Subject: Looking for tetrahedra. Searching sorted lists. Posted by cgguido on Mon, 08 Aug 2005 04:37:19 GMT

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Hi all,

I was wondering if anybody can suggest a fast algorithm (perhaps using the magic of HISTOGRAM :-o) to find tetrahedra. Let me explain.

I need to find quadruplets of mutually nearest neighbours id's in a nearest neighbour list.

I start with a list of nearest neighbours id's, NN which is a 2xn (n ~ 6e6 yep!) intarr and is sorted so that for any i:

NN[0,i] It N[1,i] and NN[0,i] le NN[0,i+1]

example input:

0.2

0 5

034

12* 13*

14*

1 56

23*

24*

34*

39 3 12

What I would like is an output of the form 4 x m (m is whatever it is) and each row contains the sorted list of ids for each quadruplet.

example output:

1 2 3 4 <-- Are all neabours to each other.

Currently my code takes (too) many hours to do this on Xeon 2GHz with 1.5GB ram and idl 6.0.

Any help or suggestions would be much appreciated!!

Gianguido

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by cgguido on Thu, 11 Aug 2005 14:33:18 GMT

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Anybody??:(

Let me know if the description of my problem is not very clear...

thanks, Gianguido

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by Karl Schultz on Mon, 15 Aug 2005 16:43:13 GMT View Forum Message <> Reply to Message

On Sun, 07 Aug 2005 21:37:19 -0700, cgguido wrote:

```
> Hi all,
> I was wondering if anybody can suggest a fast algorithm (perhaps using
> the magic of HISTOGRAM :- o ) to find tetrahedra. Let me explain.
> I need to find quadruplets of mutually nearest neighbours id's in a
> nearest neighbour list.
> I start with a list of nearest neighbours id's, NN which is a 2xn (n ~
  6e6 yep!) intarr and is sorted so that for any i:
> NN[0,i] It N[1,i] and
> NN[0,i] le NN[0,i+1]
> example input:
> 02
> 05
> 034
> 12*
> 13*
> 14*
> 156
```

> 23* > 24*

```
> 34*
> 39
> 312
> ...
>
> What I would like is an output of the form 4 x m (m is whatever it is)
  and each row contains the sorted list of ids for each quadruplet.
>
 example output:
>
 1 2 3 4 <-- Are all neabours to each other.
>
>
> Currently my code takes (too) many hours to do this on Xeon 2GHz with
  1.5GB ram and idl 6.0.
>
  Any help or suggestions would be much appreciated!!
>
> Gianguido
> PS: I can post my code if you think it might help.
```

One thing worth pointing out is that nearly all mesh-related functions in IDL are implemented in C because those algorithms call for a lot of looping and other operations that are not efficient in IDL.

Since you've got an algorithm implemented in IDL and an apparent need to run it repeatedly on lots of data that takes hours to process with IDL, this may be a good example of something to translate to C and package up as a DLM.

You might post the IDL code to see if anyone can spot any obvious "low-hanging fruit". There may be some simple operations that you are doing that are very expensive and can be addressed without understanding or changing the main algorithm. For example, how are you collecting the quads? If you are just appending them to an array to create a new array, that can be costly.

I also can't understand your problem well enough to suggest that IDL code might be able to do it fast enough. The code might better describe what you are doing.

But my gut feel after making a lot of guesses and assumptions is that you may need a C DLM to get more than two or three orders of magnitude improvement.

Karl

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by cgguido on Tue, 16 Aug 2005 02:53:32 GMT

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Hi Karl,

thanks for replying.

- > One thing worth pointing out is that nearly all mesh-related functions
- > in IDL are implemented in C because those algorithms call for a lot of
- > looping and other operations that are not efficient in IDL.

Am not sure what you mean by mesh-related... my data comes from the 3D positions of ~5000 brownian particles diffusing around (each tagged with an id). I can determine whether particles are nearest neighbours two by two (which gives me the input matrix I mention in the original post) and now am looking for quadruplets of mutually nearest neighbours particles...

- > Since you've got an algorithm implemented in IDL and an apparent need to
- > run it repeatedly on lots of data that takes hours to process with IDL,
- > this may be a good example of something to translate to C and package up
- > as a DLM.

That's a possibility I would have never thought of, thanks! Although I extensively use 'where' and 'uniq' and I don't know if they exist in C. (at the very least, they must be available as a library...)

- > You might post the IDL code to see if anyone can spot any obvious
- > "low-hanging fruit". There may be some simple operations that you are
- > doing that are very expensive and can be addressed without understanding
- > or changing the main algorithm. For example, how are you collecting the
- > quads? If you are just appending them to an array to create a new array,
- > that can be costly.

Code appended. Yeah, I originally was appending each line one at a time... got rid of that pretty fast! :-)

- > I also can't understand your problem well enough to suggest that IDL code
- > might be able to do it fast enough. The code might better describe what
- > you are doing.

Am not sure what else to say to explain the problem, do you have questions? The header on the code might help too...

Many thanks again, and appologies for the long code that follows.

Here is the code:

NAME: **TETRAHEDRA WARNING:** Input must be sorted and each entry unique! See below. : PURPOSE:

Calculates all possible tetrahedra formed by nearest neighbours. Tetrahedra are defined as quadruplets (obviously) of mutually nearest-neighbour particles.

INPUT:

Uses the output of urstrtri.pro which is formated as follows: [id0, id1, zero, timestamp] (with id0 < id1). Each line is unique!

PARAMS:

VERBOSE: Set /verbose to print out usefull information during execution.

CHRONO: Set /chrono to print out duration of calculations in seconds.

DEBUG: Set /debug to only run the function on the first time stamp and the first reference particle. You can then manually check that *all* triangles were found.

OUTPUT:

Outputs an array with one line per tetrahedron formatted as follows:

[id0, id1, id2, id3, timestamp]

The list is sorted in ascending id order along both dimensions. Outputs [-1,-1,-1] if no tetrahedra are found.

EXAMPLE:

To get all tetrahedra formed by particles in 'tri' and store the output in 'a' while printing out some information about what's going on and while timing the execution type:

a = tetrahedra(tri, /verbose, /chrono)

HISTORY:

7-26-04 Written by Gianguido Cianci

7-28-04 Gianguido Cianci

- changed how the list of tetrahedra is created and updated.
- added chrono option to measure times of execution.

```
FUNCTION tetrahedra, tri, verbose=verbose, debug=debug, $
chrono=chrono, countbonds=countbonds
Compile_Opt IDL2
::initialise timer
IF keyword_set(chrono) THEN BEGIN
 t0=systime(/seconds)
 currentt=t0
ENDIF
;find list of unique time stamps in tri
ut=uniq(tri[3,*])
utimes=tri[3,ut]
tmax=n_elements(ut[*])
IF keyword_set(debug) THEN tmax = 1
;;initialise tetrahedra list and tetrahedra counters
a = intarr(5,50000L*tmax)
row = 0L
old row = row
;loop over time stamps
FOR tstampi = 0,tmax-1 DO BEGIN
 tstamp=utimes[tstampi]
 IF keyword set(verbose) THEN $
 message, /inf,' Doing time stamp
'+strcompress(tstampi+1)+'/'+strcompress(tmax)
 ;;get all neighbours at t = tstamp
 wt = where(tri[3,*] EQ tstamp)
 trt = tri[*,wt]
 ;; get index id -> tri row
 trindex=i2p(trt, /track)
 ;;find list of particles with at least one neighbour
 u = uniq(trt[0,*])
 npart = n elements(u)
 refid = trt[0,u]
 ;;debug using first particle with neighbours
 IF keyword set(debug) THEN npart = 1
```

;;loop over particles with neighbours

```
FOR i1 = 0,npart-1 DO BEGIN
   IF (keyword_set(verbose)) THEN BEGIN
     IF ((i1 MOD 500) EQ 0) THEN $
     message, /inf, ' Doing particle '+strcompress(i1+1) +' /'+
$
           strcompress(npart)
   ENDIF
   ;;chose a particle
   p1 = refid[i1]
   ;;get its neighbours with id# > p1
   n1 = idneighbors(p1,trt, /gr)
   ;;;message, /inf, 'n1'+string(p1) & message, /inf, n1 ;debugging
stuff
   nneighbour = n elements(n1)
   ;;if the ref particle has at least 3 neighbours then continue
   IF (nneighbour GT 2) THEN BEGIN
     ;;loop over neighbours of p1
     FOR i2 = 0,nneighbour-1 DO BEGIN
       ;;chose a neighbour of p1
       p2 = n1[i2]
       ;;find its neighbours with id# > p2
       n2 = idneighbors(p2, trt, /gr)
       ;;;message, /inf, 'n2'+string(p2) & message, /inf, n2
;debugging stuff
       ;;if second particle has at least 2 neighbours then
continue
       IF (n_elements(n2) GT 1) THEN BEGIN
         ;;concatentate lists of neighbours and sort them
         n3 = [n1, n2]
         n3 = n3[sort(n3)]
         ;;find id#'s that appear twice (i.e. look for triangles)
         u = uniq(n3)
         su = shift(u,1)
         du = u-su
         w = where(du[*] EQ 2)
         ;;if p1 and p2 form at least one triangle
         IF (w[0] NE -1) THEN BEGIN
           jmax=n_elements(w)-1
```

```
;;loop over triangles p1 p2 p3
           FOR j = 0,jmax DO BEGIN
             ;;third particle in triangle p1 p2 p3
             p3 = n3[u[w[i]]]
             ;;it's neighbours with id# > p3
             n4 = idneighbors(p3, trt, /gr)
             ;;concatenate lists of neighbours and sort
             n5 = [n1, n2, n4]
             n5 = n5[sort(n5)]
             ;;find id#'s that appear thrice (i.e. look for
tetrahedra)
             uu = uniq(n5)
             suu = shift(uu,1)
             duu = uu-suu
             ww = where(duu[*] EQ 3)
             ;;loop over tetrahedra
             IF (ww[0] NE -1) THEN BEGIN
               kmax = n_elements(ww)-1
               FOR k = 0, kmax DO BEGIN
                 ;;fourth particle in tetrahedron p1 p2 p3 p4
                 p4 = n5[uu[ww[k]]]
                 ;;update list of tetrahedra
                 temp = [p1,p2,p3,p4,tstamp]
                 a[0,row] = temp
                 row = row + 1
                 ;; Using third col of tri to keep count
                 ;; nearest neighbour pair usage
                 IF (keyword set(countbonds)) THEN BEGIN
                   tri[2,wt[trindex[p1,p2]]]++
                   tri[2,wt[trindex[p1,p3]]]++
                   tri[2,wt[trindex[p1,p4]]]++
                   tri[2,wt[trindex[p2,p3]]]++
                   tri[2,wt[trindex[p2,p4]]]++
```

tri[2,wt[trindex[p3,p4]]]++

```
ENDIF ;END loop to count tetrahedral bonds
              ENDFOR :END loop over tetrahedra p1 p2 p3 p4
             ENDIF
                        ;END if p1, p2 and p3 form at least
one tetrahedron
           ENDFOR
                          ;END loop over triangles p1 p2 p3
                        ;END if p1 and p2 form at least one
         ENDIF
triangle
       ENDIF
                        ;END if second particle has at least 2
neighbours
     ENDFOR
                          ;END loop over neighbours of p1
   ENDIF
                        ;END if the ref particle has at least
3 neighbours
 ENDFOR
                          ;END loop over particles with
neighbours
 ;;Print info after each stack is analyzed.
 IF keyword_set(chrono) THEN BEGIN
   dt=ceil(systime(/seconds)-currentt)
   message, /inf, strcompress(dt)+ ' seconds elapsed for this
stack.'
   currentt=systime(/seconds)
   message, /inf, strcompress(ceil(currentt-t0))+ $
         ' seconds elapsed since the beginning of analysis.'
 ENDIF
 message, /inf, strcompress(row-old row)+' tetrahedra found in this
stack.'
 message, /inf, strcompress(row)+' tetrahedra found overall, this
far.'
 message, /inf, ' --'
 old row = row
ENDFOR
                         ;END loop over time stamps
:count tetrahedra
ntetrahedra = row
message, /inf, ' --'
message, /inf, 'Found '+strcompress(ntetrahedra)+ ' tetrahedra.'
IF keyword_set(chrono) THEN BEGIN
 t0=ceil(systime(/seconds)-t0)
 message, /inf, 'Time taken: ' +strcompress(t0)+ ' seconds.'
ENDIF
```

```
;if no tetrahedron are found return [-1,-1,-1,-1]
IF (ntetrahedra EQ 0) THEN BEGIN
 a = [-1, -1, -1, -1, -1]
 return, a
ENDIF
return, a[*,0:ntetrahedra-1]
END;; End of tetrahedra()
```

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by Richard French on Tue, 16 Aug 2005 03:09:45 GMT View Forum Message <> Reply to Message

Could you supply a sample of the input array? Even 100 lines would help! Ideally, we'd be able to run your routine with the test data and get the same answer you do.

Thanks.

Dick French

```
> Here is the code:
>
>
> ; NAME:
  : TETRAHEDRA
 : WARNING:
  ; Input must be sorted and each entry unique! See below.
> : PURPOSE:
 ; Calculates all possible tetrahedra formed by nearest neighbours.
   Tetrahedra are defined as quadruplets (obviously) of mutually
  ; nearest-neighbour particles.
> :-
 : INPUT:
  ; Uses the output of urstrtri.pro which is formated as follows:
    [id0, id1, zero, timestamp] (with id0 < id1). Each line is unique!
> : PARAMS:
> ; VERBOSE: Set /verbose to print out usefull information during
> : execution.
> ; CHRONO: Set /chrono to print out duration of calculations in
> seconds.
> ; DEBUG: Set /debug to only run the function on the first time stamp
> ; and the first reference particle. You can then manually check that
```

```
> ; *all* triangles were found.
>
> ; OUTPUT:
  ; Outputs an array with one line per tetrahedron formatted as
> : follows:
   [id0, id1, id2, id3, timestamp]
   The list is sorted in ascending id order along both dimensions.
  ; Outputs [-1,-1,-1] if no tetrahedra are found.
> : EXAMPLE:
> ; To get all tetrahedra formed by particles in 'tri' and store the
> ; output in 'a' while printing out some information about what's
  ; going on and while timing the execution type:
     a = tetrahedra(tri, /verbose, /chrono)
> : HISTORY:
 ; 7-26-04 Written by Gianguido Cianci
  ; 7-28-04 Gianguido Cianci
         - changed how the list of tetrahedra is created and
> ;
          updated.
         - added chrono option to measure times of execution.
> ;
>
>
> FUNCTION tetrahedra, tri, verbose=verbose, debug=debug, $
> chrono=chrono, countbonds=countbonds
>
> Compile_Opt IDL2
>
> ;;initialise timer
> IF keyword set(chrono) THEN BEGIN
    t0=systime(/seconds)
    currentt=t0
> ENDIF
>
> ;find list of unique time stamps in tri
> ut=uniq(tri[3,*])
> utimes=tri[3,ut]
> tmax=n_elements(ut[*])
>
> IF keyword set(debug) THEN tmax = 1
>
> ;;initialise tetrahedra list and tetrahedra counters
> a = intarr(5,50000L*tmax)
> row = 0L
> old_row = row
> ;loop over time stamps
```

```
> FOR tstampi = 0,tmax-1 DO BEGIN
>
    tstamp=utimes[tstampi]
>
    IF keyword_set(verbose) THEN $
>
    message, /inf,' Doing time stamp
>
  '+strcompress(tstampi+1)+'/'+strcompress(tmax)
>
    ;;get all neighbours at t = tstamp
>
    wt = where(tri[3,*] EQ tstamp)
>
    trt = tri[*,wt]
>
>
    ;; get index id -> tri row
>
    trindex=i2p(trt, /track)
>
    ;;find list of particles with at least one neighbour
>
    u = uniq(trt[0,*])
>
    npart = n_elements(u)
>
    refid = trt[0,u]
>
>
    ;;debug using first particle with neighbours
>
    IF keyword_set(debug) THEN npart = 1
>
>
>
    ;;loop over particles with neighbours
>
    FOR i1 = 0,npart-1 DO BEGIN
>
>
      IF (keyword_set(verbose)) THEN BEGIN
>
        IF ((i1 MOD 500) EQ 0) THEN $
>
        message, /inf, ' Doing particle '+strcompress(i1+1) +' /'+
>
> $
              strcompress(npart)
>
      ENDIF
>
>
      ;;chose a particle
>
      p1 = refid[i1]
>
>
      ;;get its neighbours with id# > p1
>
      n1 = idneighbors(p1,trt, /gr)
>
      ;;;message, /inf, 'n1'+string(p1) & message, /inf, n1 ;debugging
>
> stuff
      nneighbour = n_elements(n1)
>
      ;;if the ref particle has at least 3 neighbours then continue
>
      IF (nneighbour GT 2) THEN BEGIN
>
>
        ;;loop over neighbours of p1
>
        FOR i2 = 0,nneighbour-1 DO BEGIN
>
>
          ;;chose a neighbour of p1
>
          p2 = n1[i2]
```

```
>
          ;;find its neighbours with id# > p2
>
          n2 = idneighbors(p2, trt, /gr)
>
          ;;;message, /inf, 'n2'+string(p2) & message, /inf, n2
  ;debugging stuff
>
          ;;if second particle has at least 2 neighbours then
>
  continue
>
          IF (n_elements(n2) GT 1) THEN BEGIN
>
            ;;concatentate lists of neighbours and sort them
>
            n3 = [n1,n2]
>
            n3 = n3[sort(n3)]
>
>
            ;;find id#'s that appear twice (i.e. look for triangles)
>
            u = uniq(n3)
>
            su = shift(u,1)
>
            du = u-su
>
            w = where(du[*] EQ 2)
>
>
            ;;if p1 and p2 form at least one triangle
>
            IF (w[0] NE -1) THEN BEGIN
>
              jmax=n elements(w)-1
>
>
>
              ;;loop over triangles p1 p2 p3
>
              FOR j = 0,jmax DO BEGIN
>
>
                ;;third particle in triangle p1 p2 p3
                p3 = n3[u[w[j]]]
>
>
                ;;it's neighbours with id# > p3
                n4 = idneighbors(p3, trt, /gr)
>
>
                ;;concatenate lists of neighbours and sort
                n5 = [n1, n2, n4]
>
                n5 = n5[sort(n5)]
>
>
                ;;find id#'s that appear thrice (i.e. look for
>
  tetrahedra)
>
                uu = uniq(n5)
>
                suu = shift(uu,1)
>
                duu = uu-suu
>
                ww = where(duu[*] EQ 3)
>
>
                ;;loop over tetrahedra
>
                IF (ww[0] NE -1) THEN BEGIN
>
                  kmax = n elements(ww)-1
>
```

```
FOR k = 0, kmax DO BEGIN
>
>
                   ;;fourth particle in tetrahedron p1 p2 p3 p4
>
                   p4 = n5[uu[ww[k]]]
>
                   ;;update list of tetrahedra
>
                   temp = [p1,p2,p3,p4,tstamp]
>
                   a[0,row] = temp
>
                   row = row + 1
>
>
                   ;; Using third col of tri to keep count
>
                   ;; nearest neighbour pair usage
>
                   IF (keyword_set(countbonds)) THEN BEGIN
>
                     tri[2,wt[trindex[p1,p2]]]++
>
>
                     tri[2,wt[trindex[p1,p3]]]++
>
>
                     tri[2,wt[trindex[p1,p4]]]++
>
>
                     tri[2,wt[trindex[p2,p3]]]++
>
>
                     tri[2,wt[trindex[p2,p4]]]++
>
>
                     tri[2,wt[trindex[p3,p4]]]++
>
>
>
                   ENDIF; END loop to count tetrahedral bonds
>
                 ENDFOR ;END loop over tetrahedra p1 p2 p3 p4
>
                           ;END if p1, p2 and p3 form at least
               ENDIF
>
  one tetrahedron
             ENDFOR
                             ;END loop over triangles p1 p2 p3
>
                          ;END if p1 and p2 form at least one
            ENDIF
>
 triangle
                          ;END if second particle has at least 2
         ENDIF
>
> neighbours
        ENDFOR
                             :END loop over neighbours of p1
>
                           ;END if the ref particle has at least
      ENDIF
>
> 3 neighbours
    ENDFOR
                             ;END loop over particles with
 neighbours
>
>
    ;;Print info after each stack is analyzed.
>
    IF keyword_set(chrono) THEN BEGIN
>
      dt=ceil(systime(/seconds)-currentt)
>
      message, /inf, strcompress(dt)+ ' seconds elapsed for this
>
> stack.'
      currentt=systime(/seconds)
>
      message, /inf, strcompress(ceil(currentt-t0))+$
>
```

```
' seconds elapsed since the beginning of analysis.'
>
    ENDIF
>
    message, /inf, strcompress(row-old_row)+' tetrahedra found in this
>
> stack.'
    message, /inf, strcompress(row)+' tetrahedra found overall, this
> far.'
    message, /inf, ' --'
>
    old_row = row
> ENDFOR
                            ;END loop over time stamps
>
>
> :count tetrahedra
> ntetrahedra = row
>
>
> message, /inf, ' --'
 message, /inf, 'Found '+strcompress(ntetrahedra)+ ' tetrahedra.'
>
> IF keyword set(chrono) THEN BEGIN
    t0=ceil(systime(/seconds)-t0)
    message, /inf, 'Time taken: ' +strcompress(t0)+ ' seconds.'
> ENDIF
> ;if no tetrahedron are found return [-1,-1,-1,-1]
> IF (ntetrahedra EQ 0) THEN BEGIN
    a = [-1, -1, -1, -1, -1]
    return, a
> ENDIF
>
> return, a[*,0:ntetrahedra-1]
> END;; End of tetrahedra()
```

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by cgguido on Tue, 16 Aug 2005 03:12:21 GMT

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a few more comments:

- in my original post i did not mention time and really the problem is what's inside the time loop.
- Also, please ignore the lines that include the variable trindex.

thanks

Gianguido

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by cgguido on Tue, 16 Aug 2005 03:15:51 GMT

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I can do that with no problems... but how? just as a message on this forum?

Also, what about the other routines that are called by tetrahedra.pro? should I post them too?

G

Subject: Re: Looking for tetrahedra. Searching sorted lists. Posted by James Kuyper on Tue, 16 Aug 2005 14:13:48 GMT View Forum Message <> Reply to Message

cgguido wrote:

> Hi Karl,

>

> thanks for replying.

>

- >> One thing worth pointing out is that nearly all mesh-related functions
- >> in IDL are implemented in C because those algorithms call for a lot of
- >> looping and other operations that are not efficient in IDL.

>

- > Am not sure what you mean by mesh-related... my data comes from the 3D
- > positions of ~5000 brownian particles diffusing around (each tagged
- > with an id). I can determine whether particles are nearest neighbours
- > two by two (which gives me the input matrix I mention in the original
- > post) and now am looking for quadruplets of mutually nearest neighbours
- > particles...

The links you've made between nearest neighbors define a mesh.

- >> Since you've got an algorithm implemented in IDL and an apparent need to
- >> run it repeatedly on lots of data that takes hours to process with IDL,
- >> this may be a good example of something to translate to C and package up
- >> as a DLM.

>

- > That's a possibility I would have never thought of, thanks! Although I
- > extensively use 'where' and 'uniq' and I don't know if they exist in C.
- > (at the very least, they must be available as a library...)

Possibly, but nothing quite like 'where' or 'uniq' are available as part of the C standard library. That's because you don't write C code the same way you do IDL, mainly because of the huge performance penalty for explicit loops in IDL. In most instances where IDL code uses where

or uniq, C code would use a loop, and therefore usually doesn't need to store the complete list of indices; it just needs one index at a time:

```
IDL:
i = where(array eq 3)
; use 'i'
j = uniq(sorted_array)
; use 'j'
C:
int i;
for(i=0; i<n1; i++)
{
  if (array[i] == 3)
     /* use i */
int j;
for(j=0; j<n2; j++)
  if(j==n2-1 || sorted_array[j] != sorted_array[j+1])
     /* use j */
}
```

C code could store the complete list of matches, if needed, but then it would need to explicitly allocate the memory to store that list, and it would also need to explicitly deallocate it when the code is done with that list, which makes the user code more complicated than it would be in IDL. There's no free lunch here; those same issues apply to IDL, it's just handled internally by IDL itself. The cost of doing it internally is that's its done less efficiently, in some cases, than it could be if done under user control (by a sufficiently competent user!).