Femtocode: querying HEP data

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Reminder of motivation

(The last time I presented this here was December 12.)

Query systems

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Femtocode

I'm developing a query system whose performance would permit real-time analysis, but is capable of complex manipulations, such as filtering tracks, picking pairs to compute invariant masses, etc.

Three interrelated parts

Language/compiler

- As familiar as possible to the user (objects, nested loops).
- But constrained to allow restructuring for fast execution (map/filter/reduce instead of for-loops, total functions. . .).
- Extra-strength type system to eliminate runtime errors.

Execution engine

- Operate on contiguous columns of data, not objects. “Restructuring objects” becomes changing arrays of integers.
- No memory allocation at runtime; vectorizable loops.
- JIT-compiled. CPU for now, but structure is right for GPU.

Distributed server

- Vending machine: queries go in, histograms (etc.) come out.
- Referential transparency eliminates the need of tracking users.

Start with a working example: dimuons

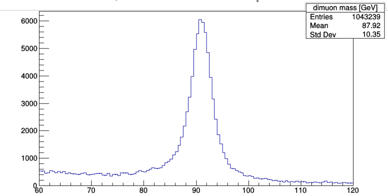
```
pending = session.source("ZZ_13TeV_pythia8")
    .define(mumass = "0.105658")      # chain of operations on source
    .toPython(mass = """
muons.map(mu1 => muons.map({mu2 =>    # doubly nested loop over muons
  p1x = mu1.pt * cos(mu1.phi);
  p1y = mu1.pt * sin(mu1.phi);        # shares scope with other steps
  p1z = mu1.pt * sinh(mu1.eta);       # in the chain (see "mumass")
  E1 = sqrt(p1x**2 + p1y**2 + p1z**2 + mumass**2);

  p2x = mu2.pt * cos(mu2.phi);
  p2y = mu2.pt * sin(mu2.phi);
  p2z = mu2.pt * sinh(mu2.eta);
  E2 = sqrt(p2x**2 + p2y**2 + p2z**2 + mumass**2);

  px = p1x + p2x; py = p1y + p2y;
  pz = p1z + p2z; E = E1 + E2;

  # "if" is required to avoid sqrt(-x)
  if E**2 - px**2 - py**2 - pz**2 >= 0:
    sqrt(E**2 - px**2 - py**2 - pz**2)
  else:
    None    # output type is nullable
}))
""").submit()                         # asynchronous submission to
final = pending.await()               # watch result accumulate
```

Yes, we see the Z peak.



Taking this example apart (1/3)

- Femtocode always appears in quotes (like SQL). It is a big-data aggregation step in the midst of a traditional analysis.
- A query is a "workflow" from source to aggregation, compiled and submitted as one unit.

  e.g. `source("dataset").define(X).define(Y).histogrammar(Z)`
- Most Femtocode expressions are tiny (hence "femto"), scattered throughout a Histogrammar aggregation:

```
session.source("dataset")
    .define(goodmuons = """...""")   # define good muons
    .filter("goodmuons.size >= 2")   # cut on them
    .define(dimuon = """..."""       # define dimuons
    .bundle(                         # plot their attributes
        mass = bin(120, 0, 12, "dimuon.mass"),
        pt = bin(100, 0, 100, "dimuon.pt"),
        eta = bin(100, -5, 5, "dimuon.eta"),
        phi = bin(314, 0, 2*pi, "dimuon.phi + pi"),
                                     # also plot the muons
        muons = loop("goodmuons", "mu", bundle(
            pt = bin(100, 0, 100, "mu.pt"),
            eta = bin(100, -5, 5, "mu.eta"),
            phi = bin(314, -pi, pi, "mu.phi"))))
```

Taking this example apart (2/3)

- Make doubly nested loops by nesting functionals:
  `"muons.map(mu1 => muons.map(mu2 => f(mu1, mu2)))"`
  is equivalent to

```
list_of_lists = []
for mu1 in muons:
    list_of_numbers = []
    for mu2 in muons:
        list_of_numbers.append(f(mu1, mu2))
    list_of_lists.append(list_of_numbers)
```

- There will someday be more convenient forms: `pairs`, `table`, `filter`, `flatten`, `flatMap`, `zip`, `permutations`, etc.

  (The dimuon example would ideally use `pairs` to avoid double-counting and `flatten` to destructure the list-of-lists. Or better yet, pick the best two by p_T to get one candidate per event.)

Taking this example apart (3/3)

- Type system requires domain of `sqrt` to be guarded:

```
sqrt(E**2 - px**2 - py**2 - pz**2)
```

```
FemtocodeError: Function "sqrt" does not accept arguments with
the given types:

    sqrt(real)

    The sqrt function can only be used on non-negative numbers.

Check line:col 19:2 (pos 401):
      sqrt(E**2 - px**2 - py**2 - pz**2)
------^
```

  To resolve this compile-time error, we write:

```
if E**2 - px**2 - py**2 - pz**2 >= 0:
    sqrt(E**2 - px**2 - py**2 - pz**2)
else:
    None
```

- The compiler tracks each subexpression's interval of validity:

  `E**2 - px**2 - py**2 - pz**2` is limited to `real(min=0, max=inf)`.

  In the future, we could use SymPy to discover this algebraically.

Another thing to notice

```
muons.map(mu1 => muons.map({mu2 =>
  p1x = mu1.pt * cos(mu1.phi);
  p1y = mu1.pt * sin(mu1.phi);
  p1z = mu1.pt * sinh(mu1.eta);
  E1 = sqrt(p1x**2 + p1y**2 + p1z**2 + mumass**2);

  p2x = mu2.pt * cos(mu2.phi);
  p2y = mu2.pt * sin(mu2.phi);
  p2z = mu2.pt * sinh(mu2.eta);
  E2 = sqrt(p2x**2 + p2y**2 + p2z**2 + mumass**2);

  px = p1x + p2x;
  py = p1y + p2y;
  pz = p1z + p2z;
  E = E1 + E2;

  if E**2 - px**2 - py**2 - pz**2 >= 0:
    sqrt(E**2 - px**2 - py**2 - pz**2)
  else:
    None
}))
```

only uses mu1

only uses mu2

uses both.

Femtocode minimizes computation

In most compilers, at least one of those two stanzas would be needlessly recomputed for every *pair* of muons. Physicists have learned to move these expressions out of the loop, possibly at the expense of readability.

Femtocode's compiler turns every loop over objects into vectorized functions on individual fields. A by-product of this is that the functions depending on just `mu1` or `mu2` decouple from the functions depending on both.

In fact, *all* duplicate subexpressions are computed exactly once. The *only* reason to use assignment is for clarity.

(It's like an executable whiteboard.)

What the dimuon example expands to

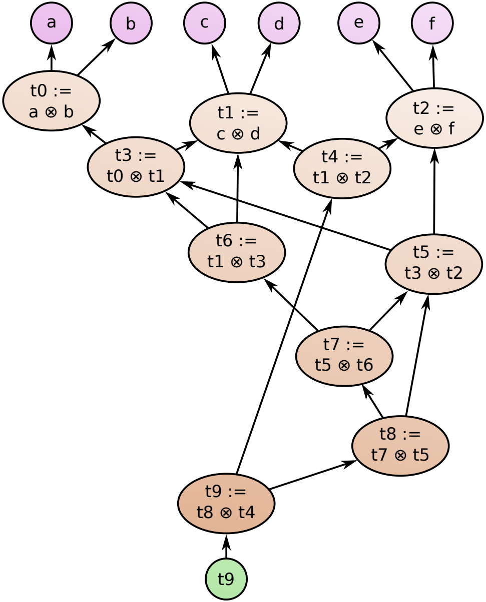
```
Sized by muons[]@size:
    #0        := cos(muons[]-phi)
    #1        := *(muons[]-pt, #0)
    #2        := **(#1, 2)
    #3        := sin(muons[]-phi)
    #4        := *(muons[]-pt, #3)
    #5        := **(#4, 2)
    #6        := sinh(muons[]-eta)
    #7        := *(muons[]-pt, #6)
    #8        := **(#7, 2)
    #9        := +(#2, #5, #8, 0.011164)
    #10       := sqrt(#9)
type(#10) == real(0.105658, almost(inf))

Sized by #11@size:
    #11@size := $explodesize(muons[], muons[])
    #11       := $explodedata(#10, #11@size, (muons[]))
    #12       := $explodedata(#10, #11@size, (muons[], muons[]))
    #13       := +(#11, #12)
    #14       := **(#13, 2)
    #15       := $explodedata(#1, #11@size, (muons[]))
    #16       := $explodedata(#1, #11@size, (muons[], muons[]))
    #17       := +(#15, #16)
    #18       := **(#17, 2)
    #19       := -(#14, #18)
    #20       := $explodedata(#4, #11@size, (muons[]))
    #21       := $explodedata(#4, #11@size, (muons[], muons[]))
    #22       := +(#20, #21)
    #23       := **(#22, 2)
    #24       := -(#19, #23)
    #25       := $explodedata(#7, #11@size, (muons[]))
    #26       := $explodedata(#7, #11@size, (muons[], muons[]))
    #27       := +(#25, #26)
    #28       := **(#27, 2)
    #29       := -(#24, #28)
    #30       := >=(#29, 0)
    #31       := <(#29, 0)
    #32       := -(#24, #28)
    #33       := sqrt(#32)
    #34       := if(#30, #31, #33, None)
type(#34) == union(null, real(0, almost(inf)))
```

`muons[]-pt`, `muons[]-phi`, `muons[]-eta`, `muons[]@size`, and everything that starts with a # is (at least conceptually) a big array of values.

All functions except `$explode*` are ideally suited to GPU acceleration.

Freedom to choose the looping structure



Suppose we have this dependency graph.

We are free to choose where to put the loops.

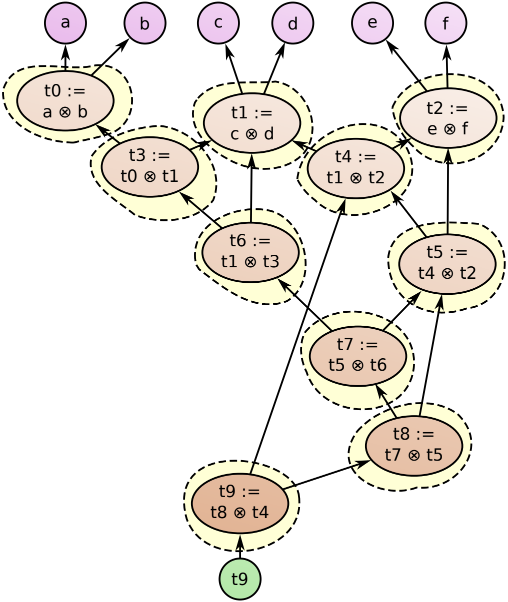
a, b, c, d, e, and f are all large arrays

t9 must also be a large array

intermediate steps need not be

(⊗ is some operation)

Freedom to choose the looping structure



At every step:

```
foreach i:
    t0[i] := a[i] ⊗ b[i]
foreach i:
    t1[i] := c[i] ⊗ d[i]
foreach i:
    t2[i] := e[i] ⊗ f[i]
foreach i:
    t3[i] := t0[i] ⊗ t1[i]
foreach i:
    t4[i] := t1[i] ⊗ t2[i]
foreach i:
    t5[i] := t4[i] ⊗ t2[i]
foreach i:
    t6[i] := t1[i] ⊗ t3[i]
foreach i:
    t7[i] := t5[i] ⊗ t6[i]
foreach i:
    t8[i] := t7[i] ⊗ t5[i]
foreach i:
    t9[i] := t8[i] ⊗ t4[i]
```

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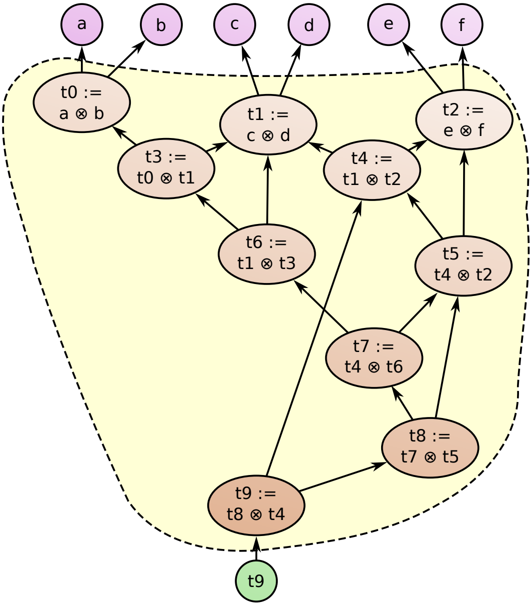

Around everything:

```
foreach i:
   t0 := a[i] ⊗ b[i]
   t1 := c[i] ⊗ d[i]
   t2 := e[i] ⊗ f[i]
   t3 := t0 ⊗ t1
   t4 := t1 ⊗ t2
   t5 := t4 ⊗ t2
   t6 := t1 ⊗ t3
   t7 := t5 ⊗ t6
   t8 := t7 ⊗ t5
   t9[i] := t8 ⊗ t4
```

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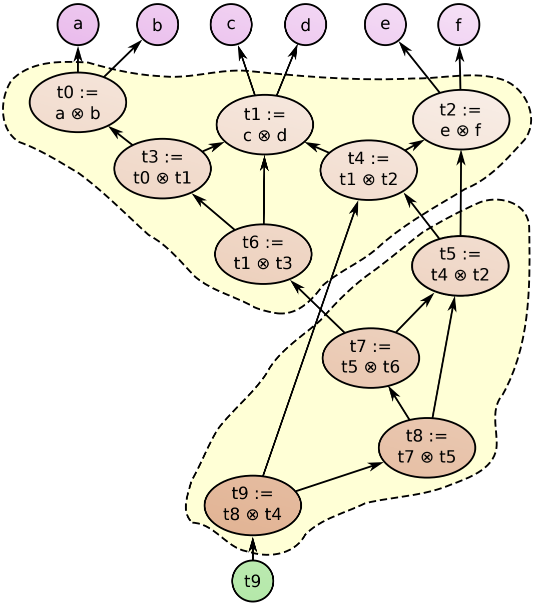


Or an intermediate case:

```
foreach i:
    t0 := a[i] ⊗ b[i]
    t1 := c[i] ⊗ d[i]
    t2[i] := e[i] ⊗ f[i]
    t3 := t0 ⊗ t1
    t4[i] := t1 ⊗ t2
    t6[i] := t1 ⊗ t3
foreach i:
    t5 := t4[i] ⊗ t2[i]
    t7 := t5 ⊗ t6
    t8 := t7 ⊗ t5
    t9[i] := t8 ⊗ t4
```

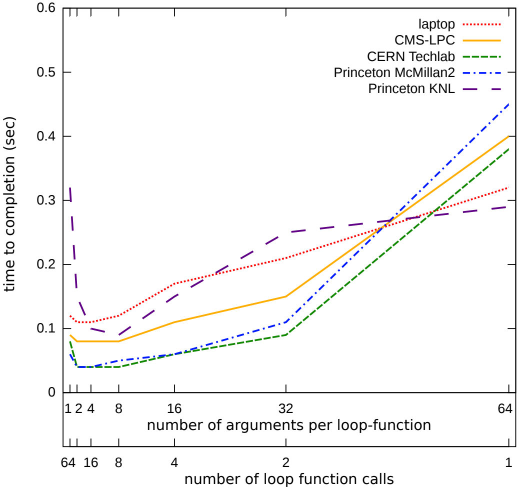
Note that this changes which intermediates are arrays and which are scalars.

What are the trade-offs?

Assuming the bottleneck to be memory bandwidth (usually true), more loops:

- increases number of memory passes and
- sometimes decreases number of arrays to stride simultaneously.

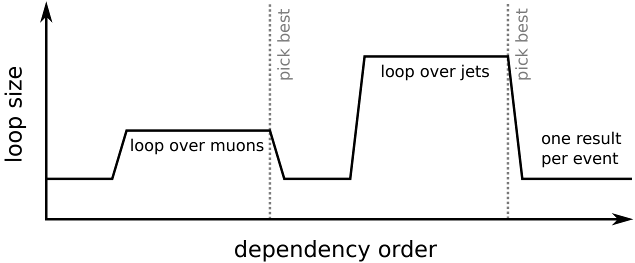
Test of splitting 1 loop over 64 variables into 64 loops over 1 variable reveals a sweet spot of about 2–32.



Sometimes you don't get to choose

Some vector operations have higher cardinality than others: e.g. a loop over jets has more steps than a loop over muons.

Operations of different cardinality can't be in the same loop, so Femtocode divides the dependency graph into "plateaus."



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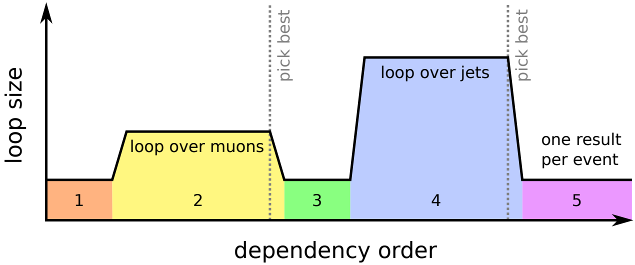

This cartoon example requires five loops (assuming each step strictly depends on the previous).

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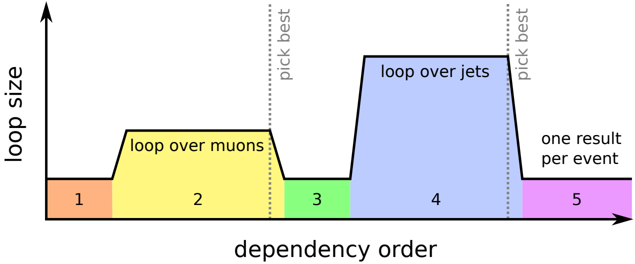
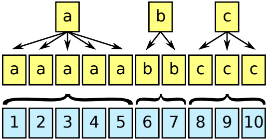


This cartoon example requires five loops (assuming each step strictly depends on the previous).

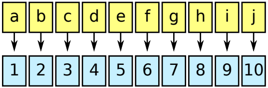
Our dimuon example naturally splits into two loops: one over muons (`muons[]@size`) and one over muons $\times$ muons (`#11@size`).

Three kinds of operations in each plateau

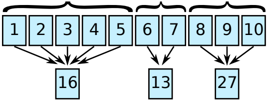
Explode: increase cardinality of one array so that it matches another. Determines the indexing of the loop, so must be first.



Flat: apply function to all members of two aligned data arrays, ignoring event boundaries. Intermediate steps need not be arrays.



Implode: combine results (sum, mean, max, etc.) to reduce cardinality of an array. Size of output arrays are not constrained by the indexing of the loop. Must be last.



Representing objects as arrays (1/2)

Muon object schema:

```
muons = collection(record(
            pt  = real(0, almost(inf)),
            eta = real,
            phi = real(-pi, pi)))
```

Physical representation:

```
input = {
    "muons[]-pt":    [31.0960, 9.7620, 8.1769, ...,
                        5.2730, 4.7240, 8.5879],      # (length 132274)
    "muons[]-phi":   [-0.4814, -0.1242, -0.1185, ...,
                        1.2469, -0.2067, -1.7541],    # (length 132274)
    "muons[]-eta":   [0.8816, 0.9243, 0.9226, ...,
                        -0.9911, 0.9532, -0.2635],    # (length 132274)
    "muons[]@size": [7, 1, 4, ..., 4, 0, 1]}          # (length 48131)
```

Dimuon run produces:

```
masses = collection(collection(union(null, real(0, almost(inf)))))

output = {
    "#34":           [0.2113, 6.2386, 5.7978, ...,
                        13.1108, 0.2113, 0.2113],     # (length 584642)
    "#11@size":      [7, 7, 7, ..., 0, 1, 1]}         # (length 180405)
```

Representing objects as arrays (2/2)

For collections of records (e.g. particles), these arrays have the same interpretation as ROOT TLeaves:

- data arrays contain all values, ignoring event boundaries,
- size array contains the size of each event's collection.

For collections of collections (of fixed, known depth), we can extend this definition recursively:

```
Given:                 [ [ a b c ] [ d e f g ] ] [ [ h ] [ i j ] ]
Data array:                a b c     d e f g           h     i j
Recursive counter:     2 3         4                 2 1   2
```

We know whether a number in the size array refers to the size of an outer collection or an inner collection via a stack of countdowns.

Looping over these recursive counters

a fully general example: "xss.map(xs => xs.map(x => ys.map(y => x + y)))"

```
entry = 0                     # entry index
deepi = 0                     # depth of collection
countdown = [0, 0, 0]         # stack of indexes
x_skip = [False, False]       # handling zero x_size
y_skip = [False]              # handling zero y_size

while entry < numEntries:     # master loop
    if deepi != 0:
        countdown[deepi - 1] -= 1

    if deepi == 0:            # xss.map(xs => ...)
        x_index[1] = x_index[0]
        countdown[deepi] = x_size[x_index[1]]
        x_index[1] += 1

        if countdown[deepi] == 0:
            x_skip[0] = True
            countdown[deepi] = 1
        else:
            x_skip[0] = False

    elif deepi == 1:          # xs.map(x => ...)
        x_index[2] = x_index[1]
        if not xskip[0]:
            countdown[deepi] = x_size[x_index[2]]
            x_index[2] += 1

        if countdown[deepi] == 0:
            x_skip[1] = True
            countdown[deepi] = 1
        else:
            x_skip[1] = False

    elif deepi == 2:          # ys.map(y => ...)
        y_index[1] = y_index[0]
        countdown[deepi] = y_size[y_index[1]]
        y_index[1] += 1

        if countdown[deepi] == 0:
            y_skip[0] = True
            countdown[deepi] = 1
        else:
            y_skip[0] = False

    elif deepi == 3:          # body of loop
        deepi -= 1

        if not x_skip[0] and not x_skip[1] \
           and not y_skip[0]:
            # put "x + y" into output array

    deepi += 1

    while deepi != 0 and countdown[deepi - 1] == 0:
        deepi -= 1            # "closing parentheses"

        if deepi == 0:
            x_index[0] = x_index[1]
            y_index[0] = y_index[1]

        elif deepi == 1:
            x_index[1] = x_index[2]

    if deepi == 0:    # master loop iterates through
        entry += 1    # deepest nesting level
```

Features of the event loop

- JIT-compiled for the specific nesting observed in query.
- Never allocates memory at runtime.
- Always two nested while-loops; the second only pops out of the stack (could be replaced with JIT-compiled if-statements).
- Walk through data controlled by stacks of fixed depth (already replaced with JIT-compiled stack variables for 30% speedup).
- Access pattern is contiguous and usually forward, though it sometimes jumps backward to emulate loops like

```
muons.map(mu1 => muons.map(mu2 => ...))
```

- Open question: would a version of this using recursion, rather than a single loop with stacks, be faster?
- Generated as Python code (previous page), compiled by Numba/LLVM into native machine code. (Easier to test.)

Why size arrays instead of runtime objects?

1. To help LLVM and the hardware optimize memory bandwidth.

Simple operation on 806177 jet p_T values (6.15 MB):	
3 ms	no-frills loop in C
7 ms	Numpy's implementation
14 ms	full generality Femtocode event loop
24 ms	allocating C++ objects on stack and iterating
64 ms	allocating C++ objects on heap, iterating, deleting
518 ms	`TTree::Draw` with `TTreeCache`
41900 ms	CMSSW EDAnalyzer (disk access)

(Note: Femtocode needs to be optimized to resemble no-frills loop in C. There's work to be done here.)

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   (Note: Femtocode needs to be optimized to resemble no-frills loop in C. There's work to be done here.)

2. With no event boundaries in the data arrays, the "flat functions" perfectly satisfy the criteria for GPU acceleration.

   Thus, we could automatically translate high-level code on physics objects into well-optimized GPU kernels!