Federated GMQL queries

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Introduction:

Here, we present the multiple version of a query described below to show possible execution strategies on different conditions. All the queries are ready to be used on the dedicated server (GeCo as LOCAL).

In this query, we showed a case study on Adenoid Cystic Carcinoma (ACC), an uncommon form of malignant neoplasm that arises within secretory glands of the head and neck. The researcher has several **MUTATION** samples in her private instance, and she likes to know the highly expressed and highly mutated genes associated with **MYC** transcription factor.

She integrates her experimental dataset with public data from TCGA and ENCODE, available in CINECA and DEIB instances respectively, by performing a Federated GMQL query. This case study shows the relevance of the Federated GMQL system and also the expressive power of GMQL in building queries of biological interest.

We present 4 distributed strategies (DIST-1 to DIST-4), 3 centralized ones (CENT-1 to CENT-3), and the BEST strategy. We also showed 1 example for protective directive and 2 examples for

Distributed 1:

In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are both executed on the DEIB instance.

```
# 1
CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
# 4
Myc = SELECT (gcm curated cell line == "H1-hESC" AND
          target name == "MYC-human" AND
          file output type == "conservative idr thresholded peaks"; at:DEIB)
                                         DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:DEIB) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:LOCAL) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:DEIB) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:DEIB) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Distributed 2:

In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are both executed on the CINECA instance.

```
# 1
AccRnaseq = SELECT (manually curated tumor tag == "acc" AND
                 manually_curated__tissue status == "tumoral"; at:CINECA)
                                              CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
# 4
Myc = SELECT(gcm_curated_cell_line == "H1-hESC" AND
            target name == "MYC-human" AND
            file_output_type == "conservative idr thresholded peaks"; at:DEIB)
                                                DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:CINECA) AccExpFilt Myc;
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:LOCAL) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:CINECA) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:CINECA) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Distributed 3:

In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are executed on the DEIB and GeCo (LOCAL) instance, respectively.

```
# 1
AccRnaseq = SELECT(manually_curated_tumor_tag == "acc" AND
                 manually_curated_tissue_status == "tumoral"; at:CINECA)
                                              CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
# 4
Myc = SELECT(gcm curated cell line == "H1-hESC" AND
           target name == "MYC-human" AND
            file output type == "conservative idr thresholded peaks"; at:DEIB)
                                                DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:DEIB) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:LOCAL) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Distributed 4:

In this example, all the unary operations are on the machine where the dataset is selected. The binary operations, JOIN and MAP, are executed on the CINECA and GeCo (LOCAL) instances, respectively.

```
# 1
AccRnaseq = SELECT(manually_curated_tumor_tag == "acc" AND
                 manually_curated_tissue_status == "tumoral"; at:CINECA)
                                             CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
# 4
Myc = SELECT(gcm curated cell line == "H1-hESC" AND
           target name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                                DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:CINECA) AccExpFilt Myc;
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:LOCAL) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Centralized 1:

In this example, all the selection operations run on the machine where the dataset is selected. All the others run on DEIB instance.

```
# 1
AccRnaseq = SELECT(manually_curated__tumor_tag == "acc" AND
                manually_curated_tissue_status == "tumoral"; at:CINECA)
                                           CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:DEIB) AccRnaseq;
#З
AccExpFilt = SELECT(region: mean exp > 1000; at:DEIB) AccExp;
# 4
Myc = SELECT(gcm_curated_cell_line == "H1-hESC" AND
           target__name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                              DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:DEIB) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example_Mutation;
# 7
myMutationMerge = MERGE(at:DEIB) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:DEIB) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:DEIB) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Centralized 2:

In this example, all the selection operations run on the machine where the dataset is selected. All the others run on CINECA instance.

```
# 1
AccRnaseq = SELECT (manually curated tumor tag == "acc" AND
                manually_curated_tissue_status == "tumoral"; at:CINECA)
                                           CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000; at:CINECA) AccExp;
# 4
Myc = SELECT(gcm_curated_cell_line == "H1-hESC" AND
           target__name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                             DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:CINECA) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:CINECA) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:CINECA) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:CINECA) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Centralized 3:

In this example, all the selection operations run on the machine where the dataset is selected. All the others run on GeCo (LOCAL) instance.

```
# 1
AccRnaseq = SELECT(manually_curated__tumor_tag == "acc" AND
                manually_curated_tissue_status == "tumoral"; at:CINECA)
                                           CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:LOCAL) AccRnaseq;
#З
AccExpFilt = SELECT(region: mean exp > 1000; at:LOCAL) AccExp;
# 4
Myc = SELECT(gcm_curated_cell_line == "H1-hESC" AND
           target__name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                              DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:LOCAL) AccExpFilt Myc;
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:LOCAL) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Best query:

In this example, all the selection operations run on the machine where the dataset is selected, and also the cover operation run on CINECA instance, i.e., where the covered dataset is selected. All the others run on GeCo (LOCAL) instance.

```
# 1
AccRnaseq = SELECT(manually_curated_tumor_tag == "acc" AND
                 manually_curated_tissue_status == "tumoral"; at:CINECA)
                                               CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count); at:CINECA)
AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000; at:LOCAL) AccExp;
# 4
Myc = SELECT(gcm curated cell line == "H1-hESC" AND
            target name == "MYC-human" AND
            file output type == "conservative idr thresholded peaks"; at:DEIB)
                                                 DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct; at:LOCAL) AccExpFilt Myc;
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE(at:LOCAL) myMutation;
# 8
GeneMycMut= MAP(count name: mut count; at:LOCAL) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0; at:LOCAL) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Protected dataset:

In this example, we set the protected dataset and the without setting any other location rather than first selection of the data, the system uses the default policy, distributed. It guaranties that the *protected* dataset will not move to other instances.

```
Oprotected Example Mutation
# 1
CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count)) AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000) AccExp;
# 4
Myc = SELECT(gcm curated cell line == "H1-hESC" AND
           target name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                            DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE() myMutation;
# 8
GeneMycMut= MAP(count name: mut count) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Distributed policy:

In this example, we set only the locations of selection of the datasets with distributed policy, which is default.

```
Opolicy distributed
# 1
AccRnaseq = SELECT(manually_curated_tumor_tag == "acc" AND
               manually_curated_tissue_status == "tumoral"; at:CINECA)
                                       CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count)) AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000) AccExp;
# 4
file output type == "conservative idr thresholded peaks"; at:DEIB)
                                          DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left_distinct) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example Mutation;
# 7
myMutationMerge = MERGE() myMutation;
# 8
GeneMycMut= MAP(count name: mut count) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```

Centralized policy:

In this example, we set only the locations of selection of the datasets with centralized policy at DEIB instance. The query is equivalent to the Centralized 1:. By changing the centralized location into CINECA and LOCAL, we will have equivalent query of Centralized 2: and Centralized 3:, respectively.

```
Opolicy centralized DEIB
# 1
AccRnaseq = SELECT (manually_curated_tumor_tag == "acc" AND
                manually_curated__tissue_status == "tumoral"; at:CINECA)
                                          CINECA.HG19 TCGA rnaseqv2 gene;
# 2
AccExp = COVER(1, ANY; aggregate: mean exp as AVG(normalized count)) AccRnaseq;
# 3
AccExpFilt = SELECT(region: mean exp > 1000) AccExp;
# 4
Myc = SELECT(gcm_curated_cell_line == "H1-hESC" AND
           target name == "MYC-human" AND
           file output type == "conservative idr thresholded peaks"; at:DEIB)
                                            DEIB.HG19 ENCODE NARROW 2019 01;
# 5
GeneMyc = JOIN(dist < 0; output: left distinct) AccExpFilt Myc;</pre>
# 6
myMutation = SELECT(at:LOCAL) Example_Mutation;
# 7
myMutationMerge = MERGE() myMutation;
# 8
GeneMycMut= MAP(count name: mut count) GeneMyc myMutationMerge;
# 9
ResGenes = SELECT(region:mut count > 0) GeneMycMut;
# 10
MATERIALIZE ResGenes INTO ResGenes;
```