
Subject: Avoiding a FOR loop in calculation of SPH potential energy

Posted by [cody](#) on Tue, 23 Jun 2009 06:48:00 GMT

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i have an SPH simulation with snapshots in time that are represented as structures in idl. the structures have mass, density, position etc. for every particle in the simulation. i'm trying to get a vector that represents the total potential energy at each snapshot. i have an outer FOR loop that loops through each snapshot file and this part is fine, i don't really want to change that. but i have an inner loop for calculating the PE that must calculate the total potential energy felt by each particle from every other particle without double counting. to do that, i just loop over a dummy variable j from 0 to the maximum particle ident -1 and make a sub list of particles where ident > j. this way, i'm not double counting and it's not n^2 time. but it's still way too slow for a 100k particle sim.

now i'm fairly certain there's a way to speed this up considerably using IDL's strengths, but i'm a c++ programmer, so that's the way i think. can someone help me out?

here's my code as it stands now:

PRO exportenergy, enditer=enditer, deliter=deliter, root=root

```
;first get the total number of particles
```

```
startiter = 1000
```

```
n = (enditer - startiter)/deliter
```

```
m=0
```

```
G=3.93935d-7 ;SPH units
```

```
arr = DBLARR(5, n)
```

```
for i=0L,(n-1) do begin
```

```
    iter = i*deliter + startiter
```

```
    filename = root + '.' + STRING(iter,format='(I0)')
```

```
    readsdf,filename,s
```

```
    arr[0,i] = sdf_getdouble(filename,"tpos")
```

```
    arr[1,i] = 0.5*total(s.mass*s.vx^2)
```

```
    arr[2,i] = 0.5*total(s.mass*s.vy^2)
```

```
    arr[3,i] = 0.5*total(s.mass*s.vz^2)
```

```
;PE part starts here
```

```
pn = max(s.ident)
```

```
PE = 0.0
```

```
for j=0L,pn-1 do begin
```

```
    sub = where(s.ident gt j)
```

```
    PE = PE + G*s[j].mass*total(s[sub].mass/sqrt((s[j].x-s[sub].x)^2+
```

```
(s[j].y-s[sub].y)^2+(s[j].z-s[sub].z)^2))  
    print,'just computed ' + string(j,format='(I0)') + ' PE=' +  
string(PE)  
    endfor  
    arr[4,i] = PE  
endfor
```
