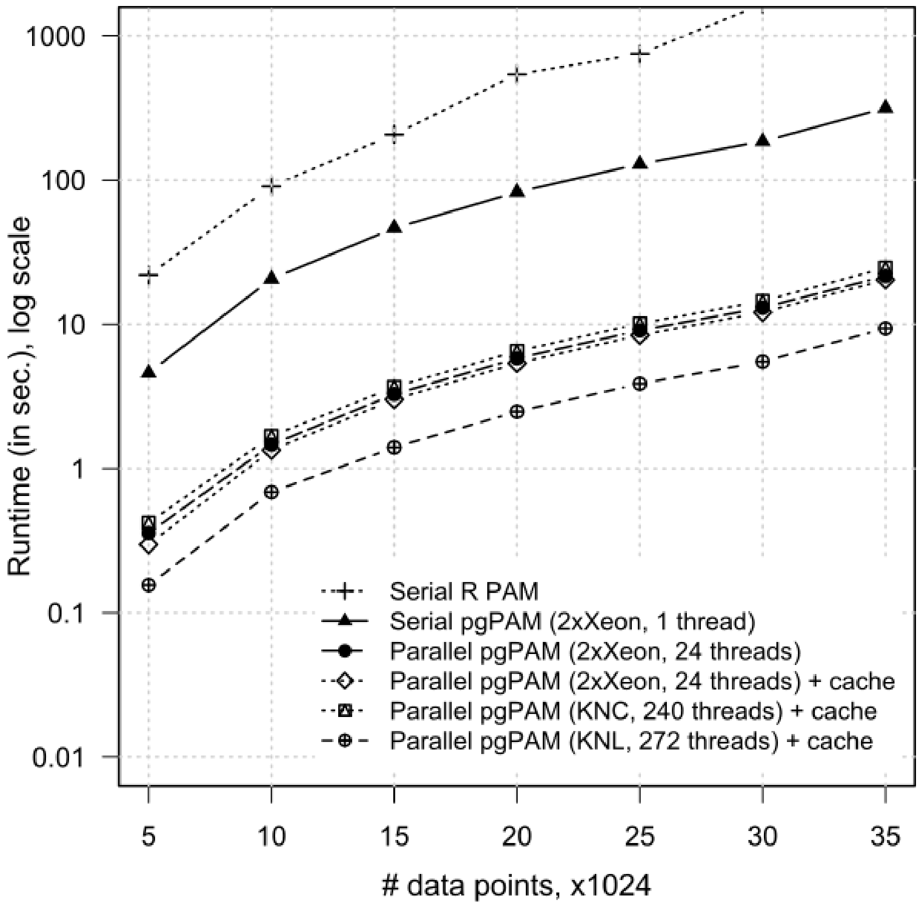
- Competitor: PAM algorithm of *R* data mining package

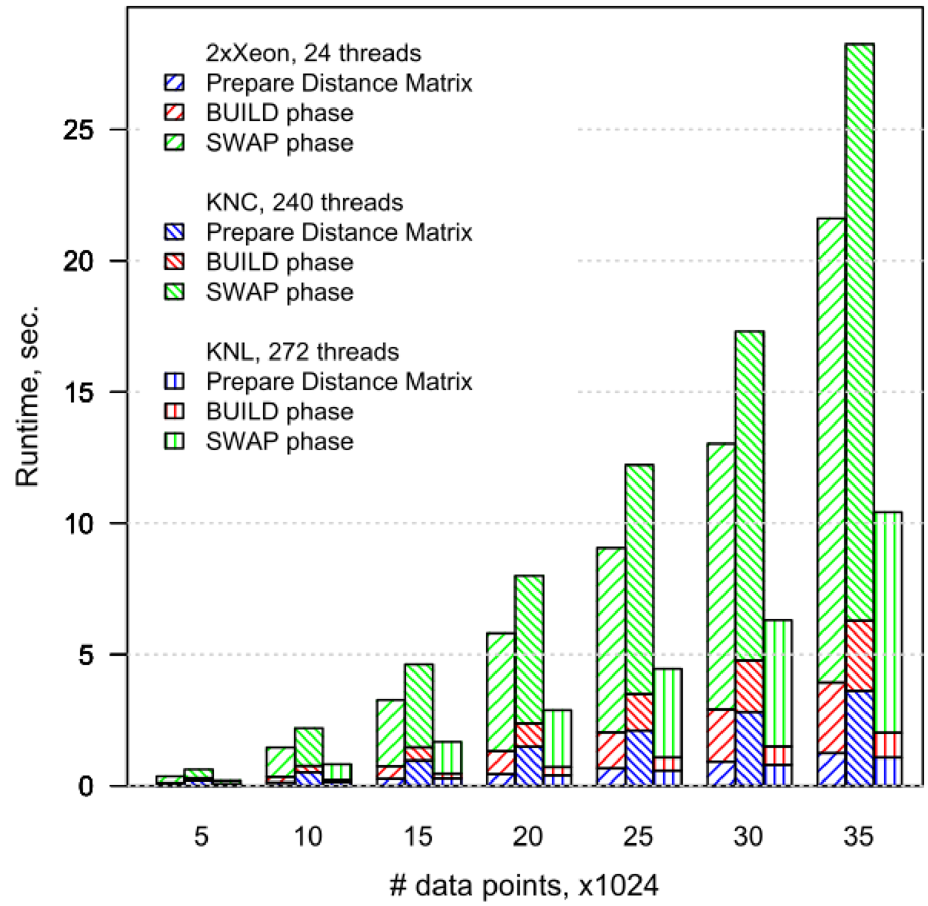
Performance: Census dataset



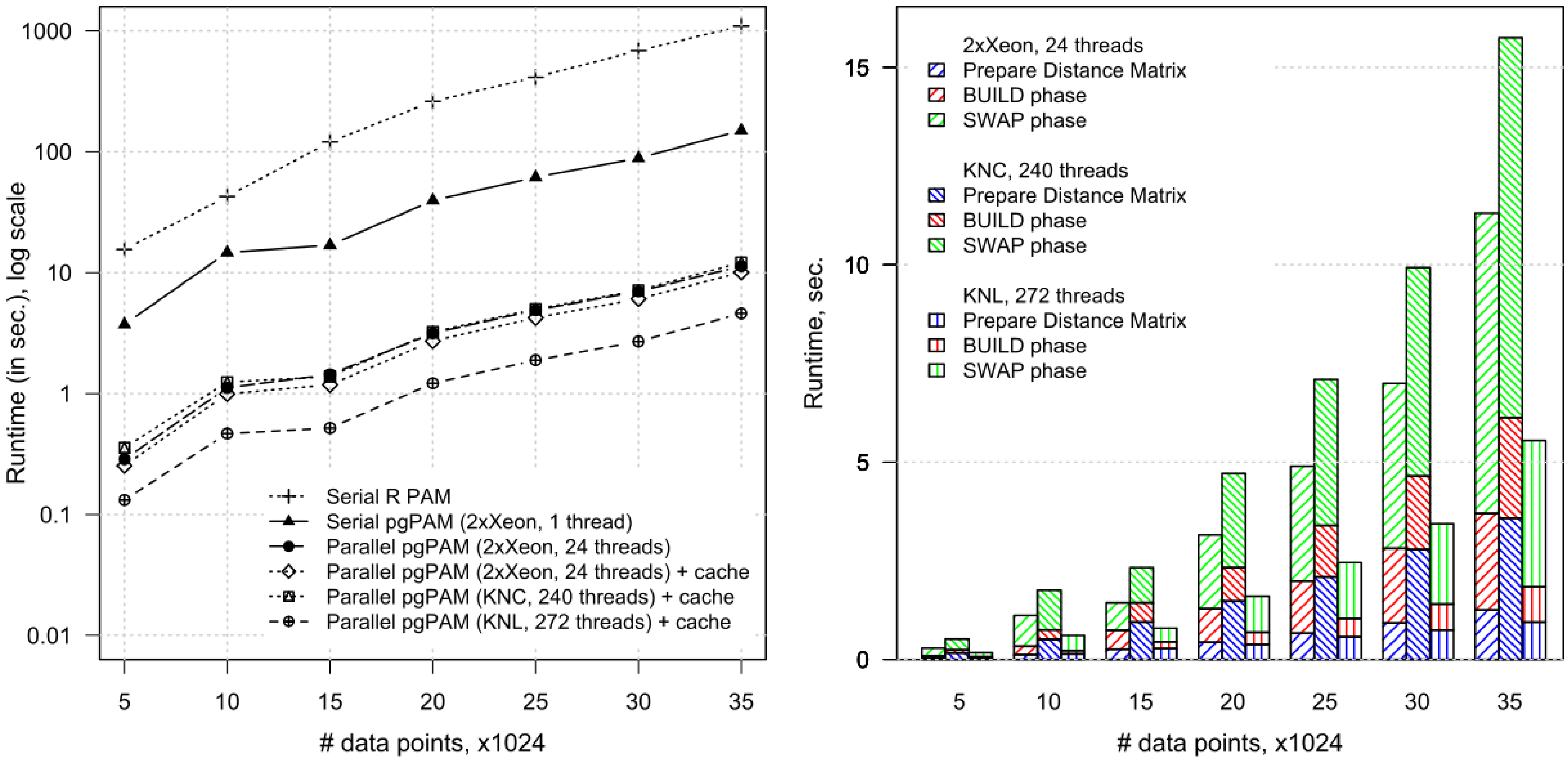


Performance: MixSim dataset

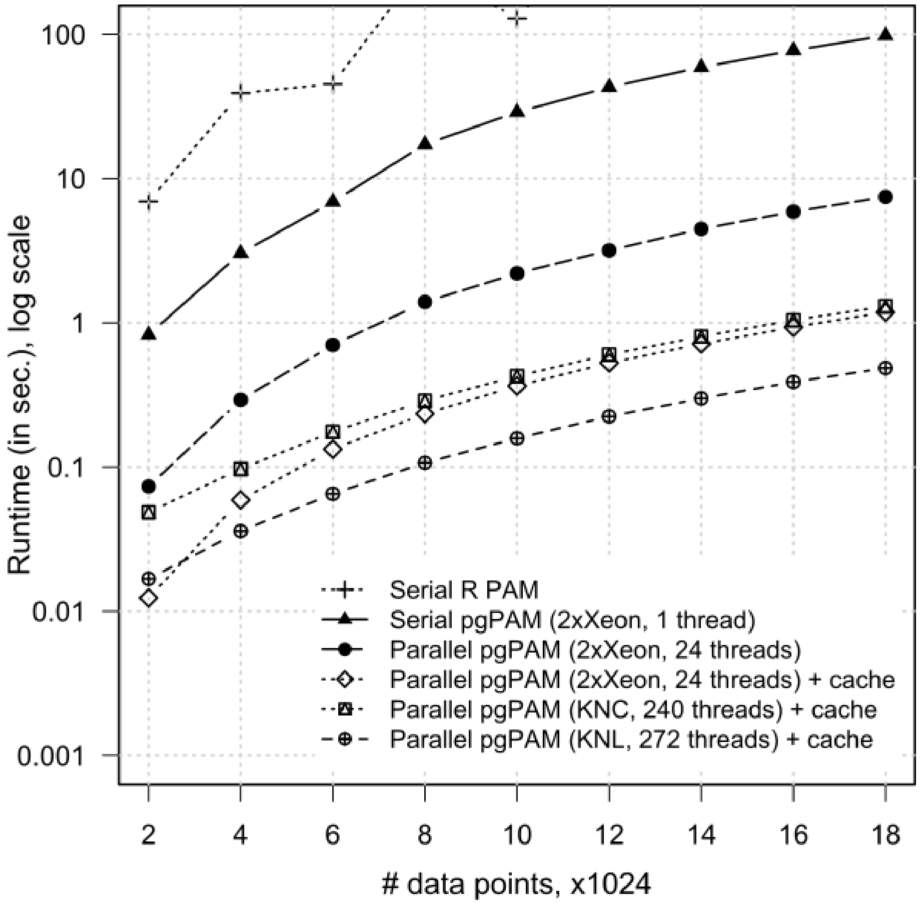


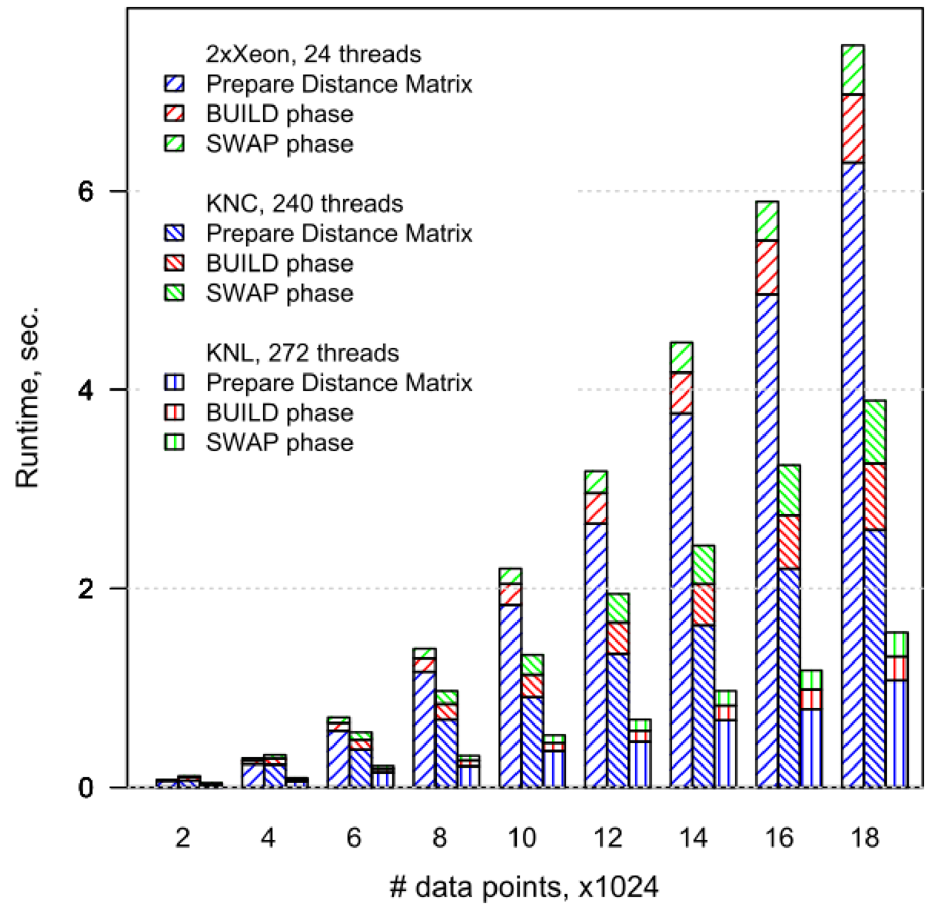


Performance: Power dataset

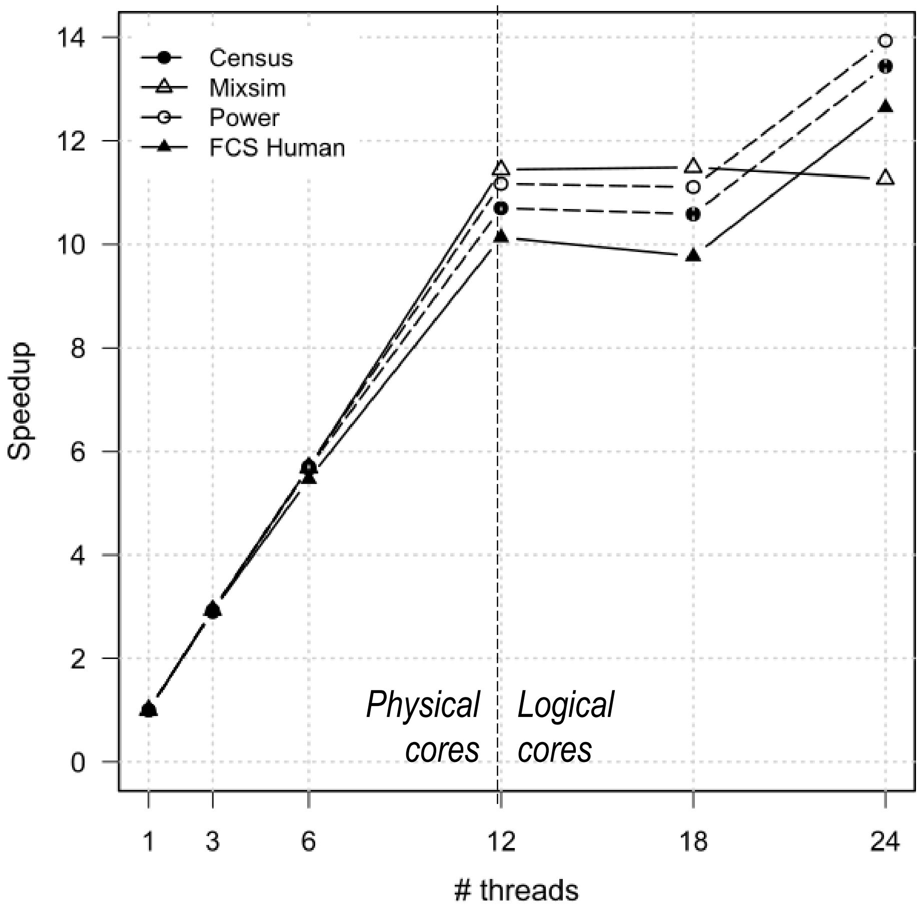


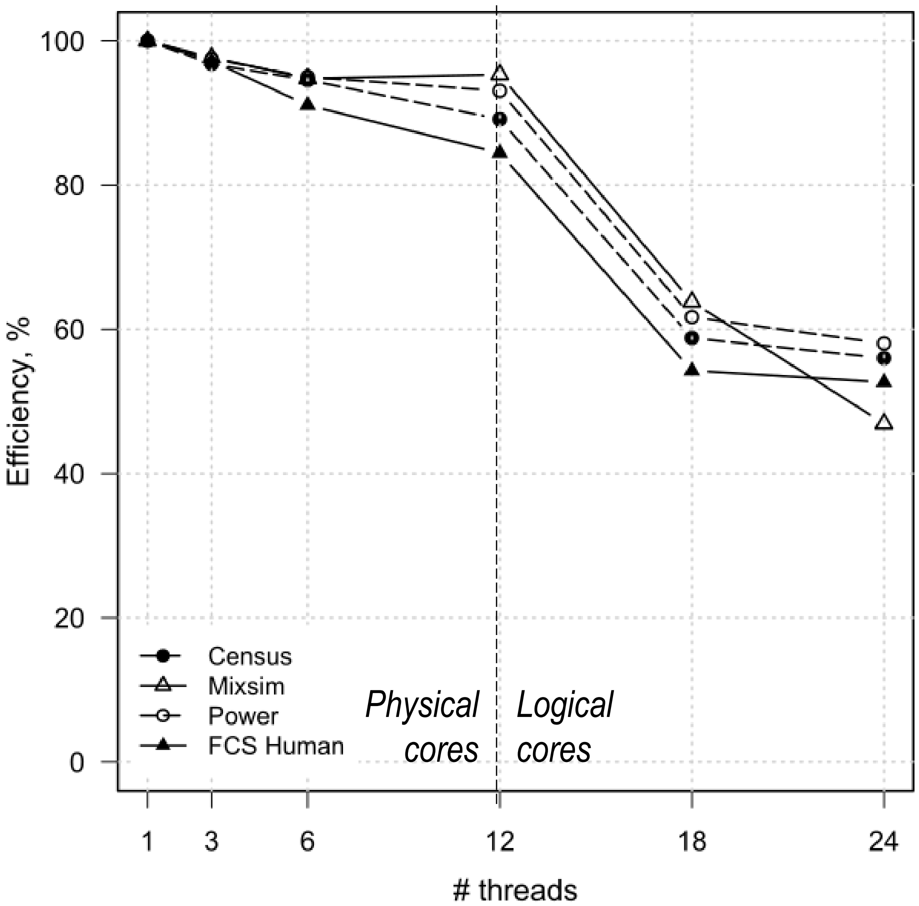
Performance: FCS Human dataset



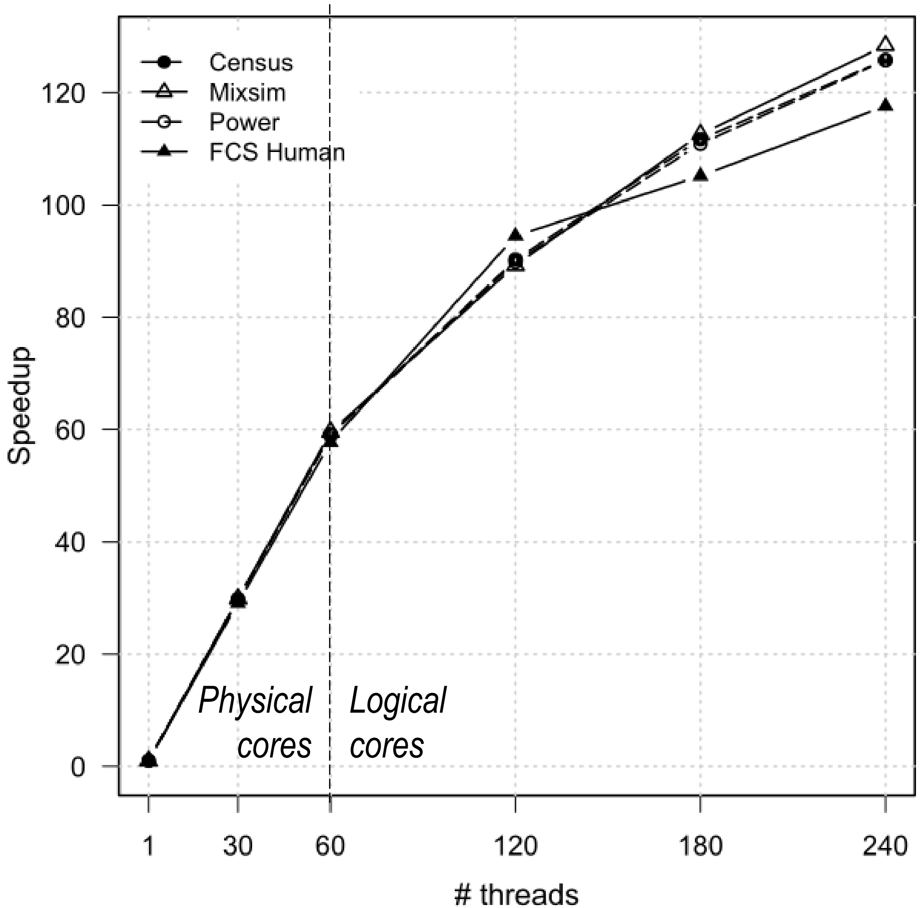


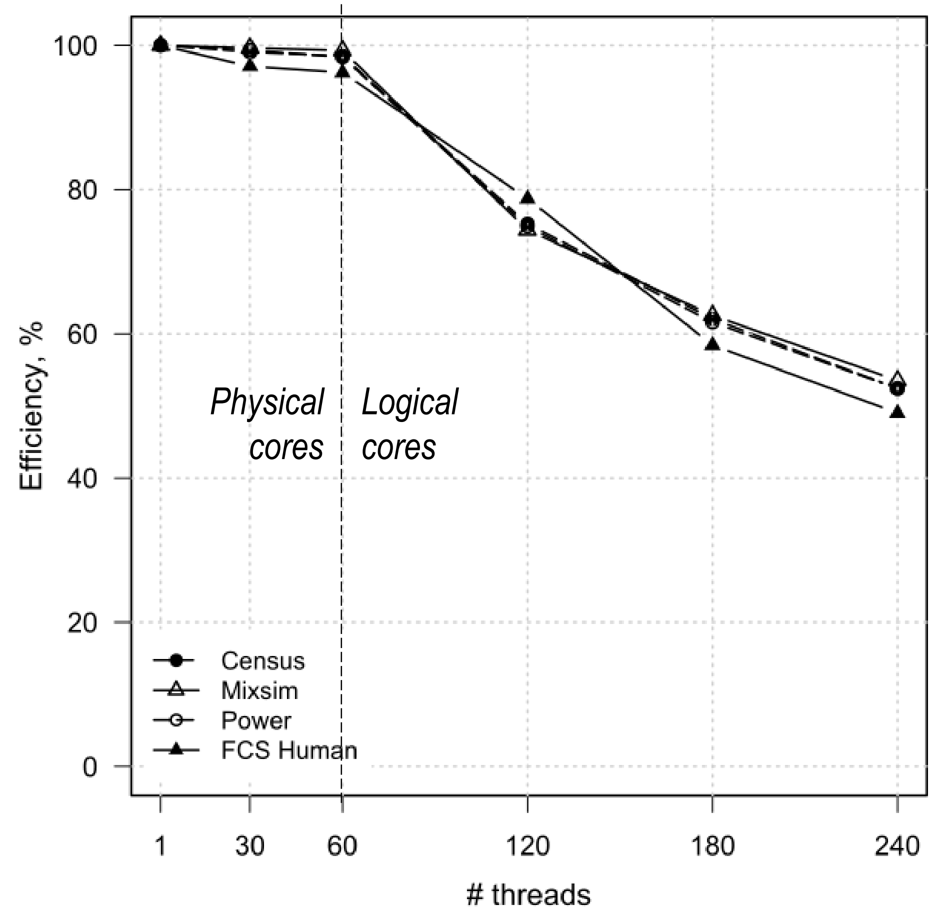
Speedup and Efficiency: 2×Xeon, 24 threads



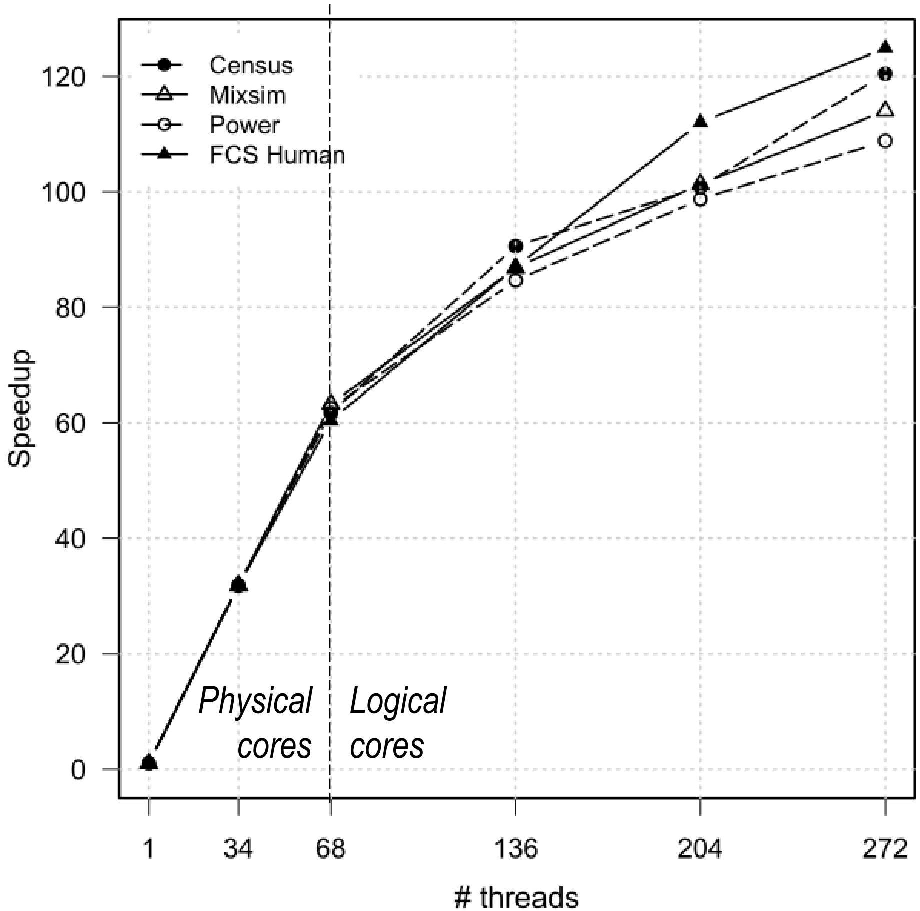


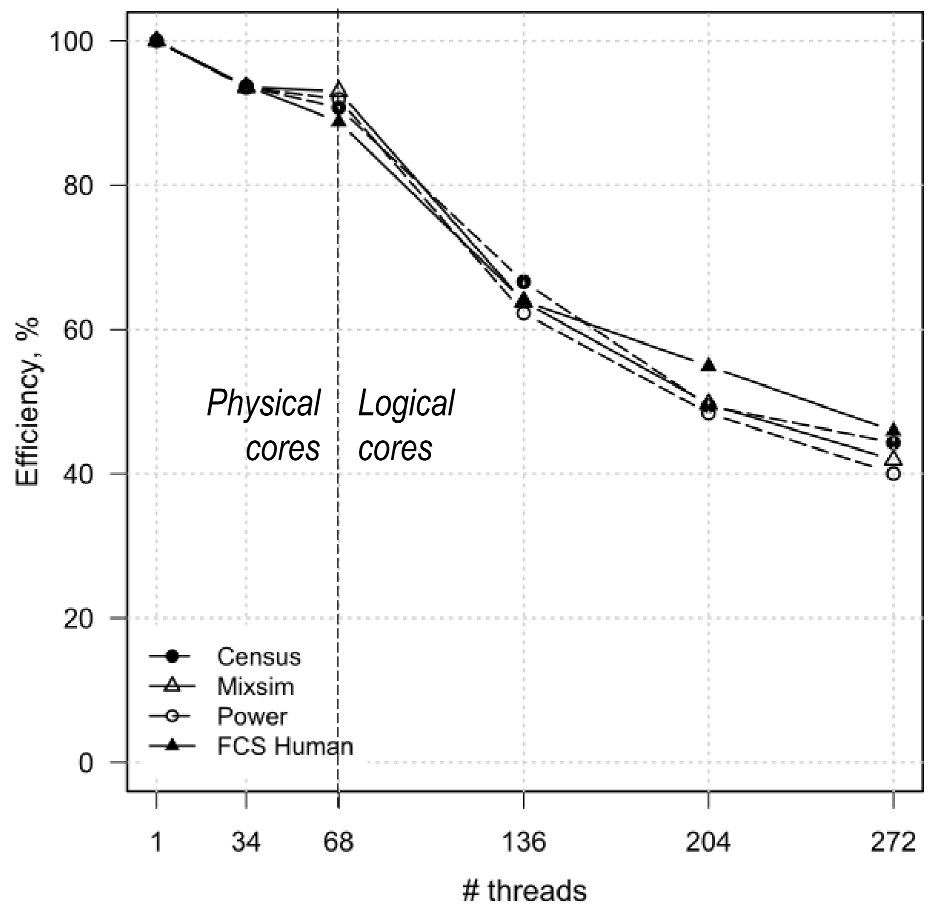
Speedup and Efficiency: KNC, 240 threads





Speedup and Efficiency: KNL, 272 threads





Conclusion

- We have proposed an approach to data mining inside DBMS based on parallel implementation of UDFs for many-core platforms
- We have implemented the approach for PostgreSQL, Intel Xeon Phi (KNC and KNL), and PAM clustering algorithm
- We have conducted experiments on synthetic and real data sets that show good scalability of our approach and overtaking analogue (*R* data mining package).

Thank you for paying attention! Questions?

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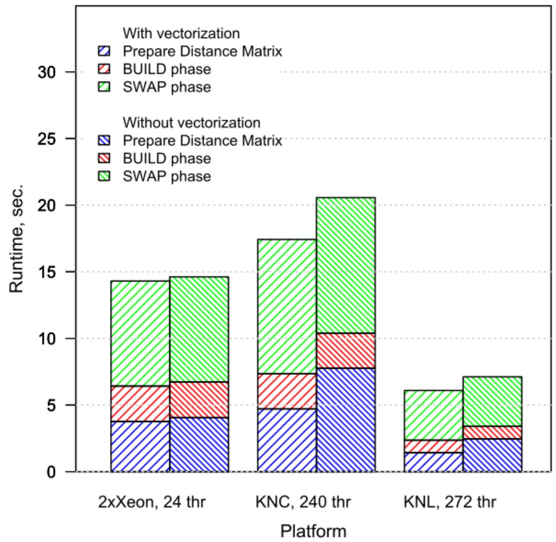
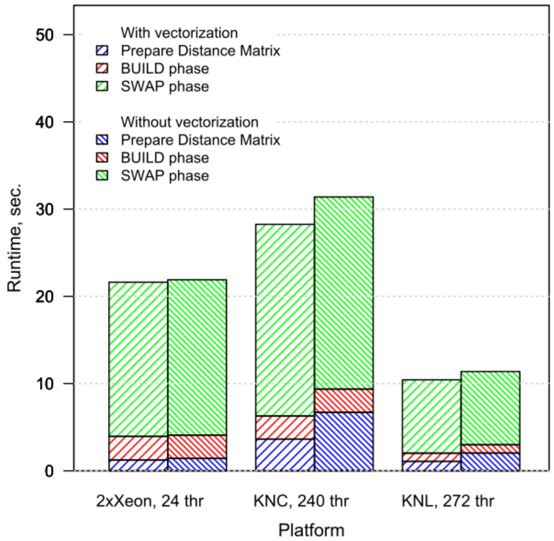
Impact of vectorization

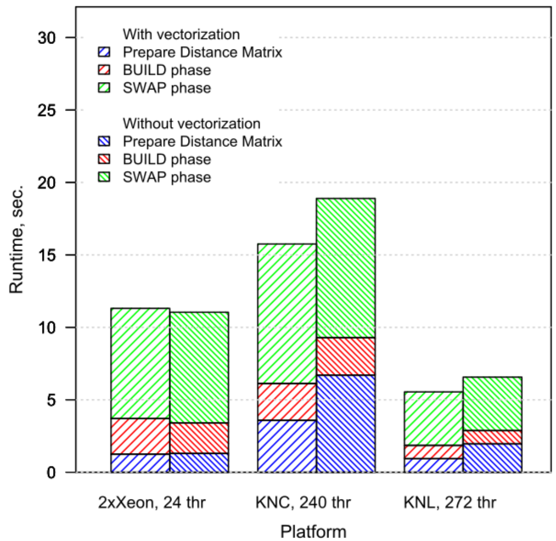
Census



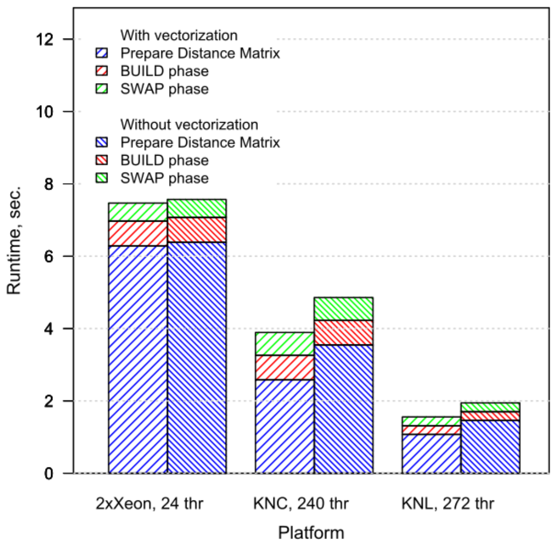
MixSim



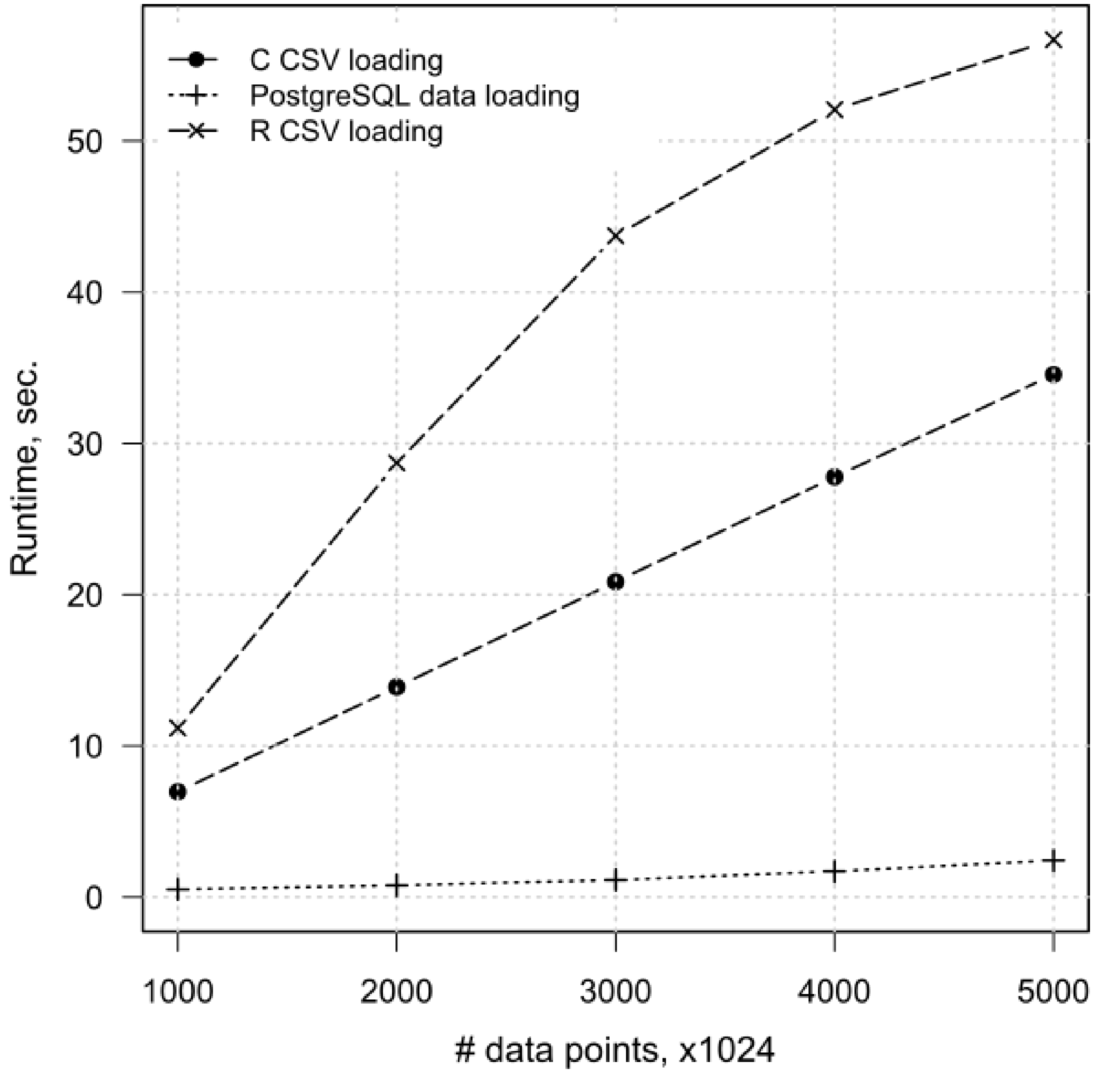
Power



FCS Human



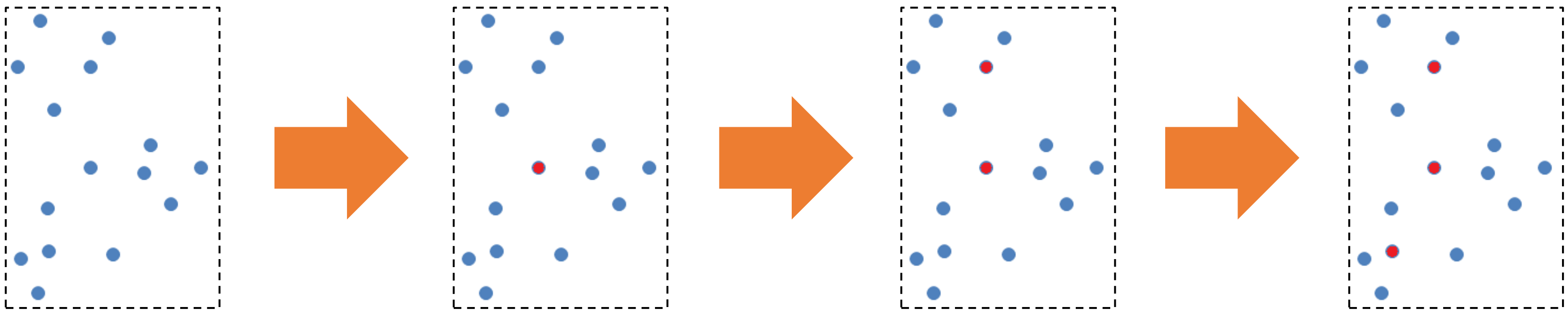
Performance of load data into RAM



PAM: Partition Around Medoids

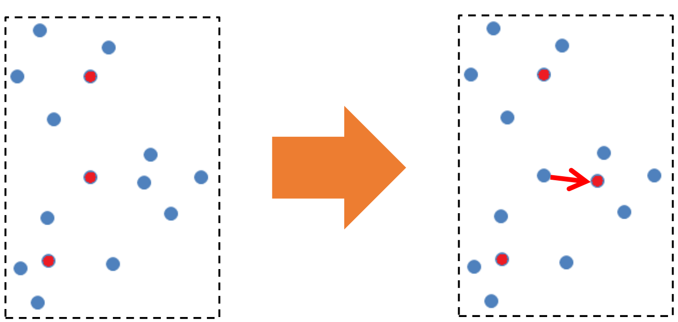
- Objective function $E = \sum_{j=1}^{n} \min_{1 \le i \le k} dist(c_i, o_j)$

  where c_i is the medoid, o_j is the clustered object, *dist* is the distance metric
- BUILD phase: complexity is $O(kn^2)$



$E=\infty$ $E= 2.250$ $E= 1.578$ $E= 1.014$

- SWAP phase: complexity is $O(k(n - k)^2)$ per iteration



$E= 1.014$ $E= 0.865$

PAM: pseudocode

```
Input: set of objects O, # of clusters k
Output: set of clusters C

// Calculation of distance matrix
distMatr ← calcDistMatr (O)
// BUILD phase
C ← BuildMedoids (distMatr)
repeat // SWAP phase
      T_min ← findBestSwap (M, C)
      Swap (c_min, o_min) for T_min
until T_min < 0
```

Rewriting loops: an example

- Vector processor unit is of 512 bits
  - 16 float elements or 8 double elements
- Rewriting loops provides vectorization of computations (SIMD, Single Instruction Multiple Data)

Scalar loop

```
for(i = 0; i < n; ++i)
    a[i] = b[i] + c[i];
```

SIMD loop

```
#ifdef DOUBLE_PRECISION
  #define LEN 8
#else
  #define LEN 16
#endif
for(i = 0; i < n; i += LEN)
    a[i:LEN] = b[i:LEN] + c[i:LEN];
```

Loop tiling: an example

Without tiling

x_1	y_1	z_1

x_1	y_1	z_1	x_2	y_2	z_2	…	x_{32}	y_{32}	z_{32}
x_{33}	y_{33}	z_{33}	x_{34}	y_{34}	z_{34}	…	x_{64}	y_{64}	z_{64}

With tiling

x_1	y_1	z_1

x_1	x_2	…	x_{32}	y_1	y_2	…	y_{32}	z_1	z_2	…	z_{32}
x_{33}	x_{34}	…	x_{64}	y_{33}	y_{34}	…	y_{64}	z_{33}	z_{34}	…	z_{64}