Vectorized Processing of Nested Data

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Intersection of three topics

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Operations on nested data structures

Often hard to vectorize or even express with array programming.

Examples of physics problems involving nested data operations

1. Compute the ϕ difference between each jet and its event's MET.

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for event in dataset:
    for jet in event.jets:
        jet.phidiff = jet.phi - event.phi    # N(jets) != N(events)
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2. Compute mass of all particles from two collections, subjet to a cut.

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for event in dataset:
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3. Find the "best" candidate per event or per subcollection.

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for event in dataset:
    event.best = None
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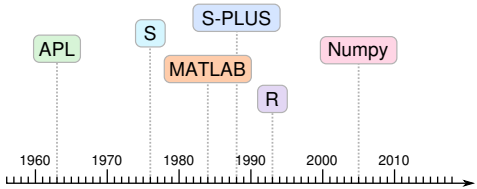
Primarily for data analysis languages

Express regular operations over rectangular data structures in shorthand.



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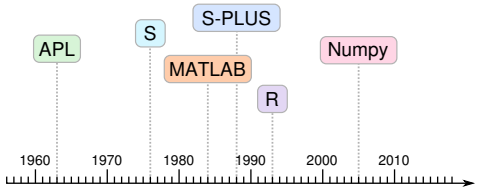

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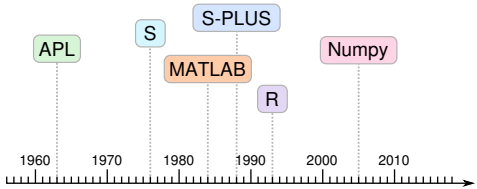

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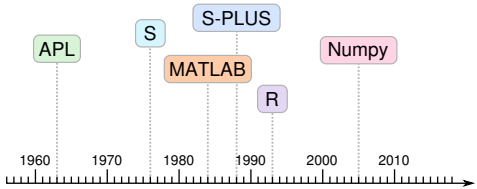

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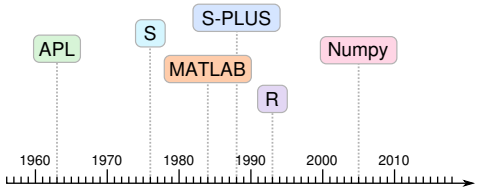

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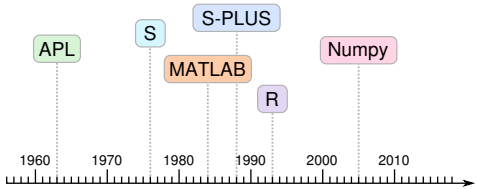

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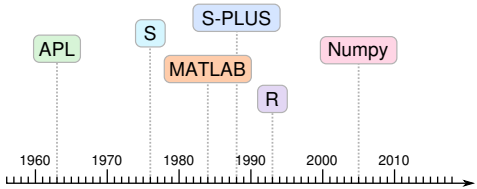

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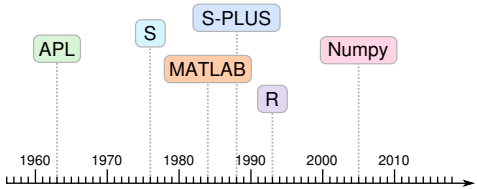

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- Array reduction: `array.sum()` → scalar

Extension to variable-sized, nested structures

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Logical structure: [[0, 1, 2], [], [3, 4], [5, 6, 7, 8, 9]]
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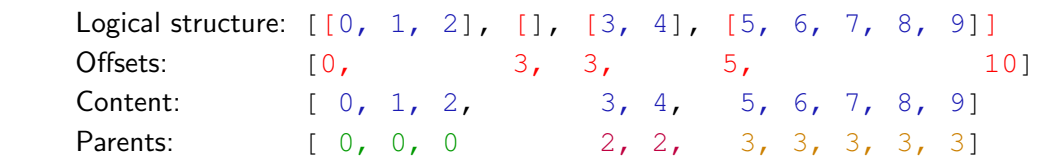

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When combined with a table type (column names → arrays), this is as expressive as any combination of `std::vector` and `struct` (i.e. as expressive as ProtoBuf).

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- Jagged array reduction: `jetpt.max()` → array of max jet p_T per event

Problem 1: Compute the ϕ difference between each jet and its event's MET.

```
for event in dataset:
    for jet in event.jets:
        jet.phidiff = jet.phi - event.phi
```

Jagged array solution:

```
# because of extended broadcasting rules
events["jets"]["phidiff"] = (
                          events["jets"]["phi"] - events["MET"]["phi"])
```

Problem 2: Compute mass of all particles from two collections, subjet to a cut.

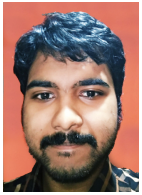
```
for event in dataset:
    event.leptoquarks = []
    for jet in event.jets:
        for lepton in event.leptons:
            if cut(jet, lepton):
                event.pairs.append(mass(jet, lepton))
```

Jagged array solution:

```
# jagged cross-join makes (jet, lepton) pairs per event
pairs = events["jets"].cross(events["leptons"])

events["leptoquarks"] = mass(pairs[cut(pairs)])
```

Jagged cross-join has a fully vectorizable implementation (Jaydeep)



```
def cross(self, other):
    offsets = counts2offsets(self.counts * other.counts)
    parents = offsets2parents(offsets)
    indexes = numpy.arange(offsets[-1], dtype=int)

    # fancy indexing get -> SIMD gather
    ocp = other.counts[parents]
    iop = indexes - offsets[parents]
    iop_ocp = iop // ocp

    left = self.content[self.starts[parents] + iop_ocp]
    right = other.content[other.starts[parents] + iop - ocp * iop_ocp]

    return JaggedArray.fromoffsets(offsets, Table(left, right))
```

(There's also a solution for non-repeating pairs of a collection with itself.)

Problem 3: Find the "best" candidate per event or per subcollection.

```
for event in dataset:
    event.best = []
    for leptoquark in leptoquarks:
        if event.best == [] or \
            quality(leptoquark) > quality(event.best[0]):
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Jagged array solution:

```
# jagged argmax makes empty lists [] or singleton lists [N]
argbest = quality(events["leptoquarks"]).argmax()

# jagged fancy indexing transforms [] -> [] and [i] -> [sublist[i]]
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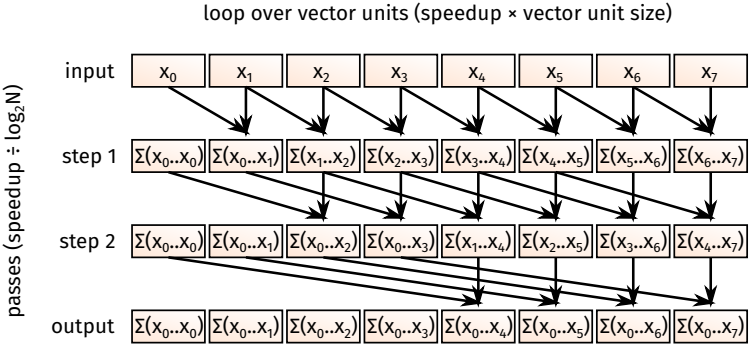
# jagged fancy indexing transforms [] -> [] and [i] -> [sublist[i]]
events["best"] = events["leptoquarks"][argbest]

# remove empty lists and concatenate singletons by dropping offsets
nonempty_best = events["best"].flatten()
```

Surprisingly, jagged reducers are fully vectorizable, too (Jaydeep)



This is known as the Hillis-Steele algorithm: creates a cumulative sum in parallel.

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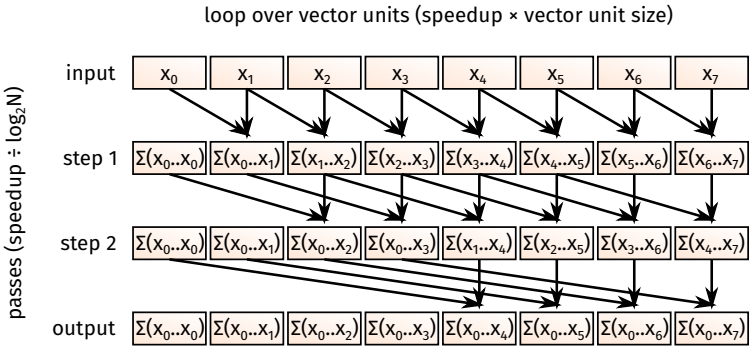

example

input	1.1	2.2	3.3	4.0	5.0	−10.0	0.0	5.0
step 1	1.1	3.3	5.5	7.3	9.0	−5.0	−10.0	5.0
step 2	1.1	3.3	6.6	10.6	14.5	2.3	−1.0	0.0
output	1.1	3.3	6.6	10.6	15.6	5.6	5.6	10.6

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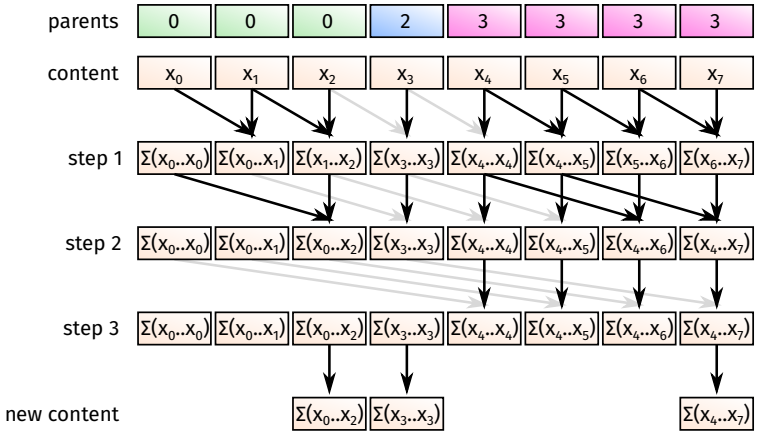
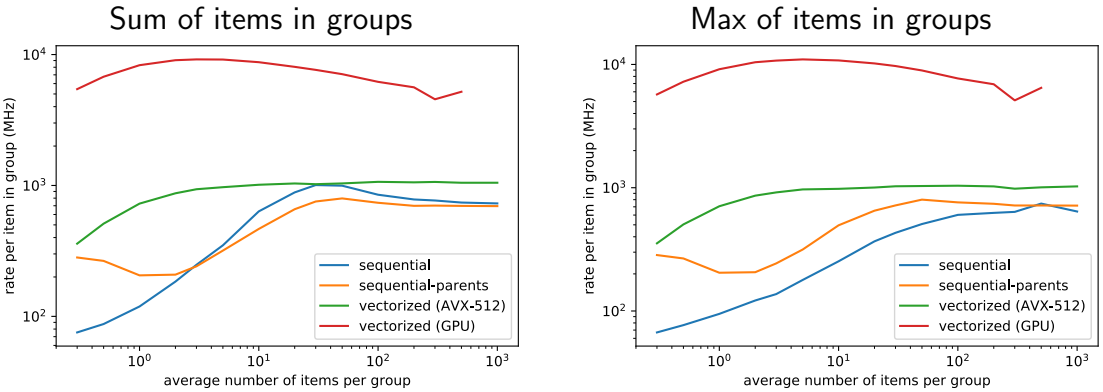


Modification of the Hillis-Steele algorithm: only combine pairs in the same event (by checking parents) and then take the last value in each event.

Performance of modified Hillis-Steele



cmslpcgpu3.fnal.gov (Xeon Silver 4110 CPU, Tesla P100 GPU)

https://github.com/jpivarski/jupyter-performance-studies/blob/master/2018-09-10-jagged-reduction.ipynb

Working examples in an interactive notebook: try it out!

https://mybinder.org/v2/gh/scikit-hep/uproot/master?filepath=binder%2Fversion-3-features.ipynb

In [66]:
```
# compute jets × muons, add the pairs to get leptoquark TLorentzVectors, then compute mass
jetp4.cross(muonp4).apply(lambda a, b: a + b).mass()
```

Out[66]:
```
<JaggedArray [[] [61.49117266] [] ... [99.96350949], [ 73.10963363 106.82646499], []] at 7f305cf8ada0>
```

In [67]:
```
# the same except compute mass in the apply— the apply can return anything
jetp4.cross(muonp4).apply(lambda a, b: (a + b).mass())
```

Out[67]:
```
<JaggedArray [[] [61.49117266] [] ... [99.96350949], [ 73.10963363 106.82646499], []] at 7f305cf9b208>
```

In [69]:
```
# compute muons × muons, make Z candidates, and only consider Z candidates with pT > 40
muonp4.pairs(same=False).apply(lambda a, b: a + b).filter(lambda z: z.pt() > 40)
```

Out[69]:
```
<JaggedArrayMethods [[] [] [TLorentzVector(49.815, 8.0774, 48.133, 102.23)] ... [], [], []] at 7f305cf9b3c8>
```

In [70]:
```
# now only consider events that have at least one Z candidate with pT > 40
muonp4.pairs(same=False).apply(lambda a, b: a + b).filter(lambda z: z.pt().max() > 40)
```

Out[70]:
```
<JaggedArrayMethods [[TLorentzVector(49.815, 8.0774, 48.133, 102.23)] [TLorentzVector(98.78, -99.792, 738.94, 757.
5)] [TLorentzVector(84.922, 92.652, -69.581, 172.15)] ... [TLorentzVector(59.597, 72.155, 35.339, 135.72)], [TLorent
zVector(52.18, 58.075, 53.209, 129.65)], [TLorentzVector(53.845, 8.6018, -227.56, 254.94)]] at 7f305cf9b668>
```

In [71]:
```
# get the mass of the Z candidate with the highest pT
muonp4.pairs(same=False).apply(lambda a, b: a + b).maxby(lambda z: z.pt()).mass()
```

Out[71]:
```
<JaggedArray [[90.22779777] [] [74.74654928] ... [], [], []] at 7f305d0011d0>
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Relevance to ROOT

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- The jagged array structure aligns perfectly with the RForest concept.
- An array programming model could be supported by RTensor.
- VecOps::RVec provides one-in-one-out vectorization; it could be extended to provide vectorized jagged operations as well.

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- An array programming model could be supported by RTensor.
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- It could fit into RDataFrame if applied to clusters ("map partitions").
- Doing so would provide a "C++ story" for how physicists can use BulkIO.

Where to find implementations and example code

- awkward-array: https://github.com/scikit-hep/awkward-array

  Implementations of jagged arrays and tables in pure Numpy. Vectorized accelerators will appear as `awkward-array-cpu` and `awkward-array-gpu`.

- Jaydeep's report on vectorized algorithms for cross ("combinations"), pairs, jagged reduction ("global argmin"):

  https://gitlab.com/Jayd_1234/GSoC_vectorized_proof_of_concepts

  Algorithms are demonstrated in Jupyter notebooks; final writeup is in Markdown.
  Earlier work:

  https://github.com/Jayd-1234/GSoC_vectorized_proof_of_concepts

- awkward-array is now used heavily by uproot and uproot-methods. Examples include array programming with TLorentzVectors and jagged arrays of TLorentzVectors.