Subject: Re: Can my big for loop exploit array operations? Posted by Dick Jackson on Tue, 20 Oct 2015 15:51:01 GMT

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JTMHD wrote on 2015-10-20 5:35am:> Hi,
> I'm writing a little post-processing procedure and need help avoiding a hefty for loop, which will
typically require 1000<sup>3</sup> iterations.
>
> Its purpose is to take data from a simulation, which expresses three components of a vector
field at a different position s.t.
>
> x - component is defined on cell boundary in x-direction, cell center in other directions (xb,yc,zc(
> y - component is defined on cell boundary in y-direction, cell center in other directions (xc,yb,zc)
> z - component is defined on cell boundary inz-direction, cell center in other directions (xc,yc,zb)
  and express the field as defined in the cell center for all components (xc,yc,zc).
> Rather than using interpolation, I think the best way will be to simply average the values across
the cell face to head off errors down the line.
> The problem is im not sure how to avoid a hefty for loop which goes through all elements taking
the desired average as follows....
>
>
 FUNCTION reformat_bcomponents_1,t
> data = getdata(t,/BX,/BY,/BZ,/GRID)
>
> bx = DBLARR(SIZE(data.x,/N ELEMENTS),SIZE(data.y,/N ELEMENTS),SIZ
E(data.z,/N ELEMENTS))
> by = DBLARR(SIZE(data.x,/N_ELEMENTS),SIZE(data.y,/N_ELEMENTS),SIZ
E(data.z,/N_ELEMENTS))
> bz = DBLARR(SIZE(data.x,/N_ELEMENTS),SIZE(data.y,/N_ELEMENTS),SIZ
E(data.z,/N ELEMENTS))
>
> FOR iz = 0,SIZE(data.z,/N ELEMENTS) -1 DO BEGIN
> FOR iy = 0,SIZE(data.y,/N ELEMENTS) -1 DO BEGIN
> FOR ix = 0,SIZE(data.x,/N ELEMENTS) -1 DO BEGIN
>
    bx[ix,iy,iz] = MEAN([data.bx[ix,iy,iz], data.bx[ix+1,iy,iz]],/DOUBLE)
>
    by[ix,iy,iz] = MEAN([data.by[ix,iy,iz], data.by[ix,iy+1,iz]],/DOUBLE)
>
    bz[ix,iy,iz] = MEAN([data.bz[ix,iy,iz], data.bz[ix,iy,iz+1]],/DOUBLE)
>
> ENDFOR
> ENDFOR
> ENDFOR
```

```
> mag_str = CREATE_STRUCT('bxp',bx,'byp',by,'bzp',bz)
> RETURN,mag_str
> END
> If anyone can point me in the direction of how to do this exploiting array operations I'd be grateful.
> Thanks in advance,
> Jonathan
```

Hi Jonathan,

I love a well-written question! I hope I've understood you correctly.

I think the middle 12 lines of code can be reduced to three (and execution time likely reduced by a factor of 10 or 20):

```
FUNCTION reformat_bcomponents_1,t
```

```
data = getdata(t,/BX,/BY,/BZ,/GRID)
```

```
bx = (data.bx[0:-2, *, *] + data.bx[1:*, *, *]) / 2
by = (data.by[*, 0:-2, *] + data.by[*, 1:*, *]) / 2
bz = (data.bz[*, *, 0:-2] + data.bz[*, *, 1:*]) / 2
```

mag_str = CREATE_STRUCT('bxp',bx,'byp',by,'bzp',bz)

RETURN,mag_str END

If you like, this may be even faster, partly because IDL needs to do less indexing (expanding the "*"s behind the scenes). Also, peak memory usage will be lower, for the same reason:

Aside:

Making 2-element kernels for convolution in a 3-D array is tricky in IDL. REPLICATE() may indeed create an array with "1" as a trailing dimension, but when you actually look at it (or pass it into a function call), it collapses. (something to do with quantum physics, I think :-)...

```
IDL> help,replicate(0.5, [2, 1, 1])
<Expression> FLOAT = Array[2]
IDL> help,replicate(0.5, [1, 2, 1])
<Expression> FLOAT = Array[1, 2]; This one would cause CONVOL to fail, below IDL> help,replicate(0.5, [1, 1, 2])
```

```
= Array[1, 1, 2]
I'll cast them all to three dimensions for consistency.
----
So, the three lines above become these six:
bx = CONVOL(data.bx, REFORM(REPLICATE(0.5, [2, 1, 1]), [2, 1, 1]))
bx = bx[1:*, *, *]
by = CONVOL(data.by, REFORM(REPLICATE(0.5, [1, 2, 1]), [1, 2, 1]))
by = by[*, 1:*, *]
bz = CONVOL(data.bz, REFORM(REPLICATE(0.5, [1, 1, 2]), [1, 1, 2]))
bz = bz[*, *, 1:*]
These timings and memory metrics are typical for my experiments with arrays of size 100<sup>3</sup>. You
may need some special handling if you have 1000\dagger3, but this work can be easily divided into slabs
of, say, 100 columns/rows/planes at a time. (sorry for line wrapping):
IDL> help,/memory
heap memory used: 61573317, max: 61591749, gets: 466522324, frees: 466429302
                      ^^^^
                      ("max:" my base memory usage)
IDL> tic & bx = (data.bx[0:-2, *, *] + data.bx[1:*, *, *]) / 2 & toc & help,/memory
% Time elapsed: 0.20199990 seconds.
heap memory used: 61573305, max: 85333785, gets: 466522291, frees: 466429269
                      ^^^^
                      ("max:" peak memory used for (a+b)/2 method)
IDL> tic & bx2 = CONVOL(data.bx, REPLICATE(0.5, [2, 1, 1])) & bx2 = bx2[1:*,*,*] & toc &
help,/memory
% Time elapsed: 0.16899991 seconds.
heap memory used: 61573189, max: 77574061, gets: 466522197, frees: 466429175
                      ("max:" peak memory used for CONVOL method)
And yes, these give the same results: :-)
IDL> array equal(bx,bx2)
 1
Hope this helps!
Cheers,
-Dick
Dick Jackson Software Consulting Inc.
```

<Expression>

FLOAT

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