Efficient, Optimal MPI Datatype Reconstruction for Vector and Index Types

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MPI Derived datatypes

…you all know about them

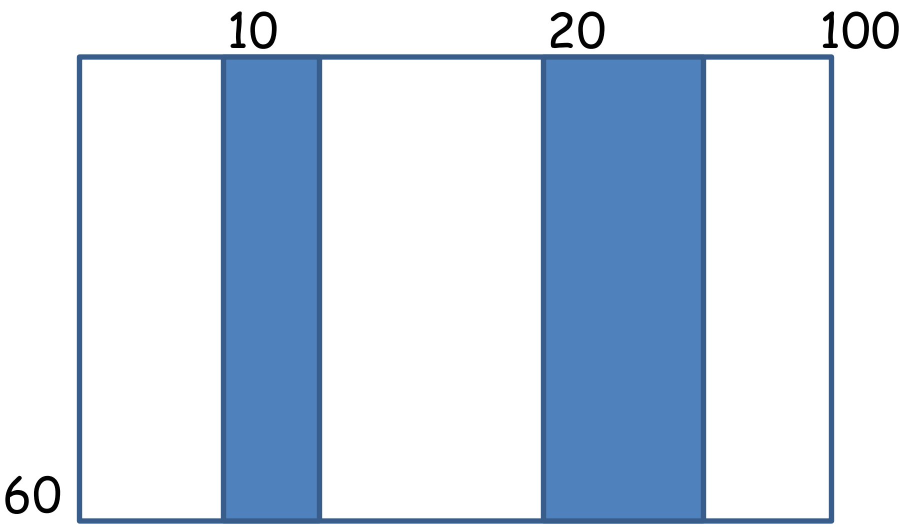
Mechanism for describing application data layouts that are

- Non-consecutive (sub-matrices, parts of buffers, …)
- Non-homogeneous: different basetypes (MPI_CHAR, MPI_DOUBLE, MPI_INT, …)

Derived (user-defined) datatypes orthogonal to communication mode: works for point-to-point, collective, one-sided, extremely important for MPI-IO specification, …

Unique feature of MPI (could be useful for other interfaces!)

Example: Receive two matrix-column blocks…



Column1 =
MPI_Vector

Column2 =
MPI_Vector

BlocksType' =
MPI_Struct(Colum1,Column2)

Rowtype =
MPI_Indexed

BlocksType =
MPI_Contig(Rowtype)

Note:
BlocksType ≠ BlocksType'

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Derived datatype describes the layout of data, and fixes the order in which data are accessed

Layout: Ordered sequence of <displacement,basetype> pairs

aka MPI type map

Example: The row-wise layout of matrix-columns:

<10,DOUBLE>, <11,DOUBLE>, <20,DOUBLE>, <21,DOUBLE>,
<22,DOUBLE>, <110,DOUBLE>,<111,DOUBLE>,<120,DOUBLE>,
<121,DOUBLE>, <122,DOUBLE>, …

Note: BlocksType ≠ BlocksType'

Derived datatype describes the layout of data, and fixes the order in which data are accessed

Layout: Ordered sequence of <displacement,basetype> pairs

Homogeneous: same basetype for all pairs

aka MPI type map

Example: Row-wise layout of matrix-columns, basetype DOUBLE

<10,11,20,21,22,110,111,120,121,122, …>

Displacement sequence: list of displacements (in access order)

Displacements themselves not necessarily ordered!

Note: BlocksType ≠ BlocksType'

Derived datatype describes the layout of data, and fixes the order in which data are accessed

Layout: Ordered sequence of <displacement,basetype> pairs

Homogeneous: same basetype for all pairs

aka MPI type map

Example: Column-wise layout of matrix-columns

<10,11,110,111,210,211,…,20,21,22,120,121,122,220,221,222, …>

Displacement sequence: list of displacements (in access order)

Displacements themselves not necessarily ordered!

Datatype representation

Tree (or DAG) like structure:

- Internal type nodes describe how child nodes are repeated (how often, where)
- Leaf nodes describe basetype

Semantics:
There is a function flatten(T) that generates the type map from datatype T, i.e., flatten(T) = D

MPI usage:
Derived datatype explicitly constructed by application using type constructor operations, MPI library maintains some convenient and efficient internal representation

Derived datatype representation of displacement sequence

MPI_Contig(60)

↓

MPI_Indexed(2,<2,3>)

↓

MPI_DOUBLE

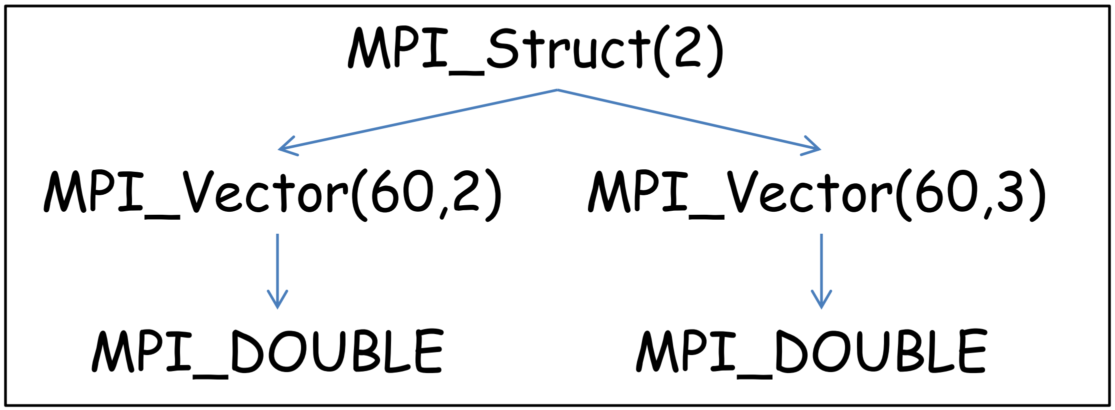
Type nodes:

- MPI_Contig
- MPI_Vector
- MPI_IndexBlock
- MPI_Indexed

MPI datatype constructors

- MPI_Type_contiguous(oldtype, …, &newtype);
- MPI_Type_vector(oldtype,…,&newtype);
- MPI_Type_create_indexed_block(oldtype,. …, &newtype);
- MPI_Type_indexed(oldtype, …, &newtype);

Derived datatype representation of heterogeneous type map



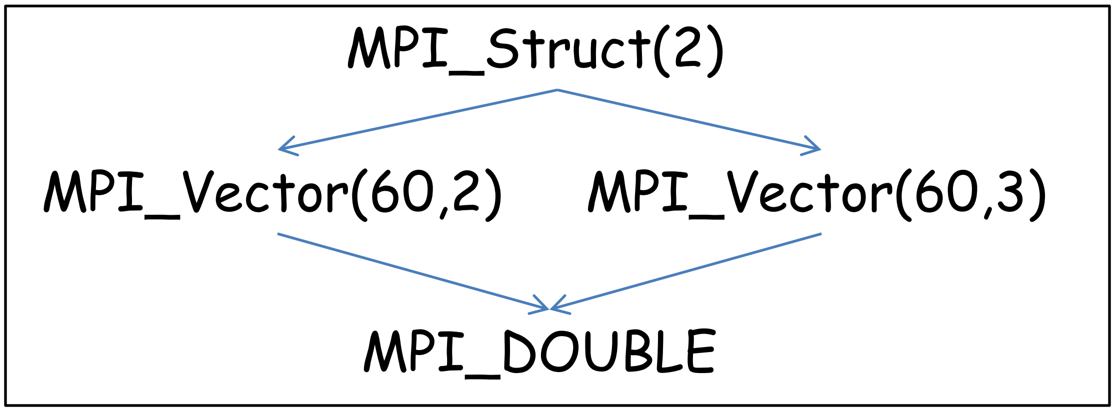
Type nodes:

- MPI_Contig
- MPI_Vector
- MPI_IndexBlock
- MPI_Indexed
- MPI_Struct

MPI datatype constructors

- MPI_Type_contiguous(oldtype, …, &newtype);
- MPI_Type_vector(oldtype,…,&newtype);
- MPI_Type_create_indexed_block(oldtype,. …, &newtype);
- MPI_Type_indexed(oldtype, …, &newtype);
- MPI_Type_create_struct(oldtypes[], …, &newtype);

Derived datatype representation of heterogeneous type map



Type nodes:

- MPI_Contig
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- MPI_Struct

MPI datatype constructors

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- MPI_Type_indexed(oldtype, …, &newtype);
- MPI_Type_create_struct(oldtypes[], …, &newtype);

Our internal representation (not very important here)

- leaf(B): basetype B at displacement 0
- vec(c,d,C): regular, strided repetition of subtype C at displacements 0, d, 2d, 3d, … (c-1)d
- idx(c,<i0,i1,i2,…,i(c-1)>,C): repetition of subtype C at displacements i0, i1, i2, …, i(c-1)

- strc(c,<i0,i1,i2,…,i(c-1)>,<C0,C1,C2,…,C(c-1)>): subtypes C0, C1, C2, …, C(c-1) at displacements i0, i1, i2, …, i(c-1)

- Can easily represent the MPI constructors (for now, we omit MPI_Type_indexed)
- Avoids some tedious problems with extents and "true extents"

Datatype representation

Tree (or DAG) like structure:

- Internal type nodes describe how child nodes are repeated (how often, where)
- Leaf nodes describe basetype

Semantics:
There is a function flatten(T) that generates the type map from datatype T, i.e., flatten(T) = D

Note:
There are (infinitely) many ways T to describe a given D

Some may be better than others

Some natural questions

- What is the best way to describe given displacement sequence (homogeneous type map) as derived datatype?
- What is the best way to describe heterogeneous type map as derived datatype?
- How do the set of constructors affect complexity and quality?

Depends on what is meant by "best" (cost function)

Abstract cost function:
Account for space consumption and (indirectly) processing cost

Real "best" depends on MPI library and (communication) system

Cost model

•cost(leaf(B)): some constant K
•cost(vec(c,d,C)): some (other) constant K'
•cost(idx(c,<i0,i1,i2,…,i(c-1)>,C)): some constant K''+c (non-constant)

•cost(strc(c,<i0,i1,i2,…,i(c-1)>,<C0,C1,C2,…,C(c-1)>)): some constant K'''+2c (non-constant)

Justification:
leaf, vec: only constant information needed to process
idx, struc: space proportional to displacement and type lists required, must be traversed on processing

cost(T): sum of costs of all nodes in T (additive cost model)

Problems

Given:
- set of constructors (leaf, vec, idx, struc, …)
- cost function cost(T)

Type reconstruction problem: Find cost-optimal representation for given type map

Type normalization problem: Find cost-optimal representation for given, user-defined datatype

William Gropp, Torsten Hoefler, Rajeev Thakur, Jesper Larsson Träff: Performance Expectations and Guidelines for MPI Derived Datatypes. EuroMPI 2011: 150-159

Known facts

MPI libraries use heuristics (folklore) to improve internal datatype representation (MPI_Struct => MPI_Indexed => MPI_Vector => MPI_Contig): type normalization, see, e.g.,

Fredrik Kjolstad, Torsten Hoefler, Marc Snir: Automatic datatype generation and optimization. PPOPP 2012: 327-328 (and more extentsive TR!)

Homogeneous type maps of size n, leaf, vec and idx nodes: $O(n\sqrt{n})$ time reconstruction, normalization in time O(size(T))

Jesper Larsson Träff: Optimal MPI Datatype Normalization for Vector and Index-block Types. EuroMPI/ASIA 2014: 33

New results

Homogeneous type maps of size n, leaf, vec and idx nodes: Better algorithm for finding all repeated prefixes, O(n log n/log log n) time type reconstruction

- Prefix algorithm can be used for normalization
- MPI_Index (idxbuc node) can be incorporated in O(n^2 log^2 n) time

Not here:

Arbitrary type maps of size n, all type nodes leaf, vec, idx, struc, type reconstruction into trees is polynomial but O(n^4)

Robert Ganian, Martin Kalany, Stefan Szeider, Jesper Larsson Träff: Polynomial-time Construction of Optimal Tree-structured Communication Data Layout Descriptions. CoRR abs/1506.09100 (2015)

and Master's Thesis by Martin Kalany

Type reconstruction strategy

Derived datatype nodes describe structured repetition of subtype

↓

To compute datatype from *given* displacement sequence: look for all possible repetitions

↓

Use dynamic programming to compute best datatype

From now on: homogeneous type maps = displacement sequences

Terminology

Displacement sequence:
Array D[] of n integer displacements , D[i] i'th displacement in sequence (D[i] can be >0, <0, =0, repetitions allowed)

D[] = <10,11,20,21,22,110,111,120,121,122, …>

…can trivially be represented as derived datatype

idx(n,<10,11,20,21,22,110,111,120,121,122, …>)
↓
DOUBLE

Cost = n+K"+K

Terminology

Displacement sequence:
Array D[] of n integer displacements , D[i] i'th displacement in sequence (D[i] can be >0, <0, =0, repetitions allowed)

D[] = <10,11,20,21,22,110,111,120,121,122, …>

D[i,j]: Segment of displacement sequence from i to j (inclusive)

D[2,4] = <20,21,22>

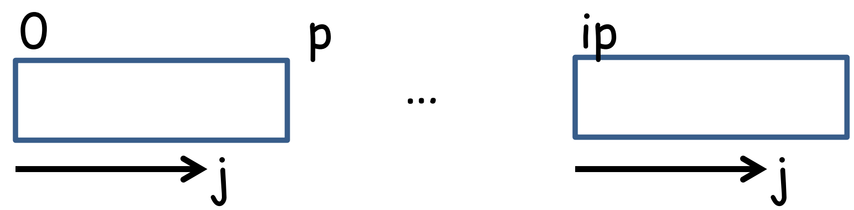
D[0,2] = <10,11,20>

D[0,p-1]: Prefix of length p

Definition:
Prefix of length p is repeated in D if

$D[j]-D[0] = D[ip+j]-D[ip]$

for $0 \le j < p$ and $1 \le i < n/p$



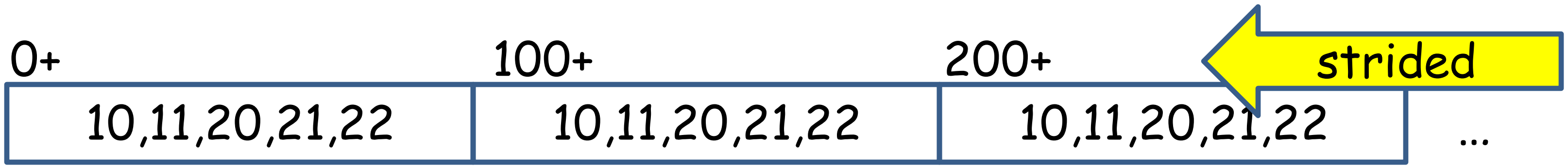
Observation: A prefix of length p can be repeated only if $p|n$, trivial prefixes $D[0,0]$ of length 1 and $D[0,n-1]$ of length 1

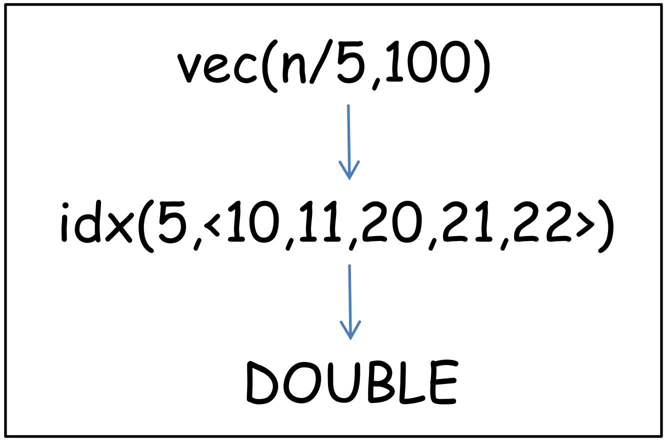
Definition: A repeated prefix of length p is strided if additionally

$D[p]-D[0] = D[(i+1)p]-D[ip]$

Prefix D[0,4] = <10,11,20,21,22> is repeated (and strided) in

D[] = <10,11,20,21,22,110,111,120,121,122, …>





Cost = K'+5+K''+K

Finding repeated prefixes

Finding strided prefixes is easy (EuroMPI 2014): longest repeated prefix in arbitrary D can be found in one scan in O(n) time

Finding repeated, non-strided prefixes; trivial approach:

Try all divisors p of n, for each check by scan of D whether prefix D[0,p-1] is repeated: total time $O(n\sqrt{n})$

At most $2\sqrt{n}$ divisors in n to check

Observation:
If D[0,p-1] is repeated prefix of D, checking whether D[0,p-1] is a strided prefix takes O(n/p) time

Claim:
Let p divisor of n. All repeated prefixes of length q where q is a divisor of p (including q=p) can be found in linear time

Idea:
To find all repeated prefixes of D, let

$n = (p1^{a1}) (p2^{a2}) (p3^{a3}) \ldots (pk^{ak})$

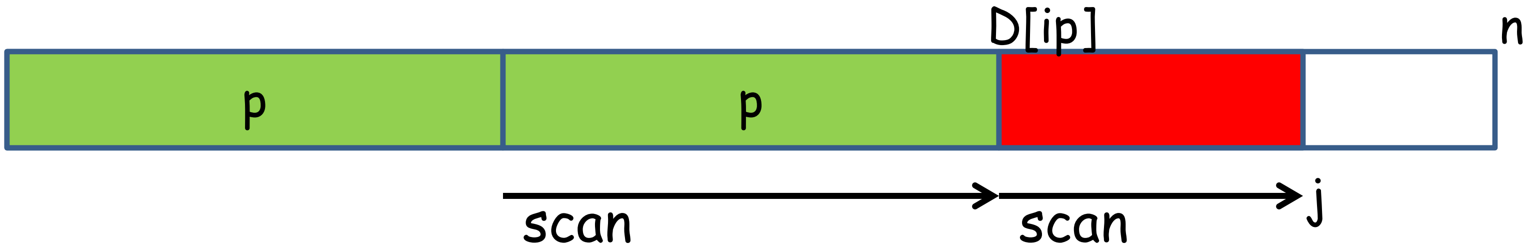
be prime factorization of n. Apply claim for all $p = (n/pi)$

Result from number theory (Robin, 1983):

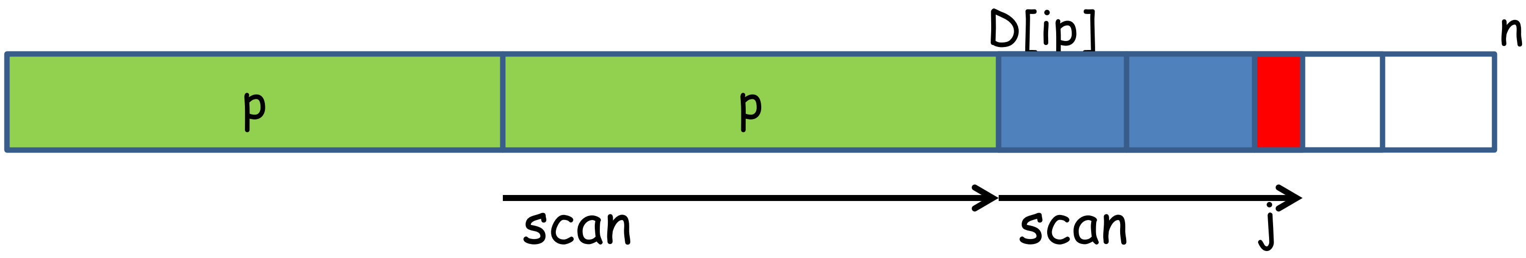
Number of distinct prime factors of n is $O(\log n/\log \log n)$

Proposition:
All repeated prefixes of given displacement sequence D of length n can be found in O(n log n/log log n) time

Proof of claim:
Pick (largest) divisor p of n, check if D[0,p-1] is repeated prefix



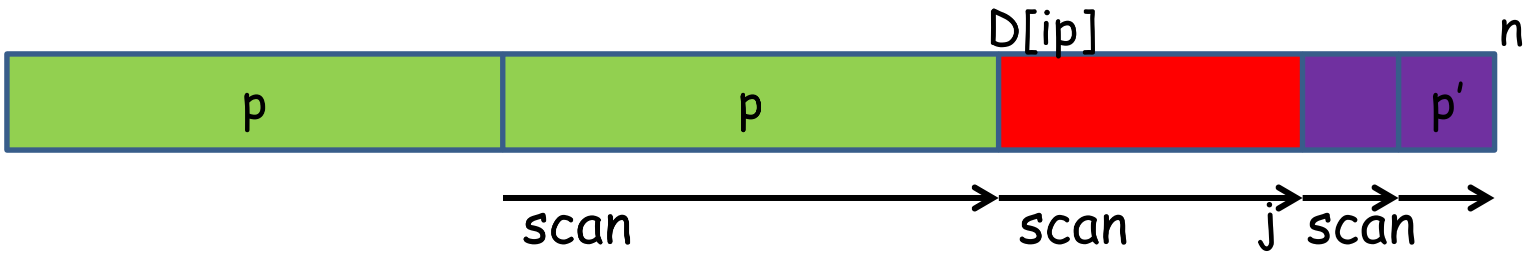
Prefix mismatch:
$D[ip+j]-D[ip] \neq D[j]-D[0]$



Prefix mismatch:
D[ip+j]-D[ip] ≠ D[j]-D[0]

1. Choose p' = gcd(p,j), continue scan for repeated prefix D[0,p'-1] from j

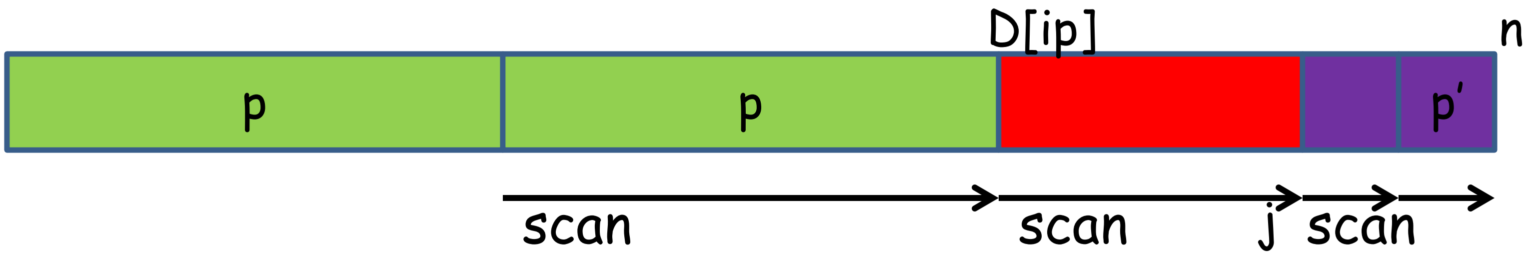
Prefix that is divisor of p but not j cannot be repeated prefix



Prefix mismatch:
D[ip+j]-D[ip] ≠ D[j]-D[0]

1. Choose p' = gcd(p,j), continue scan for repeated prefix D[0,p'-1] from j
2. Check whether prefix D[0,p'-1] is repeated in D[0,p-1]

Step 2: recurse on 

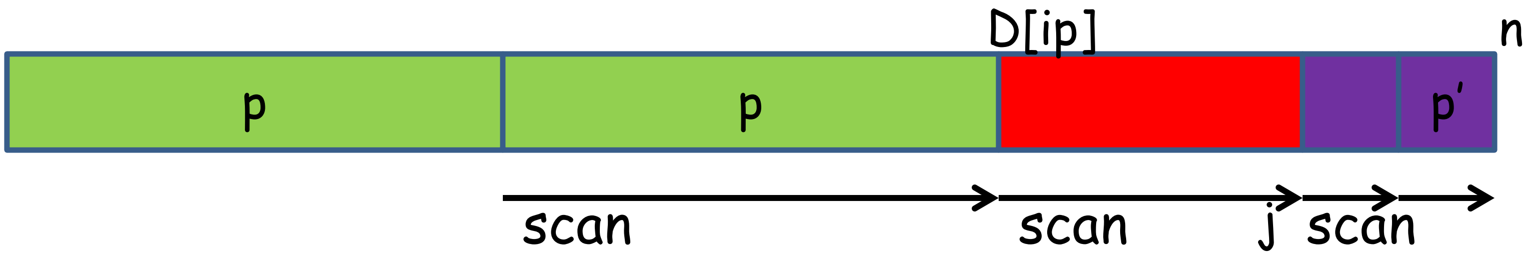


Prefix mismatch:
$D[ip+j]-D[ip] \neq D[j]-D[0]$

Step 1: linear scan, always increasing index order: $O(n)$

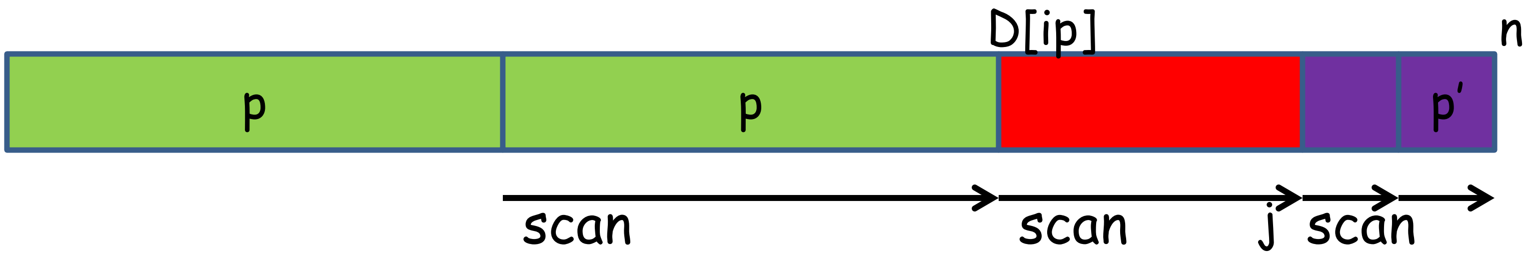
Step 2: recurse on p′ in p so $O(p)$

Total time: $O(n)$



Prefix mismatch:
D[ip+j]-D[ip] ≠ D[j]-D[0]

Algorithm determines largest p' that is a divisor of p where D[0,p'-1] is repeated prefix of D



Prefix mismatch:
D[ip+j]-D[ip] ≠ D[j]-D[0]

To find all repeated prefixes of length q where q divisor of p: recurse on q in p.

Observation:
If D[0,q-1] is repeated prefix of D[0,p-1], and D[0,p-1] is repeated prefix of D, then D[0,q-1] is repeated prefix of D

Structure of optimal path

Observations:
With leaf, vec, idx nodes (no struc), datatypes are simple paths. Each constructor has only one child

Call index node ixd(c,<i0,i1,…>) where i0≠0 a shifted node. A type tree with at most one shifted node is nice. For any datatype path T there exists nice T' (describing the same displacement sequence) with cost(T')≤cost(T)

Cost-optimal T has at most one node with count=1 (a shifted idx)

Cost optimal T has depth (log n)

Cost optimal T's have optimal substructure:
dynamic programming principle applies

idx(1,<0>)
↓
idx(3,<27,2,55>)
↓
idx(2,<0,7,13>)
↓
idx(3,<1,2,4>)
↓
DOUBLE

⇒

Nice type path

idx(1,<28>)
↓
idx(3,<0,-25,28>)
↓
idx(2,<0,7,13>)
↓
idx(3,<0,1,3>)
↓
DOUBLE

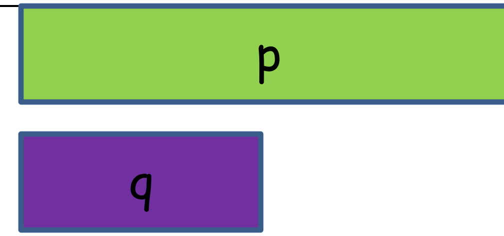
Full algorithm

Precompute: all repeated prefixes and longest strides

1. Find all repeated prefixes p
2. For each p, find largest s(p)≤n such that D[0,p-1] is strided in D[0,s(p)-1]
3. Optimal datatype representation for segment D[0,0] of length 1 is T(0) = leaf(basetype)

Technicality:
Algorithm for aligned displacement sequences with D[0] = 0

Step 4: dynamic programming




```
for all repeated prefixes D[0,p-1]:
    BestCost = ∞
    for all repeated prefixes q of D[0,p-1]:

        VecCost = K'+cost(T(q))  // cost of vec node
        if VecCost<BestCost and p≤s(q)
          T(p) = vec(p/q,stride,T(q)) where stride = D[q]-D[0]
          BestCost = VecCost

        IdxCost = K''+p/q+cost(T(q)) // cost of idx node
        if IdxCost<BestCost
          indices = <D[0],D[q],D[2q],…>
          T(p) = idx(p/q,indices,T(q))
          BestCost = IdxCost
```

Complexity

Steps 1 takes $O(n \log n/\log \log n)$ time by the proposition on repeated prefixes

Step 2 requires $O(n/p)$ time for each divisor $p|n$. By a theorem from number theory (Divisor summatory function, Gronwall, 1913)

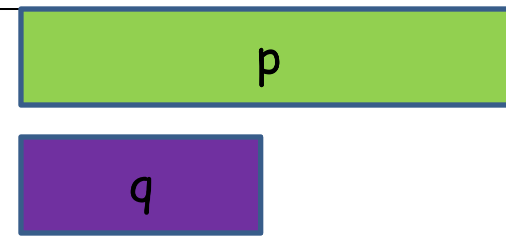
$\sum(p|n): n/p = \sum(p|n): p = O(n \log n/\log \log n)$

In step 4, both loops are over repeated prefixes. There can be at most $2\sqrt{n}$, so if body of inner loop can be implemented in constant time, total time is $O(n)$

```
for all repeated prefixes D[0,p-1]:
    BestCost = ∞
    for all repeated prefixes q of D[0,p-1]:

        VecCost = K'+cost(T(q))  // cost of vec node
        if VecCost<BestCost and p≤s(q)
          T(p) = vec(p/q,stride,T(q)) where stride = D[q]-D[0]
          BestCost = VecCost

        IdxCost = K''+p/q+cost(T(q)) // cost of idx node
        if IdxCost<BestCost
          indices = <D[0],D[q],D[2q],...>
          T(p) = idx(p/q,indices,T(q))
          BestCost = IdxCost
```



Fill in indices later

Theorem:
Cost optimal datatype path representing displacement sequence D of length n using constructors leaf, vec, idx can be computed in $O(n \log n/\log \log n)$ time

Additional constructors

idx node corresponds to MPI_Type_create_indexed_block constructor.

MPI_Type_indexed needs list of displacements and list of block sizes, represented by additional constructor

- idxbuc(c,d,<i0,i1,i2,…,i(c-1)>,<b0,b1,b2,…,b(c-1)>) with cost K'''+2c

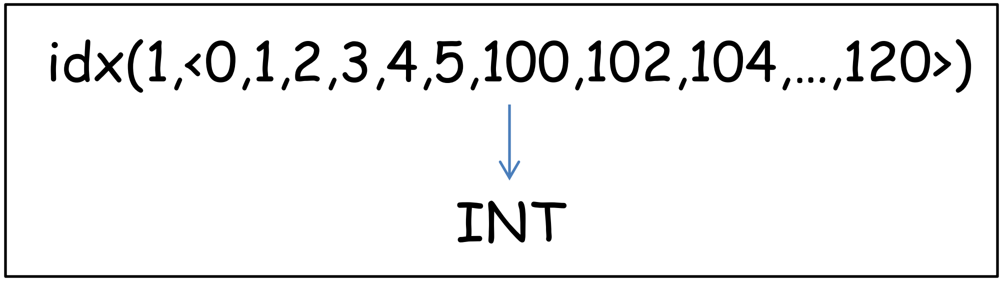
Extra check in inner loop of dynamic programming algorithm needed, requires sorting (to find best block size), total time O(√n n log n)

Outlook, summary

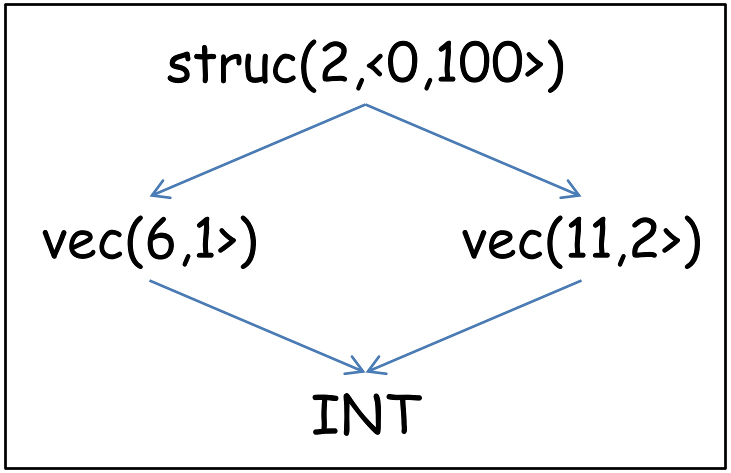
- Simple algorithm to find all repeated prefixes much faster than trivial $O(n\sqrt{n})$ approach
- Much better algorithm for type reconstruction with restricted set of constructors leaf, vec, idx, now $O(n \log n/\log \log n)$
- Can be used in algorithm for type normalization (EuroMPI 2014)
- Can incorporate additional constructors: idxbuc (MPI_Type_indexed), triangular types (see tomorrow), …, but not for type normalization

Note:

struc() node does give more power, even for (homogeneous) displacement sequences



Cost = $K''+17+K$



Cost = $K'''+2+2K'+K$

Makes sense to look for constructors inbetween idx() and struc()

This work was supported by

EPiGRAM